



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:08 PM EST

PDB ID : 7TGW
EMDB ID : EMD-25887
Title : Omicron spike at 3.0 Å (open form)
Authors : Ye, G.; Liu, B.; Li, F.
Deposited on : 2022-01-09
Resolution : 3.00 Å (reported)
Based on initial model : 7KRR

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) : 2.39

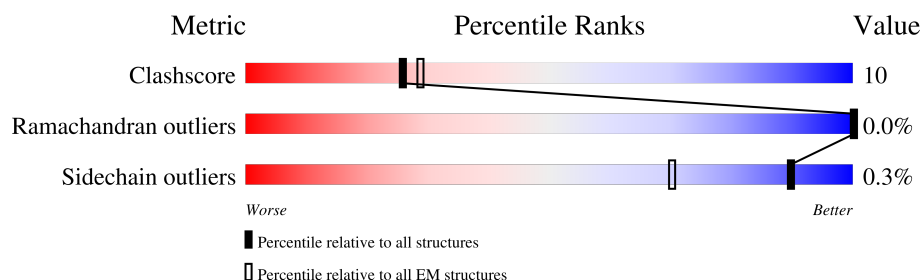
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.






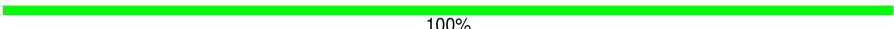
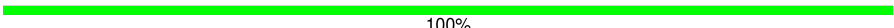

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1231	
1	B	1231	
1	C	1231	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1308	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26617 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	1113	Total	C	N	O	S	2	0
			8741	5593	1460	1648	40		
1	B	1091	Total	C	N	O	S	2	0
			8579	5493	1431	1616	39		
1	C	1103	Total	C	N	O	S	2	0
			8667	5547	1447	1633	40		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	336	ASP	GLY	conflict	UNP P0DTC2
A	368	LEU	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2
A	481	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ARG	GLN	conflict	UNP P0DTC2
A	495	ARG	GLN	conflict	UNP P0DTC2
A	498	TYR	ASN	conflict	UNP P0DTC2
A	502	HIS	TYR	conflict	UNP P0DTC2
A	544	LYS	THR	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	652	TYR	HIS	conflict	UNP P0DTC2
A	676	LYS	ASN	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	761	LYS	ASN	conflict	UNP P0DTC2
A	793	TYR	ASP	conflict	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	conflict	UNP P0DTC2
A	966	LYS	ASN	conflict	UNP P0DTC2
A	978	PHE	LEU	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	conflict	UNP P0DTC2
B	206	ILE	-	insertion	UNP P0DTC2
B	207	VAL	-	insertion	UNP P0DTC2
B	208	ARG	ASN	conflict	UNP P0DTC2
B	209	GLU	LEU	conflict	UNP P0DTC2
B	210	PRO	VAL	conflict	UNP P0DTC2
B	211	GLU	ARG	conflict	UNP P0DTC2
B	336	ASP	GLY	conflict	UNP P0DTC2
B	368	LEU	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	474	ASN	SER	conflict	UNP P0DTC2
B	475	LYS	THR	conflict	UNP P0DTC2
B	481	ALA	GLU	conflict	UNP P0DTC2
B	490	ARG	GLN	conflict	UNP P0DTC2
B	495	ARG	GLN	conflict	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	502	HIS	TYR	conflict	UNP P0DTC2
B	544	LYS	THR	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	652	TYR	HIS	conflict	UNP P0DTC2
B	676	LYS	ASN	conflict	UNP P0DTC2
B	678	HIS	PRO	conflict	UNP P0DTC2
B	761	LYS	ASN	conflict	UNP P0DTC2
B	793	TYR	ASP	conflict	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	853	LYS	ASN	conflict	UNP P0DTC2
B	889	PRO	ALA	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	939	PRO	ALA	conflict	UNP P0DTC2
B	951	HIS	GLN	conflict	UNP P0DTC2
B	966	LYS	ASN	conflict	UNP P0DTC2
B	978	PHE	LEU	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	conflict	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	conflict	UNP P0DTC2
C	206	ILE	-	insertion	UNP P0DTC2
C	207	VAL	-	insertion	UNP P0DTC2
C	208	ARG	ASN	conflict	UNP P0DTC2
C	209	GLU	LEU	conflict	UNP P0DTC2
C	210	PRO	VAL	conflict	UNP P0DTC2
C	211	GLU	ARG	conflict	UNP P0DTC2
C	336	ASP	GLY	conflict	UNP P0DTC2
C	368	LEU	SER	conflict	UNP P0DTC2
C	370	PRO	SER	conflict	UNP P0DTC2
C	372	PHE	SER	conflict	UNP P0DTC2
C	414	ASN	LYS	conflict	UNP P0DTC2
C	437	LYS	ASN	conflict	UNP P0DTC2
C	443	SER	GLY	conflict	UNP P0DTC2
C	474	ASN	SER	conflict	UNP P0DTC2
C	475	LYS	THR	conflict	UNP P0DTC2
C	481	ALA	GLU	conflict	UNP P0DTC2
C	490	ARG	GLN	conflict	UNP P0DTC2
C	495	ARG	GLN	conflict	UNP P0DTC2
C	498	TYR	ASN	conflict	UNP P0DTC2
C	502	HIS	TYR	conflict	UNP P0DTC2
C	544	LYS	THR	conflict	UNP P0DTC2
C	611	GLY	ASP	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	652	TYR	HIS	conflict	UNP P0DTC2
C	676	LYS	ASN	conflict	UNP P0DTC2
C	678	HIS	PRO	conflict	UNP P0DTC2
C	761	LYS	ASN	conflict	UNP P0DTC2
C	793	TYR	ASP	conflict	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	conflict	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	conflict	UNP P0DTC2
C	966	LYS	ASN	conflict	UNP P0DTC2
C	978	PHE	LEU	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	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
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

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

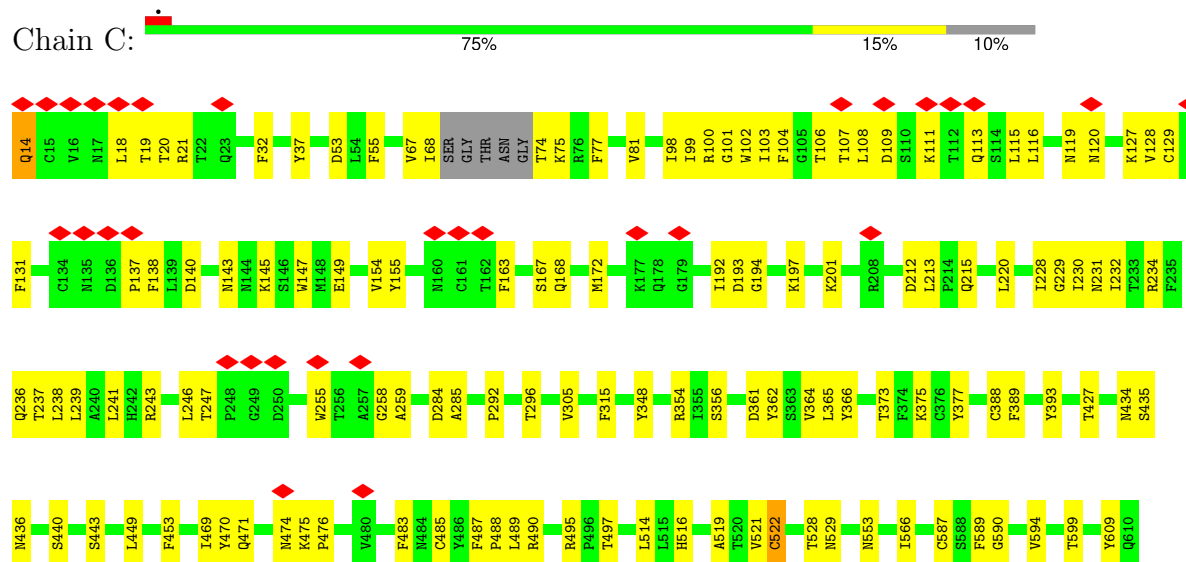


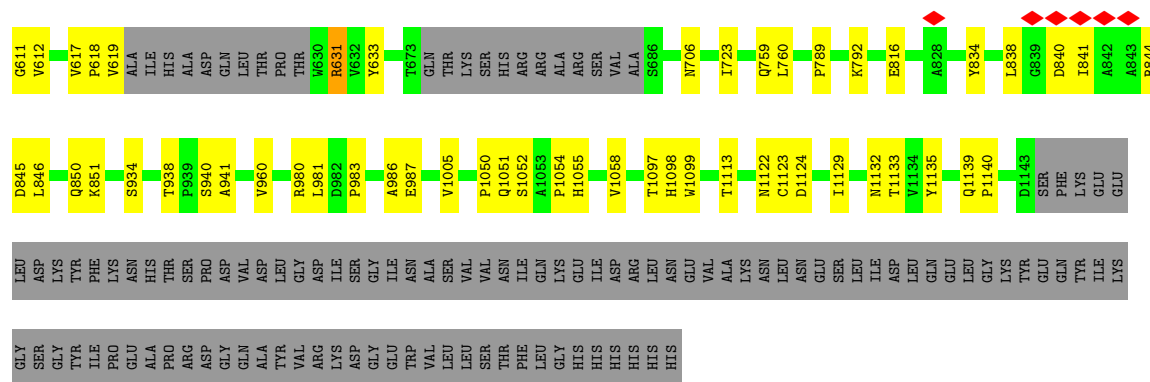
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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

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





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

Chain D: 50%



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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 50%



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

Chain I:  100%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain O:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	554951	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.336	Depositor
Minimum map value	-0.552	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.146	Depositor
Map size (Å)	341.76, 341.76, 341.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	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	0.39	1/8960 (0.0%)	0.54	0/12197
1	B	0.38	1/8793 (0.0%)	0.54	2/11965 (0.0%)
1	C	0.39	0/8883	0.54	2/12088 (0.0%)
All	All	0.39	2/26636 (0.0%)	0.54	4/36250 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	646	CYS	CB-SG	-6.29	1.71	1.82
1	A	646	CYS	CB-SG	-5.01	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	522	CYS	CA-CB-SG	14.63	140.33	114.00
1	B	587	CYS	CA-CB-SG	5.82	124.48	114.00
1	B	140	ASP	N-CA-CB	-5.05	101.51	110.60
1	C	587	CYS	CA-CB-SG	5.01	123.01	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	CYS	Peptide
1	B	139	LEU	Peptide
1	B	614	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8741	0	8553	188	0
1	B	8579	0	8403	167	0
1	C	8667	0	8485	152	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	3	0
2	I	28	0	25	3	0
2	J	28	0	25	3	0
2	K	28	0	25	2	0
2	L	28	0	25	3	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	3	0
3	A	112	0	104	10	0
3	B	98	0	91	7	0
3	C	84	0	78	6	0
All	All	26617	0	26014	528	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 10.

All (528) 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:A:61:ASN:HD22	3:A:1308:NAG:C1	1.22	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:ND2	3:A:1308:NAG:C1	1.89	1.31
1:C:840:ASP:OD2	1:C:844:ARG:NH1	2.03	0.92
1:B:808:LYS:NZ	1:B:817:ASP:OD2	2.01	0.92
1:C:115:LEU:HD21	1:C:228:ILE:HG21	1.51	0.90
1:B:208:ARG:NH1	1:B:209:GLU:O	2.09	0.85
1:B:19:THR:HG22	1:B:20:THR:H	1.44	0.83
2:I:2:NAG:O7	2:I:2:NAG:O3	1.98	0.81
1:C:14:GLN:HE21	1:C:14:GLN:N	1.78	0.81
1:B:14:GLN:HE21	1:B:14:GLN:N	1.76	0.81
3:C:1304:NAG:H82	3:C:1304:NAG:H3	1.64	0.79
1:C:115:LEU:HD21	1:C:228:ILE:CG2	2.12	0.79
1:A:362:TYR:HD2	1:A:384:LEU:HD13	1.49	0.78
2:K:2:NAG:O7	2:K:2:NAG:O3	2.02	0.77
1:A:390:THR:HG22	1:A:391:ASN:H	1.53	0.74
1:A:401:GLY:O	1:A:404:VAL:HG22	1.88	0.74
1:A:362:TYR:CD2	1:A:384:LEU:HD13	2.23	0.73
1:A:613:ASN:O	1:A:616:GLU:N	2.22	0.73
1:B:848:CYS:SG	1:B:849:ALA:N	2.62	0.73
1:A:317:VAL:HG13	1:A:318:GLN:H	1.52	0.73
1:A:337:GLU:O	1:A:353:LYS:NZ	2.21	0.73
1:B:1113:THR:HG22	1:B:1135:TYR:HB3	1.71	0.73
1:A:24:LEU:HD22	1:A:76:ARG:HH12	1.53	0.72
1:C:77:PHE:CZ	1:C:239:LEU:HD13	2.25	0.72
2:H:2:NAG:H3	2:H:2:NAG:H83	1.72	0.71
1:A:454:ARG:NH1	1:A:464:ASP:OD2	2.23	0.71
1:B:347:VAL:HG22	1:B:398:VAL:O	1.90	0.70
1:B:419:ASN:N	1:B:458:LEU:HD21	2.07	0.70
2:O:2:NAG:H83	2:O:2:NAG:H3	1.73	0.70
1:A:336:ASP:OD1	1:A:337:GLU:N	2.25	0.69
1:B:243:ARG:HE	1:B:255:TRP:HB3	1.56	0.69
1:C:21:ARG:NH1	1:C:77:PHE:O	2.25	0.69
1:A:400:ARG:NH1	1:A:402:ASP:OD2	2.26	0.69
1:C:388:CYS:HA	1:C:522:CYS:HB3	1.75	0.69
2:L:2:NAG:H83	2:L:2:NAG:H3	1.75	0.69
1:A:1113:THR:HG22	1:A:1135:TYR:HB3	1.75	0.68
1:B:376:CYS:SG	1:B:429:CYS:N	2.67	0.68
1:A:129:CYS:HA	1:A:161:CYS:HB3	1.77	0.67
1:B:76:ARG:NE	1:B:78:ASP:OD2	2.27	0.67
1:C:115:LEU:HD23	1:C:128:VAL:HG12	1.76	0.67
1:A:406:GLN:OE1	1:A:416:ALA:HB2	1.94	0.67
1:C:388:CYS:HA	1:C:522:CYS:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:THR:OG1	1:B:75:LYS:N	2.28	0.67
1:B:339:PHE:HE1	1:B:508:VAL:HG11	1.59	0.67
1:A:364:VAL:HG12	1:A:364:VAL:O	1.95	0.67
1:A:384:LEU:HD12	1:A:385:ASN:N	2.09	0.67
3:B:1306:NAG:H82	3:B:1306:NAG:C1	2.25	0.66
2:I:2:NAG:HO3	2:I:2:NAG:C7	2.06	0.66
1:B:14:GLN:N	1:B:14:GLN:NE2	2.44	0.65
1:B:94:GLU:OE2	1:B:98:ILE:N	2.23	0.65
1:B:98:ILE:HG22	1:B:239:LEU:HD12	1.77	0.65
1:B:142:LYS:HB2	1:B:150:SER:HB2	1.78	0.65
1:A:324:VAL:HG12	1:A:324:VAL:O	1.97	0.65
1:B:399:ILE:HD12	1:B:415:ILE:HD13	1.79	0.64
1:B:138:PHE:C	1:B:139:LEU:HD22	2.18	0.64
1:B:255:TRP:CZ3	1:B:257:ALA:HB2	2.33	0.64
1:B:1123:CYS:HB2	1:B:1129:ILE:HD13	1.80	0.64
1:A:614:CYS:HA	1:A:617:VAL:HG23	1.80	0.63
1:B:34:ARG:NH1	1:B:186:GLU:OE2	2.30	0.63
1:B:339:PHE:O	1:B:506:ARG:NH1	2.31	0.63
1:C:566:ILE:HD12	1:C:566:ILE:H	1.63	0.63
1:A:284:ASP:OD1	1:A:285:ALA:N	2.32	0.63
1:B:465:ILE:HG22	1:B:465:ILE:O	1.97	0.63
1:B:463:ARG:NH1	1:C:113:GLN:OE1	2.31	0.63
1:C:284:ASP:OD1	1:C:285:ALA:N	2.31	0.63
3:B:1306:NAG:C1	3:B:1306:NAG:C8	2.77	0.62
1:A:700:ASN:OD1	1:A:701:SER:N	2.33	0.62
1:A:840:ASP:OD1	1:A:844:ARG:NH1	2.30	0.62
1:B:139:LEU:HD12	1:B:239:LEU:O	2.00	0.62
1:B:284:ASP:OD1	1:B:285:ALA:N	2.32	0.62
1:C:354:ARG:NH1	1:C:393:TYR:OH	2.31	0.62
1:A:354:ARG:O	1:A:355:ILE:HD13	1.99	0.62
1:A:1116:ASN:O	1:A:1116:ASN:ND2	2.32	0.62
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.82	0.62
1:A:362:TYR:HB3	1:A:365:LEU:HB3	1.82	0.62
1:B:96:SER:OG	1:B:98:ILE:HD11	1.99	0.61
3:C:1304:NAG:H5	3:C:1304:NAG:N2	2.14	0.61
1:B:849:ALA:O	1:B:853:LYS:HG2	2.01	0.61
1:C:723:ILE:CD1	1:C:1058:VAL:HG22	2.31	0.60
1:A:352:ARG:NE	1:A:393:TYR:HB3	2.17	0.60
1:A:142:LYS:HG2	1:A:242:HIS:HA	1.82	0.60
1:A:146:SER:OG	1:A:148:MET:SD	2.57	0.60
1:A:431:ILE:HB	1:A:508:VAL:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLN:N	1:C:14:GLN:NE2	2.49	0.59
1:B:406:GLN:OE1	1:B:415:ILE:N	2.31	0.59
1:C:514:LEU:O	1:C:516:HIS:ND1	2.32	0.59
1:B:614:CYS:HA	1:B:617:VAL:HG12	1.83	0.59
1:A:368:LEU:HD12	1:A:371:PHE:HE1	1.67	0.59
1:B:228:ILE:HD12	1:B:230:ILE:HG12	1.84	0.59
1:B:611:GLY:O	1:B:612:VAL:HG13	2.03	0.59
1:A:19:THR:O	1:A:20:THR:OG1	2.16	0.58
1:B:415:ILE:HD11	1:B:419:ASN:HD22	1.68	0.58
1:A:61:ASN:HD21	3:A:1308:NAG:H5	1.66	0.58
1:B:469:ILE:H	1:B:469:ILE:HD12	1.68	0.58
1:B:513:GLU:OE2	1:B:516:HIS:ND1	2.36	0.58
1:C:497:THR:HG22	1:C:497:THR:O	2.03	0.58
1:A:321:GLU:HG3	1:A:536:VAL:HG12	1.85	0.58
1:A:376:CYS:HA	1:A:429:CYS:HB2	1.86	0.58
1:C:103:ILE:HG12	1:C:238:LEU:HD11	1.86	0.58
1:A:437:LYS:HG3	1:A:438:LEU:HD12	1.86	0.57
1:B:445:ASN:OD1	1:B:447:ASN:ND2	2.38	0.57
1:A:760:LEU:HD22	1:A:1005:VAL:HG21	1.87	0.57
1:B:242:HIS:O	1:B:256:THR:N	2.35	0.57
1:C:212:ASP:OD1	1:C:213:LEU:N	2.36	0.57
1:B:613:ASN:O	1:B:616:GLU:HB3	2.05	0.57
1:A:180:ASN:OD1	1:A:207:VAL:HG12	2.04	0.56
1:A:390:THR:HG22	1:A:391:ASN:N	2.20	0.56
1:C:115:LEU:HD12	1:C:232:ILE:HD11	1.87	0.56
1:C:609:TYR:OH	1:C:631:ARG:NH2	2.38	0.56
1:A:335:PHE:CE1	1:A:355:ILE:HG21	2.40	0.56
1:B:182:LYS:O	1:B:204:PRO:HA	2.04	0.56
1:A:142:LYS:HD2	1:A:142:LYS:O	2.04	0.56
1:C:128:VAL:HG23	1:C:128:VAL:O	2.04	0.56
1:C:77:PHE:HZ	1:C:239:LEU:HD22	1.70	0.56
1:C:983:PRO:O	1:C:987:GLU:OE1	2.23	0.56
1:A:449:LEU:HG	1:A:489:LEU:HD21	1.87	0.56
1:B:406:GLN:HB2	1:B:415:ILE:HG22	1.88	0.56
1:B:19:THR:HG22	1:B:20:THR:N	2.19	0.56
1:C:99:ILE:HG23	1:C:99:ILE:O	2.05	0.56
2:E:1:NAG:O7	2:E:1:NAG:O3	2.23	0.56
1:A:22:THR:HG23	1:A:74:THR:HA	1.88	0.56
1:B:63:THR:HG22	1:B:64:TRP:N	2.21	0.56
1:C:1113:THR:HG22	1:C:1135:TYR:HB3	1.86	0.56
1:A:405:ARG:NH2	1:A:411:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH2	1:B:78:ASP:OD1	2.39	0.55
1:C:305:VAL:HG22	1:C:599:THR:HG23	1.88	0.55
1:C:845:ASP:OD1	1:C:846:LEU:N	2.39	0.55
1:B:68:ILE:C	1:B:257:ALA:HB3	2.26	0.55
1:A:329:ILE:O	1:A:329:ILE:HG13	2.07	0.54
1:B:243:ARG:NE	1:B:254:GLY:O	2.40	0.54
1:B:714:ASN:OD1	2:I:1:NAG:O5	2.24	0.54
1:C:723:ILE:HD13	1:C:1058:VAL:HG22	1.89	0.54
1:A:376:CYS:HA	1:A:429:CYS:CB	2.38	0.54
1:C:618:PRO:O	1:C:619:VAL:HG13	2.08	0.54
1:B:407:ILE:HG23	1:B:407:ILE:O	2.08	0.54
1:C:243:ARG:HA	1:C:247:THR:HG21	1.89	0.54
1:A:143:ASN:HD22	1:A:144:ASN:N	2.05	0.54
1:A:352:ARG:HD3	1:A:395:ASP:OD1	2.07	0.54
1:C:236:GLN:NE2	1:C:237:THR:O	2.40	0.54
2:J:1:NAG:O7	2:J:1:NAG:C3	2.56	0.54
1:B:399:ILE:CD1	1:B:415:ILE:HD13	2.38	0.54
1:C:167:SER:OG	1:C:168:GLN:N	2.41	0.54
1:B:66:HIS:CE1	1:B:68:ILE:HG23	2.43	0.53
1:C:115:LEU:HD12	1:C:232:ILE:CG1	2.38	0.53
1:B:243:ARG:HG2	1:B:255:TRP:HA	1.89	0.53
1:A:520:THR:HG22	1:A:520:THR:O	2.08	0.53
1:A:635:THR:HG23	1:A:636:GLY:N	2.24	0.53
1:A:317:VAL:HG22	1:A:319:PRO:HD3	1.90	0.53
1:C:115:LEU:HD23	1:C:128:VAL:CG1	2.37	0.53
1:B:67:VAL:CG1	1:B:257:ALA:HB1	2.39	0.53
1:C:427:THR:HG23	1:C:427:THR:O	2.08	0.53
1:A:143:ASN:ND2	1:A:144:ASN:N	2.56	0.53
1:A:290:LEU:O	1:A:629:THR:OG1	2.22	0.53
1:B:845:ASP:OD1	1:B:846:LEU:N	2.41	0.53
1:B:113:GLN:NE2	1:B:128:VAL:O	2.42	0.52
1:B:208:ARG:HD2	1:B:209:GLU:N	2.24	0.52
1:A:673:THR:O	1:A:673:THR:HG22	2.08	0.52
1:B:19:THR:CG2	1:B:20:THR:H	2.21	0.52
1:B:175:GLU:OE1	1:B:175:GLU:N	2.39	0.52
1:B:436:ASN:ND2	1:B:503:GLN:OE1	2.42	0.52
1:C:292:PRO:HG3	1:C:633:TYR:CE2	2.44	0.52
1:A:535:CYS:HB3	1:A:548:VAL:HG22	1.91	0.52
1:A:623:ALA:HA	1:A:626:LEU:HD13	1.92	0.52
1:B:375:LYS:NZ	1:B:377:TYR:OH	2.43	0.52
1:C:103:ILE:CD1	1:C:116:LEU:HD23	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ASN:OD1	1:C:475:LYS:N	2.39	0.52
1:C:488:PRO:HG2	1:C:489:LEU:HD12	1.91	0.52
1:A:723:ILE:CD1	1:A:1058:VAL:HG22	2.39	0.52
1:C:470:TYR:CD1	1:C:471:GLN:N	2.78	0.52
1:C:315:PHE:CE2	1:C:590:GLY:HA3	2.45	0.52
1:A:714:ASN:HB2	1:A:1067:ALA:HB3	1.91	0.51
1:C:113:GLN:NE2	1:C:128:VAL:HG23	2.25	0.51
1:B:851:LYS:HZ1	1:B:856:THR:HG23	1.74	0.51
1:C:453:PHE:HB3	1:C:470:TYR:CD2	2.45	0.51
1:B:24:LEU:HB3	1:B:76:ARG:HH12	1.74	0.51
1:B:305:VAL:HG22	1:B:599:THR:HG23	1.92	0.51
1:A:471:GLN:HG2	1:A:475:LYS:O	2.11	0.51
1:C:107:THR:HG23	1:C:109:ASP:H	1.76	0.51
1:B:851:LYS:NZ	1:B:856:THR:HG23	2.25	0.51
1:B:255:TRP:HZ3	1:B:257:ALA:HB2	1.74	0.51
2:J:1:NAG:O7	2:J:1:NAG:H3	2.09	0.51
1:A:437:LYS:CG	1:A:438:LEU:HD12	2.41	0.51
1:B:151:GLU:OE2	1:B:153:ARG:HD3	2.10	0.51
1:B:537:ASN:OD1	1:B:537:ASN:O	2.28	0.51
1:B:565:ASP:HB3	1:B:571:ASP:OD2	2.10	0.51
1:A:24:LEU:HD22	1:A:76:ARG:NH1	2.24	0.51
1:B:517:ALA:HB1	1:B:518:PRO:HD2	1.92	0.51
1:A:405:ARG:NH1	1:A:412:THR:O	2.42	0.51
1:A:451:ARG:NH1	1:A:464:ASP:OD2	2.44	0.51
1:B:168:GLN:NE2	1:B:169:PRO:O	2.44	0.51
1:C:983:PRO:O	1:C:986:ALA:N	2.43	0.51
1:C:113:GLN:HG3	1:C:129:CYS:HA	1.92	0.50
1:A:459:LYS:HD2	1:A:460:PRO:HD2	1.93	0.50
1:B:401:GLY:O	1:B:404:VAL:HG22	2.11	0.50
1:C:388:CYS:HA	1:C:522:CYS:HB2	1.93	0.50
1:A:348:TYR:HA	1:A:419:ASN:HB3	1.92	0.50
1:A:356:SER:HA	1:A:521:VAL:HG21	1.93	0.50
1:A:497:THR:HG22	1:A:497:THR:O	2.12	0.50
1:B:617:VAL:HG13	1:B:618:PRO:HD3	1.92	0.50
1:A:987:GLU:OE1	1:A:987:GLU:HA	2.12	0.50
1:B:442:VAL:O	1:B:495:ARG:NE	2.44	0.50
1:C:192:ILE:HD11	1:C:197:LYS:NZ	2.27	0.50
1:B:140:ASP:OD2	1:B:153:ARG:HB2	2.12	0.50
1:B:339:PHE:CE1	1:B:508:VAL:HG11	2.43	0.50
1:A:402:ASP:N	1:A:501:GLY:O	2.45	0.50
1:A:435:SER:OG	1:A:506:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:CYS:HB2	1:A:1129:ILE:HD13	1.94	0.50
1:C:19:THR:HG22	1:C:20:THR:N	2.26	0.50
1:A:1089:GLU:O	1:A:1089:GLU:HG3	2.11	0.50
1:C:98:ILE:HG22	1:C:98:ILE:O	2.11	0.50
1:B:295:GLU:OE1	1:B:631:ARG:NH2	2.43	0.49
1:C:81:VAL:HG12	1:C:234:ARG:CD	2.42	0.49
1:C:834:TYR:CE1	1:C:851:LYS:HE3	2.46	0.49
1:C:1054:PRO:O	1:C:1055:HIS:HB2	2.12	0.49
1:B:160:ASN:OD1	1:B:160:ASN:O	2.30	0.49
1:A:32:PHE:O	1:A:33:THR:OG1	2.24	0.49
1:B:98:ILE:HG22	1:B:239:LEU:CD1	2.42	0.49
1:B:938:THR:O	1:B:940:SER:N	2.41	0.49
1:C:760:LEU:HD22	1:C:1005:VAL:HG21	1.94	0.49
1:A:61:ASN:HD21	3:A:1308:NAG:C1	2.10	0.49
1:C:706:ASN:OD1	1:C:706:ASN:N	2.34	0.49
1:C:940:SER:OG	1:C:941:ALA:N	2.43	0.49
1:C:18:LEU:HD11	1:C:138:PHE:CE1	2.47	0.49
1:C:201:LYS:HB2	1:C:220:LEU:HD23	1.93	0.49
1:A:53:ASP:OD1	1:A:54:LEU:N	2.43	0.49
1:B:98:ILE:HA	1:B:240:ALA:HB3	1.94	0.49
1:C:100:ARG:O	1:C:119:ASN:HB3	2.13	0.49
1:A:628:PRO:HG3	3:A:1308:NAG:H82	1.93	0.49
1:B:208:ARG:NH2	1:B:212:ASP:O	2.45	0.49
1:B:431:ILE:HB	1:B:508:VAL:CG1	2.43	0.49
1:C:789:PRO:O	1:C:792:LYS:NZ	2.45	0.49
1:A:340:ASN:OD1	1:A:340:ASN:O	2.31	0.49
1:A:372:PHE:HD2	1:A:373:THR:HG23	1.77	0.49
1:A:416:ALA:HA	1:A:420:TYR:O	2.13	0.49
1:C:443:SER:O	1:C:495:ARG:NH2	2.46	0.49
1:A:247:THR:HG22	1:A:256:THR:OG1	2.13	0.48
1:C:129:CYS:HB2	1:C:131:PHE:CZ	2.49	0.48
1:A:95:LYS:HD3	1:A:181:PHE:HD1	1.78	0.48
1:C:115:LEU:HG	1:C:230:ILE:HD11	1.94	0.48
3:C:1304:NAG:H3	3:C:1304:NAG:C8	2.39	0.48
1:A:223:LEU:HG	1:A:224:VAL:HG23	1.95	0.48
1:A:432:ALA:HB2	1:A:507:VAL:HG22	1.95	0.48
1:A:180:ASN:HD21	1:A:206:ILE:HG23	1.78	0.48
1:A:464:ASP:OD1	1:A:464:ASP:O	2.30	0.48
1:B:173:ASP:HB2	1:B:175:GLU:OE1	2.12	0.48
1:C:113:GLN:O	1:C:230:ILE:HD12	2.14	0.48
1:C:436:ASN:O	1:C:440:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:NH2	1:A:498:TYR:OH	2.46	0.48
1:C:37:TYR:HB3	1:C:220:LEU:HB2	1.95	0.48
1:C:81:VAL:HG12	1:C:234:ARG:HG2	1.95	0.48
1:C:434:ASN:OD1	1:C:435:SER:N	2.47	0.48
1:A:463:ARG:HD2	1:A:465:ILE:HD11	1.96	0.48
1:A:635:THR:HG23	1:A:636:GLY:H	1.79	0.48
1:B:406:GLN:OE1	1:B:414:ASN:N	2.47	0.48
1:B:398:VAL:HG23	1:B:448:TYR:CE2	2.48	0.48
1:C:1132:ASN:OD1	1:C:1133:THR:N	2.44	0.48
1:B:632:VAL:HG22	1:B:632:VAL:O	2.14	0.48
1:C:1122:ASN:ND2	1:C:1124:ASP:OD2	2.46	0.48
1:A:305:VAL:H	1:A:599:THR:HG22	1.79	0.48
1:A:827:ASP:O	1:A:827:ASP:OD1	2.32	0.48
1:C:140:ASP:O	1:C:149:GLU:HG2	2.13	0.48
1:C:528:THR:HG22	1:C:529:ASN:N	2.29	0.48
1:A:840:ASP:OD1	1:A:844:ARG:NH2	2.45	0.47
1:A:1071:ASN:OD1	3:A:1307:NAG:N2	2.46	0.47
1:B:328:ASN:OD1	1:B:328:ASN:O	2.32	0.47
1:C:113:GLN:HE21	1:C:128:VAL:HG23	1.79	0.47
1:A:342:THR:O	1:A:343:ARG:CZ	2.62	0.47
1:A:344:PHE:HE2	1:A:508:VAL:HG13	1.78	0.47
1:A:613:ASN:OD1	1:A:613:ASN:N	2.46	0.47
1:A:1054:PRO:O	1:A:1055:HIS:HB2	2.13	0.47
1:A:992:ARG:HH22	1:B:988:VAL:HG12	1.79	0.47
1:A:243:ARG:NH2	1:A:251:SER:O	2.48	0.47
1:C:115:LEU:HD12	1:C:232:ILE:HG13	1.97	0.47
1:C:201:LYS:CB	1:C:220:LEU:HD23	2.44	0.47
1:A:247:THR:O	1:A:247:THR:OG1	2.31	0.47
1:B:243:ARG:HA	1:B:247:THR:HG21	1.96	0.47
1:B:417:ASP:OD1	1:B:418:TYR:N	2.48	0.47
1:A:355:ILE:HB	1:A:392:VAL:HB	1.97	0.47
1:A:368:LEU:HD12	1:A:371:PHE:CE1	2.50	0.47
1:A:449:LEU:HD13	1:A:491:SER:HA	1.97	0.47
1:B:405:ARG:O	1:B:411:GLN:NE2	2.48	0.47
1:B:498:TYR:HB2	1:B:502:HIS:HB2	1.95	0.47
1:B:706:ASN:ND2	3:B:1306:NAG:C1	2.78	0.47
1:C:103:ILE:O	1:C:104:PHE:CG	2.68	0.47
1:C:375:LYS:NZ	1:C:377:TYR:CZ	2.83	0.47
1:C:487:PHE:O	1:C:490:ARG:NH1	2.44	0.47
1:C:1050:PRO:O	1:C:1051:GLN:NE2	2.42	0.47
1:A:451:ARG:CD	1:A:488:PRO:HB2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:MET:HG2	1:C:589:PHE:HE2	1.80	0.46
1:C:119:ASN:OD1	1:C:172:MET:SD	2.73	0.46
3:B:1303:NAG:C1	3:B:1303:NAG:H82	2.45	0.46
1:C:145:LYS:O	1:C:145:LYS:HG2	2.15	0.46
1:A:317:VAL:HG13	1:A:318:GLN:N	2.25	0.46
1:A:369:ALA:N	1:A:370:PRO:HD2	2.31	0.46
1:B:110:SER:HB3	1:B:132:GLN:HB2	1.96	0.46
1:C:364:VAL:HG23	1:C:365:LEU:HD12	1.97	0.46
1:A:723:ILE:HD13	1:A:1058:VAL:HG22	1.98	0.46
3:A:1308:NAG:O7	3:A:1308:NAG:H3	2.16	0.46
1:B:798:ASN:OD1	2:J:1:NAG:N2	2.48	0.46
1:C:102:TRP:HA	1:C:238:LEU:HD13	1.98	0.46
1:A:21:ARG:NH1	1:A:77:PHE:O	2.48	0.46
1:B:432:ALA:HA	1:B:506:ARG:O	2.16	0.46
1:C:489:LEU:O	1:C:490:ARG:CZ	2.64	0.46
3:C:1304:NAG:N2	3:C:1304:NAG:C5	2.72	0.46
1:A:372:PHE:CD2	1:A:373:THR:HG23	2.50	0.46
1:A:385:ASN:HA	1:A:523:GLY:HA3	1.97	0.46
1:B:115:LEU:CD1	1:B:228:ILE:HD13	2.46	0.46
1:A:95:LYS:HB3	1:A:177:LYS:HB3	1.97	0.46
1:A:352:ARG:HE	1:A:393:TYR:HB3	1.78	0.46
1:B:331:ASN:OD1	1:B:331:ASN:O	2.33	0.46
1:C:81:VAL:HG22	1:C:236:GLN:HG3	1.98	0.46
1:A:419:ASN:OD1	1:A:451:ARG:HB3	2.16	0.46
1:A:737:MET:HG2	1:C:589:PHE:CE2	2.50	0.46
1:A:242:HIS:O	1:A:256:THR:N	2.40	0.45
1:B:611:GLY:O	1:B:612:VAL:CG1	2.64	0.45
1:C:611:GLY:O	1:C:612:VAL:HG23	2.15	0.45
1:C:1139:GLN:N	1:C:1140:PRO:CD	2.79	0.45
1:B:454:ARG:NH1	1:B:455:LYS:HB3	2.31	0.45
1:B:631:ARG:HA	1:B:631:ARG:HH11	1.80	0.45
1:C:106:THR:HG23	1:C:107:THR:N	2.31	0.45
1:C:192:ILE:O	1:C:193:ASP:OD1	2.35	0.45
1:C:631:ARG:HG2	1:C:633:TYR:CE1	2.51	0.45
1:A:103:ILE:HG23	1:A:238:LEU:HD11	1.99	0.45
1:A:329:ILE:HD13	1:A:524:PRO:HB3	1.99	0.45
1:A:613:ASN:HB2	1:A:616:GLU:OE1	2.16	0.45
1:B:985:GLU:O	1:B:988:VAL:HG22	2.16	0.45
1:C:113:GLN:HG3	1:C:129:CYS:CA	2.45	0.45
1:B:376:CYS:HA	1:B:429:CYS:HA	1.98	0.45
1:C:115:LEU:CD2	1:C:128:VAL:HG12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:HG3	1:A:415:ILE:HD12	1.98	0.45
1:B:438:LEU:HD23	1:B:438:LEU:H	1.82	0.45
1:C:115:LEU:HD12	1:C:232:ILE:CD1	2.45	0.45
2:K:2:NAG:O7	2:K:2:NAG:C3	2.62	0.45
2:E:2:NAG:H2	2:E:2:NAG:C6	2.47	0.45
1:B:119:ASN:O	1:B:172:MET:HE1	2.17	0.45
1:C:129:CYS:O	1:C:131:PHE:N	2.48	0.45
1:A:436:ASN:HA	1:A:504:PRO:HG2	1.99	0.45
1:B:19:THR:O	1:B:20:THR:HG22	2.17	0.45
1:B:435:SER:O	1:B:439:ASP:OD1	2.35	0.45
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.52	0.45
1:A:326:PHE:O	1:A:577:GLN:NE2	2.43	0.44
1:B:344:PHE:CD2	1:B:398:VAL:HG13	2.51	0.44
1:B:714:ASN:HB3	1:B:1067:ALA:HB3	1.98	0.44
1:C:103:ILE:HG22	1:C:104:PHE:N	2.32	0.44
1:A:341:ALA:HB3	1:A:344:PHE:CE1	2.52	0.44
1:A:933:ASP:C	1:A:933:ASP:OD2	2.56	0.44
1:B:489:LEU:O	1:B:490:ARG:NH1	2.38	0.44
1:A:390:THR:CG2	1:A:391:ASN:H	2.27	0.44
1:A:983:PRO:N	1:A:984:PRO:HD2	2.32	0.44
1:C:74:THR:OG1	1:C:75:LYS:N	2.50	0.44
1:C:362:TYR:HH	1:C:366:TYR:HE1	1.57	0.44
1:A:331:ASN:O	1:A:359:VAL:HG23	2.17	0.44
1:A:867:ILE:O	1:A:871:THR:HG23	2.18	0.44
1:B:578:THR:HG22	1:B:578:THR:O	2.17	0.44
1:B:589:PHE:O	1:C:834:TYR:HE2	1.99	0.44
1:C:471:GLN:HG2	1:C:476:PRO:HA	1.99	0.44
1:C:128:VAL:HG22	1:C:163:PHE:HB3	1.99	0.44
1:A:61:ASN:ND2	3:A:1308:NAG:O5	2.46	0.44
1:A:399:ILE:HG22	1:A:415:ILE:HD13	2.00	0.44
1:C:120:ASN:ND2	1:C:149:GLU:OE1	2.50	0.44
1:C:361:ASP:OD1	1:C:362:TYR:N	2.51	0.44
1:C:389:PHE:O	1:C:519:ALA:HB1	2.18	0.44
1:A:337:GLU:O	1:A:341:ALA:HB2	2.18	0.44
1:A:418:TYR:HA	1:A:454:ARG:HD3	2.00	0.44
1:A:938:THR:HG23	1:A:938:THR:O	2.17	0.44
1:B:79:ASN:N	1:B:80:PRO:HD3	2.32	0.44
1:B:983:PRO:N	1:B:984:PRO:HD2	2.32	0.44
1:C:77:PHE:HB3	1:C:255:TRP:HH2	1.82	0.44
1:C:296:THR:OG1	1:C:594:VAL:HG11	2.18	0.44
1:A:61:ASN:ND2	3:A:1308:NAG:C5	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ALA:CB	1:A:507:VAL:HG22	2.48	0.44
1:C:617:VAL:HG12	1:C:617:VAL:O	2.17	0.44
2:H:2:NAG:H3	2:H:2:NAG:C8	2.45	0.44
1:B:446:TYR:O	1:B:446:TYR:CD2	2.71	0.43
1:C:32:PHE:HD2	1:C:215:GLN:HG2	1.81	0.43
1:C:469:ILE:CG2	1:C:485:CYS:HB3	2.48	0.43
1:A:75:LYS:HE2	1:A:257:ALA:HB2	2.00	0.43
1:B:446:TYR:HB2	1:B:491:SER:HB3	2.00	0.43
1:B:140:ASP:O	1:B:141:HIS:C	2.56	0.43
1:B:637:SER:O	1:B:638:ASN:HB2	2.18	0.43
1:A:403:GLU:OE2	1:A:403:GLU:HA	2.19	0.43
1:B:93:ILE:O	1:B:93:ILE:HG23	2.18	0.43
1:B:617:VAL:CG1	1:B:618:PRO:HD3	2.48	0.43
1:C:99:ILE:O	1:C:99:ILE:CG2	2.67	0.43
1:C:107:THR:O	1:C:108:LEU:HB2	2.18	0.43
1:B:752:GLN:OE1	1:B:752:GLN:HA	2.19	0.43
1:C:107:THR:HG21	1:C:111:LYS:HB3	2.01	0.43
1:C:938:THR:OG1	1:C:941:ALA:HB2	2.18	0.43
1:C:1097:THR:HG1	1:C:1098:HIS:CE1	2.35	0.43
1:A:61:ASN:HD21	3:A:1308:NAG:C5	2.30	0.43
1:A:207:VAL:HG13	1:A:208:ARG:H	1.84	0.43
1:B:213:LEU:HD23	1:B:213:LEU:H	1.84	0.43
1:B:398:VAL:HG12	1:B:506:ARG:HG2	1.99	0.43
1:C:81:VAL:HG12	1:C:234:ARG:CG	2.49	0.43
1:A:458:LEU:HD21	1:A:462:GLU:O	2.18	0.43
1:B:98:ILE:N	1:B:98:ILE:HD12	2.34	0.43
1:B:142:LYS:HZ2	1:B:243:ARG:NH1	2.16	0.43
1:C:67:VAL:O	1:C:259:ALA:HA	2.17	0.43
1:C:934:SER:O	1:C:938:THR:HG23	2.17	0.43
1:A:344:PHE:CE2	1:A:508:VAL:HG13	2.52	0.43
1:A:364:VAL:HG12	1:A:368:LEU:HD21	2.01	0.43
1:A:398:VAL:HG21	1:A:448:TYR:CE2	2.53	0.43
1:B:66:HIS:O	1:B:76:ARG:HG3	2.18	0.43
1:B:243:ARG:HH12	1:B:251:SER:HA	1.84	0.43
1:A:74:THR:O	1:A:75:LYS:HB2	2.19	0.43
1:A:507:VAL:HG12	1:A:509:VAL:HG23	2.00	0.43
1:A:927:ALA:O	1:A:931:ILE:HG12	2.19	0.43
1:B:30:ASN:HD22	1:B:32:PHE:HE1	1.67	0.43
1:B:847:ILE:O	1:B:847:ILE:HG22	2.18	0.43
1:C:137:PRO:CB	1:C:154:VAL:HG13	2.48	0.43
1:C:246:LEU:O	1:C:246:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HG22	1:A:420:TYR:HB3	2.01	0.43
1:A:550:THR:HG22	1:A:551:GLU:N	2.34	0.43
1:B:349:ALA:HA	1:B:465:ILE:HD11	2.00	0.43
1:B:375:LYS:O	1:B:429:CYS:HA	2.19	0.43
1:C:231:ASN:O	1:C:232:ILE:HD13	2.18	0.43
1:C:348:TYR:HE1	1:C:449:LEU:HB2	1.84	0.43
1:A:34:ARG:NH1	1:A:186:GLU:OE2	2.51	0.42
1:A:474:ASN:OD1	1:A:474:ASN:O	2.37	0.42
1:B:400:ARG:HG2	1:B:494:PHE:CE1	2.54	0.42
1:C:980:ARG:O	1:C:981:LEU:HG	2.18	0.42
1:A:96:SER:O	1:A:96:SER:OG	2.30	0.42
1:A:392:VAL:HG22	1:A:512:PHE:CD1	2.53	0.42
1:A:451:ARG:HD3	1:A:488:PRO:O	2.19	0.42
1:B:223:LEU:HG	1:B:224:VAL:HG23	2.01	0.42
1:B:337:GLU:OE2	1:B:337:GLU:N	2.52	0.42
1:B:614:CYS:CA	1:B:617:VAL:HG12	2.49	0.42
1:C:850:GLN:HG2	1:C:960:VAL:HG21	2.00	0.42
1:B:733:VAL:HG23	1:B:855:LEU:HD23	2.02	0.42
1:C:127:LYS:HD2	1:C:155:TYR:OH	2.20	0.42
1:C:231:ASN:OD1	1:C:232:ILE:N	2.53	0.42
2:L:2:NAG:C1	2:L:2:NAG:H82	2.48	0.42
1:A:173:ASP:HB2	1:A:175:GLU:OE1	2.19	0.42
1:B:958:THR:HG21	1:C:759:GLN:HE21	1.84	0.42
1:C:143:ASN:ND2	1:C:147:TRP:CZ2	2.88	0.42
1:A:348:TYR:CE1	1:A:449:LEU:HB2	2.54	0.42
1:A:535:CYS:HB3	1:A:548:VAL:CG2	2.50	0.42
1:B:273:LEU:HB3	1:B:286:VAL:HG12	2.02	0.42
1:B:348:TYR:CD2	1:B:464:ASP:O	2.72	0.42
1:B:991:ASP:O	1:B:995:THR:HG23	2.20	0.42
1:C:194:GLY:HA2	1:C:229:GLY:HA2	2.01	0.42
1:C:469:ILE:HD12	1:C:469:ILE:H	1.85	0.42
1:C:553:ASN:OD1	1:C:553:ASN:O	2.37	0.42
1:A:364:VAL:O	1:A:364:VAL:CG1	2.66	0.42
1:A:627:THR:HG22	1:A:629:THR:H	1.84	0.42
1:A:614:CYS:CA	1:A:617:VAL:HG23	2.49	0.42
1:B:174:LEU:HG	1:B:174:LEU:O	2.19	0.42
1:B:1141:GLU:HA	1:B:1141:GLU:OE1	2.19	0.42
1:C:67:VAL:O	1:C:67:VAL:HG23	2.20	0.42
1:A:787:LYS:HE3	1:A:787:LYS:HB3	1.90	0.42
1:B:63:THR:CG2	1:B:64:TRP:N	2.82	0.42
1:B:364:VAL:HG23	1:B:365:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LYS:HD3	1:B:456:SER:HB3	2.01	0.42
1:C:373:THR:HG22	1:C:373:THR:O	2.20	0.42
1:C:497:THR:O	1:C:497:THR:CG2	2.67	0.42
1:A:143:ASN:HD22	1:A:144:ASN:H	1.68	0.42
1:A:367:ASN:OD1	1:A:367:ASN:O	2.38	0.42
1:A:619:VAL:HG12	1:A:619:VAL:O	2.20	0.42
1:A:761:LYS:HE3	1:A:761:LYS:HB3	1.79	0.42
3:B:1306:NAG:H83	3:B:1306:NAG:O4	2.20	0.42
1:C:723:ILE:HD12	1:C:1058:VAL:HG22	2.02	0.42
1:C:1099:TRP:HB2	1:C:1132:ASN:ND2	2.35	0.42
1:A:95:LYS:HD3	1:A:179:GLY:O	2.20	0.41
1:C:101:GLY:HA2	1:C:102:TRP:CE3	2.55	0.41
1:B:140:ASP:OD2	1:B:153:ARG:N	2.53	0.41
1:C:838:LEU:O	1:C:841:ILE:HB	2.19	0.41
1:A:143:ASN:ND2	1:A:143:ASN:C	2.73	0.41
1:A:578:THR:O	1:A:578:THR:HG22	2.19	0.41
1:B:126:ILE:HD13	1:B:165:TYR:HD2	1.85	0.41
1:B:801:GLN:OE1	1:B:932:GLN:OE1	2.37	0.41
1:A:368:LEU:O	1:C:483:PHE:HE2	2.04	0.41
1:A:441:LYS:HB2	1:A:445:ASN:HB2	2.03	0.41
1:C:816:GLU:OE2	1:C:1052:SER:OG	2.38	0.41
2:O:2:NAG:H3	2:O:2:NAG:C8	2.46	0.41
2:O:2:NAG:C1	2:O:2:NAG:H82	2.50	0.41
1:B:375:LYS:O	1:B:375:LYS:HG3	2.19	0.41
1:A:110:SER:HB2	1:A:132:GLN:HB2	2.03	0.41
1:A:845:ASP:OD1	1:A:846:LEU:N	2.54	0.41
1:A:21:ARG:HD2	1:A:77:PHE:O	2.20	0.41
1:A:336:ASP:O	1:A:340:ASN:N	2.48	0.41
1:A:469:ILE:CD1	1:A:485:CYS:SG	3.08	0.41
1:A:871:THR:O	1:A:875:LEU:HD13	2.21	0.41
1:B:450:TYR:HB3	1:B:492:TYR:CE1	2.56	0.41
3:C:1301:NAG:O7	3:C:1301:NAG:O3	2.31	0.41
1:A:818:LEU:O	1:A:822:LYS:HG3	2.21	0.41
1:B:364:VAL:HG23	1:B:365:LEU:N	2.35	0.41
1:C:1139:GLN:N	1:C:1140:PRO:HD2	2.36	0.41
2:H:2:NAG:C1	2:H:2:NAG:H82	2.50	0.41
1:A:386:ASP:HA	1:A:525:LYS:HG2	2.02	0.41
1:A:449:LEU:HD12	1:A:489:LEU:HD23	2.02	0.41
1:A:459:LYS:HD2	1:A:460:PRO:CD	2.50	0.41
1:A:808:LYS:NZ	1:A:817:ASP:OD2	2.53	0.41
1:A:933:ASP:OD2	1:A:933:ASP:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:HD3	1:B:502:HIS:HA	2.02	0.41
1:B:482:GLY:N	1:B:485:CYS:HB2	2.36	0.41
1:B:611:GLY:C	1:B:612:VAL:HG13	2.41	0.41
1:B:742:ASP:OD1	1:B:742:ASP:O	2.38	0.41
1:B:927:ALA:O	1:B:931:ILE:HG12	2.21	0.41
1:C:1123:CYS:HB2	1:C:1129:ILE:HD13	2.01	0.41
1:B:139:LEU:HD22	1:B:139:LEU:N	2.35	0.41
1:B:348:TYR:OH	1:B:489:LEU:HD22	2.21	0.41
1:B:368:LEU:HD23	1:B:369:ALA:HB2	2.03	0.41
1:C:103:ILE:HD12	1:C:116:LEU:HD23	2.02	0.41
1:C:128:VAL:O	1:C:128:VAL:CG2	2.68	0.41
1:C:241:LEU:O	1:C:243:ARG:N	2.54	0.41
2:L:2:NAG:H3	2:L:2:NAG:C8	2.48	0.41
1:A:146:SER:OG	1:A:148:MET:HG3	2.21	0.40
1:A:421:LYS:HE3	1:A:458:LEU:O	2.20	0.40
1:A:801:GLN:OE1	1:A:932:GLN:OE1	2.38	0.40
1:B:140:ASP:OD2	1:B:153:ARG:CB	2.69	0.40
1:C:113:GLN:HB3	1:C:230:ILE:HG21	2.03	0.40
1:C:1132:ASN:CG	1:C:1133:THR:H	2.23	0.40
3:C:1302:NAG:O4	3:C:1303:NAG:C1	2.70	0.40
1:A:143:ASN:HB3	1:A:148:MET:HE2	2.02	0.40
1:A:373:THR:O	1:A:373:THR:OG1	2.39	0.40
1:B:452:LEU:C	1:B:452:LEU:HD23	2.41	0.40
1:B:706:ASN:HD21	3:B:1306:NAG:C1	2.35	0.40
3:B:1303:NAG:O4	3:B:1303:NAG:H83	2.21	0.40
1:C:68:ILE:HD12	1:C:258:GLY:O	2.21	0.40
1:C:356:SER:HA	1:C:521:VAL:CG2	2.51	0.40
1:A:228:ILE:HG13	1:A:229:GLY:N	2.36	0.40
1:A:911:ASN:OD1	1:A:912:VAL:N	2.54	0.40
1:B:1136:ASP:O	1:B:1138:LEU:N	2.49	0.40
1:B:1025:LYS:NZ	1:B:1039:PHE:O	2.55	0.40
1:A:967:PHE:HA	1:B:753:TYR:HE1	1.87	0.40
1:B:167:SER:OG	1:B:168:GLN:N	2.54	0.40
1:B:296:THR:HA	1:B:299:THR:HG22	2.04	0.40
1:C:192:ILE:O	1:C:192:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1109/1231 (90%)	1026 (92%)	82 (7%)	1 (0%)	48	81
1	B	1083/1231 (88%)	1015 (94%)	68 (6%)	0	100	100
1	C	1097/1231 (89%)	1006 (92%)	91 (8%)	0	100	100
All	All	3289/3693 (89%)	3047 (93%)	241 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	HIS

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	975/1075 (91%)	970 (100%)	5 (0%)	86	94
1	B	959/1075 (89%)	957 (100%)	2 (0%)	92	97
1	C	967/1075 (90%)	965 (100%)	2 (0%)	92	97
All	All	2901/3225 (90%)	2892 (100%)	9 (0%)	90	96

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

Mol	Chain	Res	Type
1	A	142	LYS
1	A	143	ASN

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Mol	Chain	Res	Type
1	A	613	ASN
1	A	761	LYS
1	A	1116	ASN
1	B	14	GLN
1	B	631	ARG
1	C	14	GLN
1	C	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	503	GLN
1	A	801	GLN
1	B	434	ASN
1	B	436	ASN
1	B	447	ASN
1	B	503	GLN
1	B	560	GLN
1	B	706	ASN
1	C	951	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
2	NAG	D	2	2	14,14,15	0.20	0	17,19,21	0.50	0
2	NAG	E	1	1,2	14,14,15	0.77	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	1.47	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.25	0	17,19,21	0.54	0
2	NAG	F	2	2	14,14,15	0.17	0	17,19,21	0.49	0
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.44	0
2	NAG	G	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	H	1	1,2	14,14,15	0.24	0	17,19,21	0.53	0
2	NAG	H	2	2	14,14,15	0.26	0	17,19,21	0.91	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.84	1 (7%)	17,19,21	0.80	0
2	NAG	I	2	2	14,14,15	0.85	1 (7%)	17,19,21	2.04	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.17	0	17,19,21	0.84	1 (5%)
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	K	2	2	14,14,15	0.62	0	17,19,21	0.69	0
2	NAG	L	1	1,2	14,14,15	0.30	0	17,19,21	0.48	0
2	NAG	L	2	2	14,14,15	0.19	0	17,19,21	0.92	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.22	0	17,19,21	0.56	0
2	NAG	M	2	2	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	N	1	1,2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	O	1	1,2	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	O	2	2	14,14,15	0.30	0	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	6/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	6/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O5-C1	-2.86	1.38	1.43
2	I	1	NAG	O5-C1	2.69	1.48	1.43
2	E	1	NAG	O5-C1	-2.22	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C1-O5-C5	7.57	122.33	112.19
2	E	2	NAG	C1-O5-C5	5.62	119.72	112.19
2	J	2	NAG	C1-O5-C5	4.80	118.61	112.19
2	E	1	NAG	C1-O5-C5	3.44	116.80	112.19
2	O	2	NAG	C2-N2-C7	2.93	126.83	122.90
2	H	2	NAG	C2-N2-C7	2.82	126.68	122.90
2	L	2	NAG	C2-N2-C7	2.77	126.61	122.90
2	I	2	NAG	C3-C4-C5	2.72	115.16	110.23
2	D	1	NAG	C1-O5-C5	2.09	114.98	112.19
2	J	1	NAG	C2-N2-C7	2.03	125.62	122.90
2	J	2	NAG	C3-C4-C5	2.01	113.88	110.23

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7

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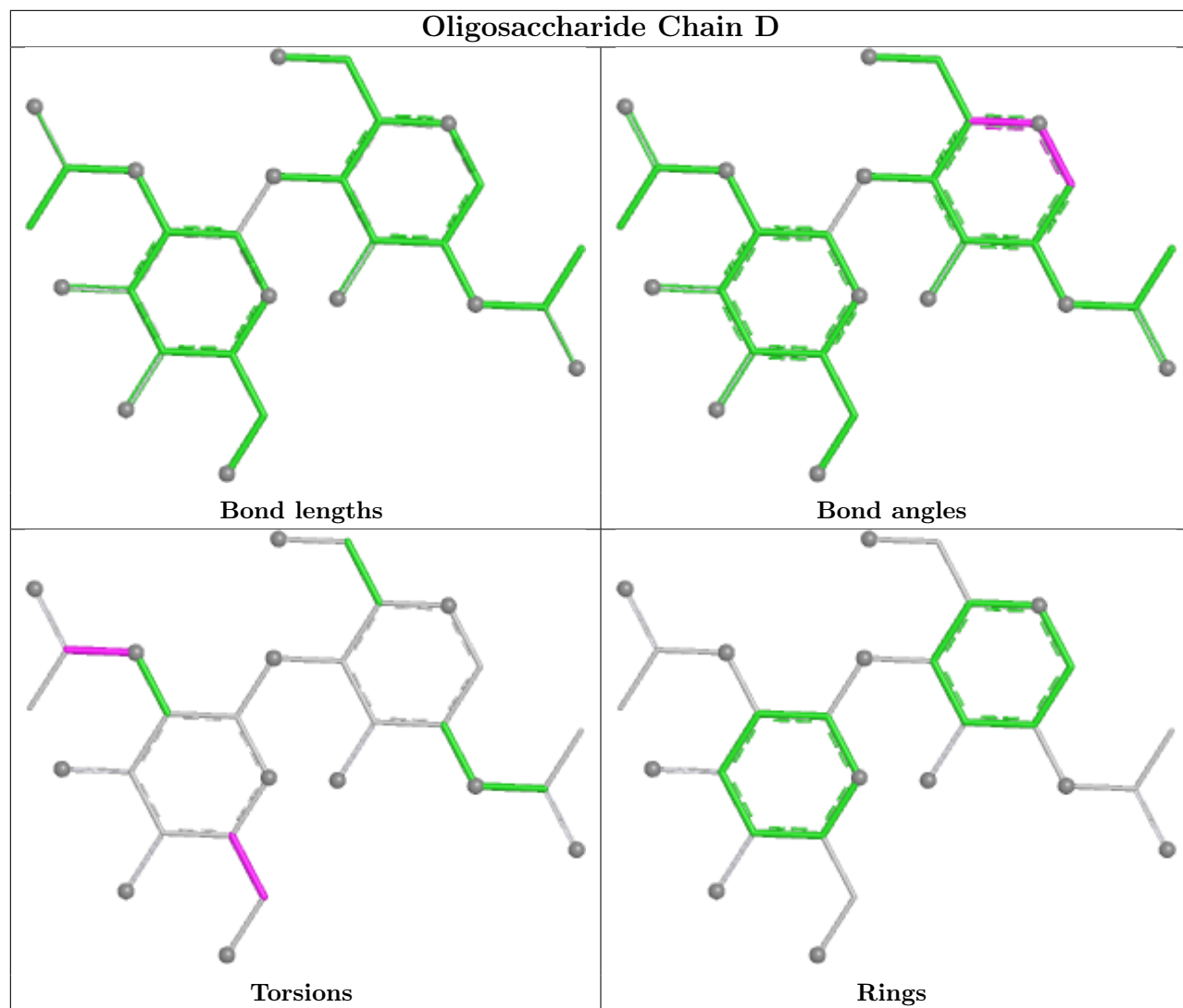
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7
2	M	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6

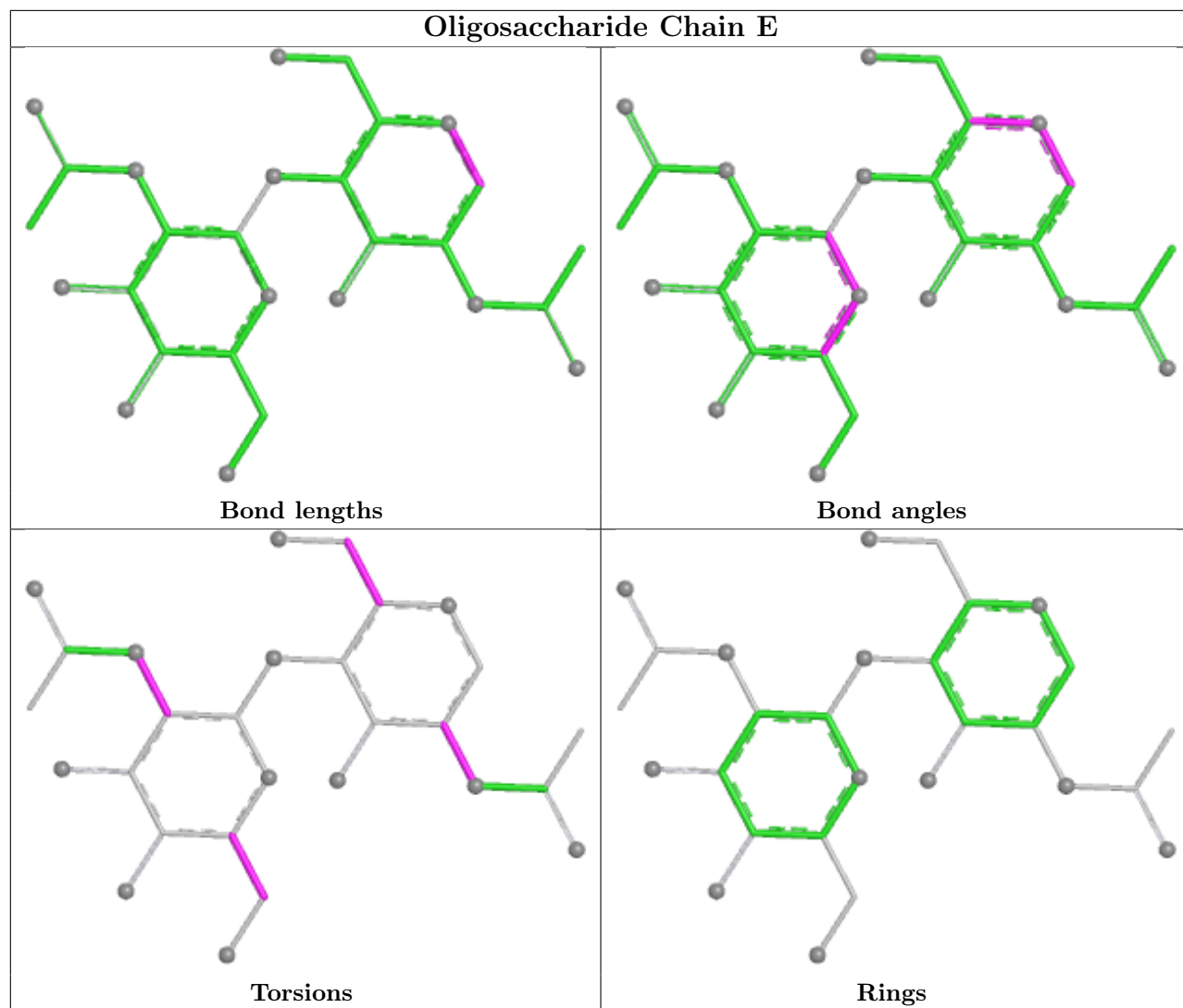
There are no ring outliers.

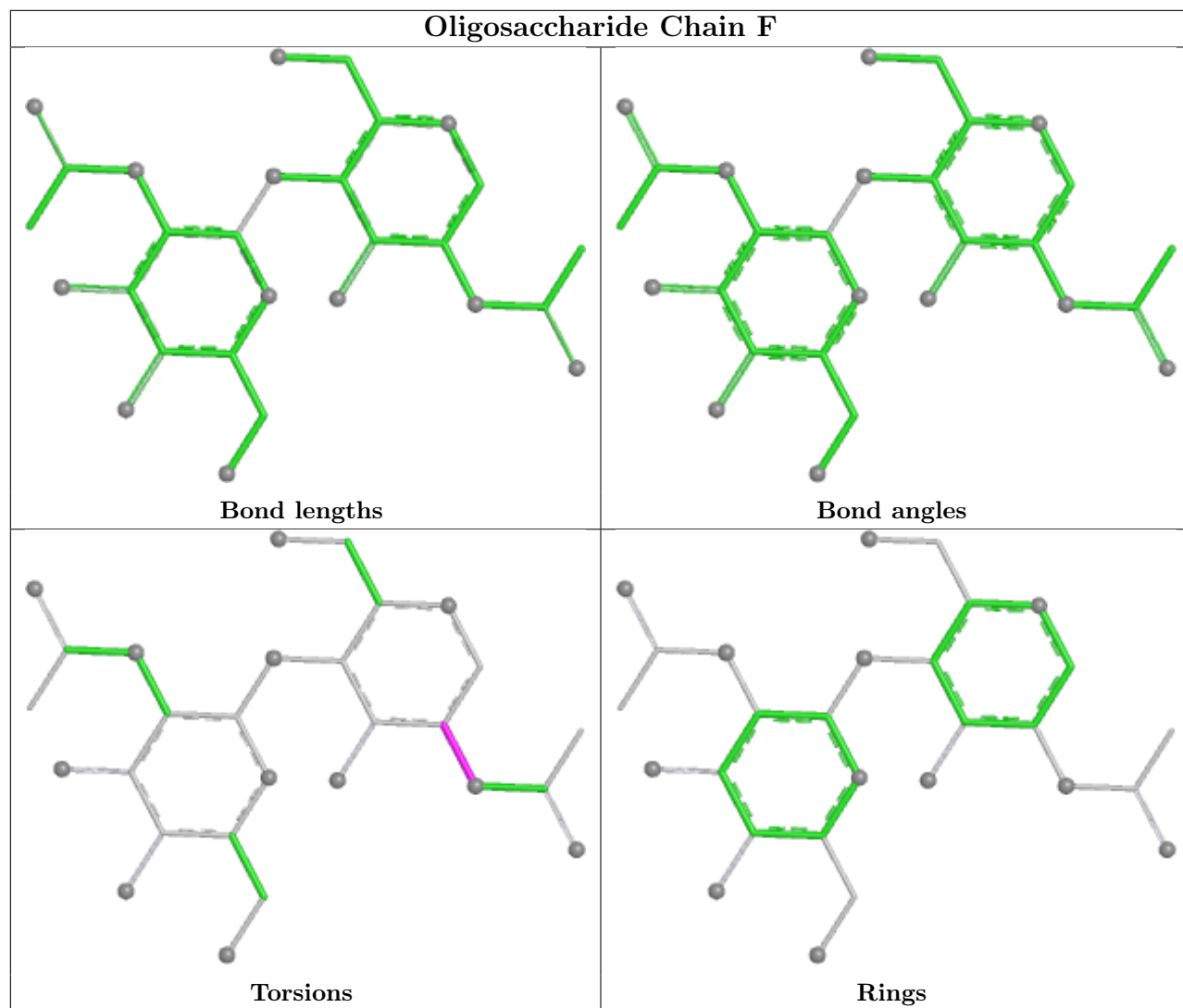
9 monomers are involved in 19 short contacts:

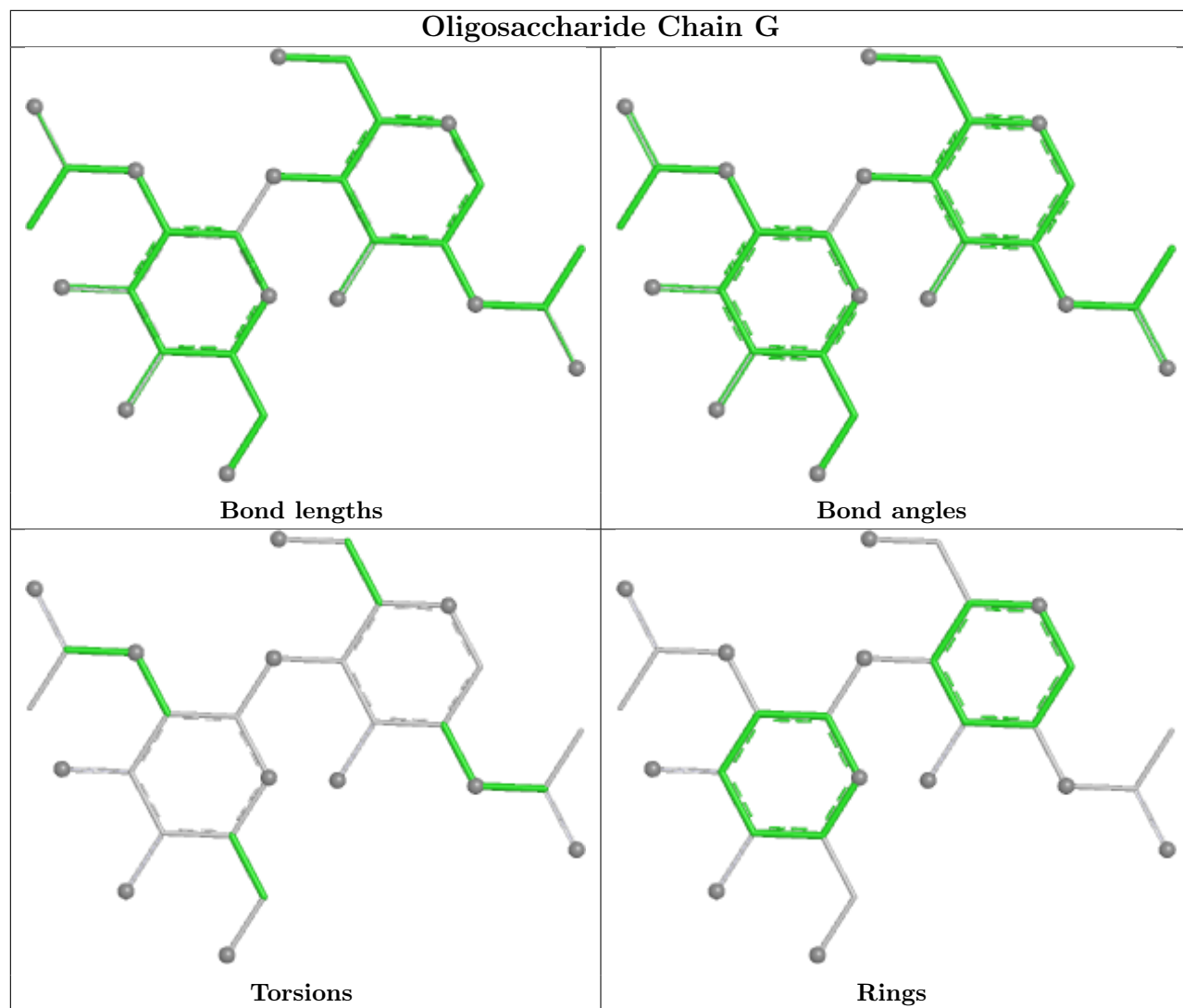
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	3	0
2	E	1	NAG	1	0
2	I	1	NAG	1	0
2	E	2	NAG	1	0
2	O	2	NAG	3	0
2	L	2	NAG	3	0
2	K	2	NAG	2	0
2	I	2	NAG	2	0
2	H	2	NAG	3	0

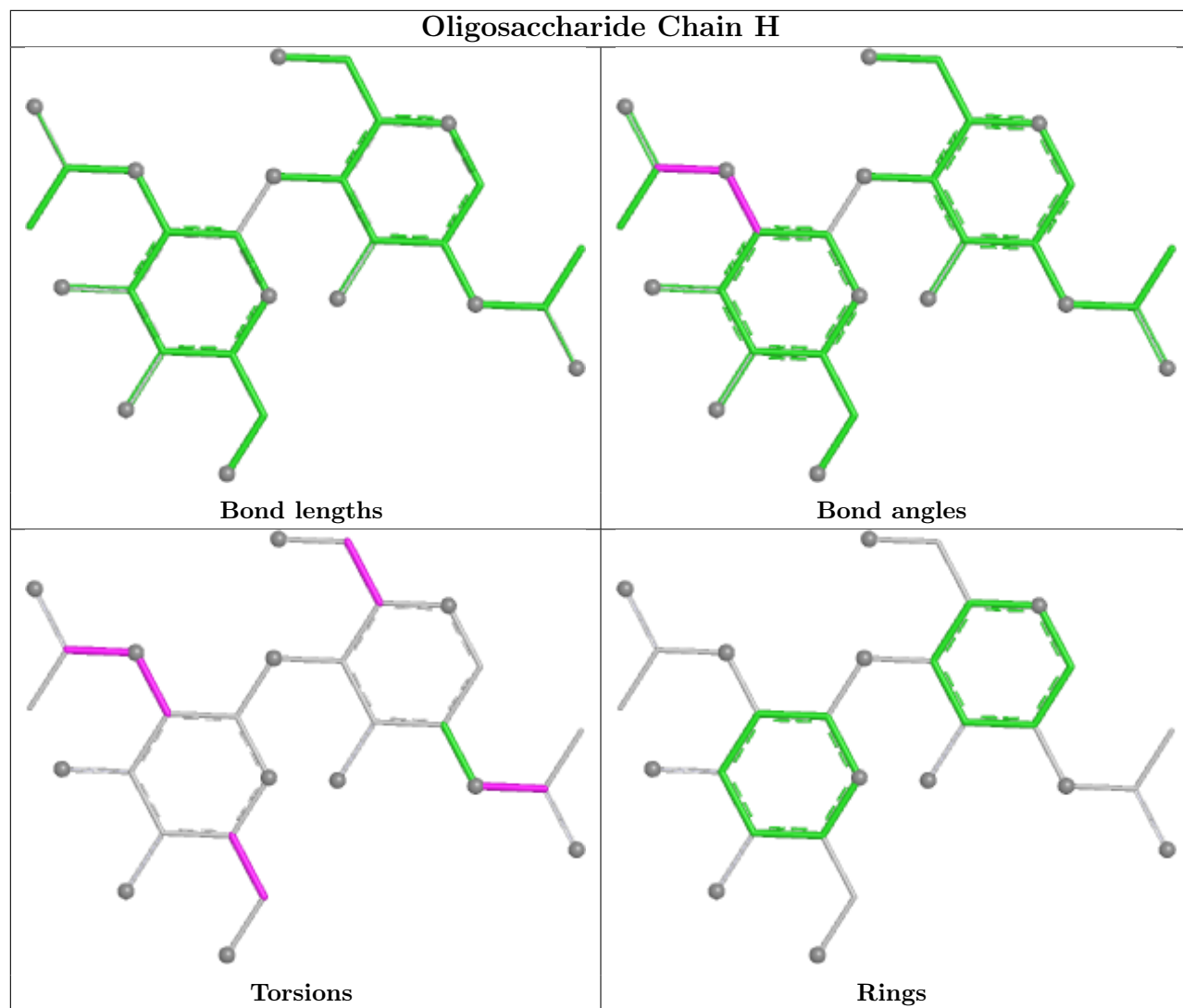
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

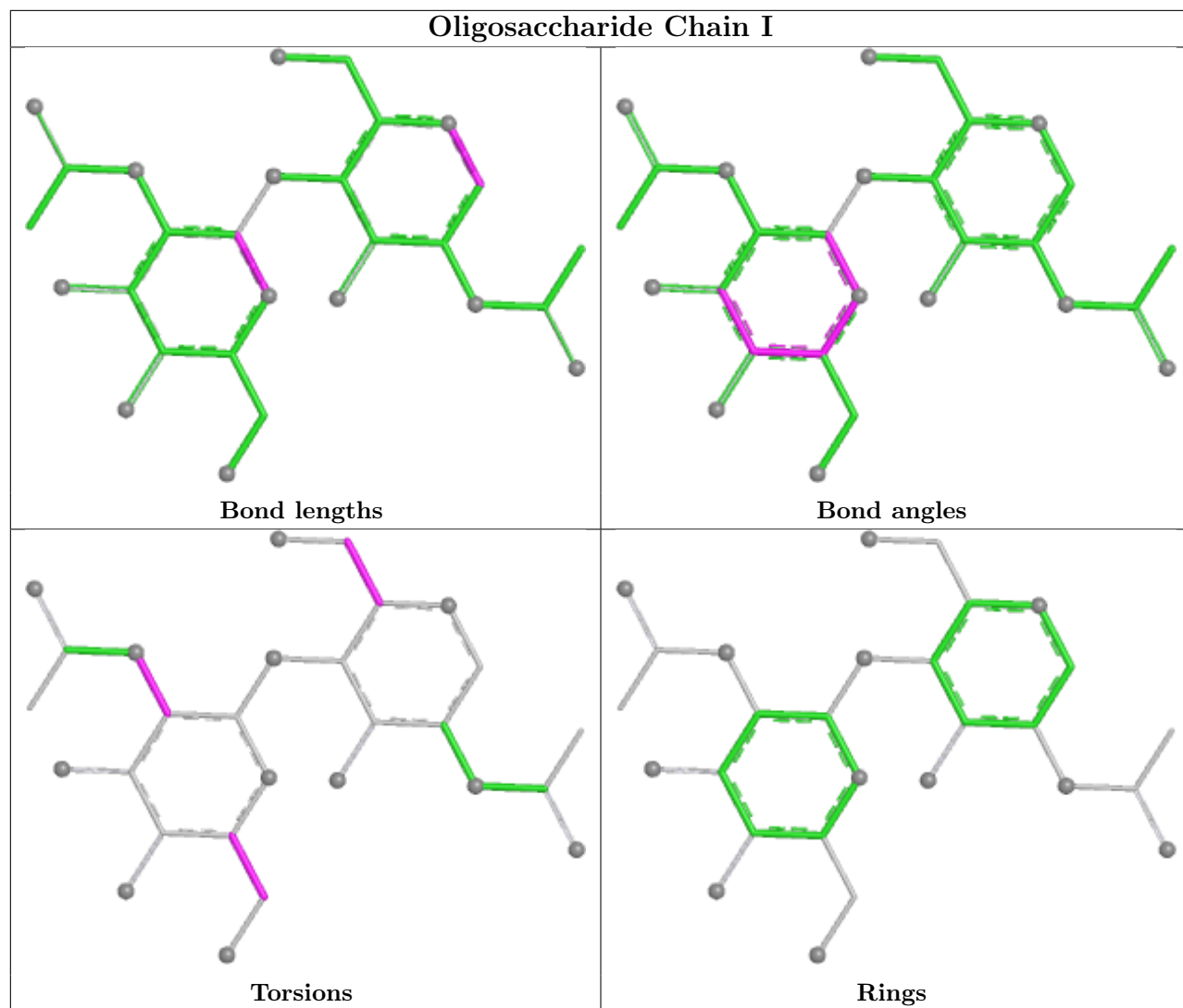


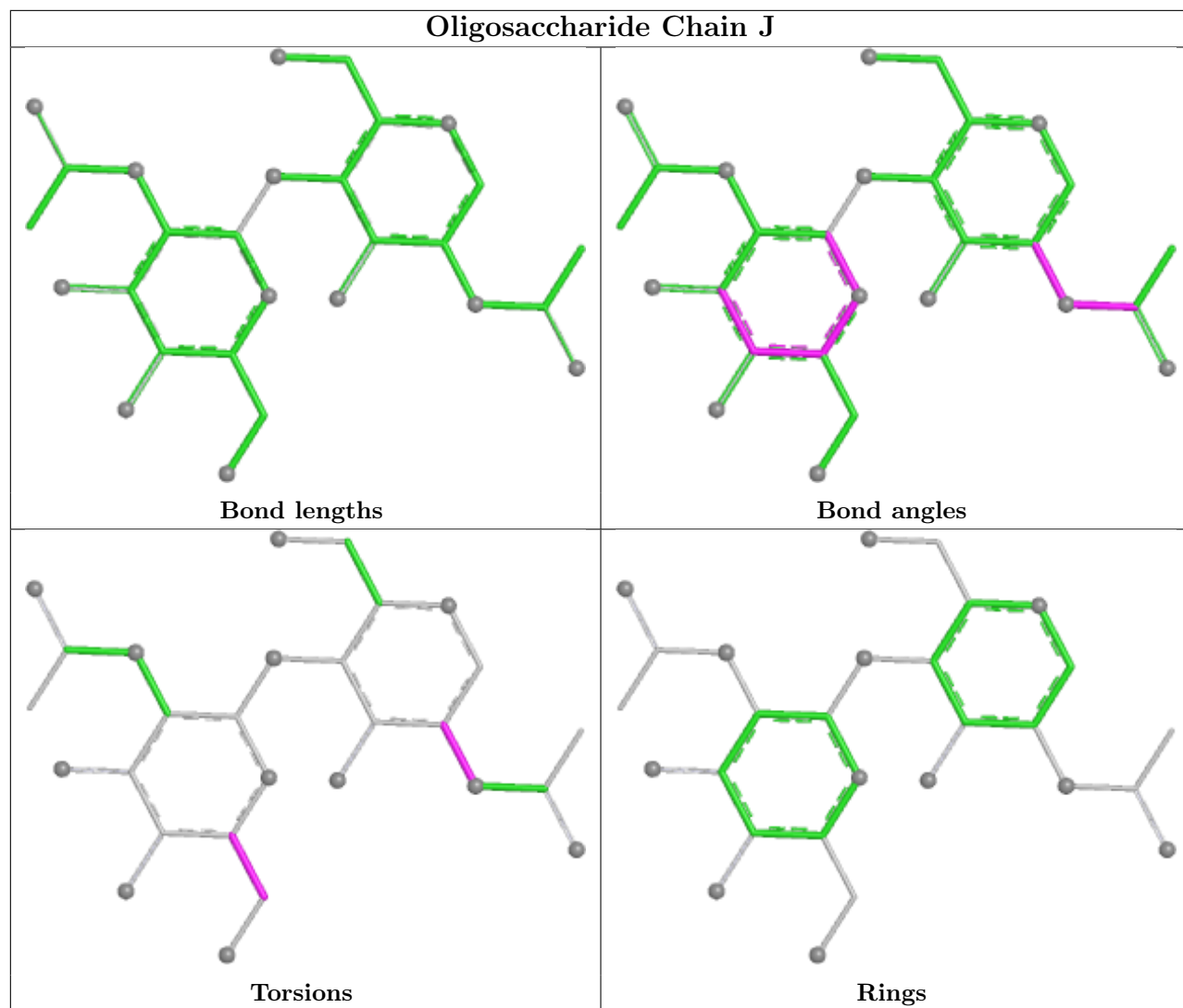


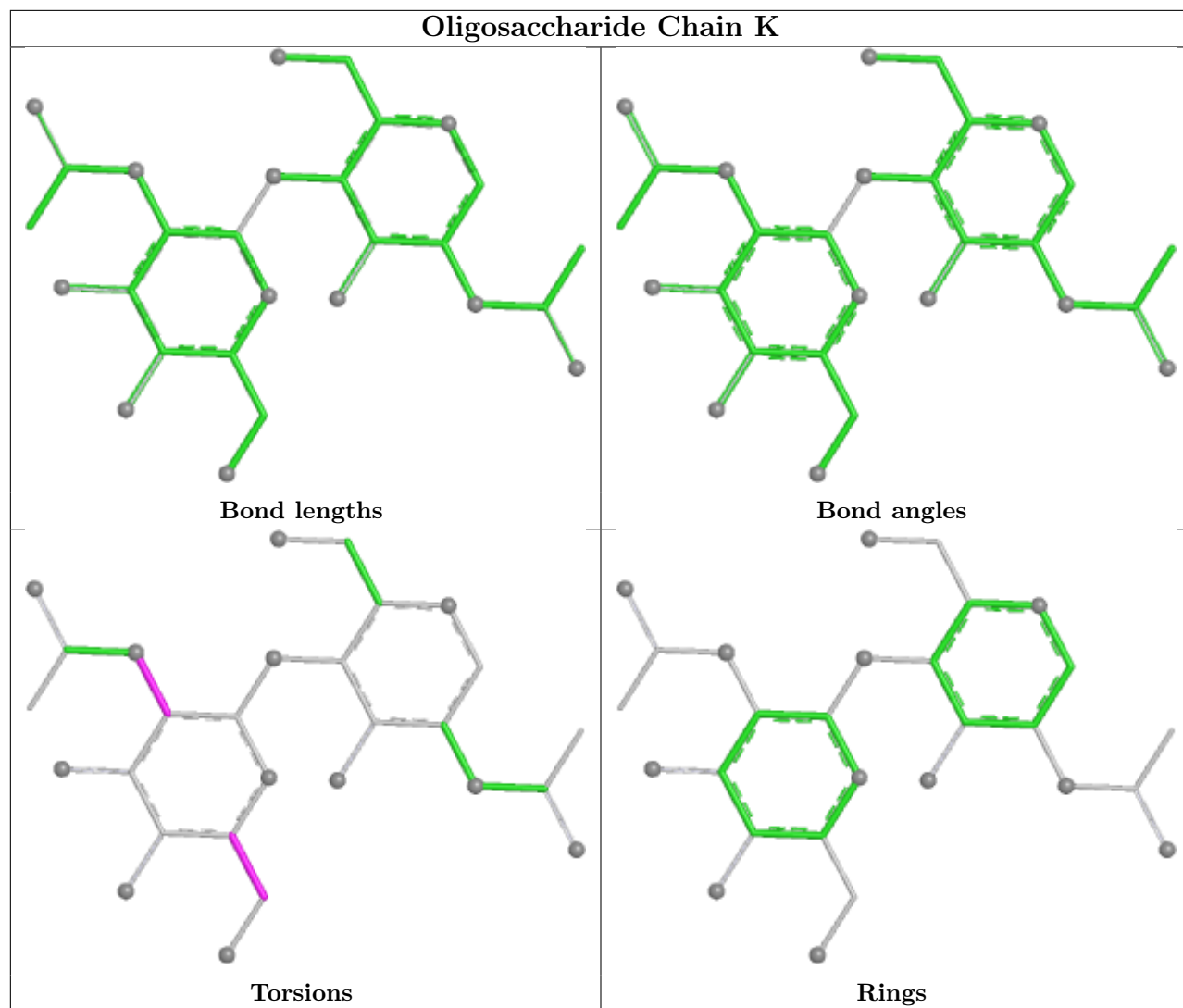


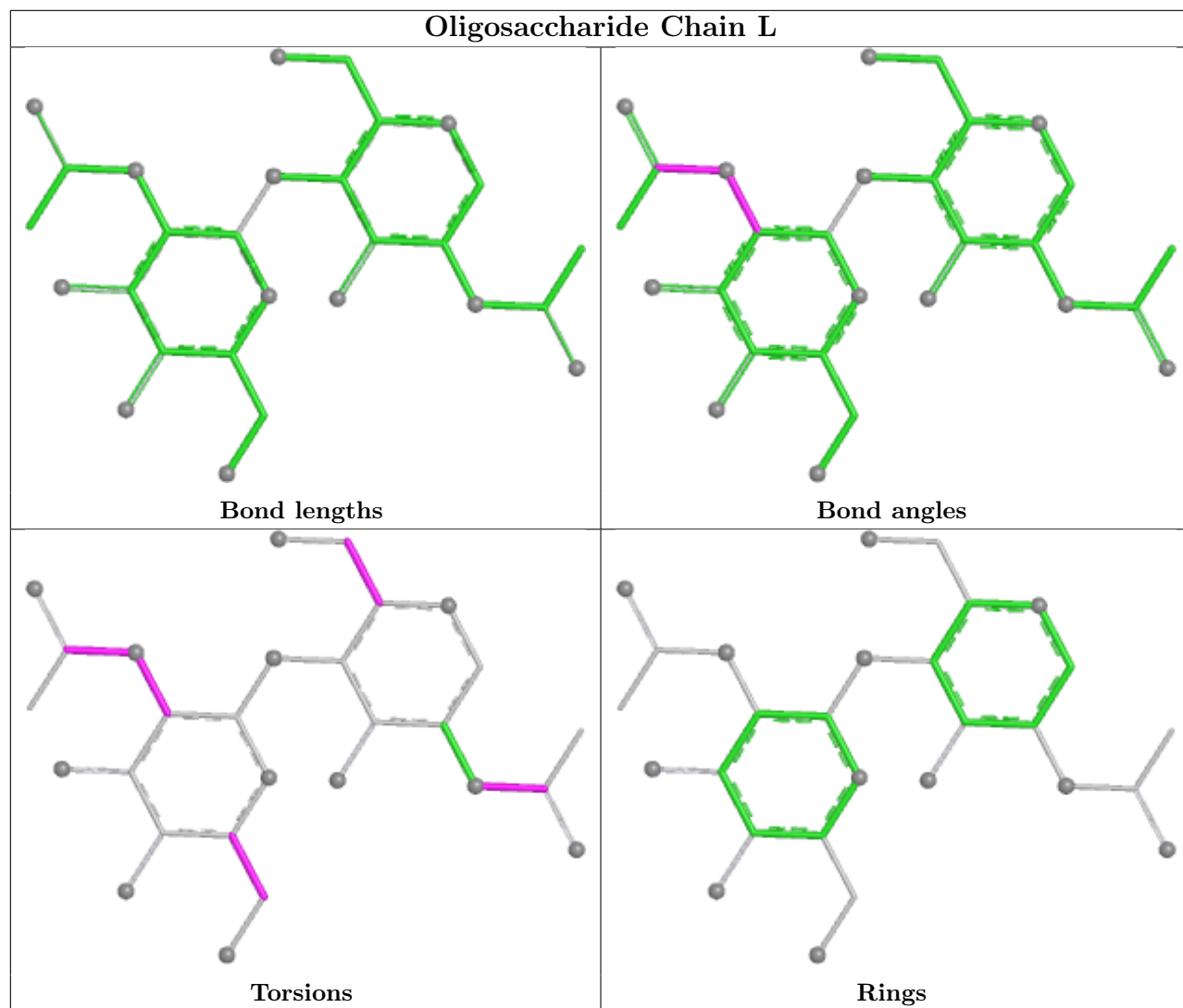


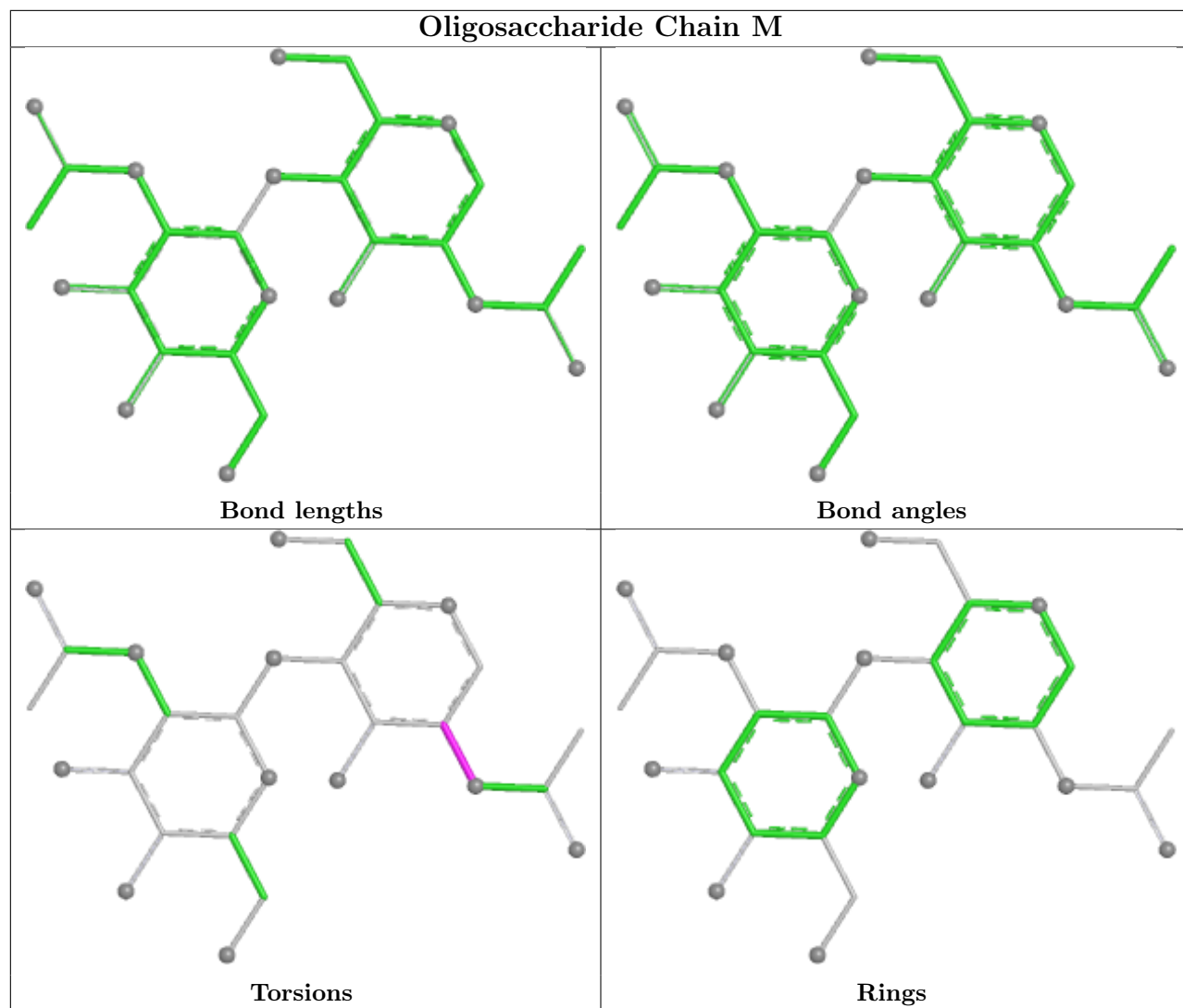


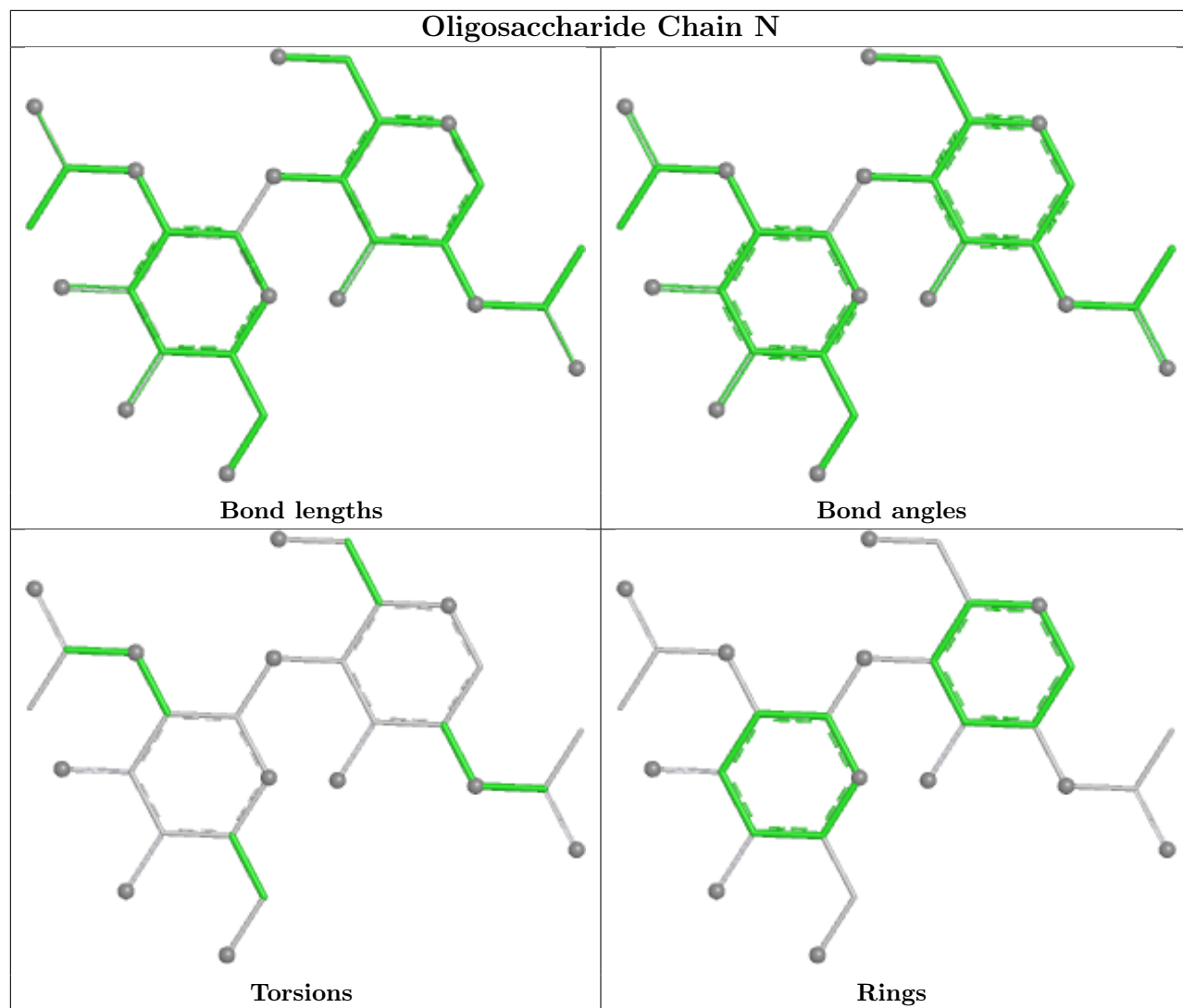


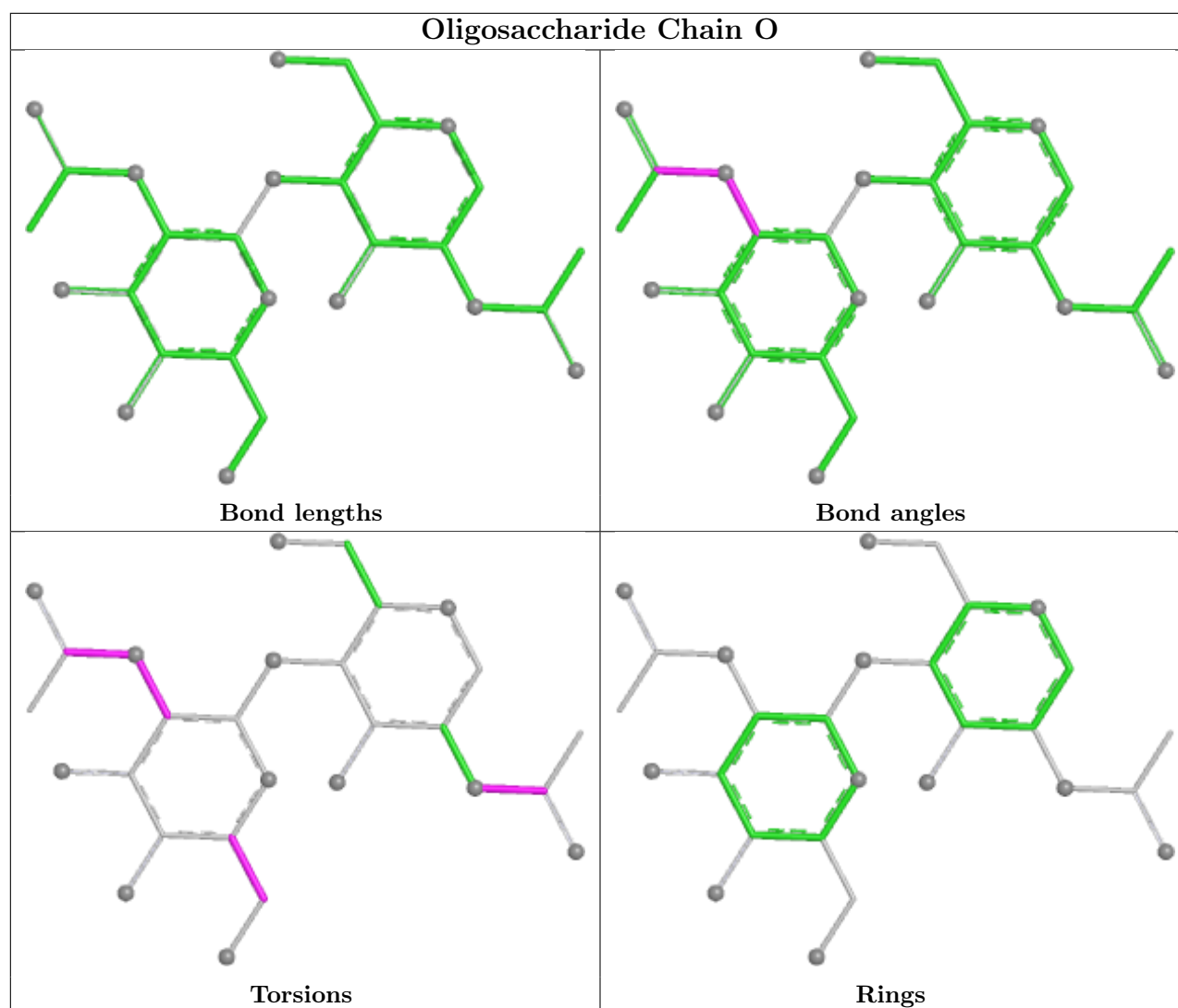












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1301	1	14,14,15	0.30	0	17,19,21	0.41	0
3	NAG	A	1308	-	14,14,15	0.34	0	17,19,21	0.45	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	A	1305	1	14,14,15	0.45	0	17,19,21	0.65	1 (5%)
3	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.91	1 (5%)
3	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.81	1 (5%)
3	NAG	B	1302	-	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	C	1306	-	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	C	1302	1	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
3	NAG	B	1301	1	14,14,15	0.33	0	17,19,21	0.68	0
3	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.76	1 (5%)
3	NAG	B	1306	-	14,14,15	1.38	1 (7%)	17,19,21	1.19	2 (11%)
3	NAG	C	1304	1	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
3	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.60	0
3	NAG	A	1301	1	14,14,15	0.35	0	17,19,21	0.36	0
3	NAG	A	1306	1	14,14,15	2.34	2 (14%)	17,19,21	2.00	2 (11%)
3	NAG	A	1307	1	14,14,15	0.37	0	17,19,21	0.57	0
3	NAG	B	1304	-	14,14,15	0.19	0	17,19,21	0.47	0
3	NAG	C	1303	-	14,14,15	1.08	1 (7%)	17,19,21	0.60	0
3	NAG	B	1303	-	14,14,15	1.29	1 (7%)	17,19,21	1.43	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
3	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	-	-	5/6/23/26	0/1/1/1

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NAG	O5-C1	7.86	1.56	1.43
3	B	1306	NAG	O5-C1	-4.99	1.35	1.43
3	B	1303	NAG	O5-C1	-4.47	1.36	1.43
3	C	1303	NAG	O5-C1	-3.87	1.37	1.43
3	A	1306	NAG	C1-C2	3.70	1.57	1.52
3	C	1302	NAG	O5-C1	-2.82	1.39	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1306	NAG	C1-O5-C5	7.72	122.53	112.19
3	B	1303	NAG	C2-N2-C7	3.85	128.06	122.90
3	B	1307	NAG	C1-O5-C5	3.38	116.71	112.19
3	B	1306	NAG	C2-N2-C7	3.30	127.32	122.90
3	C	1304	NAG	C1-O5-C5	3.06	116.29	112.19
3	C	1305	NAG	C1-O5-C5	2.91	116.08	112.19
3	C	1304	NAG	C2-N2-C7	2.75	126.58	122.90
3	A	1303	NAG	C1-O5-C5	2.66	115.75	112.19
3	A	1306	NAG	C3-C4-C5	-2.63	105.45	110.23
3	B	1303	NAG	C3-C4-C5	2.58	114.92	110.23
3	A	1305	NAG	C1-O5-C5	2.12	115.03	112.19
3	B	1306	NAG	C3-C4-C5	2.03	113.91	110.23

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1304	NAG	C1-C2-N2-C7
3	B	1306	NAG	C1-C2-N2-C7
3	B	1303	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	B	1306	NAG	C8-C7-N2-C2
3	B	1306	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	A	1307	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1308	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	B	1302	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	A	1304	NAG	C1-C2-N2-C7
3	B	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	C3-C2-N2-C7
3	C	1304	NAG	C3-C2-N2-C7
3	C	1303	NAG	O5-C5-C6-O6
3	C	1304	NAG	C1-C2-N2-C7
3	A	1304	NAG	C3-C2-N2-C7
3	B	1304	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	C	1303	NAG	C3-C2-N2-C7
3	A	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	NAG	1	0
3	A	1308	NAG	9	0
3	C	1302	NAG	1	0
3	B	1306	NAG	5	0
3	C	1304	NAG	4	0
3	A	1307	NAG	1	0
3	C	1303	NAG	1	0
3	B	1303	NAG	2	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.

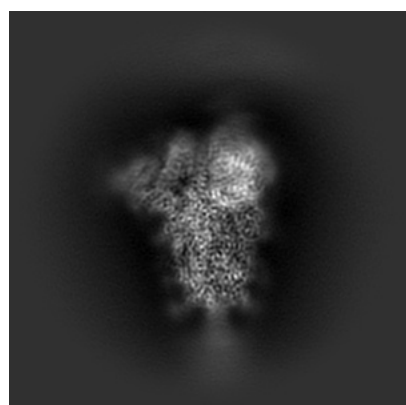
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25887. These allow visual inspection of the internal detail of the map and identification of artifacts.

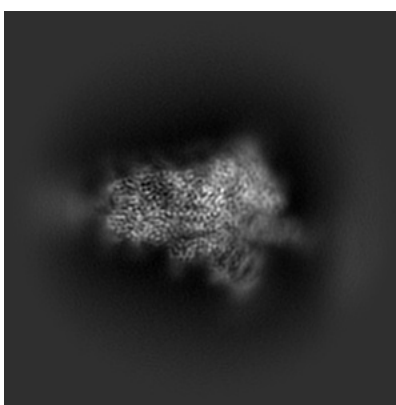
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

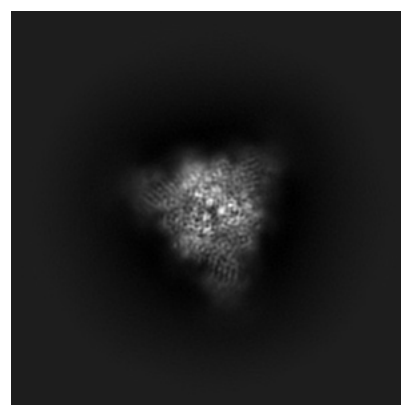
6.1.1 Primary map



X



Y

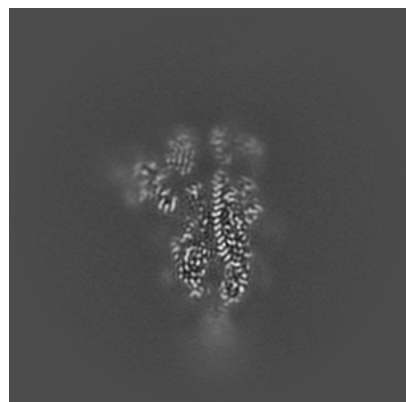


Z

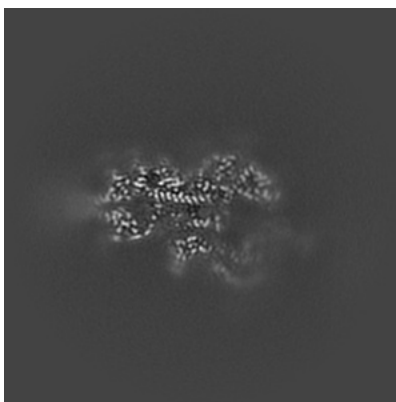
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

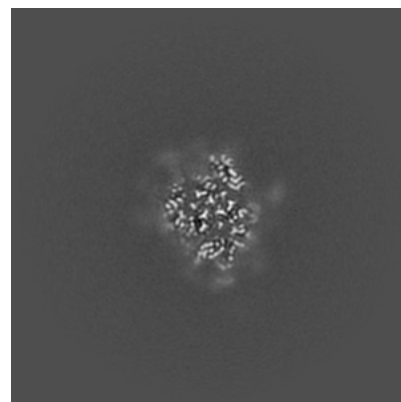
6.2.1 Primary map



X Index: 192



Y Index: 192

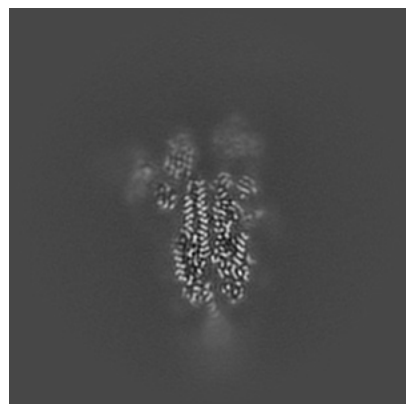


Z Index: 192

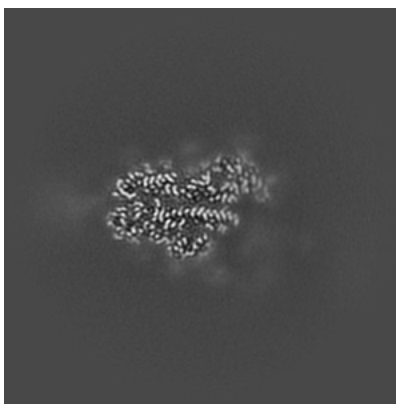
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

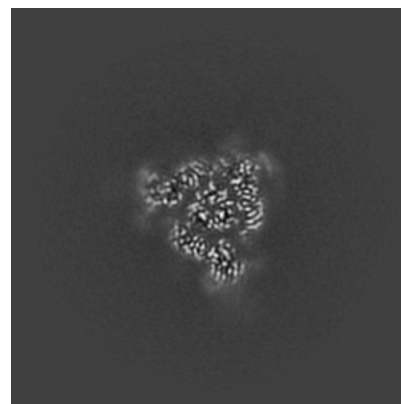
6.3.1 Primary map



X Index: 187



Y Index: 184

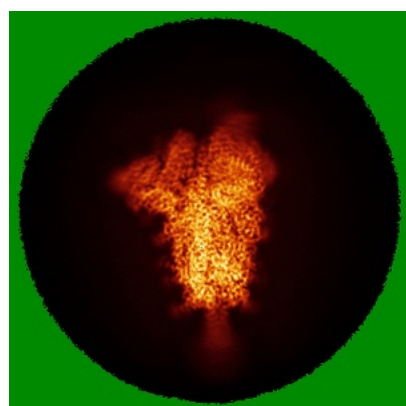


Z Index: 205

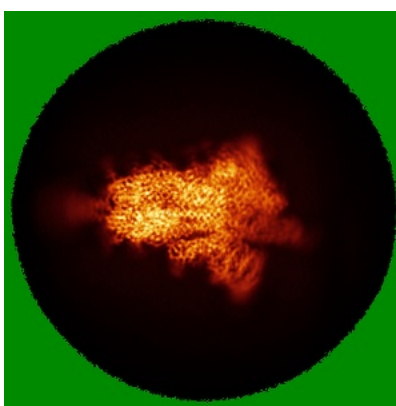
The images above show the largest variance slices of the map in three orthogonal directions.

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

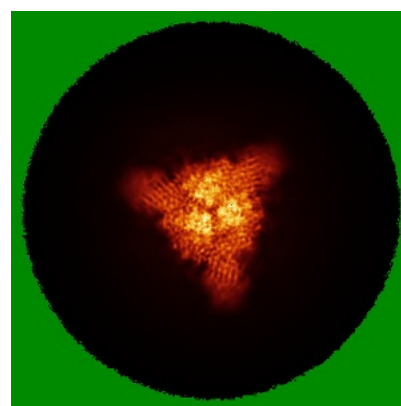
6.4.1 Primary map



X



Y

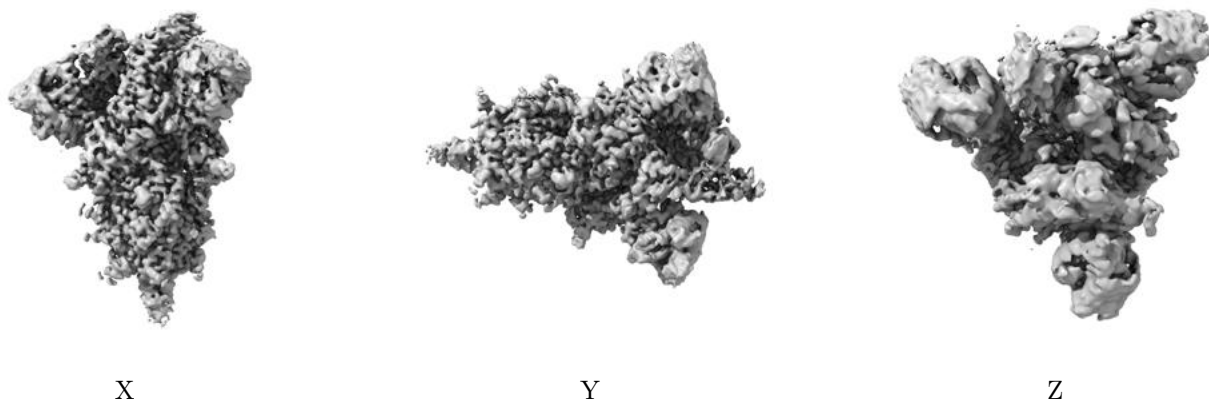


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.146. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

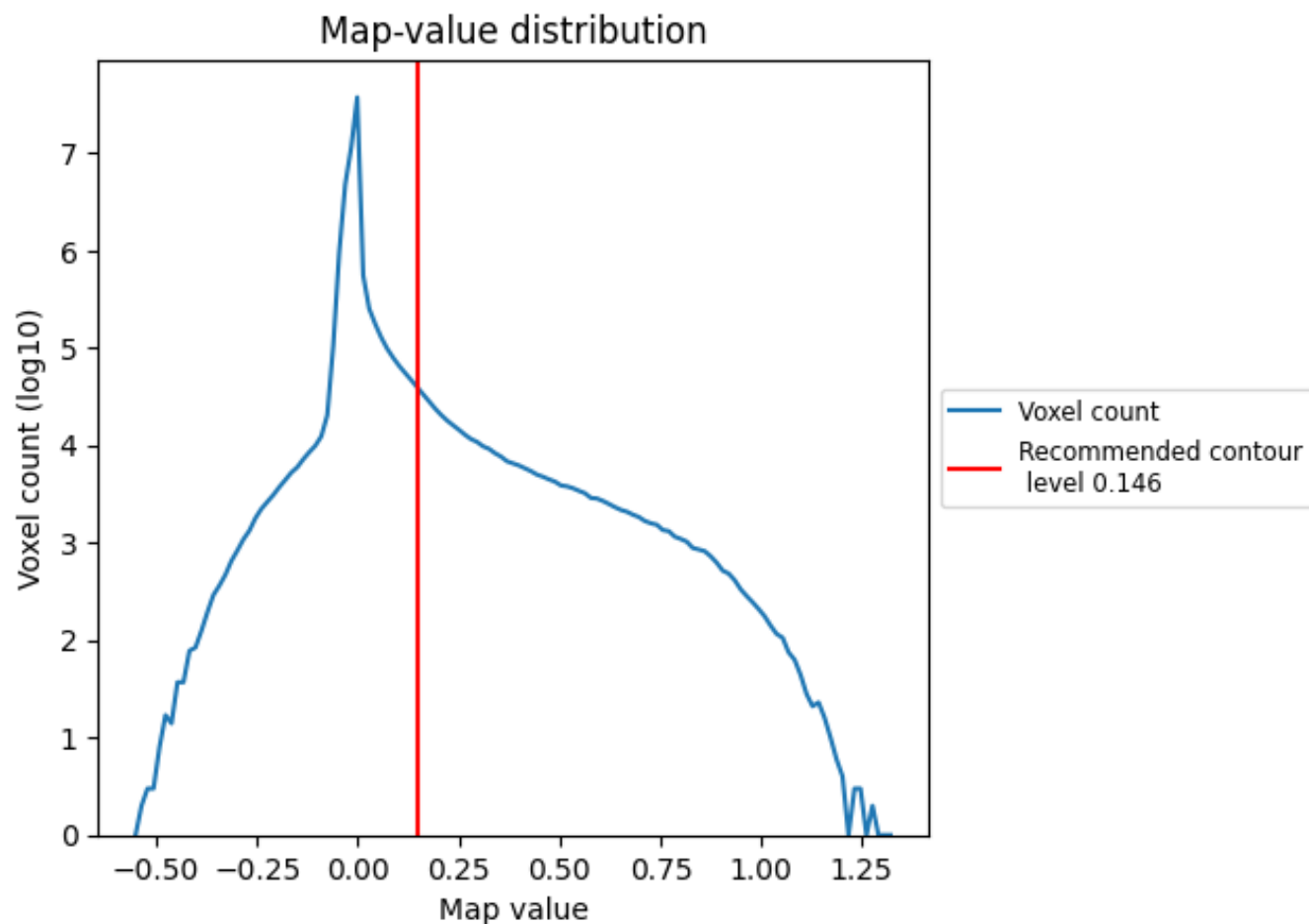
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

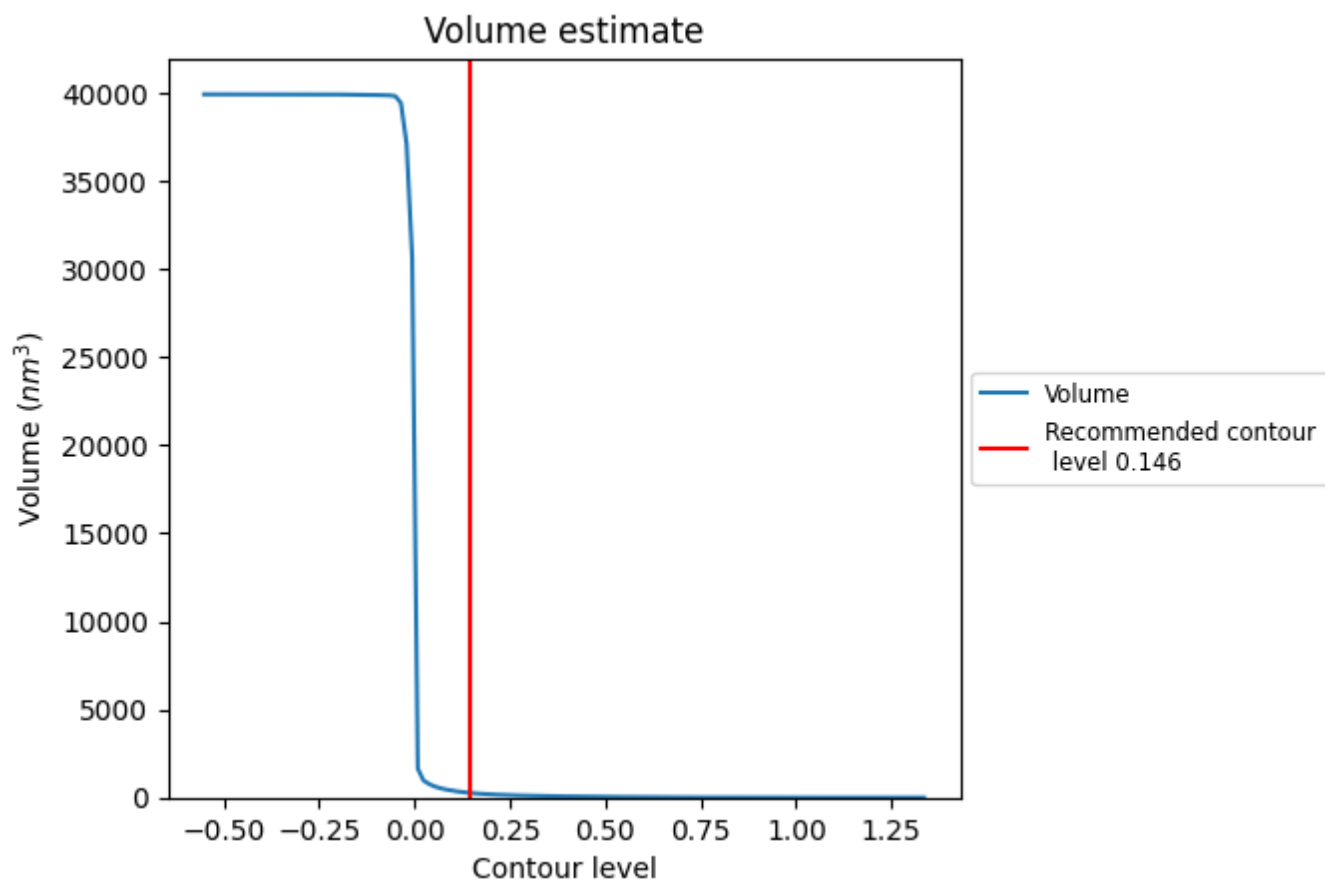
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

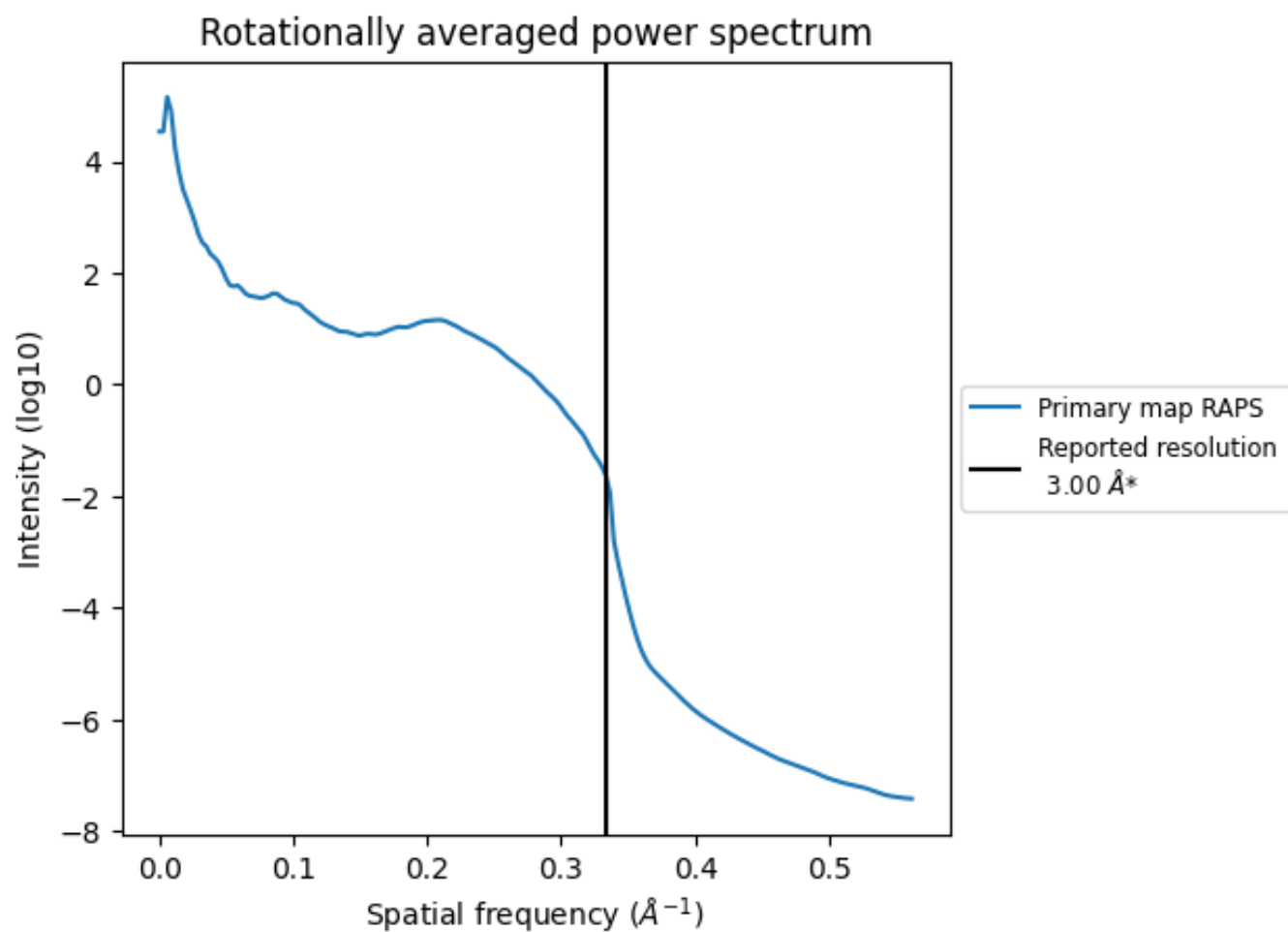
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm^3 ; this corresponds to an approximate mass of 238 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 ⓘ

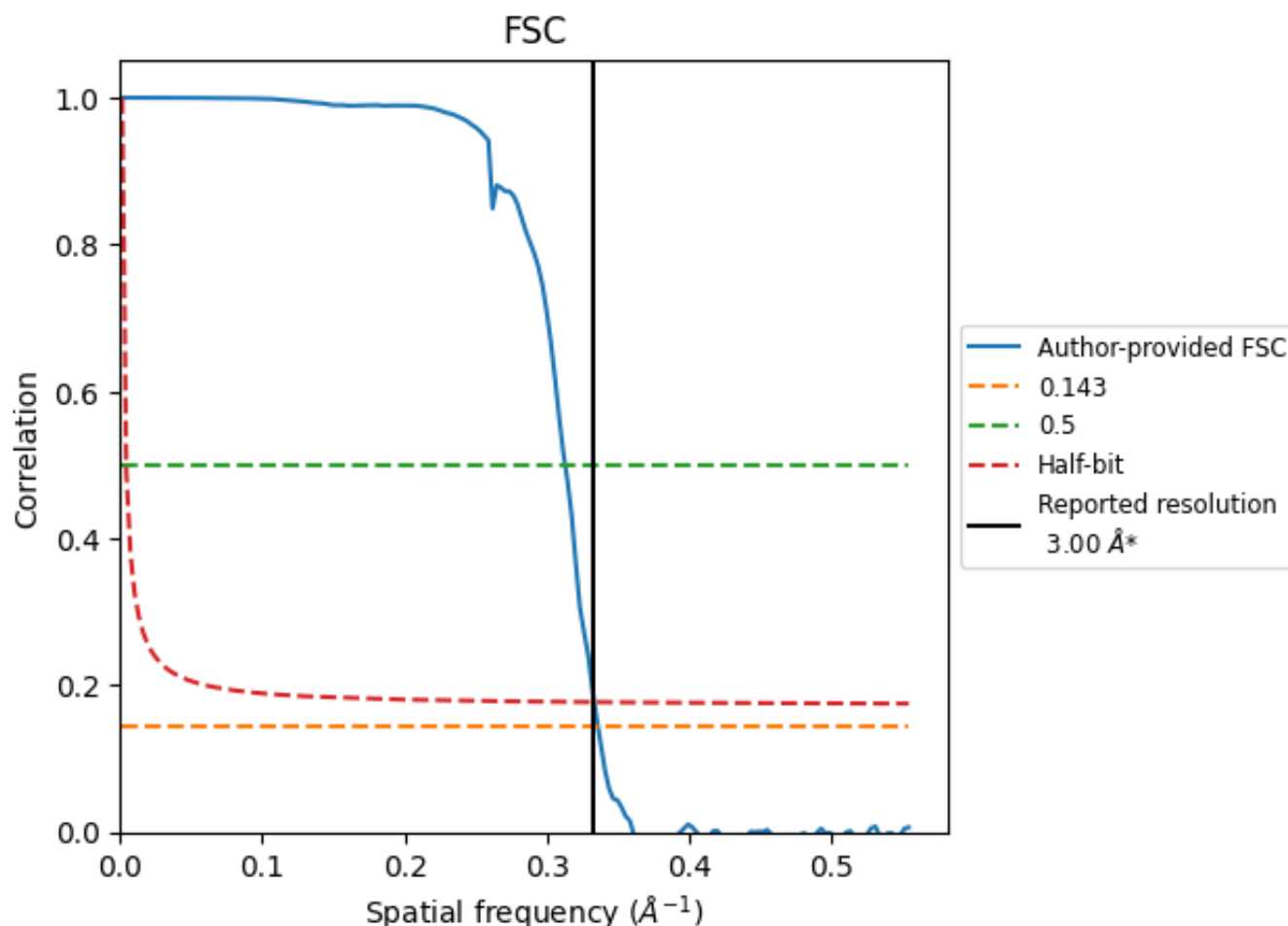


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

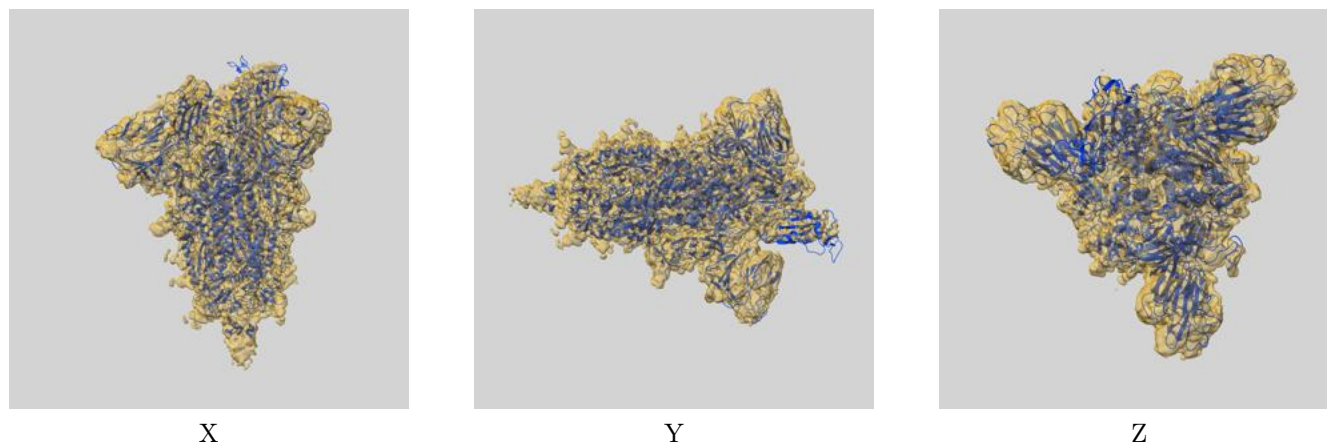
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.19	3.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

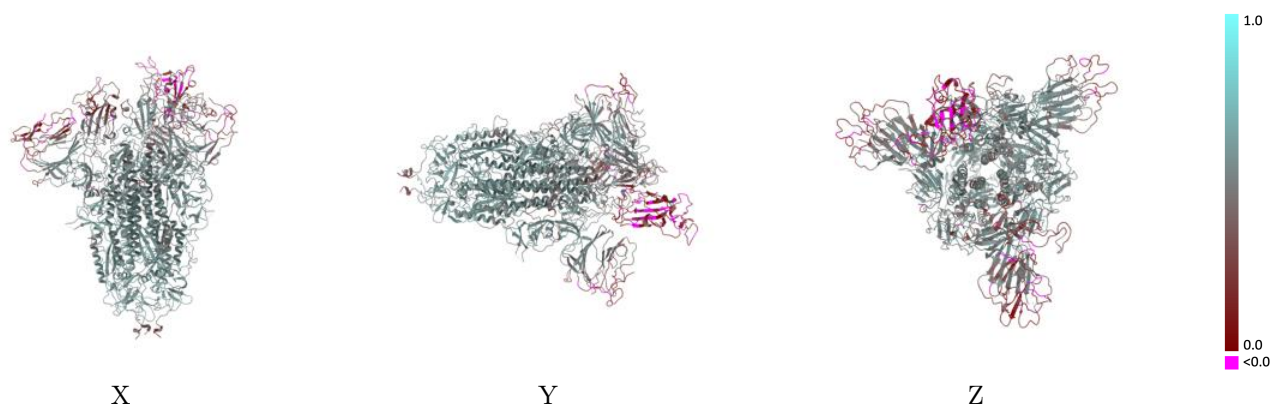
This section contains information regarding the fit between EMDB map EMD-25887 and PDB model 7TGW. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.146 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](#)



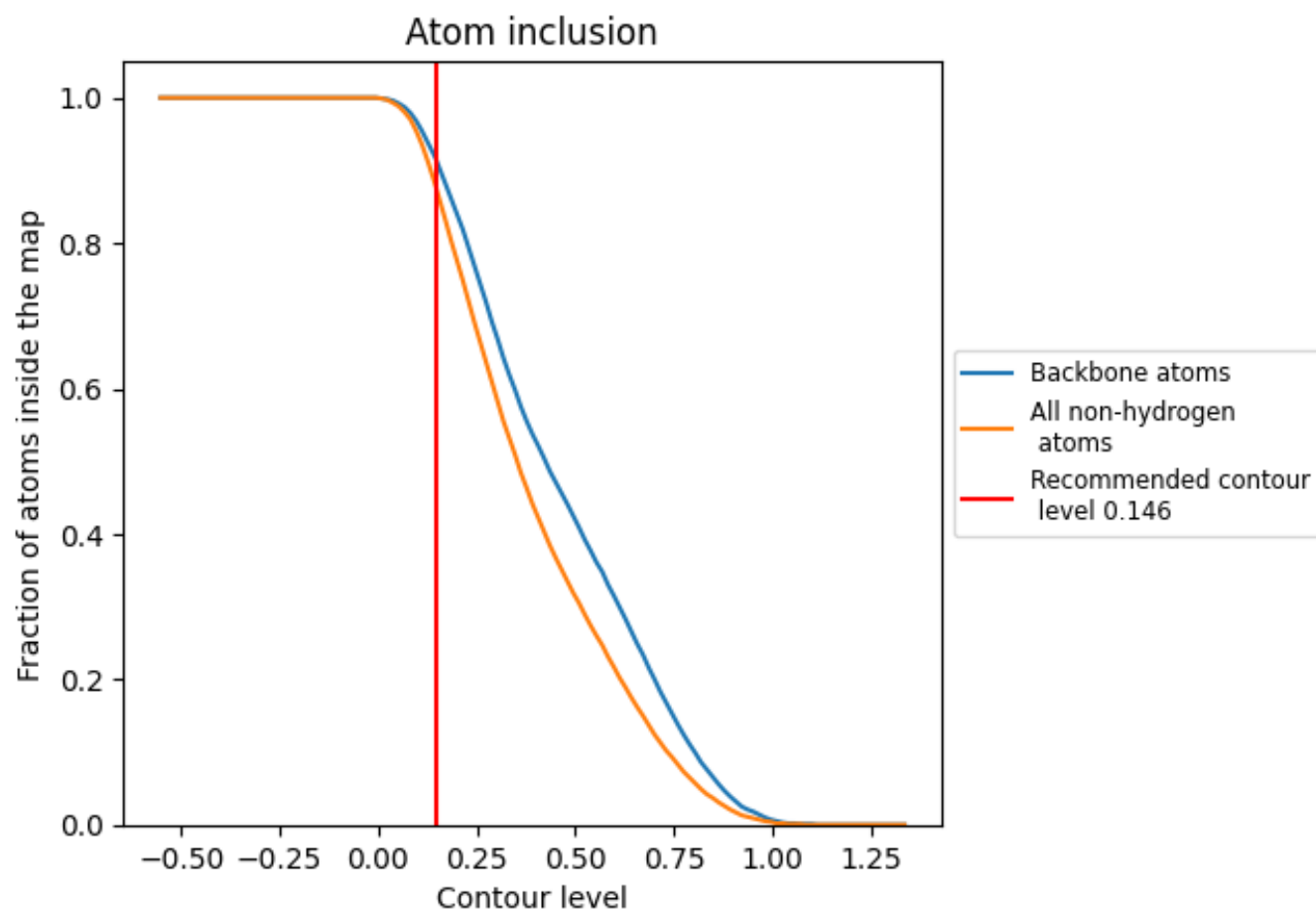
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.146).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.4710
A	 0.8120	 0.4450
B	 0.9060	 0.4760
C	 0.9170	 0.4940
D	 0.6430	 0.3000
E	 0.9290	 0.4760
F	 0.9290	 0.4920
G	 0.9290	 0.4850
H	 0.8930	 0.4550
I	 0.9640	 0.4830
J	 0.9640	 0.4870
K	 0.8570	 0.4810
L	 0.8930	 0.4260
M	 0.9290	 0.4990
N	 0.9640	 0.5190
O	 0.8930	 0.4400

