Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 05:09 AM EST

PDB ID	:	6U7K
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 (i) 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 (i)) were used in the production of this report:

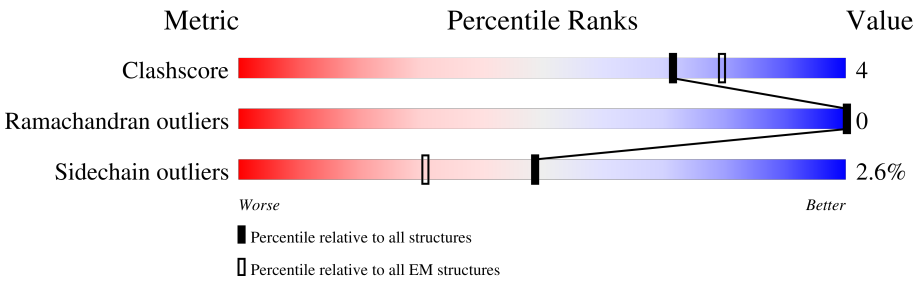
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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%
2	I	6	17% 67% 33%
2	N	6	17% 50% 50%
3	E	2	50% 100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	100%
3	J	2	50% 100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%
3	O	2	50% 50% 50%
3	P	2	100%
3	Q	2	100%
3	R	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-
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
			Total	C	N	O	S		
1	A	1064	8139	5189	1320	1594	36	0	0
1	B	1064	8139	5189	1320	1594	36	0	0
1	C	1064	8139	5189	1320	1594	36	0	0

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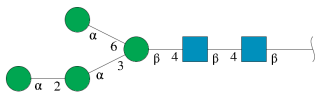
Chain	Residue	Modelled	Actual	Comment	Reference
C	1394	HIS	-	expression tag	UNP Q91AV1
C	1395	PRO	-	expression tag	UNP Q91AV1
C	1396	GLN	-	expression tag	UNP Q91AV1
C	1397	PHE	-	expression tag	UNP Q91AV1
C	1398	GLU	-	expression tag	UNP Q91AV1
C	1399	LYS	-	expression tag	UNP Q91AV1

- 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
			Total	C	N	O		
2	D	6	72	40	2	30	0	0
2	I	6	72	40	2	30	0	0
2	N	6	72	40	2	30	0	0

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

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

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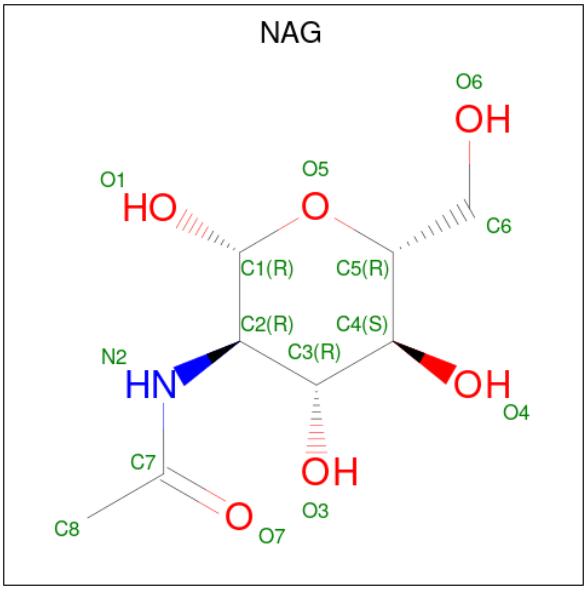
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	K	2	28	16	2	10	0	0
			Total	C	N	O		
3	L	2	28	16	2	10	0	0
			Total	C	N	O		
3	M	2	28	16	2	10	0	0
			Total	C	N	O		
3	O	2	28	16	2	10	0	0
			Total	C	N	O		
3	P	2	28	16	2	10	0	0
			Total	C	N	O		
3	Q	2	28	16	2	10	0	0
			Total	C	N	O		
3	R	2	28	16	2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

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	182	104	13	65	0
			Total	C	N	O	
4	A	1	182	104	13	65	0
			Total	C	N	O	
4	A	1	182	104	13	65	0
			Total	C	N	O	
4	A	1	182	104	13	65	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0
4	B	1	182	104	13	65	0

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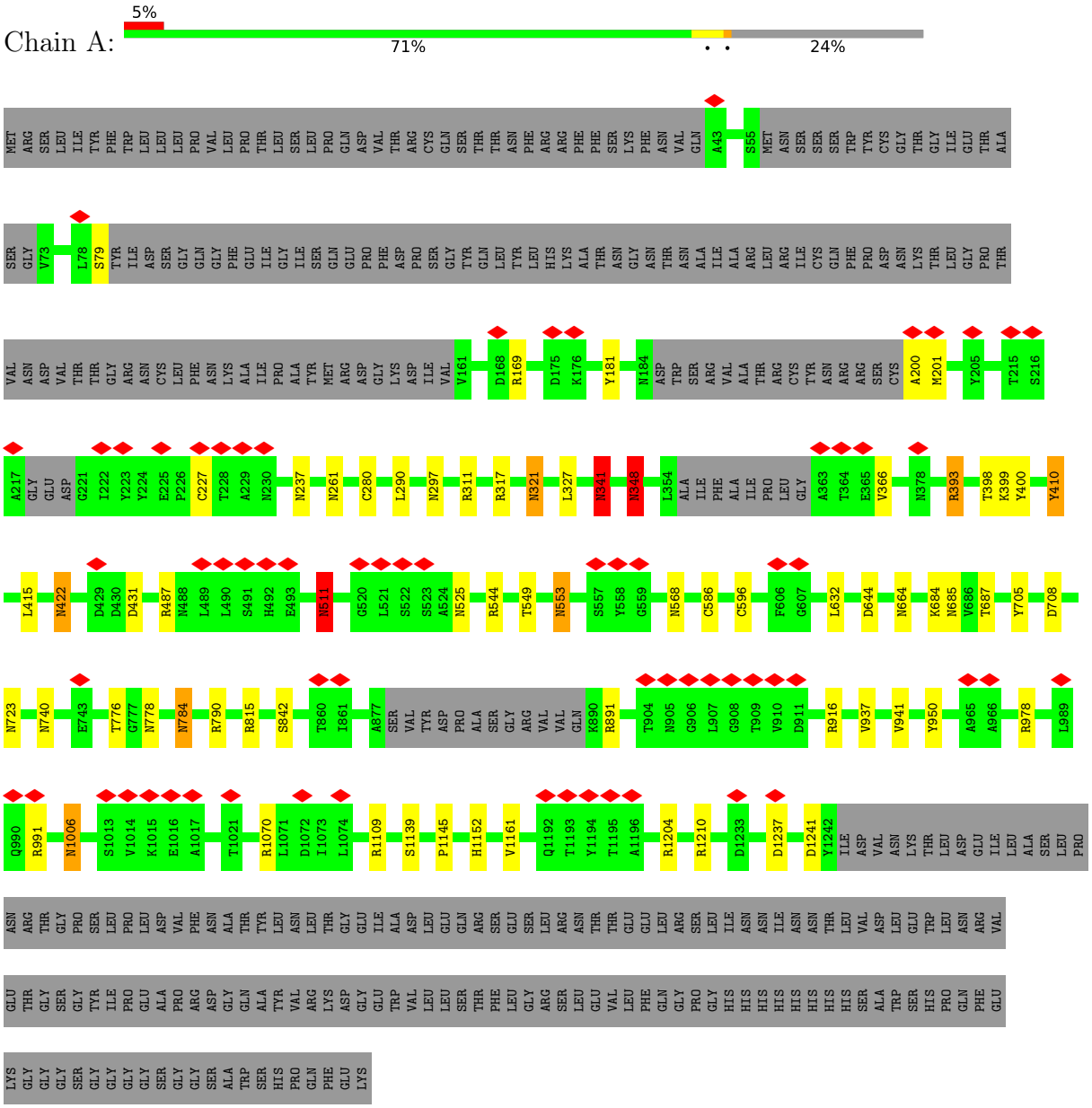
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0

3 Residue-property plots (i)

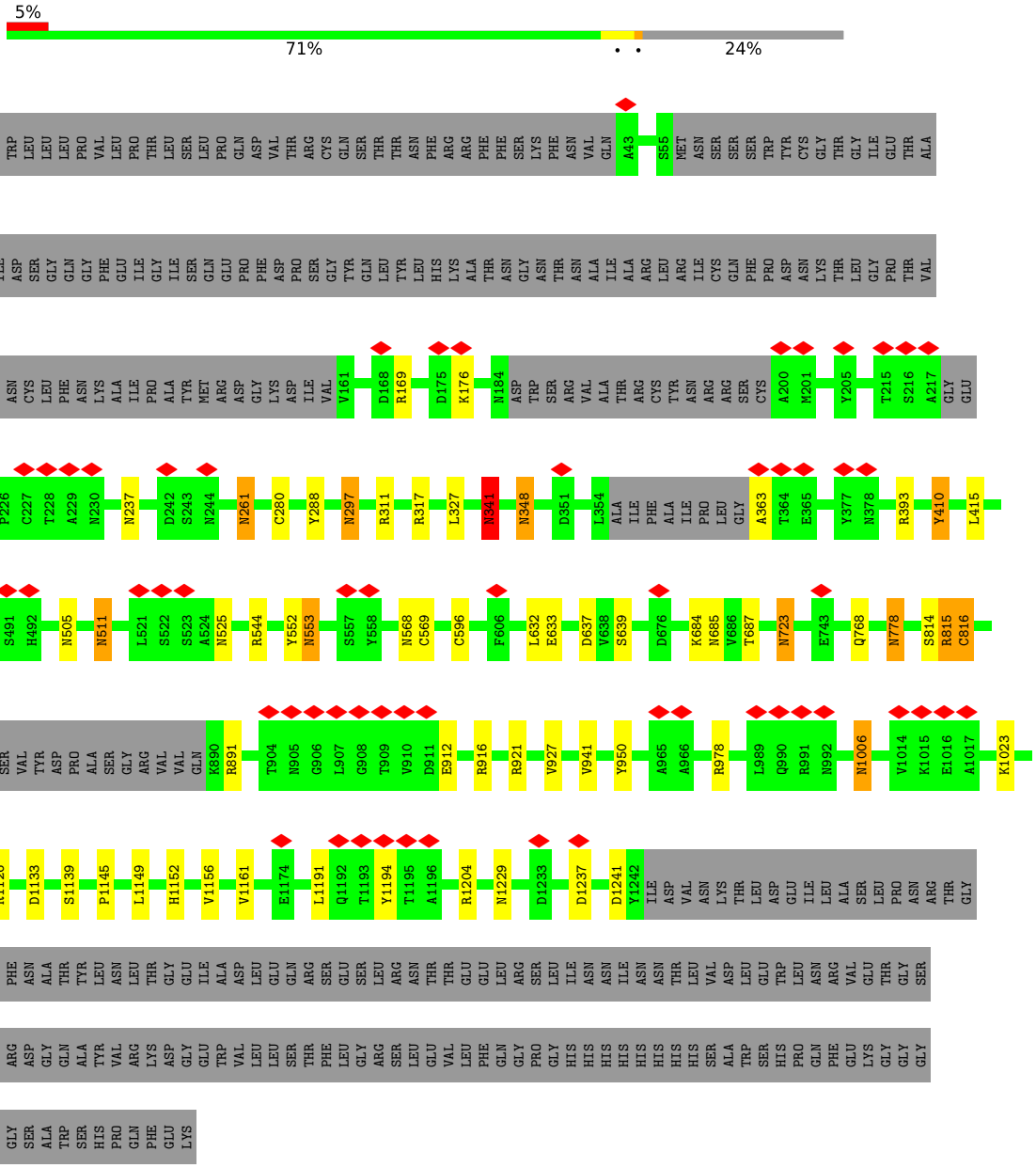
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike glycoprotein



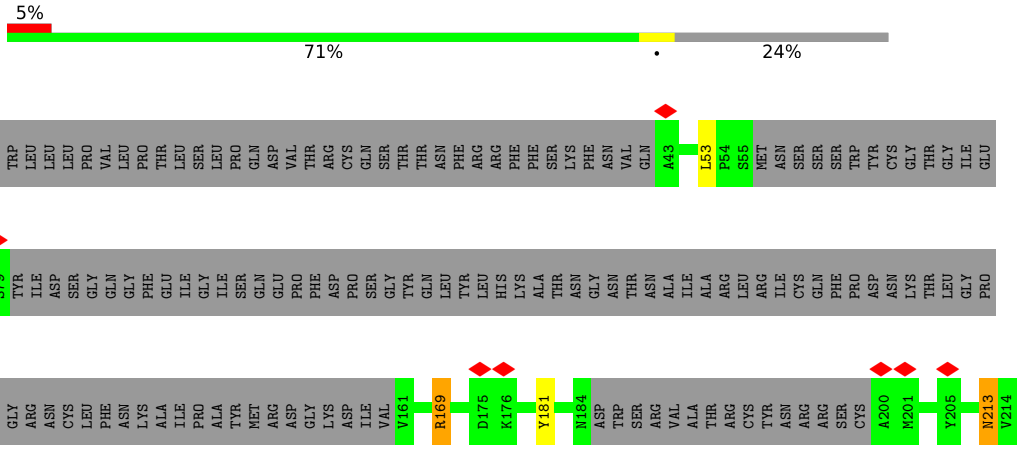
- Molecule 1: Spike glycoprotein

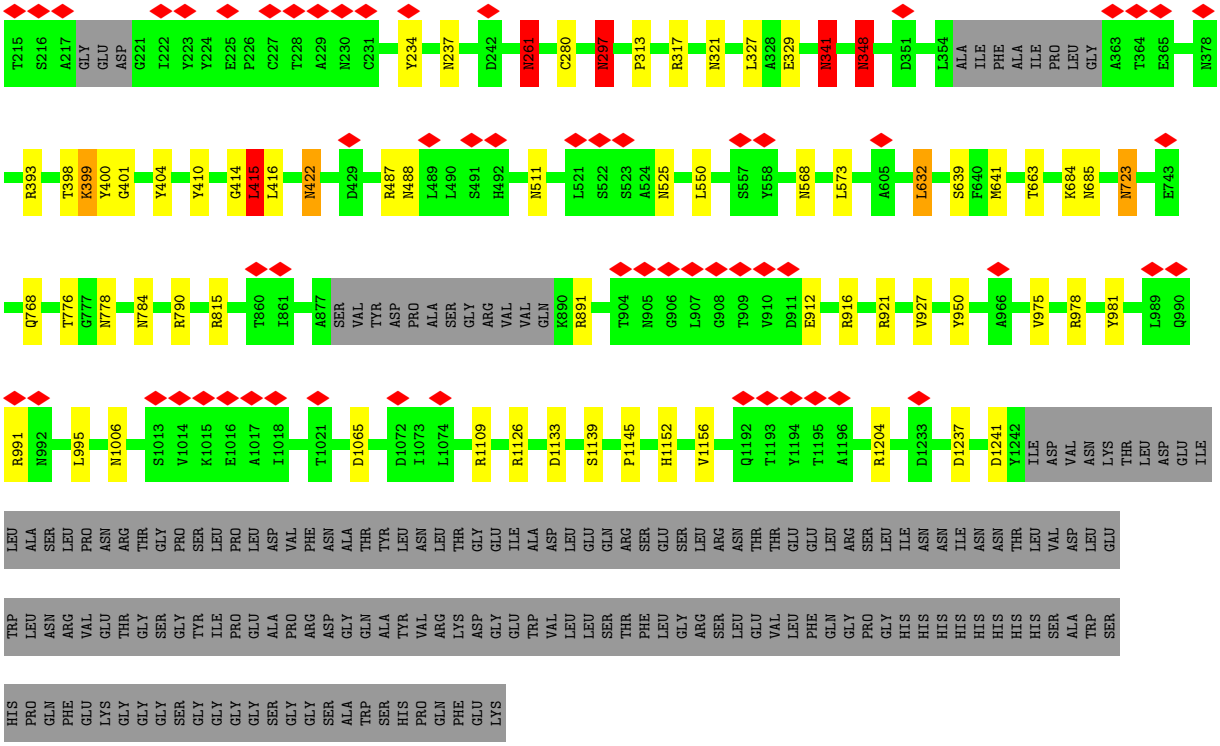
Chain B:



• Molecule 1: Spike glycoprotein

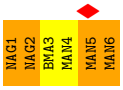
Chain C:





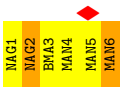
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



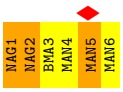
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

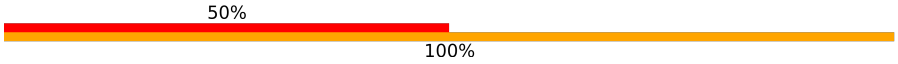


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain E: 

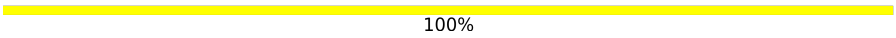
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:

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

Chain H: 

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

Chain J:

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

Chain K:

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

Chain L: 100%

NAG1 NAG2

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

Chain M: 100%

NAG1 NAG2

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

Chain O: 50% 50% 50%

NAG1 NAG2

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

Chain P: 100%

NAG1 NAG2

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

Chain Q: 100%

NAG1 NAG2

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

Chain R: 100%

NAG1 NAG2

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	464.40002, 464.40002, 464.40002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.075, 1.075, 1.075	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.76	18/8305 (0.2%)	1.05	27/11318 (0.2%)
1	B	0.78	16/8305 (0.2%)	1.06	25/11318 (0.2%)
1	C	0.80	21/8305 (0.3%)	1.07	30/11318 (0.3%)
All	All	0.78	55/24915 (0.2%)	1.06	82/33954 (0.2%)

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 (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ASN	C-O	-9.12	1.06	1.23
1	B	79	SER	CB-OG	-8.26	1.31	1.42
1	C	401	GLY	C-O	-7.94	1.10	1.23
1	C	422	ASN	C-O	-7.78	1.08	1.23
1	B	816	CYS	CB-SG	-7.68	1.69	1.82
1	C	399	LYS	C-O	-6.88	1.10	1.23
1	B	778	ASN	CB-CG	-6.84	1.35	1.51
1	C	511	ASN	C-O	-6.68	1.10	1.23
1	A	422	ASN	C-O	-6.61	1.10	1.23
1	A	511	ASN	CG-OD1	-6.43	1.09	1.24
1	B	685	ASN	CA-CB	-6.42	1.36	1.53
1	C	348	ASN	N-CA	-6.38	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ASN	CB-CG	-6.21	1.36	1.51
1	B	816	CYS	CA-CB	-6.11	1.40	1.53
1	C	511	ASN	CB-CG	-6.05	1.37	1.51
1	A	341	ASN	CB-CG	-6.01	1.37	1.51
1	B	1006	ASN	C-O	-5.96	1.12	1.23
1	B	422	ASN	C-O	-5.95	1.12	1.23
1	A	348	ASN	N-CA	-5.93	1.34	1.46
1	A	778	ASN	CB-CG	-5.92	1.37	1.51
1	A	784	ASN	C-O	-5.89	1.12	1.23
1	B	341	ASN	CB-CG	-5.84	1.37	1.51
1	B	685	ASN	CG-OD1	-5.83	1.11	1.24
1	C	784	ASN	C-O	-5.81	1.12	1.23
1	C	685	ASN	CG-ND2	-5.78	1.18	1.32
1	B	814	SER	C-O	-5.76	1.12	1.23
1	C	778	ASN	CB-CG	-5.71	1.38	1.51
1	A	685	ASN	CG-OD1	-5.64	1.11	1.24
1	C	723	ASN	CA-C	-5.62	1.38	1.52
1	B	814	SER	CA-C	-5.56	1.38	1.52
1	C	685	ASN	CG-OD1	-5.49	1.11	1.24
1	A	723	ASN	C-O	-5.48	1.12	1.23
1	B	685	ASN	CB-CG	-5.48	1.38	1.51
1	B	685	ASN	CG-ND2	-5.47	1.19	1.32
1	A	341	ASN	CG-ND2	-5.45	1.19	1.32
1	C	341	ASN	CB-CG	-5.44	1.38	1.51
1	C	416	LEU	C-O	-5.38	1.13	1.23
1	C	1006	ASN	C-O	-5.33	1.13	1.23
1	B	1073	ILE	C-O	-5.33	1.13	1.23
1	A	685	ASN	CG-ND2	-5.30	1.19	1.32
1	C	261	ASN	CB-CG	-5.30	1.38	1.51
1	A	422	ASN	CB-CG	-5.29	1.38	1.51
1	A	341	ASN	C-O	-5.28	1.13	1.23
1	C	511	ASN	CG-OD1	-5.22	1.12	1.24
1	A	685	ASN	CA-CB	-5.20	1.39	1.53
1	A	422	ASN	N-CA	-5.16	1.36	1.46
1	A	348	ASN	C-O	-5.16	1.13	1.23
1	A	321	ASN	CB-CG	-5.15	1.39	1.51
1	C	723	ASN	C-O	-5.14	1.13	1.23
1	C	321	ASN	CB-CG	-5.13	1.39	1.51
1	C	415	LEU	C-O	-5.07	1.13	1.23
1	C	414	GLY	C-O	-5.04	1.15	1.23
1	B	723	ASN	CA-C	-5.03	1.39	1.52
1	C	511	ASN	CG-ND2	-5.02	1.20	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	511	ASN	C-O	-5.01	1.13	1.23

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1109	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	B	348	ASN	N-CA-CB	-10.10	92.42	110.60
1	C	348	ASN	CB-CA-C	9.48	129.36	110.40
1	A	916	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	B	978	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	511	ASN	CB-CA-C	-7.79	94.82	110.40
1	A	978	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	348	ASN	N-CA-CB	-7.48	97.14	110.60
1	C	1109	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	422	ASN	N-CA-CB	-7.22	97.61	110.60
1	A	1204	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	B	393	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	916	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	685	ASN	N-CA-C	-7.12	91.78	111.00
1	C	978	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	916	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	685	ASN	N-CA-C	-7.07	91.90	111.00
1	B	778	ASN	CB-CA-C	-6.92	96.57	110.40
1	B	685	ASN	N-CA-C	-6.81	92.61	111.00
1	B	1204	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	511	ASN	CB-CA-C	-6.66	97.09	110.40
1	C	393	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	790	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	169	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	213	ASN	N-CA-CB	-6.49	98.92	110.60
1	A	393	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	1073	ILE	CG1-CB-CG2	-6.31	97.52	111.40
1	A	815	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	410	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	991	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	317	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	487	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	341	ASN	CB-CA-C	-6.08	98.23	110.40
1	A	410	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	B	778	ASN	N-CA-CB	6.05	121.49	110.60
1	B	723	ASN	N-CA-C	6.05	127.33	111.00
1	B	1070	ARG	NE-CZ-NH1	6.05	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	790	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	169	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	341	ASN	CB-CA-C	-5.90	98.60	110.40
1	C	1126	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	C	723	ASN	N-CA-C	5.88	126.88	111.00
1	A	1070	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	778	ASN	CB-CA-C	-5.86	98.68	110.40
1	C	1204	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	511	ASN	N-CA-CB	5.75	120.96	110.60
1	A	317	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	778	ASN	CB-CA-C	-5.72	98.96	110.40
1	A	891	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	C	891	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	487	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	553	ASN	N-CA-CB	-5.60	100.53	110.60
1	A	553	ASN	N-CA-CB	-5.58	100.55	110.60
1	C	511	ASN	N-CA-CB	5.55	120.59	110.60
1	B	1126	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	422	ASN	N-CA-CB	-5.50	100.71	110.60
1	C	815	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	169	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	723	ASN	N-CA-C	5.46	125.75	111.00
1	C	415	LEU	CB-CA-C	-5.46	99.82	110.20
1	C	317	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	341	ASN	CB-CA-C	-5.45	99.51	110.40
1	B	891	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	288	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	311	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	991	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	348	ASN	N-CA-CB	-5.33	101.00	110.60
1	C	422	ASN	N-CA-CB	-5.32	101.02	110.60
1	A	1006	ASN	CB-CA-C	-5.29	99.82	110.40
1	C	297	ASN	CB-CA-C	-5.29	99.83	110.40
1	C	921	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	1109	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	C	778	ASN	N-CA-C	-5.17	97.05	111.00
1	A	348	ASN	CB-CG-OD1	-5.15	111.29	121.60
1	B	1229	ASN	N-CA-CB	-5.15	101.33	110.60
1	A	586	CYS	CA-CB-SG	5.12	123.21	114.00
1	A	321	ASN	N-CA-CB	-5.11	101.39	110.60
1	B	410	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	B	511	ASN	CB-CG-OD1	-5.09	111.42	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	181	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	921	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	1210	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	TYR	Sidechain
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	60	0
1	B	8139	0	7923	42	0
1	C	8139	0	7922	39	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	12	0
3	F	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	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	10	0
3	R	28	0	25	0	0
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	176	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 (176) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:641:MET:HE1	3:Q:1:NAG:O7	1.46	1.08
1:C:641:MET:HE2	3:Q:1:NAG:O7	1.49	1.07
1:A:431:ASP:OD2	3:E:1:NAG:H62	1.52	1.05
1:A:321:ASN:CG	3:E:1:NAG:C1	2.25	1.05
1:A:341:ASN:CG	4:A:1411:NAG:C1	2.26	1.02
1:B:511:ASN:CG	3:K:1:NAG:C1	2.27	1.01
1:B:341:ASN:CG	4:B:1411:NAG:C1	2.29	1.01
1:A:348:ASN:CG	4:A:1412:NAG:C1	2.30	0.99
1:C:341:ASN:CG	4:C:1411:NAG:C1	2.33	0.95
1:C:639:SER:HB2	3:Q:1:NAG:H83	1.57	0.86
1:C:348:ASN:CG	4:C:1412:NAG:C1	2.44	0.86
1:A:664:ASN:CG	4:A:1417:NAG:C1	2.44	0.85
1:A:297:ASN:CG	4:A:1408:NAG:C1	2.43	0.85
1:A:431:ASP:CG	3:E:1:NAG:H62	1.97	0.85
1:C:297:ASN:CG	4:C:1408:NAG:C1	2.45	0.84
1:C:213:ASN:CG	4:C:1401:NAG:C1	2.45	0.83
1:B:297:ASN:CG	4:B:1408:NAG:C1	2.46	0.83
1:A:321:ASN:OD1	3:E:1:NAG:C1	2.28	0.82
1:A:784:ASN:CG	4:A:1423:NAG:C1	2.48	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:A:431:ASP:CG	3:E:1:NAG:C6	2.49	0.79
1:A:740:ASN:CG	4:A:1421:NAG:C1	2.50	0.79
1:B:422:ASN:CG	4:B:1413:NAG:C1	2.49	0.79
1:B:348:ASN:CG	4:B:1412:NAG:C1	2.50	0.78
1:A:431:ASP:CG	3:E:1:NAG:O6	2.22	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:1401:NAG:O3	4:C:1401:NAG:O7	2.05	0.75
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
1:B:1074:LEU:HD23	1:B:1074:LEU:O	1.89	0.73
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:A:422:ASN:CG	4:A:1413:NAG:C1	2.58	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
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
4:A:1426:NAG:O6	4:A:1426:NAG:O4	2.00	0.63
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:553:ASN:CG	4:A:1416:NAG:C1	2.60	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: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
1:B:553:ASN:CG	4:B:1416:NAG:C1	2.62	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:A:1006:ASN:CG	4:A:1426:NAG:C1	2.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:297:ASN:OD1	4:A:1408:NAG:C1	2.58	0.52
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
3:L:1:NAG:C7	3:L:1:NAG:HO3	2.17	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:B:297:ASN:OD1	4:B:1408:NAG:C1	2.60	0.49
1:C:297:ASN:OD1	4:C:1408:NAG:C1	2.60	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:B:1139:SER:HG	1:B:1152:HIS:HD1	0.49	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:363:ALA:N	4:B:1412:NAG:HO3	2.18	0.42
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: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
4:C:1420:NAG:O6	4:C:1420:NAG:O4	2.31	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	914/1200 (76%)	895 (98%)	19 (2%)	53	78
1	B	914/1200 (76%)	888 (97%)	26 (3%)	43	71
1	C	914/1200 (76%)	888 (97%)	26 (3%)	43	71
All	All	2742/3600 (76%)	2671 (97%)	71 (3%)	49	73

All (71) 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	280	CYS

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Mol	Chain	Res	Type
1	A	290	LEU
1	A	327	LEU
1	A	341	ASN
1	A	348	ASN
1	A	525	ASN
1	A	568	ASN
1	A	596	CYS
1	A	632	LEU
1	A	644	ASP
1	A	937	VAL
1	A	1145	PRO
1	A	1161	VAL
1	A	1237	ASP
1	A	1241	ASP
1	B	176	LYS
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	505	ASN
1	B	525	ASN
1	B	568	ASN
1	B	569	CYS
1	B	596	CYS
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	1133	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

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Mol	Chain	Res	Type
1	C	234	TYR
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
1	C	415	LEU
1	C	488	ASN
1	C	525	ASN
1	C	568	ASN
1	C	632	LEU
1	C	663	THR
1	C	723	ASN
1	C	912	GLU
1	C	927	VAL
1	C	975	VAL
1	C	995	LEU
1	C	1065	ASP
1	C	1133	ASP
1	C	1145	PRO
1	C	1237	ASP
1	C	1241	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1006	ASN
1	B	1006	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	3.16	12 (85%)	17,19,21	3.47	11 (64%)
2	NAG	D	2	2	14,14,15	2.92	7 (50%)	17,19,21	3.58	11 (64%)
2	BMA	D	3	2	11,11,12	2.99	6 (54%)	15,15,17	2.40	5 (33%)
2	MAN	D	4	2	11,11,12	1.62	2 (18%)	15,15,17	2.28	6 (40%)
2	MAN	D	5	2	11,11,12	1.03	0	15,15,17	2.09	6 (40%)
2	MAN	D	6	2	11,11,12	1.46	2 (18%)	15,15,17	1.85	5 (33%)
3	NAG	E	1	3	14,14,15	1.91	1 (7%)	17,19,21	2.55	6 (35%)
3	NAG	E	2	3	14,14,15	0.73	0	17,19,21	2.16	4 (23%)
3	NAG	F	1	3	14,14,15	2.15	6 (42%)	17,19,21	2.85	7 (41%)
3	NAG	F	2	3	14,14,15	1.64	3 (21%)	17,19,21	1.62	4 (23%)
3	NAG	G	1	3	14,14,15	3.70	11 (78%)	17,19,21	5.53	11 (64%)
3	NAG	G	2	3	14,14,15	1.96	6 (42%)	17,19,21	2.96	10 (58%)
3	NAG	H	1	3	14,14,15	2.40	6 (42%)	17,19,21	4.03	8 (47%)
3	NAG	H	2	3	14,14,15	1.37	2 (14%)	17,19,21	1.79	5 (29%)
2	NAG	I	1	2	14,14,15	2.66	10 (71%)	17,19,21	3.02	8 (47%)
2	NAG	I	2	2	14,14,15	2.77	8 (57%)	17,19,21	3.19	8 (47%)
2	BMA	I	3	2	11,11,12	2.72	6 (54%)	15,15,17	2.38	4 (26%)
2	MAN	I	4	2	11,11,12	1.63	4 (36%)	15,15,17	2.52	8 (53%)
2	MAN	I	5	2	11,11,12	1.17	1 (9%)	15,15,17	2.16	5 (33%)
2	MAN	I	6	2	11,11,12	1.35	1 (9%)	15,15,17	1.88	6 (40%)
3	NAG	J	1	3	14,14,15	1.66	1 (7%)	17,19,21	2.55	6 (35%)
3	NAG	J	2	3	14,14,15	0.74	0	17,19,21	1.52	5 (29%)
3	NAG	K	1	3	14,14,15	1.80	5 (35%)	17,19,21	5.60	9 (52%)
3	NAG	K	2	3	14,14,15	1.77	4 (28%)	17,19,21	1.32	2 (11%)
3	NAG	L	1	3	14,14,15	3.49	11 (78%)	17,19,21	6.32	14 (82%)
3	NAG	L	2	3	14,14,15	2.12	7 (50%)	17,19,21	2.06	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	M	1	3	14,14,15	2.59	7 (50%)	17,19,21	3.27	9 (52%)
3	NAG	M	2	3	14,14,15	1.31	3 (21%)	17,19,21	1.89	4 (23%)
2	NAG	N	1	2,1	14,14,15	3.14	10 (71%)	17,19,21	3.09	6 (35%)
2	NAG	N	2	2	14,14,15	2.51	7 (50%)	17,19,21	3.26	8 (47%)
2	BMA	N	3	2	11,11,12	1.43	2 (18%)	15,15,17	1.82	3 (20%)
2	MAN	N	4	2	11,11,12	0.97	0	15,15,17	1.79	5 (33%)
2	MAN	N	5	2	11,11,12	0.54	0	15,15,17	1.69	3 (20%)
2	MAN	N	6	2	11,11,12	1.50	2 (18%)	15,15,17	1.95	4 (26%)
3	NAG	O	1	3	14,14,15	1.88	2 (14%)	17,19,21	5.26	7 (41%)
3	NAG	O	2	3	14,14,15	0.85	0	17,19,21	1.95	6 (35%)
3	NAG	P	1	3	14,14,15	2.22	8 (57%)	17,19,21	3.29	7 (41%)
3	NAG	P	2	3	14,14,15	1.80	2 (14%)	17,19,21	1.44	2 (11%)
3	NAG	Q	1	3	14,14,15	3.40	11 (78%)	17,19,21	3.49	9 (52%)
3	NAG	Q	2	3	14,14,15	2.12	6 (42%)	17,19,21	2.44	6 (35%)
3	NAG	R	1	3	14,14,15	2.59	6 (42%)	17,19,21	3.82	9 (52%)
3	NAG	R	2	3	14,14,15	1.42	3 (21%)	17,19,21	1.74	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	-	4/6/23/26	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	-	2/6/23/26	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	-	4/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-	3/6/23/26	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	-	4/6/23/26	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	-	4/6/23/26	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 (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	C2-N2	-8.64	1.31	1.46
3	E	1	NAG	C1-C2	6.49	1.62	1.52
2	D	2	NAG	C1-C2	-6.17	1.43	1.52
2	I	2	NAG	C1-C2	-6.07	1.43	1.52
2	N	1	NAG	O5-C1	-5.95	1.34	1.43
3	Q	1	NAG	O5-C1	-5.71	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C1-C2	5.60	1.60	1.52
2	N	2	NAG	C1-C2	-5.51	1.44	1.52
3	L	1	NAG	O5-C1	-5.37	1.35	1.43
3	L	1	NAG	C2-N2	-5.28	1.37	1.46
3	R	1	NAG	O5-C1	-5.07	1.35	1.43
2	D	1	NAG	O5-C5	-5.03	1.33	1.43
3	Q	1	NAG	C4-C5	-4.99	1.42	1.53
2	I	3	BMA	O5-C1	-4.95	1.35	1.43
3	O	1	NAG	C1-C2	4.89	1.59	1.52
2	D	1	NAG	C4-C5	-4.76	1.43	1.53
2	D	3	BMA	O5-C1	-4.72	1.36	1.43
2	N	1	NAG	O5-C5	-4.70	1.33	1.43
3	G	1	NAG	O5-C1	-4.68	1.36	1.43
3	L	1	NAG	C3-C2	-4.66	1.42	1.52
2	N	1	NAG	C2-N2	-4.56	1.38	1.46
3	Q	1	NAG	O5-C5	-4.51	1.34	1.43
3	P	2	NAG	C2-N2	-4.47	1.38	1.46
3	R	1	NAG	O5-C5	-4.41	1.34	1.43
2	D	2	NAG	O5-C1	-4.39	1.36	1.43
3	L	1	NAG	C7-N2	-4.34	1.19	1.34
3	H	1	NAG	O5-C1	-4.34	1.36	1.43
2	D	3	BMA	C2-C3	-4.31	1.46	1.52
3	Q	1	NAG	C1-C2	4.28	1.58	1.52
2	I	1	NAG	C2-N2	-4.27	1.39	1.46
3	L	1	NAG	C4-C5	-4.27	1.44	1.53
3	G	1	NAG	C7-N2	-4.18	1.20	1.34
2	D	1	NAG	O5-C1	-4.16	1.37	1.43
3	M	1	NAG	O5-C1	-4.15	1.37	1.43
2	N	1	NAG	C3-C2	-4.12	1.43	1.52
3	Q	1	NAG	O7-C7	-4.12	1.13	1.23
2	D	1	NAG	C2-N2	-3.97	1.39	1.46
2	I	1	NAG	O5-C1	-3.88	1.37	1.43
3	G	1	NAG	C4-C5	-3.87	1.44	1.53
3	R	1	NAG	C4-C5	-3.86	1.44	1.53
3	O	1	NAG	O5-C1	-3.84	1.37	1.43
3	H	1	NAG	O5-C5	-3.83	1.35	1.43
3	F	2	NAG	C2-N2	-3.81	1.39	1.46
3	L	1	NAG	O5-C5	-3.81	1.35	1.43
3	M	1	NAG	C4-C5	-3.73	1.45	1.53
3	M	1	NAG	C2-N2	-3.72	1.40	1.46
3	Q	2	NAG	O5-C1	-3.72	1.37	1.43
2	I	2	NAG	O5-C1	-3.70	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C5	-3.69	1.36	1.43
2	D	3	BMA	O5-C5	-3.68	1.36	1.43
2	I	3	BMA	C2-C3	-3.67	1.47	1.52
2	D	2	NAG	O5-C5	-3.66	1.36	1.43
3	M	1	NAG	O5-C5	-3.66	1.36	1.43
2	D	3	BMA	C4-C5	-3.64	1.45	1.53
2	D	2	NAG	C4-C5	-3.64	1.45	1.53
3	F	1	NAG	O5-C1	-3.62	1.37	1.43
3	L	1	NAG	O7-C7	-3.58	1.15	1.23
3	H	1	NAG	C2-N2	-3.56	1.40	1.46
3	L	2	NAG	O5-C1	-3.56	1.38	1.43
3	M	1	NAG	C1-C2	3.55	1.57	1.52
3	R	1	NAG	C2-N2	-3.51	1.40	1.46
3	P	1	NAG	C1-C2	3.50	1.57	1.52
3	K	2	NAG	O5-C1	-3.49	1.38	1.43
3	G	1	NAG	O5-C5	-3.44	1.36	1.43
2	I	2	NAG	C4-C5	-3.38	1.45	1.53
2	I	3	BMA	O5-C5	-3.37	1.36	1.43
3	L	1	NAG	O4-C4	-3.36	1.35	1.43
3	L	2	NAG	C2-N2	-3.35	1.40	1.46
2	D	2	NAG	C3-C2	-3.31	1.45	1.52
2	N	2	NAG	O5-C1	-3.31	1.38	1.43
2	N	2	NAG	C3-C2	-3.29	1.45	1.52
3	G	1	NAG	C3-C2	-3.28	1.45	1.52
3	G	1	NAG	C4-C3	-3.26	1.44	1.52
3	F	1	NAG	C4-C5	-3.23	1.46	1.53
2	I	3	BMA	C4-C5	-3.21	1.46	1.53
2	I	2	NAG	C3-C2	-3.21	1.45	1.52
3	K	2	NAG	C1-C2	-3.19	1.47	1.52
3	Q	2	NAG	C2-N2	-3.17	1.40	1.46
2	D	3	BMA	C4-C3	-3.17	1.44	1.52
3	G	1	NAG	O7-C7	-3.16	1.16	1.23
2	N	2	NAG	C4-C5	-3.13	1.46	1.53
2	I	1	NAG	C4-C5	-3.13	1.46	1.53
2	I	1	NAG	O7-C7	-3.13	1.16	1.23
2	D	3	BMA	O2-C2	-3.12	1.36	1.43
3	H	1	NAG	C4-C5	-3.09	1.46	1.53
3	P	1	NAG	O5-C1	-3.06	1.38	1.43
2	D	4	MAN	C2-C3	-3.04	1.48	1.52
3	P	2	NAG	C1-C2	-3.03	1.47	1.52
3	P	1	NAG	O5-C5	-2.99	1.37	1.43
2	D	1	NAG	C4-C3	-2.94	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	C3-C2	-2.93	1.46	1.52
2	I	2	NAG	O5-C5	-2.91	1.37	1.43
3	Q	2	NAG	C1-C2	-2.88	1.48	1.52
3	F	1	NAG	C2-N2	-2.87	1.41	1.46
2	D	1	NAG	O4-C4	-2.87	1.36	1.43
3	Q	1	NAG	C4-C3	-2.86	1.45	1.52
3	K	2	NAG	C2-N2	-2.86	1.41	1.46
3	G	2	NAG	O5-C1	-2.85	1.39	1.43
2	I	4	MAN	C2-C3	-2.85	1.48	1.52
3	P	1	NAG	O7-C7	-2.84	1.16	1.23
2	D	1	NAG	C7-N2	-2.84	1.24	1.34
3	F	1	NAG	O5-C5	-2.83	1.37	1.43
3	M	1	NAG	C3-C2	-2.83	1.46	1.52
2	D	1	NAG	C3-C2	-2.83	1.46	1.52
3	F	2	NAG	C1-C2	-2.83	1.48	1.52
2	D	4	MAN	O5-C5	-2.83	1.37	1.43
3	K	1	NAG	C3-C2	-2.82	1.46	1.52
2	I	1	NAG	C8-C7	-2.82	1.44	1.50
3	G	2	NAG	C2-N2	-2.81	1.41	1.46
2	I	1	NAG	C3-C2	-2.77	1.46	1.52
2	N	6	MAN	C2-C3	-2.76	1.48	1.52
3	Q	2	NAG	C3-C2	-2.75	1.46	1.52
2	D	1	NAG	C1-C2	2.74	1.56	1.52
3	R	2	NAG	O5-C5	-2.72	1.37	1.43
3	Q	1	NAG	C7-N2	-2.71	1.25	1.34
3	Q	1	NAG	C8-C7	-2.70	1.44	1.50
3	P	1	NAG	C2-N2	-2.70	1.41	1.46
3	G	2	NAG	C1-C2	-2.70	1.48	1.52
3	Q	1	NAG	C3-C2	-2.69	1.46	1.52
3	H	1	NAG	C1-C2	2.69	1.56	1.52
2	I	3	BMA	C4-C3	-2.66	1.45	1.52
3	P	1	NAG	C4-C5	-2.65	1.47	1.53
3	R	1	NAG	C3-C2	-2.64	1.46	1.52
3	G	2	NAG	C3-C2	-2.63	1.46	1.52
2	I	3	BMA	O2-C2	-2.63	1.37	1.43
3	Q	1	NAG	C2-N2	-2.61	1.41	1.46
2	N	1	NAG	O7-C7	-2.60	1.17	1.23
2	N	1	NAG	O4-C4	-2.59	1.36	1.43
3	L	2	NAG	C1-C2	-2.56	1.48	1.52
2	N	1	NAG	C8-C7	-2.55	1.45	1.50
3	L	2	NAG	C4-C5	-2.54	1.47	1.53
3	K	1	NAG	O5-C1	-2.53	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	MAN	O5-C5	-2.53	1.38	1.43
2	N	1	NAG	C4-C3	-2.52	1.45	1.52
2	D	6	MAN	O5-C1	-2.51	1.39	1.43
3	L	2	NAG	C3-C2	-2.50	1.47	1.52
2	D	1	NAG	C8-C7	-2.49	1.45	1.50
2	D	1	NAG	O7-C7	-2.48	1.17	1.23
2	N	6	MAN	C1-C2	-2.48	1.46	1.52
2	I	6	MAN	C2-C3	-2.47	1.48	1.52
3	G	2	NAG	O7-C7	-2.46	1.17	1.23
3	K	1	NAG	O5-C5	-2.45	1.38	1.43
2	I	2	NAG	O3-C3	-2.45	1.37	1.43
3	F	1	NAG	O7-C7	-2.43	1.17	1.23
2	I	1	NAG	O4-C4	-2.42	1.37	1.43
3	K	1	NAG	C2-N2	-2.41	1.42	1.46
3	G	1	NAG	C1-C2	2.40	1.55	1.52
2	N	3	BMA	O5-C1	-2.39	1.39	1.43
3	M	1	NAG	C4-C3	-2.38	1.46	1.52
2	D	6	MAN	C2-C3	-2.38	1.49	1.52
2	N	2	NAG	C4-C3	-2.37	1.46	1.52
2	I	4	MAN	C4-C5	-2.35	1.48	1.53
3	L	2	NAG	O7-C7	-2.35	1.17	1.23
3	K	1	NAG	O3-C3	-2.34	1.37	1.43
3	L	1	NAG	C8-C7	-2.34	1.45	1.50
3	H	2	NAG	C3-C2	-2.34	1.47	1.52
3	R	2	NAG	C3-C2	-2.29	1.47	1.52
3	M	2	NAG	C3-C2	-2.29	1.47	1.52
3	Q	2	NAG	O5-C5	-2.29	1.38	1.43
3	G	1	NAG	C8-C7	-2.29	1.45	1.50
3	R	2	NAG	C4-C5	-2.27	1.48	1.53
2	N	1	NAG	C4-C5	-2.25	1.48	1.53
2	I	2	NAG	C4-C3	-2.24	1.46	1.52
3	P	1	NAG	C4-C3	-2.24	1.46	1.52
3	H	2	NAG	C4-C5	-2.23	1.48	1.53
2	D	2	NAG	O3-C3	-2.22	1.37	1.43
3	Q	1	NAG	O4-C4	-2.21	1.37	1.43
3	L	1	NAG	C4-C3	-2.20	1.46	1.52
2	N	2	NAG	O3-C3	-2.20	1.37	1.43
3	K	2	NAG	C3-C2	-2.20	1.47	1.52
2	D	1	NAG	C6-C5	-2.20	1.44	1.51
3	M	2	NAG	O5-C5	-2.19	1.39	1.43
2	I	1	NAG	C7-N2	-2.18	1.26	1.34
3	R	1	NAG	C1-C2	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C3-C2	-2.16	1.47	1.52
3	L	1	NAG	O3-C3	-2.16	1.37	1.43
2	I	1	NAG	C4-C3	-2.16	1.46	1.52
2	N	2	NAG	O5-C5	-2.16	1.39	1.43
3	Q	2	NAG	C4-C5	-2.16	1.48	1.53
2	I	5	MAN	O5-C1	-2.16	1.40	1.43
3	P	1	NAG	C3-C2	-2.14	1.48	1.52
3	M	2	NAG	C4-C5	-2.14	1.48	1.53
2	N	3	BMA	C2-C3	-2.12	1.49	1.52
3	G	1	NAG	C6-C5	-2.12	1.44	1.51
2	D	2	NAG	C4-C3	-2.09	1.47	1.52
2	I	2	NAG	C2-N2	-2.06	1.42	1.46
3	F	1	NAG	C4-C3	-2.05	1.47	1.52
2	N	1	NAG	C7-N2	-2.05	1.27	1.34
3	L	2	NAG	O5-C5	-2.04	1.39	1.43
3	G	2	NAG	O5-C5	-2.04	1.39	1.43
2	I	4	MAN	O5-C1	-2.02	1.40	1.43

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	1	NAG	O5-C5-C6	-16.92	80.67	107.20
3	G	1	NAG	C1-C2-N2	-14.74	85.31	110.49
3	K	1	NAG	O5-C1-C2	-13.08	90.63	111.29
3	L	1	NAG	O5-C1-C2	-12.44	91.64	111.29
3	L	1	NAG	C1-C2-N2	-11.76	90.41	110.49
3	G	1	NAG	O5-C1-C2	-10.80	94.23	111.29
3	K	1	NAG	C2-N2-C7	10.27	137.52	122.90
3	L	1	NAG	O3-C3-C2	-9.99	88.80	109.47
3	H	1	NAG	O5-C1-C2	-8.97	97.12	111.29
3	P	1	NAG	O5-C1-C2	-8.70	97.55	111.29
3	R	1	NAG	O5-C1-C2	-8.66	97.61	111.29
3	K	1	NAG	C1-C2-N2	-8.61	95.78	110.49
3	Q	1	NAG	O5-C1-C2	-8.55	97.78	111.29
2	D	2	NAG	O3-C3-C2	-8.43	92.02	109.47
2	N	2	NAG	O3-C3-C2	-8.34	92.22	109.47
2	D	1	NAG	O5-C1-C2	-8.14	98.43	111.29
3	G	1	NAG	O5-C5-C6	8.13	119.95	107.20
3	O	1	NAG	O5-C1-C2	-8.12	98.47	111.29
3	K	1	NAG	O3-C3-C2	-8.09	92.72	109.47
3	L	1	NAG	C4-C3-C2	-8.08	99.18	111.02
3	F	1	NAG	O5-C1-C2	-7.87	98.86	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	NAG	C1-O5-C5	7.47	122.31	112.19
3	H	1	NAG	C2-N2-C7	-7.46	112.29	122.90
2	N	1	NAG	C4-C3-C2	-7.38	100.20	111.02
3	L	1	NAG	O4-C4-C5	-7.30	91.17	109.30
2	D	1	NAG	O6-C6-C5	-7.22	86.53	111.29
2	I	2	NAG	O3-C3-C2	-7.16	94.65	109.47
3	M	1	NAG	O5-C1-C2	-7.10	100.07	111.29
3	R	1	NAG	C2-N2-C7	-6.96	113.00	122.90
3	M	1	NAG	C1-C2-N2	-6.86	98.76	110.49
2	I	1	NAG	O5-C1-C2	-6.85	100.47	111.29
2	D	2	NAG	O4-C4-C5	-6.58	92.96	109.30
3	K	1	NAG	C1-O5-C5	6.52	121.03	112.19
3	H	1	NAG	C1-C2-N2	-6.03	100.19	110.49
3	O	1	NAG	O4-C4-C5	6.01	124.22	109.30
2	N	1	NAG	C1-O5-C5	-6.00	104.06	112.19
2	I	2	NAG	O4-C4-C5	-5.95	94.53	109.30
3	L	1	NAG	O7-C7-C8	5.88	132.97	122.06
3	P	1	NAG	C3-C4-C5	-5.83	99.84	110.24
3	R	1	NAG	C1-C2-N2	-5.80	100.57	110.49
3	G	2	NAG	C1-C2-N2	-5.76	100.66	110.49
3	O	1	NAG	C4-C3-C2	-5.64	102.76	111.02
2	D	3	BMA	O4-C4-C3	-5.60	97.39	110.35
3	J	1	NAG	O5-C1-C2	-5.56	102.52	111.29
3	H	1	NAG	C1-O5-C5	5.52	119.68	112.19
2	N	1	NAG	O6-C6-C5	-5.49	92.46	111.29
2	I	3	BMA	O4-C4-C3	-5.49	97.66	110.35
3	R	1	NAG	C1-O5-C5	5.47	119.60	112.19
3	Q	2	NAG	O5-C5-C6	-5.30	98.90	107.20
3	G	1	NAG	C2-N2-C7	-5.29	115.37	122.90
3	G	2	NAG	O3-C3-C4	-5.25	98.22	110.35
2	I	3	BMA	O4-C4-C5	-5.17	96.45	109.30
3	E	1	NAG	O5-C1-C2	-5.15	103.16	111.29
3	Q	1	NAG	O5-C5-C6	5.12	115.22	107.20
3	E	2	NAG	C2-N2-C7	5.09	130.15	122.90
2	I	1	NAG	O5-C5-C6	5.08	115.17	107.20
3	F	1	NAG	C1-O5-C5	5.08	119.07	112.19
3	L	1	NAG	O5-C5-C6	-5.06	99.27	107.20
2	I	1	NAG	C1-C2-N2	-5.03	101.89	110.49
3	G	2	NAG	C2-N2-C7	4.93	129.93	122.90
2	D	2	NAG	C2-N2-C7	-4.93	115.89	122.90
2	N	2	NAG	O4-C4-C5	-4.86	97.24	109.30
3	K	1	NAG	O4-C4-C5	-4.84	97.29	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C4-C3-C2	-4.81	103.97	111.02
3	H	2	NAG	O3-C3-C2	-4.79	99.54	109.47
2	D	3	BMA	O4-C4-C5	-4.79	97.41	109.30
3	Q	1	NAG	C3-C4-C5	-4.74	101.78	110.24
3	Q	1	NAG	C1-C2-N2	4.66	118.45	110.49
2	N	6	MAN	O3-C3-C2	-4.62	101.15	109.99
3	G	1	NAG	C3-C4-C5	-4.60	102.04	110.24
2	I	5	MAN	O3-C3-C4	-4.51	99.93	110.35
3	M	1	NAG	C1-O5-C5	4.49	118.28	112.19
3	E	1	NAG	C1-C2-N2	4.48	118.15	110.49
3	E	1	NAG	O4-C4-C5	4.46	120.36	109.30
3	H	1	NAG	C4-C3-C2	-4.45	104.49	111.02
2	D	4	MAN	O4-C4-C5	-4.44	98.26	109.30
2	I	2	NAG	C3-C4-C5	-4.43	102.34	110.24
2	I	4	MAN	O4-C4-C5	-4.42	98.31	109.30
2	I	2	NAG	C1-C2-N2	-4.42	102.94	110.49
3	Q	2	NAG	C6-C5-C4	-4.41	102.67	113.00
3	E	2	NAG	O3-C3-C4	-4.40	100.18	110.35
3	Q	1	NAG	O3-C3-C4	-4.36	100.28	110.35
3	P	1	NAG	C1-O5-C5	4.35	118.09	112.19
2	I	1	NAG	C3-C4-C5	-4.33	102.51	110.24
3	K	1	NAG	C3-C4-C5	-4.33	102.51	110.24
2	I	5	MAN	C6-C5-C4	-4.30	102.94	113.00
3	K	1	NAG	C4-C3-C2	-4.29	104.73	111.02
2	N	2	NAG	C2-N2-C7	-4.17	116.97	122.90
2	D	5	MAN	O3-C3-C4	-4.17	100.71	110.35
3	R	2	NAG	O3-C3-C2	-4.15	100.88	109.47
3	J	1	NAG	C1-C2-N2	4.14	117.56	110.49
2	N	3	BMA	O4-C4-C3	-4.09	100.88	110.35
3	E	1	NAG	O5-C5-C6	4.06	113.57	107.20
3	G	1	NAG	O6-C6-C5	-4.05	97.41	111.29
2	N	5	MAN	O5-C5-C6	4.04	113.53	107.20
3	M	2	NAG	O3-C3-C2	-4.03	101.13	109.47
3	R	1	NAG	O6-C6-C5	-4.02	97.50	111.29
2	I	4	MAN	C6-C5-C4	-3.98	103.68	113.00
3	J	1	NAG	O5-C5-C6	3.96	113.42	107.20
2	N	2	NAG	C3-C4-C5	-3.96	103.18	110.24
2	D	4	MAN	C1-C2-C3	-3.96	104.80	109.67
3	O	1	NAG	C1-C2-N2	3.90	117.16	110.49
3	F	1	NAG	C3-C4-C5	-3.85	103.37	110.24
3	M	1	NAG	O5-C5-C6	3.83	113.20	107.20
2	D	2	NAG	O5-C5-C6	-3.83	101.21	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	O4-C4-C3	3.82	119.18	110.35
3	G	1	NAG	C1-O5-C5	3.82	117.36	112.19
3	G	2	NAG	O5-C5-C6	3.82	113.19	107.20
3	O	2	NAG	C1-O5-C5	3.79	117.33	112.19
3	F	2	NAG	O4-C4-C3	-3.77	101.64	110.35
2	N	2	NAG	O3-C3-C4	-3.76	101.66	110.35
3	M	2	NAG	C2-N2-C7	3.75	128.24	122.90
3	Q	1	NAG	O6-C6-C5	-3.71	98.57	111.29
2	D	5	MAN	C6-C5-C4	-3.71	104.32	113.00
2	I	2	NAG	C2-N2-C7	-3.69	117.65	122.90
3	L	1	NAG	O5-C5-C4	-3.69	101.86	110.83
3	H	1	NAG	O4-C4-C5	-3.67	100.19	109.30
3	P	1	NAG	C1-C2-N2	-3.67	104.23	110.49
2	N	2	NAG	O5-C1-C2	-3.66	105.51	111.29
3	H	1	NAG	O3-C3-C2	-3.65	101.91	109.47
3	G	1	NAG	C4-C3-C2	-3.64	105.69	111.02
3	O	2	NAG	O3-C3-C2	3.63	116.98	109.47
3	Q	2	NAG	O4-C4-C3	-3.63	101.97	110.35
3	J	1	NAG	C4-C3-C2	-3.62	105.71	111.02
2	D	2	NAG	C3-C4-C5	-3.61	103.80	110.24
3	G	2	NAG	C8-C7-N2	3.58	122.16	116.10
3	E	1	NAG	C4-C3-C2	-3.57	105.78	111.02
2	D	2	NAG	O5-C1-C2	-3.57	105.64	111.29
2	N	1	NAG	O5-C5-C6	3.56	112.79	107.20
3	O	1	NAG	C1-O5-C5	3.56	117.01	112.19
3	Q	2	NAG	O3-C3-C4	-3.47	102.32	110.35
3	L	2	NAG	O5-C5-C6	3.47	112.64	107.20
2	I	4	MAN	O4-C4-C3	-3.43	102.42	110.35
3	M	1	NAG	C2-N2-C7	-3.42	118.03	122.90
2	D	2	NAG	C1-C2-N2	-3.37	104.73	110.49
2	D	1	NAG	C1-O5-C5	3.36	116.74	112.19
3	L	1	NAG	O7-C7-N2	-3.33	115.83	121.95
3	Q	2	NAG	O3-C3-C2	-3.32	102.59	109.47
3	R	1	NAG	C4-C3-C2	-3.28	106.22	111.02
2	D	6	MAN	C6-C5-C4	3.27	120.67	113.00
3	E	2	NAG	C1-O5-C5	3.27	116.62	112.19
3	P	2	NAG	O4-C4-C3	-3.26	102.80	110.35
2	I	2	NAG	O5-C1-C2	-3.26	106.14	111.29
3	P	1	NAG	O4-C4-C5	-3.25	101.22	109.30
2	D	3	BMA	O3-C3-C4	-3.25	102.83	110.35
3	O	2	NAG	O5-C1-C2	-3.25	106.15	111.29
2	N	1	NAG	C2-N2-C7	-3.25	118.28	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	2	NAG	O6-C6-C5	-3.24	100.18	111.29
3	M	1	NAG	O6-C6-C5	-3.23	100.19	111.29
2	I	6	MAN	O4-C4-C3	-3.18	102.99	110.35
3	J	2	NAG	C2-N2-C7	3.17	127.42	122.90
2	I	1	NAG	O3-C3-C4	3.17	117.68	110.35
3	F	1	NAG	O4-C4-C5	-3.14	101.49	109.30
2	D	4	MAN	O5-C5-C6	-3.11	102.33	107.20
2	N	2	NAG	O4-C4-C3	-3.10	103.17	110.35
2	N	6	MAN	C3-C4-C5	-3.10	104.71	110.24
2	I	4	MAN	O2-C2-C3	-3.09	103.96	110.14
2	N	4	MAN	O2-C2-C3	-3.08	103.96	110.14
2	I	6	MAN	C6-C5-C4	3.07	120.19	113.00
2	I	4	MAN	C1-C2-C3	-3.06	105.91	109.67
2	I	3	BMA	O5-C1-C2	-3.03	106.10	110.77
2	D	2	NAG	O4-C4-C3	-3.02	103.36	110.35
3	L	2	NAG	O3-C3-C4	-3.02	103.36	110.35
3	L	2	NAG	O4-C4-C3	-3.01	103.39	110.35
3	R	1	NAG	O4-C4-C5	-3.00	101.84	109.30
3	P	1	NAG	C2-N2-C7	3.00	127.18	122.90
3	K	2	NAG	O3-C3-C2	-3.00	103.26	109.47
3	E	2	NAG	C6-C5-C4	-2.96	106.06	113.00
3	L	1	NAG	C8-C7-N2	-2.96	111.09	116.10
3	H	1	NAG	O4-C4-C3	2.94	117.15	110.35
2	I	4	MAN	O5-C5-C6	-2.94	102.59	107.20
3	P	1	NAG	O5-C5-C6	2.93	111.80	107.20
2	N	5	MAN	C2-C3-C4	-2.93	105.83	110.89
3	F	2	NAG	C1-O5-C5	-2.92	108.24	112.19
2	D	4	MAN	O3-C3-C2	-2.91	104.41	109.99
3	K	2	NAG	O4-C4-C3	-2.89	103.67	110.35
2	N	4	MAN	C2-C3-C4	-2.89	105.90	110.89
3	G	1	NAG	O4-C4-C3	2.88	117.01	110.35
3	R	2	NAG	C1-O5-C5	2.88	116.09	112.19
3	G	2	NAG	O3-C3-C2	-2.85	103.58	109.47
2	N	3	BMA	O4-C4-C5	-2.84	102.25	109.30
3	J	1	NAG	O3-C3-C4	2.83	116.89	110.35
2	D	6	MAN	O2-C2-C1	-2.82	103.39	109.15
2	D	1	NAG	C8-C7-N2	-2.80	111.35	116.10
3	J	1	NAG	O4-C4-C5	2.80	116.25	109.30
2	D	5	MAN	O2-C2-C3	-2.79	104.56	110.14
2	N	5	MAN	C6-C5-C4	-2.77	106.51	113.00
2	N	4	MAN	C6-C5-C4	-2.76	106.55	113.00
2	I	6	MAN	O2-C2-C1	-2.75	103.52	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	6	MAN	O5-C5-C4	-2.75	104.13	110.83
2	D	1	NAG	O7-C7-C8	2.73	127.13	122.06
2	D	2	NAG	O6-C6-C5	-2.72	101.97	111.29
2	I	5	MAN	C2-C3-C4	-2.71	106.21	110.89
3	F	1	NAG	C1-C2-N2	-2.71	105.87	110.49
2	D	6	MAN	O4-C4-C3	-2.70	104.11	110.35
2	D	6	MAN	C2-C3-C4	-2.70	106.23	110.89
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
2	N	1	NAG	O4-C4-C3	2.69	116.57	110.35
2	D	5	MAN	C2-C3-C4	-2.68	106.26	110.89
2	I	1	NAG	C2-N2-C7	-2.68	119.09	122.90
3	Q	1	NAG	C4-C3-C2	-2.66	107.11	111.02
3	O	1	NAG	C2-N2-C7	-2.66	119.11	122.90
2	D	5	MAN	O5-C1-C2	-2.66	106.67	110.77
3	O	2	NAG	O3-C3-C4	-2.64	104.25	110.35
3	G	2	NAG	C1-O5-C5	-2.62	108.64	112.19
3	L	1	NAG	C2-N2-C7	2.61	126.61	122.90
2	I	1	NAG	C4-C3-C2	-2.60	107.21	111.02
3	M	2	NAG	C1-C2-N2	-2.57	106.10	110.49
2	N	2	NAG	C1-C2-N2	-2.57	106.10	110.49
2	I	4	MAN	O3-C3-C2	-2.57	105.07	109.99
3	Q	1	NAG	O3-C3-C2	-2.56	104.17	109.47
2	N	4	MAN	O5-C1-C2	-2.55	106.83	110.77
3	J	2	NAG	C1-O5-C5	2.53	115.62	112.19
2	I	5	MAN	O2-C2-C3	-2.52	105.10	110.14
3	L	2	NAG	C8-C7-N2	2.51	120.35	116.10
2	D	3	BMA	C1-C2-C3	-2.49	106.60	109.67
2	I	6	MAN	O5-C5-C6	2.49	111.11	107.20
3	R	1	NAG	C3-C4-C5	-2.47	105.84	110.24
3	P	2	NAG	C4-C3-C2	-2.46	107.41	111.02
3	J	2	NAG	O3-C3-C4	-2.46	104.67	110.35
2	D	4	MAN	O2-C2-C3	-2.45	105.23	110.14
3	F	2	NAG	C2-N2-C7	-2.44	119.42	122.90
3	L	2	NAG	C1-O5-C5	-2.43	108.91	112.19
3	R	2	NAG	C6-C5-C4	-2.42	107.33	113.00
3	G	1	NAG	C8-C7-N2	2.42	120.19	116.10
2	I	5	MAN	O5-C1-C2	-2.38	107.10	110.77
3	H	2	NAG	C1-C2-N2	-2.38	106.42	110.49
3	F	1	NAG	C6-C5-C4	-2.38	107.43	113.00
3	H	2	NAG	O3-C3-C4	-2.38	104.85	110.35
3	O	2	NAG	C2-N2-C7	-2.38	119.52	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	NAG	C4-C3-C2	-2.37	107.55	111.02
2	I	2	NAG	O6-C6-C5	-2.36	103.19	111.29
3	G	2	NAG	O7-C7-C8	-2.36	117.68	122.06
3	L	1	NAG	C6-C5-C4	-2.35	107.49	113.00
2	I	3	BMA	C2-C3-C4	-2.34	106.84	110.89
3	L	1	NAG	O6-C6-C5	2.32	119.24	111.29
2	N	3	BMA	C2-C3-C4	-2.30	106.92	110.89
3	J	2	NAG	O5-C1-C2	-2.28	107.68	111.29
2	D	4	MAN	C2-C3-C4	-2.28	106.95	110.89
2	D	1	NAG	O3-C3-C2	2.27	114.15	109.47
3	E	1	NAG	O3-C3-C4	2.25	115.54	110.35
3	Q	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	H	2	NAG	C2-N2-C7	2.23	126.08	122.90
2	I	6	MAN	C2-C3-C4	-2.23	107.03	110.89
3	M	1	NAG	C3-C4-C5	-2.21	106.29	110.24
3	G	2	NAG	O6-C6-C5	-2.21	103.70	111.29
3	M	1	NAG	C8-C7-N2	-2.21	112.36	116.10
3	F	1	NAG	O5-C5-C6	2.21	110.66	107.20
3	K	1	NAG	O4-C4-C3	2.19	115.42	110.35
2	N	6	MAN	C1-O5-C5	2.17	115.14	112.19
2	D	1	NAG	O5-C5-C6	2.16	110.59	107.20
3	G	2	NAG	O4-C4-C3	-2.15	105.37	110.35
2	D	5	MAN	C1-O5-C5	2.15	115.10	112.19
3	F	2	NAG	C4-C3-C2	-2.15	107.87	111.02
2	I	4	MAN	O5-C1-C2	-2.13	107.49	110.77
2	D	3	BMA	C2-C3-C4	-2.12	107.22	110.89
2	I	2	NAG	O4-C4-C3	-2.10	105.50	110.35
2	D	1	NAG	O3-C3-C4	2.09	115.18	110.35
3	H	2	NAG	C6-C5-C4	-2.08	108.12	113.00
3	M	2	NAG	C6-C5-C4	-2.07	108.15	113.00
3	R	1	NAG	C8-C7-N2	-2.06	112.61	116.10
3	L	2	NAG	C3-C4-C5	-2.06	106.56	110.24
2	D	2	NAG	C1-O5-C5	2.06	114.98	112.19
3	G	1	NAG	O7-C7-N2	-2.05	118.19	121.95
2	N	6	MAN	C1-C2-C3	-2.04	107.16	109.67
3	M	1	NAG	C4-C3-C2	-2.04	108.03	111.02
2	I	1	NAG	O4-C4-C5	-2.04	104.24	109.30
3	O	2	NAG	C6-C5-C4	-2.03	108.24	113.00
2	D	2	NAG	O3-C3-C4	-2.03	105.65	110.35
2	D	1	NAG	C3-C4-C5	-2.00	106.67	110.24
2	N	4	MAN	O3-C3-C2	-2.00	106.16	109.99

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 (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
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	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	O	1	NAG	C8-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-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	C4-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
2	N	6	MAN	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-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	F	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-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
3	F	2	NAG	C1-C2-N2-C7
3	O	2	NAG	C1-C2-N2-C7
2	N	1	NAG	O7-C7-N2-C2
2	I	5	MAN	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
2	N	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	P	2	NAG	O5-C5-C6-O6
2	N	5	MAN	O5-C5-C6-O6
3	O	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	R	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C1-C2-N2-C7
2	D	5	MAN	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	O	1	NAG	C1-C2-N2-C7
2	I	1	NAG	O7-C7-N2-C2
2	D	5	MAN	C4-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	F	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7

There are no ring outliers.

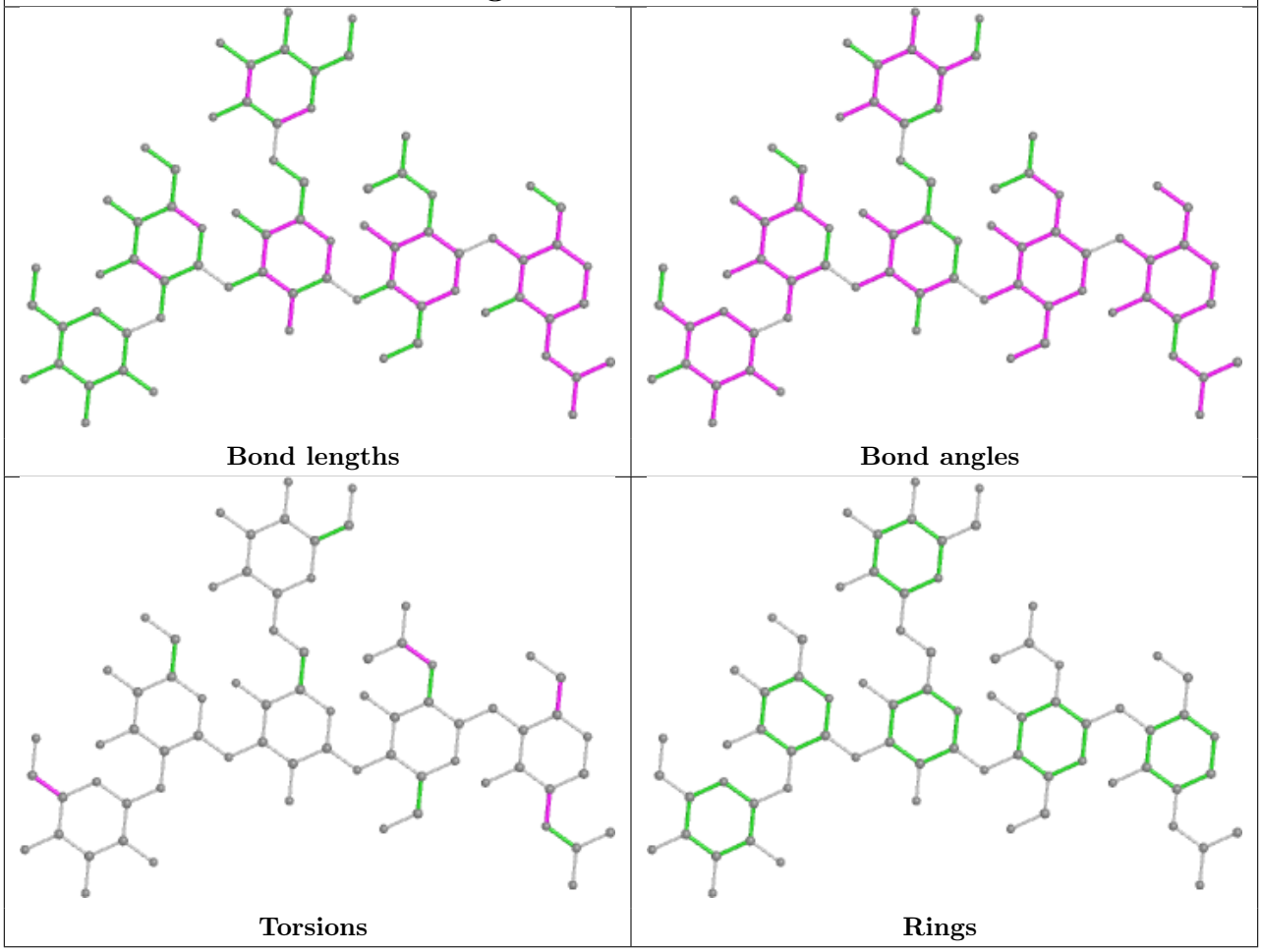
23 monomers are involved in 59 short contacts:

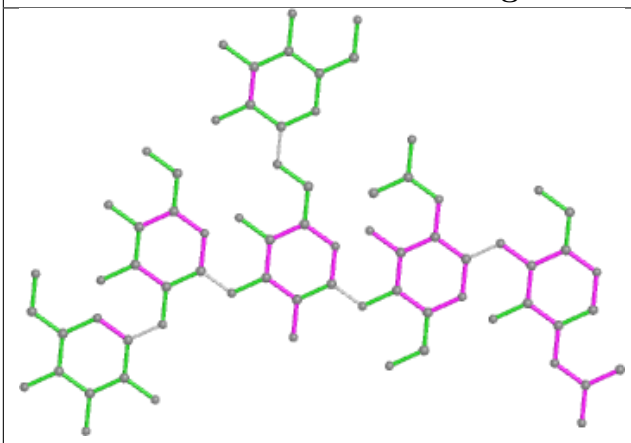
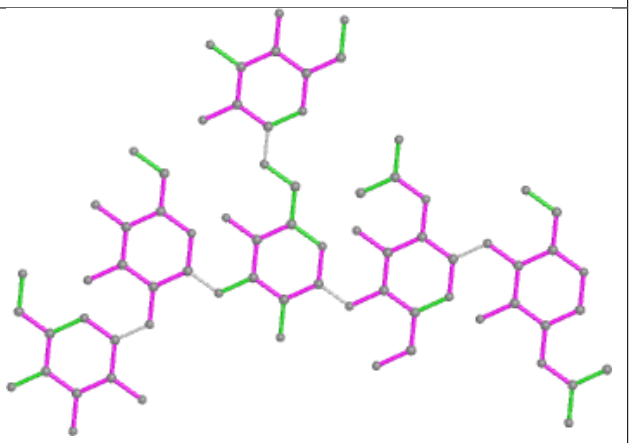
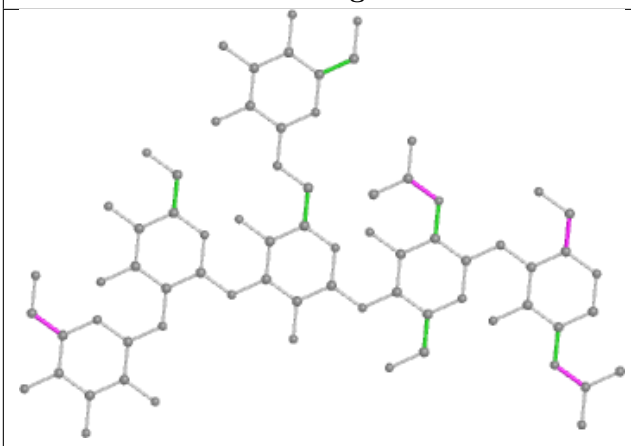
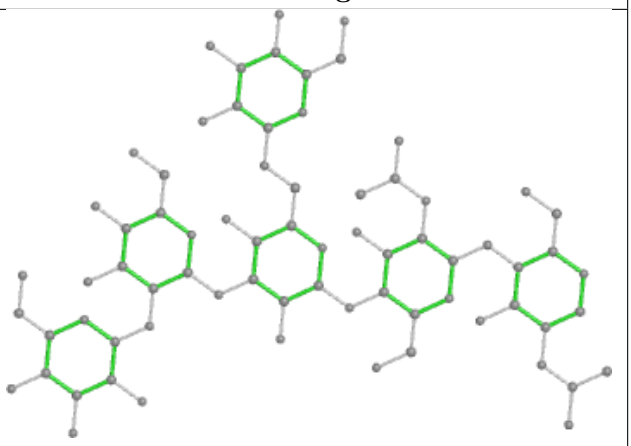
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	5	0
2	D	6	MAN	1	0
3	O	2	NAG	2	0
3	F	1	NAG	1	0
2	N	2	NAG	2	0
3	E	1	NAG	11	0
3	E	2	NAG	1	0
2	I	6	MAN	1	0
3	L	1	NAG	5	0
3	P	2	NAG	1	0
3	G	2	NAG	1	0
2	N	5	MAN	1	0
2	I	2	NAG	2	0
3	Q	2	NAG	5	0
3	L	2	NAG	1	0
2	D	5	MAN	5	0
2	D	2	NAG	2	0
3	P	1	NAG	1	0
3	Q	1	NAG	6	0
2	D	1	NAG	1	0
3	F	2	NAG	2	0
3	G	1	NAG	5	0
2	N	1	NAG	1	0

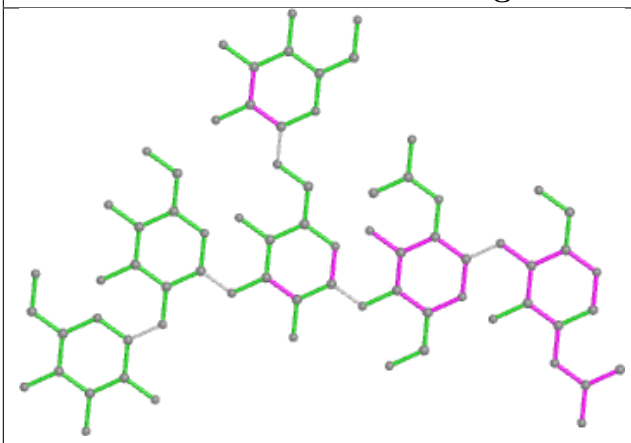
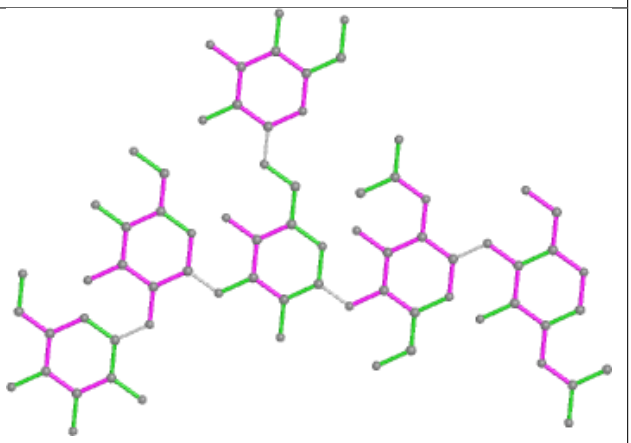
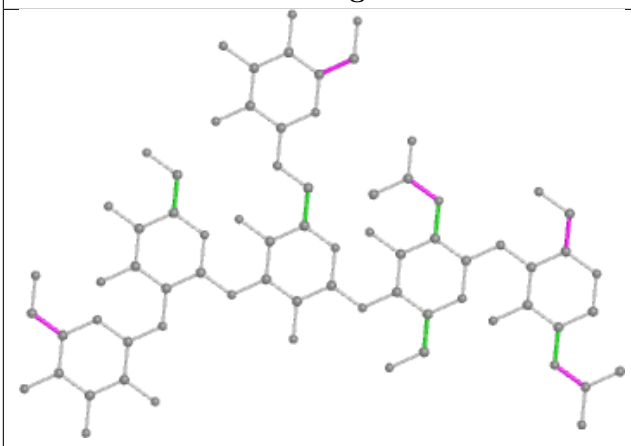
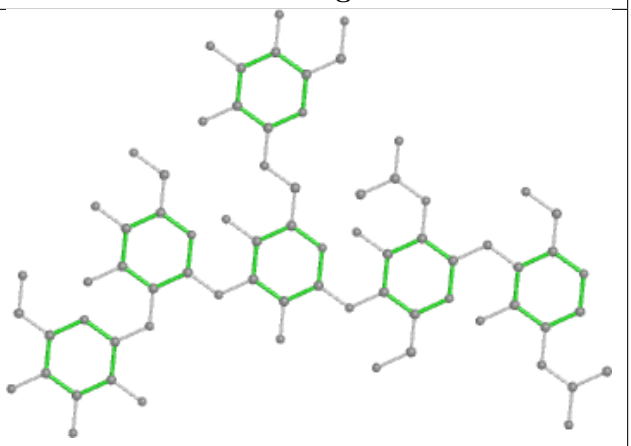
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

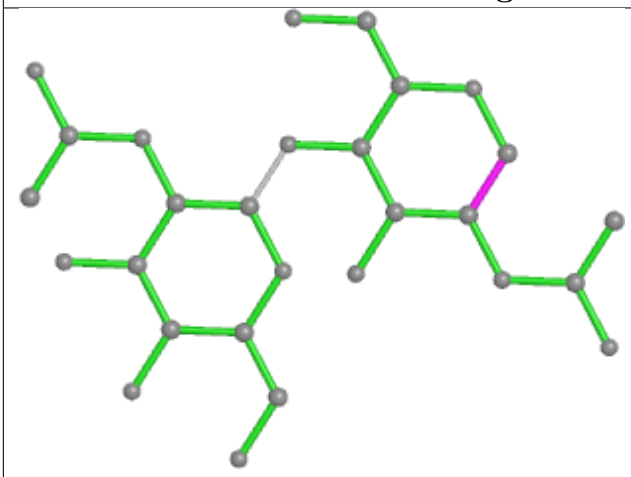
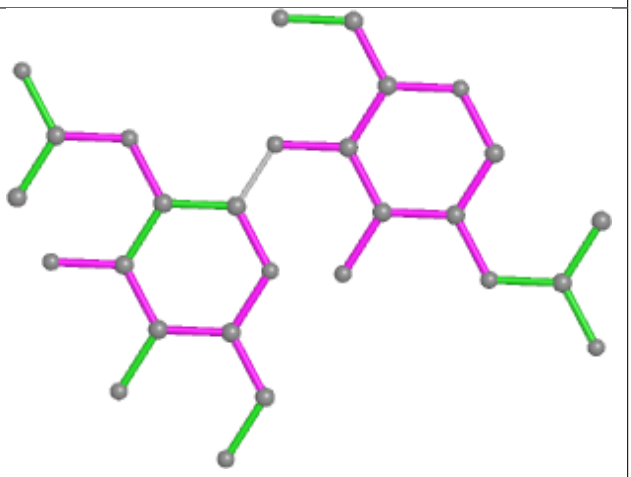
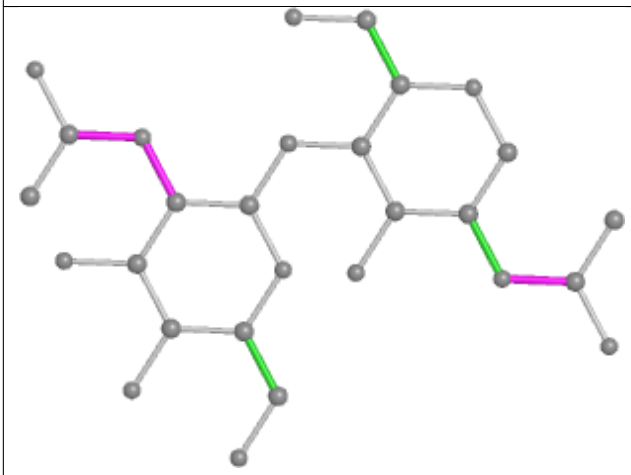
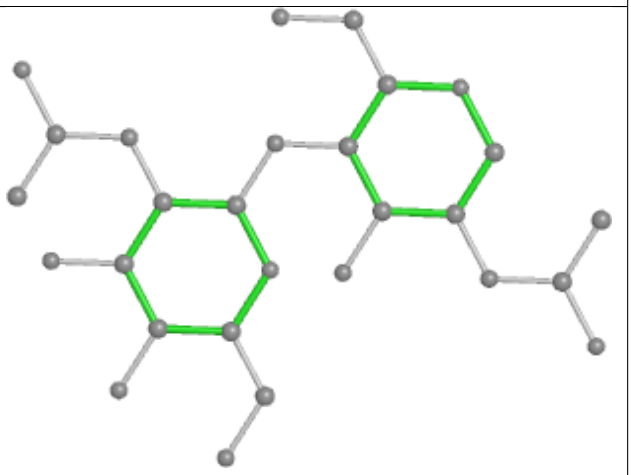
bond angles, torsion angles, and ring geometry for oligosaccharide.

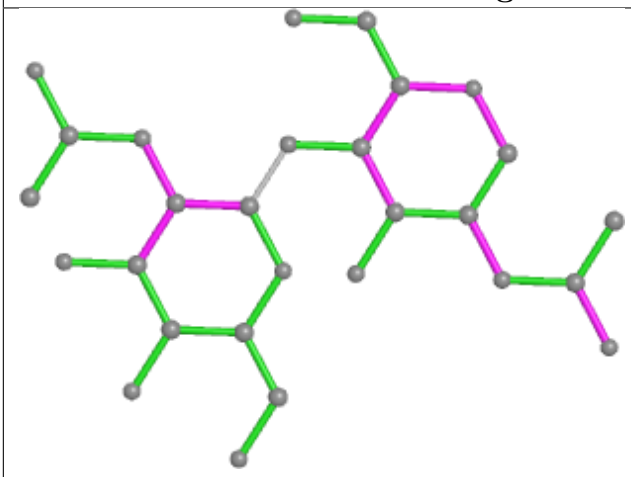
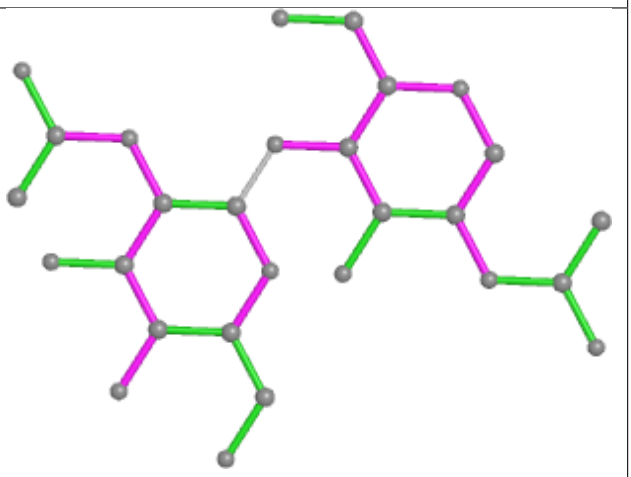
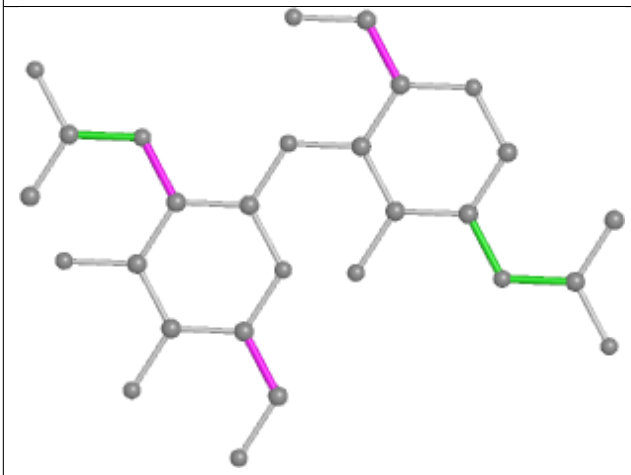
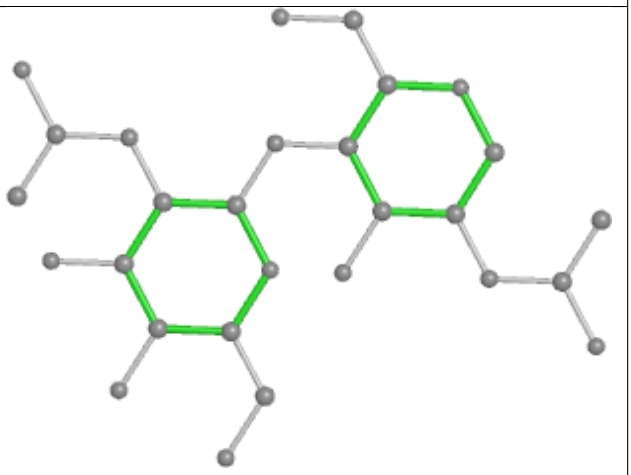
Oligosaccharide Chain D

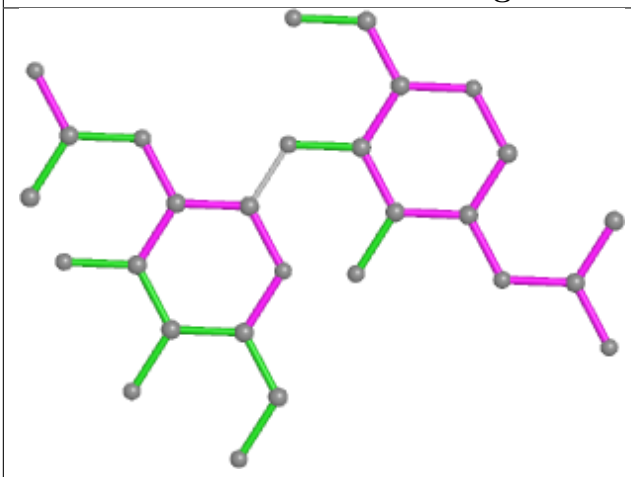
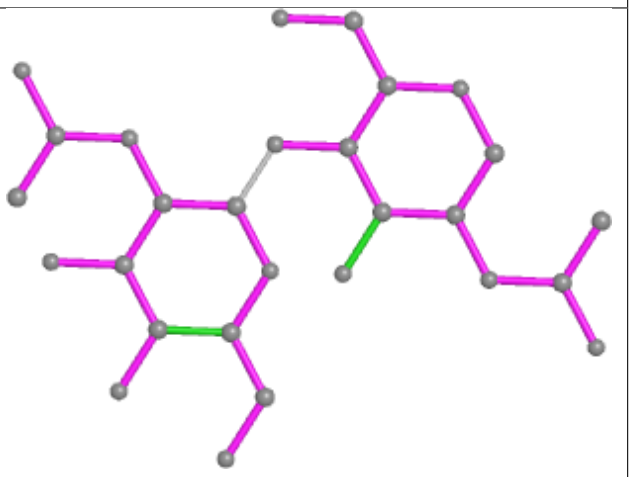
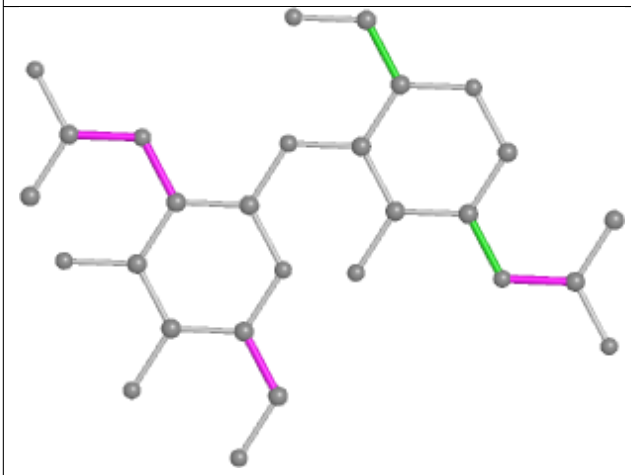
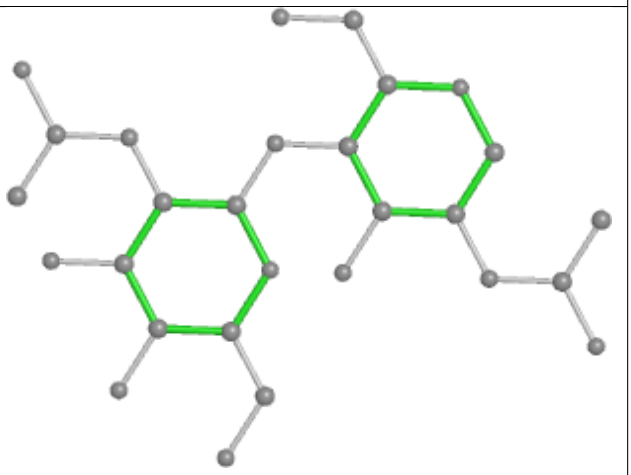


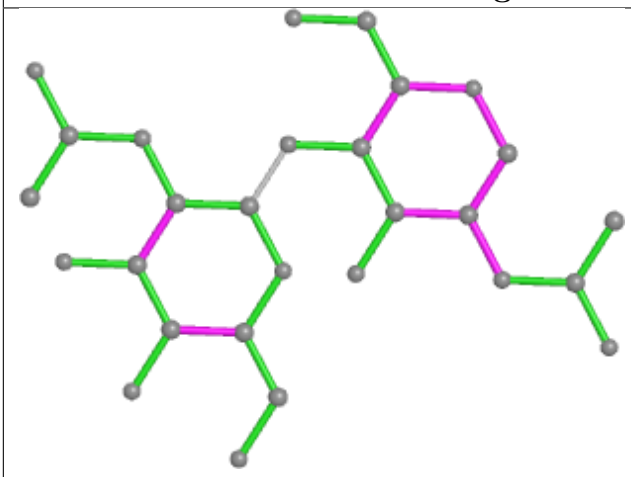
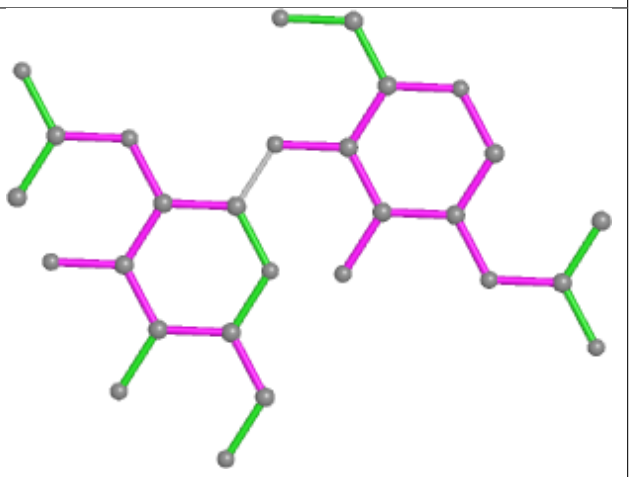
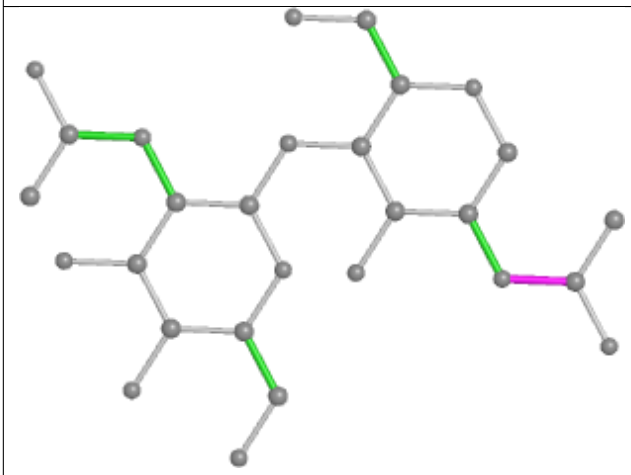
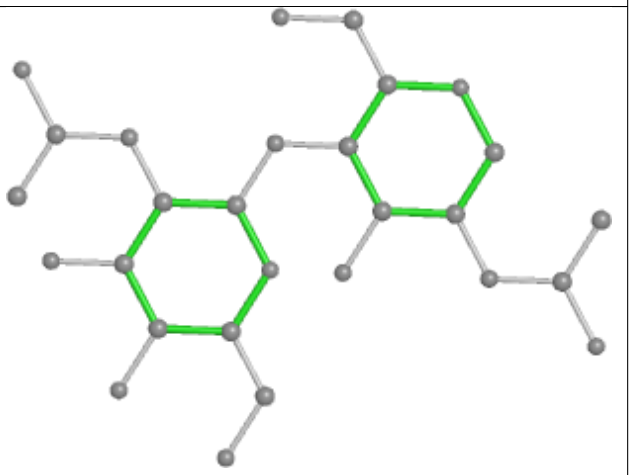
Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

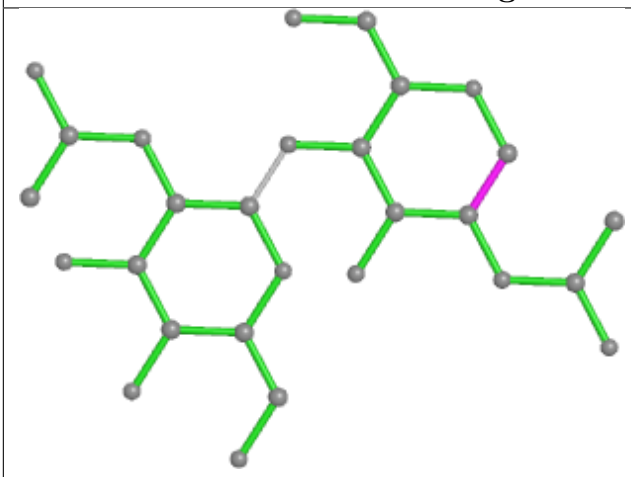
Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

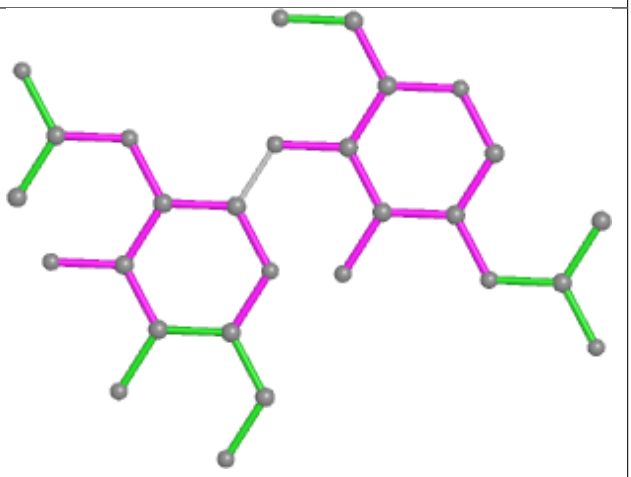
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

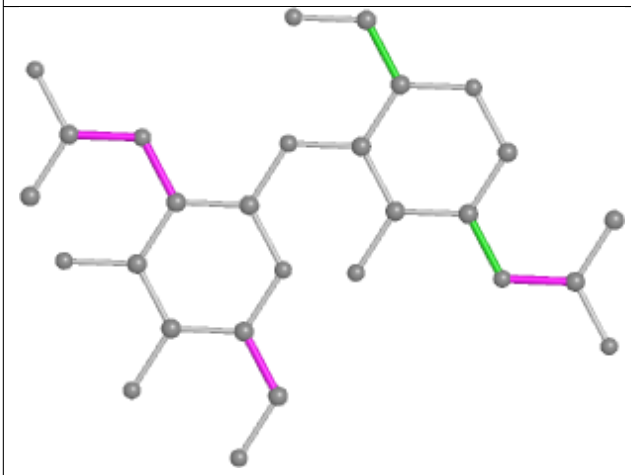
Oligosaccharide Chain J



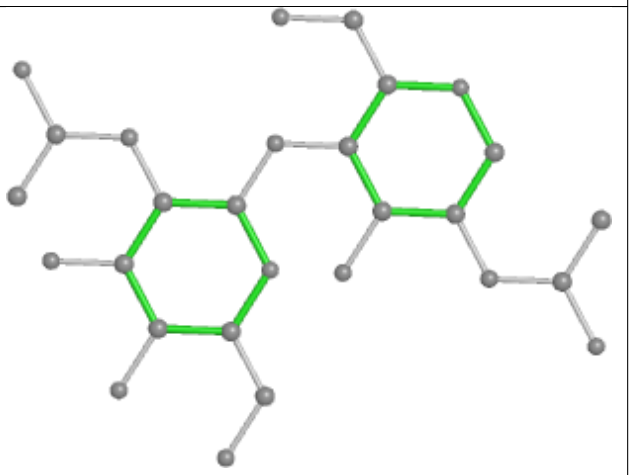
Bond lengths



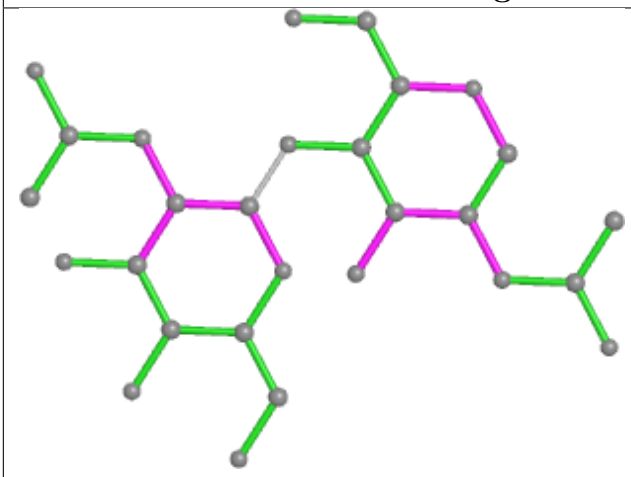
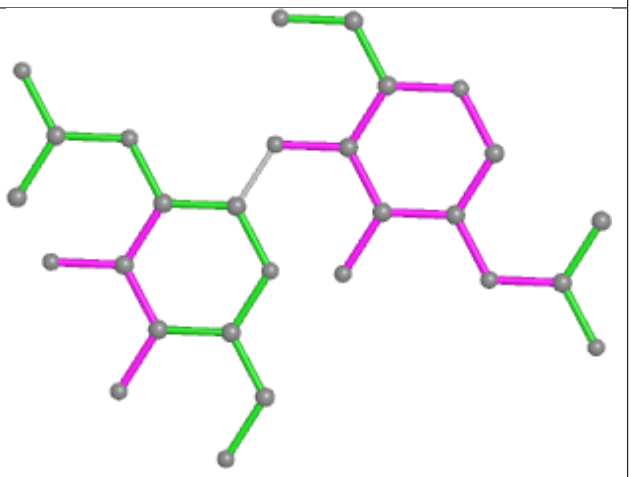
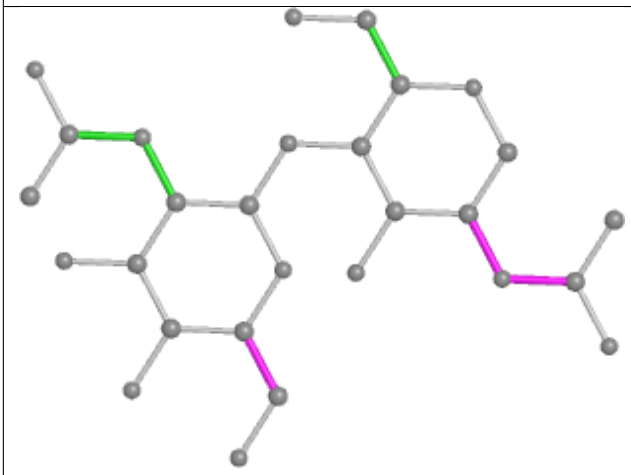
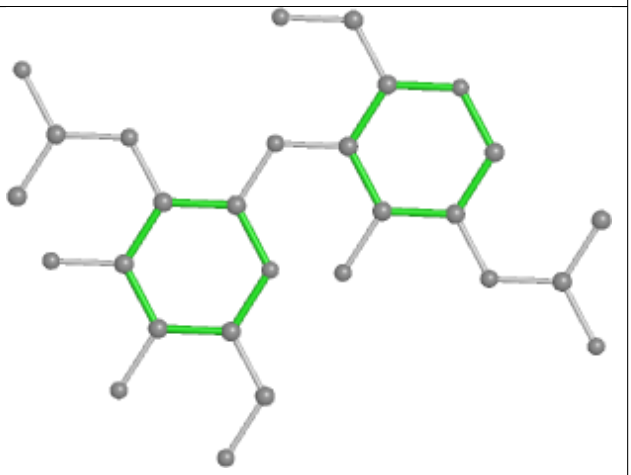
Bond angles

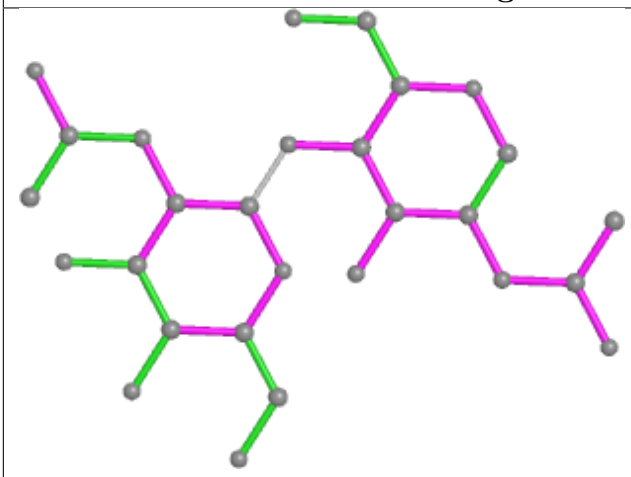
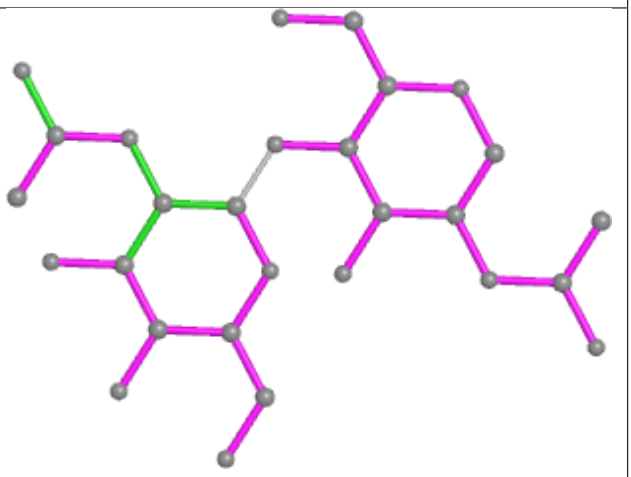
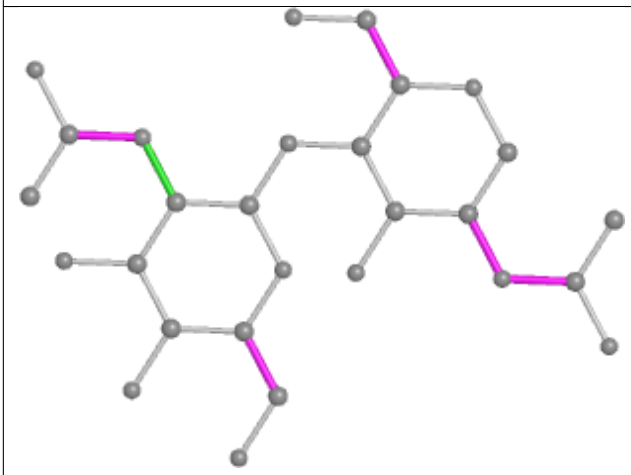
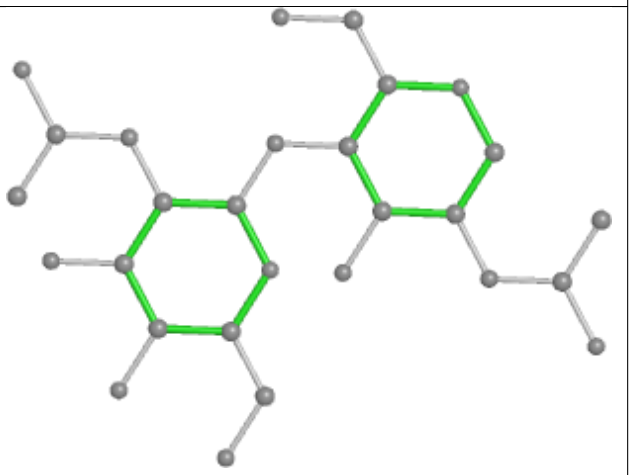


Torsions

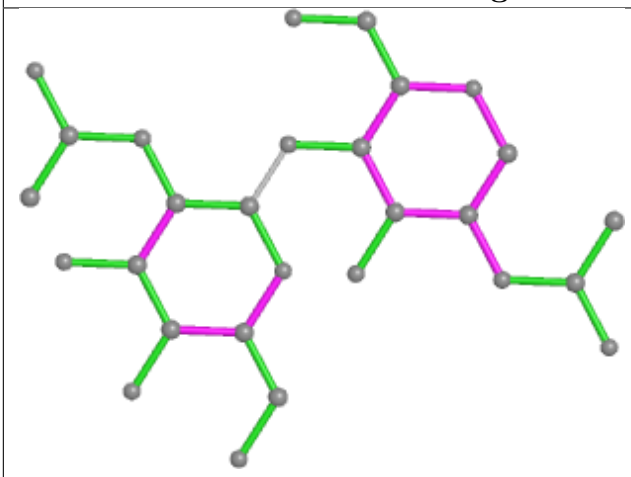


Rings

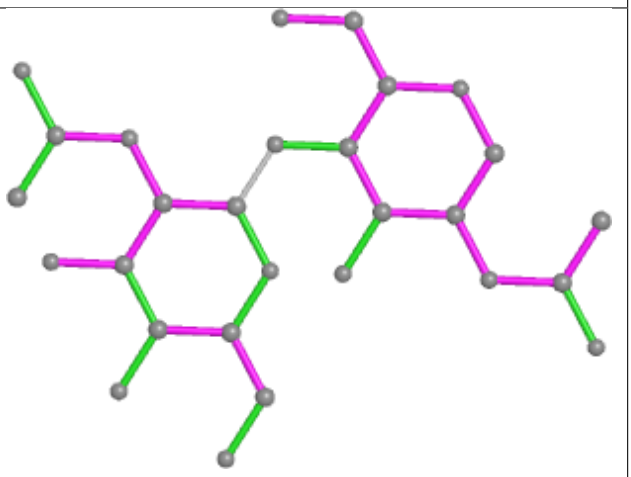
Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

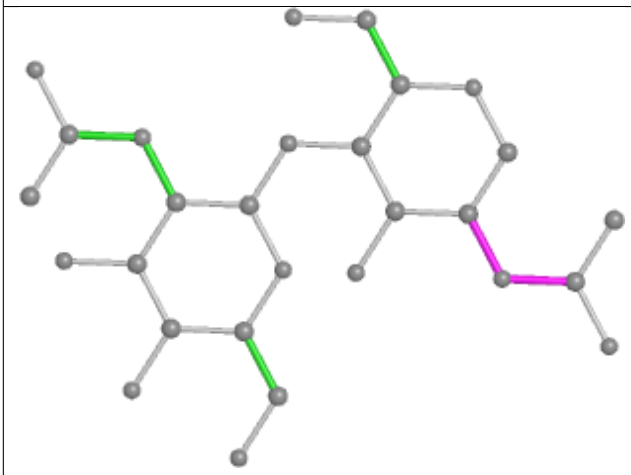
Oligosaccharide Chain M



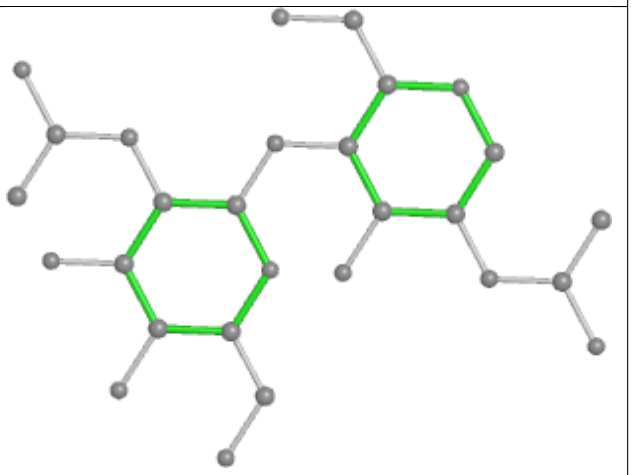
Bond lengths



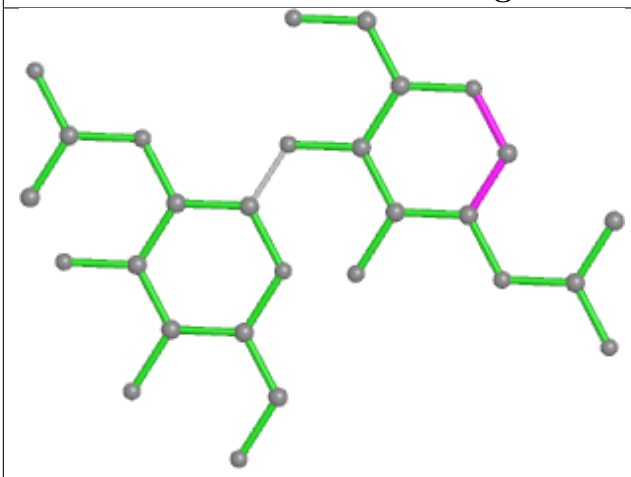
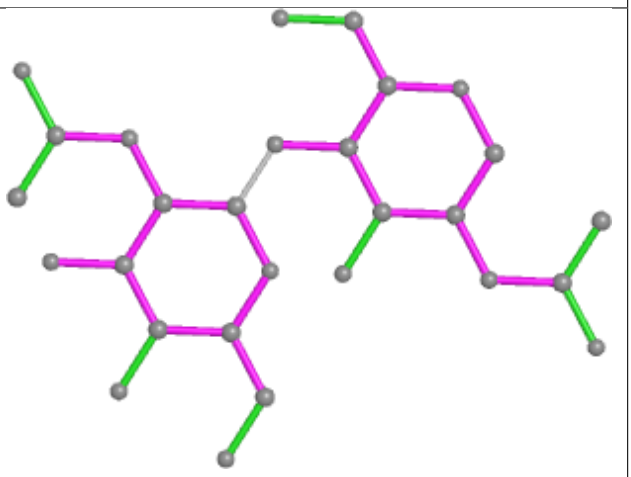
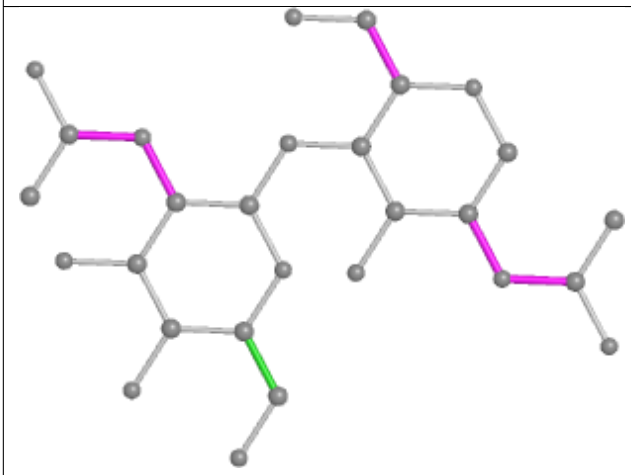
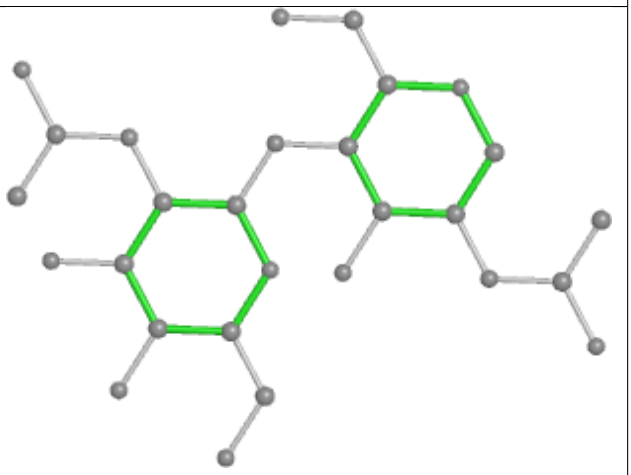
Bond angles

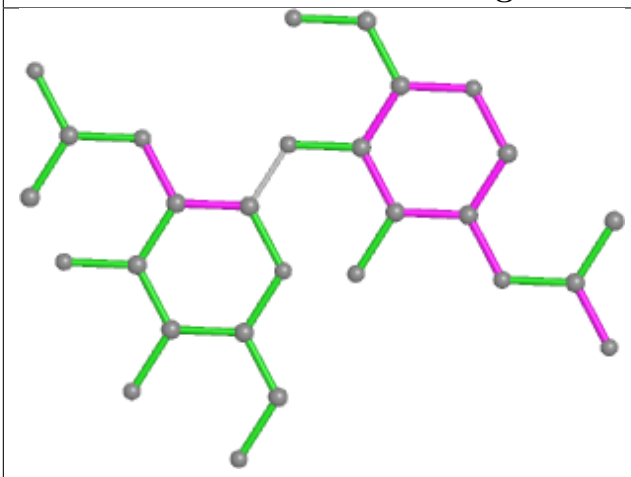
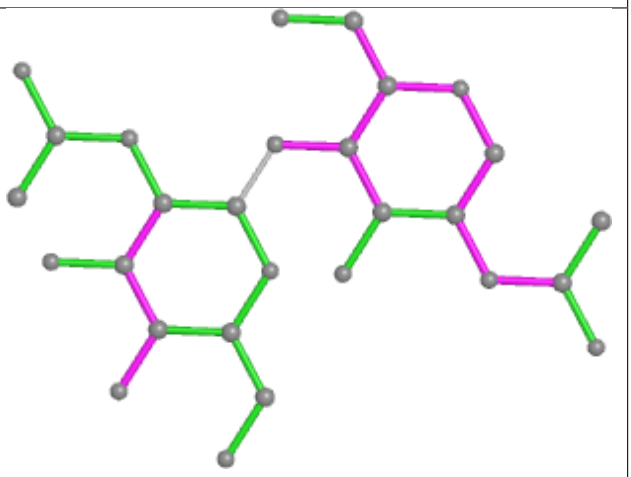
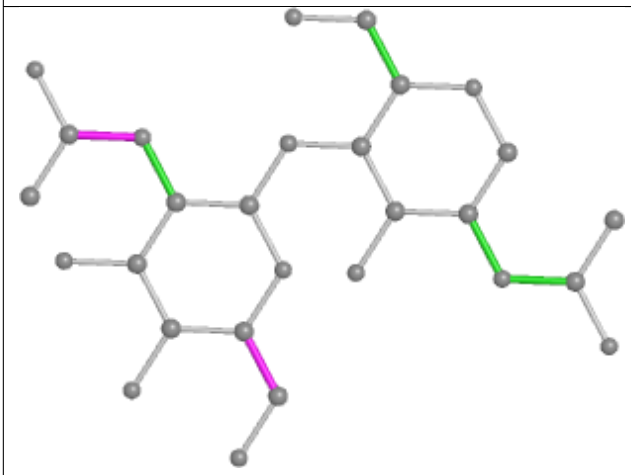
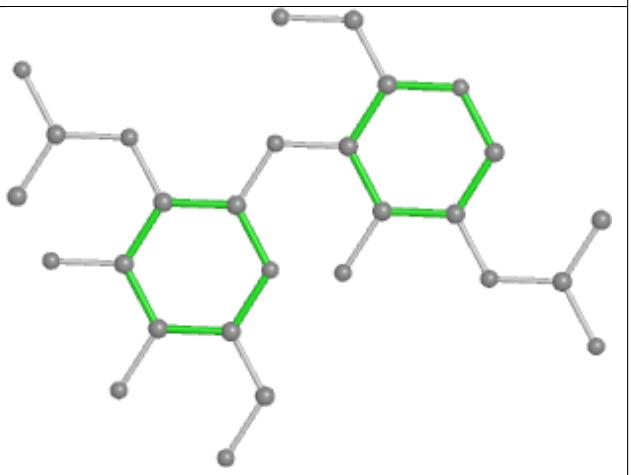


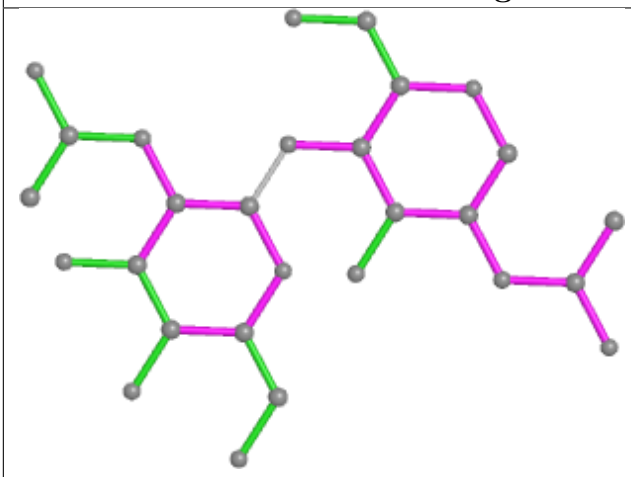
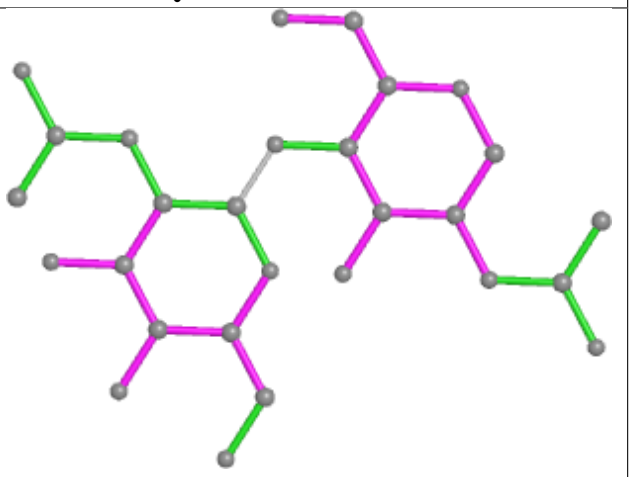
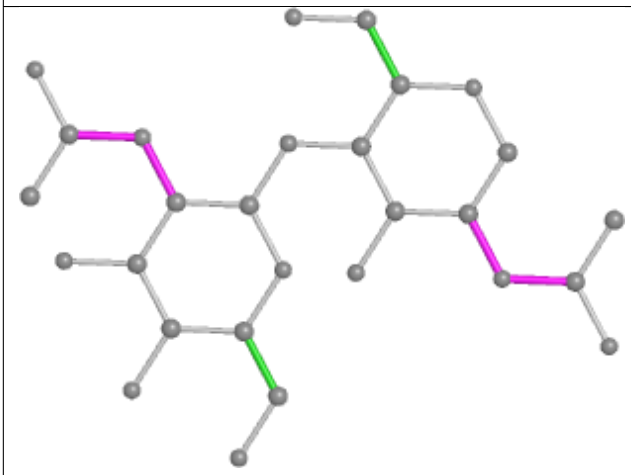
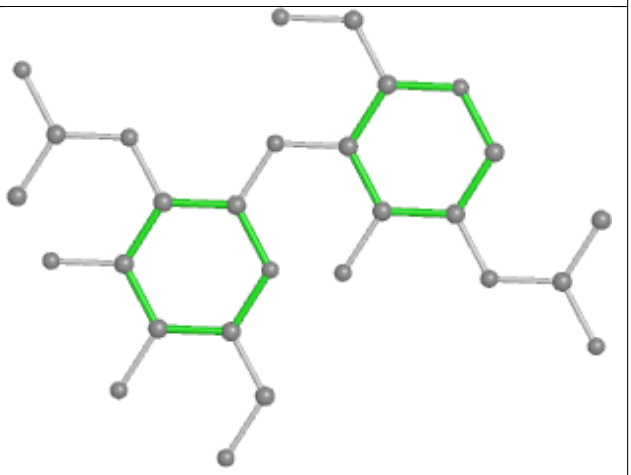
Torsions



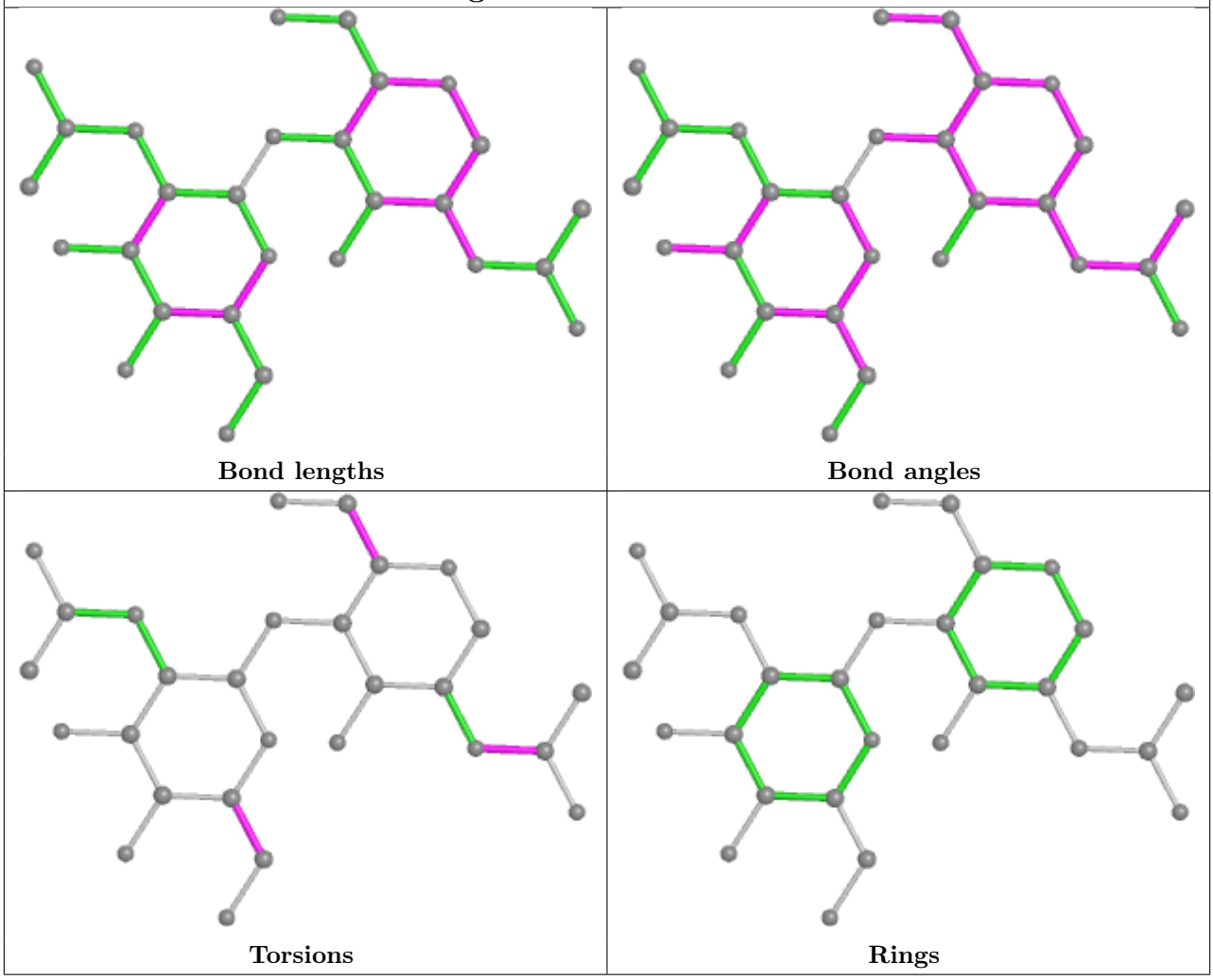
Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R



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	A	1408	-	14,14,15	1.64	1 (7%)	17,19,21	1.80	6 (35%)
4	NAG	B	1423	-	14,14,15	2.10	5 (35%)	17,19,21	4.54	9 (52%)
4	NAG	A	1411	-	14,14,15	2.30	3 (21%)	17,19,21	3.21	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1416	-	14,14,15	1.90	1 (7%)	17,19,21	2.67	5 (29%)
4	NAG	B	1427	-	14,14,15	1.77	3 (21%)	17,19,21	4.32	6 (35%)
4	NAG	B	1412	-	14,14,15	1.47	1 (7%)	17,19,21	2.44	3 (17%)
4	NAG	B	1421	-	14,14,15	1.77	3 (21%)	17,19,21	2.42	7 (41%)
4	NAG	C	1412	-	14,14,15	1.76	2 (14%)	17,19,21	2.58	7 (41%)
4	NAG	C	1416	-	14,14,15	1.14	1 (7%)	17,19,21	1.80	3 (17%)
4	NAG	B	1417	-	14,14,15	1.20	2 (14%)	17,19,21	2.29	5 (29%)
4	NAG	A	1420	-	14,14,15	1.74	6 (42%)	17,19,21	2.86	7 (41%)
4	NAG	A	1426	-	14,14,15	1.39	1 (7%)	17,19,21	3.38	8 (47%)
4	NAG	C	1420	-	14,14,15	1.81	5 (35%)	17,19,21	3.00	8 (47%)
4	NAG	C	1401	-	14,14,15	1.65	1 (7%)	17,19,21	2.44	6 (35%)
4	NAG	C	1413	-	14,14,15	2.41	2 (14%)	17,19,21	3.07	12 (70%)
4	NAG	C	1421	-	14,14,15	1.60	4 (28%)	17,19,21	2.80	4 (23%)
4	NAG	B	1413	-	14,14,15	2.74	6 (42%)	17,19,21	3.25	6 (35%)
4	NAG	C	1411	-	14,14,15	2.20	4 (28%)	17,19,21	3.35	10 (58%)
4	NAG	A	1412	-	14,14,15	1.85	2 (14%)	17,19,21	3.25	5 (29%)
4	NAG	B	1422	-	14,14,15	1.83	4 (28%)	17,19,21	2.99	7 (41%)
4	NAG	A	1423	-	14,14,15	2.18	4 (28%)	17,19,21	4.16	9 (52%)
4	NAG	C	1408	-	14,14,15	1.06	1 (7%)	17,19,21	2.03	4 (23%)
4	NAG	B	1408	-	14,14,15	1.10	1 (7%)	17,19,21	2.11	4 (23%)
4	NAG	B	1411	-	14,14,15	2.24	3 (21%)	17,19,21	3.14	11 (64%)
4	NAG	C	1427	1	14,14,15	1.14	1 (7%)	17,19,21	3.11	8 (47%)
4	NAG	A	1422	-	14,14,15	2.00	3 (21%)	17,19,21	3.42	9 (52%)
4	NAG	A	1416	-	14,14,15	1.91	1 (7%)	17,19,21	2.90	6 (35%)
4	NAG	C	1423	-	14,14,15	2.03	4 (28%)	17,19,21	4.36	9 (52%)
4	NAG	A	1427	-	14,14,15	1.65	4 (28%)	17,19,21	4.01	8 (47%)
4	NAG	A	1421	-	14,14,15	1.76	3 (21%)	17,19,21	2.79	6 (35%)
4	NAG	C	1417	-	14,14,15	1.17	2 (14%)	17,19,21	2.37	6 (35%)
4	NAG	B	1420	-	14,14,15	1.79	6 (42%)	17,19,21	2.97	8 (47%)
4	NAG	A	1417	-	14,14,15	1.43	2 (14%)	17,19,21	2.33	5 (29%)
4	NAG	C	1426	-	14,14,15	1.72	4 (28%)	17,19,21	1.82	5 (29%)
4	NAG	A	1401	-	14,14,15	1.03	1 (7%)	17,19,21	2.85	7 (41%)
4	NAG	A	1413	-	14,14,15	2.26	5 (35%)	17,19,21	3.46	5 (29%)
4	NAG	B	1426	-	14,14,15	1.40	2 (14%)	17,19,21	4.12	8 (47%)
4	NAG	C	1422	-	14,14,15	1.91	3 (21%)	17,19,21	3.24	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1401	-	14,14,15	1.25	1 (7%)	17,19,21	2.90	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1408	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1423	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1416	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1427	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1412	-	-	5/6/23/26	0/1/1/1
4	NAG	B	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1412	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1416	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1417	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1420	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1426	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1420	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1413	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1413	-	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	C	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1412	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1422	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1423	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1408	-	-	5/6/23/26	0/1/1/1
4	NAG	B	1411	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1427	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1422	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1416	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1423	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1427	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1421	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1417	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1420	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1417	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1426	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1413	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1426	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1422	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	-	-	4/6/23/26	0/1/1/1

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1413	NAG	C1-C2	8.31	1.64	1.52
4	A	1411	NAG	C1-C2	6.75	1.62	1.52
4	B	1411	NAG	C1-C2	6.46	1.62	1.52
4	B	1416	NAG	C1-C2	6.33	1.61	1.52
4	C	1411	NAG	C1-C2	6.21	1.61	1.52
4	A	1416	NAG	C1-C2	6.09	1.61	1.52
4	B	1413	NAG	C3-C2	-6.03	1.39	1.52
4	C	1412	NAG	C1-C2	5.75	1.60	1.52
4	A	1413	NAG	C1-C2	5.67	1.60	1.52
4	A	1412	NAG	C1-C2	5.59	1.60	1.52
4	C	1401	NAG	C1-C2	5.45	1.60	1.52
4	A	1408	NAG	C1-C2	5.38	1.60	1.52
4	B	1413	NAG	C1-C2	5.30	1.60	1.52
4	B	1412	NAG	C1-C2	4.97	1.59	1.52
4	A	1422	NAG	C1-C2	4.69	1.59	1.52
4	B	1427	NAG	C1-C2	4.66	1.59	1.52
4	A	1423	NAG	C1-C2	4.50	1.59	1.52
4	A	1423	NAG	O5-C1	-4.48	1.36	1.43
4	A	1421	NAG	C1-C2	4.47	1.59	1.52
4	C	1423	NAG	O5-C1	-4.42	1.36	1.43
4	A	1426	NAG	C1-C2	4.32	1.58	1.52
4	C	1422	NAG	C1-C2	4.29	1.58	1.52
4	B	1421	NAG	C1-C2	4.25	1.58	1.52
4	B	1423	NAG	C1-C2	4.13	1.58	1.52
4	A	1417	NAG	C1-C2	4.07	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1413	NAG	C4-C3	-4.03	1.42	1.52
4	A	1427	NAG	C1-C2	4.02	1.58	1.52
4	B	1423	NAG	O5-C1	-3.98	1.37	1.43
4	B	1401	NAG	C1-C2	3.96	1.58	1.52
4	C	1421	NAG	C1-C2	3.80	1.58	1.52
4	C	1426	NAG	C1-C2	3.69	1.57	1.52
4	C	1416	NAG	C1-C2	3.58	1.57	1.52
4	B	1408	NAG	C1-C2	3.54	1.57	1.52
4	B	1426	NAG	C1-C2	3.51	1.57	1.52
4	C	1423	NAG	C1-C2	3.38	1.57	1.52
4	A	1422	NAG	C3-C2	-3.37	1.45	1.52
4	B	1422	NAG	C1-C2	3.32	1.57	1.52
4	C	1408	NAG	C1-C2	3.30	1.57	1.52
4	B	1417	NAG	C1-C2	3.16	1.57	1.52
4	B	1422	NAG	C3-C2	-3.14	1.45	1.52
4	B	1423	NAG	O5-C5	-3.11	1.37	1.43
4	A	1427	NAG	C2-N2	-3.08	1.41	1.46
4	A	1413	NAG	C2-N2	-3.02	1.41	1.46
4	C	1422	NAG	C3-C2	-3.01	1.46	1.52
4	A	1420	NAG	C1-C2	3.01	1.56	1.52
4	A	1413	NAG	C3-C2	-3.00	1.46	1.52
4	B	1427	NAG	O5-C1	-2.96	1.39	1.43
4	C	1420	NAG	O5-C1	-2.90	1.39	1.43
4	B	1420	NAG	O5-C5	-2.90	1.37	1.43
4	B	1422	NAG	C2-N2	-2.90	1.41	1.46
4	B	1420	NAG	O5-C1	-2.88	1.39	1.43
4	C	1420	NAG	C1-C2	2.87	1.56	1.52
4	C	1420	NAG	O5-C5	-2.86	1.37	1.43
4	A	1413	NAG	O5-C5	-2.86	1.37	1.43
4	B	1421	NAG	O5-C1	-2.85	1.39	1.43
4	C	1422	NAG	C2-N2	-2.84	1.41	1.46
4	C	1417	NAG	C1-C2	2.84	1.56	1.52
4	A	1412	NAG	C2-N2	-2.81	1.41	1.46
4	A	1422	NAG	C2-N2	-2.80	1.41	1.46
4	C	1423	NAG	O5-C5	-2.72	1.37	1.43
4	C	1426	NAG	O5-C1	-2.71	1.39	1.43
4	B	1413	NAG	C2-N2	-2.64	1.41	1.46
4	A	1423	NAG	O5-C5	-2.62	1.38	1.43
4	B	1420	NAG	C2-N2	-2.59	1.41	1.46
4	B	1420	NAG	C1-C2	2.57	1.56	1.52
4	C	1413	NAG	O5-C5	-2.53	1.38	1.43
4	C	1420	NAG	C2-N2	-2.52	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1420	NAG	C2-N2	-2.52	1.42	1.46
4	A	1401	NAG	C1-C2	2.50	1.56	1.52
4	C	1423	NAG	C4-C5	-2.49	1.47	1.53
4	B	1423	NAG	O7-C7	-2.47	1.17	1.23
4	B	1413	NAG	O3-C3	-2.45	1.37	1.43
4	B	1421	NAG	O5-C5	-2.44	1.38	1.43
4	C	1427	NAG	C2-N2	-2.42	1.42	1.46
4	A	1420	NAG	O5-C5	-2.42	1.38	1.43
4	B	1426	NAG	O5-C5	-2.42	1.38	1.43
4	A	1421	NAG	O5-C1	-2.39	1.39	1.43
4	B	1411	NAG	O5-C1	-2.37	1.39	1.43
4	C	1417	NAG	C2-N2	-2.34	1.42	1.46
4	A	1413	NAG	C4-C5	-2.34	1.48	1.53
4	C	1411	NAG	O5-C1	-2.33	1.40	1.43
4	B	1417	NAG	C2-N2	-2.31	1.42	1.46
4	B	1423	NAG	C4-C5	-2.30	1.48	1.53
4	A	1421	NAG	O5-C5	-2.26	1.38	1.43
4	A	1420	NAG	O5-C1	-2.24	1.40	1.43
4	B	1422	NAG	O5-C1	-2.23	1.40	1.43
4	C	1420	NAG	C3-C2	-2.23	1.47	1.52
4	A	1417	NAG	C2-N2	-2.22	1.42	1.46
4	A	1420	NAG	C3-C2	-2.22	1.47	1.52
4	A	1411	NAG	O5-C1	-2.19	1.40	1.43
4	B	1427	NAG	C2-N2	-2.19	1.42	1.46
4	C	1411	NAG	C4-C5	-2.18	1.48	1.53
4	C	1426	NAG	O5-C5	-2.18	1.39	1.43
4	B	1420	NAG	C3-C2	-2.17	1.47	1.52
4	A	1423	NAG	O7-C7	-2.16	1.18	1.23
4	A	1411	NAG	O5-C5	-2.16	1.39	1.43
4	C	1411	NAG	C2-N2	-2.15	1.42	1.46
4	B	1413	NAG	O5-C1	2.12	1.47	1.43
4	C	1421	NAG	O5-C5	-2.12	1.39	1.43
4	C	1421	NAG	C2-N2	-2.09	1.42	1.46
4	B	1411	NAG	C2-N2	-2.09	1.42	1.46
4	A	1427	NAG	O7-C7	-2.08	1.18	1.23
4	C	1421	NAG	O5-C1	-2.08	1.40	1.43
4	B	1420	NAG	C4-C5	-2.07	1.48	1.53
4	C	1412	NAG	O5-C1	-2.06	1.40	1.43
4	A	1420	NAG	C4-C5	-2.03	1.48	1.53
4	A	1427	NAG	C4-C3	-2.01	1.47	1.52
4	C	1426	NAG	C3-C2	-2.00	1.48	1.52

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1426	NAG	O5-C1-C2	-12.70	91.23	111.29
4	A	1427	NAG	O5-C1-C2	-10.90	94.08	111.29
4	A	1412	NAG	C2-N2-C7	-10.78	107.56	122.90
4	B	1423	NAG	O5-C1-C2	-9.84	95.76	111.29
4	A	1423	NAG	O5-C1-C2	-9.78	95.85	111.29
4	B	1427	NAG	C2-N2-C7	-9.77	109.00	122.90
4	C	1423	NAG	C2-N2-C7	-9.50	109.38	122.90
4	B	1427	NAG	C4-C3-C2	-9.35	97.31	111.02
4	A	1426	NAG	O5-C1-C2	-9.12	96.88	111.29
4	B	1420	NAG	C1-C2-N2	-8.87	95.34	110.49
4	C	1423	NAG	O5-C1-C2	-8.74	97.49	111.29
4	A	1411	NAG	C1-O5-C5	8.61	123.85	112.19
4	C	1411	NAG	C1-O5-C5	8.36	123.52	112.19
4	B	1413	NAG	C4-C3-C2	8.34	123.24	111.02
4	B	1423	NAG	C2-N2-C7	-8.26	111.14	122.90
4	C	1427	NAG	O5-C1-C2	-8.18	98.37	111.29
4	B	1427	NAG	O5-C1-C2	-8.08	98.53	111.29
4	B	1411	NAG	C1-O5-C5	7.97	122.98	112.19
4	C	1420	NAG	C1-C2-N2	-7.94	96.92	110.49
4	B	1423	NAG	C4-C3-C2	-7.77	99.63	111.02
4	A	1413	NAG	C1-C2-N2	-7.74	97.27	110.49
4	B	1401	NAG	O5-C1-C2	-7.72	99.09	111.29
4	A	1423	NAG	C4-C3-C2	-7.66	99.79	111.02
4	A	1416	NAG	O5-C1-C2	-7.64	99.23	111.29
4	B	1426	NAG	C1-O5-C5	7.57	122.45	112.19
4	C	1423	NAG	C4-C3-C2	-7.57	99.93	111.02
4	C	1413	NAG	C1-C2-N2	-7.56	97.57	110.49
4	A	1423	NAG	C2-N2-C7	-7.53	112.18	122.90
4	A	1413	NAG	C1-O5-C5	7.48	122.32	112.19
4	A	1401	NAG	O5-C1-C2	-7.38	99.63	111.29
4	B	1412	NAG	O5-C5-C6	7.38	118.78	107.20
4	B	1413	NAG	C3-C4-C5	-7.27	97.27	110.24
4	C	1411	NAG	O5-C1-C2	-7.18	99.95	111.29
4	C	1422	NAG	C1-O5-C5	7.12	121.84	112.19
4	A	1427	NAG	C2-N2-C7	-6.91	113.07	122.90
4	C	1401	NAG	O5-C1-C2	-6.88	100.42	111.29
4	B	1416	NAG	O5-C1-C2	-6.84	100.48	111.29
4	C	1412	NAG	O4-C4-C3	-6.80	94.64	110.35
4	A	1422	NAG	C1-O5-C5	6.75	121.33	112.19
4	C	1421	NAG	O5-C1-C2	-6.61	100.85	111.29
4	A	1417	NAG	O5-C1-C2	-6.31	101.33	111.29
4	B	1408	NAG	O5-C1-C2	-6.29	101.36	111.29
4	B	1417	NAG	O5-C1-C2	-6.28	101.37	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1421	NAG	C2-N2-C7	-6.28	113.97	122.90
4	C	1417	NAG	O5-C1-C2	-6.27	101.39	111.29
4	A	1422	NAG	C1-C2-N2	-6.25	99.81	110.49
4	A	1413	NAG	O5-C1-C2	-6.13	101.61	111.29
4	C	1408	NAG	O5-C1-C2	-6.10	101.66	111.29
4	B	1411	NAG	O5-C1-C2	-6.09	101.67	111.29
4	C	1422	NAG	O5-C1-C2	-6.07	101.70	111.29
4	B	1422	NAG	O3-C3-C2	-6.06	96.92	109.47
4	B	1423	NAG	C6-C5-C4	-6.06	98.81	113.00
4	A	1421	NAG	O5-C1-C2	-6.05	101.74	111.29
4	A	1426	NAG	C3-C4-C5	-6.04	99.47	110.24
4	B	1423	NAG	C1-O5-C5	6.02	120.35	112.19
4	A	1427	NAG	C1-O5-C5	6.02	120.34	112.19
4	A	1421	NAG	C2-N2-C7	-6.02	114.33	122.90
4	A	1411	NAG	O5-C1-C2	-6.01	101.80	111.29
4	A	1420	NAG	C1-C2-N2	-6.01	100.23	110.49
4	A	1422	NAG	O3-C3-C2	-5.85	97.36	109.47
4	A	1420	NAG	O5-C1-C2	-5.83	102.08	111.29
4	C	1423	NAG	C6-C5-C4	-5.77	99.50	113.00
4	A	1401	NAG	C2-N2-C7	-5.72	114.77	122.90
4	C	1420	NAG	O5-C1-C2	-5.34	102.85	111.29
4	A	1426	NAG	O5-C5-C6	5.34	115.57	107.20
4	A	1423	NAG	C1-O5-C5	5.30	119.37	112.19
4	A	1422	NAG	O5-C1-C2	-5.22	103.04	111.29
4	B	1422	NAG	O5-C5-C6	5.10	115.20	107.20
4	A	1423	NAG	C6-C5-C4	-5.00	101.30	113.00
4	B	1427	NAG	C1-C2-N2	4.99	119.01	110.49
4	A	1412	NAG	O5-C1-C2	-4.95	103.47	111.29
4	C	1427	NAG	C2-N2-C7	-4.88	115.96	122.90
4	C	1426	NAG	C1-C2-N2	-4.78	102.32	110.49
4	A	1427	NAG	C4-C3-C2	-4.78	104.01	111.02
4	C	1422	NAG	C1-C2-N2	-4.76	102.36	110.49
4	B	1421	NAG	C2-N2-C7	-4.71	116.20	122.90
4	C	1422	NAG	O3-C3-C2	-4.69	99.76	109.47
4	B	1421	NAG	O5-C1-C2	-4.62	103.99	111.29
4	B	1412	NAG	O5-C1-C2	-4.61	104.00	111.29
4	C	1423	NAG	C1-O5-C5	4.61	118.44	112.19
4	A	1416	NAG	C1-O5-C5	4.61	118.43	112.19
4	A	1420	NAG	C2-N2-C7	-4.60	116.35	122.90
4	B	1423	NAG	O5-C5-C6	-4.58	100.03	107.20
4	A	1401	NAG	C4-C3-C2	-4.56	104.33	111.02
4	C	1427	NAG	O4-C4-C3	-4.54	99.86	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1417	NAG	C2-N2-C7	-4.50	116.49	122.90
4	B	1422	NAG	O5-C1-C2	-4.47	104.23	111.29
4	B	1427	NAG	O5-C5-C6	-4.46	100.21	107.20
4	B	1422	NAG	C1-O5-C5	4.44	118.20	112.19
4	B	1426	NAG	C3-C4-C5	-4.42	102.35	110.24
4	B	1401	NAG	C2-N2-C7	-4.41	116.62	122.90
4	B	1417	NAG	C2-N2-C7	-4.41	116.63	122.90
4	C	1420	NAG	C4-C3-C2	-4.40	104.56	111.02
4	B	1401	NAG	C1-C2-N2	4.39	117.98	110.49
4	C	1412	NAG	C2-N2-C7	4.33	129.06	122.90
4	A	1413	NAG	C2-N2-C7	-4.31	116.76	122.90
4	B	1416	NAG	C1-O5-C5	4.31	118.03	112.19
4	C	1416	NAG	C4-C3-C2	-4.28	104.75	111.02
4	B	1420	NAG	O5-C1-C2	-4.27	104.55	111.29
4	A	1420	NAG	C4-C3-C2	-4.24	104.81	111.02
4	A	1413	NAG	O4-C4-C5	-4.22	98.81	109.30
4	A	1416	NAG	O3-C3-C4	-4.19	100.67	110.35
4	B	1411	NAG	C6-C5-C4	-4.14	103.30	113.00
4	C	1413	NAG	C2-N2-C7	4.14	128.79	122.90
4	A	1417	NAG	C2-N2-C7	-4.11	117.06	122.90
4	C	1421	NAG	C4-C3-C2	-4.07	105.05	111.02
4	C	1416	NAG	O5-C1-C2	-4.00	104.98	111.29
4	C	1420	NAG	C2-N2-C7	-3.98	117.23	122.90
4	B	1413	NAG	O5-C5-C6	3.98	113.45	107.20
4	C	1427	NAG	C1-O5-C5	3.81	117.36	112.19
4	B	1416	NAG	O3-C3-C4	-3.81	101.53	110.35
4	C	1411	NAG	C6-C5-C4	-3.80	104.11	113.00
4	A	1422	NAG	O5-C5-C4	-3.79	101.60	110.83
4	A	1421	NAG	C1-O5-C5	3.74	117.26	112.19
4	B	1421	NAG	C1-O5-C5	3.73	117.24	112.19
4	B	1427	NAG	O4-C4-C3	-3.72	101.74	110.35
4	A	1421	NAG	C4-C3-C2	-3.72	105.57	111.02
4	C	1401	NAG	C1-C2-N2	3.70	116.80	110.49
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	A	1416	NAG	C2-N2-C7	-3.64	117.72	122.90
4	B	1401	NAG	C4-C3-C2	-3.63	105.70	111.02
4	C	1413	NAG	C1-O5-C5	3.62	117.09	112.19
4	B	1408	NAG	O5-C5-C6	3.60	112.84	107.20
4	C	1416	NAG	C2-N2-C7	-3.60	117.78	122.90
4	B	1416	NAG	C6-C5-C4	-3.57	104.64	113.00
4	C	1422	NAG	O5-C5-C4	-3.55	102.19	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1416	NAG	C4-C3-C2	-3.55	105.82	111.02
4	B	1413	NAG	C2-N2-C7	-3.55	117.85	122.90
4	B	1420	NAG	C2-N2-C7	-3.50	117.92	122.90
4	B	1422	NAG	C1-C2-N2	-3.49	104.52	110.49
4	C	1423	NAG	O7-C7-C8	-3.47	115.62	122.06
4	A	1411	NAG	O5-C5-C4	-3.46	102.40	110.83
4	C	1423	NAG	O5-C5-C6	-3.46	101.79	107.20
4	C	1411	NAG	C4-C3-C2	-3.45	105.97	111.02
4	A	1426	NAG	O6-C6-C5	-3.44	99.50	111.29
4	B	1426	NAG	C6-C5-C4	3.43	121.04	113.00
4	A	1408	NAG	O5-C5-C6	3.41	112.55	107.20
4	A	1408	NAG	O5-C1-C2	-3.40	105.93	111.29
4	B	1401	NAG	C1-O5-C5	3.31	116.68	112.19
4	C	1421	NAG	C1-O5-C5	3.31	116.67	112.19
4	C	1413	NAG	C8-C7-N2	3.31	121.70	116.10
4	A	1408	NAG	C2-N2-C7	3.30	127.61	122.90
4	B	1420	NAG	C4-C3-C2	-3.30	106.19	111.02
4	A	1423	NAG	O5-C5-C6	-3.26	102.09	107.20
4	B	1408	NAG	C1-O5-C5	3.26	116.61	112.19
4	A	1427	NAG	O4-C4-C3	-3.24	102.86	110.35
4	B	1423	NAG	C8-C7-N2	3.18	121.48	116.10
4	C	1422	NAG	O4-C4-C5	3.16	117.14	109.30
4	C	1423	NAG	C8-C7-N2	3.13	121.40	116.10
4	B	1422	NAG	O5-C5-C4	-3.12	103.24	110.83
4	A	1411	NAG	C6-C5-C4	-3.09	105.77	113.00
4	C	1408	NAG	O5-C5-C6	3.08	112.04	107.20
4	B	1417	NAG	C3-C4-C5	-3.08	104.75	110.24
4	A	1411	NAG	O3-C3-C4	-3.08	103.23	110.35
4	B	1413	NAG	C1-O5-C5	-3.06	108.05	112.19
4	A	1427	NAG	C6-C5-C4	-3.06	105.84	113.00
4	C	1411	NAG	O3-C3-C4	-3.06	103.28	110.35
4	A	1416	NAG	C6-C5-C4	-3.04	105.88	113.00
4	C	1411	NAG	O5-C5-C4	-3.04	103.43	110.83
4	B	1423	NAG	O4-C4-C3	3.03	117.36	110.35
4	B	1421	NAG	O3-C3-C4	-3.02	103.36	110.35
4	B	1423	NAG	O7-C7-C8	-3.00	116.49	122.06
4	A	1426	NAG	C6-C5-C4	2.99	120.02	113.00
4	A	1412	NAG	O4-C4-C3	-2.99	103.44	110.35
4	C	1408	NAG	C1-O5-C5	2.98	116.22	112.19
4	C	1412	NAG	C6-C5-C4	-2.96	106.07	113.00
4	B	1412	NAG	C3-C4-C5	-2.96	104.96	110.24
4	C	1427	NAG	C3-C4-C5	-2.96	104.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1413	NAG	O5-C5-C4	2.94	117.99	110.83
4	C	1413	NAG	O3-C3-C4	-2.93	103.56	110.35
4	C	1413	NAG	C6-C5-C4	2.93	119.87	113.00
4	B	1426	NAG	C4-C3-C2	-2.92	106.73	111.02
4	A	1422	NAG	C4-C3-C2	-2.90	106.77	111.02
4	B	1421	NAG	C4-C3-C2	-2.89	106.78	111.02
4	C	1417	NAG	C1-C2-N2	-2.87	105.58	110.49
4	C	1412	NAG	O3-C3-C4	-2.85	103.76	110.35
4	B	1426	NAG	O3-C3-C2	2.85	115.36	109.47
4	B	1422	NAG	C4-C3-C2	-2.84	106.85	111.02
4	A	1411	NAG	C4-C3-C2	-2.84	106.86	111.02
4	A	1422	NAG	O4-C4-C5	2.82	116.31	109.30
4	A	1411	NAG	C3-C4-C5	2.82	115.26	110.24
4	A	1427	NAG	O3-C3-C4	-2.80	103.87	110.35
4	B	1411	NAG	O3-C3-C4	-2.80	103.87	110.35
4	B	1411	NAG	O5-C5-C4	-2.76	104.11	110.83
4	C	1417	NAG	C1-O5-C5	2.75	115.91	112.19
4	C	1426	NAG	O4-C4-C3	-2.75	104.00	110.35
4	A	1421	NAG	O3-C3-C4	-2.74	104.00	110.35
4	C	1426	NAG	C3-C4-C5	-2.74	105.34	110.24
4	A	1420	NAG	O3-C3-C4	-2.74	104.01	110.35
4	C	1417	NAG	C3-C4-C5	-2.73	105.37	110.24
4	B	1401	NAG	O4-C4-C3	-2.69	104.12	110.35
4	C	1413	NAG	O3-C3-C2	-2.68	103.93	109.47
4	A	1423	NAG	O4-C4-C3	2.67	116.52	110.35
4	B	1413	NAG	C1-C2-N2	-2.67	105.93	110.49
4	C	1413	NAG	O5-C5-C6	2.66	111.38	107.20
4	C	1426	NAG	O3-C3-C2	-2.66	103.97	109.47
4	A	1427	NAG	C8-C7-N2	2.63	120.55	116.10
4	A	1401	NAG	O4-C4-C5	-2.62	102.79	109.30
4	C	1401	NAG	C4-C3-C2	-2.58	107.23	111.02
4	B	1426	NAG	O3-C3-C4	-2.58	104.38	110.35
4	C	1412	NAG	O5-C5-C6	-2.58	103.16	107.20
4	A	1408	NAG	O4-C4-C3	-2.57	104.42	110.35
4	B	1411	NAG	C1-C2-N2	-2.52	106.19	110.49
4	C	1401	NAG	C1-O5-C5	2.50	115.58	112.19
4	A	1401	NAG	C1-C2-N2	2.49	114.75	110.49
4	B	1411	NAG	C4-C3-C2	-2.48	107.38	111.02
4	A	1420	NAG	O5-C5-C6	2.48	111.10	107.20
4	C	1401	NAG	C3-C4-C5	-2.48	105.81	110.24
4	B	1411	NAG	C2-N2-C7	2.48	126.43	122.90
4	C	1412	NAG	C4-C3-C2	-2.48	107.39	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1420	NAG	O3-C3-C2	-2.48	104.34	109.47
4	C	1413	NAG	O7-C7-N2	-2.48	117.40	121.95
4	C	1427	NAG	O7-C7-C8	2.45	126.61	122.06
4	C	1427	NAG	C4-C3-C2	-2.45	107.42	111.02
4	A	1426	NAG	O4-C4-C3	2.45	116.01	110.35
4	C	1411	NAG	O5-C5-C6	2.43	111.01	107.20
4	B	1420	NAG	O5-C5-C6	2.42	111.00	107.20
4	B	1401	NAG	C6-C5-C4	-2.41	107.35	113.00
4	A	1417	NAG	O3-C3-C2	-2.41	104.49	109.47
4	B	1421	NAG	O4-C4-C3	-2.40	104.80	110.35
4	A	1423	NAG	O7-C7-C8	-2.39	117.62	122.06
4	C	1413	NAG	O5-C1-C2	-2.38	107.52	111.29
4	A	1420	NAG	O3-C3-C2	-2.37	104.57	109.47
4	C	1411	NAG	C1-C2-N2	-2.35	106.48	110.49
4	B	1417	NAG	C4-C3-C2	-2.32	107.62	111.02
4	C	1417	NAG	C4-C3-C2	-2.30	107.64	111.02
4	B	1420	NAG	O3-C3-C4	-2.30	105.03	110.35
4	C	1420	NAG	O3-C3-C4	-2.30	105.03	110.35
4	C	1423	NAG	O4-C4-C3	2.29	115.64	110.35
4	C	1422	NAG	C4-C3-C2	-2.29	107.66	111.02
4	C	1413	NAG	O4-C4-C3	-2.26	105.12	110.35
4	A	1421	NAG	O5-C5-C6	-2.26	103.67	107.20
4	B	1426	NAG	O4-C4-C5	2.24	114.87	109.30
4	A	1426	NAG	C8-C7-N2	2.24	119.90	116.10
4	B	1408	NAG	C3-C4-C5	-2.24	106.24	110.24
4	A	1411	NAG	O5-C5-C6	2.23	110.70	107.20
4	A	1412	NAG	C1-C2-N2	-2.23	106.68	110.49
4	C	1426	NAG	O5-C1-C2	-2.22	107.78	111.29
4	A	1422	NAG	C3-C4-C5	2.22	114.20	110.24
4	C	1420	NAG	O3-C3-C2	-2.20	104.91	109.47
4	C	1401	NAG	O4-C4-C5	-2.19	103.86	109.30
4	B	1421	NAG	O3-C3-C2	-2.19	104.94	109.47
4	B	1411	NAG	O5-C5-C6	2.16	110.60	107.20
4	A	1401	NAG	C1-O5-C5	2.16	115.12	112.19
4	B	1420	NAG	O6-C6-C5	-2.16	103.89	111.29
4	A	1417	NAG	C3-C4-C5	-2.13	106.44	110.24
4	A	1423	NAG	C8-C7-N2	2.13	119.71	116.10
4	C	1420	NAG	O6-C6-C5	-2.11	104.04	111.29
4	C	1412	NAG	O4-C4-C5	-2.11	104.05	109.30
4	C	1427	NAG	C1-C2-N2	-2.11	106.89	110.49
4	B	1417	NAG	C1-O5-C5	2.11	115.05	112.19
4	A	1412	NAG	C1-O5-C5	2.10	115.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1411	NAG	C3-C4-C5	2.08	113.95	110.24
4	A	1426	NAG	O4-C4-C5	-2.07	104.14	109.30
4	C	1420	NAG	O4-C4-C5	-2.07	104.16	109.30
4	B	1411	NAG	O3-C3-C2	-2.05	105.22	109.47
4	C	1408	NAG	C3-C4-C5	-2.05	106.58	110.24
4	A	1408	NAG	C4-C3-C2	-2.04	108.02	111.02
4	A	1408	NAG	C6-C5-C4	-2.04	108.22	113.00
4	A	1422	NAG	O7-C7-N2	-2.04	118.21	121.95
4	A	1401	NAG	O4-C4-C3	-2.03	105.67	110.35
4	C	1411	NAG	O4-C4-C3	2.01	115.00	110.35
4	B	1411	NAG	C3-C4-C5	2.01	113.82	110.24

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	1412	NAG	C8-C7-N2-C2
4	A	1412	NAG	O7-C7-N2-C2
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	C8-C7-N2-C2
4	B	1412	NAG	O7-C7-N2-C2
4	B	1413	NAG	C3-C2-N2-C7
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	1417	NAG	C3-C2-N2-C7
4	B	1420	NAG	C8-C7-N2-C2
4	B	1420	NAG	O7-C7-N2-C2
4	B	1426	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1426	NAG	O7-C7-N2-C2
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	1417	NAG	C3-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	1413	NAG	C8-C7-N2-C2
4	A	1421	NAG	C8-C7-N2-C2
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	C	1412	NAG	C8-C7-N2-C2
4	C	1421	NAG	C8-C7-N2-C2
4	B	1427	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1413	NAG	O5-C5-C6-O6
4	A	1411	NAG	C4-C5-C6-O6
4	C	1411	NAG	C4-C5-C6-O6
4	A	1413	NAG	O7-C7-N2-C2
4	A	1423	NAG	O7-C7-N2-C2
4	C	1412	NAG	O7-C7-N2-C2
4	B	1421	NAG	C1-C2-N2-C7
4	B	1426	NAG	C1-C2-N2-C7

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

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Mol	Chain	Res	Type	Atoms
4	A	1427	NAG	O5-C5-C6-O6
4	A	1417	NAG	C1-C2-N2-C7
4	C	1417	NAG	C1-C2-N2-C7
4	B	1417	NAG	C1-C2-N2-C7
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	A	1408	NAG	3	0
4	A	1411	NAG	4	0
4	B	1416	NAG	5	0
4	B	1412	NAG	4	0
4	C	1412	NAG	4	0
4	A	1426	NAG	4	0
4	C	1420	NAG	1	0
4	C	1401	NAG	7	0
4	C	1413	NAG	3	0
4	B	1413	NAG	4	0
4	C	1411	NAG	4	0
4	A	1412	NAG	3	0
4	A	1423	NAG	4	0
4	C	1408	NAG	3	0
4	B	1408	NAG	4	0
4	B	1411	NAG	4	0
4	A	1416	NAG	3	0
4	A	1421	NAG	3	0
4	B	1420	NAG	1	0
4	A	1417	NAG	4	0
4	A	1413	NAG	5	0
4	B	1426	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

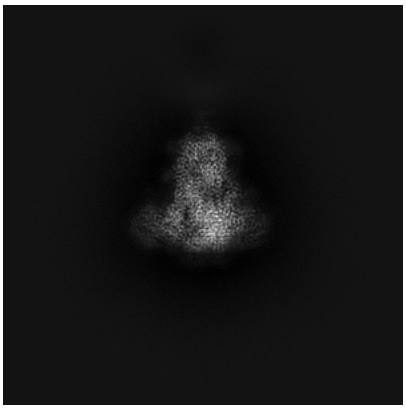
6 Map visualisation (i)

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

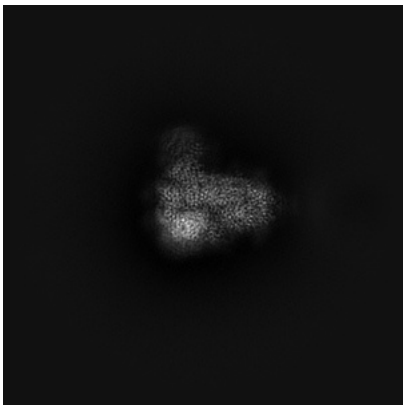
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

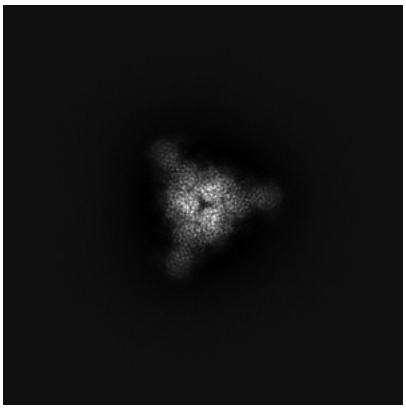
6.1.1 Primary map



X

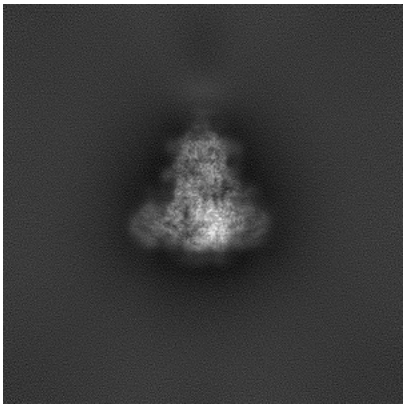


Y

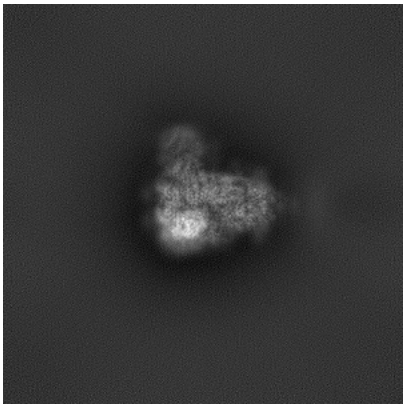


Z

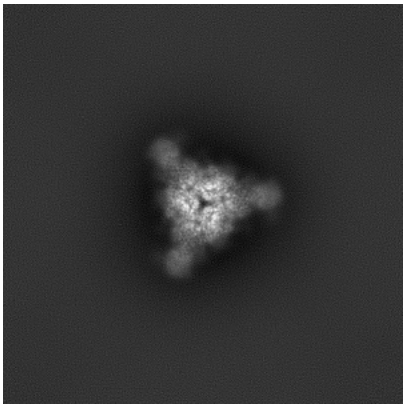
6.1.2 Raw map



X



Y



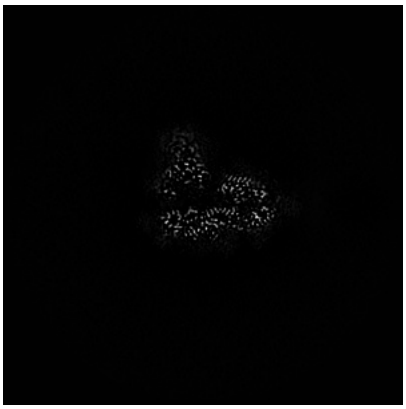
Z

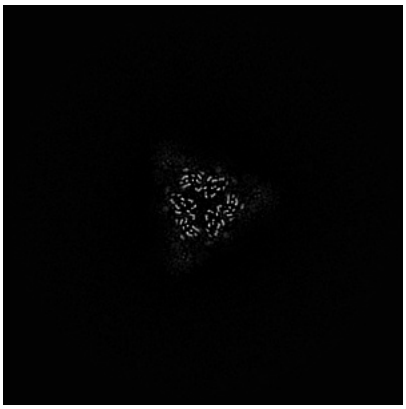
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

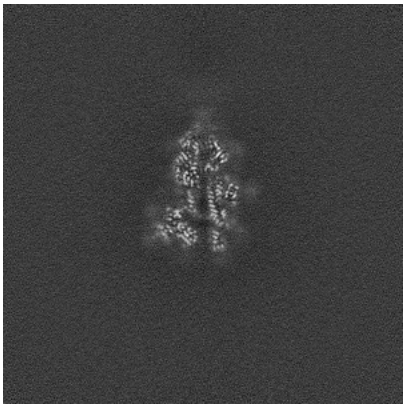
6.2.1 Primary map

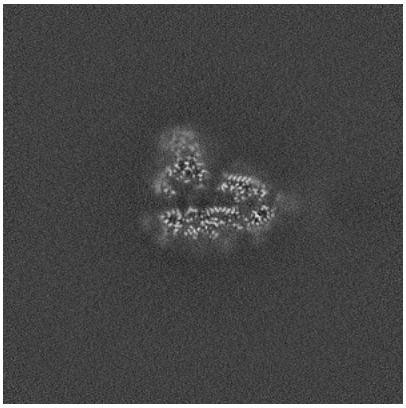
X Index: 216

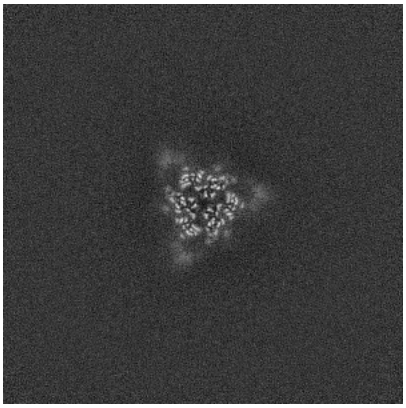

Y Index: 216


Z Index: 216

6.2.2 Raw map


X Index: 216


Y Index: 216


Z Index: 216

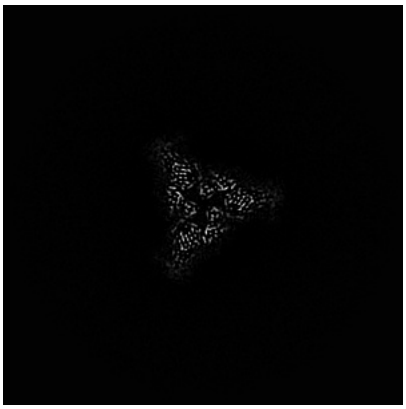
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

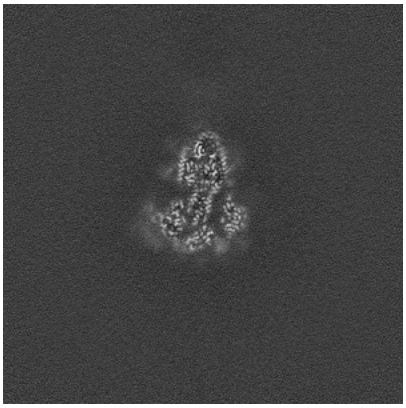
6.3.1 Primary map

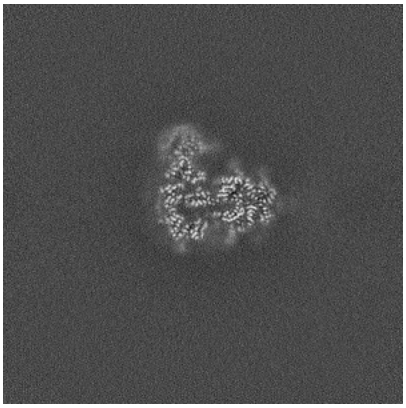
X Index: 225

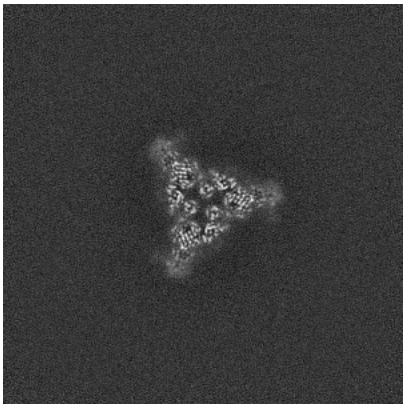
Y Index: 226


Z Index: 199

6.3.2 Raw map


X Index: 204

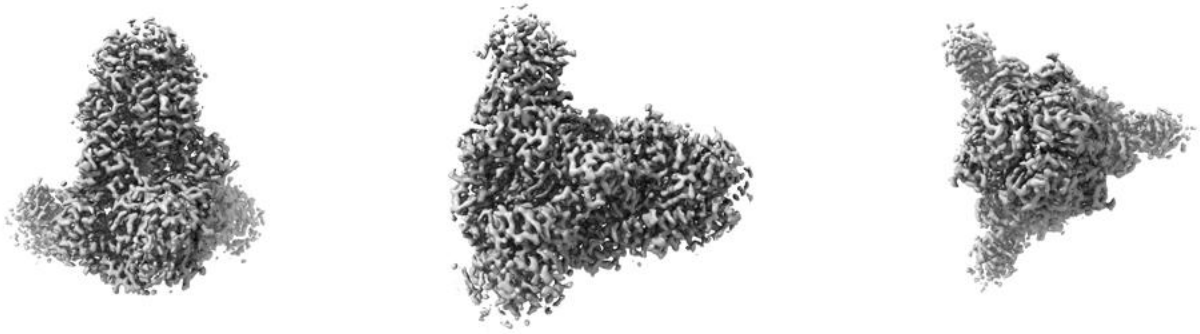

Y Index: 226


Z Index: 199

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

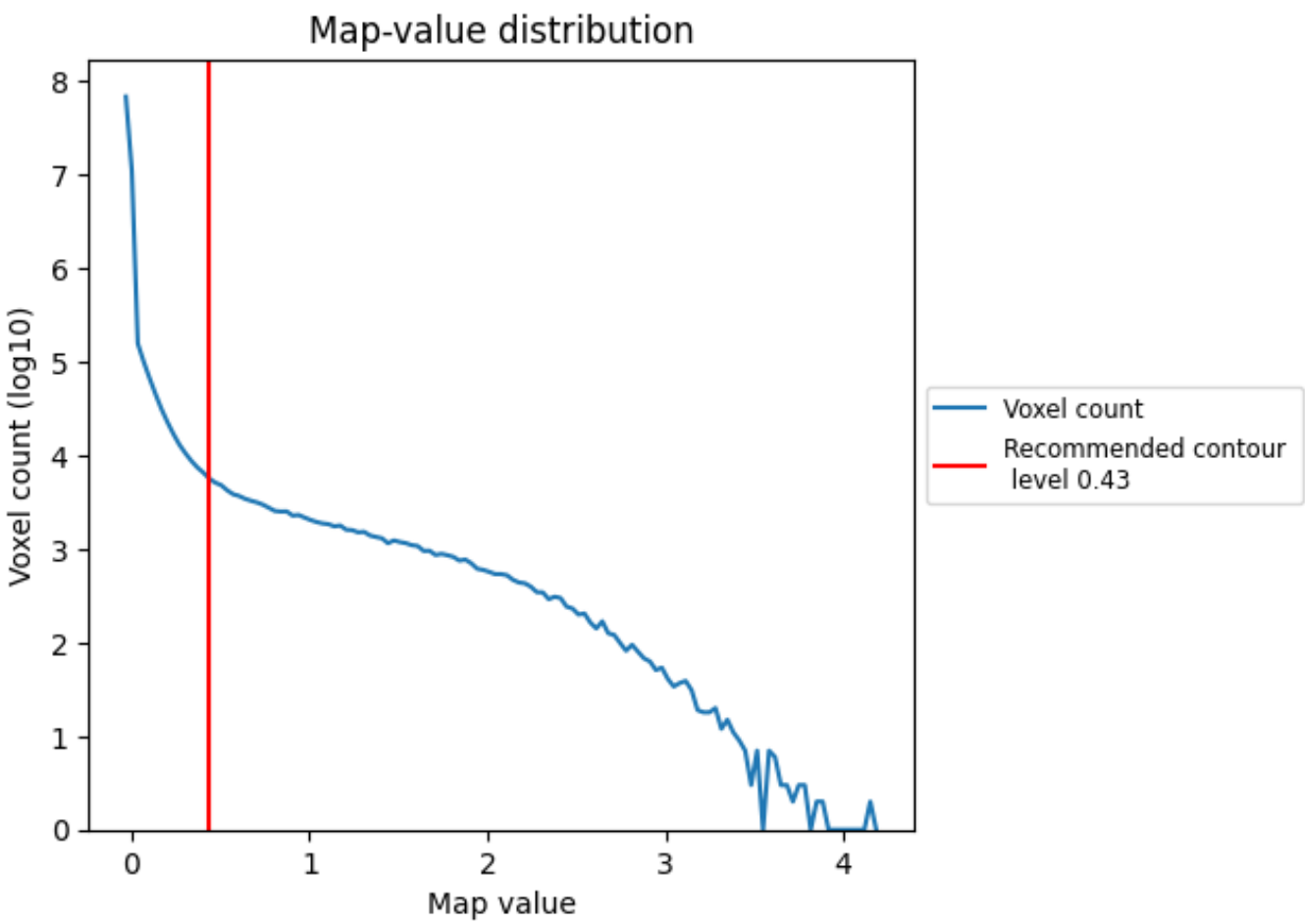
6.5 Mask visualisation (i)

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

7 Map analysis (i)

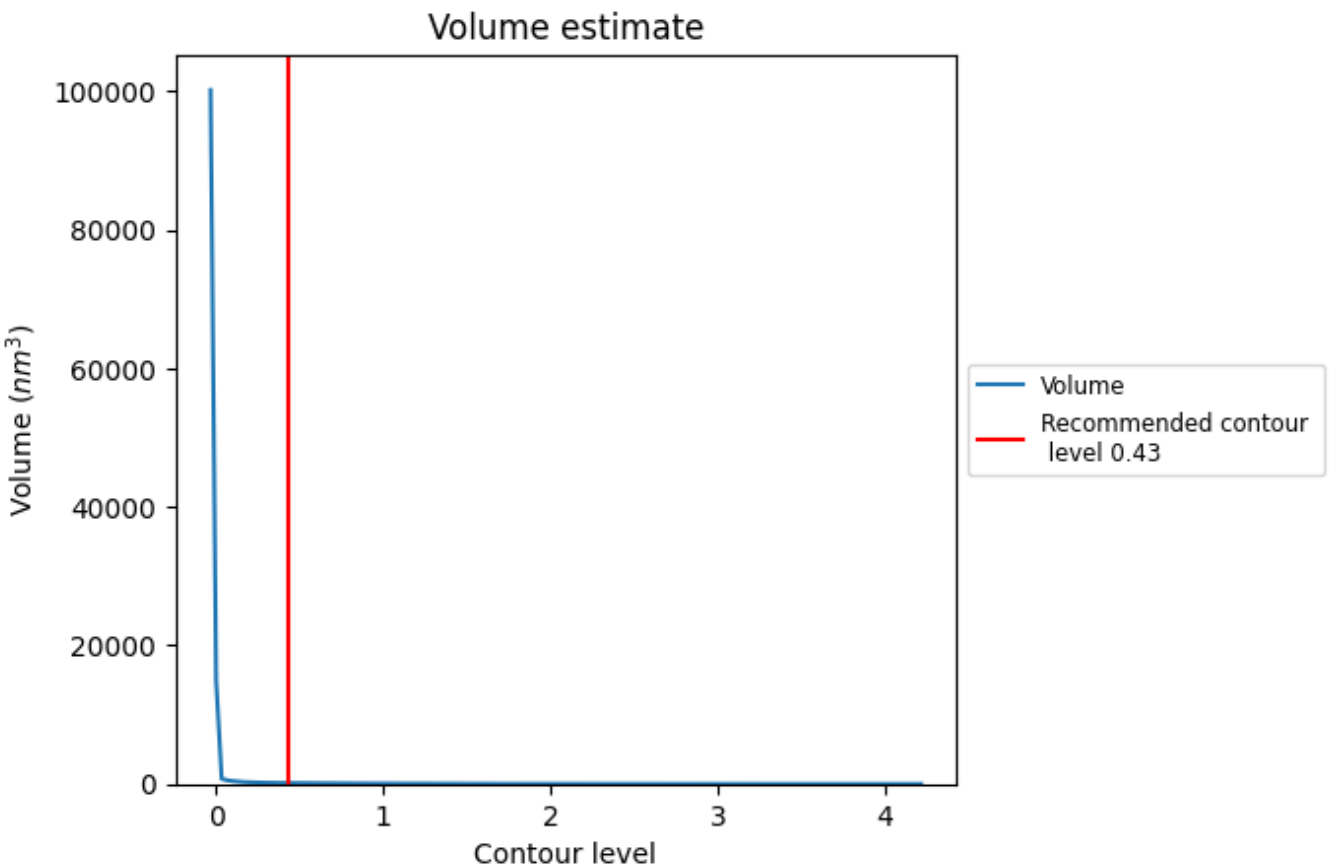
This section contains the results of statistical analysis of the map.

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.

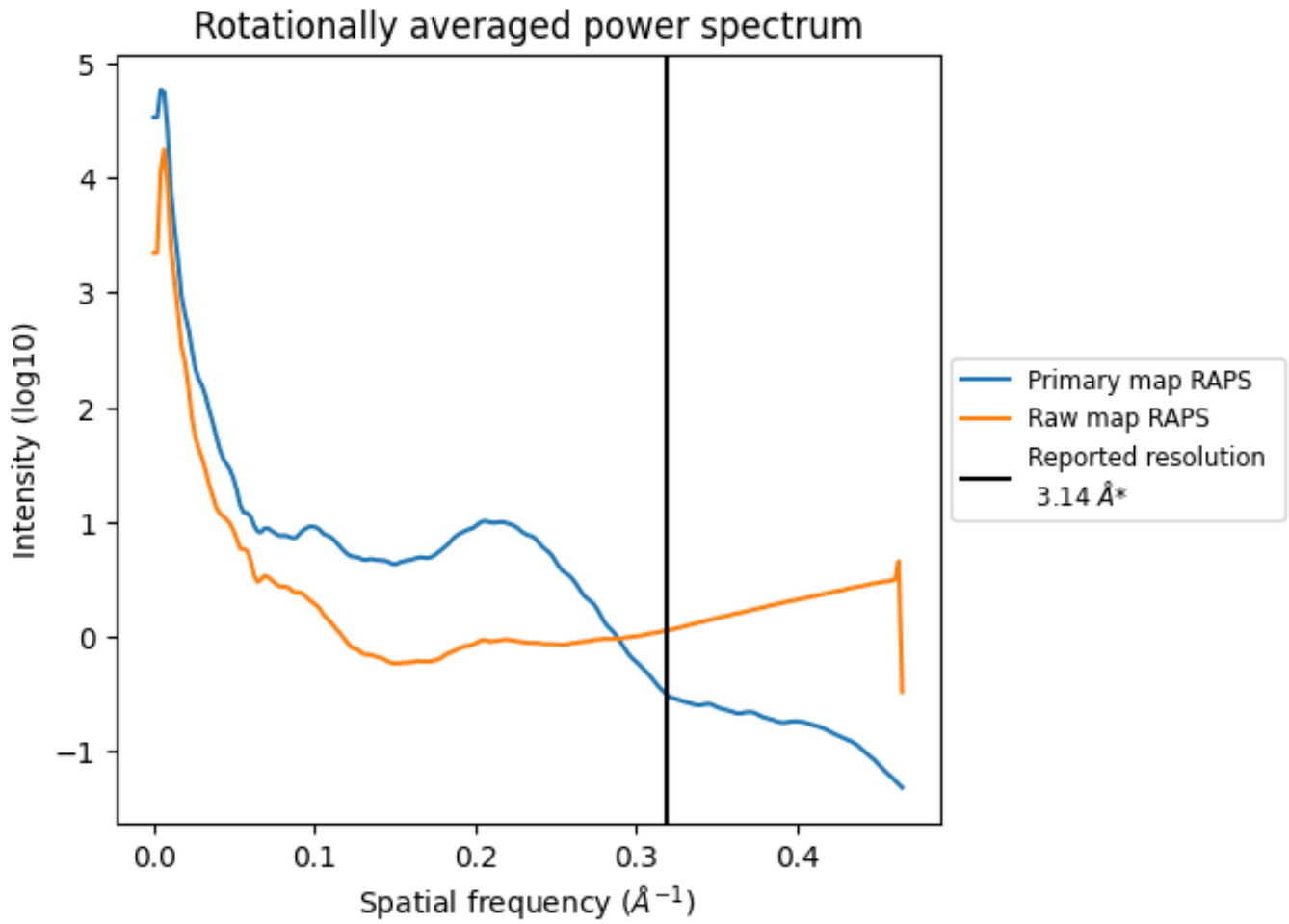
7.2 Volume estimate (i)



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 (i)

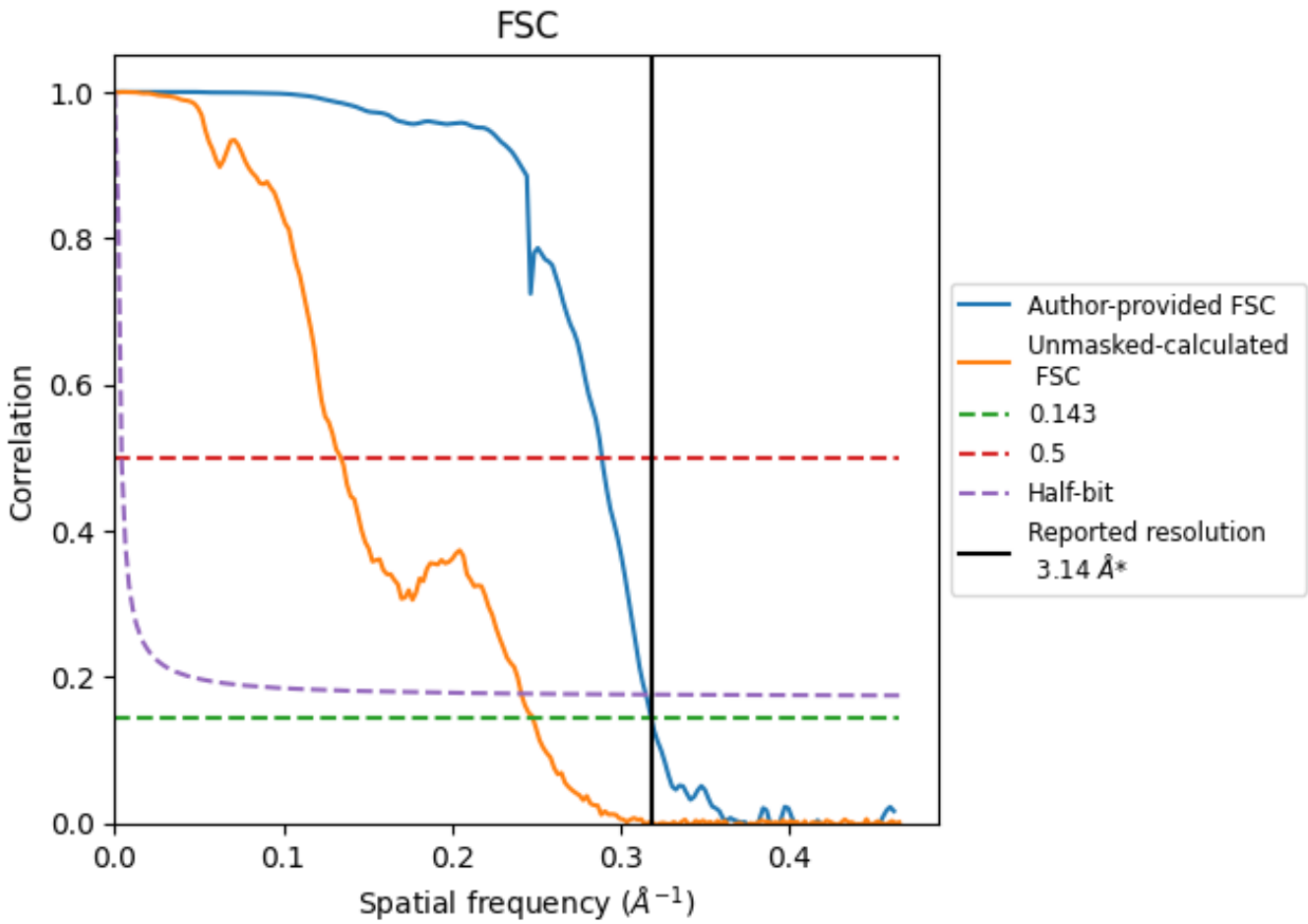


*Reported resolution corresponds to spatial frequency of 0.318 Å^{-1}

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 Å^{-1}

8.2 Resolution estimates (i)

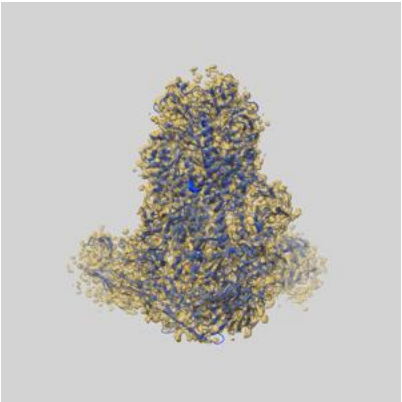
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.46	3.18
Unmasked-calculated*	4.03	7.46	4.15

*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 %

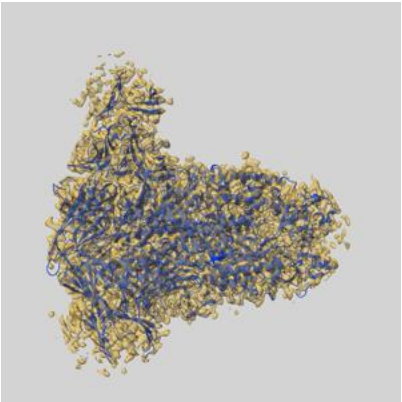
9 Map-model fit (i)

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.

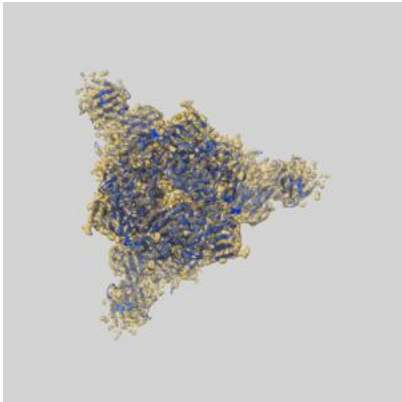
9.1 Map-model overlay (i)



X



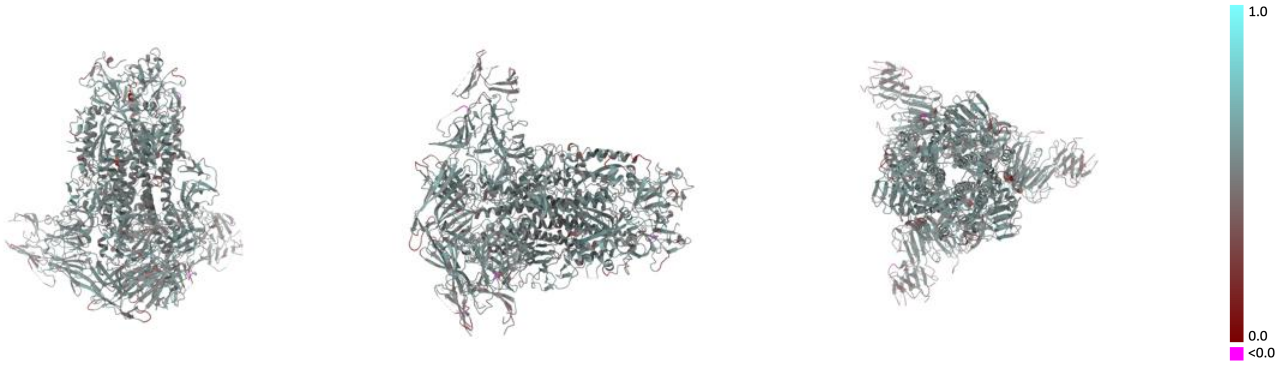
Y



Z

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.

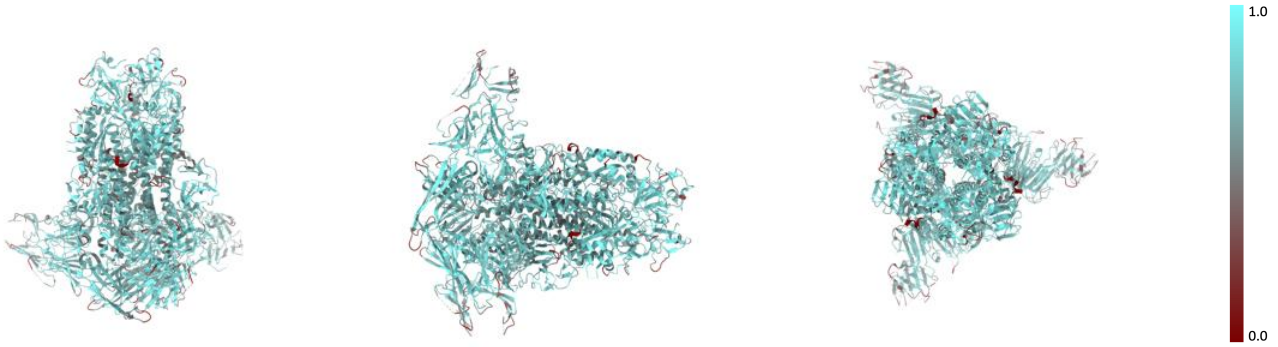
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

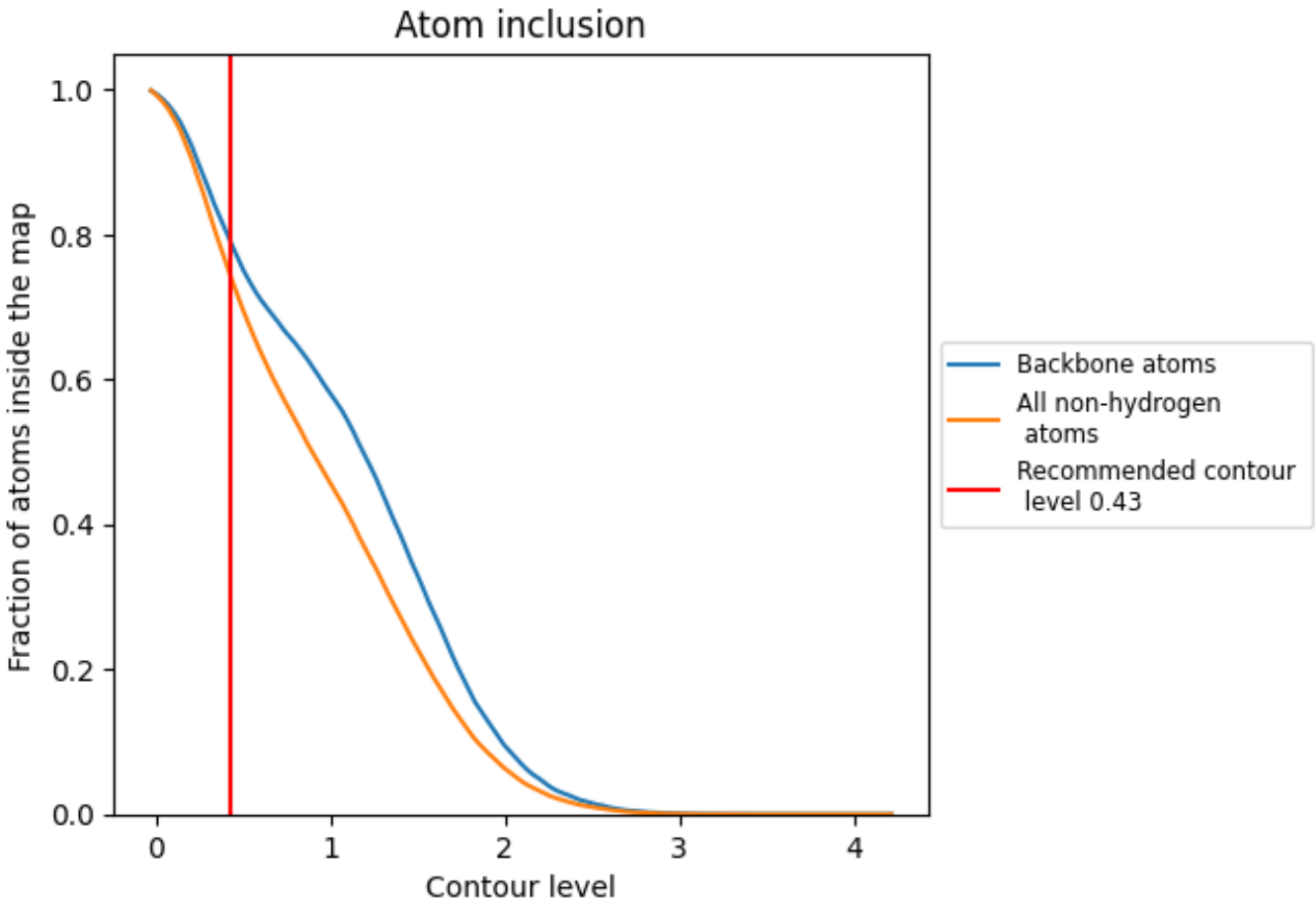
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

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 (i)

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	0.7398	0.5180
A	0.7401	0.5170
B	0.7412	0.5180
C	0.7414	0.5160
D	0.7917	0.5830
E	0.3929	0.5010
F	0.7143	0.6030
G	0.7857	0.5750
H	0.6429	0.5460
I	0.7778	0.5820
J	0.3929	0.4920
K	0.6786	0.6060
L	0.7857	0.6010
M	0.6786	0.5640
N	0.7917	0.5570
O	0.2500	0.5480
P	0.7500	0.5960
Q	0.8571	0.5980
R	0.6429	0.5610