



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:02 PM UTC

PDB ID : 6U7K / pdb_00006u7k
EMDB ID : EMD-20672
Title : Prefusion structure of PEDV spike
Authors : Wrapp, D.; McLellan, J.S.
Deposited on : 2019-09-03
Resolution : 3.14 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

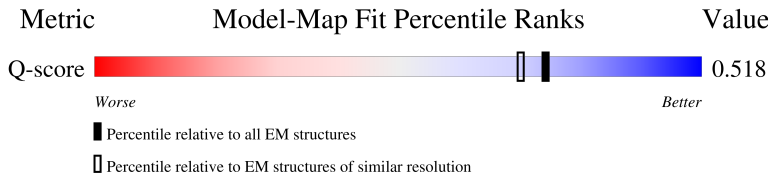
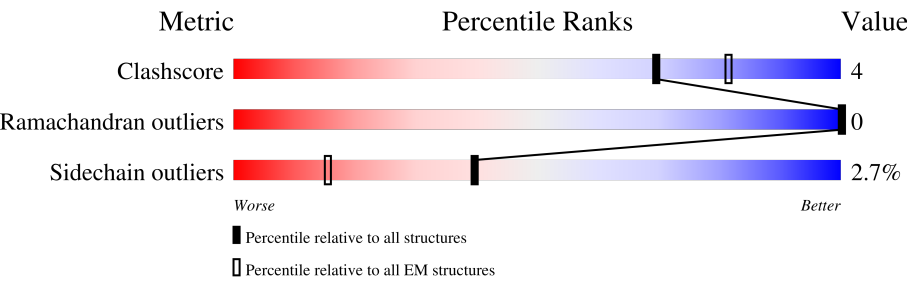
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.14 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	1399	5% 71% 24%
1	B	1399	5% 71% 24%
1	C	1399	5% 71% 24%
2	D	6	17% 33% 67%

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Mol	Chain	Length	Quality of chain
2	I	6	
2	N	6	
3	E	2	
3	F	2	
3	G	2	
3	H	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	-	X	-	-
2	NAG	N	1	X	-	-	-
3	NAG	E	1	-	-	X	-
3	NAG	F	2	X	-	-	-
3	NAG	G	1	-	X	-	-
3	NAG	K	2	X	-	-	-
3	NAG	L	1	-	X	-	-
3	NAG	P	2	X	-	-	-
3	NAG	Q	1	-	X	X	-
4	NAG	B	1413	X	-	-	-
4	NAG	C	1401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25515 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	1064	Total	C	N	O	S	0	0
			8139	5189	1320	1594	36		
1	B	1064	Total	C	N	O	S	0	0
			8139	5189	1320	1594	36		
1	C	1064	Total	C	N	O	S	0	0
			8139	5189	1320	1594	36		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1320	GLY	-	expression tag	UNP Q91AV1
A	1321	SER	-	expression tag	UNP Q91AV1
A	1322	GLY	-	expression tag	UNP Q91AV1
A	1323	TYR	-	expression tag	UNP Q91AV1
A	1324	ILE	-	expression tag	UNP Q91AV1
A	1325	PRO	-	expression tag	UNP Q91AV1
A	1326	GLU	-	expression tag	UNP Q91AV1
A	1327	ALA	-	expression tag	UNP Q91AV1
A	1328	PRO	-	expression tag	UNP Q91AV1
A	1329	ARG	-	expression tag	UNP Q91AV1
A	1330	ASP	-	expression tag	UNP Q91AV1
A	1331	GLY	-	expression tag	UNP Q91AV1
A	1332	GLN	-	expression tag	UNP Q91AV1
A	1333	ALA	-	expression tag	UNP Q91AV1
A	1334	TYR	-	expression tag	UNP Q91AV1
A	1335	VAL	-	expression tag	UNP Q91AV1
A	1336	ARG	-	expression tag	UNP Q91AV1
A	1337	LYS	-	expression tag	UNP Q91AV1
A	1338	ASP	-	expression tag	UNP Q91AV1
A	1339	GLY	-	expression tag	UNP Q91AV1
A	1340	GLU	-	expression tag	UNP Q91AV1
A	1341	TRP	-	expression tag	UNP Q91AV1
A	1342	VAL	-	expression tag	UNP Q91AV1
A	1343	LEU	-	expression tag	UNP Q91AV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1344	LEU	-	expression tag	UNP Q91AV1
A	1345	SER	-	expression tag	UNP Q91AV1
A	1346	THR	-	expression tag	UNP Q91AV1
A	1347	PHE	-	expression tag	UNP Q91AV1
A	1348	LEU	-	expression tag	UNP Q91AV1
A	1349	GLY	-	expression tag	UNP Q91AV1
A	1350	ARG	-	expression tag	UNP Q91AV1
A	1351	SER	-	expression tag	UNP Q91AV1
A	1352	LEU	-	expression tag	UNP Q91AV1
A	1353	GLU	-	expression tag	UNP Q91AV1
A	1354	VAL	-	expression tag	UNP Q91AV1
A	1355	LEU	-	expression tag	UNP Q91AV1
A	1356	PHE	-	expression tag	UNP Q91AV1
A	1357	GLN	-	expression tag	UNP Q91AV1
A	1358	GLY	-	expression tag	UNP Q91AV1
A	1359	PRO	-	expression tag	UNP Q91AV1
A	1360	GLY	-	expression tag	UNP Q91AV1
A	1361	HIS	-	expression tag	UNP Q91AV1
A	1362	HIS	-	expression tag	UNP Q91AV1
A	1363	HIS	-	expression tag	UNP Q91AV1
A	1364	HIS	-	expression tag	UNP Q91AV1
A	1365	HIS	-	expression tag	UNP Q91AV1
A	1366	HIS	-	expression tag	UNP Q91AV1
A	1367	HIS	-	expression tag	UNP Q91AV1
A	1368	HIS	-	expression tag	UNP Q91AV1
A	1369	SER	-	expression tag	UNP Q91AV1
A	1370	ALA	-	expression tag	UNP Q91AV1
A	1371	TRP	-	expression tag	UNP Q91AV1
A	1372	SER	-	expression tag	UNP Q91AV1
A	1373	HIS	-	expression tag	UNP Q91AV1
A	1374	PRO	-	expression tag	UNP Q91AV1
A	1375	GLN	-	expression tag	UNP Q91AV1
A	1376	PHE	-	expression tag	UNP Q91AV1
A	1377	GLU	-	expression tag	UNP Q91AV1
A	1378	LYS	-	expression tag	UNP Q91AV1
A	1379	GLY	-	expression tag	UNP Q91AV1
A	1380	GLY	-	expression tag	UNP Q91AV1
A	1381	GLY	-	expression tag	UNP Q91AV1
A	1382	SER	-	expression tag	UNP Q91AV1
A	1383	GLY	-	expression tag	UNP Q91AV1
A	1384	GLY	-	expression tag	UNP Q91AV1
A	1385	GLY	-	expression tag	UNP Q91AV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1386	GLY	-	expression tag	UNP Q91AV1
A	1387	SER	-	expression tag	UNP Q91AV1
A	1388	GLY	-	expression tag	UNP Q91AV1
A	1389	GLY	-	expression tag	UNP Q91AV1
A	1390	SER	-	expression tag	UNP Q91AV1
A	1391	ALA	-	expression tag	UNP Q91AV1
A	1392	TRP	-	expression tag	UNP Q91AV1
A	1393	SER	-	expression tag	UNP Q91AV1
A	1394	HIS	-	expression tag	UNP Q91AV1
A	1395	PRO	-	expression tag	UNP Q91AV1
A	1396	GLN	-	expression tag	UNP Q91AV1
A	1397	PHE	-	expression tag	UNP Q91AV1
A	1398	GLU	-	expression tag	UNP Q91AV1
A	1399	LYS	-	expression tag	UNP Q91AV1
B	1320	GLY	-	expression tag	UNP Q91AV1
B	1321	SER	-	expression tag	UNP Q91AV1
B	1322	GLY	-	expression tag	UNP Q91AV1
B	1323	TYR	-	expression tag	UNP Q91AV1
B	1324	ILE	-	expression tag	UNP Q91AV1
B	1325	PRO	-	expression tag	UNP Q91AV1
B	1326	GLU	-	expression tag	UNP Q91AV1
B	1327	ALA	-	expression tag	UNP Q91AV1
B	1328	PRO	-	expression tag	UNP Q91AV1
B	1329	ARG	-	expression tag	UNP Q91AV1
B	1330	ASP	-	expression tag	UNP Q91AV1
B	1331	GLY	-	expression tag	UNP Q91AV1
B	1332	GLN	-	expression tag	UNP Q91AV1
B	1333	ALA	-	expression tag	UNP Q91AV1
B	1334	TYR	-	expression tag	UNP Q91AV1
B	1335	VAL	-	expression tag	UNP Q91AV1
B	1336	ARG	-	expression tag	UNP Q91AV1
B	1337	LYS	-	expression tag	UNP Q91AV1
B	1338	ASP	-	expression tag	UNP Q91AV1
B	1339	GLY	-	expression tag	UNP Q91AV1
B	1340	GLU	-	expression tag	UNP Q91AV1
B	1341	TRP	-	expression tag	UNP Q91AV1
B	1342	VAL	-	expression tag	UNP Q91AV1
B	1343	LEU	-	expression tag	UNP Q91AV1
B	1344	LEU	-	expression tag	UNP Q91AV1
B	1345	SER	-	expression tag	UNP Q91AV1
B	1346	THR	-	expression tag	UNP Q91AV1
B	1347	PHE	-	expression tag	UNP Q91AV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1348	LEU	-	expression tag	UNP Q91AV1
B	1349	GLY	-	expression tag	UNP Q91AV1
B	1350	ARG	-	expression tag	UNP Q91AV1
B	1351	SER	-	expression tag	UNP Q91AV1
B	1352	LEU	-	expression tag	UNP Q91AV1
B	1353	GLU	-	expression tag	UNP Q91AV1
B	1354	VAL	-	expression tag	UNP Q91AV1
B	1355	LEU	-	expression tag	UNP Q91AV1
B	1356	PHE	-	expression tag	UNP Q91AV1
B	1357	GLN	-	expression tag	UNP Q91AV1
B	1358	GLY	-	expression tag	UNP Q91AV1
B	1359	PRO	-	expression tag	UNP Q91AV1
B	1360	GLY	-	expression tag	UNP Q91AV1
B	1361	HIS	-	expression tag	UNP Q91AV1
B	1362	HIS	-	expression tag	UNP Q91AV1
B	1363	HIS	-	expression tag	UNP Q91AV1
B	1364	HIS	-	expression tag	UNP Q91AV1
B	1365	HIS	-	expression tag	UNP Q91AV1
B	1366	HIS	-	expression tag	UNP Q91AV1
B	1367	HIS	-	expression tag	UNP Q91AV1
B	1368	HIS	-	expression tag	UNP Q91AV1
B	1369	SER	-	expression tag	UNP Q91AV1
B	1370	ALA	-	expression tag	UNP Q91AV1
B	1371	TRP	-	expression tag	UNP Q91AV1
B	1372	SER	-	expression tag	UNP Q91AV1
B	1373	HIS	-	expression tag	UNP Q91AV1
B	1374	PRO	-	expression tag	UNP Q91AV1
B	1375	GLN	-	expression tag	UNP Q91AV1
B	1376	PHE	-	expression tag	UNP Q91AV1
B	1377	GLU	-	expression tag	UNP Q91AV1
B	1378	LYS	-	expression tag	UNP Q91AV1
B	1379	GLY	-	expression tag	UNP Q91AV1
B	1380	GLY	-	expression tag	UNP Q91AV1
B	1381	GLY	-	expression tag	UNP Q91AV1
B	1382	SER	-	expression tag	UNP Q91AV1
B	1383	GLY	-	expression tag	UNP Q91AV1
B	1384	GLY	-	expression tag	UNP Q91AV1
B	1385	GLY	-	expression tag	UNP Q91AV1
B	1386	GLY	-	expression tag	UNP Q91AV1
B	1387	SER	-	expression tag	UNP Q91AV1
B	1388	GLY	-	expression tag	UNP Q91AV1
B	1389	GLY	-	expression tag	UNP Q91AV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1390	SER	-	expression tag	UNP Q91AV1
B	1391	ALA	-	expression tag	UNP Q91AV1
B	1392	TRP	-	expression tag	UNP Q91AV1
B	1393	SER	-	expression tag	UNP Q91AV1
B	1394	HIS	-	expression tag	UNP Q91AV1
B	1395	PRO	-	expression tag	UNP Q91AV1
B	1396	GLN	-	expression tag	UNP Q91AV1
B	1397	PHE	-	expression tag	UNP Q91AV1
B	1398	GLU	-	expression tag	UNP Q91AV1
B	1399	LYS	-	expression tag	UNP Q91AV1
C	1320	GLY	-	expression tag	UNP Q91AV1
C	1321	SER	-	expression tag	UNP Q91AV1
C	1322	GLY	-	expression tag	UNP Q91AV1
C	1323	TYR	-	expression tag	UNP Q91AV1
C	1324	ILE	-	expression tag	UNP Q91AV1
C	1325	PRO	-	expression tag	UNP Q91AV1
C	1326	GLU	-	expression tag	UNP Q91AV1
C	1327	ALA	-	expression tag	UNP Q91AV1
C	1328	PRO	-	expression tag	UNP Q91AV1
C	1329	ARG	-	expression tag	UNP Q91AV1
C	1330	ASP	-	expression tag	UNP Q91AV1
C	1331	GLY	-	expression tag	UNP Q91AV1
C	1332	GLN	-	expression tag	UNP Q91AV1
C	1333	ALA	-	expression tag	UNP Q91AV1
C	1334	TYR	-	expression tag	UNP Q91AV1
C	1335	VAL	-	expression tag	UNP Q91AV1
C	1336	ARG	-	expression tag	UNP Q91AV1
C	1337	LYS	-	expression tag	UNP Q91AV1
C	1338	ASP	-	expression tag	UNP Q91AV1
C	1339	GLY	-	expression tag	UNP Q91AV1
C	1340	GLU	-	expression tag	UNP Q91AV1
C	1341	TRP	-	expression tag	UNP Q91AV1
C	1342	VAL	-	expression tag	UNP Q91AV1
C	1343	LEU	-	expression tag	UNP Q91AV1
C	1344	LEU	-	expression tag	UNP Q91AV1
C	1345	SER	-	expression tag	UNP Q91AV1
C	1346	THR	-	expression tag	UNP Q91AV1
C	1347	PHE	-	expression tag	UNP Q91AV1
C	1348	LEU	-	expression tag	UNP Q91AV1
C	1349	GLY	-	expression tag	UNP Q91AV1
C	1350	ARG	-	expression tag	UNP Q91AV1
C	1351	SER	-	expression tag	UNP Q91AV1

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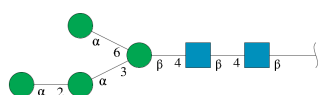
Chain	Residue	Modelled	Actual	Comment	Reference
C	1352	LEU	-	expression tag	UNP Q91AV1
C	1353	GLU	-	expression tag	UNP Q91AV1
C	1354	VAL	-	expression tag	UNP Q91AV1
C	1355	LEU	-	expression tag	UNP Q91AV1
C	1356	PHE	-	expression tag	UNP Q91AV1
C	1357	GLN	-	expression tag	UNP Q91AV1
C	1358	GLY	-	expression tag	UNP Q91AV1
C	1359	PRO	-	expression tag	UNP Q91AV1
C	1360	GLY	-	expression tag	UNP Q91AV1
C	1361	HIS	-	expression tag	UNP Q91AV1
C	1362	HIS	-	expression tag	UNP Q91AV1
C	1363	HIS	-	expression tag	UNP Q91AV1
C	1364	HIS	-	expression tag	UNP Q91AV1
C	1365	HIS	-	expression tag	UNP Q91AV1
C	1366	HIS	-	expression tag	UNP Q91AV1
C	1367	HIS	-	expression tag	UNP Q91AV1
C	1368	HIS	-	expression tag	UNP Q91AV1
C	1369	SER	-	expression tag	UNP Q91AV1
C	1370	ALA	-	expression tag	UNP Q91AV1
C	1371	TRP	-	expression tag	UNP Q91AV1
C	1372	SER	-	expression tag	UNP Q91AV1
C	1373	HIS	-	expression tag	UNP Q91AV1
C	1374	PRO	-	expression tag	UNP Q91AV1
C	1375	GLN	-	expression tag	UNP Q91AV1
C	1376	PHE	-	expression tag	UNP Q91AV1
C	1377	GLU	-	expression tag	UNP Q91AV1
C	1378	LYS	-	expression tag	UNP Q91AV1
C	1379	GLY	-	expression tag	UNP Q91AV1
C	1380	GLY	-	expression tag	UNP Q91AV1
C	1381	GLY	-	expression tag	UNP Q91AV1
C	1382	SER	-	expression tag	UNP Q91AV1
C	1383	GLY	-	expression tag	UNP Q91AV1
C	1384	GLY	-	expression tag	UNP Q91AV1
C	1385	GLY	-	expression tag	UNP Q91AV1
C	1386	GLY	-	expression tag	UNP Q91AV1
C	1387	SER	-	expression tag	UNP Q91AV1
C	1388	GLY	-	expression tag	UNP Q91AV1
C	1389	GLY	-	expression tag	UNP Q91AV1
C	1390	SER	-	expression tag	UNP Q91AV1
C	1391	ALA	-	expression tag	UNP Q91AV1
C	1392	TRP	-	expression tag	UNP Q91AV1
C	1393	SER	-	expression tag	UNP Q91AV1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1394	HIS	-	expression tag	UNP Q91AV1
C	1395	PRO	-	expression tag	UNP Q91AV1
C	1396	GLN	-	expression tag	UNP Q91AV1
C	1397	PHE	-	expression tag	UNP Q91AV1
C	1398	GLU	-	expression tag	UNP Q91AV1
C	1399	LYS	-	expression tag	UNP Q91AV1

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	I	6	Total	C	N	O	0	0
			72	40	2	30		
2	N	6	Total	C	N	O	0	0
			72	40	2	30		

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



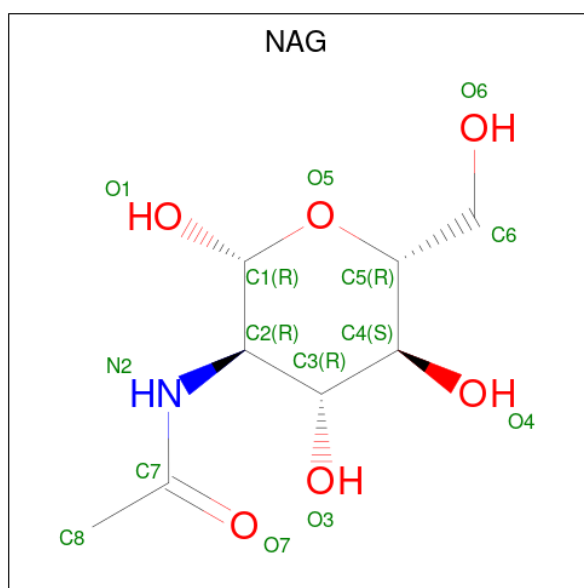
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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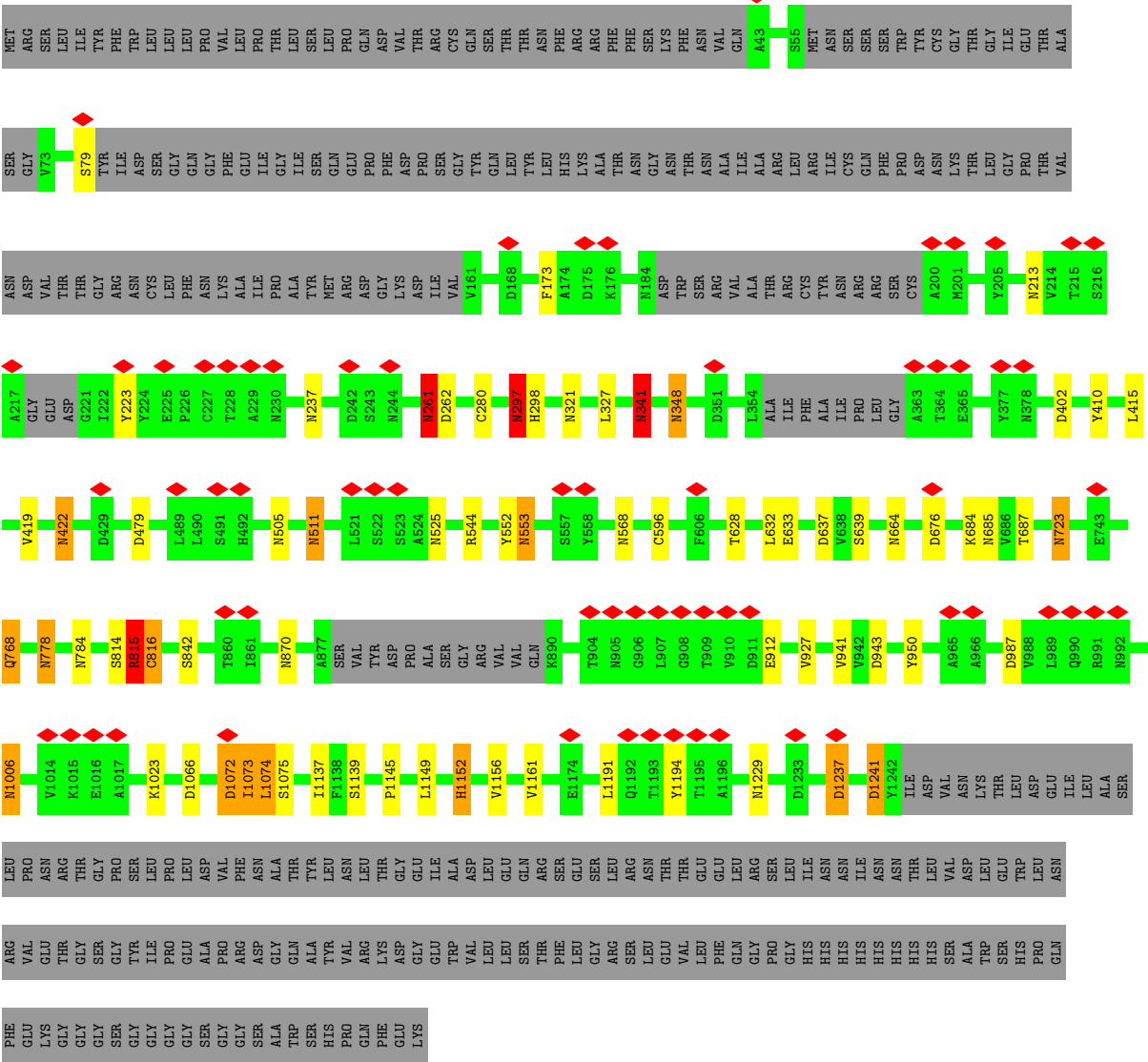
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C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

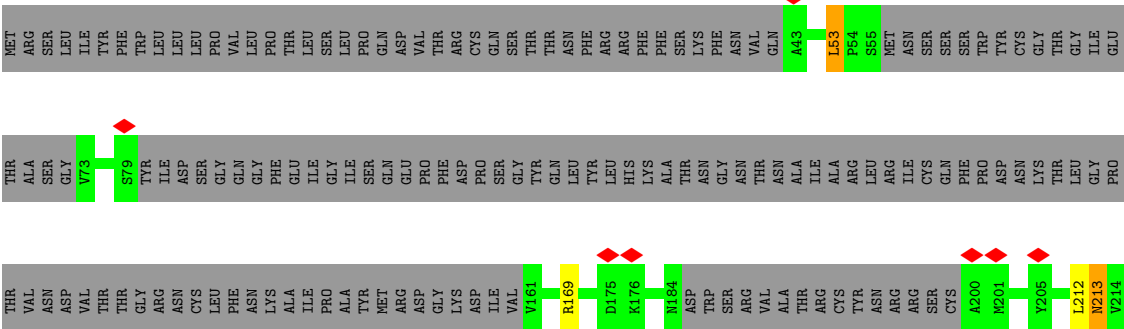
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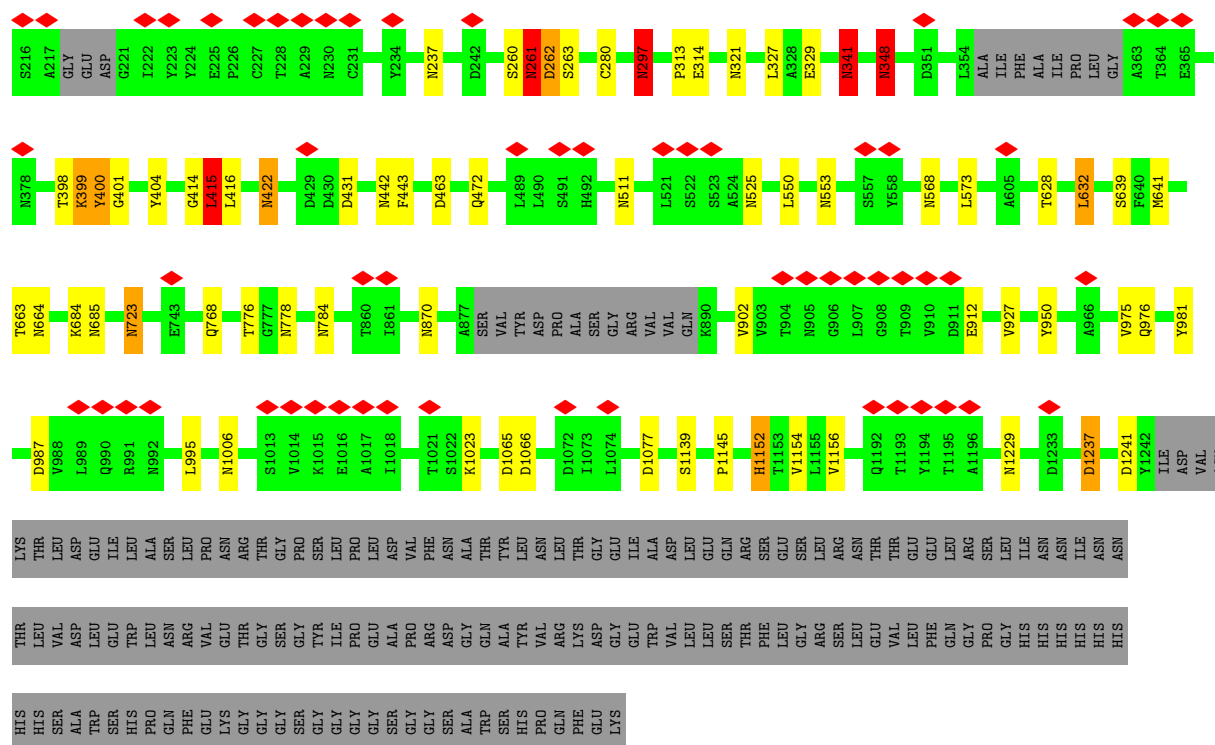
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

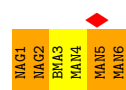


• Molecule 1: Spike glycoprotein





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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



- 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



- 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 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 O:  50% 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

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	112655	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.217	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.43	Depositor
Map size ($\text{\AA}$)	464.40002, 464.40002, 464.40002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.075, 1.075, 1.075	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.98	52/8305 (0.6%)	1.41	39/11318 (0.3%)
1	B	1.00	56/8305 (0.7%)	1.43	41/11318 (0.4%)
1	C	1.04	64/8305 (0.8%)	1.42	44/11318 (0.4%)
All	All	1.00	172/24915 (0.7%)	1.42	124/33954 (0.4%)

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	5
1	B	0	7
1	C	0	4
All	All	0	16

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ASN	C-O	-14.53	1.06	1.24
1	C	422	ASN	C-O	-13.46	1.08	1.23
1	A	422	ASN	C-O	-12.68	1.10	1.23
1	B	422	ASN	CA-CB	-12.58	1.43	1.53
1	C	511	ASN	C-O	-11.22	1.10	1.23
1	C	399	LYS	C-O	-10.88	1.10	1.24
1	A	784	ASN	CA-C	-10.53	1.40	1.52
1	C	723	ASN	CA-C	-10.48	1.38	1.52
1	B	814	SER	CA-C	-10.05	1.38	1.52
1	C	685	ASN	CA-CB	-9.97	1.40	1.53
1	C	784	ASN	C-O	-9.68	1.12	1.24
1	C	401	GLY	C-O	-9.61	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	ASN	C-O	-9.59	1.12	1.24
1	C	348	ASN	N-CA	-9.43	1.33	1.46
1	A	511	ASN	CA-C	-9.37	1.41	1.52
1	B	1006	ASN	C-O	-9.14	1.12	1.24
1	B	723	ASN	CA-C	-9.11	1.39	1.52
1	B	814	SER	C-O	-9.09	1.12	1.24
1	A	348	ASN	N-CA	-8.86	1.34	1.46
1	C	416	LEU	C-O	-8.81	1.13	1.24
1	A	341	ASN	C-O	-8.66	1.13	1.24
1	C	414	GLY	C-O	-8.64	1.15	1.23
1	A	784	ASN	CA-CB	-8.60	1.41	1.53
1	C	415	LEU	C-O	-8.52	1.13	1.23
1	C	1006	ASN	C-O	-8.46	1.13	1.24
1	B	511	ASN	C-O	-8.44	1.13	1.24
1	A	723	ASN	C-O	-8.30	1.12	1.24
1	B	816	CYS	CA-CB	-8.26	1.40	1.53
1	C	778	ASN	C-O	-8.20	1.14	1.24
1	C	341	ASN	C-O	-8.16	1.14	1.24
1	B	1073	ILE	C-O	-8.11	1.13	1.24
1	A	778	ASN	C-O	-8.11	1.14	1.24
1	A	348	ASN	C-O	-8.00	1.13	1.24
1	B	553	ASN	CA-CB	-7.99	1.42	1.53
1	C	723	ASN	C-O	-7.97	1.13	1.24
1	B	341	ASN	C-O	-7.92	1.14	1.24
1	B	784	ASN	CA-C	-7.82	1.43	1.52
1	C	422	ASN	CA-CB	-7.81	1.45	1.53
1	A	422	ASN	CA-CB	-7.81	1.41	1.53
1	A	870	ASN	N-CA	-7.81	1.36	1.46
1	A	723	ASN	CA-C	-7.80	1.40	1.52
1	A	870	ASN	CA-CB	-7.63	1.43	1.52
1	B	348	ASN	C-O	-7.63	1.14	1.24
1	C	784	ASN	CA-C	-7.61	1.43	1.52
1	B	816	CYS	N-CA	-7.59	1.36	1.46
1	C	399	LYS	CA-C	-7.57	1.42	1.52
1	C	341	ASN	CA-CB	-7.53	1.42	1.53
1	A	664	ASN	N-CA	-7.52	1.37	1.46
1	B	1075	SER	C-O	-7.41	1.14	1.24
1	A	870	ASN	C-O	-7.39	1.14	1.23
1	B	778	ASN	CA-CB	-7.39	1.42	1.53
1	C	553	ASN	CA-CB	-7.26	1.43	1.53
1	A	511	ASN	CG-OD1	-7.24	1.09	1.23
1	B	778	ASN	C-O	-7.21	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	870	ASN	C-O	-7.18	1.14	1.23
1	C	1006	ASN	CA-CB	-7.14	1.42	1.53
1	B	1006	ASN	CA-C	-7.11	1.42	1.52
1	B	685	ASN	CA-C	-7.10	1.43	1.53
1	C	685	ASN	CG-ND2	-7.08	1.18	1.33
1	A	348	ASN	CA-CB	-7.06	1.41	1.53
1	C	778	ASN	C-N	-7.05	1.25	1.33
1	B	870	ASN	C-O	-7.04	1.14	1.23
1	C	348	ASN	C-O	-6.96	1.14	1.24
1	A	297	ASN	C-O	-6.94	1.14	1.24
1	A	422	ASN	N-CA	-6.93	1.36	1.46
1	C	399	LYS	N-CA	-6.90	1.37	1.46
1	C	870	ASN	CA-CB	-6.86	1.42	1.52
1	B	511	ASN	CA-CB	-6.76	1.43	1.53
1	B	784	ASN	CA-CB	-6.73	1.44	1.52
1	B	685	ASN	CG-ND2	-6.70	1.19	1.33
1	B	778	ASN	CB-CG	-6.69	1.35	1.52
1	A	341	ASN	CG-ND2	-6.68	1.19	1.33
1	C	685	ASN	N-CA	-6.67	1.37	1.46
1	C	870	ASN	CA-C	-6.66	1.44	1.53
1	C	261	ASN	CA-CB	-6.64	1.43	1.53
1	B	723	ASN	C-O	-6.60	1.15	1.24
1	A	341	ASN	CA-CB	-6.57	1.42	1.53
1	A	511	ASN	CA-CB	-6.57	1.44	1.53
1	A	778	ASN	C-N	-6.57	1.26	1.33
1	A	1006	ASN	CA-C	-6.55	1.43	1.52
1	B	685	ASN	CG-OD1	-6.54	1.11	1.23
1	B	297	ASN	C-O	-6.53	1.15	1.24
1	B	422	ASN	C-O	-6.52	1.12	1.23
1	A	685	ASN	CG-ND2	-6.50	1.19	1.33
1	B	784	ASN	C-O	-6.45	1.14	1.23
1	B	685	ASN	CA-CB	-6.44	1.36	1.53
1	C	723	ASN	CA-CB	-6.32	1.42	1.53
1	A	870	ASN	CA-C	-6.32	1.44	1.52
1	A	685	ASN	CG-OD1	-6.32	1.11	1.23
1	A	685	ASN	C-N	-6.29	1.27	1.34
1	C	511	ASN	CG-ND2	-6.17	1.20	1.33
1	B	1074	LEU	C-O	-6.16	1.16	1.24
1	C	685	ASN	CG-OD1	-6.15	1.11	1.23
1	A	1229	ASN	C-O	-6.13	1.16	1.24
1	A	511	ASN	CB-CG	-6.12	1.36	1.52
1	C	261	ASN	CA-C	-6.10	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	511	ASN	CA-CB	-6.08	1.44	1.53
1	B	1075	SER	C-N	-6.08	1.25	1.33
1	B	778	ASN	C-N	-6.07	1.26	1.33
1	B	815	ARG	CA-C	-6.07	1.43	1.52
1	C	778	ASN	CA-CB	-6.06	1.45	1.53
1	A	685	ASN	CA-C	-6.01	1.45	1.53
1	C	511	ASN	CB-CG	-5.96	1.37	1.52
1	B	870	ASN	CA-CB	-5.94	1.45	1.52
1	A	778	ASN	CA-CB	-5.94	1.45	1.53
1	C	870	ASN	N-CA	-5.93	1.38	1.46
1	A	341	ASN	CB-CG	-5.93	1.37	1.52
1	C	1006	ASN	CA-C	-5.92	1.44	1.52
1	A	261	ASN	CG-ND2	-5.89	1.20	1.33
1	C	341	ASN	CG-ND2	-5.89	1.20	1.33
1	B	341	ASN	CG-ND2	-5.88	1.21	1.33
1	A	321	ASN	CA-C	5.88	1.60	1.52
1	A	1229	ASN	CA-CB	-5.86	1.45	1.53
1	B	685	ASN	N-CA	-5.86	1.38	1.46
1	B	723	ASN	CA-CB	-5.85	1.43	1.53
1	A	778	ASN	CB-CG	-5.84	1.37	1.52
1	C	511	ASN	CG-OD1	-5.83	1.12	1.23
1	A	1006	ASN	CA-CB	-5.81	1.44	1.54
1	A	784	ASN	N-CA	-5.81	1.39	1.46
1	C	442	ASN	C-O	-5.79	1.16	1.23
1	C	1229	ASN	C-O	-5.78	1.17	1.24
1	B	341	ASN	CB-CG	-5.77	1.37	1.52
1	B	814	SER	N-CA	-5.73	1.38	1.46
1	C	297	ASN	C-O	-5.72	1.16	1.24
1	B	1073	ILE	CA-CB	-5.72	1.45	1.54
1	A	723	ASN	CA-CB	-5.70	1.43	1.53
1	C	553	ASN	N-CA	-5.67	1.39	1.46
1	B	341	ASN	CA-CB	-5.66	1.43	1.53
1	C	778	ASN	CB-CG	-5.65	1.38	1.52
1	C	870	ASN	C-N	-5.65	1.25	1.33
1	C	261	ASN	CG-ND2	-5.61	1.21	1.33
1	B	664	ASN	CA-CB	-5.58	1.45	1.53
1	B	348	ASN	N-CA	-5.57	1.39	1.46
1	A	740	ASN	C-O	-5.55	1.16	1.23
1	C	784	ASN	CA-CB	-5.50	1.45	1.53
1	A	1006	ASN	C-O	-5.49	1.15	1.23
1	B	870	ASN	N-CA	-5.48	1.39	1.46
1	A	664	ASN	C-O	-5.47	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	685	ASN	C-N	-5.47	1.27	1.33
1	B	685	ASN	CB-CG	-5.44	1.38	1.52
1	C	664	ASN	CA-CB	-5.44	1.45	1.53
1	C	415	LEU	CA-C	-5.43	1.46	1.52
1	C	341	ASN	CB-CG	-5.40	1.38	1.52
1	C	321	ASN	CA-C	5.39	1.59	1.52
1	B	778	ASN	CG-OD1	-5.39	1.13	1.23
1	C	443	PHE	C-O	-5.39	1.17	1.23
1	C	685	ASN	CA-C	-5.36	1.46	1.52
1	B	816	CYS	C-O	-5.36	1.15	1.23
1	C	400	TYR	CA-C	-5.34	1.45	1.52
1	B	664	ASN	C-O	-5.34	1.16	1.24
1	C	297	ASN	CA-CB	-5.33	1.45	1.53
1	B	79	SER	CB-OG	-5.32	1.31	1.42
1	B	297	ASN	CA-CB	-5.29	1.46	1.53
1	C	261	ASN	CB-CG	-5.28	1.38	1.52
1	B	261	ASN	CA-CB	-5.27	1.46	1.53
1	B	1229	ASN	C-O	-5.27	1.17	1.24
1	A	422	ASN	CB-CG	-5.26	1.38	1.52
1	B	511	ASN	N-CA	-5.25	1.39	1.46
1	A	348	ASN	CA-C	-5.25	1.45	1.52
1	A	685	ASN	CA-CB	-5.23	1.39	1.53
1	B	815	ARG	C-O	-5.20	1.17	1.24
1	A	321	ASN	CB-CG	-5.14	1.39	1.52
1	C	778	ASN	CG-ND2	-5.13	1.22	1.33
1	B	870	ASN	CA-C	-5.12	1.47	1.53
1	C	321	ASN	CB-CG	-5.12	1.39	1.52
1	C	314	GLU	CA-CB	-5.09	1.47	1.54
1	C	1229	ASN	CA-CB	-5.08	1.46	1.53
1	A	723	ASN	N-CA	-5.06	1.39	1.46
1	A	664	ASN	CA-CB	-5.03	1.46	1.53
1	B	664	ASN	N-CA	-5.03	1.40	1.46
1	A	740	ASN	CA-CB	-5.02	1.45	1.53
1	C	415	LEU	CA-CB	-5.02	1.44	1.53

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	723	ASN	N-CA-C	11.68	127.33	113.20
1	C	723	ASN	N-CA-C	11.32	126.88	113.18
1	A	723	ASN	N-CA-C	10.61	125.75	113.02
1	B	348	ASN	N-CA-CB	-10.53	92.42	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	685	ASN	N-CA-C	-9.60	91.78	108.20
1	B	816	CYS	N-CA-C	-9.54	101.53	113.55
1	C	348	ASN	CB-CA-C	9.27	129.36	109.99
1	A	348	ASN	CA-CB-CG	8.76	121.36	112.60
1	C	511	ASN	CB-CA-C	-8.73	94.82	109.48
1	C	348	ASN	N-CA-CB	-8.13	97.14	110.40
1	B	778	ASN	CB-CA-C	-8.07	96.57	109.80
1	B	511	ASN	CB-CA-C	-8.05	97.09	110.29
1	C	314	GLU	N-CA-C	-7.93	104.08	114.31
1	A	987	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	685	ASN	N-CA-C	-7.68	91.90	107.41
1	B	422	ASN	N-CA-CB	-7.62	97.61	110.79
1	A	778	ASN	CB-CA-C	-7.56	98.68	110.78
1	B	685	ASN	N-CA-C	-7.33	92.61	107.41
1	C	213	ASN	N-CA-CB	-7.31	98.92	110.69
1	B	553	ASN	N-CA-CB	-7.26	100.53	111.64
1	C	778	ASN	N-CA-C	-7.16	97.05	108.73
1	B	422	ASN	CA-C-N	7.02	130.83	120.87
1	B	422	ASN	C-N-CA	7.02	130.83	120.87
1	C	987	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	1237	ASP	CA-CB-CG	7.00	119.61	112.60
1	A	553	ASN	N-CA-CB	-6.98	100.55	111.23
1	A	664	ASN	CA-C-N	6.93	132.48	122.08
1	A	664	ASN	C-N-CA	6.93	132.48	122.08
1	C	778	ASN	CB-CA-C	-6.93	98.96	110.19
1	C	422	ASN	N-CA-CB	-6.92	101.02	111.19
1	B	778	ASN	N-CA-CB	6.87	121.49	110.16
1	B	987	ASP	CA-CB-CG	6.87	119.47	112.60
1	C	568	ASN	CA-CB-CG	6.70	119.30	112.60
1	B	1066	ASP	CA-CB-CG	6.68	119.28	112.60
1	B	778	ASN	N-CA-C	-6.63	98.46	109.46
1	A	511	ASN	N-CA-C	6.59	119.44	108.96
1	B	1237	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	511	ASN	N-CA-CB	6.42	120.96	110.17
1	C	1241	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	1237	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	553	ASN	CA-C-N	6.32	130.89	122.93
1	A	553	ASN	C-N-CA	6.32	130.89	122.93
1	B	553	ASN	CA-C-N	6.29	130.85	122.93
1	B	553	ASN	C-N-CA	6.29	130.85	122.93
1	B	511	ASN	CA-CB-CG	6.26	118.86	112.60
1	C	341	ASN	CB-CA-C	-6.21	99.51	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASN	CB-CA-C	-6.19	98.23	109.38
1	C	511	ASN	N-CA-CB	6.11	120.59	110.52
1	B	511	ASN	CB-CG-ND2	6.09	125.53	116.40
1	A	1241	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	341	ASN	CB-CA-C	-5.99	98.60	109.38
1	C	553	ASN	N-CA-CB	-5.98	102.06	111.39
1	C	415	LEU	CB-CA-C	-5.96	99.82	109.72
1	A	321	ASN	N-CA-CB	-5.94	101.39	110.01
1	A	778	ASN	N-CA-C	-5.93	98.05	108.20
1	B	943	ASP	CA-CB-CG	5.91	118.50	112.60
1	C	1066	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	348	ASN	N-CA-C	-5.86	105.63	112.89
1	C	297	ASN	CB-CA-C	-5.84	99.83	109.99
1	B	1241	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	416	LEU	CD1-CG-CD2	-5.80	98.03	110.80
1	A	422	ASN	CA-C-N	5.79	129.50	120.75
1	A	422	ASN	C-N-CA	5.79	129.50	120.75
1	A	262	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	348	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	297	ASN	N-CA-CB	-5.65	101.89	111.27
1	A	511	ASN	CA-C-O	-5.63	114.12	120.43
1	A	422	ASN	N-CA-CB	-5.61	100.71	111.53
1	A	348	ASN	N-CA-CB	-5.60	101.00	110.41
1	B	1073	ILE	N-CA-C	5.56	119.90	111.89
1	C	553	ASN	CA-C-N	5.56	127.95	120.50
1	C	553	ASN	C-N-CA	5.56	127.95	120.50
1	A	1152	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	A	913	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	1066	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	422	ASN	CB-CG-ND2	-5.51	108.13	116.40
1	C	431	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	1077	ASP	CA-CB-CG	5.50	118.09	112.60
1	A	341	ASN	CA-C-N	5.49	130.75	123.00
1	A	341	ASN	C-N-CA	5.49	130.75	123.00
1	B	1152	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	B	1006	ASN	N-CA-C	5.48	120.03	113.23
1	A	321	ASN	N-CA-C	5.45	116.91	111.07
1	B	1137	ILE	N-CA-C	5.44	115.92	111.62
1	C	422	ASN	CA-C-N	5.41	128.40	120.71
1	C	422	ASN	C-N-CA	5.41	128.40	120.71
1	A	297	ASN	CB-CA-C	-5.38	101.40	110.44
1	B	479	ASP	CA-CB-CG	5.37	117.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	SER	O-C-N	-5.37	116.83	123.33
1	B	297	ASN	CB-CA-C	-5.37	100.65	109.99
1	B	262	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	341	ASN	CA-C-N	5.33	130.68	123.11
1	B	341	ASN	C-N-CA	5.33	130.68	123.11
1	C	463	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	173	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	321	ASN	N-CA-C	5.30	116.74	111.07
1	C	422	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	765	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	1006	ASN	CB-CA-C	-5.24	99.82	109.15
1	B	1229	ASN	N-CA-CB	-5.24	101.33	109.87
1	C	414	GLY	CA-C-O	-5.22	116.54	122.33
1	B	768	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	511	ASN	CA-C-N	5.14	129.41	122.93
1	A	511	ASN	C-N-CA	5.14	129.41	122.93
1	B	298	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	B	987	ASP	CA-C-N	5.14	129.44	120.86
1	B	987	ASP	C-N-CA	5.14	129.44	120.86
1	B	213	ASN	CB-CA-C	5.12	119.49	109.35
1	C	1152	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	C	262	ASP	CA-C-N	5.12	128.34	120.82
1	C	262	ASP	C-N-CA	5.12	128.34	120.82
1	C	976	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	C	53	LEU	CA-C-N	5.10	126.21	119.84
1	C	53	LEU	C-N-CA	5.10	126.21	119.84
1	C	212	LEU	CA-C-N	5.08	130.30	122.93
1	C	212	LEU	C-N-CA	5.08	130.30	122.93
1	A	53	LEU	CA-C-N	5.08	125.36	119.92
1	A	53	LEU	C-N-CA	5.08	125.36	119.92
1	C	472	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	676	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	298	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	C	778	ASN	CA-C-N	5.04	128.17	122.48
1	C	778	ASN	C-N-CA	5.04	128.17	122.48
1	B	402	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	511	ASN	Mainchain
1	A	544	ARG	Sidechain
1	A	684	LYS	Mainchain
1	A	950	TYR	Sidechain
1	B	1194	TYR	Sidechain
1	B	223	TYR	Sidechain
1	B	410	TYR	Sidechain
1	B	544	ARG	Sidechain
1	B	552	TYR	Sidechain
1	B	684	LYS	Mainchain
1	B	950	TYR	Sidechain
1	C	313	PRO	Mainchain
1	C	684	LYS	Mainchain
1	C	950	TYR	Sidechain
1	C	981	TYR	Sidechain

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	8139	0	7923	62	0
1	B	8139	0	7923	42	0
1	C	8139	0	7922	41	0
2	D	72	0	59	8	0
2	I	72	0	61	3	0
2	N	72	0	61	4	0
3	E	28	0	25	13	0
3	F	28	0	25	2	0
3	G	28	0	24	6	0
3	H	28	0	25	0	0
3	J	28	0	23	0	0
3	K	28	0	23	5	0
3	L	28	0	23	5	0
3	M	28	0	25	0	0
3	O	28	0	25	2	0
3	P	28	0	25	1	0
3	Q	28	0	24	11	0
3	R	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	182	0	168	33	0
4	B	182	0	167	24	0
4	C	182	0	168	22	0
All	All	25515	0	24744	179	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 (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:ND2	4:B:1411:NAG:C1	1.68	1.55
1:A:740:ASN:ND2	4:A:1421:NAG:C1	1.67	1.55
1:C:341:ASN:ND2	4:C:1411:NAG:C1	1.68	1.55
1:A:341:ASN:ND2	4:A:1411:NAG:C1	1.68	1.54
1:B:553:ASN:ND2	4:B:1416:NAG:C1	1.70	1.54
1:A:784:ASN:ND2	4:A:1423:NAG:C1	1.68	1.54
1:B:511:ASN:ND2	3:K:1:NAG:C1	1.68	1.54
1:A:553:ASN:ND2	4:A:1416:NAG:C1	1.70	1.53
1:C:348:ASN:ND2	4:C:1412:NAG:C1	1.68	1.53
1:C:422:ASN:ND2	4:C:1413:NAG:C1	1.70	1.53
1:A:348:ASN:ND2	4:A:1412:NAG:C1	1.69	1.53
1:B:1006:ASN:HD21	4:B:1426:NAG:C1	0.87	1.52
1:C:297:ASN:ND2	4:C:1408:NAG:C1	1.69	1.52
1:A:297:ASN:ND2	4:A:1408:NAG:C1	1.69	1.51
1:A:1006:ASN:HD21	4:A:1426:NAG:C1	0.87	1.51
1:C:213:ASN:ND2	4:C:1401:NAG:C1	1.68	1.51
1:B:297:ASN:ND2	4:B:1408:NAG:C1	1.69	1.50
1:B:348:ASN:ND2	4:B:1412:NAG:C1	1.69	1.50
1:B:422:ASN:ND2	4:B:1413:NAG:C1	1.67	1.50
1:A:321:ASN:ND2	3:E:1:NAG:C1	1.67	1.50
1:A:664:ASN:ND2	4:A:1417:NAG:C1	1.68	1.50
1:A:422:ASN:ND2	4:A:1413:NAG:C1	1.71	1.48
1:A:1006:ASN:ND2	4:A:1426:NAG:C1	1.72	1.47
1:B:1006:ASN:ND2	4:B:1426:NAG:C1	1.73	1.43
1:A:431:ASP:OD2	3:E:1:NAG:C6	1.74	1.35
1:C:641:MET:CE	3:Q:1:NAG:O7	1.75	1.31
1:C:641:MET:HE2	3:Q:1:NAG:O7	1.17	1.29
1:A:431:ASP:OD2	3:E:1:NAG:O6	1.60	1.19
1:A:399:LYS:NZ	2:D:5:MAN:O6	1.81	1.14
1:A:311:ARG:NH2	2:D:5:MAN:O3	1.85	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASN:CG	3:E:1:NAG:C1	2.25	1.10
1:A:341:ASN:CG	4:A:1411:NAG:C1	2.26	1.07
1:B:511:ASN:CG	3:K:1:NAG:C1	2.27	1.06
1:A:431:ASP:OD2	3:E:1:NAG:H62	1.52	1.05
1:B:341:ASN:CG	4:B:1411:NAG:C1	2.29	1.05
1:A:348:ASN:CG	4:A:1412:NAG:C1	2.30	1.04
1:C:341:ASN:CG	4:C:1411:NAG:C1	2.33	1.00
1:C:348:ASN:CG	4:C:1412:NAG:C1	2.44	0.90
1:A:664:ASN:CG	4:A:1417:NAG:C1	2.44	0.90
1:A:297:ASN:CG	4:A:1408:NAG:C1	2.43	0.90
1:A:431:ASP:CG	3:E:1:NAG:H62	1.97	0.90
1:C:297:ASN:CG	4:C:1408:NAG:C1	2.45	0.89
1:C:213:ASN:CG	4:C:1401:NAG:C1	2.45	0.88
1:B:297:ASN:CG	4:B:1408:NAG:C1	2.46	0.87
1:A:784:ASN:CG	4:A:1423:NAG:C1	2.48	0.87
1:C:639:SER:HB2	3:Q:1:NAG:H83	1.57	0.86
1:A:431:ASP:CG	3:E:1:NAG:C6	2.49	0.84
1:A:740:ASN:CG	4:A:1421:NAG:C1	2.50	0.84
1:B:422:ASN:CG	4:B:1413:NAG:C1	2.49	0.83
1:B:348:ASN:CG	4:B:1412:NAG:C1	2.50	0.83
1:A:321:ASN:OD1	3:E:1:NAG:C1	2.28	0.82
1:A:431:ASP:CG	3:E:1:NAG:O6	2.22	0.82
1:B:778:ASN:HD22	1:B:1191:LEU:HD22	1.44	0.82
1:B:511:ASN:OD1	3:K:1:NAG:C1	2.27	0.81
1:A:341:ASN:OD1	4:A:1411:NAG:C1	2.29	0.81
1:B:1072:ASP:OD1	1:B:1072:ASP:N	2.15	0.77
4:B:1416:NAG:C1	4:B:1416:NAG:H82	2.15	0.77
1:B:341:ASN:ND2	4:B:1411:NAG:O5	2.18	0.77
1:A:348:ASN:OD1	4:A:1412:NAG:C1	2.34	0.76
3:E:2:NAG:H82	3:E:2:NAG:O3	1.86	0.76
1:A:341:ASN:ND2	4:A:1411:NAG:O5	2.18	0.75
1:B:639:SER:HB2	3:L:1:NAG:H81	1.69	0.75
1:A:422:ASN:CG	4:A:1413:NAG:C1	2.58	0.75
4:C:1401:NAG:O3	4:C:1401:NAG:O7	2.05	0.75
1:A:553:ASN:CG	4:A:1416:NAG:C1	2.60	0.74
3:F:2:NAG:O7	3:F:2:NAG:O3	2.04	0.74
1:C:341:ASN:ND2	4:C:1411:NAG:O5	2.19	0.74
2:I:2:NAG:O7	2:I:2:NAG:O3	2.05	0.74
1:B:341:ASN:OD1	4:B:1411:NAG:C1	2.34	0.74
1:C:213:ASN:ND2	4:C:1401:NAG:O5	2.21	0.73
2:N:2:NAG:O3	2:N:2:NAG:O7	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:LEU:HD23	1:B:1074:LEU:O	1.89	0.73
4:A:1426:NAG:O6	4:A:1426:NAG:O4	2.00	0.72
1:C:641:MET:HE1	3:Q:1:NAG:O7	1.88	0.72
1:B:553:ASN:CG	4:B:1416:NAG:C1	2.62	0.71
1:C:398:THR:HG22	1:C:400:TYR:H	1.54	0.71
3:Q:2:NAG:C3	3:Q:2:NAG:H83	2.19	0.71
2:D:2:NAG:O3	2:D:2:NAG:O7	2.08	0.70
1:C:399:LYS:HG2	1:C:399:LYS:O	1.92	0.69
1:C:341:ASN:OD1	4:C:1411:NAG:C1	2.40	0.69
1:C:641:MET:HE2	3:Q:1:NAG:C7	2.14	0.69
3:F:1:NAG:H62	3:F:2:NAG:HN2	1.61	0.66
1:A:511:ASN:HB3	1:A:549:THR:OG1	1.95	0.66
3:L:2:NAG:O3	3:L:2:NAG:H83	1.96	0.65
1:A:784:ASN:ND2	4:A:1423:NAG:O5	2.29	0.64
1:A:181:TYR:CD2	4:A:1413:NAG:H3	2.33	0.64
2:N:5:MAN:O6	2:N:5:MAN:O4	2.05	0.64
1:B:1139:SER:OG	1:B:1152:HIS:ND1	1.93	0.64
1:A:311:ARG:NH2	2:D:5:MAN:C3	2.61	0.63
1:B:1073:ILE:O	1:B:1073:ILE:HG22	1.98	0.63
2:I:2:NAG:HO3	2:I:2:NAG:C7	2.00	0.62
1:A:740:ASN:ND2	4:A:1421:NAG:O5	2.30	0.62
1:C:639:SER:CB	3:Q:1:NAG:H83	2.30	0.61
1:A:415:LEU:HD21	2:D:6:MAN:O2	2.01	0.60
1:A:1006:ASN:CG	4:A:1426:NAG:C1	2.67	0.60
1:A:422:ASN:ND2	4:A:1413:NAG:O5	2.32	0.59
1:B:778:ASN:HD22	1:B:1191:LEU:CD2	2.15	0.59
4:B:1420:NAG:O6	4:B:1420:NAG:O4	2.16	0.59
1:A:311:ARG:NH2	2:D:5:MAN:O4	2.36	0.58
3:Q:2:NAG:H83	3:Q:2:NAG:O3	2.03	0.58
1:B:639:SER:CB	3:L:1:NAG:H81	2.34	0.56
3:G:2:NAG:O3	3:G:2:NAG:H83	2.05	0.56
1:A:393:ARG:HD3	3:E:1:NAG:H81	1.88	0.55
1:C:348:ASN:ND2	4:C:1412:NAG:O5	2.36	0.55
3:O:2:NAG:O3	3:O:2:NAG:H82	2.08	0.54
1:A:687:THR:HG23	3:G:1:NAG:H62	1.90	0.54
1:C:261:ASN:OD1	1:C:261:ASN:N	2.37	0.54
1:A:1139:SER:OG	1:A:1152:HIS:ND1	1.89	0.53
3:K:1:NAG:H83	3:K:1:NAG:O3	2.09	0.53
3:Q:2:NAG:H83	3:Q:2:NAG:H3	1.89	0.52
3:G:1:NAG:O3	3:G:1:NAG:H82	2.10	0.52
1:C:213:ASN:OD1	4:C:1401:NAG:C1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:OD1	4:A:1408:NAG:C1	2.58	0.52
1:B:1006:ASN:CG	4:B:1426:NAG:C1	2.73	0.51
1:A:553:ASN:ND2	4:A:1416:NAG:O5	2.40	0.51
1:B:415:LEU:HD21	2:I:6:MAN:O2	2.10	0.51
4:B:1413:NAG:O6	4:B:1413:NAG:O4	2.21	0.51
1:C:348:ASN:OD1	4:C:1412:NAG:C1	2.59	0.51
4:B:1408:NAG:O6	4:B:1408:NAG:O4	2.28	0.51
1:A:348:ASN:HB2	1:A:366:VAL:HG21	1.92	0.51
1:C:415:LEU:N	1:C:415:LEU:CD2	2.72	0.50
1:A:664:ASN:OD1	4:A:1417:NAG:C1	2.59	0.49
1:A:431:ASP:OD1	3:E:1:NAG:O6	2.30	0.49
1:C:415:LEU:N	1:C:415:LEU:HD23	2.27	0.49
1:A:311:ARG:HH22	2:D:5:MAN:C3	2.22	0.49
1:C:341:ASN:OD1	1:C:341:ASN:N	2.44	0.49
1:A:687:THR:CG2	3:G:1:NAG:H5	2.43	0.49
1:C:415:LEU:HD23	1:C:415:LEU:H	1.79	0.48
3:Q:1:NAG:H61	3:Q:2:NAG:HN2	1.78	0.48
1:C:297:ASN:OD1	4:C:1408:NAG:C1	2.60	0.47
1:B:1139:SER:HG	1:B:1152:HIS:HD1	0.49	0.47
1:B:297:ASN:OD1	4:B:1408:NAG:C1	2.60	0.47
1:C:1139:SER:OG	1:C:1152:HIS:ND1	1.83	0.47
1:C:329:GLU:O	4:C:1413:NAG:H2	2.14	0.47
4:A:1417:NAG:O6	4:A:1417:NAG:O4	2.24	0.46
1:A:687:THR:HG21	3:G:1:NAG:H5	1.96	0.46
3:P:1:NAG:H62	3:P:2:NAG:HN2	1.80	0.46
1:B:815:ARG:O	1:B:815:ARG:HD3	2.16	0.46
1:B:261:ASN:OD1	1:B:261:ASN:N	2.48	0.45
4:C:1420:NAG:O6	4:C:1420:NAG:O4	2.31	0.45
1:C:632:LEU:H	1:C:632:LEU:HD23	1.81	0.45
1:A:398:THR:HG22	1:A:400:TYR:H	1.82	0.44
1:A:79:SER:H	1:A:200:ALA:N	2.14	0.44
1:C:262:ASP:CG	1:C:263:SER:H	2.25	0.44
1:A:431:ASP:CG	3:E:1:NAG:HO6	2.06	0.44
1:A:784:ASN:OD1	4:A:1423:NAG:C1	2.65	0.44
1:C:550:LEU:HD11	1:C:573:LEU:HD12	2.00	0.44
2:D:1:NAG:H62	2:D:2:NAG:H82	1.99	0.44
1:B:553:ASN:ND2	4:B:1416:NAG:O5	2.42	0.43
1:C:768:GLN:HE22	1:C:1156:VAL:HG12	1.83	0.43
1:B:815:ARG:O	1:B:815:ARG:CG	2.66	0.43
1:C:404:TYR:OH	2:N:1:NAG:H3	2.19	0.42
1:C:399:LYS:HD3	1:C:400:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1139:SER:CB	1:C:1152:HIS:HD1	2.12	0.42
3:G:1:NAG:O3	3:G:1:NAG:C8	2.68	0.41
1:A:705:TYR:CZ	1:A:708:ASP:HA	2.55	0.41
4:C:1401:NAG:HO3	4:C:1401:NAG:C7	2.22	0.41
2:N:2:NAG:HO3	2:N:2:NAG:C7	2.07	0.41
3:O:2:NAG:O3	3:O:2:NAG:C7	2.68	0.41
1:A:842:SER:HA	1:A:941:VAL:HG13	2.02	0.41
1:B:687:THR:HG23	3:L:1:NAG:H5	2.03	0.41
1:B:1073:ILE:HD13	1:B:1073:ILE:HG21	1.70	0.41
3:K:1:NAG:O3	3:K:1:NAG:C8	2.69	0.41
1:A:201:MET:HA	1:A:201:MET:HE2	2.01	0.41
1:B:768:GLN:HE22	1:B:1156:VAL:HG12	1.86	0.41
1:B:815:ARG:O	1:B:815:ARG:CD	2.69	0.41
1:A:181:TYR:CE2	4:A:1413:NAG:H3	2.55	0.41
1:B:422:ASN:OD1	4:B:1413:NAG:C1	2.67	0.41
4:B:1416:NAG:C1	4:B:1416:NAG:C8	2.85	0.41
1:C:422:ASN:ND2	4:C:1413:NAG:H82	2.36	0.41
1:B:816:CYS:O	1:B:816:CYS:SG	2.78	0.41
1:C:213:ASN:ND2	4:C:1401:NAG:C5	2.84	0.40
3:Q:2:NAG:O3	3:Q:2:NAG:C7	2.68	0.40
1:A:341:ASN:OD1	1:A:341:ASN:N	2.52	0.40
1:A:776:THR:O	1:A:776:THR:OG1	2.34	0.40
1:B:348:ASN:OD1	4:B:1412:NAG:C1	2.68	0.40
1:B:637:ASP:OD2	3:L:1:NAG:H83	2.22	0.40
1:C:776:THR:O	1:C:776:THR:OG1	2.34	0.40
1:B:842:SER:HA	1:B:941:VAL:HG13	2.04	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	1050/1399 (75%)	994 (95%)	56 (5%)	0	100	100
1	B	1050/1399 (75%)	992 (94%)	58 (6%)	0	100	100
1	C	1050/1399 (75%)	996 (95%)	54 (5%)	0	100	100
All	All	3150/4197 (75%)	2982 (95%)	168 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	914/1200 (76%)	891 (98%)	23 (2%)	42	64
1	B	914/1200 (76%)	889 (97%)	25 (3%)	39	63
1	C	914/1200 (76%)	889 (97%)	25 (3%)	39	63
All	All	2742/3600 (76%)	2669 (97%)	73 (3%)	40	63

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	MET
1	A	227	CYS
1	A	237	ASN
1	A	261	ASN
1	A	290	LEU
1	A	326	ILE
1	A	327	LEU
1	A	341	ASN
1	A	345	VAL
1	A	348	ASN
1	A	419	VAL
1	A	525	ASN
1	A	531	THR
1	A	596	CYS
1	A	628	THR

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Mol	Chain	Res	Type
1	A	632	LEU
1	A	644	ASP
1	A	912	GLU
1	A	937	VAL
1	A	1145	PRO
1	A	1161	VAL
1	A	1237	ASP
1	A	1241	ASP
1	B	237	ASN
1	B	261	ASN
1	B	280	CYS
1	B	297	ASN
1	B	327	LEU
1	B	341	ASN
1	B	419	VAL
1	B	505	ASN
1	B	525	ASN
1	B	568	ASN
1	B	596	CYS
1	B	628	THR
1	B	632	LEU
1	B	633	GLU
1	B	723	ASN
1	B	815	ARG
1	B	912	GLU
1	B	927	VAL
1	B	1023	LYS
1	B	1072	ASP
1	B	1145	PRO
1	B	1149	LEU
1	B	1161	VAL
1	B	1237	ASP
1	B	1241	ASP
1	C	53	LEU
1	C	169	ARG
1	C	237	ASN
1	C	261	ASN
1	C	280	CYS
1	C	297	ASN
1	C	327	LEU
1	C	341	ASN
1	C	348	ASN

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Mol	Chain	Res	Type
1	C	415	LEU
1	C	525	ASN
1	C	628	THR
1	C	632	LEU
1	C	663	THR
1	C	723	ASN
1	C	902	VAL
1	C	912	GLU
1	C	927	VAL
1	C	975	VAL
1	C	995	LEU
1	C	1023	LYS
1	C	1065	ASP
1	C	1145	PRO
1	C	1154	VAL
1	C	1237	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	292	GLN
1	A	451	GLN
1	A	488	ASN
1	A	507	HIS
1	A	702	GLN
1	A	724	ASN
1	A	835	GLN
1	A	980	ASN
1	A	985	GLN
1	A	1006	ASN
1	A	1097	GLN
1	A	1114	GLN
1	A	1234	GLN
1	B	237	ASN
1	B	279	ASN
1	B	292	GLN
1	B	451	GLN
1	B	488	ASN
1	B	507	HIS
1	B	545	GLN
1	B	565	GLN

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Mol	Chain	Res	Type
1	B	724	ASN
1	B	768	GLN
1	B	813	ASN
1	B	818	GLN
1	B	835	GLN
1	B	980	ASN
1	B	992	ASN
1	B	1006	ASN
1	B	1030	HIS
1	B	1042	GLN
1	B	1097	GLN
1	B	1146	GLN
1	B	1192	GLN
1	C	237	ASN
1	C	244	ASN
1	C	255	ASN
1	C	426	HIS
1	C	451	GLN
1	C	768	GLN
1	C	795	GLN
1	C	835	GLN
1	C	980	ASN
1	C	1097	GLN
1	C	1114	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

42 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	2	14,14,15	3.18	12 (85%)	17,19,21	3.48	9 (52%)
2	NAG	D	2	2	14,14,15	2.99	7 (50%)	17,19,21	3.58	11 (64%)
2	BMA	D	3	2	11,11,12	2.92	6 (54%)	15,15,17	2.33	5 (33%)
2	MAN	D	4	2	11,11,12	1.59	2 (18%)	15,15,17	2.14	6 (40%)
2	MAN	D	5	2	11,11,12	1.00	0	15,15,17	1.96	5 (33%)
2	MAN	D	6	2	11,11,12	1.43	2 (18%)	15,15,17	1.77	5 (33%)
3	NAG	E	1	3	14,14,15	2.06	1 (7%)	17,19,21	2.52	6 (35%)
3	NAG	E	2	3	14,14,15	0.74	0	17,19,21	2.18	4 (23%)
3	NAG	F	1	3	14,14,15	2.14	6 (42%)	17,19,21	2.87	6 (35%)
3	NAG	F	2	3	14,14,15	1.69	3 (21%)	17,19,21	1.63	4 (23%)
3	NAG	G	1	3	14,14,15	3.75	11 (78%)	17,19,21	5.63	11 (64%)
3	NAG	G	2	3	14,14,15	1.99	6 (42%)	17,19,21	2.97	10 (58%)
3	NAG	H	1	3	14,14,15	2.41	6 (42%)	17,19,21	4.16	8 (47%)
3	NAG	H	2	3	14,14,15	1.39	3 (21%)	17,19,21	1.78	4 (23%)
2	NAG	I	1	2	14,14,15	2.67	10 (71%)	17,19,21	2.97	8 (47%)
2	NAG	I	2	2	14,14,15	2.85	8 (57%)	17,19,21	3.23	8 (47%)
2	BMA	I	3	2	11,11,12	2.65	6 (54%)	15,15,17	2.28	3 (20%)
2	MAN	I	4	2	11,11,12	1.59	3 (27%)	15,15,17	2.38	7 (46%)
2	MAN	I	5	2	11,11,12	1.13	1 (9%)	15,15,17	2.03	4 (26%)
2	MAN	I	6	2	11,11,12	1.31	1 (9%)	15,15,17	1.75	5 (33%)
3	NAG	J	1	3	14,14,15	1.79	1 (7%)	17,19,21	2.52	6 (35%)
3	NAG	J	2	3	14,14,15	0.74	0	17,19,21	1.55	5 (29%)
3	NAG	K	1	3	14,14,15	1.80	6 (42%)	17,19,21	5.76	9 (52%)
3	NAG	K	2	3	14,14,15	1.81	5 (35%)	17,19,21	1.31	2 (11%)
3	NAG	L	1	3	14,14,15	3.50	11 (78%)	17,19,21	6.45	14 (82%)
3	NAG	L	2	3	14,14,15	2.14	7 (50%)	17,19,21	1.99	7 (41%)
3	NAG	M	1	3	14,14,15	2.62	7 (50%)	17,19,21	3.32	9 (52%)
3	NAG	M	2	3	14,14,15	1.33	3 (21%)	17,19,21	1.93	3 (17%)
2	NAG	N	1	2,1	14,14,15	3.13	10 (71%)	17,19,21	3.06	6 (35%)
2	NAG	N	2	2	14,14,15	2.58	7 (50%)	17,19,21	3.29	8 (47%)
2	BMA	N	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.74	3 (20%)
2	MAN	N	4	2	11,11,12	0.95	0	15,15,17	1.68	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	N	5	2	11,11,12	0.53	0	15,15,17	1.51	3 (20%)
2	MAN	N	6	2	11,11,12	1.45	2 (18%)	15,15,17	1.83	3 (20%)
3	NAG	O	1	3	14,14,15	1.95	2 (14%)	17,19,21	4.75	7 (41%)
3	NAG	O	2	3	14,14,15	0.84	0	17,19,21	1.97	5 (29%)
3	NAG	P	1	3	14,14,15	2.25	8 (57%)	17,19,21	3.30	7 (41%)
3	NAG	P	2	3	14,14,15	1.86	3 (21%)	17,19,21	1.43	2 (11%)
3	NAG	Q	1	3	14,14,15	3.42	11 (78%)	17,19,21	3.45	9 (52%)
3	NAG	Q	2	3	14,14,15	2.14	6 (42%)	17,19,21	2.31	6 (35%)
3	NAG	R	1	3	14,14,15	2.58	6 (42%)	17,19,21	3.94	9 (52%)
3	NAG	R	2	3	14,14,15	1.44	3 (21%)	17,19,21	1.73	3 (17%)

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	2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	1	3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	NAG	K	1	3	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	5/6/23/26	0/1/1/1
3	NAG	L	2	3	-	4/6/23/26	0/1/1/1
3	NAG	M	1	3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	0/1/1/1
2	MAN	N	5	2	-	1/2/19/22	0/1/1/1
2	MAN	N	6	2	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	C2-N2	-8.86	1.31	1.46
3	E	1	NAG	C1-C2	7.12	1.62	1.52
2	D	2	NAG	C1-C2	-6.78	1.43	1.52
2	I	2	NAG	C1-C2	-6.67	1.43	1.52
3	J	1	NAG	C1-C2	6.14	1.60	1.52
2	N	2	NAG	C1-C2	-6.06	1.44	1.52
2	N	1	NAG	O5-C1	-5.64	1.34	1.43
3	Q	1	NAG	O5-C1	-5.42	1.34	1.43
3	L	1	NAG	C2-N2	-5.40	1.37	1.46
3	O	1	NAG	C1-C2	5.35	1.59	1.52
2	D	1	NAG	O5-C5	-5.22	1.33	1.43
3	L	1	NAG	O5-C1	-5.09	1.35	1.43
3	Q	1	NAG	C4-C5	-4.91	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O5-C5	-4.88	1.33	1.43
3	R	1	NAG	O5-C1	-4.80	1.35	1.43
3	L	1	NAG	C3-C2	-4.73	1.42	1.52
2	I	3	BMA	O5-C1	-4.70	1.35	1.43
2	D	1	NAG	C4-C5	-4.70	1.43	1.53
3	Q	1	NAG	C1-C2	4.69	1.58	1.52
3	Q	1	NAG	O5-C5	-4.68	1.34	1.43
2	N	1	NAG	C2-N2	-4.66	1.38	1.46
3	L	1	NAG	C7-N2	-4.62	1.19	1.34
3	R	1	NAG	O5-C5	-4.58	1.34	1.43
3	P	2	NAG	C2-N2	-4.57	1.38	1.46
2	D	3	BMA	O5-C1	-4.48	1.36	1.43
3	G	1	NAG	C7-N2	-4.45	1.20	1.34
3	G	1	NAG	O5-C1	-4.44	1.36	1.43
2	I	1	NAG	C2-N2	-4.36	1.39	1.46
3	L	1	NAG	C4-C5	-4.20	1.44	1.53
2	N	1	NAG	C3-C2	-4.18	1.43	1.52
2	D	2	NAG	O5-C1	-4.16	1.36	1.43
3	Q	1	NAG	O7-C7	-4.16	1.13	1.23
2	D	3	BMA	C2-C3	-4.12	1.46	1.52
3	H	1	NAG	O5-C1	-4.12	1.36	1.43
2	D	1	NAG	C2-N2	-4.05	1.39	1.46
3	H	1	NAG	O5-C5	-3.98	1.35	1.43
3	L	1	NAG	O5-C5	-3.95	1.35	1.43
2	D	1	NAG	O5-C1	-3.95	1.37	1.43
3	M	1	NAG	O5-C1	-3.93	1.37	1.43
3	M	1	NAG	C1-C2	3.89	1.57	1.52
3	F	2	NAG	C2-N2	-3.89	1.39	1.46
2	I	1	NAG	O5-C5	-3.83	1.36	1.43
3	P	1	NAG	C1-C2	3.83	1.57	1.52
2	D	3	BMA	O5-C5	-3.82	1.36	1.43
3	G	1	NAG	C4-C5	-3.82	1.44	1.53
3	R	1	NAG	C4-C5	-3.81	1.44	1.53
2	D	2	NAG	O5-C5	-3.80	1.36	1.43
3	M	1	NAG	O5-C5	-3.80	1.36	1.43
3	M	1	NAG	C2-N2	-3.79	1.40	1.46
2	I	1	NAG	O5-C1	-3.68	1.37	1.43
3	M	1	NAG	C4-C5	-3.68	1.45	1.53
3	O	1	NAG	O5-C1	-3.63	1.37	1.43
3	H	1	NAG	C2-N2	-3.63	1.40	1.46
3	L	1	NAG	O7-C7	-3.62	1.15	1.23
2	D	3	BMA	C4-C5	-3.59	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C4-C5	-3.58	1.45	1.53
3	R	1	NAG	C2-N2	-3.58	1.40	1.46
3	G	1	NAG	O5-C5	-3.58	1.36	1.43
3	Q	2	NAG	O5-C1	-3.52	1.37	1.43
2	I	3	BMA	C2-C3	-3.51	1.47	1.52
3	K	2	NAG	C1-C2	-3.51	1.47	1.52
2	I	2	NAG	O5-C1	-3.51	1.37	1.43
2	I	3	BMA	O5-C5	-3.50	1.36	1.43
3	F	1	NAG	O5-C1	-3.43	1.37	1.43
3	L	2	NAG	C2-N2	-3.41	1.40	1.46
3	L	2	NAG	O5-C1	-3.37	1.38	1.43
2	D	2	NAG	C3-C2	-3.36	1.45	1.52
3	P	2	NAG	C1-C2	-3.34	1.47	1.52
2	N	2	NAG	C3-C2	-3.34	1.45	1.52
2	I	2	NAG	C4-C5	-3.33	1.45	1.53
3	G	1	NAG	C3-C2	-3.33	1.45	1.52
3	K	2	NAG	O5-C1	-3.31	1.38	1.43
2	I	2	NAG	C3-C2	-3.25	1.45	1.52
3	Q	2	NAG	C2-N2	-3.23	1.40	1.46
3	G	1	NAG	C4-C3	-3.20	1.44	1.52
3	G	1	NAG	O7-C7	-3.20	1.16	1.23
3	L	1	NAG	O4-C4	-3.19	1.35	1.43
3	F	1	NAG	C4-C5	-3.19	1.46	1.53
3	Q	2	NAG	C1-C2	-3.17	1.48	1.52
2	I	1	NAG	O7-C7	-3.16	1.16	1.23
2	I	3	BMA	C4-C5	-3.16	1.46	1.53
2	D	3	BMA	O2-C2	-3.14	1.36	1.43
2	N	2	NAG	O5-C1	-3.13	1.38	1.43
2	D	3	BMA	C4-C3	-3.12	1.44	1.52
3	F	2	NAG	C1-C2	-3.11	1.48	1.52
3	P	1	NAG	O5-C5	-3.10	1.37	1.43
2	N	2	NAG	C4-C5	-3.08	1.46	1.53
2	I	1	NAG	C4-C5	-3.08	1.46	1.53
3	H	1	NAG	C4-C5	-3.04	1.46	1.53
2	D	1	NAG	C7-N2	-3.02	1.24	1.34
2	I	2	NAG	O5-C5	-3.02	1.37	1.43
2	D	1	NAG	C1-C2	2.99	1.56	1.52
3	H	1	NAG	C3-C2	-2.97	1.46	1.52
3	G	2	NAG	C1-C2	-2.97	1.48	1.52
3	H	1	NAG	C1-C2	2.94	1.56	1.52
3	F	1	NAG	O5-C5	-2.94	1.37	1.43
2	D	4	MAN	O5-C5	-2.93	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C2-N2	-2.92	1.41	1.46
3	K	2	NAG	C2-N2	-2.91	1.41	1.46
3	P	1	NAG	O5-C1	-2.90	1.38	1.43
2	D	4	MAN	C2-C3	-2.90	1.48	1.52
2	D	1	NAG	C4-C3	-2.89	1.44	1.52
3	Q	1	NAG	C7-N2	-2.88	1.25	1.34
3	P	1	NAG	O7-C7	-2.87	1.16	1.23
3	M	1	NAG	C3-C2	-2.87	1.46	1.52
2	D	1	NAG	C3-C2	-2.87	1.46	1.52
3	K	1	NAG	C3-C2	-2.86	1.46	1.52
3	G	2	NAG	C2-N2	-2.86	1.41	1.46
2	I	1	NAG	C8-C7	-2.83	1.44	1.50
3	R	2	NAG	O5-C5	-2.82	1.37	1.43
3	L	2	NAG	C1-C2	-2.82	1.48	1.52
3	Q	1	NAG	C4-C3	-2.82	1.45	1.52
2	I	1	NAG	C3-C2	-2.81	1.46	1.52
3	Q	2	NAG	C3-C2	-2.79	1.46	1.52
3	P	1	NAG	C2-N2	-2.75	1.41	1.46
3	Q	1	NAG	C3-C2	-2.73	1.46	1.52
2	I	4	MAN	C2-C3	-2.72	1.48	1.52
2	D	1	NAG	O4-C4	-2.72	1.36	1.43
3	Q	1	NAG	C8-C7	-2.71	1.44	1.50
3	G	2	NAG	O5-C1	-2.70	1.39	1.43
3	R	1	NAG	C3-C2	-2.68	1.46	1.52
3	G	2	NAG	C3-C2	-2.67	1.46	1.52
3	Q	1	NAG	C2-N2	-2.66	1.41	1.46
2	I	3	BMA	O2-C2	-2.65	1.37	1.43
2	N	6	MAN	C2-C3	-2.64	1.48	1.52
3	G	1	NAG	C1-C2	2.63	1.55	1.52
2	I	4	MAN	O5-C5	-2.63	1.38	1.43
2	N	1	NAG	O7-C7	-2.63	1.17	1.23
2	I	3	BMA	C4-C3	-2.61	1.45	1.52
3	P	1	NAG	C4-C5	-2.60	1.47	1.53
2	N	1	NAG	C8-C7	-2.56	1.45	1.50
3	K	1	NAG	O5-C5	-2.54	1.38	1.43
3	L	2	NAG	C3-C2	-2.54	1.47	1.52
2	D	1	NAG	O7-C7	-2.51	1.17	1.23
2	D	1	NAG	C8-C7	-2.50	1.45	1.50
3	L	2	NAG	C4-C5	-2.50	1.47	1.53
3	G	2	NAG	O7-C7	-2.49	1.17	1.23
2	N	1	NAG	C4-C3	-2.48	1.45	1.52
3	F	1	NAG	O7-C7	-2.46	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O4-C4	-2.46	1.36	1.43
3	K	1	NAG	C2-N2	-2.45	1.42	1.46
3	K	1	NAG	O5-C1	-2.40	1.39	1.43
3	Q	2	NAG	O5-C5	-2.38	1.38	1.43
3	L	2	NAG	O7-C7	-2.38	1.17	1.23
2	D	6	MAN	O5-C1	-2.38	1.39	1.43
3	R	1	NAG	C1-C2	2.37	1.55	1.52
3	H	2	NAG	C3-C2	-2.37	1.47	1.52
2	N	6	MAN	C1-C2	-2.37	1.46	1.52
2	I	6	MAN	C2-C3	-2.36	1.48	1.52
3	L	1	NAG	C8-C7	-2.35	1.45	1.50
3	M	1	NAG	C4-C3	-2.34	1.46	1.52
2	N	2	NAG	C4-C3	-2.33	1.46	1.52
3	R	2	NAG	C3-C2	-2.33	1.47	1.52
3	M	2	NAG	C3-C2	-2.33	1.47	1.52
2	I	1	NAG	C7-N2	-2.32	1.26	1.34
2	I	2	NAG	O3-C3	-2.32	1.37	1.43
2	I	4	MAN	C4-C5	-2.31	1.48	1.53
3	G	1	NAG	C8-C7	-2.30	1.45	1.50
2	I	1	NAG	O4-C4	-2.29	1.37	1.43
3	M	2	NAG	O5-C5	-2.27	1.39	1.43
2	D	6	MAN	C2-C3	-2.27	1.49	1.52
2	N	3	BMA	O5-C1	-2.26	1.39	1.43
2	N	2	NAG	O5-C5	-2.24	1.39	1.43
3	R	2	NAG	C4-C5	-2.23	1.48	1.53
3	K	2	NAG	C3-C2	-2.23	1.47	1.52
3	K	1	NAG	O3-C3	-2.22	1.37	1.43
2	N	1	NAG	C4-C5	-2.21	1.48	1.53
2	I	2	NAG	C4-C3	-2.20	1.46	1.52
3	P	1	NAG	C4-C3	-2.20	1.46	1.52
3	F	2	NAG	C3-C2	-2.20	1.47	1.52
3	H	2	NAG	C4-C5	-2.19	1.48	1.53
2	D	1	NAG	C6-C5	-2.18	1.44	1.51
2	N	1	NAG	C7-N2	-2.18	1.27	1.34
3	P	1	NAG	C3-C2	-2.17	1.48	1.52
3	H	2	NAG	C1-C2	-2.17	1.49	1.52
3	K	1	NAG	C1-C2	2.17	1.55	1.52
3	L	1	NAG	C4-C3	-2.17	1.46	1.52
2	I	1	NAG	C4-C3	-2.13	1.46	1.52
3	Q	2	NAG	C4-C5	-2.13	1.48	1.53
3	L	2	NAG	O5-C5	-2.11	1.39	1.43
3	G	2	NAG	O5-C5	-2.11	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O3-C3	-2.10	1.37	1.43
3	G	1	NAG	C6-C5	-2.10	1.44	1.51
3	M	2	NAG	C4-C5	-2.10	1.48	1.53
3	Q	1	NAG	O4-C4	-2.10	1.37	1.43
2	I	2	NAG	C2-N2	-2.09	1.42	1.46
2	N	2	NAG	O3-C3	-2.09	1.37	1.43
3	P	2	NAG	O5-C5	-2.06	1.39	1.43
2	D	2	NAG	C4-C3	-2.06	1.47	1.52
3	L	1	NAG	O3-C3	-2.05	1.37	1.43
2	I	5	MAN	O5-C1	-2.04	1.40	1.43
2	N	3	BMA	C2-C3	-2.02	1.49	1.52
3	F	1	NAG	C4-C3	-2.02	1.47	1.52
3	K	2	NAG	O5-C5	-2.01	1.39	1.43

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-C2-N2	-15.94	85.31	110.43
3	O	1	NAG	O5-C5-C6	-13.87	80.67	107.66
3	K	1	NAG	O5-C1-C2	-13.35	90.63	111.29
3	L	1	NAG	C1-C2-N2	-12.71	90.41	110.43
3	L	1	NAG	O5-C1-C2	-12.70	91.64	111.29
3	G	1	NAG	O5-C1-C2	-11.02	94.23	111.29
3	K	1	NAG	C2-N2-C7	10.91	137.52	122.90
3	L	1	NAG	O3-C3-C2	-9.92	88.80	109.40
3	K	1	NAG	C1-C2-N2	-9.30	95.78	110.43
3	H	1	NAG	O5-C1-C2	-9.16	97.12	111.29
3	P	1	NAG	O5-C1-C2	-8.88	97.55	111.29
3	R	1	NAG	O5-C1-C2	-8.84	97.61	111.29
3	Q	1	NAG	O5-C1-C2	-8.73	97.78	111.29
2	D	2	NAG	O3-C3-C2	-8.37	92.02	109.40
2	D	1	NAG	O5-C1-C2	-8.31	98.43	111.29
3	O	1	NAG	O5-C1-C2	-8.29	98.47	111.29
2	N	2	NAG	O3-C3-C2	-8.27	92.22	109.40
3	L	1	NAG	C4-C3-C2	-8.08	99.18	111.02
3	F	1	NAG	O5-C1-C2	-8.04	98.86	111.29
3	K	1	NAG	O3-C3-C2	-8.03	92.72	109.40
3	H	1	NAG	C2-N2-C7	-7.92	112.29	122.90
3	L	1	NAG	C1-O5-C5	7.55	122.31	112.19
3	M	1	NAG	C1-C2-N2	-7.41	98.76	110.43
3	R	1	NAG	C2-N2-C7	-7.39	113.00	122.90
2	N	1	NAG	C4-C3-C2	-7.38	100.20	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	O4-C4-C5	-7.37	91.17	109.32
2	D	1	NAG	O6-C6-C5	-7.29	86.53	111.33
3	M	1	NAG	O5-C1-C2	-7.25	100.07	111.29
2	I	2	NAG	O3-C3-C2	-7.10	94.65	109.40
2	I	1	NAG	O5-C1-C2	-7.00	100.47	111.29
2	D	2	NAG	O4-C4-C5	-6.64	92.96	109.32
3	K	1	NAG	C1-O5-C5	6.60	121.03	112.19
3	H	1	NAG	C1-C2-N2	-6.50	100.19	110.43
3	G	1	NAG	O5-C5-C6	6.31	119.95	107.66
3	R	1	NAG	C1-C2-N2	-6.26	100.57	110.43
3	G	2	NAG	C1-C2-N2	-6.20	100.66	110.43
3	L	1	NAG	O7-C7-C8	6.13	132.97	122.05
2	N	1	NAG	C1-O5-C5	-6.06	104.06	112.19
3	O	1	NAG	O4-C4-C5	6.05	124.22	109.32
2	I	2	NAG	O4-C4-C5	-6.01	94.53	109.32
3	P	1	NAG	C3-C4-C5	-5.73	99.84	110.23
3	J	1	NAG	O5-C1-C2	-5.67	102.52	111.29
3	O	1	NAG	C4-C3-C2	-5.64	102.76	111.02
3	G	1	NAG	C2-N2-C7	-5.62	115.37	122.90
3	H	1	NAG	C1-O5-C5	5.59	119.68	112.19
2	N	1	NAG	O6-C6-C5	-5.54	92.46	111.33
3	R	1	NAG	C1-O5-C5	5.53	119.60	112.19
2	D	3	BMA	O4-C4-C3	-5.51	97.39	110.38
2	I	1	NAG	C1-C2-N2	-5.42	101.89	110.43
3	E	2	NAG	C2-N2-C7	5.41	130.15	122.90
2	I	3	BMA	O4-C4-C3	-5.39	97.66	110.38
3	E	1	NAG	O5-C1-C2	-5.26	103.16	111.29
3	G	2	NAG	C2-N2-C7	5.24	129.93	122.90
2	D	2	NAG	C2-N2-C7	-5.23	115.89	122.90
2	I	3	BMA	O4-C4-C5	-5.23	96.45	109.32
3	G	2	NAG	O3-C3-C4	-5.16	98.22	110.38
3	F	1	NAG	C1-O5-C5	5.14	119.07	112.19
3	Q	1	NAG	C1-C2-N2	5.09	118.45	110.43
2	N	2	NAG	O4-C4-C5	-4.91	97.24	109.32
3	E	1	NAG	C1-C2-N2	4.90	118.15	110.43
3	K	1	NAG	O4-C4-C5	-4.89	97.29	109.32
2	D	3	BMA	O4-C4-C5	-4.84	97.41	109.32
2	D	1	NAG	C4-C3-C2	-4.81	103.97	111.02
2	I	2	NAG	C1-C2-N2	-4.76	102.94	110.43
3	H	2	NAG	O3-C3-C2	-4.75	99.54	109.40
3	Q	1	NAG	C3-C4-C5	-4.66	101.78	110.23
3	M	1	NAG	C1-O5-C5	4.54	118.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C1-C2-N2	4.52	117.56	110.43
3	G	1	NAG	C3-C4-C5	-4.52	102.04	110.23
3	Q	2	NAG	O5-C5-C6	-4.50	98.90	107.66
2	D	4	MAN	O4-C4-C5	-4.49	98.26	109.32
3	E	1	NAG	O4-C4-C5	4.48	120.36	109.32
2	I	4	MAN	O4-C4-C5	-4.47	98.31	109.32
3	H	1	NAG	C4-C3-C2	-4.45	104.49	111.02
2	I	5	MAN	O3-C3-C4	-4.43	99.93	110.38
2	N	2	NAG	C2-N2-C7	-4.43	116.97	122.90
3	P	1	NAG	C1-O5-C5	4.40	118.09	112.19
2	N	6	MAN	O3-C3-C2	-4.37	101.15	110.05
2	I	2	NAG	C3-C4-C5	-4.35	102.34	110.23
3	E	2	NAG	O3-C3-C4	-4.33	100.18	110.38
3	L	1	NAG	O5-C5-C6	-4.31	99.27	107.66
3	K	1	NAG	C4-C3-C2	-4.29	104.73	111.02
3	Q	1	NAG	O3-C3-C4	-4.28	100.28	110.38
3	O	1	NAG	C1-C2-N2	4.27	117.16	110.43
2	I	1	NAG	C3-C4-C5	-4.26	102.51	110.23
3	K	1	NAG	C3-C4-C5	-4.26	102.51	110.23
3	Q	2	NAG	C6-C5-C4	-4.21	102.67	113.02
2	I	5	MAN	C6-C5-C4	-4.11	102.94	113.02
3	R	2	NAG	O3-C3-C2	-4.10	100.88	109.40
2	D	5	MAN	O3-C3-C4	-4.10	100.71	110.38
3	G	1	NAG	O6-C6-C5	-4.09	97.41	111.33
3	R	1	NAG	O6-C6-C5	-4.06	97.50	111.33
2	N	3	BMA	O4-C4-C3	-4.03	100.88	110.38
3	M	2	NAG	C2-N2-C7	3.98	128.24	122.90
3	M	2	NAG	O3-C3-C2	-3.98	101.13	109.40
3	P	1	NAG	C1-C2-N2	-3.94	104.23	110.43
2	I	2	NAG	C2-N2-C7	-3.91	117.65	122.90
2	N	2	NAG	C3-C4-C5	-3.89	103.18	110.23
3	Q	1	NAG	O5-C5-C6	3.88	115.22	107.66
3	G	1	NAG	C1-O5-C5	3.86	117.36	112.19
2	I	1	NAG	O5-C5-C6	3.86	115.17	107.66
3	O	2	NAG	C1-O5-C5	3.83	117.33	112.19
2	I	4	MAN	C6-C5-C4	-3.80	103.68	113.02
3	F	1	NAG	C3-C4-C5	-3.79	103.37	110.23
3	Q	1	NAG	O6-C6-C5	-3.75	98.57	111.33
2	D	1	NAG	O4-C4-C3	3.74	119.18	110.38
2	N	2	NAG	O5-C1-C2	-3.73	105.51	111.29
3	H	1	NAG	O4-C4-C5	-3.71	100.19	109.32
3	F	2	NAG	O4-C4-C3	-3.71	101.64	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	NAG	O3-C3-C4	-3.70	101.66	110.38
3	L	1	NAG	O5-C5-C4	-3.69	101.86	110.83
2	D	2	NAG	O5-C1-C2	-3.65	105.64	111.29
3	O	2	NAG	O3-C3-C2	3.65	116.98	109.40
3	G	2	NAG	C8-C7-N2	3.64	122.16	116.12
3	G	1	NAG	C4-C3-C2	-3.64	105.69	111.02
3	M	1	NAG	C2-N2-C7	-3.64	118.03	122.90
3	J	1	NAG	C4-C3-C2	-3.62	105.71	111.02
2	D	2	NAG	C1-C2-N2	-3.62	104.73	110.43
3	H	1	NAG	O3-C3-C2	-3.60	101.91	109.40
3	O	1	NAG	C1-O5-C5	3.60	117.01	112.19
3	E	1	NAG	C4-C3-C2	-3.57	105.78	111.02
3	Q	2	NAG	O4-C4-C3	-3.57	101.97	110.38
2	D	2	NAG	C3-C4-C5	-3.55	103.80	110.23
2	D	5	MAN	C6-C5-C4	-3.54	104.32	113.02
3	L	1	NAG	O7-C7-N2	-3.48	115.83	121.98
2	N	1	NAG	C2-N2-C7	-3.45	118.28	122.90
3	Q	2	NAG	O3-C3-C4	-3.42	102.32	110.38
2	D	1	NAG	C1-O5-C5	3.40	116.74	112.19
2	I	4	MAN	O4-C4-C3	-3.38	102.42	110.38
3	J	2	NAG	C2-N2-C7	3.37	127.42	122.90
2	I	2	NAG	O5-C1-C2	-3.33	106.14	111.29
2	D	4	MAN	C1-C2-C3	-3.33	104.80	109.64
3	O	2	NAG	O5-C1-C2	-3.32	106.15	111.29
2	D	2	NAG	O5-C5-C6	-3.32	101.21	107.66
3	E	2	NAG	C1-O5-C5	3.31	116.62	112.19
3	P	1	NAG	O4-C4-C5	-3.29	101.22	109.32
3	Q	2	NAG	O3-C3-C2	-3.28	102.59	109.40
3	R	1	NAG	C4-C3-C2	-3.28	106.22	111.02
3	L	2	NAG	O6-C6-C5	-3.28	100.18	111.33
3	M	1	NAG	O6-C6-C5	-3.27	100.19	111.33
3	P	2	NAG	O4-C4-C3	-3.21	102.80	110.38
2	D	3	BMA	O3-C3-C4	-3.20	102.83	110.38
3	P	1	NAG	C2-N2-C7	3.19	127.18	122.90
3	F	1	NAG	O4-C4-C5	-3.18	101.49	109.32
2	I	6	MAN	O4-C4-C3	-3.13	102.99	110.38
2	D	6	MAN	C6-C5-C4	3.12	120.67	113.02
2	I	1	NAG	O3-C3-C4	3.10	117.68	110.38
2	N	2	NAG	O4-C4-C3	-3.05	103.17	110.38
2	N	6	MAN	C3-C4-C5	-3.05	104.71	110.23
3	R	1	NAG	O4-C4-C5	-3.04	101.84	109.32
3	E	1	NAG	O5-C5-C6	3.04	113.57	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C8-C7-N2	-3.03	111.09	116.12
2	N	5	MAN	O5-C5-C6	3.02	113.53	107.66
2	I	4	MAN	O2-C2-C3	-2.99	103.96	110.15
2	N	4	MAN	O2-C2-C3	-2.99	103.96	110.15
2	D	2	NAG	O4-C4-C3	-2.98	103.36	110.38
3	L	2	NAG	O3-C3-C4	-2.98	103.36	110.38
3	L	2	NAG	O4-C4-C3	-2.96	103.39	110.38
3	K	2	NAG	O3-C3-C2	-2.96	103.26	109.40
3	J	1	NAG	O5-C5-C6	2.96	113.42	107.66
3	F	2	NAG	C1-O5-C5	-2.94	108.24	112.19
2	I	6	MAN	C6-C5-C4	2.92	120.19	113.02
3	R	2	NAG	C1-O5-C5	2.91	116.09	112.19
3	F	1	NAG	C1-C2-N2	-2.90	105.87	110.43
3	H	1	NAG	O4-C4-C3	2.87	117.15	110.38
2	D	1	NAG	C8-C7-N2	-2.87	111.35	116.12
2	N	3	BMA	O4-C4-C5	-2.87	102.25	109.32
2	N	5	MAN	C2-C3-C4	-2.86	105.83	110.86
2	D	1	NAG	O7-C7-C8	2.85	127.13	122.05
3	M	1	NAG	O5-C5-C6	2.85	113.20	107.66
3	K	2	NAG	O4-C4-C3	-2.84	103.67	110.38
2	I	1	NAG	C2-N2-C7	-2.84	119.09	122.90
3	G	2	NAG	O5-C5-C6	2.84	113.19	107.66
3	E	2	NAG	C6-C5-C4	-2.83	106.06	113.02
3	O	1	NAG	C2-N2-C7	-2.83	119.11	122.90
2	N	4	MAN	C2-C3-C4	-2.82	105.90	110.86
3	G	1	NAG	O4-C4-C3	2.81	117.01	110.38
3	J	1	NAG	O4-C4-C5	2.81	116.25	109.32
3	G	2	NAG	O3-C3-C2	-2.80	103.58	109.40
3	L	1	NAG	C2-N2-C7	2.77	126.61	122.90
2	D	4	MAN	O3-C3-C2	-2.76	104.41	110.05
3	J	1	NAG	O3-C3-C4	2.76	116.89	110.38
3	M	2	NAG	C1-C2-N2	-2.75	106.10	110.43
2	D	6	MAN	O5-C5-C4	-2.75	104.13	110.83
2	N	2	NAG	C1-C2-N2	-2.75	106.10	110.43
2	D	2	NAG	O6-C6-C5	-2.75	101.97	111.33
2	D	4	MAN	O5-C5-C6	-2.74	102.33	107.66
2	D	5	MAN	O2-C2-C3	-2.70	104.56	110.15
2	I	6	MAN	O5-C5-C4	-2.70	104.27	110.83
3	Q	2	NAG	C4-C3-C2	-2.69	107.07	111.02
3	Q	1	NAG	C4-C3-C2	-2.66	107.11	111.02
2	D	6	MAN	O4-C4-C3	-2.66	104.11	110.38
2	N	5	MAN	C6-C5-C4	-2.65	106.51	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	MAN	C2-C3-C4	-2.65	106.21	110.86
3	G	2	NAG	C1-O5-C5	-2.64	108.64	112.19
2	N	4	MAN	C6-C5-C4	-2.64	106.55	113.02
2	D	6	MAN	C2-C3-C4	-2.63	106.23	110.86
2	N	1	NAG	O5-C5-C6	2.63	112.79	107.66
2	N	1	NAG	O4-C4-C3	2.63	116.57	110.38
2	D	5	MAN	C2-C3-C4	-2.62	106.26	110.86
2	I	4	MAN	O5-C5-C6	-2.61	102.59	107.66
3	O	2	NAG	O3-C3-C4	-2.60	104.25	110.38
2	I	1	NAG	C4-C3-C2	-2.60	107.21	111.02
3	F	2	NAG	C2-N2-C7	-2.59	119.42	122.90
3	J	2	NAG	C1-O5-C5	2.57	115.62	112.19
2	I	4	MAN	C1-C2-C3	-2.57	105.91	109.64
3	L	2	NAG	O5-C5-C6	2.56	112.64	107.66
3	L	2	NAG	C8-C7-N2	2.55	120.35	116.12
2	D	6	MAN	O2-C2-C1	-2.55	103.39	109.22
3	H	2	NAG	C1-C2-N2	-2.54	106.42	110.43
3	O	2	NAG	C2-N2-C7	-2.52	119.52	122.90
3	Q	1	NAG	O3-C3-C2	-2.52	104.17	109.40
2	I	6	MAN	O2-C2-C1	-2.49	103.52	109.22
3	P	2	NAG	C4-C3-C2	-2.46	107.41	111.02
3	G	2	NAG	O7-C7-C8	-2.46	117.68	122.05
3	G	1	NAG	C8-C7-N2	2.46	120.19	116.12
3	L	2	NAG	C1-O5-C5	-2.45	108.91	112.19
2	I	4	MAN	O3-C3-C2	-2.44	105.07	110.05
2	I	5	MAN	O2-C2-C3	-2.44	105.10	110.15
3	R	1	NAG	C3-C4-C5	-2.42	105.84	110.23
3	J	2	NAG	O3-C3-C4	-2.42	104.67	110.38
2	I	2	NAG	O6-C6-C5	-2.39	103.19	111.33
2	D	4	MAN	O2-C2-C3	-2.38	105.23	110.15
3	H	2	NAG	C2-N2-C7	2.37	126.08	122.90
3	J	2	NAG	C4-C3-C2	-2.37	107.55	111.02
3	H	2	NAG	O3-C3-C4	-2.34	104.85	110.38
3	J	2	NAG	O5-C1-C2	-2.33	107.68	111.29
3	L	1	NAG	O6-C6-C5	2.32	119.24	111.33
3	R	2	NAG	C6-C5-C4	-2.32	107.33	113.02
2	D	1	NAG	O3-C3-C2	2.29	114.15	109.40
2	I	3	BMA	C2-C3-C4	-2.28	106.84	110.86
3	F	1	NAG	C6-C5-C4	-2.27	107.43	113.02
3	Q	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	M	1	NAG	C8-C7-N2	-2.27	112.36	116.12
3	L	1	NAG	C6-C5-C4	-2.25	107.49	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	3	BMA	C2-C3-C4	-2.24	106.92	110.86
3	G	2	NAG	O6-C6-C5	-2.24	103.70	111.33
2	D	4	MAN	C2-C3-C4	-2.22	106.95	110.86
2	N	6	MAN	C1-O5-C5	2.20	115.14	112.19
3	E	1	NAG	O3-C3-C4	2.19	115.54	110.38
2	I	6	MAN	C2-C3-C4	-2.18	107.03	110.86
2	D	5	MAN	C1-O5-C5	2.18	115.10	112.19
3	M	1	NAG	C3-C4-C5	-2.17	106.29	110.23
3	F	2	NAG	C4-C3-C2	-2.15	107.87	111.02
3	G	1	NAG	O7-C7-N2	-2.15	118.19	121.98
3	K	1	NAG	O4-C4-C3	2.14	115.42	110.38
3	P	1	NAG	O5-C5-C6	2.12	111.80	107.66
3	G	2	NAG	O4-C4-C3	-2.12	105.37	110.38
3	R	1	NAG	C8-C7-N2	-2.12	112.61	116.12
2	D	3	BMA	C1-C2-C3	-2.09	106.60	109.64
2	D	2	NAG	C1-O5-C5	2.08	114.98	112.19
2	D	3	BMA	C2-C3-C4	-2.07	107.22	110.86
2	I	2	NAG	O4-C4-C3	-2.07	105.50	110.38
2	I	1	NAG	O4-C4-C5	-2.06	104.24	109.32
2	D	1	NAG	O3-C3-C4	2.04	115.18	110.38
3	M	1	NAG	C4-C3-C2	-2.04	108.03	111.02
3	L	2	NAG	C3-C4-C5	-2.02	106.56	110.23
2	D	2	NAG	O3-C3-C4	-2.00	105.65	110.38

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	1	NAG	C1
3	F	2	NAG	C1
3	K	2	NAG	C1
3	P	2	NAG	C1

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C3-C2-N2-C7
3	L	1	NAG	C3-C2-N2-C7
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
3	O	1	NAG	C1-C2-N2-C7
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C3-C2-N2-C7
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
2	I	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C8-C7-N2-C2
2	N	6	MAN	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
2	N	6	MAN	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
3	R	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
2	I	5	MAN	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O7-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
2	I	5	MAN	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
3	O	2	NAG	C3-C2-N2-C7
2	N	5	MAN	O5-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C1-C2-N2-C7
3	R	1	NAG	O7-C7-N2-C2
2	D	5	MAN	O5-C5-C6-O6
2	I	1	NAG	O7-C7-N2-C2
2	D	5	MAN	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2

There are no ring outliers.

23 monomers are involved in 60 short contacts:

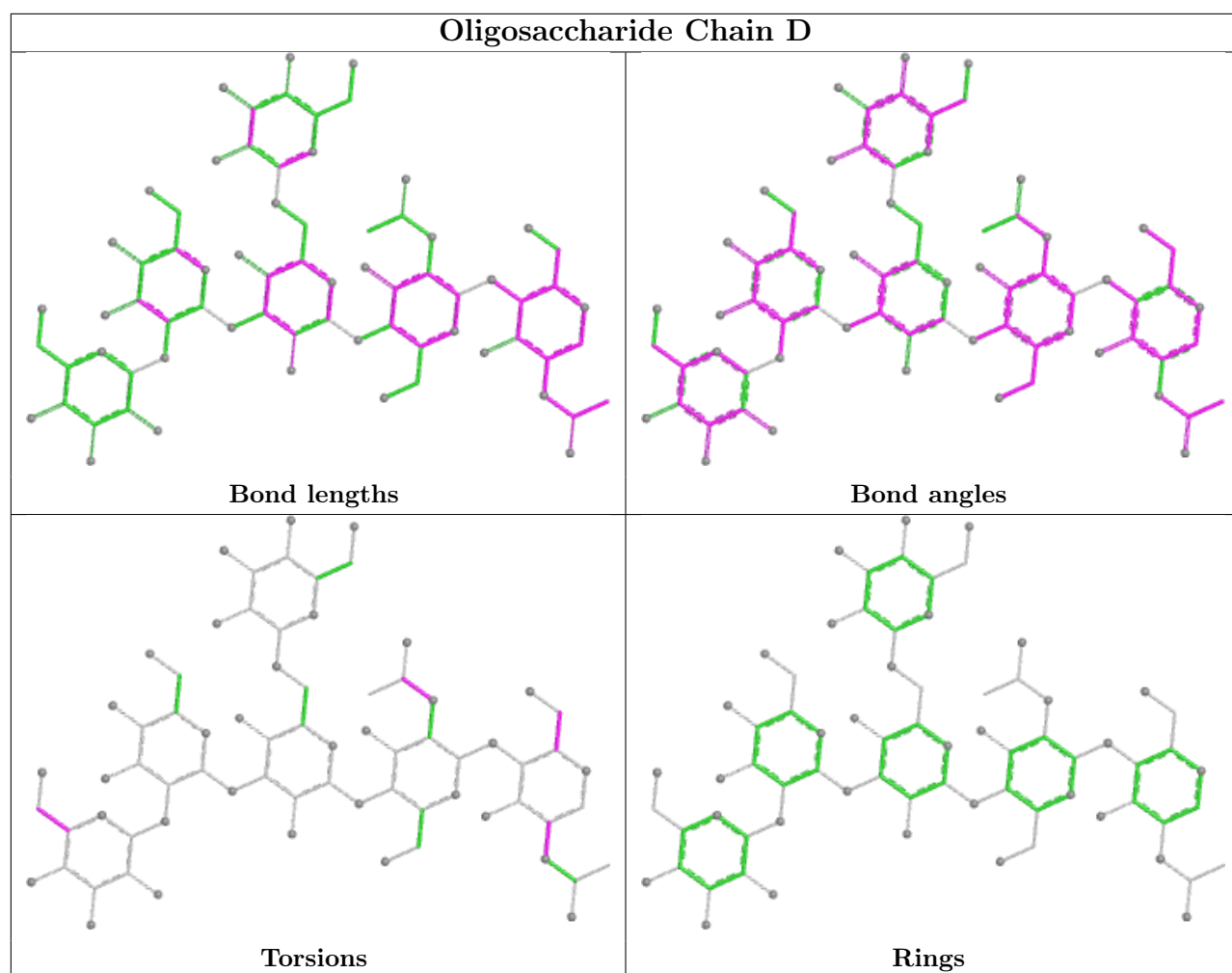
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	4	0

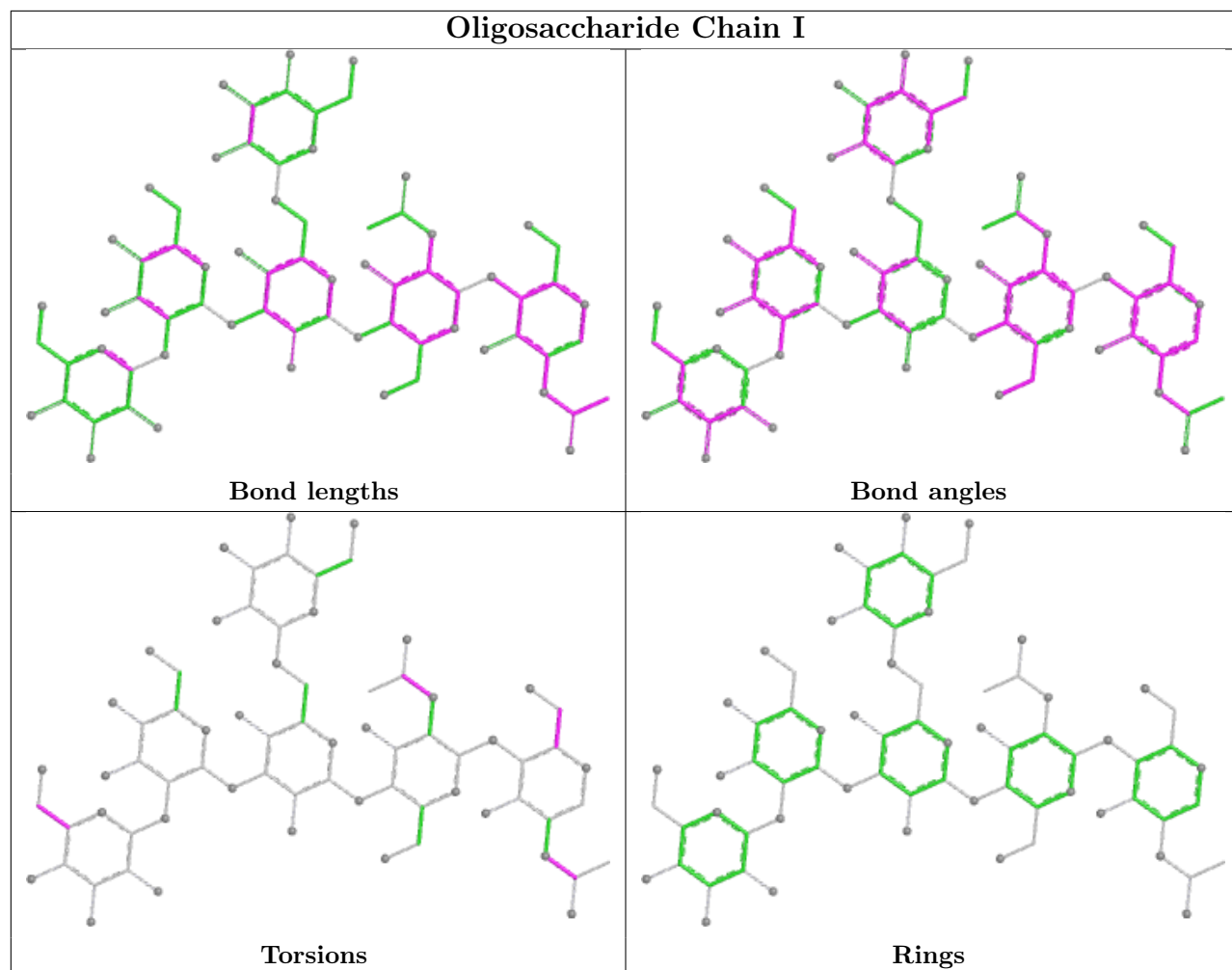
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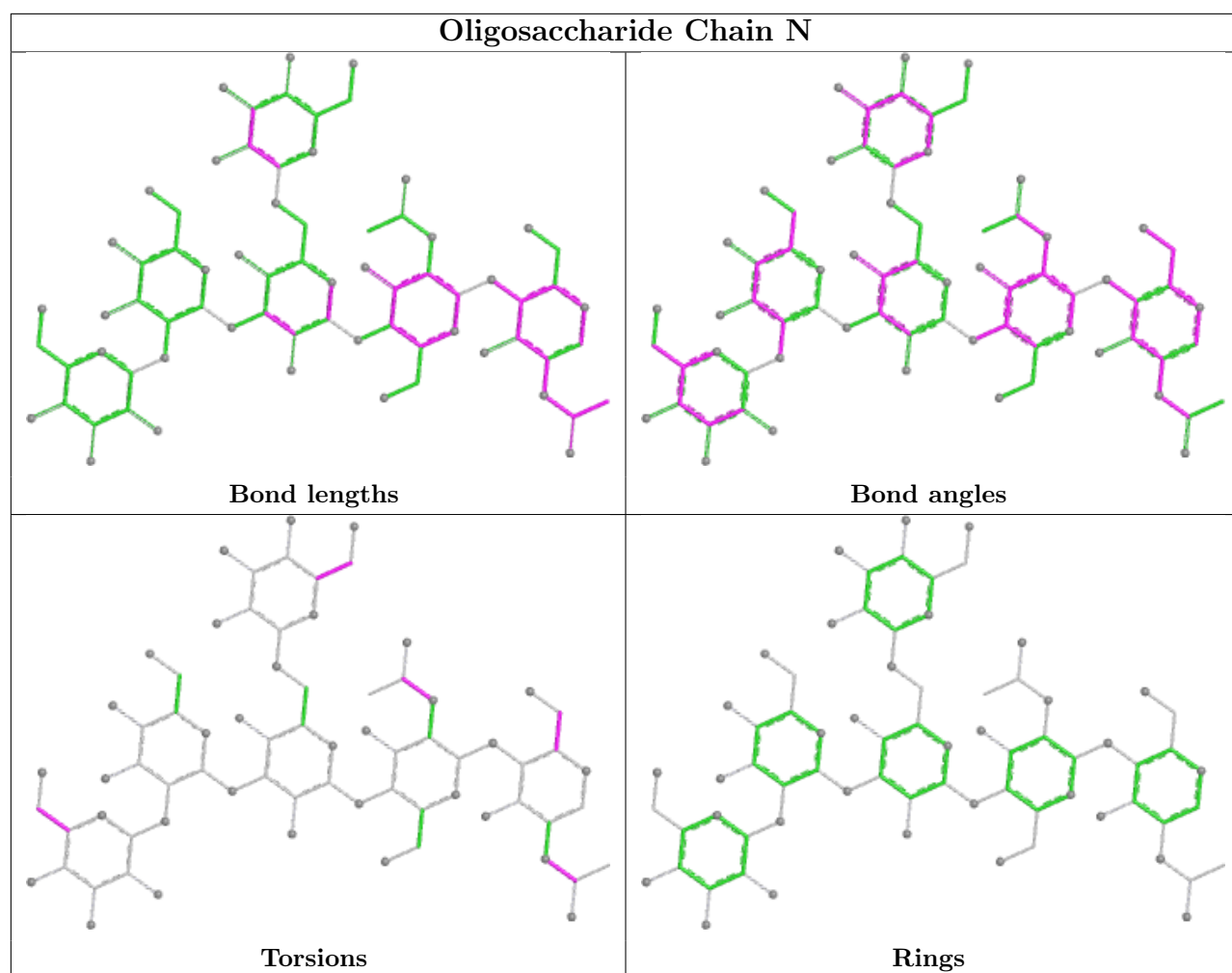
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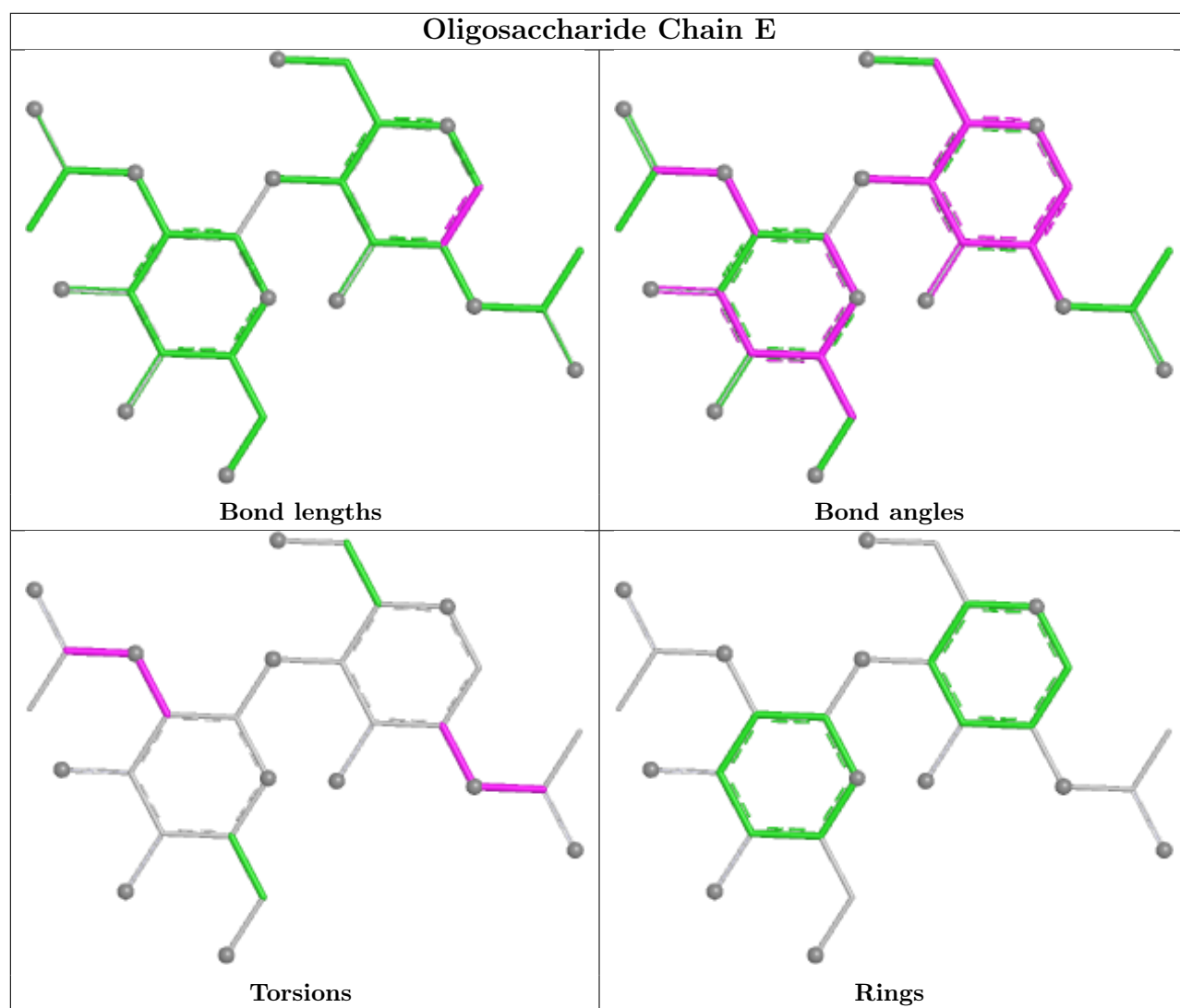
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	N	5	MAN	1	0
3	F	1	NAG	1	0
2	N	2	NAG	2	0
2	I	6	MAN	1	0
3	G	2	NAG	1	0
3	P	2	NAG	1	0
2	D	6	MAN	1	0
3	Q	1	NAG	7	0
3	E	1	NAG	12	0
3	Q	2	NAG	5	0
2	N	1	NAG	1	0
3	P	1	NAG	1	0
3	G	1	NAG	5	0
3	E	2	NAG	1	0
3	L	2	NAG	1	0
2	I	2	NAG	2	0
3	O	2	NAG	2	0
2	D	2	NAG	2	0
2	D	5	MAN	5	0
3	F	2	NAG	2	0
3	K	1	NAG	5	0

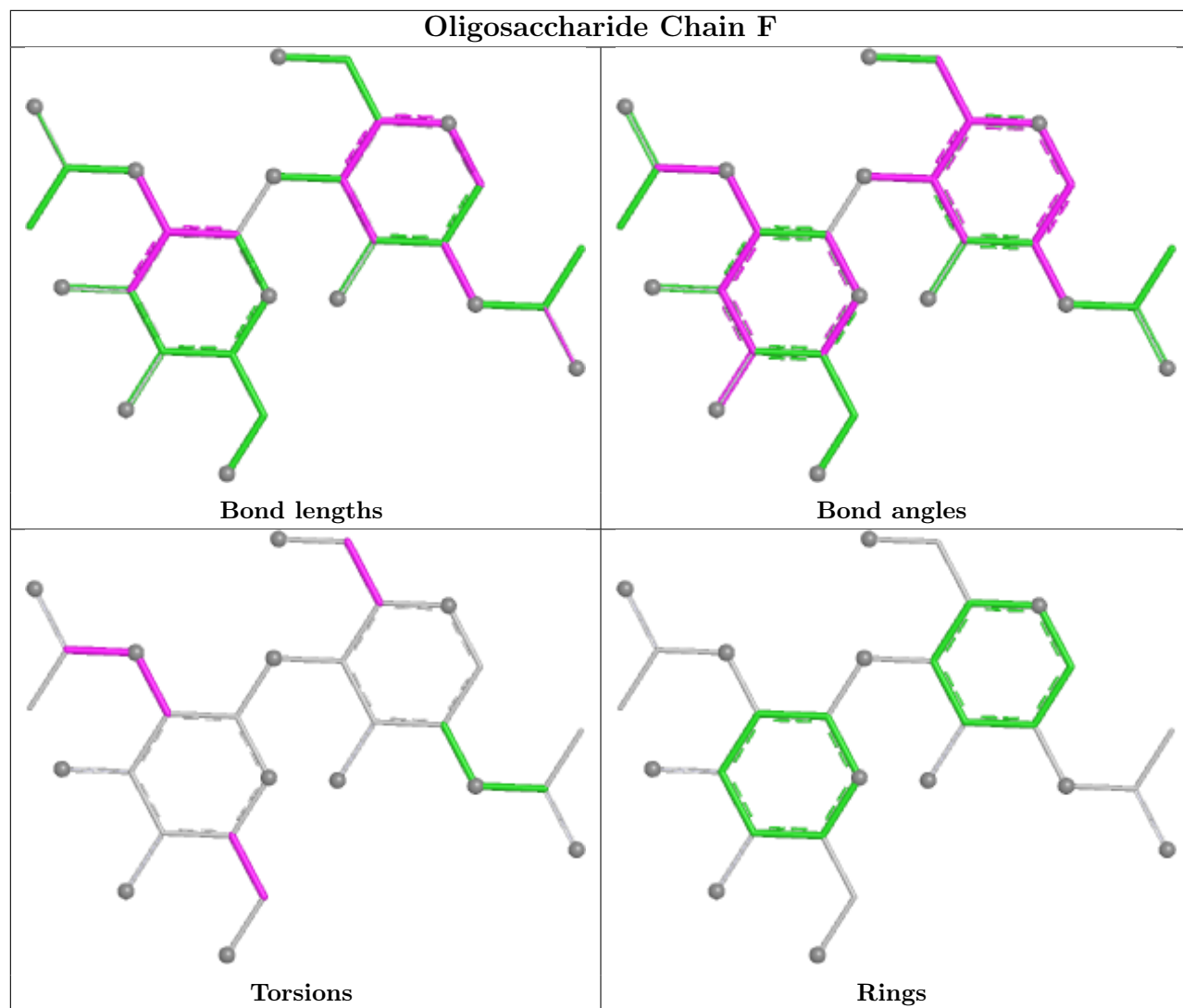
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

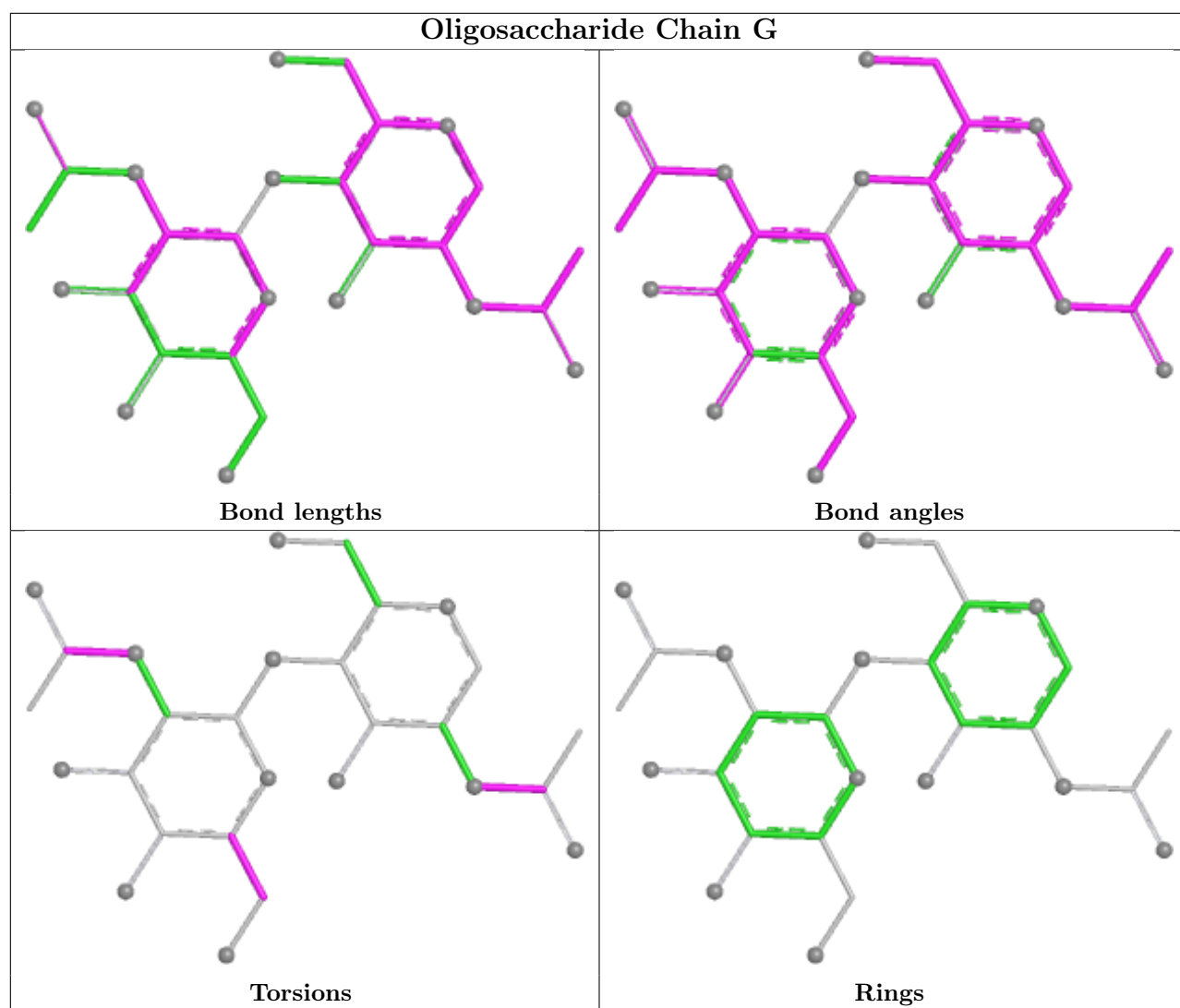


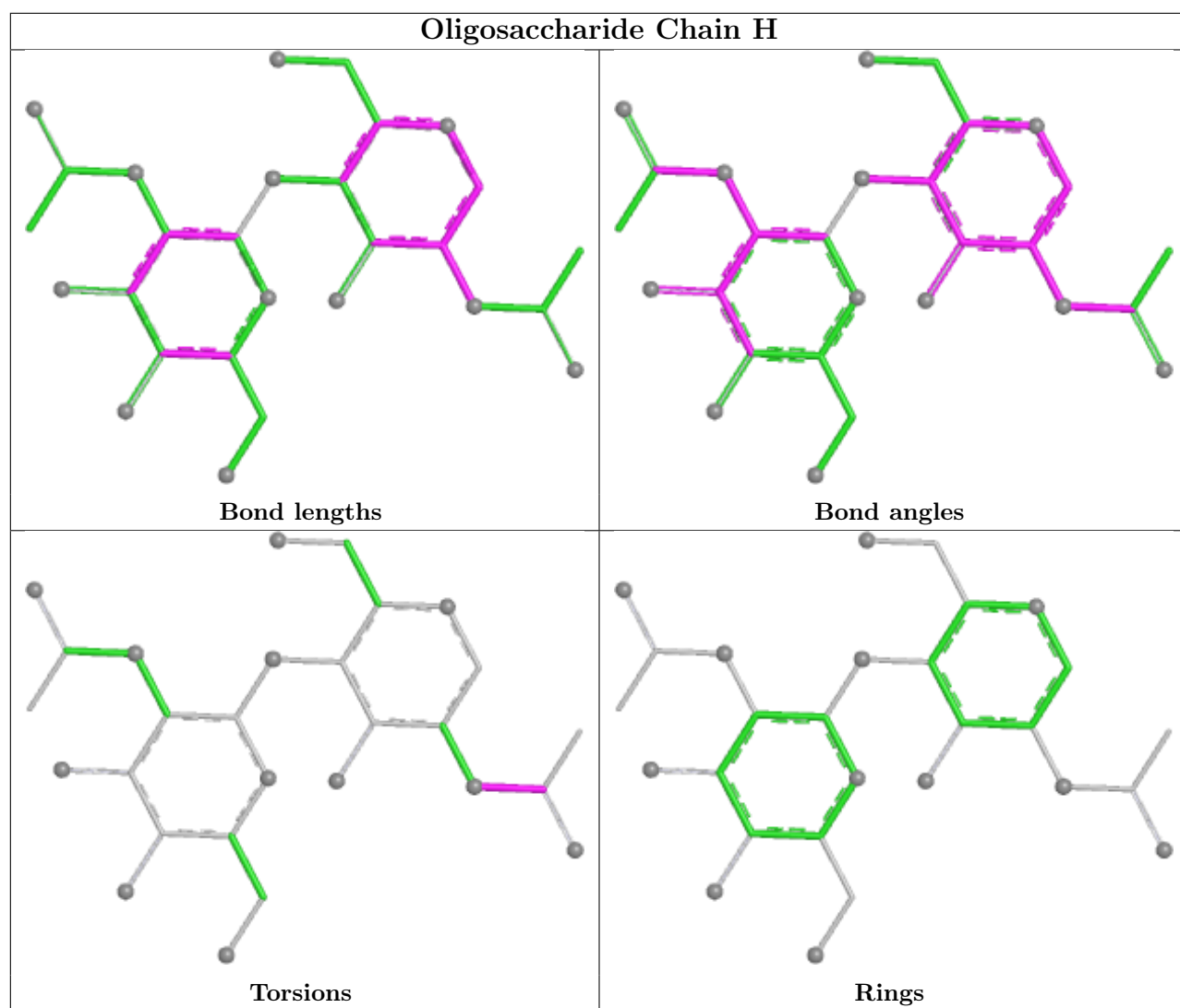


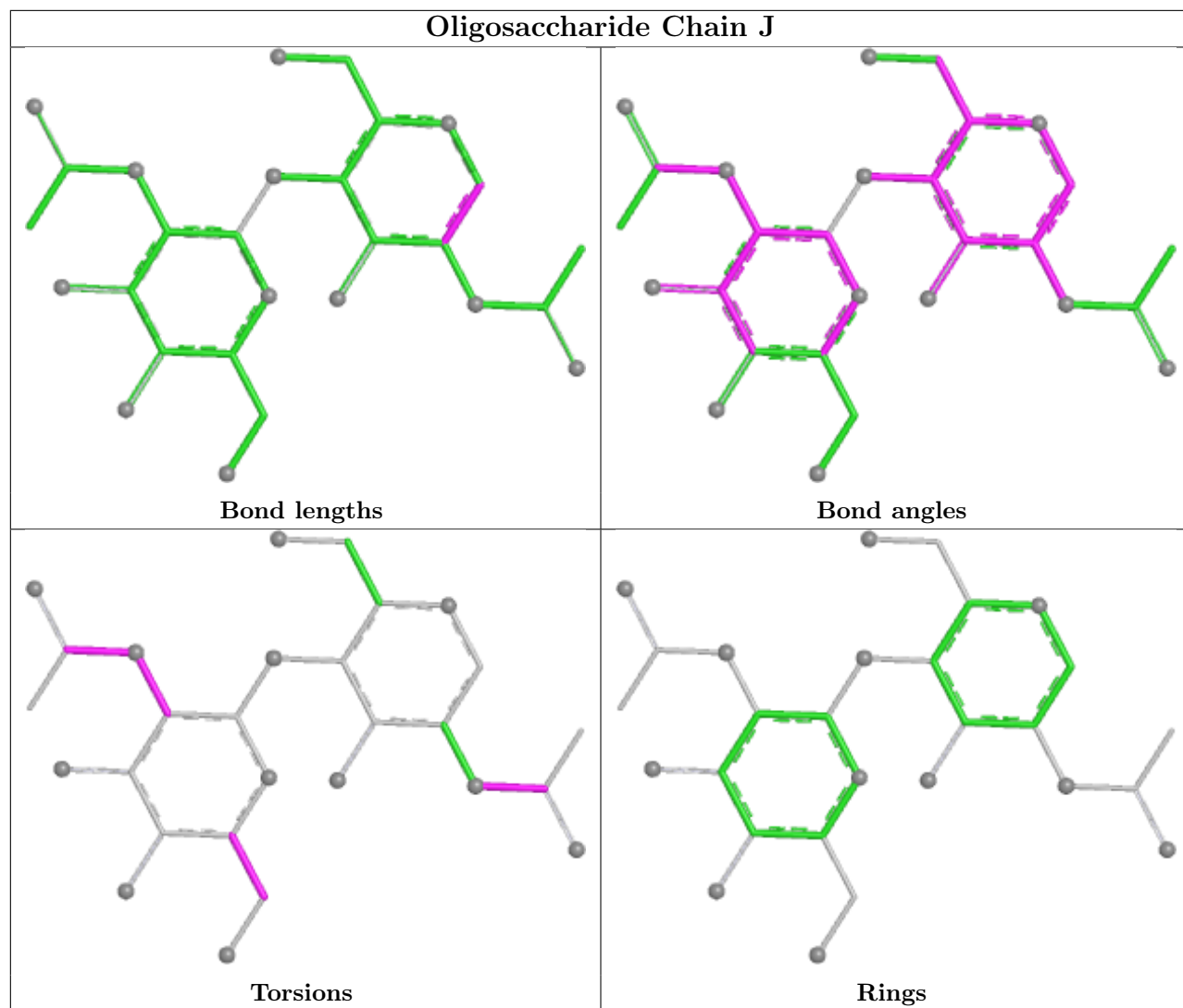


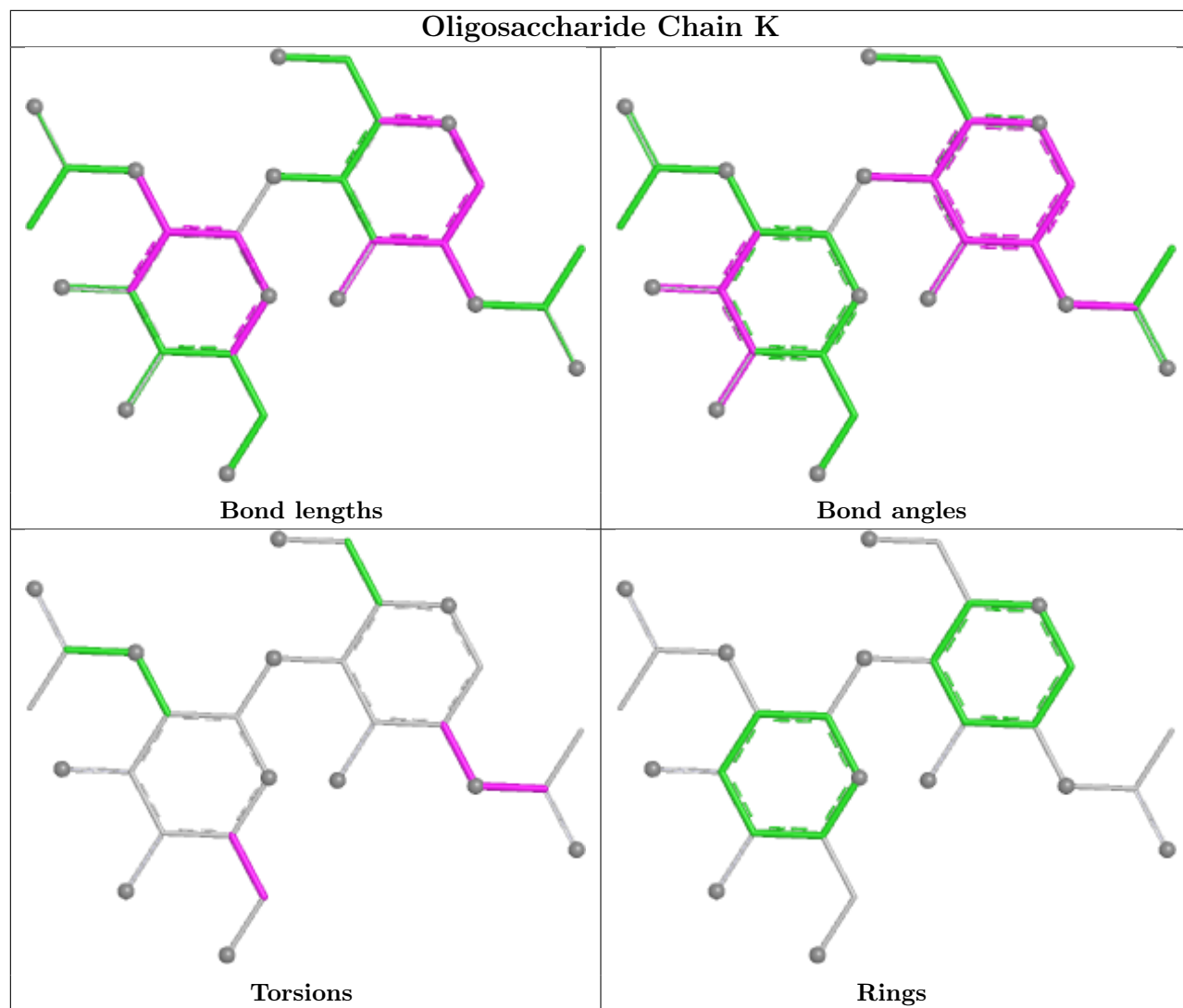


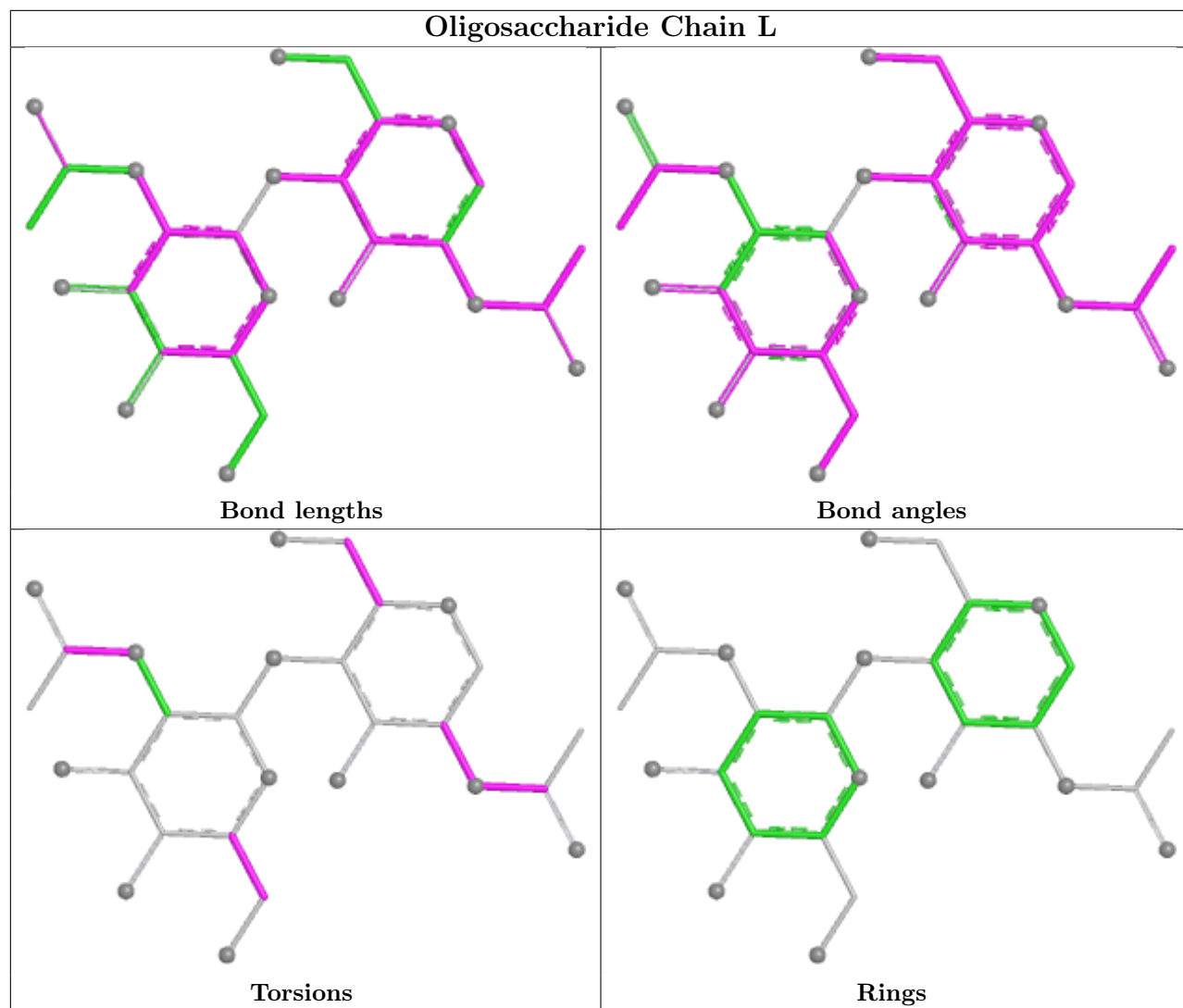


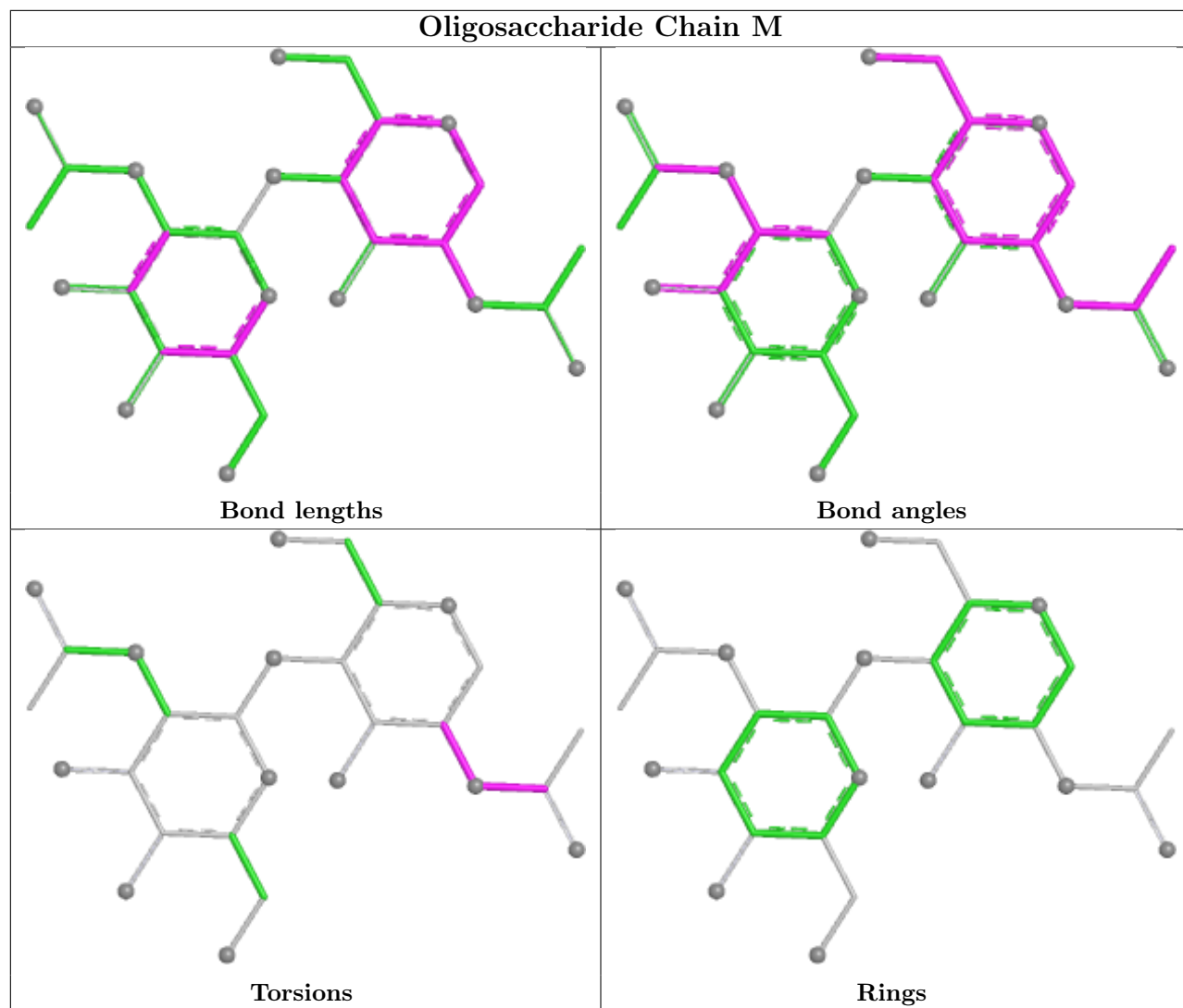


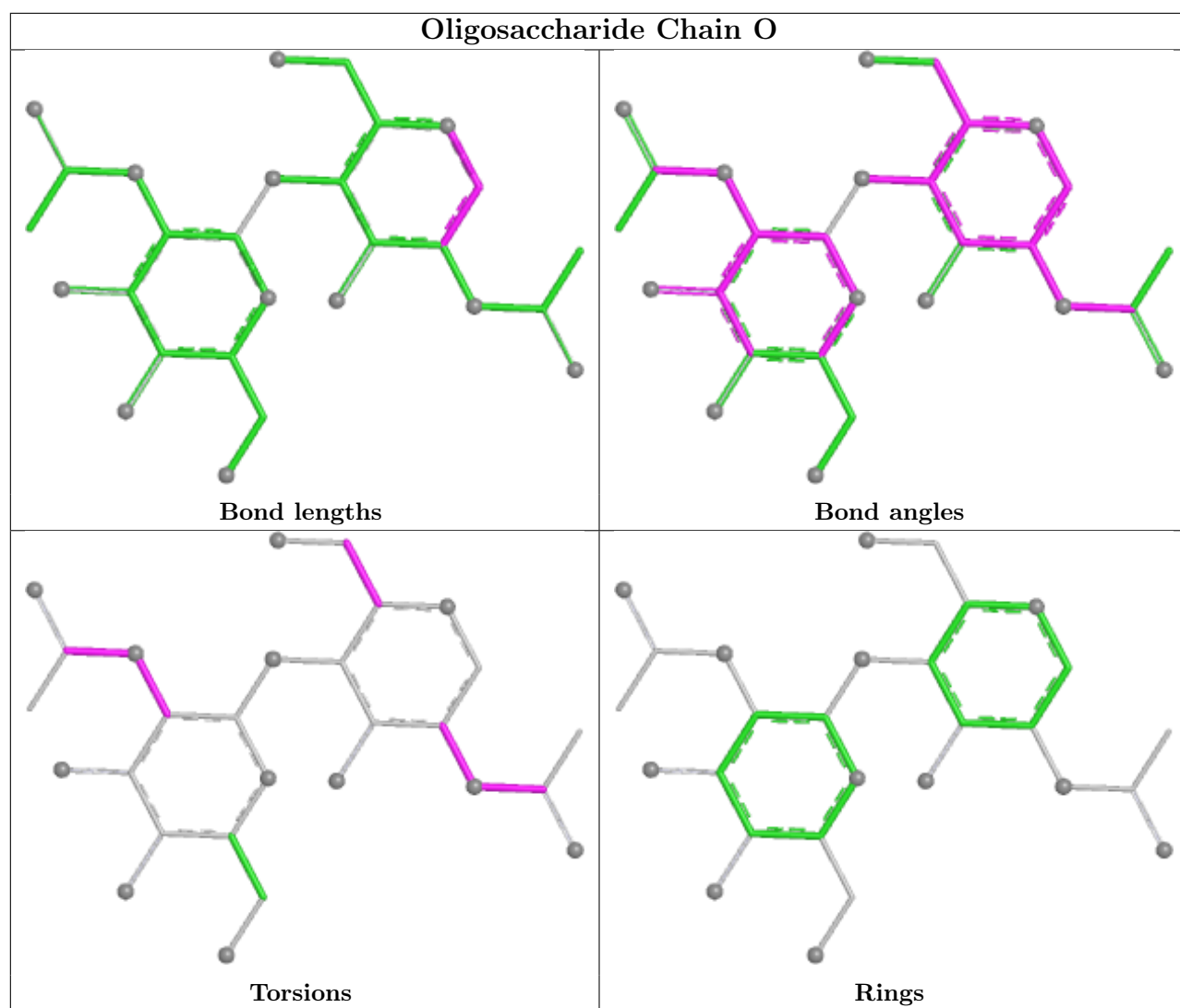


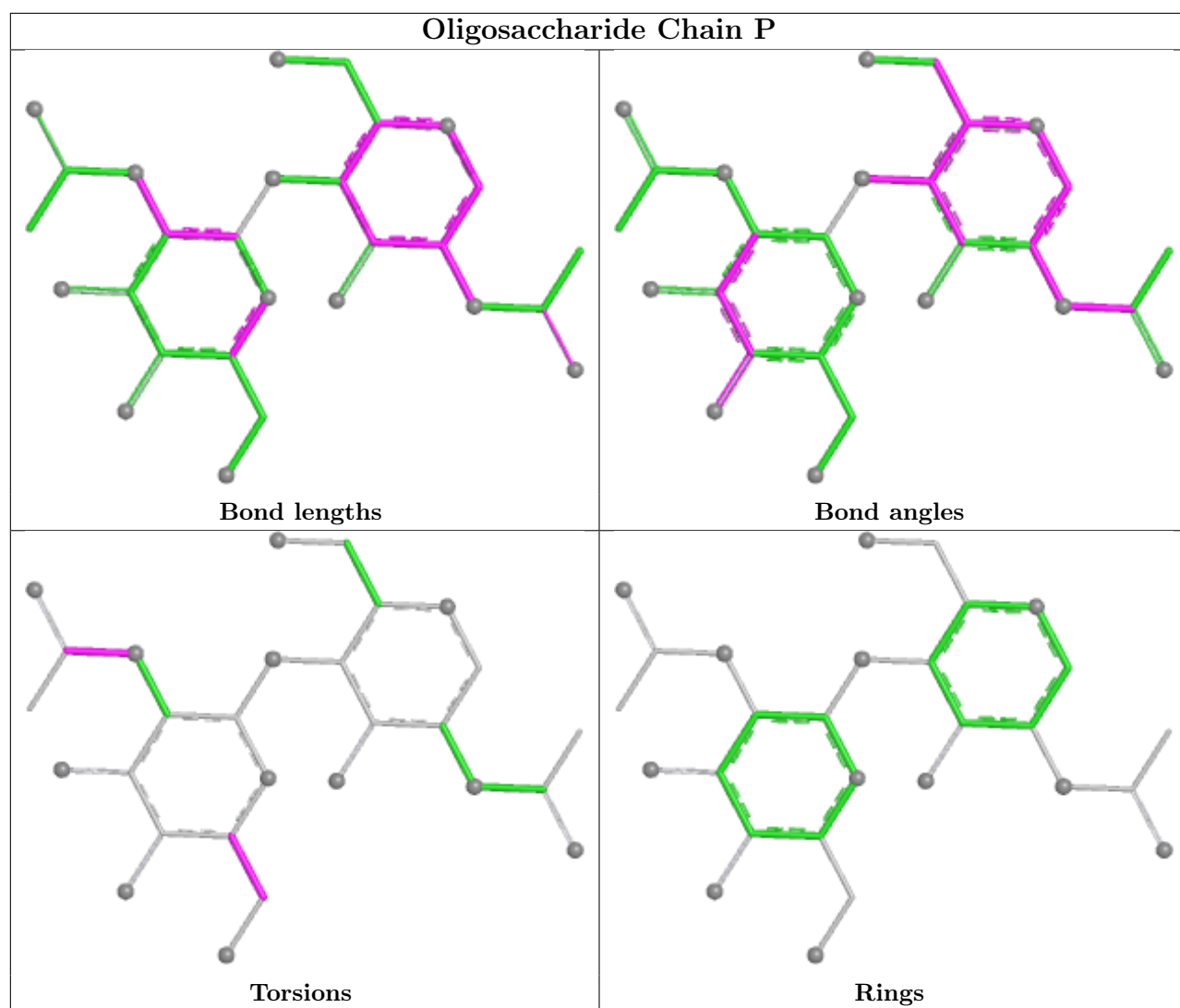


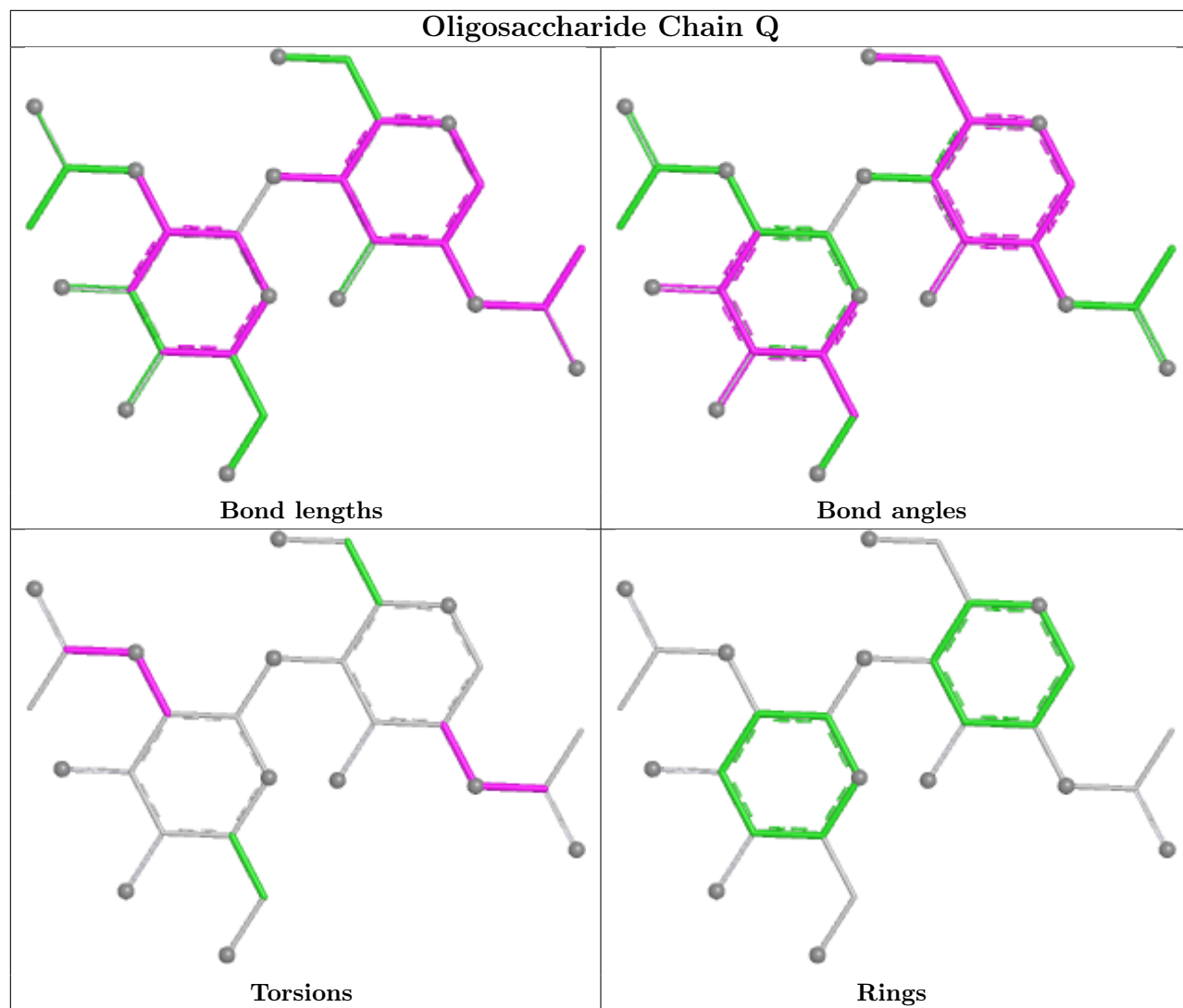


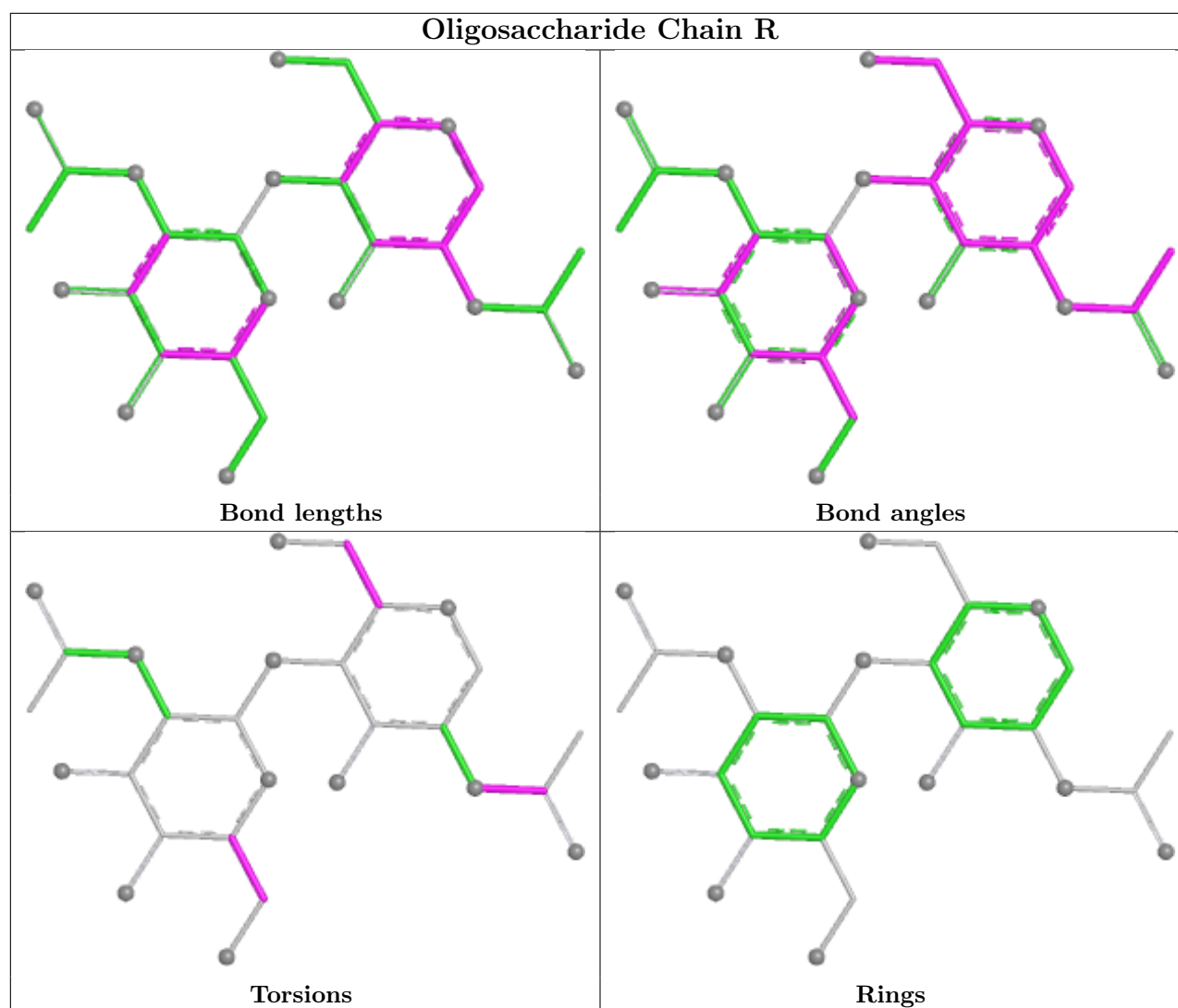












5.6 Ligand geometry [i](#)

39 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	C	1413	-	14,14,15	2.62	2 (14%)	17,19,21	3.15	11 (64%)
4	NAG	A	1417	-	14,14,15	1.52	2 (14%)	17,19,21	2.35	5 (29%)
4	NAG	A	1413	-	14,14,15	2.38	5 (35%)	17,19,21	3.58	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1412	-	14,14,15	1.89	1 (7%)	17,19,21	2.57	7 (41%)
4	NAG	B	1422	-	14,14,15	1.87	4 (28%)	17,19,21	2.91	8 (47%)
4	NAG	B	1401	-	14,14,15	1.33	1 (7%)	17,19,21	2.97	7 (41%)
4	NAG	B	1427	-	14,14,15	1.85	3 (21%)	17,19,21	4.41	6 (35%)
4	NAG	C	1417	-	14,14,15	1.22	2 (14%)	17,19,21	2.43	6 (35%)
4	NAG	B	1421	-	14,14,15	1.83	3 (21%)	17,19,21	2.47	7 (41%)
4	NAG	C	1421	-	14,14,15	1.66	3 (21%)	17,19,21	2.88	5 (29%)
4	NAG	B	1411	-	14,14,15	2.37	4 (28%)	17,19,21	3.15	9 (52%)
4	NAG	A	1426	-	14,14,15	1.49	1 (7%)	17,19,21	3.29	8 (47%)
4	NAG	C	1416	-	14,14,15	1.22	1 (7%)	17,19,21	1.83	3 (17%)
4	NAG	B	1408	-	14,14,15	1.18	1 (7%)	17,19,21	2.05	4 (23%)
4	NAG	A	1416	-	14,14,15	2.05	1 (7%)	17,19,21	2.93	6 (35%)
4	NAG	C	1408	-	14,14,15	1.13	1 (7%)	17,19,21	1.99	4 (23%)
4	NAG	C	1423	-	14,14,15	2.04	4 (28%)	17,19,21	4.43	9 (52%)
4	NAG	B	1417	-	14,14,15	1.26	2 (14%)	17,19,21	2.34	5 (29%)
4	NAG	A	1423	-	14,14,15	2.23	4 (28%)	17,19,21	4.21	9 (52%)
4	NAG	B	1413	-	14,14,15	2.81	6 (42%)	17,19,21	3.20	6 (35%)
4	NAG	B	1420	-	14,14,15	1.82	6 (42%)	17,19,21	3.09	7 (41%)
4	NAG	C	1420	-	14,14,15	1.84	5 (35%)	17,19,21	3.11	8 (47%)
4	NAG	B	1412	-	14,14,15	1.59	1 (7%)	17,19,21	2.17	3 (17%)
4	NAG	A	1420	-	14,14,15	1.77	6 (42%)	17,19,21	2.93	6 (35%)
4	NAG	C	1426	-	14,14,15	1.77	4 (28%)	17,19,21	1.87	5 (29%)
4	NAG	A	1408	-	14,14,15	1.76	1 (7%)	17,19,21	1.73	5 (29%)
4	NAG	C	1422	-	14,14,15	1.98	3 (21%)	17,19,21	3.28	7 (41%)
4	NAG	B	1426	-	14,14,15	1.47	2 (14%)	17,19,21	4.17	8 (47%)
4	NAG	C	1401	-	14,14,15	1.77	1 (7%)	17,19,21	2.48	7 (41%)
4	NAG	A	1422	-	14,14,15	2.09	3 (21%)	17,19,21	3.47	9 (52%)
4	NAG	C	1427	1	14,14,15	1.15	1 (7%)	17,19,21	3.17	8 (47%)
4	NAG	C	1411	-	14,14,15	2.32	5 (35%)	17,19,21	3.35	8 (47%)
4	NAG	A	1401	-	14,14,15	1.06	1 (7%)	17,19,21	2.93	6 (35%)
4	NAG	A	1412	-	14,14,15	1.98	2 (14%)	17,19,21	3.40	5 (29%)
4	NAG	B	1416	-	14,14,15	2.04	1 (7%)	17,19,21	2.69	5 (29%)
4	NAG	A	1411	-	14,14,15	2.44	3 (21%)	17,19,21	3.21	8 (47%)
4	NAG	A	1421	-	14,14,15	1.83	3 (21%)	17,19,21	2.85	6 (35%)
4	NAG	A	1427	-	14,14,15	1.72	3 (21%)	17,19,21	4.10	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1423	-	14,14,15	2.14	5 (35%)	17,19,21	4.58	9 (52%)

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	C	1413	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1417	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1413	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1412	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1422	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1427	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1417	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1426	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1416	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1408	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1416	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1423	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1417	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1423	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1413	-	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	B	1420	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1420	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1412	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1420	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1426	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1422	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1426	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1401	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1422	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1427	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1412	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1416	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1427	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1423	-	-	2/6/23/26	0/1/1/1

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1413	NAG	C1-C2	9.11	1.64	1.52
4	A	1411	NAG	C1-C2	7.40	1.62	1.52
4	B	1411	NAG	C1-C2	7.08	1.62	1.52
4	B	1416	NAG	C1-C2	6.94	1.61	1.52
4	C	1411	NAG	C1-C2	6.81	1.61	1.52
4	A	1416	NAG	C1-C2	6.68	1.61	1.52
4	C	1412	NAG	C1-C2	6.30	1.60	1.52
4	A	1413	NAG	C1-C2	6.22	1.60	1.52
4	A	1412	NAG	C1-C2	6.13	1.60	1.52
4	B	1413	NAG	C3-C2	-6.12	1.39	1.52
4	C	1401	NAG	C1-C2	5.97	1.60	1.52
4	A	1408	NAG	C1-C2	5.90	1.60	1.52
4	B	1413	NAG	C1-C2	5.81	1.60	1.52
4	B	1412	NAG	C1-C2	5.45	1.59	1.52
4	A	1422	NAG	C1-C2	5.14	1.59	1.52
4	B	1427	NAG	C1-C2	5.11	1.59	1.52
4	A	1423	NAG	C1-C2	4.93	1.59	1.52
4	A	1421	NAG	C1-C2	4.89	1.59	1.52
4	A	1426	NAG	C1-C2	4.74	1.58	1.52
4	C	1422	NAG	C1-C2	4.70	1.58	1.52
4	B	1421	NAG	C1-C2	4.66	1.58	1.52
4	B	1423	NAG	C1-C2	4.53	1.58	1.52
4	A	1417	NAG	C1-C2	4.46	1.58	1.52
4	A	1427	NAG	C1-C2	4.41	1.58	1.52
4	B	1401	NAG	C1-C2	4.34	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1423	NAG	O5-C1	-4.25	1.36	1.43
4	C	1423	NAG	O5-C1	-4.20	1.36	1.43
4	C	1421	NAG	C1-C2	4.17	1.58	1.52
4	C	1426	NAG	C1-C2	4.04	1.57	1.52
4	B	1413	NAG	C4-C3	-3.96	1.42	1.52
4	C	1416	NAG	C1-C2	3.93	1.57	1.52
4	B	1408	NAG	C1-C2	3.88	1.57	1.52
4	B	1426	NAG	C1-C2	3.85	1.57	1.52
4	B	1423	NAG	O5-C1	-3.77	1.37	1.43
4	C	1423	NAG	C1-C2	3.70	1.57	1.52
4	B	1422	NAG	C1-C2	3.64	1.57	1.52
4	C	1408	NAG	C1-C2	3.62	1.57	1.52
4	B	1417	NAG	C1-C2	3.46	1.57	1.52
4	A	1422	NAG	C3-C2	-3.42	1.45	1.52
4	A	1420	NAG	C1-C2	3.29	1.56	1.52
4	B	1423	NAG	O5-C5	-3.22	1.37	1.43
4	B	1422	NAG	C3-C2	-3.19	1.45	1.52
4	C	1420	NAG	C1-C2	3.14	1.56	1.52
4	A	1427	NAG	C2-N2	-3.14	1.41	1.46
4	C	1417	NAG	C1-C2	3.11	1.56	1.52
4	A	1413	NAG	C2-N2	-3.07	1.41	1.46
4	C	1422	NAG	C3-C2	-3.05	1.46	1.52
4	A	1413	NAG	C3-C2	-3.05	1.46	1.52
4	B	1420	NAG	O5-C5	-3.01	1.37	1.43
4	C	1420	NAG	O5-C5	-2.97	1.37	1.43
4	A	1413	NAG	O5-C5	-2.96	1.37	1.43
4	B	1422	NAG	C2-N2	-2.95	1.41	1.46
4	C	1422	NAG	C2-N2	-2.89	1.41	1.46
4	A	1412	NAG	C2-N2	-2.86	1.41	1.46
4	A	1422	NAG	C2-N2	-2.85	1.41	1.46
4	C	1423	NAG	O5-C5	-2.83	1.37	1.43
4	B	1420	NAG	C1-C2	2.81	1.56	1.52
4	B	1427	NAG	O5-C1	-2.81	1.39	1.43
4	C	1420	NAG	O5-C1	-2.74	1.39	1.43
4	A	1401	NAG	C1-C2	2.74	1.56	1.52
4	B	1420	NAG	O5-C1	-2.73	1.39	1.43
4	A	1423	NAG	O5-C5	-2.72	1.38	1.43
4	B	1421	NAG	O5-C1	-2.70	1.39	1.43
4	B	1413	NAG	C2-N2	-2.69	1.41	1.46
4	B	1420	NAG	C2-N2	-2.64	1.41	1.46
4	C	1413	NAG	O5-C5	-2.62	1.38	1.43
4	C	1426	NAG	O5-C1	-2.57	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1420	NAG	C2-N2	-2.56	1.42	1.46
4	A	1420	NAG	C2-N2	-2.56	1.42	1.46
4	B	1421	NAG	O5-C5	-2.53	1.38	1.43
4	A	1420	NAG	O5-C5	-2.51	1.38	1.43
4	B	1426	NAG	O5-C5	-2.51	1.38	1.43
4	B	1423	NAG	O7-C7	-2.49	1.17	1.23
4	C	1427	NAG	C2-N2	-2.46	1.42	1.46
4	C	1423	NAG	C4-C5	-2.45	1.47	1.53
4	C	1417	NAG	C2-N2	-2.38	1.42	1.46
4	A	1421	NAG	O5-C5	-2.35	1.38	1.43
4	B	1417	NAG	C2-N2	-2.34	1.42	1.46
4	B	1413	NAG	O3-C3	-2.32	1.37	1.43
4	A	1413	NAG	C4-C5	-2.30	1.48	1.53
4	C	1426	NAG	O5-C5	-2.26	1.39	1.43
4	B	1423	NAG	C4-C5	-2.26	1.48	1.53
4	C	1420	NAG	C3-C2	-2.26	1.47	1.52
4	A	1421	NAG	O5-C1	-2.26	1.39	1.43
4	A	1417	NAG	C2-N2	-2.25	1.42	1.46
4	A	1420	NAG	C3-C2	-2.25	1.47	1.52
4	B	1411	NAG	O5-C1	-2.24	1.39	1.43
4	A	1411	NAG	O5-C5	-2.24	1.39	1.43
4	B	1427	NAG	C2-N2	-2.22	1.42	1.46
4	C	1411	NAG	O5-C1	-2.21	1.40	1.43
4	B	1420	NAG	C3-C2	-2.20	1.47	1.52
4	C	1421	NAG	O5-C5	-2.20	1.39	1.43
4	A	1423	NAG	O7-C7	-2.19	1.18	1.23
4	C	1411	NAG	C2-N2	-2.18	1.42	1.46
4	C	1411	NAG	C4-C5	-2.15	1.48	1.53
4	A	1420	NAG	O5-C1	-2.12	1.40	1.43
4	C	1421	NAG	C2-N2	-2.12	1.42	1.46
4	B	1411	NAG	C2-N2	-2.11	1.42	1.46
4	B	1422	NAG	O5-C1	-2.11	1.40	1.43
4	A	1427	NAG	O7-C7	-2.11	1.18	1.23
4	A	1411	NAG	O5-C1	-2.07	1.40	1.43
4	B	1420	NAG	C4-C5	-2.04	1.48	1.53
4	C	1411	NAG	O5-C5	-2.04	1.39	1.43
4	B	1413	NAG	O5-C1	2.03	1.47	1.43
4	C	1426	NAG	C3-C2	-2.03	1.48	1.52
4	B	1411	NAG	O5-C5	-2.03	1.39	1.43
4	A	1420	NAG	C4-C5	-2.00	1.48	1.53

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1426	NAG	O5-C1-C2	-12.97	91.23	111.29
4	A	1412	NAG	C2-N2-C7	-11.45	107.56	122.90
4	A	1427	NAG	O5-C1-C2	-11.13	94.08	111.29
4	B	1427	NAG	C2-N2-C7	-10.37	109.00	122.90
4	C	1423	NAG	C2-N2-C7	-10.09	109.38	122.90
4	B	1423	NAG	O5-C1-C2	-10.04	95.76	111.29
4	A	1423	NAG	O5-C1-C2	-9.98	95.85	111.29
4	B	1420	NAG	C1-C2-N2	-9.58	95.34	110.43
4	B	1427	NAG	C4-C3-C2	-9.35	97.31	111.02
4	A	1426	NAG	O5-C1-C2	-9.31	96.88	111.29
4	C	1423	NAG	O5-C1-C2	-8.92	97.49	111.29
4	B	1423	NAG	C2-N2-C7	-8.78	111.14	122.90
4	A	1411	NAG	C1-O5-C5	8.70	123.85	112.19
4	C	1420	NAG	C1-C2-N2	-8.57	96.92	110.43
4	C	1411	NAG	C1-O5-C5	8.46	123.52	112.19
4	A	1413	NAG	C1-C2-N2	-8.35	97.27	110.43
4	C	1427	NAG	O5-C1-C2	-8.35	98.37	111.29
4	B	1413	NAG	C4-C3-C2	8.34	123.24	111.02
4	B	1427	NAG	O5-C1-C2	-8.24	98.53	111.29
4	C	1413	NAG	C1-C2-N2	-8.16	97.57	110.43
4	B	1411	NAG	C1-O5-C5	8.06	122.98	112.19
4	A	1423	NAG	C2-N2-C7	-8.00	112.18	122.90
4	B	1401	NAG	O5-C1-C2	-7.88	99.09	111.29
4	A	1416	NAG	O5-C1-C2	-7.79	99.23	111.29
4	B	1423	NAG	C4-C3-C2	-7.77	99.63	111.02
4	A	1423	NAG	C4-C3-C2	-7.66	99.79	111.02
4	B	1426	NAG	C1-O5-C5	7.66	122.45	112.19
4	C	1423	NAG	C4-C3-C2	-7.57	99.93	111.02
4	A	1413	NAG	C1-O5-C5	7.56	122.32	112.19
4	A	1401	NAG	O5-C1-C2	-7.54	99.63	111.29
4	A	1427	NAG	C2-N2-C7	-7.34	113.07	122.90
4	C	1411	NAG	O5-C1-C2	-7.33	99.95	111.29
4	C	1422	NAG	C1-O5-C5	7.20	121.84	112.19
4	B	1413	NAG	C3-C4-C5	-7.15	97.27	110.23
4	C	1401	NAG	O5-C1-C2	-7.03	100.42	111.29
4	B	1416	NAG	O5-C1-C2	-6.98	100.48	111.29
4	A	1422	NAG	C1-O5-C5	6.82	121.33	112.19
4	C	1421	NAG	O5-C1-C2	-6.75	100.85	111.29
4	A	1422	NAG	C1-C2-N2	-6.74	99.81	110.43
4	C	1412	NAG	O4-C4-C3	-6.68	94.64	110.38
4	C	1421	NAG	C2-N2-C7	-6.67	113.97	122.90
4	A	1420	NAG	C1-C2-N2	-6.48	100.23	110.43
4	A	1417	NAG	O5-C1-C2	-6.44	101.33	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1408	NAG	O5-C1-C2	-6.42	101.36	111.29
4	B	1417	NAG	O5-C1-C2	-6.41	101.37	111.29
4	C	1417	NAG	O5-C1-C2	-6.40	101.39	111.29
4	A	1421	NAG	C2-N2-C7	-6.39	114.33	122.90
4	A	1413	NAG	O5-C1-C2	-6.26	101.61	111.29
4	C	1408	NAG	O5-C1-C2	-6.22	101.66	111.29
4	B	1411	NAG	O5-C1-C2	-6.22	101.67	111.29
4	C	1422	NAG	O5-C1-C2	-6.20	101.70	111.29
4	A	1421	NAG	O5-C1-C2	-6.17	101.74	111.29
4	A	1411	NAG	O5-C1-C2	-6.13	101.80	111.29
4	B	1423	NAG	C1-O5-C5	6.09	120.35	112.19
4	A	1427	NAG	C1-O5-C5	6.09	120.34	112.19
4	A	1401	NAG	C2-N2-C7	-6.07	114.77	122.90
4	B	1422	NAG	O3-C3-C2	-6.01	96.92	109.40
4	A	1420	NAG	O5-C1-C2	-5.96	102.08	111.29
4	A	1426	NAG	C3-C4-C5	-5.93	99.47	110.23
4	A	1422	NAG	O3-C3-C2	-5.80	97.36	109.40
4	B	1423	NAG	C6-C5-C4	-5.79	98.81	113.02
4	B	1412	NAG	O5-C5-C6	5.71	118.78	107.66
4	C	1423	NAG	C6-C5-C4	-5.51	99.50	113.02
4	C	1420	NAG	O5-C1-C2	-5.45	102.85	111.29
4	B	1427	NAG	C1-C2-N2	5.44	119.01	110.43
4	A	1423	NAG	C1-O5-C5	5.36	119.37	112.19
4	A	1422	NAG	O5-C1-C2	-5.33	103.04	111.29
4	C	1427	NAG	C2-N2-C7	-5.18	115.96	122.90
4	C	1426	NAG	C1-C2-N2	-5.15	102.32	110.43
4	C	1422	NAG	C1-C2-N2	-5.12	102.36	110.43
4	A	1412	NAG	O5-C1-C2	-5.06	103.47	111.29
4	B	1421	NAG	C2-N2-C7	-5.00	116.20	122.90
4	A	1420	NAG	C2-N2-C7	-4.89	116.35	122.90
4	B	1401	NAG	C1-C2-N2	4.79	117.98	110.43
4	A	1427	NAG	C4-C3-C2	-4.78	104.01	111.02
4	C	1417	NAG	C2-N2-C7	-4.78	116.49	122.90
4	A	1423	NAG	C6-C5-C4	-4.77	101.30	113.02
4	B	1421	NAG	O5-C1-C2	-4.72	103.99	111.29
4	B	1412	NAG	O5-C1-C2	-4.71	104.00	111.29
4	B	1401	NAG	C2-N2-C7	-4.69	116.62	122.90
4	B	1417	NAG	C2-N2-C7	-4.68	116.63	122.90
4	C	1423	NAG	C1-O5-C5	4.66	118.44	112.19
4	A	1416	NAG	C1-O5-C5	4.66	118.43	112.19
4	C	1422	NAG	O3-C3-C2	-4.64	99.76	109.40
4	C	1412	NAG	C2-N2-C7	4.60	129.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1413	NAG	C2-N2-C7	-4.58	116.76	122.90
4	B	1422	NAG	O5-C1-C2	-4.56	104.23	111.29
4	A	1401	NAG	C4-C3-C2	-4.56	104.33	111.02
4	B	1422	NAG	C1-O5-C5	4.49	118.20	112.19
4	C	1427	NAG	O4-C4-C3	-4.46	99.86	110.38
4	C	1420	NAG	C4-C3-C2	-4.40	104.56	111.02
4	C	1413	NAG	C2-N2-C7	4.40	128.79	122.90
4	A	1417	NAG	C2-N2-C7	-4.36	117.06	122.90
4	B	1420	NAG	O5-C1-C2	-4.36	104.55	111.29
4	B	1416	NAG	C1-O5-C5	4.36	118.03	112.19
4	B	1426	NAG	C3-C4-C5	-4.35	102.35	110.23
4	C	1416	NAG	C4-C3-C2	-4.28	104.75	111.02
4	A	1413	NAG	O4-C4-C5	-4.27	98.81	109.32
4	A	1420	NAG	C4-C3-C2	-4.24	104.81	111.02
4	C	1420	NAG	C2-N2-C7	-4.23	117.23	122.90
4	A	1416	NAG	O3-C3-C4	-4.12	100.67	110.38
4	C	1416	NAG	O5-C1-C2	-4.08	104.98	111.29
4	C	1421	NAG	C4-C3-C2	-4.07	105.05	111.02
4	A	1426	NAG	O5-C5-C6	4.06	115.57	107.66
4	C	1401	NAG	C1-C2-N2	4.04	116.80	110.43
4	B	1411	NAG	C6-C5-C4	-3.96	103.30	113.02
4	B	1423	NAG	O5-C5-C6	-3.92	100.03	107.66
4	B	1422	NAG	O5-C5-C6	3.87	115.20	107.66
4	A	1416	NAG	C2-N2-C7	-3.87	117.72	122.90
4	C	1427	NAG	C1-O5-C5	3.86	117.36	112.19
4	B	1427	NAG	O5-C5-C6	-3.83	100.21	107.66
4	C	1416	NAG	C2-N2-C7	-3.82	117.78	122.90
4	A	1422	NAG	O5-C5-C4	-3.79	101.60	110.83
4	A	1421	NAG	C1-O5-C5	3.79	117.26	112.19
4	B	1421	NAG	C1-O5-C5	3.77	117.24	112.19
4	B	1413	NAG	C2-N2-C7	-3.77	117.85	122.90
4	B	1422	NAG	C1-C2-N2	-3.75	104.52	110.43
4	B	1416	NAG	O3-C3-C4	-3.75	101.53	110.38
4	A	1421	NAG	C4-C3-C2	-3.72	105.57	111.02
4	B	1420	NAG	C2-N2-C7	-3.71	117.92	122.90
4	A	1417	NAG	C4-C3-C2	-3.69	105.61	111.02
4	A	1416	NAG	C4-C3-C2	-3.68	105.63	111.02
4	B	1427	NAG	O4-C4-C3	-3.66	101.74	110.38
4	C	1413	NAG	C1-O5-C5	3.66	117.09	112.19
4	B	1401	NAG	C4-C3-C2	-3.63	105.70	111.02
4	C	1411	NAG	C6-C5-C4	-3.63	104.11	113.02
4	C	1423	NAG	O7-C7-C8	-3.61	115.62	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1422	NAG	O5-C5-C4	-3.55	102.19	110.83
4	B	1416	NAG	C4-C3-C2	-3.55	105.82	111.02
4	A	1408	NAG	C2-N2-C7	3.51	127.61	122.90
4	A	1426	NAG	O6-C6-C5	-3.48	99.50	111.33
4	A	1408	NAG	O5-C1-C2	-3.47	105.93	111.29
4	A	1411	NAG	O5-C5-C4	-3.46	102.40	110.83
4	C	1411	NAG	C4-C3-C2	-3.45	105.97	111.02
4	B	1416	NAG	C6-C5-C4	-3.41	104.64	113.02
4	C	1413	NAG	C8-C7-N2	3.36	121.70	116.12
4	B	1401	NAG	C1-O5-C5	3.35	116.68	112.19
4	C	1421	NAG	C1-O5-C5	3.35	116.67	112.19
4	B	1408	NAG	C1-O5-C5	3.30	116.61	112.19
4	B	1420	NAG	C4-C3-C2	-3.30	106.19	111.02
4	B	1426	NAG	C6-C5-C4	3.27	121.04	113.02
4	B	1423	NAG	C8-C7-N2	3.24	121.48	116.12
4	A	1427	NAG	O4-C4-C3	-3.19	102.86	110.38
4	C	1423	NAG	C8-C7-N2	3.19	121.40	116.12
4	C	1422	NAG	O4-C4-C5	3.17	117.14	109.32
4	B	1423	NAG	O7-C7-C8	-3.12	116.49	122.05
4	B	1422	NAG	O5-C5-C4	-3.12	103.24	110.83
4	B	1413	NAG	C1-O5-C5	-3.09	108.05	112.19
4	C	1417	NAG	C1-C2-N2	-3.08	105.58	110.43
4	C	1411	NAG	O5-C5-C4	-3.04	103.43	110.83
4	A	1411	NAG	O3-C3-C4	-3.03	103.23	110.38
4	B	1417	NAG	C3-C4-C5	-3.03	104.75	110.23
4	C	1423	NAG	O5-C5-C6	-3.02	101.79	107.66
4	C	1408	NAG	C1-O5-C5	3.01	116.22	112.19
4	C	1411	NAG	O3-C3-C4	-3.01	103.28	110.38
4	B	1421	NAG	O3-C3-C4	-2.98	103.36	110.38
4	B	1413	NAG	O5-C5-C6	2.97	113.45	107.66
4	B	1423	NAG	O4-C4-C3	2.96	117.36	110.38
4	A	1411	NAG	C6-C5-C4	-2.95	105.77	113.02
4	A	1412	NAG	O4-C4-C3	-2.94	103.44	110.38
4	C	1413	NAG	O5-C5-C4	2.94	117.99	110.83
4	A	1427	NAG	C6-C5-C4	-2.92	105.84	113.02
4	B	1426	NAG	C4-C3-C2	-2.92	106.73	111.02
4	A	1416	NAG	C6-C5-C4	-2.91	105.88	113.02
4	B	1412	NAG	C3-C4-C5	-2.91	104.96	110.23
4	C	1427	NAG	C3-C4-C5	-2.91	104.96	110.23
4	A	1422	NAG	C4-C3-C2	-2.90	106.77	111.02
4	C	1413	NAG	O3-C3-C4	-2.89	103.56	110.38
4	B	1421	NAG	C4-C3-C2	-2.89	106.78	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1426	NAG	O3-C3-C2	2.87	115.36	109.40
4	A	1423	NAG	O5-C5-C6	-2.86	102.09	107.66
4	B	1413	NAG	C1-C2-N2	-2.86	105.93	110.43
4	A	1426	NAG	C6-C5-C4	2.85	120.02	113.02
4	B	1422	NAG	C4-C3-C2	-2.84	106.85	111.02
4	A	1422	NAG	O4-C4-C5	2.84	116.31	109.32
4	A	1411	NAG	C4-C3-C2	-2.84	106.86	111.02
4	C	1412	NAG	C6-C5-C4	-2.83	106.07	113.02
4	C	1412	NAG	O3-C3-C4	-2.81	103.76	110.38
4	C	1413	NAG	C6-C5-C4	2.79	119.87	113.02
4	C	1417	NAG	C1-O5-C5	2.78	115.91	112.19
4	A	1411	NAG	C3-C4-C5	2.77	115.26	110.23
4	A	1427	NAG	O3-C3-C4	-2.76	103.87	110.38
4	B	1411	NAG	O5-C5-C4	-2.76	104.11	110.83
4	B	1411	NAG	O3-C3-C4	-2.76	103.87	110.38
4	A	1401	NAG	C1-C2-N2	2.74	114.75	110.43
4	C	1426	NAG	O4-C4-C3	-2.70	104.00	110.38
4	A	1421	NAG	O3-C3-C4	-2.70	104.00	110.38
4	A	1420	NAG	O3-C3-C4	-2.70	104.01	110.38
4	C	1426	NAG	C3-C4-C5	-2.70	105.34	110.23
4	B	1411	NAG	C1-C2-N2	-2.70	106.19	110.43
4	C	1417	NAG	C3-C4-C5	-2.68	105.37	110.23
4	A	1427	NAG	C8-C7-N2	2.67	120.55	116.12
4	B	1408	NAG	O5-C5-C6	2.66	112.84	107.66
4	A	1401	NAG	O4-C4-C5	-2.65	102.79	109.32
4	B	1401	NAG	O4-C4-C3	-2.65	104.12	110.38
4	B	1411	NAG	C2-N2-C7	2.64	126.43	122.90
4	C	1413	NAG	O3-C3-C2	-2.63	103.93	109.40
4	C	1426	NAG	O3-C3-C2	-2.61	103.97	109.40
4	A	1423	NAG	O4-C4-C3	2.61	116.52	110.38
4	C	1413	NAG	O7-C7-N2	-2.59	117.40	121.98
4	C	1401	NAG	C4-C3-C2	-2.58	107.23	111.02
4	C	1427	NAG	O7-C7-C8	2.56	126.61	122.05
4	B	1426	NAG	O3-C3-C4	-2.54	104.38	110.38
4	C	1401	NAG	C1-O5-C5	2.53	115.58	112.19
4	A	1408	NAG	O4-C4-C3	-2.53	104.42	110.38
4	A	1408	NAG	O5-C5-C6	2.51	112.55	107.66
4	C	1411	NAG	C1-C2-N2	-2.51	106.48	110.43
4	A	1423	NAG	O7-C7-C8	-2.49	117.62	122.05
4	B	1411	NAG	C4-C3-C2	-2.48	107.38	111.02
4	C	1412	NAG	C4-C3-C2	-2.48	107.39	111.02
4	C	1427	NAG	C4-C3-C2	-2.45	107.42	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1401	NAG	C3-C4-C5	-2.44	105.81	110.23
4	B	1420	NAG	O3-C3-C2	-2.44	104.34	109.40
4	C	1413	NAG	O5-C1-C2	-2.44	107.52	111.29
4	A	1426	NAG	O4-C4-C3	2.39	116.01	110.38
4	A	1412	NAG	C1-C2-N2	-2.38	106.68	110.43
4	A	1417	NAG	O3-C3-C2	-2.37	104.49	109.40
4	B	1421	NAG	O4-C4-C3	-2.37	104.80	110.38
4	A	1420	NAG	O3-C3-C2	-2.33	104.57	109.40
4	B	1417	NAG	C4-C3-C2	-2.32	107.62	111.02
4	C	1412	NAG	O5-C5-C6	-2.32	103.16	107.66
4	B	1401	NAG	C6-C5-C4	-2.31	107.35	113.02
4	C	1417	NAG	C4-C3-C2	-2.30	107.64	111.02
4	C	1422	NAG	C4-C3-C2	-2.29	107.66	111.02
4	A	1426	NAG	C8-C7-N2	2.28	119.90	116.12
4	C	1426	NAG	O5-C1-C2	-2.27	107.78	111.29
4	B	1420	NAG	O3-C3-C4	-2.27	105.03	110.38
4	C	1420	NAG	O3-C3-C4	-2.27	105.03	110.38
4	B	1426	NAG	O4-C4-C5	2.25	114.87	109.32
4	C	1427	NAG	C1-C2-N2	-2.25	106.89	110.43
4	C	1408	NAG	O5-C5-C6	2.25	112.04	107.66
4	C	1423	NAG	O4-C4-C3	2.24	115.64	110.38
4	C	1413	NAG	O4-C4-C3	-2.23	105.12	110.38
4	C	1401	NAG	O4-C4-C5	-2.22	103.86	109.32
4	B	1408	NAG	C3-C4-C5	-2.20	106.24	110.23
4	A	1422	NAG	C3-C4-C5	2.19	114.20	110.23
4	A	1401	NAG	C1-O5-C5	2.19	115.12	112.19
4	B	1420	NAG	O6-C6-C5	-2.19	103.89	111.33
4	C	1420	NAG	O3-C3-C2	-2.16	104.91	109.40
4	A	1423	NAG	C8-C7-N2	2.16	119.71	116.12
4	B	1421	NAG	O3-C3-C2	-2.15	104.94	109.40
4	C	1420	NAG	O6-C6-C5	-2.14	104.04	111.33
4	C	1412	NAG	O4-C4-C5	-2.14	104.05	109.32
4	A	1422	NAG	O7-C7-N2	-2.14	118.21	121.98
4	B	1417	NAG	C1-O5-C5	2.13	115.05	112.19
4	A	1412	NAG	C1-O5-C5	2.12	115.03	112.19
4	A	1426	NAG	O4-C4-C5	-2.10	104.14	109.32
4	C	1420	NAG	O4-C4-C5	-2.10	104.16	109.32
4	A	1427	NAG	O7-C7-N2	-2.10	118.28	121.98
4	A	1417	NAG	C3-C4-C5	-2.09	106.44	110.23
4	A	1421	NAG	O5-C5-C6	-2.05	103.67	107.66
4	C	1411	NAG	C3-C4-C5	2.05	113.95	110.23
4	A	1408	NAG	C4-C3-C2	-2.04	108.02	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1411	NAG	C1-C2-N2	-2.03	107.23	110.43
4	C	1408	NAG	C3-C4-C5	-2.01	106.58	110.23
4	C	1421	NAG	O6-C6-C5	-2.01	104.48	111.33
4	B	1411	NAG	O3-C3-C2	-2.01	105.22	109.40
4	C	1401	NAG	C2-N2-C7	-2.01	120.21	122.90
4	B	1422	NAG	O7-C7-C8	2.00	125.62	122.05
4	A	1427	NAG	C1-C2-N2	-2.00	107.28	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1413	NAG	C3

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1401	NAG	C8-C7-N2-C2
4	A	1401	NAG	O7-C7-N2-C2
4	A	1408	NAG	C1-C2-N2-C7
4	A	1412	NAG	C8-C7-N2-C2
4	A	1412	NAG	O7-C7-N2-C2
4	A	1421	NAG	C1-C2-N2-C7
4	A	1426	NAG	C1-C2-N2-C7
4	A	1426	NAG	C8-C7-N2-C2
4	A	1426	NAG	O7-C7-N2-C2
4	B	1401	NAG	C8-C7-N2-C2
4	B	1401	NAG	O7-C7-N2-C2
4	B	1408	NAG	C1-C2-N2-C7
4	B	1408	NAG	C8-C7-N2-C2
4	B	1408	NAG	O7-C7-N2-C2
4	B	1412	NAG	C1-C2-N2-C7
4	B	1412	NAG	C8-C7-N2-C2
4	B	1412	NAG	O7-C7-N2-C2
4	B	1416	NAG	C1-C2-N2-C7
4	B	1416	NAG	C8-C7-N2-C2
4	B	1416	NAG	O7-C7-N2-C2
4	B	1420	NAG	C8-C7-N2-C2
4	B	1420	NAG	O7-C7-N2-C2
4	B	1421	NAG	C1-C2-N2-C7
4	B	1426	NAG	C1-C2-N2-C7
4	B	1426	NAG	C8-C7-N2-C2
4	B	1426	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1427	NAG	C8-C7-N2-C2
4	B	1427	NAG	O7-C7-N2-C2
4	C	1408	NAG	C1-C2-N2-C7
4	C	1408	NAG	C8-C7-N2-C2
4	C	1408	NAG	O7-C7-N2-C2
4	C	1412	NAG	C3-C2-N2-C7
4	C	1413	NAG	C8-C7-N2-C2
4	C	1413	NAG	O7-C7-N2-C2
4	C	1421	NAG	C1-C2-N2-C7
4	C	1426	NAG	C8-C7-N2-C2
4	C	1426	NAG	O7-C7-N2-C2
4	C	1427	NAG	O7-C7-N2-C2
4	A	1408	NAG	C8-C7-N2-C2
4	A	1408	NAG	O7-C7-N2-C2
4	A	1416	NAG	C8-C7-N2-C2
4	A	1416	NAG	O7-C7-N2-C2
4	B	1421	NAG	C8-C7-N2-C2
4	B	1423	NAG	C8-C7-N2-C2
4	B	1423	NAG	O7-C7-N2-C2
4	C	1423	NAG	C8-C7-N2-C2
4	C	1423	NAG	O7-C7-N2-C2
4	C	1427	NAG	C8-C7-N2-C2
4	B	1427	NAG	C4-C5-C6-O6
4	A	1423	NAG	C8-C7-N2-C2
4	B	1421	NAG	O7-C7-N2-C2
4	C	1401	NAG	C8-C7-N2-C2
4	C	1401	NAG	O7-C7-N2-C2
4	B	1427	NAG	O5-C5-C6-O6
4	C	1413	NAG	O5-C5-C6-O6
4	A	1411	NAG	C4-C5-C6-O6
4	A	1413	NAG	C8-C7-N2-C2
4	A	1413	NAG	O7-C7-N2-C2
4	A	1421	NAG	C8-C7-N2-C2
4	A	1423	NAG	O7-C7-N2-C2
4	C	1412	NAG	C8-C7-N2-C2
4	C	1421	NAG	C8-C7-N2-C2
4	B	1408	NAG	O5-C5-C6-O6
4	A	1411	NAG	O5-C5-C6-O6
4	C	1411	NAG	O5-C5-C6-O6
4	C	1411	NAG	C4-C5-C6-O6
4	B	1411	NAG	C4-C5-C6-O6
4	C	1412	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1401	NAG	O5-C5-C6-O6
4	B	1411	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	C	1427	NAG	O5-C5-C6-O6
4	A	1421	NAG	O7-C7-N2-C2
4	A	1427	NAG	C8-C7-N2-C2
4	A	1427	NAG	O7-C7-N2-C2
4	C	1421	NAG	O7-C7-N2-C2
4	C	1427	NAG	C4-C5-C6-O6
4	B	1412	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	B	1413	NAG	C8-C7-N2-C2
4	A	1417	NAG	O5-C5-C6-O6
4	B	1413	NAG	O7-C7-N2-C2
4	A	1401	NAG	O5-C5-C6-O6
4	A	1420	NAG	O5-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	A	1426	NAG	O5-C5-C6-O6
4	B	1413	NAG	O5-C5-C6-O6
4	A	1413	NAG	O5-C5-C6-O6
4	C	1420	NAG	O5-C5-C6-O6
4	B	1413	NAG	C3-C2-N2-C7
4	B	1417	NAG	C3-C2-N2-C7
4	C	1417	NAG	C3-C2-N2-C7
4	B	1420	NAG	O5-C5-C6-O6
4	A	1417	NAG	C1-C2-N2-C7
4	B	1417	NAG	C1-C2-N2-C7
4	C	1417	NAG	C1-C2-N2-C7
4	C	1422	NAG	O5-C5-C6-O6
4	B	1412	NAG	O5-C5-C6-O6
4	C	1416	NAG	C8-C7-N2-C2
4	C	1416	NAG	C4-C5-C6-O6
4	C	1422	NAG	C4-C5-C6-O6
4	A	1422	NAG	O5-C5-C6-O6
4	B	1417	NAG	O5-C5-C6-O6
4	C	1416	NAG	O7-C7-N2-C2
4	A	1417	NAG	C3-C2-N2-C7
4	A	1422	NAG	C4-C5-C6-O6
4	C	1420	NAG	C8-C7-N2-C2
4	A	1427	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1420	NAG	C8-C7-N2-C2

There are no ring outliers.

22 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1413	NAG	3	0
4	A	1417	NAG	4	0
4	A	1413	NAG	5	0
4	C	1412	NAG	4	0
4	B	1411	NAG	4	0
4	A	1426	NAG	4	0
4	B	1408	NAG	4	0
4	A	1416	NAG	3	0
4	C	1408	NAG	3	0
4	A	1423	NAG	4	0
4	B	1413	NAG	4	0
4	B	1420	NAG	1	0
4	C	1420	NAG	1	0
4	B	1412	NAG	3	0
4	A	1408	NAG	3	0
4	B	1426	NAG	3	0
4	C	1401	NAG	7	0
4	C	1411	NAG	4	0
4	A	1412	NAG	3	0
4	B	1416	NAG	5	0
4	A	1411	NAG	4	0
4	A	1421	NAG	3	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.

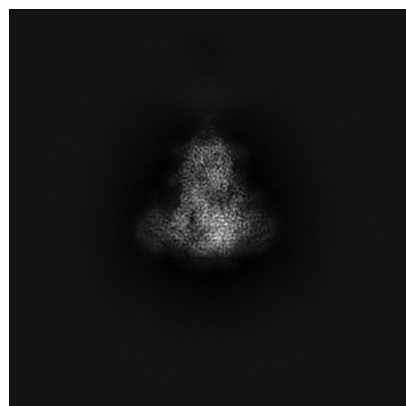
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20672. These allow visual inspection of the internal detail of the map and identification of artifacts.

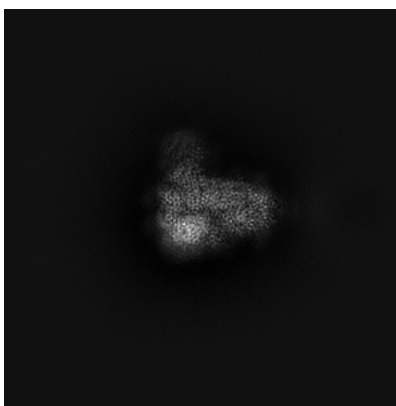
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

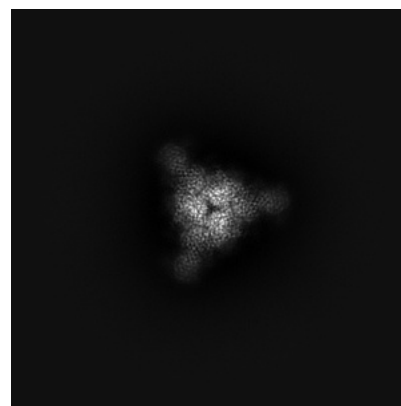
6.1.1 Primary map



X

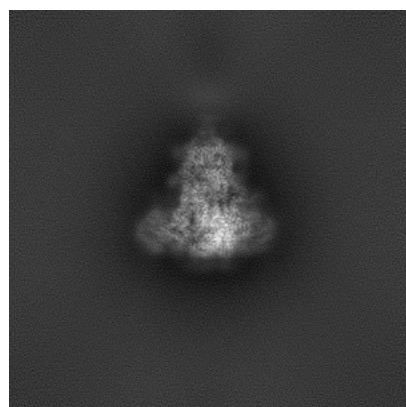


Y

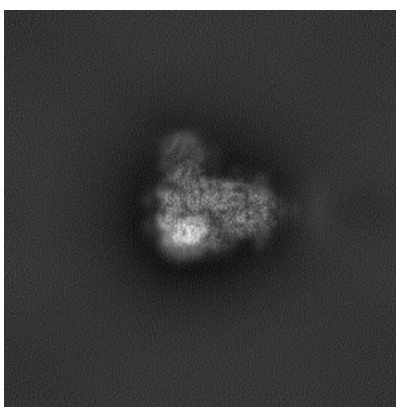


Z

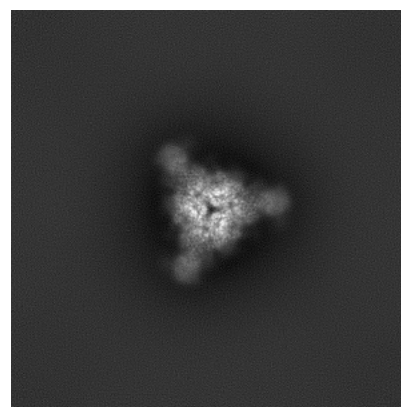
6.1.2 Raw map



X



Y

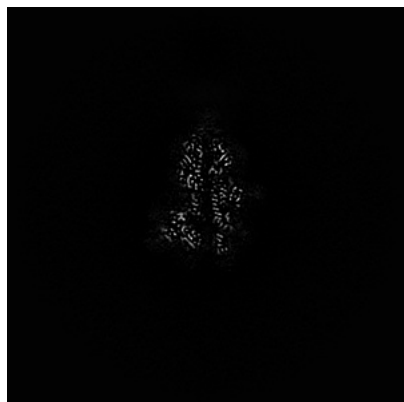


Z

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

6.2 Central slices [i](#)

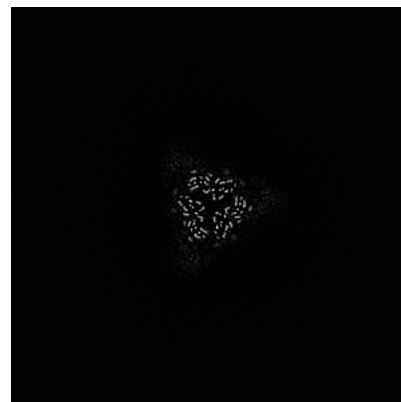
6.2.1 Primary map



X Index: 216

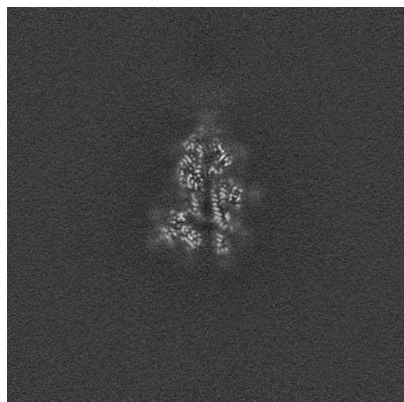


Y Index: 216

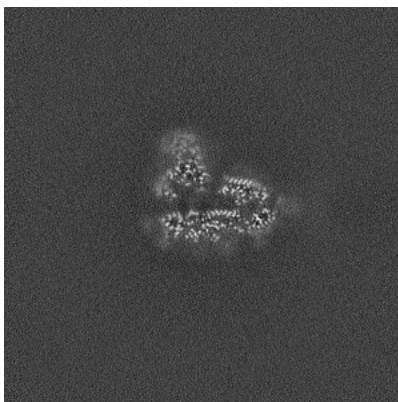


Z Index: 216

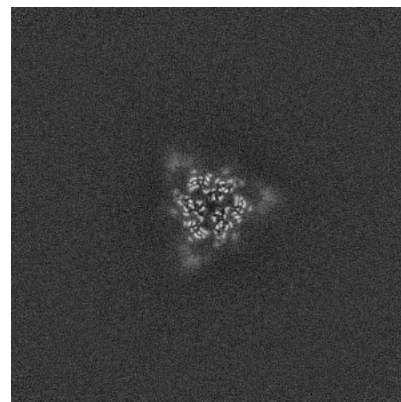
6.2.2 Raw map



X Index: 216



Y Index: 216

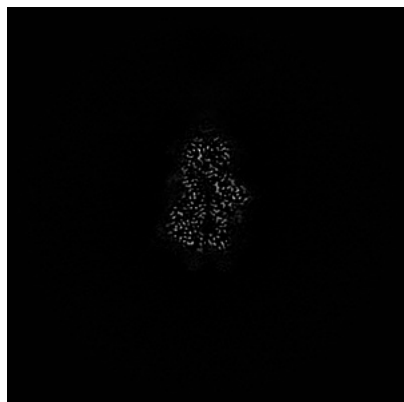


Z Index: 216

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

6.3 Largest variance slices [i](#)

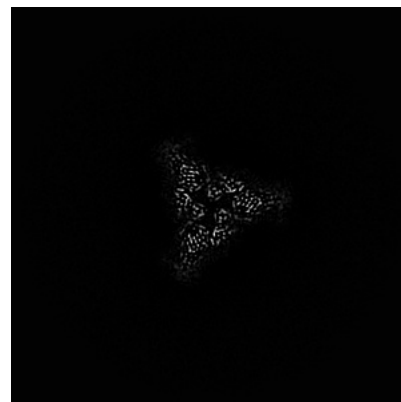
6.3.1 Primary map



X Index: 225

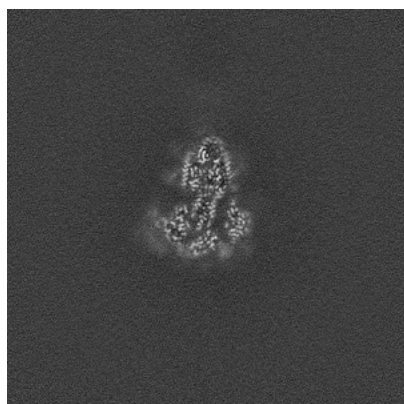


Y Index: 226

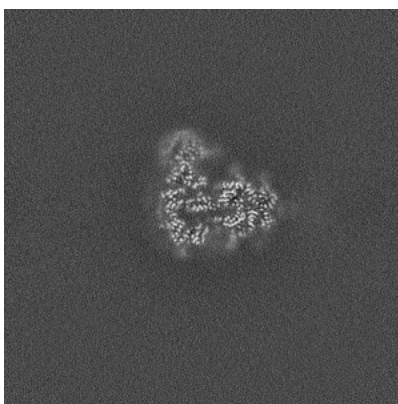


Z Index: 199

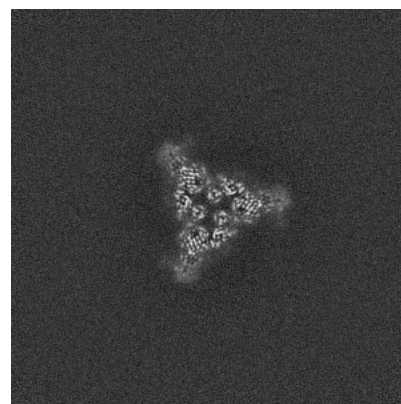
6.3.2 Raw map



X Index: 204



Y Index: 226

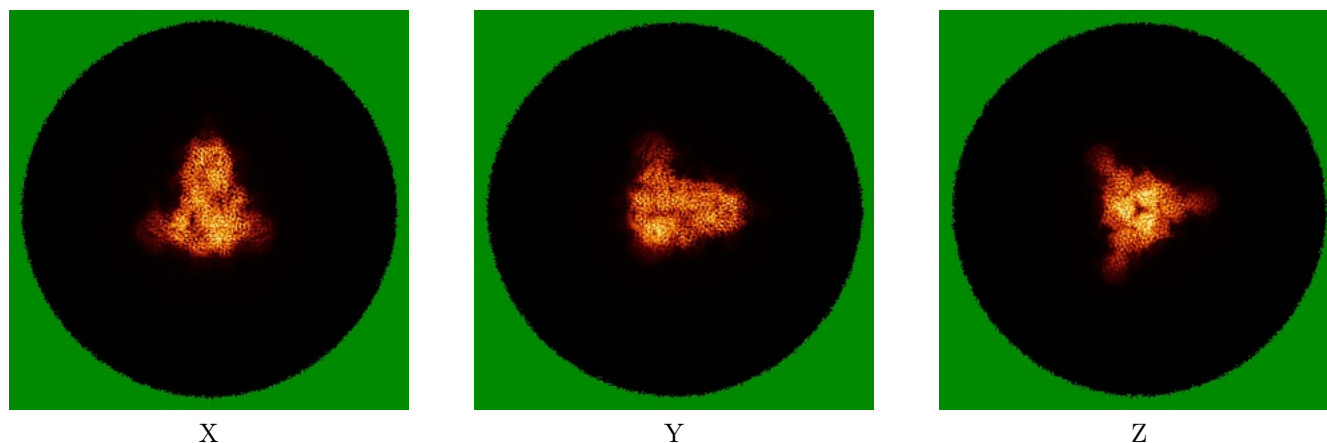


Z Index: 199

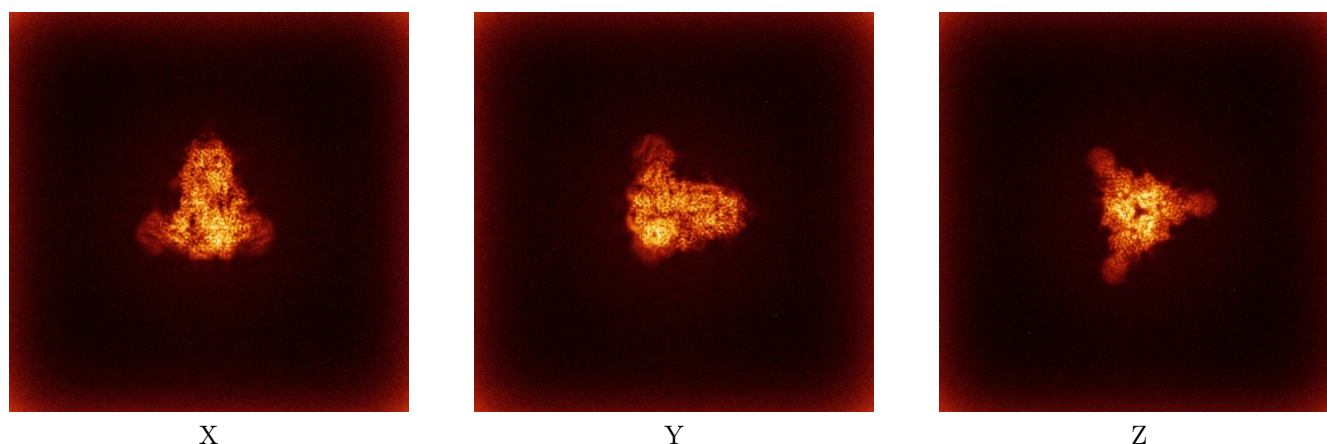
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

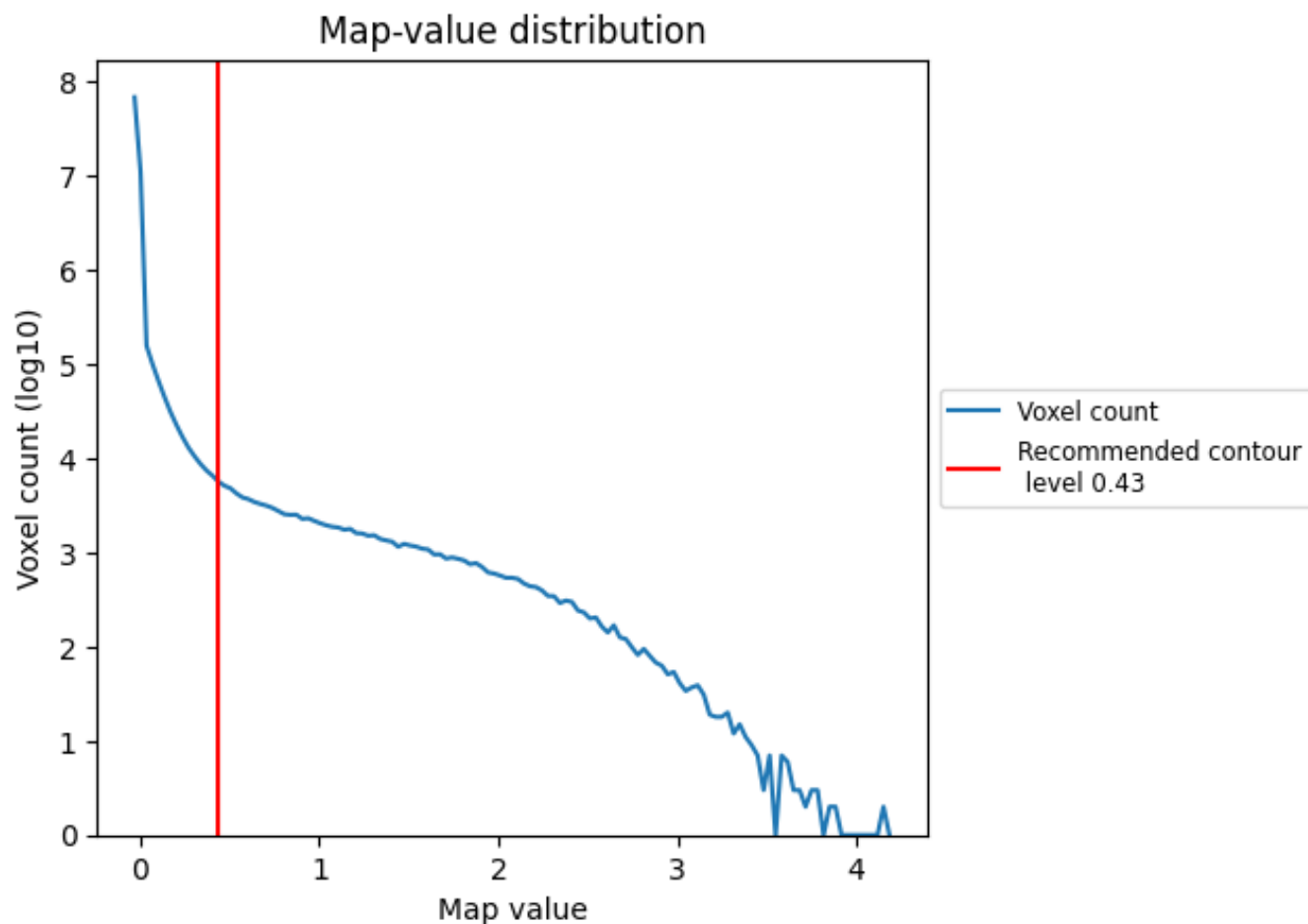
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

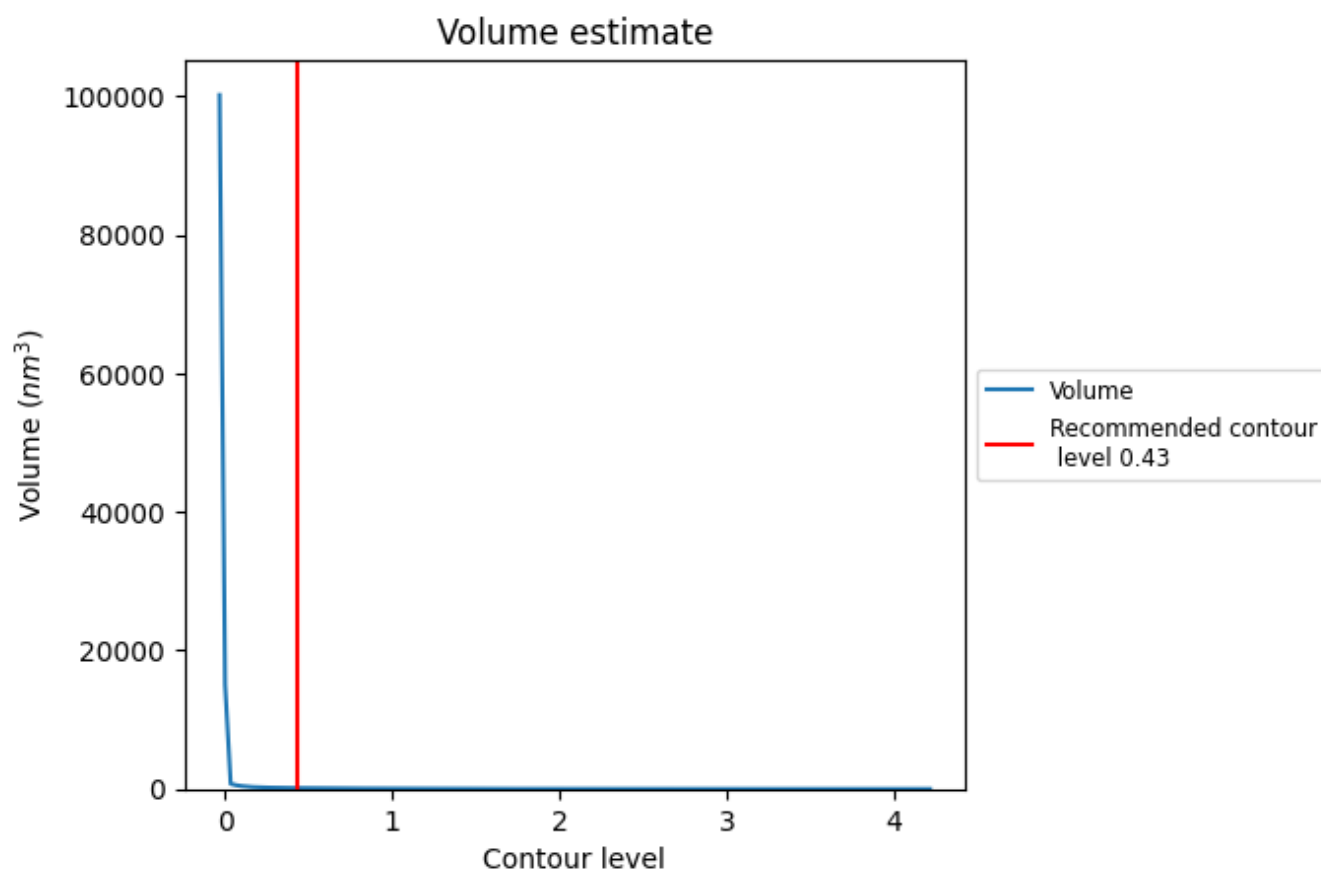
This section contains the results of statistical analysis of the map.

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.

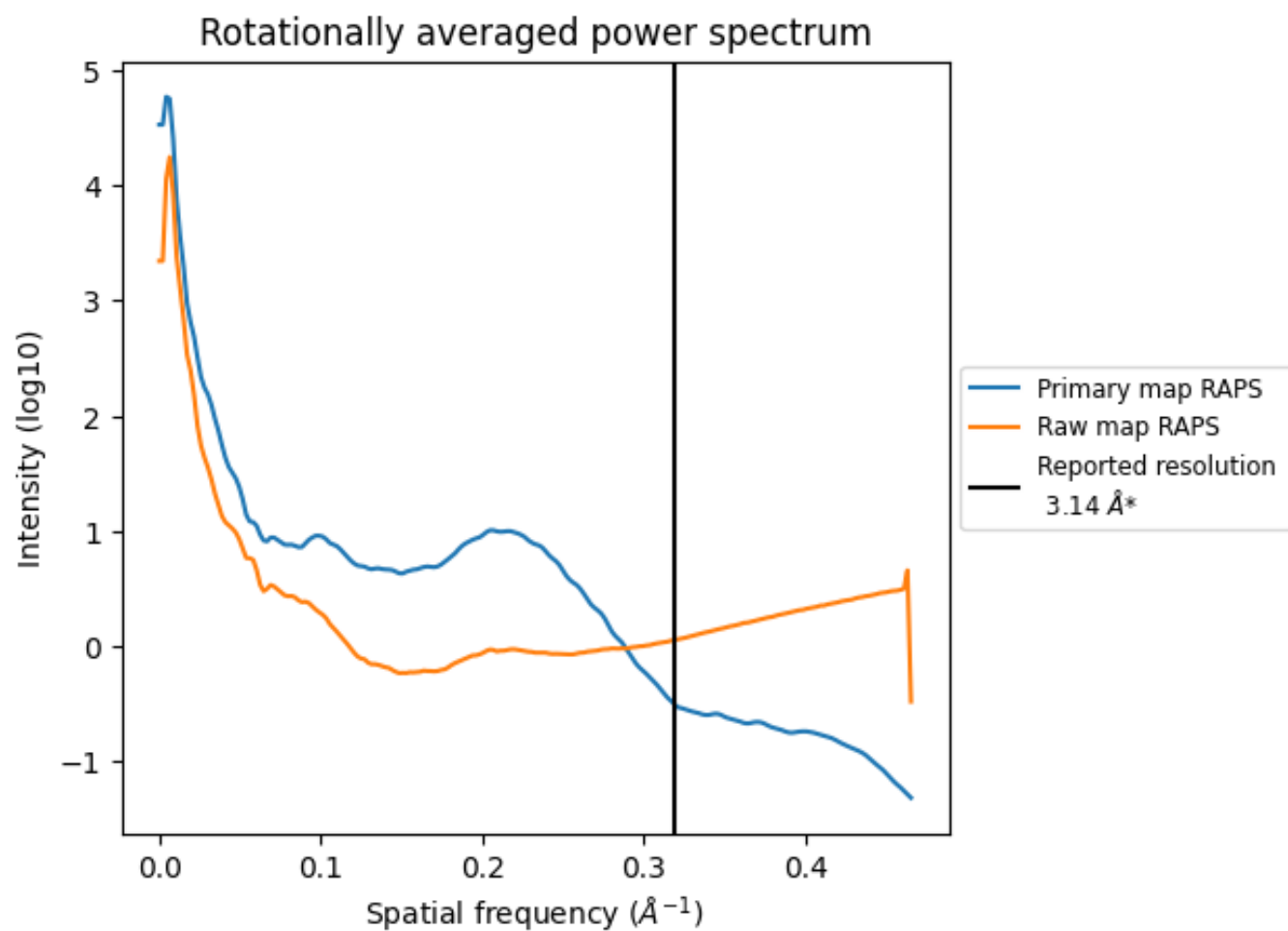
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm^3 ; this corresponds to an approximate mass of 117 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 ⓘ

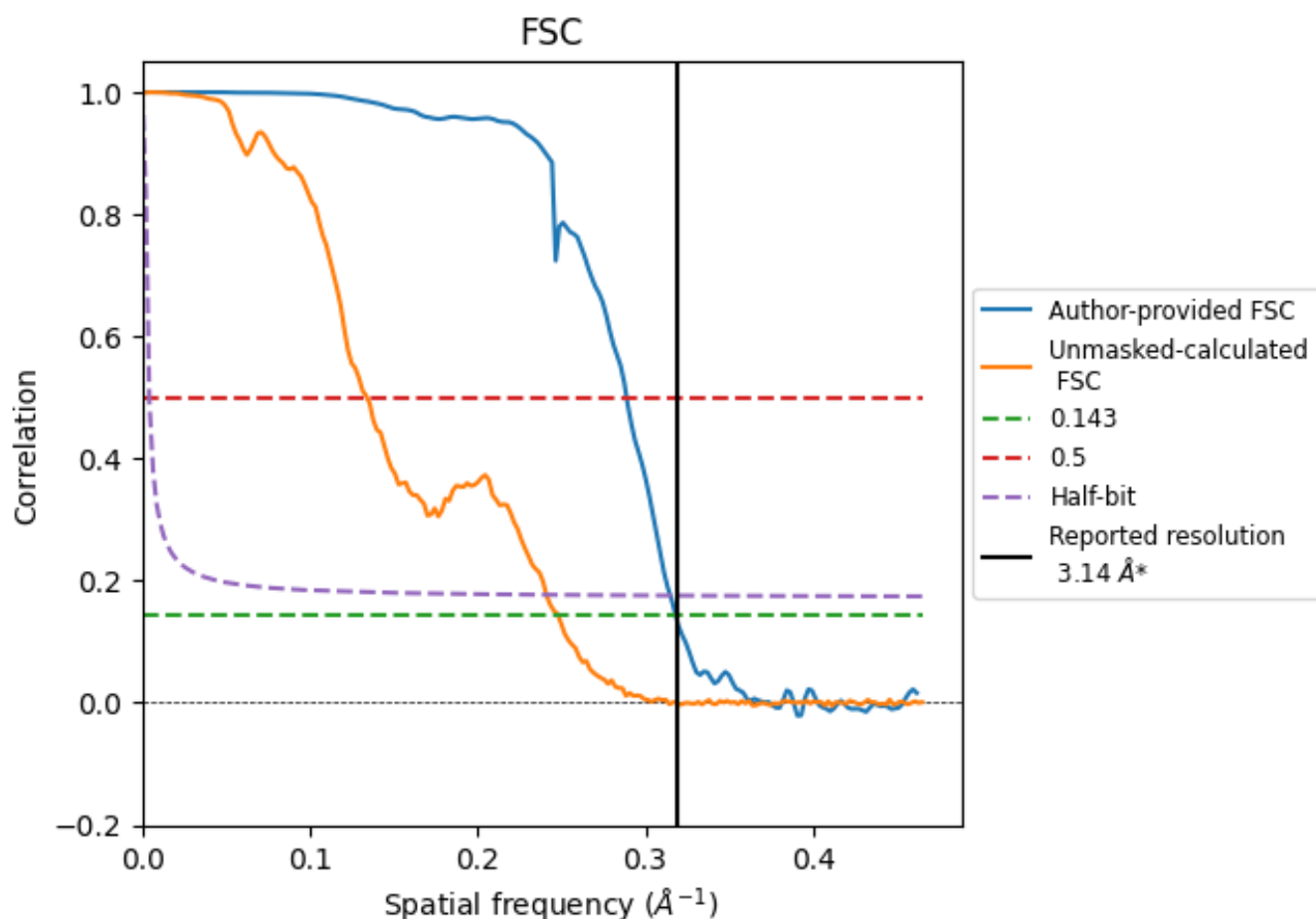


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 $0.318 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

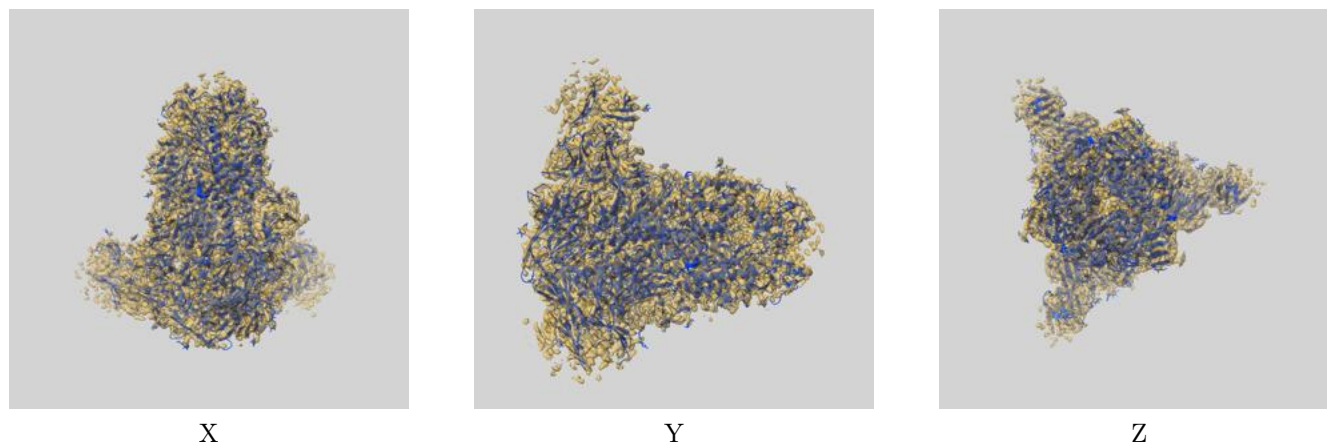
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.46	3.18
Unmasked-calculated*	4.03	7.46	4.15

*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 4.03 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

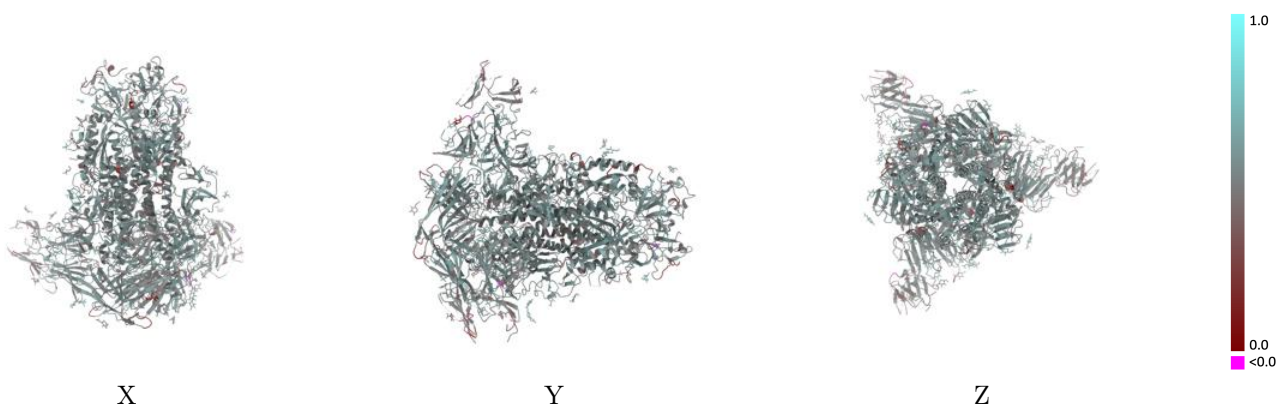
This section contains information regarding the fit between EMDB map EMD-20672 and PDB model 6U7K. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.43 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](#)

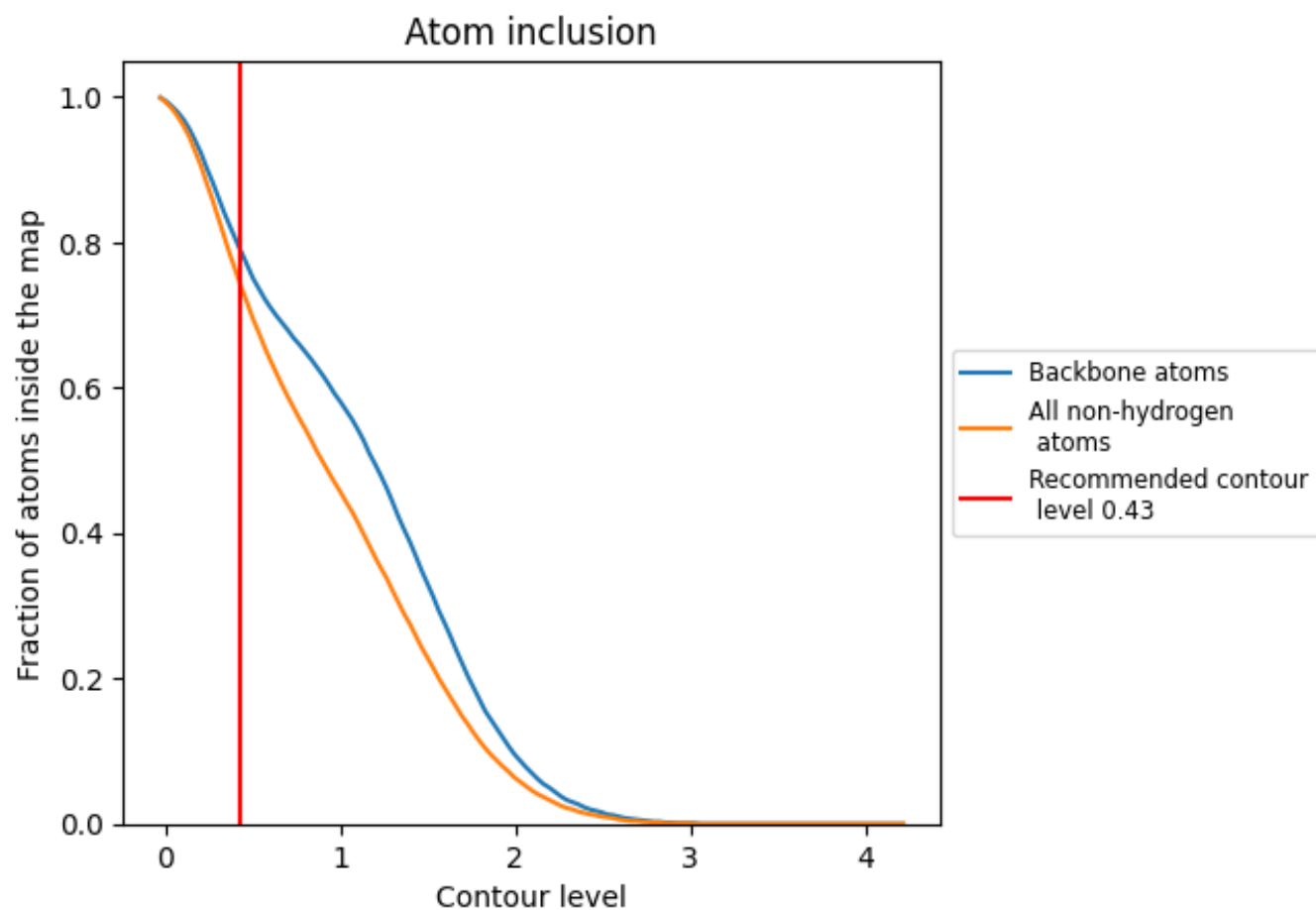


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.5180
A	 0.7400	 0.5170
B	 0.7410	 0.5180
C	 0.7410	 0.5160
D	 0.7920	 0.5830
E	 0.3930	 0.5010
F	 0.7140	 0.6030
G	 0.7860	 0.5750
H	 0.6430	 0.5460
I	 0.7780	 0.5820
J	 0.3930	 0.4920
K	 0.6790	 0.6060
L	 0.7860	 0.6010
M	 0.6790	 0.5640
N	 0.7920	 0.5570
O	 0.2500	 0.5480
P	 0.7500	 0.5960
Q	 0.8570	 0.5980
R	 0.6430	 0.5610

