Full wwPDB EM Validation Report ⓘ

May 31, 2025 – 01:20 PM EDT

PDB ID	:	9D4T / pdb_00009d4t
EMDB ID	:	EMD-46569
Title	:	Structure of HKU5-20s spike glycoprotein
Authors	:	Wu, Z.; Fan, C.; Bjorkman, P.J.
Deposited on	:	2024-08-12
Resolution	:	2.80 Å(reported)
Based on initial model	:	6NB3

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

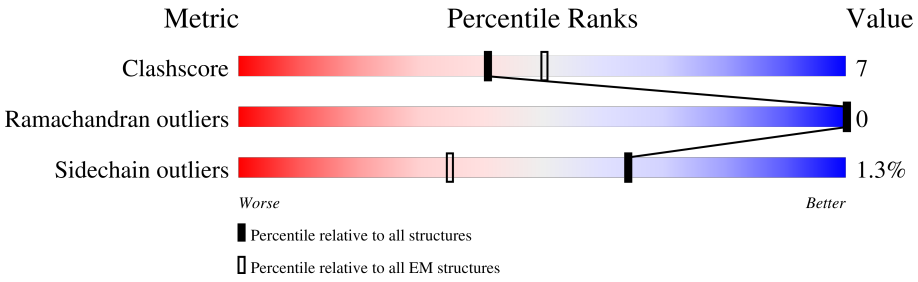
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1344	73% 15% 12%
1	B	1344	72% 16% 12%
1	C	1344	72% 16% 12%
2	D	2	50% 50%
2	F	2	100%
2	G	2	50% 50%
2	H	2	50% 50%
2	J	2	100%

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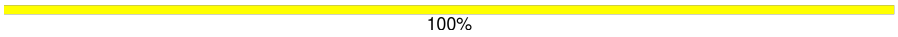
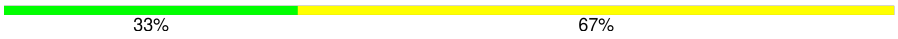
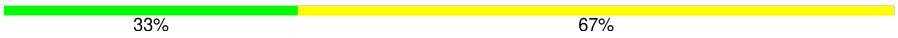
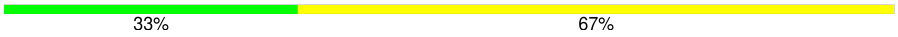
Mol	Chain	Length	Quality of chain
2	K	2	
2	L	2	
2	N	2	
2	O	2	
3	E	3	
3	I	3	
3	M	3	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1183	Total	C	N	O	S	0	0
			9189	5834	1521	1781	53		
1	B	1183	Total	C	N	O	S	0	0
			9189	5834	1521	1781	53		
1	C	1183	Total	C	N	O	S	0	0
			9189	5834	1521	1781	53		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	748	ALA	ARG	conflict	UNP S4X419
A	749	SER	PHE	conflict	UNP S4X419
A	750	VAL	ARG	conflict	UNP S4X419
A	751	GLY	ARG	conflict	UNP S4X419
A	1063	PRO	THR	conflict	UNP S4X419
A	1064	PRO	VAL	conflict	UNP S4X419
A	1302	GLY	-	expression tag	UNP S4X419
A	1303	SER	-	expression tag	UNP S4X419
A	1304	GLY	-	expression tag	UNP S4X419
A	1305	ARG	-	expression tag	UNP S4X419
A	1306	GLU	-	expression tag	UNP S4X419
A	1307	ASN	-	expression tag	UNP S4X419
A	1308	LEU	-	expression tag	UNP S4X419
A	1309	TYR	-	expression tag	UNP S4X419
A	1310	PHE	-	expression tag	UNP S4X419
A	1311	GLN	-	expression tag	UNP S4X419
A	1312	GLY	-	expression tag	UNP S4X419
A	1313	GLY	-	expression tag	UNP S4X419
A	1314	GLY	-	expression tag	UNP S4X419
A	1315	GLY	-	expression tag	UNP S4X419
A	1316	SER	-	expression tag	UNP S4X419
A	1317	GLY	-	expression tag	UNP S4X419
A	1318	TYR	-	expression tag	UNP S4X419
A	1319	ILE	-	expression tag	UNP S4X419

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1320	PRO	-	expression tag	UNP S4X419
A	1321	GLU	-	expression tag	UNP S4X419
A	1322	ALA	-	expression tag	UNP S4X419
A	1323	PRO	-	expression tag	UNP S4X419
A	1324	ARG	-	expression tag	UNP S4X419
A	1325	ASP	-	expression tag	UNP S4X419
A	1326	GLY	-	expression tag	UNP S4X419
A	1327	GLN	-	expression tag	UNP S4X419
A	1328	ALA	-	expression tag	UNP S4X419
A	1329	TYR	-	expression tag	UNP S4X419
A	1330	VAL	-	expression tag	UNP S4X419
A	1331	ARG	-	expression tag	UNP S4X419
A	1332	LYS	-	expression tag	UNP S4X419
A	1333	ASP	-	expression tag	UNP S4X419
A	1334	GLY	-	expression tag	UNP S4X419
A	1335	GLU	-	expression tag	UNP S4X419
A	1336	TRP	-	expression tag	UNP S4X419
A	1337	VAL	-	expression tag	UNP S4X419
A	1338	LEU	-	expression tag	UNP S4X419
A	1339	LEU	-	expression tag	UNP S4X419
A	1340	SER	-	expression tag	UNP S4X419
A	1341	THR	-	expression tag	UNP S4X419
A	1342	PHE	-	expression tag	UNP S4X419
A	1343	LEU	-	expression tag	UNP S4X419
A	1344	GLY	-	expression tag	UNP S4X419
A	1345	HIS	-	expression tag	UNP S4X419
A	1346	HIS	-	expression tag	UNP S4X419
A	1347	HIS	-	expression tag	UNP S4X419
A	1348	HIS	-	expression tag	UNP S4X419
A	1349	HIS	-	expression tag	UNP S4X419
A	1350	HIS	-	expression tag	UNP S4X419
A	1351	HIS	-	expression tag	UNP S4X419
A	1352	HIS	-	expression tag	UNP S4X419
A	1353	GLY	-	expression tag	UNP S4X419
A	1354	LEU	-	expression tag	UNP S4X419
A	1355	ASN	-	expression tag	UNP S4X419
A	1356	ASP	-	expression tag	UNP S4X419
A	1357	ILE	-	expression tag	UNP S4X419
A	1358	PHE	-	expression tag	UNP S4X419
A	1359	GLU	-	expression tag	UNP S4X419
A	1360	ALA	-	expression tag	UNP S4X419
A	1361	GLN	-	expression tag	UNP S4X419

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1362	LYS	-	expression tag	UNP S4X419
A	1363	ILE	-	expression tag	UNP S4X419
A	1364	GLU	-	expression tag	UNP S4X419
A	1365	TRP	-	expression tag	UNP S4X419
A	1366	HIS	-	expression tag	UNP S4X419
A	1367	GLU	-	expression tag	UNP S4X419
B	748	ALA	ARG	conflict	UNP S4X419
B	749	SER	PHE	conflict	UNP S4X419
B	750	VAL	ARG	conflict	UNP S4X419
B	751	GLY	ARG	conflict	UNP S4X419
B	1063	PRO	THR	conflict	UNP S4X419
B	1064	PRO	VAL	conflict	UNP S4X419
B	1302	GLY	-	expression tag	UNP S4X419
B	1303	SER	-	expression tag	UNP S4X419
B	1304	GLY	-	expression tag	UNP S4X419
B	1305	ARG	-	expression tag	UNP S4X419
B	1306	GLU	-	expression tag	UNP S4X419
B	1307	ASN	-	expression tag	UNP S4X419
B	1308	LEU	-	expression tag	UNP S4X419
B	1309	TYR	-	expression tag	UNP S4X419
B	1310	PHE	-	expression tag	UNP S4X419
B	1311	GLN	-	expression tag	UNP S4X419
B	1312	GLY	-	expression tag	UNP S4X419
B	1313	GLY	-	expression tag	UNP S4X419
B	1314	GLY	-	expression tag	UNP S4X419
B	1315	GLY	-	expression tag	UNP S4X419
B	1316	SER	-	expression tag	UNP S4X419
B	1317	GLY	-	expression tag	UNP S4X419
B	1318	TYR	-	expression tag	UNP S4X419
B	1319	ILE	-	expression tag	UNP S4X419
B	1320	PRO	-	expression tag	UNP S4X419
B	1321	GLU	-	expression tag	UNP S4X419
B	1322	ALA	-	expression tag	UNP S4X419
B	1323	PRO	-	expression tag	UNP S4X419
B	1324	ARG	-	expression tag	UNP S4X419
B	1325	ASP	-	expression tag	UNP S4X419
B	1326	GLY	-	expression tag	UNP S4X419
B	1327	GLN	-	expression tag	UNP S4X419
B	1328	ALA	-	expression tag	UNP S4X419
B	1329	TYR	-	expression tag	UNP S4X419
B	1330	VAL	-	expression tag	UNP S4X419
B	1331	ARG	-	expression tag	UNP S4X419

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1332	LYS	-	expression tag	UNP S4X419
B	1333	ASP	-	expression tag	UNP S4X419
B	1334	GLY	-	expression tag	UNP S4X419
B	1335	GLU	-	expression tag	UNP S4X419
B	1336	TRP	-	expression tag	UNP S4X419
B	1337	VAL	-	expression tag	UNP S4X419
B	1338	LEU	-	expression tag	UNP S4X419
B	1339	LEU	-	expression tag	UNP S4X419
B	1340	SER	-	expression tag	UNP S4X419
B	1341	THR	-	expression tag	UNP S4X419
B	1342	PHE	-	expression tag	UNP S4X419
B	1343	LEU	-	expression tag	UNP S4X419
B	1344	GLY	-	expression tag	UNP S4X419
B	1345	HIS	-	expression tag	UNP S4X419
B	1346	HIS	-	expression tag	UNP S4X419
B	1347	HIS	-	expression tag	UNP S4X419
B	1348	HIS	-	expression tag	UNP S4X419
B	1349	HIS	-	expression tag	UNP S4X419
B	1350	HIS	-	expression tag	UNP S4X419
B	1351	HIS	-	expression tag	UNP S4X419
B	1352	HIS	-	expression tag	UNP S4X419
B	1353	GLY	-	expression tag	UNP S4X419
B	1354	LEU	-	expression tag	UNP S4X419
B	1355	ASN	-	expression tag	UNP S4X419
B	1356	ASP	-	expression tag	UNP S4X419
B	1357	ILE	-	expression tag	UNP S4X419
B	1358	PHE	-	expression tag	UNP S4X419
B	1359	GLU	-	expression tag	UNP S4X419
B	1360	ALA	-	expression tag	UNP S4X419
B	1361	GLN	-	expression tag	UNP S4X419
B	1362	LYS	-	expression tag	UNP S4X419
B	1363	ILE	-	expression tag	UNP S4X419
B	1364	GLU	-	expression tag	UNP S4X419
B	1365	TRP	-	expression tag	UNP S4X419
B	1366	HIS	-	expression tag	UNP S4X419
B	1367	GLU	-	expression tag	UNP S4X419
C	748	ALA	ARG	conflict	UNP S4X419
C	749	SER	PHE	conflict	UNP S4X419
C	750	VAL	ARG	conflict	UNP S4X419
C	751	GLY	ARG	conflict	UNP S4X419
C	1063	PRO	THR	conflict	UNP S4X419
C	1064	PRO	VAL	conflict	UNP S4X419

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	GLY	-	expression tag	UNP S4X419
C	1303	SER	-	expression tag	UNP S4X419
C	1304	GLY	-	expression tag	UNP S4X419
C	1305	ARG	-	expression tag	UNP S4X419
C	1306	GLU	-	expression tag	UNP S4X419
C	1307	ASN	-	expression tag	UNP S4X419
C	1308	LEU	-	expression tag	UNP S4X419
C	1309	TYR	-	expression tag	UNP S4X419
C	1310	PHE	-	expression tag	UNP S4X419
C	1311	GLN	-	expression tag	UNP S4X419
C	1312	GLY	-	expression tag	UNP S4X419
C	1313	GLY	-	expression tag	UNP S4X419
C	1314	GLY	-	expression tag	UNP S4X419
C	1315	GLY	-	expression tag	UNP S4X419
C	1316	SER	-	expression tag	UNP S4X419
C	1317	GLY	-	expression tag	UNP S4X419
C	1318	TYR	-	expression tag	UNP S4X419
C	1319	ILE	-	expression tag	UNP S4X419
C	1320	PRO	-	expression tag	UNP S4X419
C	1321	GLU	-	expression tag	UNP S4X419
C	1322	ALA	-	expression tag	UNP S4X419
C	1323	PRO	-	expression tag	UNP S4X419
C	1324	ARG	-	expression tag	UNP S4X419
C	1325	ASP	-	expression tag	UNP S4X419
C	1326	GLY	-	expression tag	UNP S4X419
C	1327	GLN	-	expression tag	UNP S4X419
C	1328	ALA	-	expression tag	UNP S4X419
C	1329	TYR	-	expression tag	UNP S4X419
C	1330	VAL	-	expression tag	UNP S4X419
C	1331	ARG	-	expression tag	UNP S4X419
C	1332	LYS	-	expression tag	UNP S4X419
C	1333	ASP	-	expression tag	UNP S4X419
C	1334	GLY	-	expression tag	UNP S4X419
C	1335	GLU	-	expression tag	UNP S4X419
C	1336	TRP	-	expression tag	UNP S4X419
C	1337	VAL	-	expression tag	UNP S4X419
C	1338	LEU	-	expression tag	UNP S4X419
C	1339	LEU	-	expression tag	UNP S4X419
C	1340	SER	-	expression tag	UNP S4X419
C	1341	THR	-	expression tag	UNP S4X419
C	1342	PHE	-	expression tag	UNP S4X419
C	1343	LEU	-	expression tag	UNP S4X419

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1344	GLY	-	expression tag	UNP S4X419
C	1345	HIS	-	expression tag	UNP S4X419
C	1346	HIS	-	expression tag	UNP S4X419
C	1347	HIS	-	expression tag	UNP S4X419
C	1348	HIS	-	expression tag	UNP S4X419
C	1349	HIS	-	expression tag	UNP S4X419
C	1350	HIS	-	expression tag	UNP S4X419
C	1351	HIS	-	expression tag	UNP S4X419
C	1352	HIS	-	expression tag	UNP S4X419
C	1353	GLY	-	expression tag	UNP S4X419
C	1354	LEU	-	expression tag	UNP S4X419
C	1355	ASN	-	expression tag	UNP S4X419
C	1356	ASP	-	expression tag	UNP S4X419
C	1357	ILE	-	expression tag	UNP S4X419
C	1358	PHE	-	expression tag	UNP S4X419
C	1359	GLU	-	expression tag	UNP S4X419
C	1360	ALA	-	expression tag	UNP S4X419
C	1361	GLN	-	expression tag	UNP S4X419
C	1362	LYS	-	expression tag	UNP S4X419
C	1363	ILE	-	expression tag	UNP S4X419
C	1364	GLU	-	expression tag	UNP S4X419
C	1365	TRP	-	expression tag	UNP S4X419
C	1366	HIS	-	expression tag	UNP S4X419
C	1367	GLU	-	expression tag	UNP S4X419

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

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

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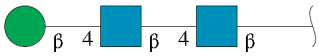
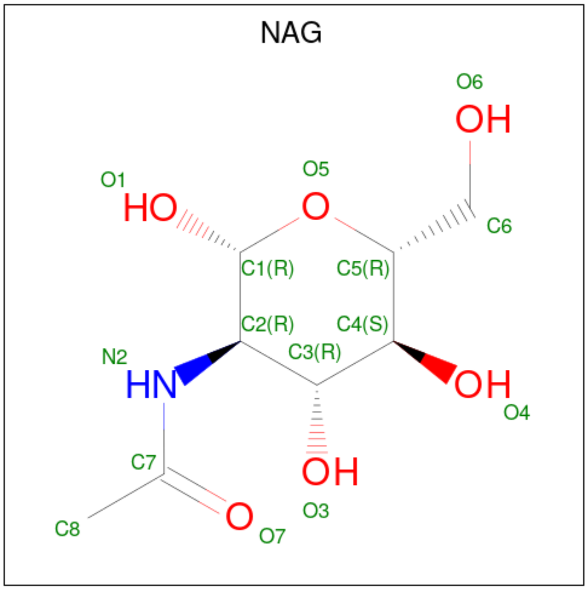
Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 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
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

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

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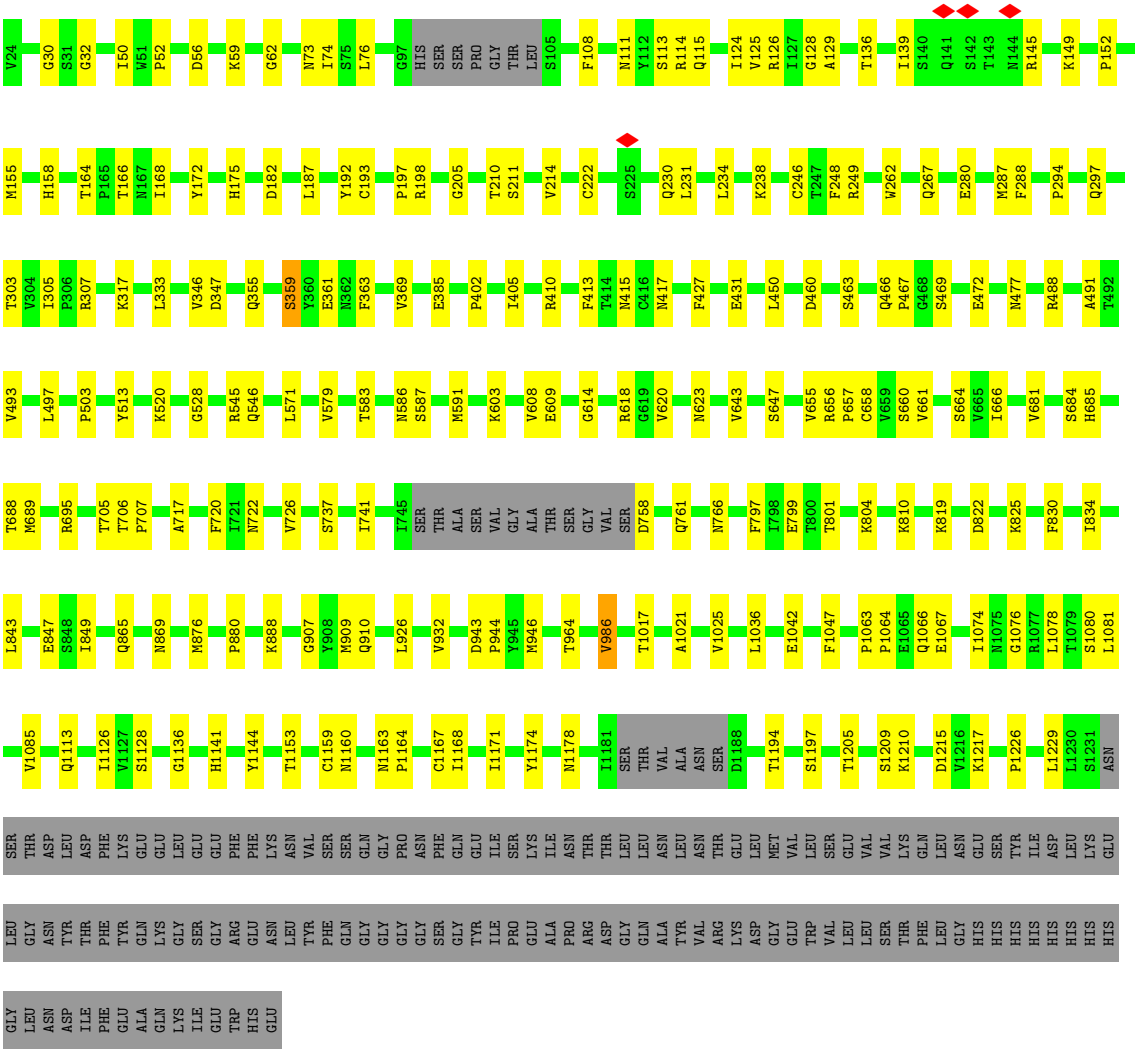
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	

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.

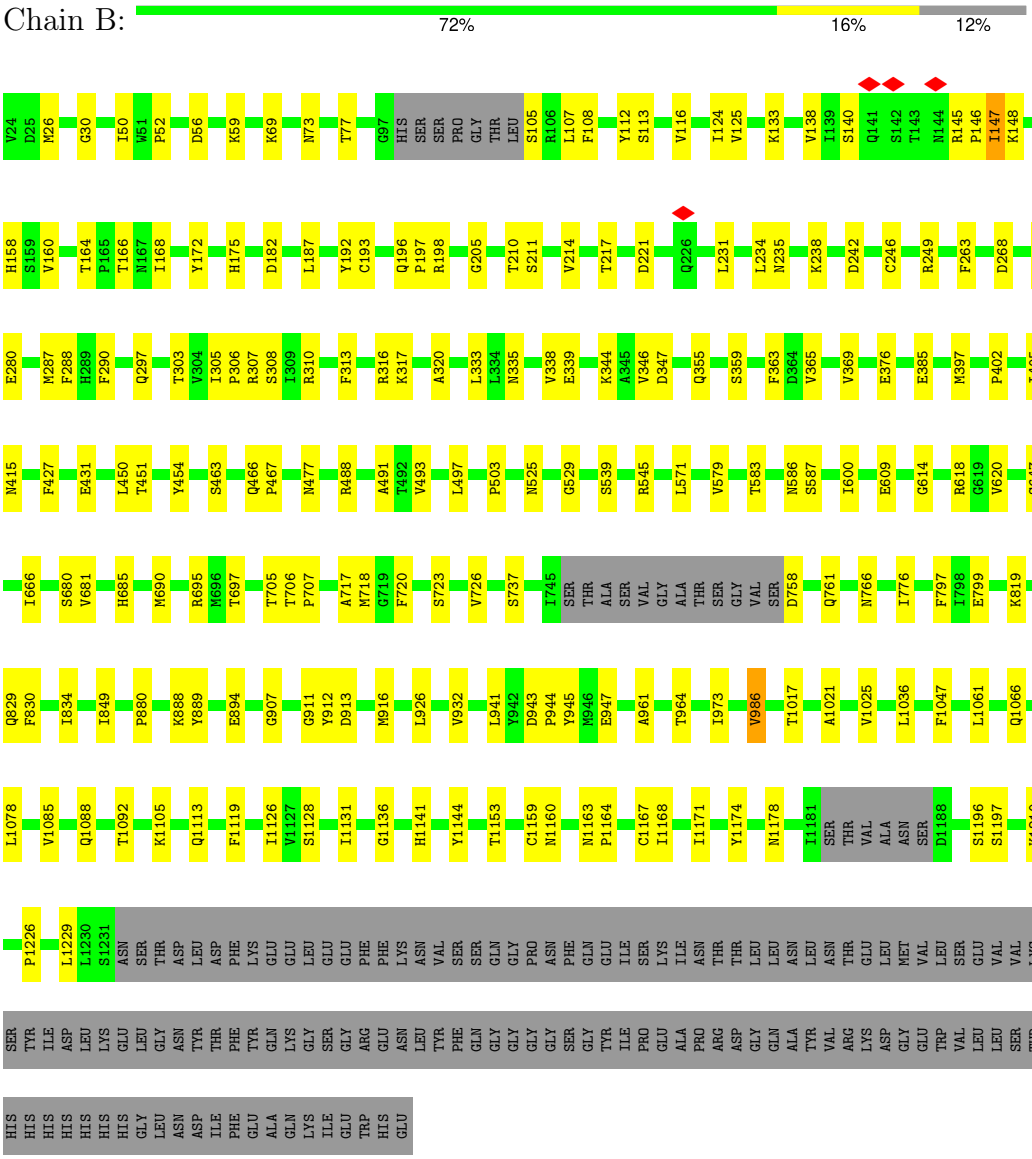
• Molecule 1: Spike glycoprotein

Chain A:



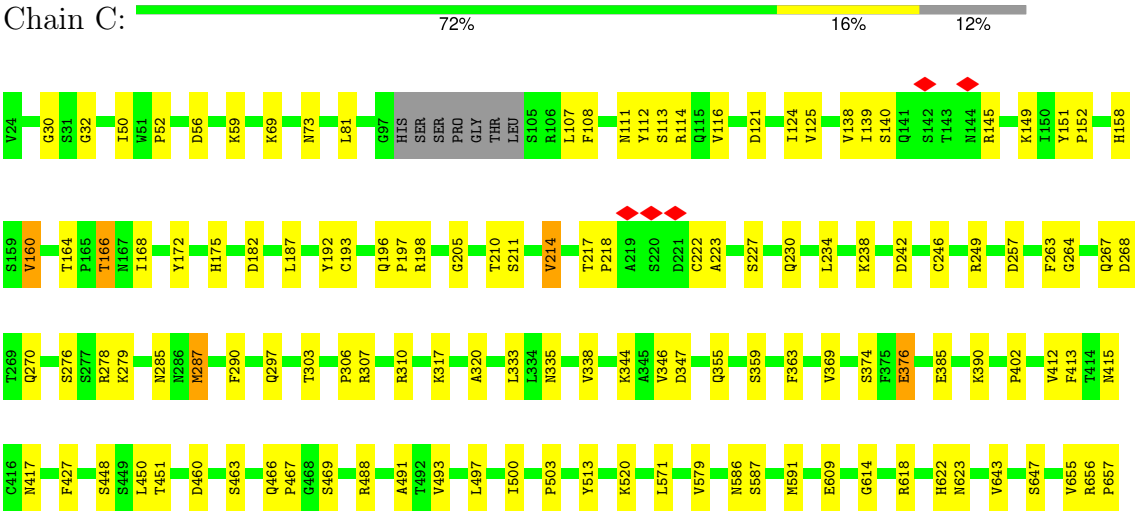
• Molecule 1: Spike glycoprotein

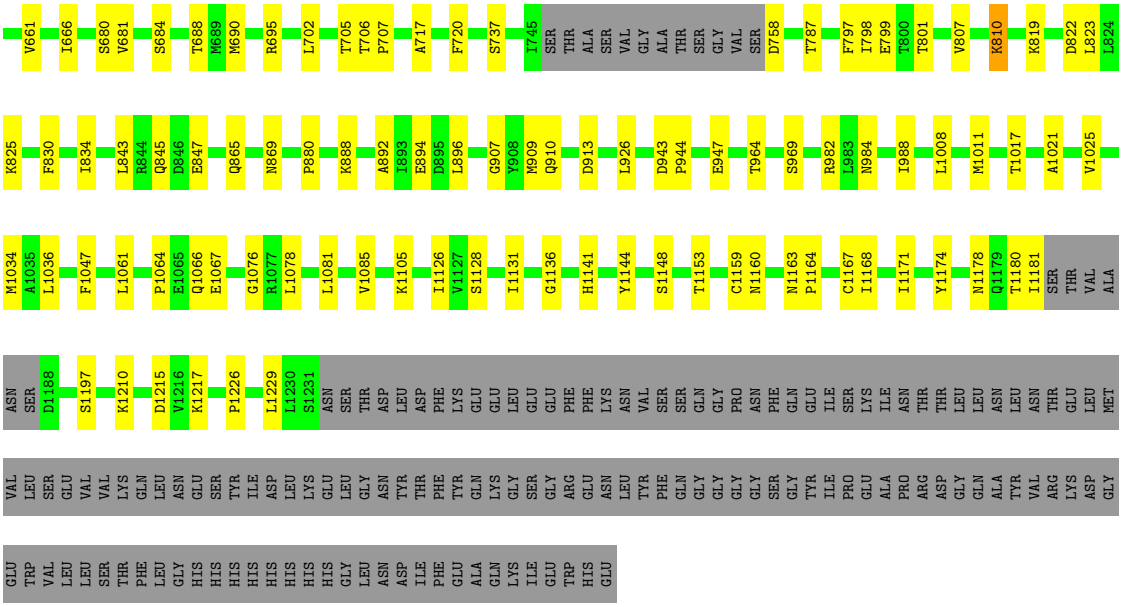
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



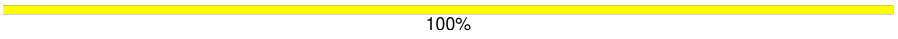


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain F:



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

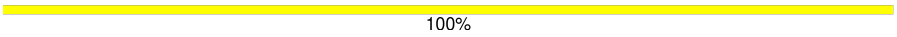
Chain G:

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

Chain H:

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

Chain J:



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

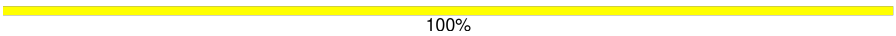
Chain K:

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

Chain L:

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

Chain N:

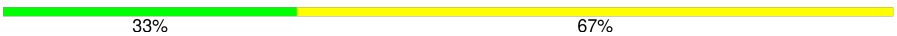


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

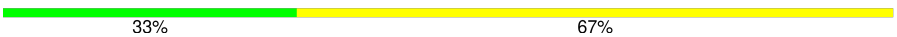
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



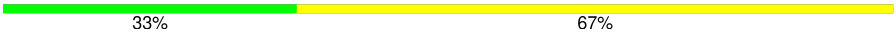
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	270453	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0649	Depositor
Map size (Å)	312.84, 312.84, 312.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.10	0/9408	0.26	0/12813
1	B	0.10	0/9408	0.26	0/12813
1	C	0.10	0/9408	0.27	0/12813
All	All	0.10	0/28224	0.26	0/38439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9189	0	8851	127	0
1	B	9189	0	8851	127	0
1	C	9189	0	8851	140	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	E	39	0	34	0	0
3	I	39	0	34	0	0
3	M	39	0	34	0	0
4	A	182	0	169	4	0
4	B	168	0	156	3	0
4	C	154	0	143	3	0
All	All	28440	0	27348	373	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 7.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:CYS:HB3	1:A:1167:CYS:HA	1.51	0.93
1:B:1159:CYS:HB3	1:B:1167:CYS:HA	1.52	0.91
1:C:1159:CYS:HB3	1:C:1167:CYS:HA	1.54	0.87
1:A:193:CYS:HB3	1:A:246:CYS:HA	1.57	0.84
1:C:193:CYS:HB3	1:C:246:CYS:HA	1.64	0.80
1:B:193:CYS:HB3	1:B:246:CYS:HA	1.65	0.78
1:C:417:ASN:HB3	1:C:591:MET:HG3	1.71	0.72
1:A:661:VAL:HG13	1:A:681:VAL:HG21	1.73	0.70
1:B:405:ILE:HG12	1:B:477:ASN:HB3	1.73	0.70
1:A:405:ILE:HG12	1:A:477:ASN:HB3	1.73	0.69
1:A:125:VAL:HG11	1:A:152:PRO:HG3	1.75	0.68
1:C:125:VAL:HG11	1:C:152:PRO:HG3	1.74	0.68
1:B:1226:PRO:HD2	1:B:1229:LEU:HD12	1.74	0.68
1:A:1226:PRO:HD2	1:A:1229:LEU:HD12	1.77	0.67
1:A:1215:ASP:OD2	1:A:1217:LYS:NZ	2.29	0.66
1:B:138:VAL:HG12	1:B:140:SER:H	1.61	0.66
1:A:819:LYS:HZ1	1:A:1067:GLU:HG3	1.61	0.65
1:B:145:ARG:HG2	1:B:317:LYS:HA	1.77	0.65
1:C:138:VAL:HG12	1:C:140:SER:H	1.61	0.65
1:C:415:ASN:HA	1:C:587:SER:HB2	1.79	0.64
1:B:125:VAL:HG11	1:B:152:PRO:HG3	1.80	0.64
1:A:843:LEU:O	1:A:847:GLU:HG3	1.99	0.63
1:C:1226:PRO:HD2	1:C:1229:LEU:HD12	1.80	0.63
1:B:197:PRO:HB2	1:B:205:GLY:HA3	1.81	0.62
1:C:586:ASN:HB2	1:C:614:GLY:HA3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLU:HG2	1:B:618:ARG:HG2	1.82	0.62
1:A:347:ASP:OD2	1:A:695:ARG:NH2	2.33	0.62
1:A:1178:ASN:HA	4:A:1412:NAG:H2	1.82	0.62
1:C:1178:ASN:HA	4:C:1411:NAG:H2	1.82	0.62
1:C:158:HIS:NE2	1:C:192:TYR:OH	2.28	0.61
1:B:586:ASN:HB2	1:B:614:GLY:HA3	1.82	0.61
1:B:1178:ASN:HA	4:B:1412:NAG:H2	1.82	0.61
1:A:880:PRO:HG2	1:A:888:LYS:HD2	1.81	0.61
1:C:609:GLU:HG3	1:C:618:ARG:HG2	1.82	0.61
1:A:586:ASN:HB2	1:A:614:GLY:HA3	1.83	0.61
1:B:427:PHE:HB3	1:B:491:ALA:HB1	1.83	0.60
1:A:427:PHE:HB3	1:A:491:ALA:HB1	1.83	0.60
1:B:661:VAL:HG13	1:B:681:VAL:HG21	1.82	0.60
1:B:431:GLU:OE2	1:B:488:ARG:NH1	2.35	0.60
1:C:822:ASP:HA	1:C:825:LYS:HE3	1.83	0.60
1:B:217:THR:HG22	1:B:310:ARG:HB2	1.82	0.60
1:C:218:PRO:HA	1:C:222:CYS:HB3	1.83	0.60
1:A:609:GLU:HG2	1:A:618:ARG:HG2	1.83	0.60
1:C:347:ASP:OD2	1:C:695:ARG:NH2	2.35	0.60
1:C:234:LEU:HG	1:C:238:LYS:HE2	1.83	0.59
1:C:843:LEU:O	1:C:847:GLU:HG3	2.02	0.59
1:A:450:LEU:HD12	1:A:579:VAL:HG12	1.84	0.59
1:B:347:ASP:OD2	1:B:695:ARG:NH2	2.35	0.59
1:A:197:PRO:HB2	1:A:205:GLY:HA3	1.85	0.59
1:C:427:PHE:HB3	1:C:491:ALA:HB1	1.85	0.59
1:B:234:LEU:HG	1:B:238:LYS:HE2	1.84	0.59
1:B:268:ASP:OD1	1:B:273:HIS:NE2	2.35	0.59
1:B:830:PHE:CE2	1:B:1078:LEU:HD22	2.37	0.58
1:B:706:THR:HG23	1:B:707:PRO:HD3	1.85	0.58
1:C:333:LEU:HB3	1:C:346:VAL:HB	1.85	0.58
1:C:1215:ASP:OD2	1:C:1217:LYS:NZ	2.37	0.58
1:B:1047:PHE:CD2	1:B:1076:GLY:HA3	2.38	0.58
1:C:145:ARG:HG2	1:C:317:LYS:HA	1.83	0.58
1:C:880:PRO:HG2	1:C:888:LYS:HD2	1.85	0.58
1:B:1061:LEU:O	1:B:1066:GLN:NE2	2.36	0.58
1:B:943:ASP:OD2	1:B:944:PRO:HD2	2.04	0.58
1:A:741:ILE:HB	1:A:761:GLN:HB2	1.87	0.57
1:C:830:PHE:CE1	1:C:1078:LEU:HD22	2.40	0.57
1:A:333:LEU:HB3	1:A:346:VAL:HB	1.86	0.57
1:A:623:ASN:HB2	4:A:1409:NAG:H2	1.86	0.57
1:B:1215:ASP:OD2	1:B:1217:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASP:OD2	1:C:59:LYS:NZ	2.38	0.57
1:A:417:ASN:HB3	1:A:591:MET:HG2	1.87	0.57
1:A:415:ASN:HA	1:A:587:SER:HB2	1.85	0.57
1:C:197:PRO:HB2	1:C:205:GLY:HA3	1.87	0.57
1:B:415:ASN:HA	1:B:587:SER:HB2	1.86	0.57
1:C:1163:ASN:HB3	1:C:1164:PRO:HD3	1.87	0.57
1:B:140:SER:HB2	1:B:316:ARG:NH2	2.20	0.56
1:C:217:THR:HG22	1:C:310:ARG:HD3	1.86	0.56
1:C:655:VAL:O	1:C:656:ARG:NH1	2.37	0.56
1:A:114:ARG:HH21	1:A:168:ILE:HG21	1.70	0.56
1:A:234:LEU:HG	1:A:238:LYS:HE2	1.87	0.56
1:B:1128:SER:OG	1:B:1141:HIS:ND1	2.33	0.56
4:A:1413:NAG:H2	1:C:623:ASN:HB2	1.86	0.56
1:A:822:ASP:HA	1:A:825:LYS:HE3	1.87	0.56
1:C:114:ARG:HH21	1:C:168:ILE:HG21	1.71	0.56
1:B:1105:LYS:NZ	1:B:1119:PHE:O	2.29	0.56
1:B:166:THR:HB	1:B:168:ILE:HG12	1.88	0.56
1:B:880:PRO:HG2	1:B:888:LYS:HD2	1.86	0.56
1:A:431:GLU:OE2	1:A:488:ARG:NH1	2.38	0.56
1:B:822:ASP:HA	1:B:825:LYS:HE3	1.86	0.56
1:B:277:SER:O	1:B:277:SER:OG	2.23	0.56
1:B:182:ASP:OD2	1:B:231:LEU:N	2.39	0.55
1:A:166:THR:HB	1:A:168:ILE:HG12	1.89	0.55
1:C:943:ASP:OD2	1:C:944:PRO:HD2	2.06	0.55
1:C:166:THR:HB	1:C:168:ILE:HG12	1.88	0.55
1:C:279:LYS:HG3	1:C:290:PHE:HB3	1.88	0.55
1:A:1163:ASN:HB3	1:A:1164:PRO:HD3	1.89	0.55
1:A:737:SER:HB2	1:B:943:ASP:HB2	1.89	0.55
1:B:333:LEU:HB3	1:B:346:VAL:HB	1.89	0.55
1:C:450:LEU:HD12	1:C:579:VAL:HG12	1.89	0.55
1:A:145:ARG:HG2	1:A:317:LYS:HA	1.89	0.54
1:B:385:GLU:OE2	1:B:647:SER:OG	2.25	0.54
1:C:661:VAL:HG13	1:C:681:VAL:HG21	1.90	0.54
1:C:1047:PHE:CD2	1:C:1076:GLY:HA3	2.42	0.54
1:C:30:GLY:O	1:C:198:ARG:NH1	2.41	0.54
1:C:801:THR:OG1	1:C:845:GLN:OE1	2.25	0.54
1:B:583:THR:HG21	1:C:69:LYS:HG3	1.89	0.54
1:A:1160:ASN:ND2	1:A:1229:LEU:O	2.41	0.54
1:A:385:GLU:OE2	1:A:647:SER:OG	2.25	0.54
1:A:108:PHE:HD2	1:A:139:ILE:HB	1.73	0.54
1:B:125:VAL:N	1:B:263:PHE:O	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:OD2	1:B:59:LYS:NZ	2.40	0.53
1:B:280:GLU:HG3	1:B:288:PHE:CG	2.43	0.53
1:A:1047:PHE:CD2	1:A:1076:GLY:HA3	2.44	0.53
1:C:1061:LEU:O	1:C:1066:GLN:NE2	2.39	0.53
1:C:1171:ILE:HD11	1:C:1210:LYS:HB3	1.90	0.53
1:A:684:SER:O	1:A:688:THR:HG23	2.08	0.53
1:C:1128:SER:OG	1:C:1141:HIS:ND1	2.32	0.53
1:B:1163:ASN:HB3	1:B:1164:PRO:HD3	1.90	0.53
1:A:705:THR:HB	1:A:707:PRO:HD2	1.91	0.52
1:B:450:LEU:HD12	1:B:579:VAL:HG12	1.90	0.52
1:C:214:VAL:HG13	1:C:307:ARG:HG2	1.90	0.52
1:C:894:GLU:HG3	1:C:1131:ILE:HB	1.91	0.52
1:A:182:ASP:N	1:A:187:LEU:O	2.36	0.52
1:A:410:ARG:NH2	1:A:528:GLY:O	2.32	0.52
1:B:1171:ILE:HD11	1:B:1210:LYS:HB3	1.92	0.52
1:C:503:PRO:HD2	1:C:571:LEU:HD13	1.92	0.52
1:C:865:GLN:O	1:C:869:ASN:ND2	2.42	0.52
1:C:1160:ASN:ND2	1:C:1229:LEU:O	2.43	0.52
1:B:30:GLY:O	1:B:198:ARG:NH1	2.42	0.52
1:B:73:ASN:HB3	4:B:1401:NAG:O5	2.10	0.52
1:A:361:GLU:OE1	1:B:829:GLN:NE2	2.29	0.52
1:A:964:THR:HG21	1:C:1174:TYR:CZ	2.45	0.52
1:C:787:THR:HG1	1:C:1148:SER:HG	1.58	0.52
1:A:124:ILE:HG22	1:A:287:MET:HE1	1.91	0.51
1:C:385:GLU:OE2	1:C:647:SER:OG	2.27	0.51
1:C:32:GLY:O	1:C:198:ARG:NH2	2.43	0.51
1:C:182:ASP:N	1:C:187:LEU:O	2.40	0.51
1:A:126:ARG:HD3	1:A:129:ALA:HB2	1.92	0.51
1:B:1126:ILE:HD11	1:B:1144:TYR:HB2	1.92	0.51
1:C:684:SER:O	1:C:688:THR:HG23	2.10	0.51
1:A:1171:ILE:HD11	1:A:1210:LYS:HB3	1.93	0.51
1:B:369:VAL:HG13	1:B:666:ILE:HG13	1.92	0.51
1:A:32:GLY:O	1:A:198:ARG:NH2	2.42	0.51
1:A:830:PHE:CE2	1:A:1078:LEU:HD22	2.46	0.51
1:A:943:ASP:HB2	1:C:737:SER:HB2	1.93	0.51
1:B:155:MET:HG3	1:B:305:ILE:HD11	1.92	0.51
1:A:545:ARG:HH11	1:A:545:ARG:HG2	1.76	0.50
1:B:463:SER:HA	1:B:466:GLN:HG3	1.92	0.50
1:A:503:PRO:HD2	1:A:571:LEU:HD13	1.93	0.50
1:A:583:THR:HG21	1:B:69:LYS:HG3	1.92	0.50
1:A:1174:TYR:CZ	1:B:964:THR:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:O	1:B:235:ASN:ND2	2.44	0.50
1:C:81:LEU:HD22	1:C:121:ASP:HB3	1.93	0.50
1:A:865:GLN:O	1:A:869:ASN:ND2	2.45	0.50
1:B:313:PHE:HA	1:B:316:ARG:HD2	1.94	0.50
1:A:355:GLN:O	1:A:359:SER:OG	2.21	0.50
1:B:402:PRO:HG3	1:B:571:LEU:HD21	1.94	0.50
1:B:685:HIS:ND1	1:C:913:ASP:OD2	2.45	0.50
1:C:758:ASP:N	1:C:758:ASP:OD1	2.44	0.50
1:B:620:VAL:N	1:B:656:ARG:O	2.31	0.50
1:B:737:SER:HB2	1:C:943:ASP:HB2	1.94	0.50
1:C:463:SER:HA	1:C:466:GLN:HG3	1.94	0.50
1:B:894:GLU:HG3	1:B:1131:ILE:HB	1.93	0.50
1:C:799:GLU:HA	1:C:1136:GLY:HA3	1.94	0.50
1:C:807:VAL:HG11	1:C:1081:LEU:HD11	1.94	0.50
1:A:657:PRO:HG3	1:B:932:VAL:HA	1.94	0.49
1:C:705:THR:HB	1:C:707:PRO:HD2	1.93	0.49
1:A:932:VAL:HA	1:C:657:PRO:HG2	1.94	0.49
1:B:124:ILE:HG22	1:B:287:MET:HE1	1.94	0.49
1:A:1168:ILE:HG12	1:A:1229:LEU:HD21	1.94	0.49
1:B:112:TYR:HB2	1:B:306:PRO:HG3	1.93	0.49
1:A:1128:SER:OG	1:A:1141:HIS:ND1	2.31	0.49
1:B:705:THR:HB	1:B:707:PRO:HD2	1.94	0.49
1:C:834:ILE:HG23	1:C:1085:VAL:HG21	1.95	0.49
1:A:907:GLY:O	1:C:680:SER:OG	2.25	0.49
1:B:355:GLN:O	1:B:359:SER:OG	2.20	0.49
1:C:276:SER:HB3	1:C:279:LYS:HG2	1.94	0.49
1:B:1168:ILE:HG12	1:B:1229:LEU:HD21	1.93	0.49
1:B:1144:TYR:OH	1:B:1197:SER:O	2.22	0.48
1:B:889:TYR:HB3	1:B:945:TYR:CD1	2.48	0.48
1:A:128:GLY:HA3	1:A:149:LYS:HB2	1.96	0.48
1:B:249:ARG:HH21	2:H:1:NAG:H2	1.77	0.48
1:B:503:PRO:HD2	1:B:571:LEU:HD13	1.94	0.48
1:B:758:ASP:OD1	1:B:758:ASP:N	2.46	0.48
1:C:193:CYS:CB	1:C:246:CYS:HA	2.40	0.48
1:C:1168:ILE:HG12	1:C:1229:LEU:HD21	1.95	0.48
1:B:986:VAL:HG21	1:B:1126:ILE:HD13	1.96	0.48
1:B:849:ILE:HG22	1:B:941:LEU:HD23	1.95	0.48
1:C:706:THR:HG23	1:C:707:PRO:HD3	1.96	0.48
1:A:50:ILE:HG22	1:A:52:PRO:HD3	1.96	0.48
1:B:1174:TYR:CZ	1:C:964:THR:HG21	2.48	0.48
1:A:463:SER:HA	1:A:466:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:HG23	1:A:658:CYS:HA	1.94	0.48
1:A:758:ASP:N	1:A:758:ASP:OD1	2.44	0.48
1:C:355:GLN:O	1:C:359:SER:OG	2.23	0.48
1:C:268:ASP:OD2	1:C:270:GLN:N	2.46	0.47
1:C:892:ALA:O	1:C:896:LEU:HD12	2.13	0.47
1:A:466:GLN:O	1:A:469:SER:OG	2.27	0.47
1:C:138:VAL:HG12	1:C:140:SER:N	2.30	0.47
1:C:402:PRO:HG3	1:C:571:LEU:HD21	1.97	0.47
1:A:726:VAL:HG13	1:A:766:ASN:HB2	1.97	0.47
1:B:726:VAL:HG13	1:B:766:ASN:HB2	1.96	0.47
1:C:622:HIS:HE1	1:C:656:ARG:HB2	1.78	0.47
1:B:151:TYR:O	1:B:307:ARG:NH1	2.47	0.47
1:B:1160:ASN:ND2	1:B:1229:LEU:O	2.47	0.47
1:C:50:ILE:HG22	1:C:52:PRO:HD3	1.97	0.47
1:A:685:HIS:CE1	1:B:916:MET:HE1	2.50	0.47
1:B:148:LYS:O	1:B:320:ALA:N	2.47	0.47
1:B:697:THR:HG23	1:B:718:MET:HE1	1.96	0.47
1:B:105:SER:O	1:B:310:ARG:NH1	2.48	0.47
1:C:466:GLN:O	1:C:469:SER:OG	2.31	0.46
1:C:1159:CYS:HB3	1:C:1167:CYS:CA	2.35	0.46
1:B:799:GLU:HA	1:B:1136:GLY:HA3	1.96	0.46
1:A:262:TRP:HB3	1:A:287:MET:SD	2.56	0.46
1:A:986:VAL:HG23	1:A:1113:GLN:HE22	1.78	0.46
1:C:222:CYS:N	1:C:230:GLN:OE1	2.45	0.46
1:A:1205:THR:O	1:A:1209:SER:OG	2.24	0.46
1:B:525:ASN:ND2	1:B:529:GLY:O	2.48	0.46
1:A:717:ALA:HB1	1:A:720:PHE:CD2	2.50	0.46
1:A:1126:ILE:HD11	1:A:1144:TYR:HB2	1.97	0.46
1:B:819:LYS:HE2	1:B:819:LYS:HB3	1.78	0.46
1:A:30:GLY:O	1:A:198:ARG:NH1	2.48	0.46
1:A:1159:CYS:HB3	1:A:1167:CYS:CA	2.36	0.46
1:B:680:SER:OG	1:C:907:GLY:O	2.26	0.46
1:B:1074:ILE:O	1:B:1078:LEU:HG	2.16	0.46
1:C:267:GLN:NE2	1:C:297:GLN:O	2.41	0.46
1:B:217:THR:OG1	1:B:221:ASP:OD2	2.33	0.46
1:C:196:GLN:HB3	1:C:242:ASP:HB2	1.98	0.46
1:C:369:VAL:HG13	1:C:666:ILE:HG13	1.96	0.46
1:A:175:HIS:HB3	1:A:192:TYR:CZ	2.50	0.46
1:A:369:VAL:HG13	1:A:666:ILE:HG13	1.98	0.46
1:C:73:ASN:OD1	1:C:338:VAL:HA	2.15	0.46
1:C:223:ALA:HB3	1:C:227:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLU:HA	1:A:1136:GLY:HA3	1.97	0.46
1:B:717:ALA:HB1	1:B:720:PHE:CD2	2.51	0.46
1:A:74:ILE:HD13	1:A:76:LEU:HD21	1.97	0.46
1:B:182:ASP:N	1:B:187:LEU:O	2.42	0.46
1:C:124:ILE:HG22	1:C:287:MET:HE1	1.98	0.45
1:C:346:VAL:HG23	1:C:363:PHE:CE2	2.52	0.45
1:A:603:LYS:HB3	1:A:608:VAL:HG11	1.98	0.45
1:A:706:THR:HG23	1:A:707:PRO:HD3	1.99	0.45
1:A:222:CYS:HA	1:A:230:GLN:HG3	1.98	0.45
1:B:1088:GLN:O	1:B:1092:THR:OG1	2.34	0.45
1:C:1021:ALA:O	1:C:1025:VAL:HG23	2.17	0.45
1:C:643:VAL:O	1:C:655:VAL:N	2.49	0.45
1:A:113:SER:HB3	1:A:211:SER:HB2	1.98	0.45
1:A:214:VAL:HG13	1:A:307:ARG:HG2	1.98	0.45
1:C:513:TYR:CZ	1:C:520:LYS:HE2	2.52	0.45
1:B:397:MET:HE2	1:B:411:LEU:HD12	1.99	0.45
1:C:520:LYS:HA	1:C:520:LYS:HD3	1.65	0.45
1:C:843:LEU:HD12	1:C:843:LEU:HA	1.85	0.45
1:C:460:ASP:N	1:C:460:ASP:OD1	2.50	0.45
1:B:50:ILE:HG22	1:B:52:PRO:HD3	1.99	0.44
1:C:984:ASN:HA	1:C:988:ILE:O	2.18	0.44
1:A:843:LEU:HD12	1:A:843:LEU:HA	1.85	0.44
1:B:797:PHE:CD1	1:B:1025:VAL:HG22	2.53	0.44
1:C:125:VAL:N	1:C:263:PHE:O	2.39	0.44
1:C:944:PRO:HA	1:C:947:GLU:HG3	1.99	0.44
1:B:723:SER:HB3	1:B:761:GLN:HB3	1.98	0.44
1:B:961:ALA:HA	1:B:973:ILE:HD12	1.98	0.44
1:A:1021:ALA:O	1:A:1025:VAL:HG23	2.18	0.44
1:B:175:HIS:HB3	1:B:192:TYR:CZ	2.53	0.44
1:C:1008:LEU:O	1:C:1011:MET:HG2	2.18	0.44
1:A:155:MET:HG3	1:A:305:ILE:HD11	1.99	0.44
1:A:158:HIS:CE1	1:A:297:GLN:HB3	2.53	0.44
1:B:73:ASN:OD1	1:B:338:VAL:HA	2.17	0.44
1:C:249:ARG:HH21	2:L:1:NAG:H2	1.81	0.44
1:C:717:ALA:HB1	1:C:720:PHE:CD1	2.53	0.44
1:C:926:LEU:HD12	1:C:1036:LEU:HB2	1.99	0.44
1:A:346:VAL:HG23	1:A:363:PHE:CE2	2.53	0.44
1:B:113:SER:HB3	1:B:211:SER:HB2	1.99	0.44
1:A:111:ASN:O	1:A:115:GLN:HG3	2.18	0.44
1:A:493:VAL:HG13	1:A:497:LEU:HD23	2.00	0.44
1:B:346:VAL:HG23	1:B:363:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASN:HB3	4:C:1401:NAG:O5	2.17	0.44
1:A:1064:PRO:HG3	1:B:467:PRO:HB3	1.99	0.43
1:B:335:ASN:HB3	1:B:344:LYS:HG3	2.00	0.43
1:B:1021:ALA:O	1:B:1025:VAL:HG23	2.17	0.43
1:A:801:THR:HG22	1:A:849:ILE:HD11	1.99	0.43
1:C:217:THR:HG22	1:C:310:ARG:HB2	2.00	0.43
1:B:172:TYR:OH	1:B:303:THR:HG23	2.18	0.43
1:C:279:LYS:HA	1:C:279:LYS:HD3	1.86	0.43
1:A:685:HIS:ND1	1:B:913:ASP:OD2	2.49	0.43
1:C:151:TYR:O	1:C:307:ARG:NH1	2.51	0.43
1:C:376:GLU:OE2	1:C:695:ARG:NH1	2.52	0.43
1:A:819:LYS:HE2	1:A:819:LYS:HB3	1.76	0.43
1:B:834:ILE:HG23	1:B:1085:VAL:HG21	1.99	0.43
1:A:249:ARG:HH21	2:D:1:NAG:H2	1.83	0.43
1:A:943:ASP:OD1	1:A:944:PRO:HD2	2.19	0.43
1:B:376:GLU:OE1	1:B:695:ARG:NH1	2.51	0.43
1:C:493:VAL:HG13	1:C:497:LEU:HD23	2.01	0.43
1:A:655:VAL:O	1:A:656:ARG:NH1	2.50	0.43
1:A:804:LYS:HE3	1:A:804:LYS:HB2	1.74	0.43
1:A:830:PHE:HZ	1:A:1081:LEU:HB3	1.84	0.43
1:A:660:SER:HB2	1:B:912:TYR:HE1	1.84	0.43
1:C:467:PRO:HD3	1:C:488:ARG:NH2	2.34	0.43
1:B:217:THR:OG1	1:B:217:THR:O	2.37	0.42
1:C:390:LYS:O	1:C:417:ASN:N	2.52	0.42
1:B:397:MET:HG3	1:B:454:TYR:CG	2.55	0.42
1:B:276:SER:HB2	1:B:290:PHE:CD1	2.55	0.42
1:B:1153:THR:H	4:B:1412:NAG:H62	1.84	0.42
1:A:1153:THR:H	4:A:1412:NAG:H62	1.84	0.42
1:B:467:PRO:HD3	1:B:488:ARG:NH2	2.34	0.42
1:C:139:ILE:HD12	1:C:139:ILE:HA	1.83	0.42
1:C:412:VAL:HG22	1:C:451:THR:HG23	2.01	0.42
1:A:1144:TYR:OH	1:A:1197:SER:O	2.26	0.42
1:B:108:PHE:O	1:B:308:SER:OG	2.38	0.42
1:C:1153:THR:H	4:C:1411:NAG:H62	1.84	0.42
1:A:722:ASN:OD1	1:A:722:ASN:N	2.50	0.42
1:B:944:PRO:HA	1:B:947:GLU:HG3	2.02	0.42
1:A:545:ARG:HG2	1:A:545:ARG:NH1	2.34	0.42
1:C:1034:MET:HE3	1:C:1034:MET:HB2	1.94	0.42
1:A:402:PRO:HG3	1:A:571:LEU:HD21	2.00	0.42
1:A:909:MET:O	1:A:910:GLN:HG2	2.20	0.42
1:C:112:TYR:HB2	1:C:306:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PRO:HD3	1:A:488:ARG:NH2	2.35	0.41
1:A:545:ARG:HD3	1:A:545:ARG:HA	1.75	0.41
1:C:149:LYS:HA	1:C:320:ALA:HB3	2.02	0.41
1:C:819:LYS:HE2	1:C:819:LYS:HB3	1.84	0.41
1:A:56:ASP:OD2	1:A:59:LYS:NZ	2.44	0.41
1:A:946:MET:HE2	1:A:946:MET:HA	2.02	0.41
1:A:986:VAL:HG21	1:A:1126:ILE:HD13	2.02	0.41
1:B:926:LEU:HD12	1:B:1036:LEU:HB2	2.02	0.41
1:C:172:TYR:OH	1:C:303:THR:HG23	2.20	0.41
1:C:413:PHE:CD2	1:C:450:LEU:HD23	2.55	0.41
1:A:797:PHE:CD1	1:A:1025:VAL:HG22	2.54	0.41
1:B:116:VAL:HG21	1:B:160:VAL:HG21	2.02	0.41
1:B:986:VAL:HG23	1:B:1113:GLN:HE22	1.85	0.41
1:C:810:LYS:HB3	1:C:810:LYS:HE3	1.97	0.41
1:C:1144:TYR:CE2	1:C:1197:SER:HB3	2.56	0.41
1:A:810:LYS:NZ	1:C:374:SER:O	2.49	0.41
1:B:133:LYS:O	1:B:147:ILE:N	2.51	0.41
1:B:907:GLY:HA3	1:B:911:GLY:HA3	2.02	0.41
1:C:1180:THR:O	1:C:1181:ILE:HG13	2.20	0.41
1:A:111:ASN:O	1:A:114:ARG:HG3	2.19	0.41
1:C:158:HIS:CE1	1:C:297:GLN:HB3	2.56	0.41
1:C:798:ILE:HD11	1:C:1105:LYS:HD2	2.02	0.41
1:C:909:MET:O	1:C:910:GLN:HG2	2.19	0.41
1:A:460:ASP:N	1:A:460:ASP:OD1	2.53	0.41
1:C:257:ASP:HB2	1:C:278:ARG:HH22	1.85	0.41
1:C:268:ASP:OD2	1:C:268:ASP:C	2.63	0.41
1:A:926:LEU:HD12	1:A:1036:LEU:HB2	2.03	0.41
1:B:600:ILE:H	1:B:600:ILE:HG13	1.73	0.41
1:C:264:GLY:HA3	1:C:287:MET:HE1	2.03	0.41
1:A:172:TYR:OH	1:A:303:THR:HG23	2.21	0.41
1:A:834:ILE:HG23	1:A:1085:VAL:HG21	2.02	0.41
1:A:1074:ILE:O	1:A:1078:LEU:HG	2.21	0.41
1:B:145:ARG:HG3	1:B:146:PRO:HD2	2.03	0.41
1:B:493:VAL:HG13	1:B:497:LEU:HD23	2.02	0.41
1:B:1196:SER:O	1:C:969:SER:HB3	2.20	0.41
1:C:107:LEU:HD21	1:C:310:ARG:HG3	2.03	0.41
1:A:248:PHE:CD2	1:A:294:PRO:HG2	2.56	0.41
1:A:280:GLU:HB2	1:A:288:PHE:CD1	2.54	0.41
1:A:413:PHE:CD2	1:A:450:LEU:HD23	2.56	0.41
1:A:467:PRO:HB3	1:C:1064:PRO:HG3	2.02	0.41
1:B:158:HIS:CE1	1:B:297:GLN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ILE:HD12	1:B:776:ILE:HA	1.92	0.41
1:C:823:LEU:HD21	1:C:1067:GLU:HA	2.02	0.41
1:C:982:ARG:HD3	1:C:1126:ILE:O	2.21	0.41
1:A:62:GLY:HA3	1:A:124:ILE:HD12	2.02	0.40
1:A:1042:GLU:HG2	1:A:1080:SER:HB2	2.03	0.40
1:C:108:PHE:HD1	1:C:108:PHE:HA	1.77	0.40
1:C:111:ASN:OD1	1:C:111:ASN:N	2.48	0.40
1:A:1063:PRO:HA	1:A:1066:GLN:HG2	2.03	0.40
1:B:107:LEU:HD21	1:B:310:ARG:HG3	2.03	0.40
1:B:196:GLN:HB3	1:B:242:ASP:HB2	2.03	0.40
1:C:113:SER:HB3	1:C:211:SER:HB2	2.02	0.40
1:C:175:HIS:HB3	1:C:192:TYR:CZ	2.56	0.40
1:C:335:ASN:HB3	1:C:344:LYS:HG3	2.03	0.40
1:A:267:GLN:NE2	1:A:297:GLN:O	2.51	0.40
1:C:116:VAL:HG21	1:C:160:VAL:HG21	2.03	0.40
1:C:797:PHE:CD1	1:C:1025:VAL:HG22	2.56	0.40
1:A:182:ASP:OD2	1:A:231:LEU:HA	2.21	0.40
1:A:513:TYR:CZ	1:A:520:LYS:HE2	2.57	0.40
1:B:412:VAL:HG22	1:B:451:THR:HG23	2.02	0.40
1:C:690:MET:SD	1:C:702:LEU:HG	2.62	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	1175/1344 (87%)	1143 (97%)	32 (3%)	0	100	100
1	B	1175/1344 (87%)	1149 (98%)	26 (2%)	0	100	100
1	C	1175/1344 (87%)	1139 (97%)	36 (3%)	0	100	100
All	All	3525/4032 (87%)	3431 (97%)	94 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1024/1163 (88%)	1010 (99%)	14 (1%)	62 87
1	B	1024/1163 (88%)	1011 (99%)	13 (1%)	65 88
1	C	1024/1163 (88%)	1012 (99%)	12 (1%)	67 89
All	All	3072/3489 (88%)	3033 (99%)	39 (1%)	64 88

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	136	THR
1	A	164	THR
1	A	210	THR
1	A	359	SER
1	A	472	GLU
1	A	546	GLN
1	A	643	VAL
1	A	664	SER
1	A	689	MET
1	A	876	MET
1	A	986	VAL
1	A	1017	THR
1	A	1194	THR
1	B	26	MET
1	B	77	THR
1	B	147	ILE
1	B	164	THR
1	B	210	THR
1	B	214	VAL
1	B	339	GLU
1	B	365	VAL
1	B	539	SER

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Mol	Chain	Res	Type
1	B	545	ARG
1	B	690	MET
1	B	986	VAL
1	B	1017	THR
1	C	160	VAL
1	C	164	THR
1	C	166	THR
1	C	210	THR
1	C	214	VAL
1	C	285	ASN
1	C	287	MET
1	C	376	GLU
1	C	448	SER
1	C	500	ILE
1	C	810	LYS
1	C	1017	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASN
1	A	335	ASN
1	A	386	GLN
1	A	415	ASN
1	A	829	GLN
1	A	881	GLN
1	A	1012	GLN
1	A	1019	ASN
1	A	1026	GLN
1	A	1066	GLN
1	A	1132	ASN
1	B	49	ASN
1	B	115	GLN
1	B	235	ASN
1	B	851	ASN
1	B	869	ASN
1	B	1019	ASN
1	B	1026	GLN
1	B	1132	ASN
1	C	49	ASN
1	C	115	GLN

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Mol	Chain	Res	Type
1	C	175	HIS
1	C	189	HIS
1	C	386	GLN
1	C	548	HIS
1	C	722	ASN
1	C	766	ASN
1	C	851	ASN
1	C	881	GLN
1	C	1019	ASN
1	C	1026	GLN
1	C	1113	GLN
1	C	1132	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)

27 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	2,1	14,14,15	0.79	0	17,19,21	2.32	3 (17%)
2	NAG	D	2	2	14,14,15	0.75	0	17,19,21	2.35	3 (17%)
3	NAG	E	1	3	14,14,15	0.73	0	17,19,21	0.75	0
3	NAG	E	2	3	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
3	BMA	E	3	3	11,11,12	0.83	0	15,15,17	2.09	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	1	2,1	14,14,15	0.72	0	17,19,21	1.27	2 (11%)
2	NAG	F	2	2	14,14,15	0.73	0	17,19,21	1.17	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.75	0	17,19,21	0.95	0
2	NAG	G	2	2	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.79	0	17,19,21	2.33	3 (17%)
2	NAG	H	2	2	14,14,15	0.75	0	17,19,21	2.35	3 (17%)
3	NAG	I	1	3	14,14,15	0.72	0	17,19,21	0.72	0
3	NAG	I	2	3	14,14,15	0.75	0	17,19,21	0.96	2 (11%)
3	BMA	I	3	3	11,11,12	0.82	0	15,15,17	2.10	4 (26%)
2	NAG	J	1	2,1	14,14,15	0.73	0	17,19,21	1.26	2 (11%)
2	NAG	J	2	2	14,14,15	0.73	0	17,19,21	1.18	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.75	0	17,19,21	0.93	0
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.78	0	17,19,21	2.32	3 (17%)
2	NAG	L	2	2	14,14,15	0.75	0	17,19,21	2.36	3 (17%)
3	NAG	M	1	3	14,14,15	0.70	0	17,19,21	0.73	0
3	NAG	M	2	3	14,14,15	0.72	0	17,19,21	1.63	3 (17%)
3	BMA	M	3	3	11,11,12	0.84	0	15,15,17	2.36	3 (20%)
2	NAG	N	1	2,1	14,14,15	0.74	0	17,19,21	1.26	2 (11%)
2	NAG	N	2	2	14,14,15	0.73	0	17,19,21	1.18	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.75	0	17,19,21	0.95	0
2	NAG	O	2	2	14,14,15	0.70	0	17,19,21	1.18	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
3	NAG	I	1	3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1
3	NAG	M	1	3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	2	NAG	C2-N2-C7	8.45	134.22	122.90
2	H	2	NAG	C2-N2-C7	8.45	134.22	122.90
2	D	2	NAG	C2-N2-C7	8.44	134.21	122.90
2	H	1	NAG	C2-N2-C7	8.19	133.87	122.90
2	L	1	NAG	C2-N2-C7	8.18	133.86	122.90
2	D	1	NAG	C2-N2-C7	8.17	133.85	122.90
3	M	3	BMA	C1-O5-C5	7.56	122.32	112.19
3	I	3	BMA	C1-O5-C5	6.19	120.48	112.19
3	E	3	BMA	C1-O5-C5	6.18	120.47	112.19
3	M	2	NAG	C1-O5-C5	4.36	118.02	112.19
2	F	1	NAG	C2-N2-C7	3.27	127.28	122.90
2	O	2	NAG	C2-N2-C7	3.26	127.27	122.90
2	N	1	NAG	C2-N2-C7	3.24	127.25	122.90
2	J	1	NAG	C2-N2-C7	3.24	127.24	122.90
2	K	2	NAG	C2-N2-C7	3.20	127.19	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C2-N2-C7	3.19	127.17	122.90
2	J	2	NAG	C2-N2-C7	3.15	127.12	122.90
2	N	2	NAG	C2-N2-C7	3.15	127.12	122.90
2	F	2	NAG	C2-N2-C7	3.15	127.12	122.90
3	I	3	BMA	C3-C4-C5	2.72	115.16	110.23
3	E	3	BMA	C3-C4-C5	2.69	115.10	110.23
2	H	1	NAG	C8-C7-N2	2.57	120.37	116.12
3	M	2	NAG	O4-C4-C5	2.56	115.63	109.32
2	D	1	NAG	C8-C7-N2	2.56	120.36	116.12
2	L	1	NAG	C8-C7-N2	2.55	120.35	116.12
2	D	2	NAG	C8-C7-N2	2.51	120.28	116.12
2	H	2	NAG	C8-C7-N2	2.50	120.27	116.12
2	L	2	NAG	C8-C7-N2	2.47	120.21	116.12
3	M	3	BMA	C2-C3-C4	2.38	115.05	110.86
2	H	1	NAG	C1-C2-N2	2.28	114.02	110.43
2	L	1	NAG	C1-C2-N2	2.27	114.01	110.43
2	D	1	NAG	C1-C2-N2	2.20	113.90	110.43
2	D	2	NAG	C1-C2-N2	2.18	113.86	110.43
2	L	2	NAG	C1-C2-N2	2.17	113.86	110.43
3	M	2	NAG	C3-C4-C5	-2.16	106.32	110.23
3	E	3	BMA	C2-C3-C4	2.15	114.64	110.86
3	I	2	NAG	C2-N2-C7	2.15	125.78	122.90
2	J	1	NAG	O5-C1-C2	-2.14	107.98	111.29
3	E	2	NAG	C2-N2-C7	2.14	125.77	122.90
2	H	2	NAG	C1-C2-N2	2.14	113.80	110.43
2	F	1	NAG	O5-C1-C2	-2.13	107.99	111.29
3	I	3	BMA	C2-C3-C4	2.12	114.60	110.86
3	M	3	BMA	C3-C4-C5	2.12	114.07	110.23
3	I	2	NAG	O5-C1-C2	-2.10	108.04	111.29
2	N	1	NAG	O5-C1-C2	-2.01	108.17	111.29
3	I	3	BMA	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2

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

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Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7

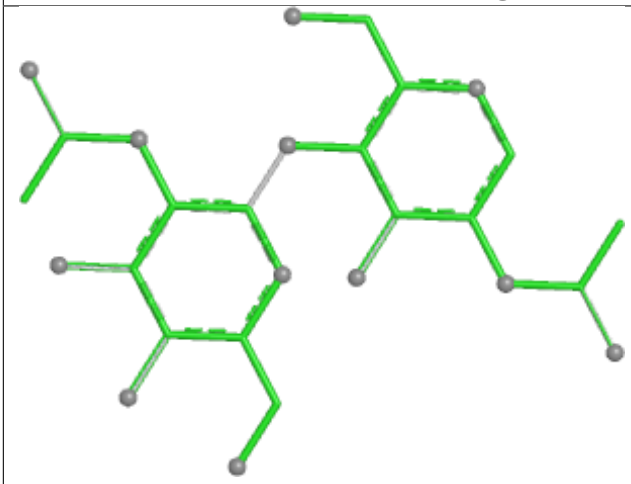
There are no ring outliers.

3 monomers are involved in 3 short contacts:

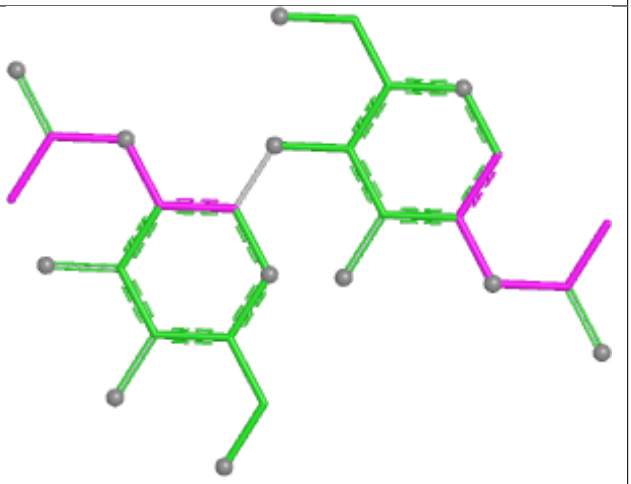
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	H	1	NAG	1	0
2	L	1	NAG	1	0

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

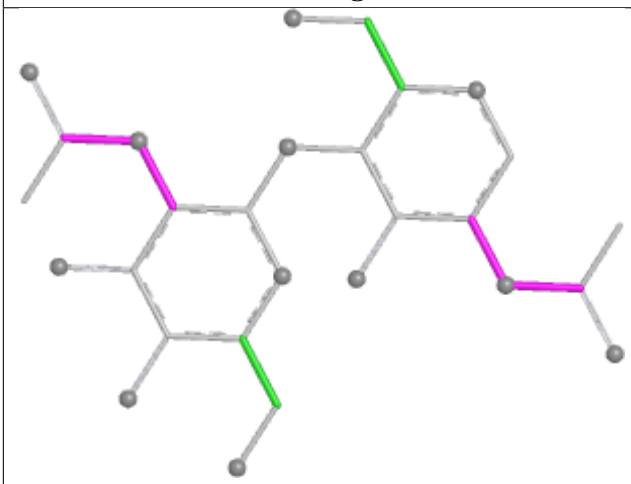
Oligosaccharide Chain D



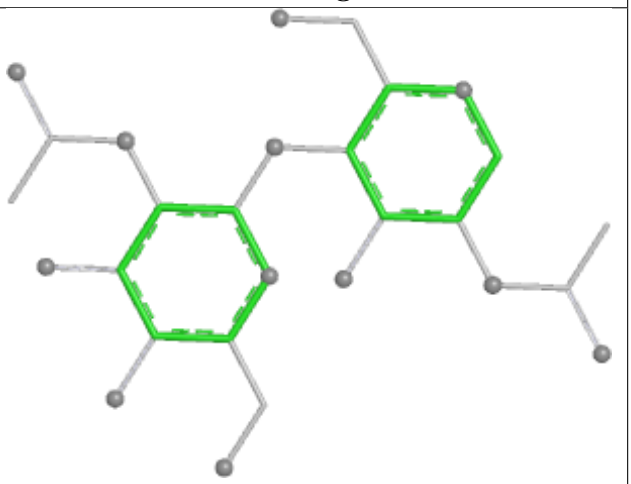
Bond lengths



Bond angles

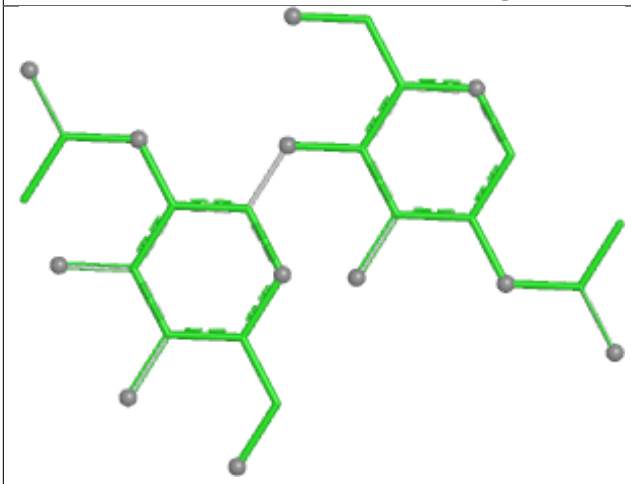


Torsions

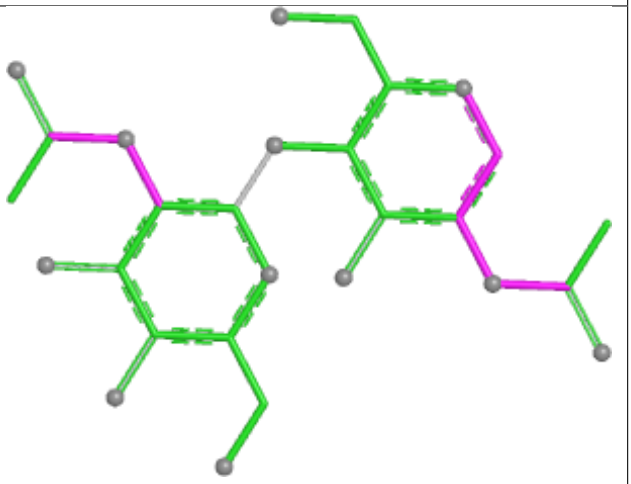


Rings

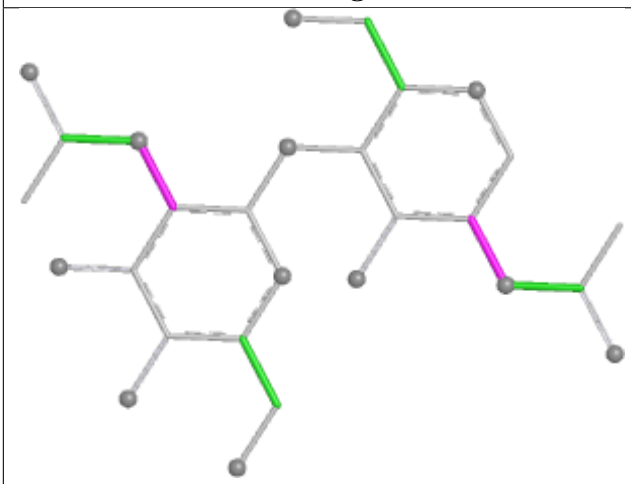
Oligosaccharide Chain F



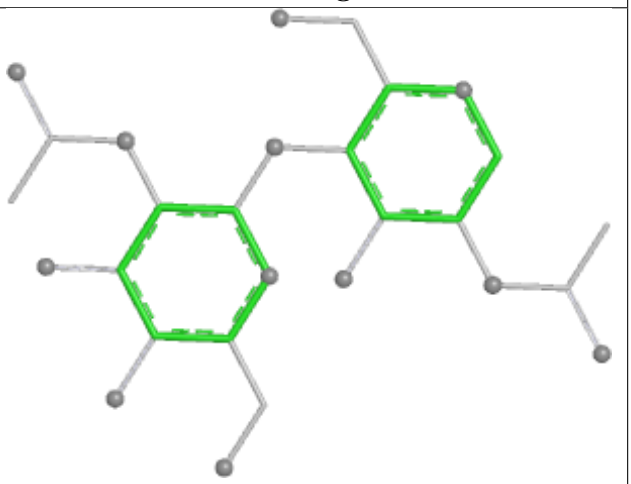
Bond lengths



Bond angles

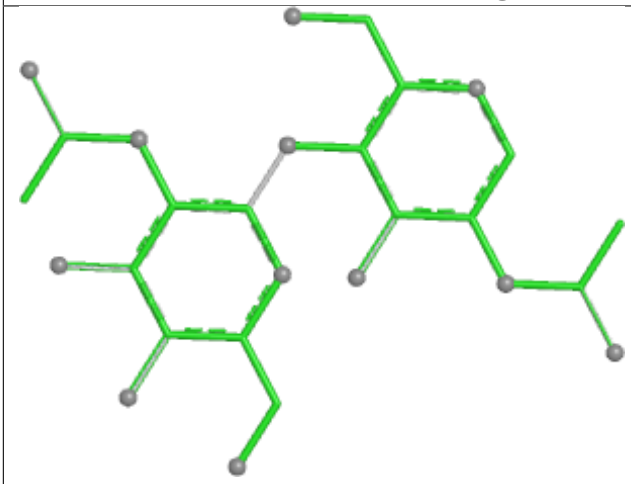


Torsions

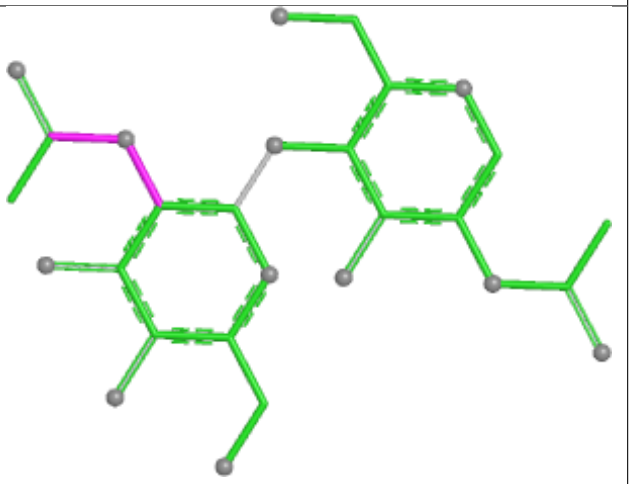


Rings

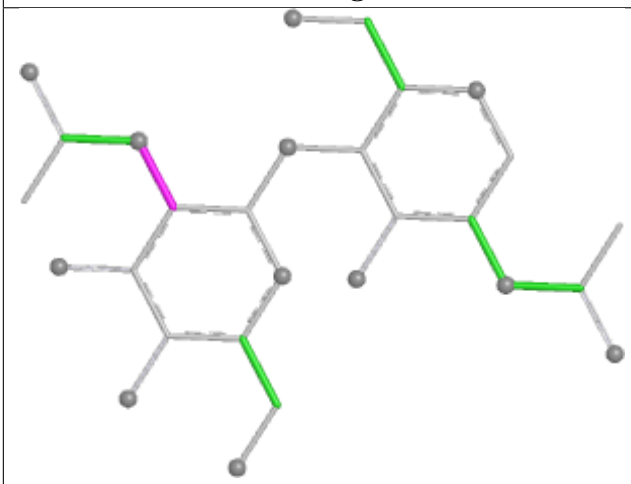
Oligosaccharide Chain G



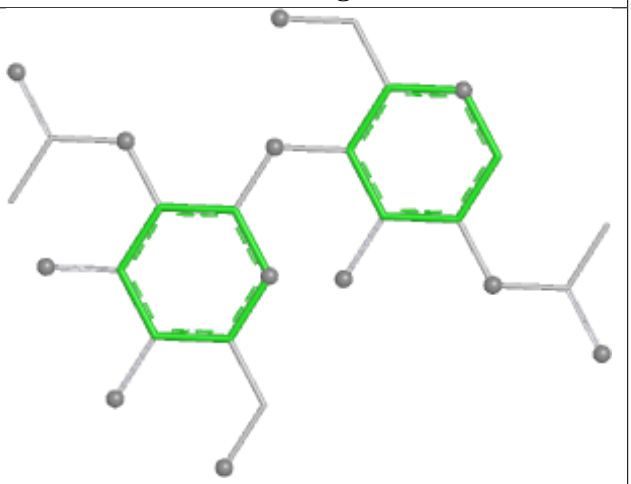
Bond lengths



Bond angles

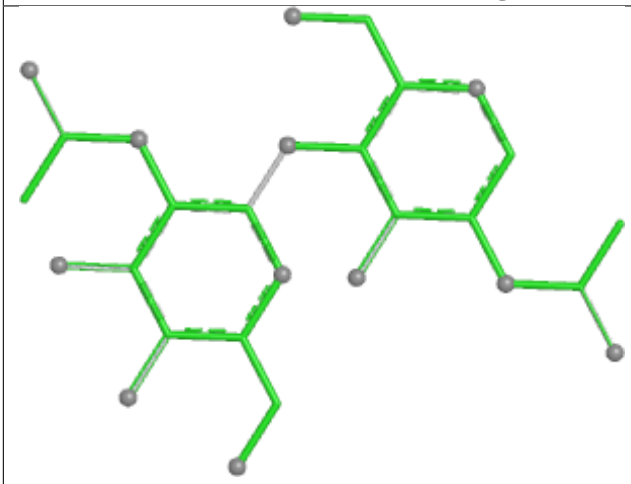


Torsions

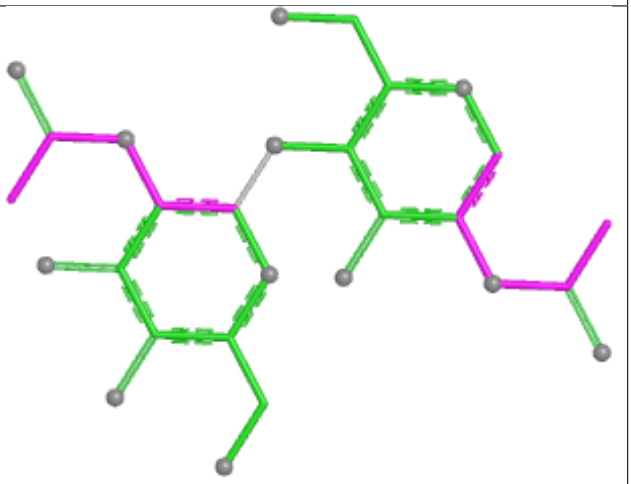


Rings

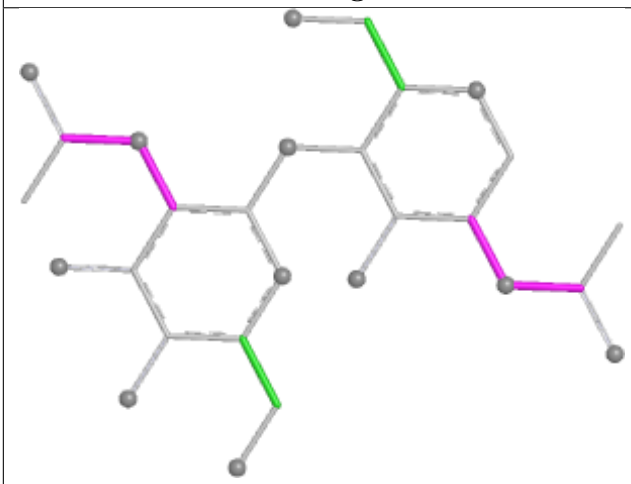
Oligosaccharide Chain H



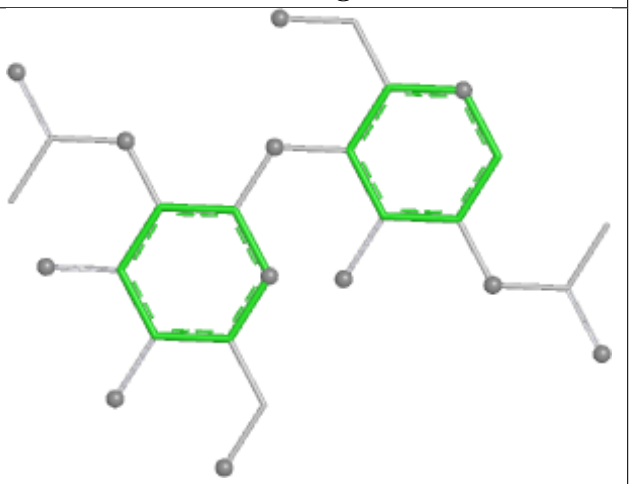
Bond lengths



Bond angles

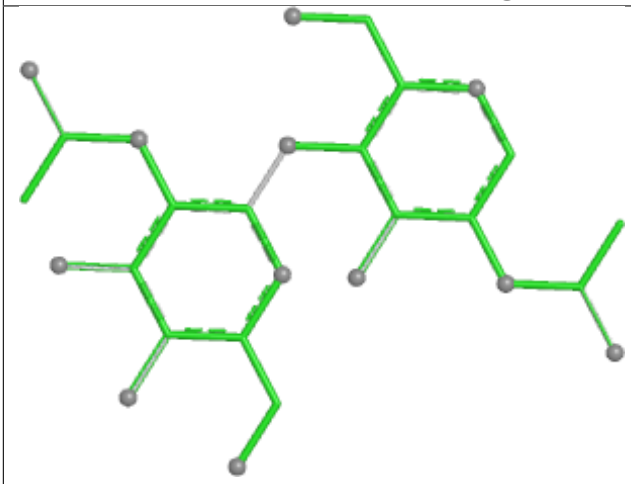


Torsions

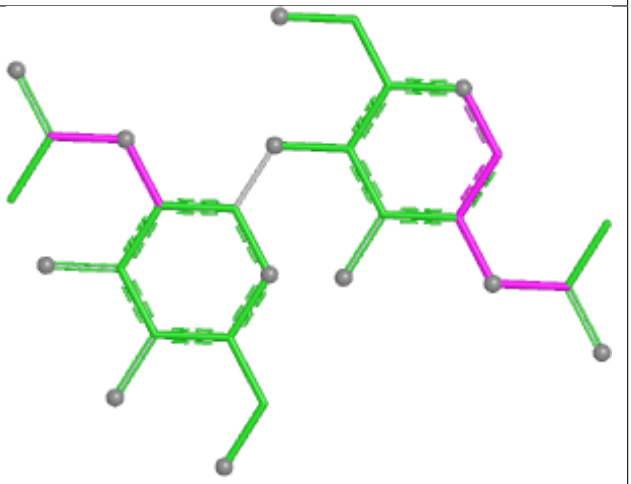


Rings

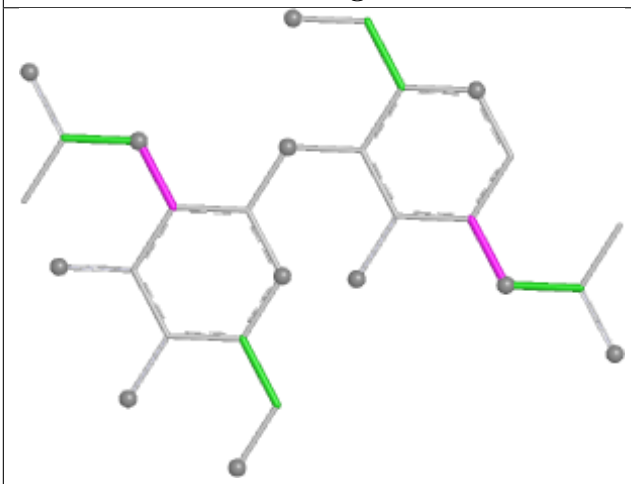
Oligosaccharide Chain J



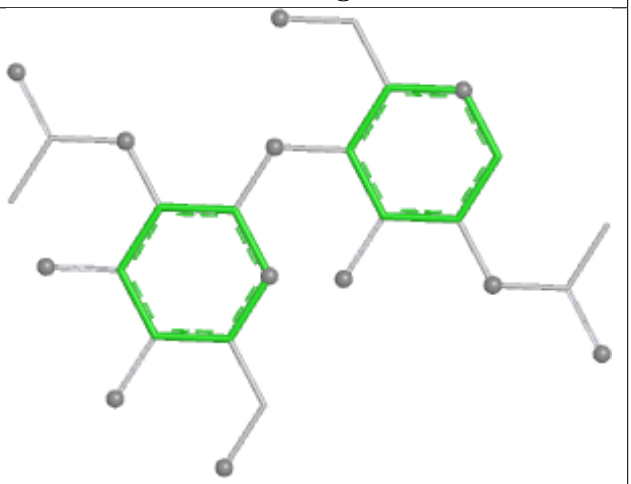
Bond lengths



Bond angles

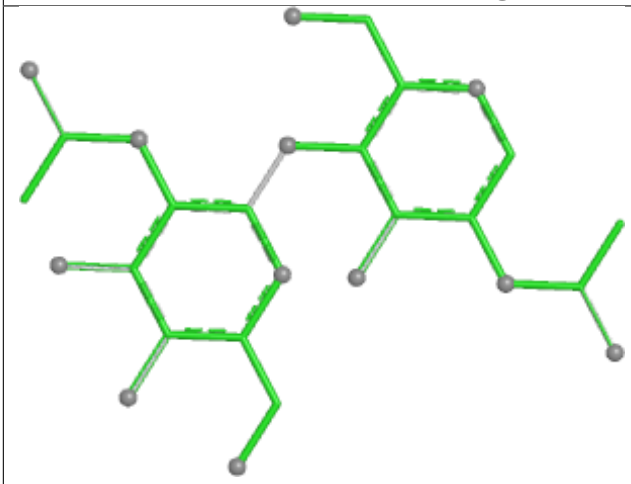


Torsions

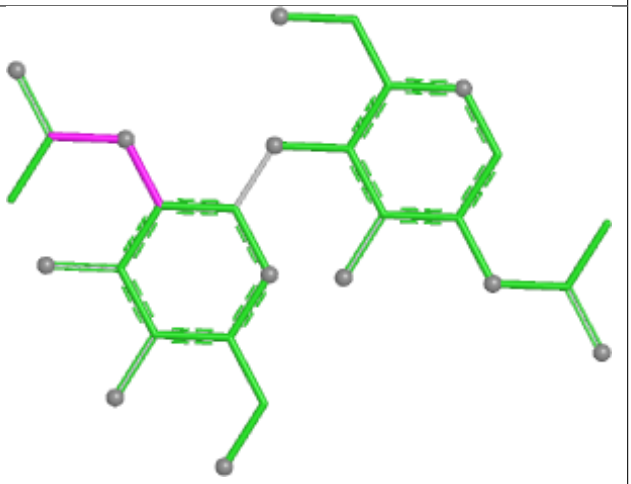


Rings

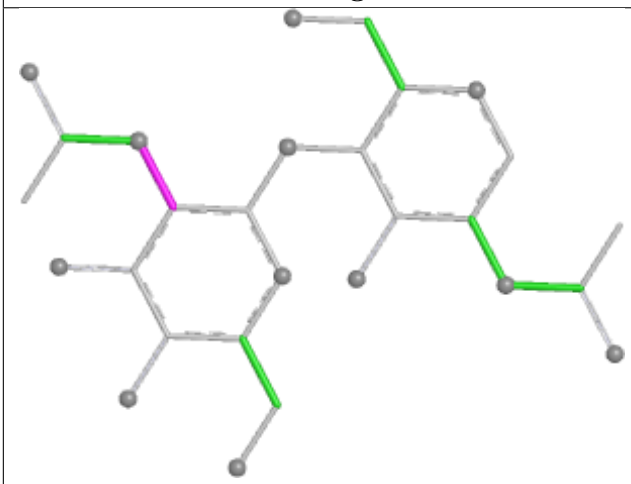
Oligosaccharide Chain K



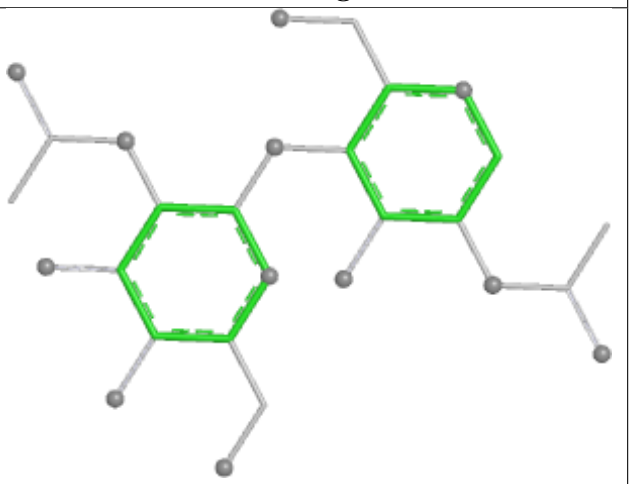
Bond lengths



Bond angles

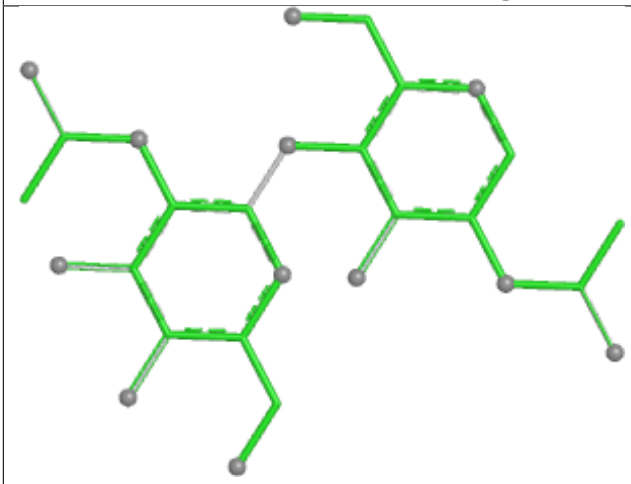


Torsions

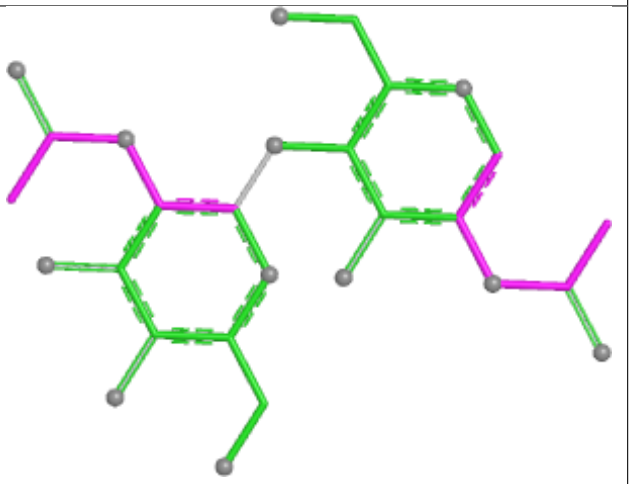


Rings

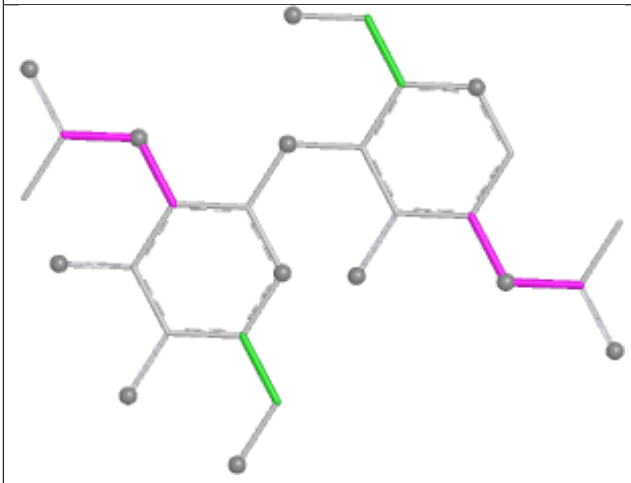
Oligosaccharide Chain L



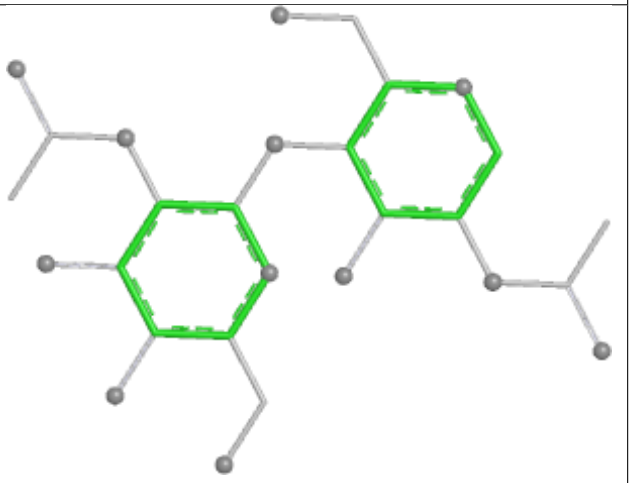
Bond lengths



Bond angles

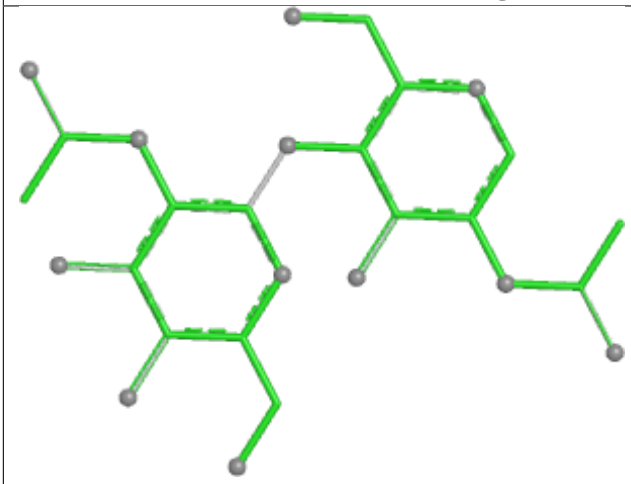


Torsions

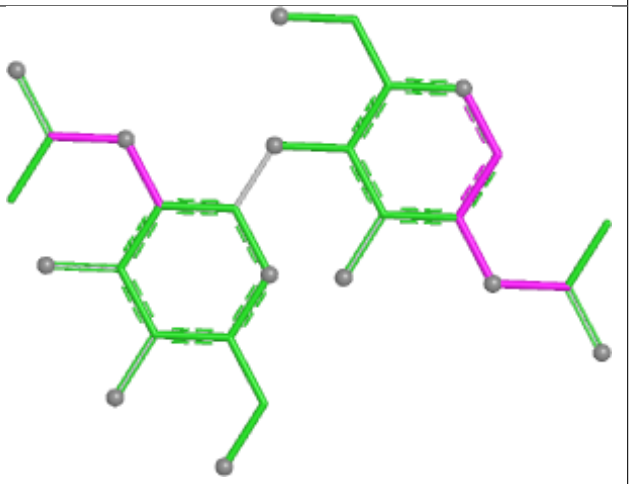


Rings

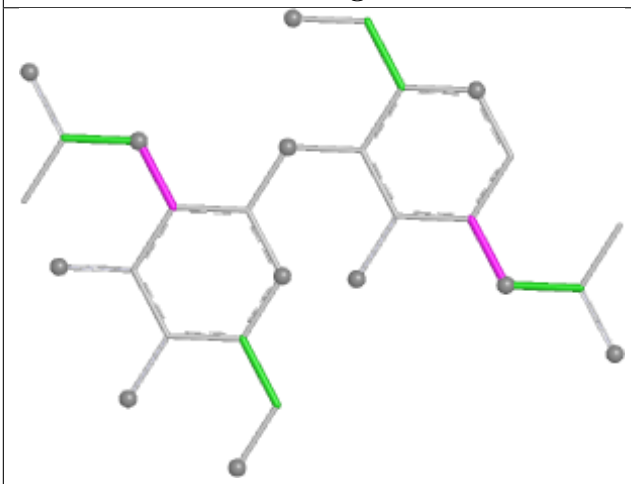
Oligosaccharide Chain N



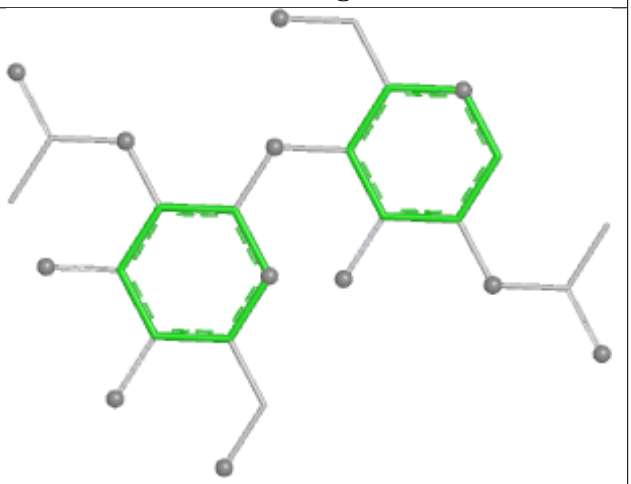
Bond lengths



Bond angles

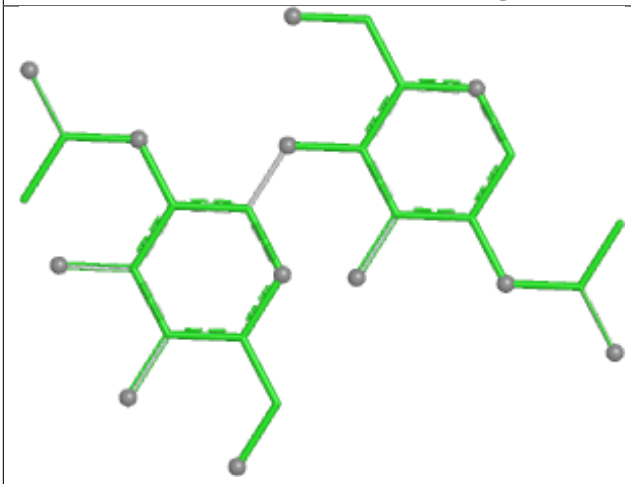


Torsions

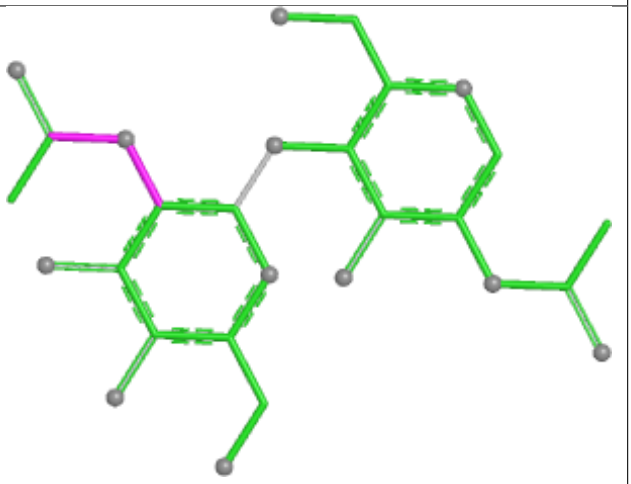


Rings

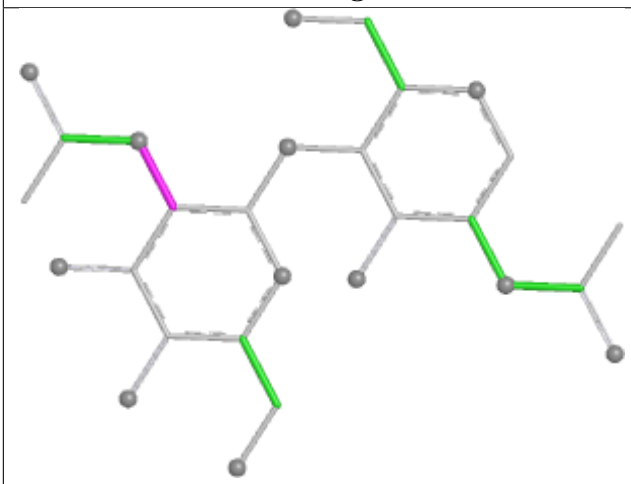
Oligosaccharide Chain O



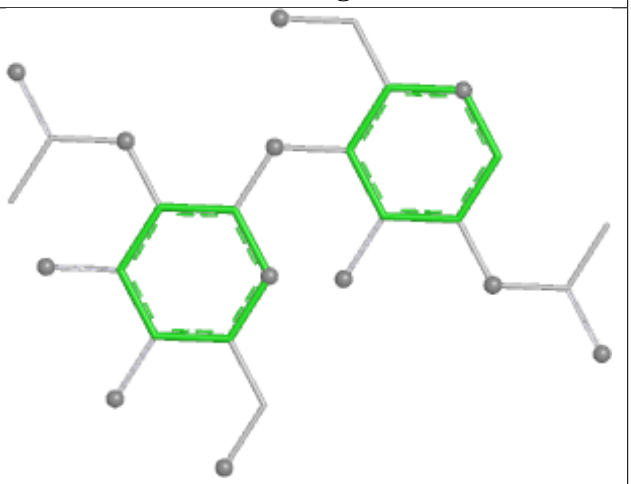
Bond lengths



Bond angles

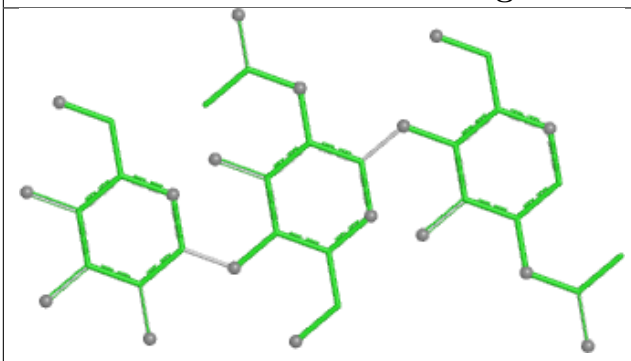


Torsions

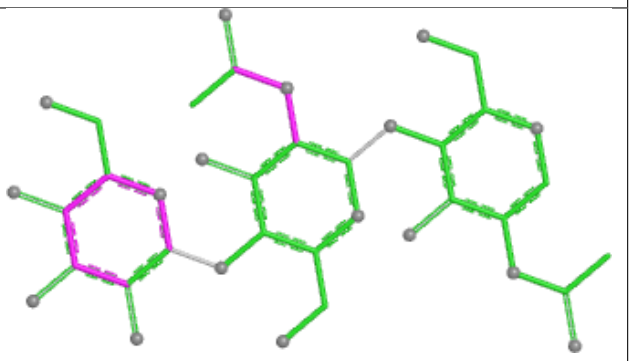


Rings

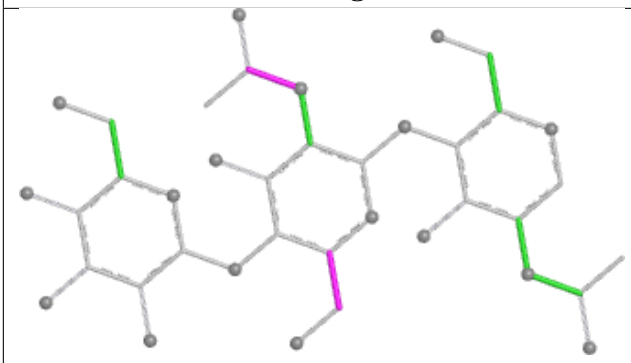
Oligosaccharide Chain E



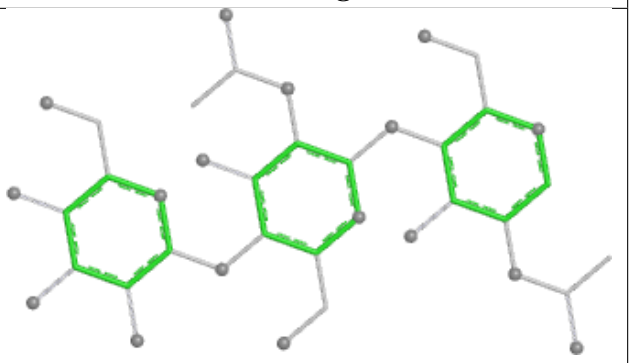
Bond lengths



Bond angles

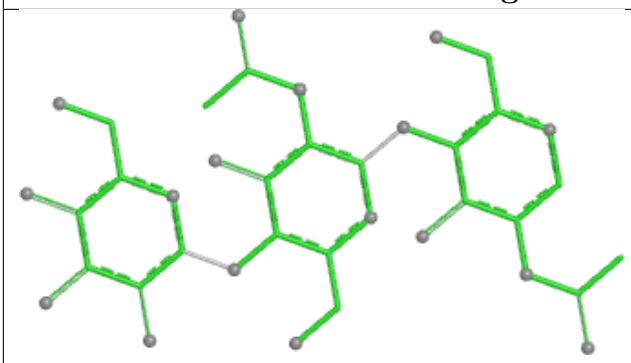


Torsions

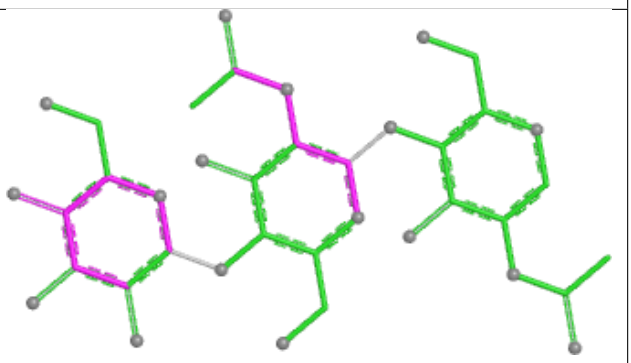


Rings

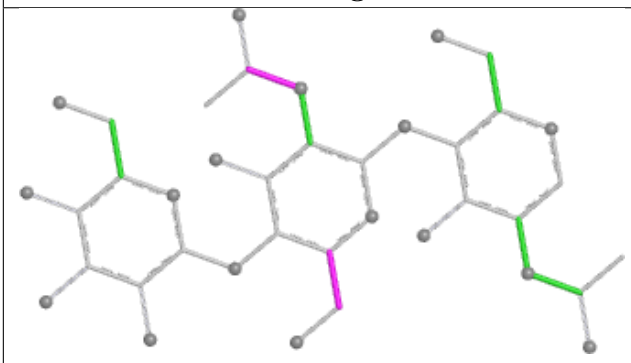
Oligosaccharide Chain I



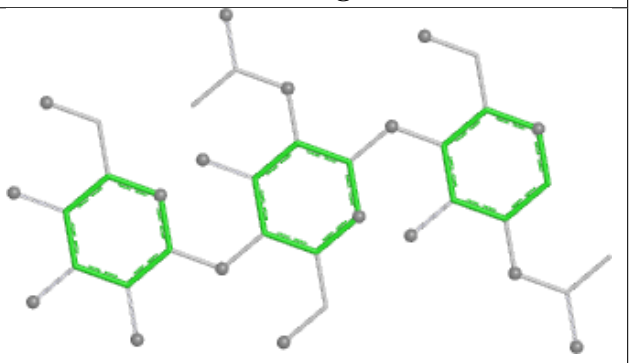
Bond lengths



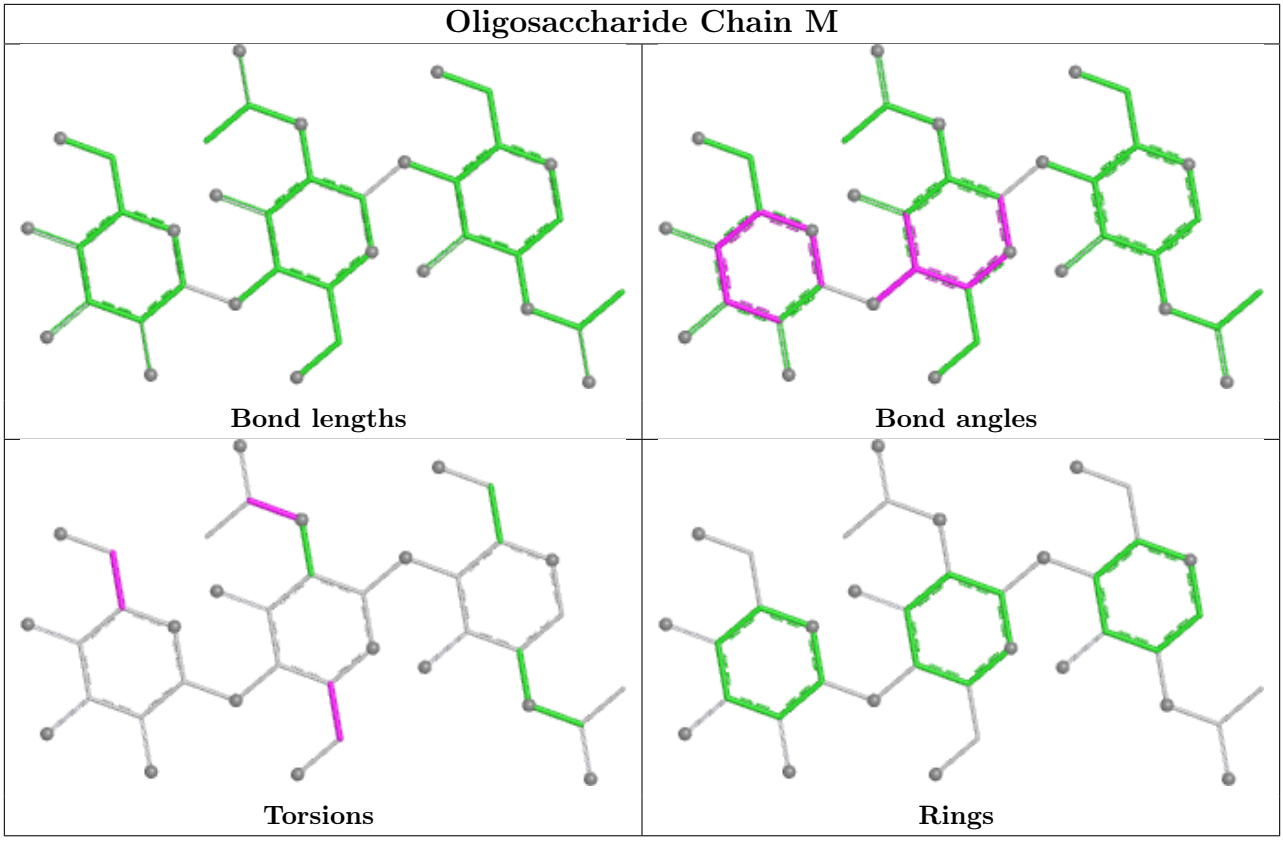
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1404	1	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	A	1409	-	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
4	NAG	A	1402	1	14,14,15	0.70	0	17,19,21	0.92	0
4	NAG	A	1407	1	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
4	NAG	C	1408	1	14,14,15	0.77	0	17,19,21	2.37	4 (23%)
4	NAG	A	1404	1	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	B	1406	1	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
4	NAG	A	1405	1	14,14,15	0.73	0	17,19,21	2.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1413	-	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
4	NAG	B	1401	1	14,14,15	0.68	0	17,19,21	0.87	1 (5%)
4	NAG	A	1401	1	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	B	1404	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	B	1405	1	14,14,15	0.74	0	17,19,21	2.33	3 (17%)
4	NAG	B	1410	1	14,14,15	0.70	0	17,19,21	0.76	0
4	NAG	B	1408	1	14,14,15	0.79	0	17,19,21	2.42	4 (23%)
4	NAG	C	1410	1	14,14,15	0.70	0	17,19,21	0.83	0
4	NAG	B	1411	1	14,14,15	0.70	0	17,19,21	0.82	0
4	NAG	A	1406	1	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
4	NAG	C	1402	1	14,14,15	0.70	0	17,19,21	0.92	0
4	NAG	B	1409	-	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
4	NAG	B	1412	1	14,14,15	0.73	0	17,19,21	0.79	0
4	NAG	A	1410	1	14,14,15	0.71	0	17,19,21	0.88	0
4	NAG	C	1406	1	14,14,15	0.71	0	17,19,21	1.19	1 (5%)
4	NAG	C	1409	1	14,14,15	0.71	0	17,19,21	0.88	1 (5%)
4	NAG	A	1412	1	14,14,15	0.73	0	17,19,21	0.79	0
4	NAG	B	1403	1	14,14,15	0.69	0	17,19,21	1.31	1 (5%)
4	NAG	C	1407	1	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
4	NAG	C	1411	1	14,14,15	0.73	0	17,19,21	0.79	0
4	NAG	A	1408	1	14,14,15	0.77	0	17,19,21	2.37	4 (23%)
4	NAG	B	1402	1	14,14,15	0.69	0	17,19,21	0.93	0
4	NAG	C	1401	1	14,14,15	0.68	0	17,19,21	0.77	0
4	NAG	C	1403	1	14,14,15	0.70	0	17,19,21	1.24	1 (5%)
4	NAG	C	1405	1	14,14,15	0.74	0	17,19,21	2.31	2 (11%)
4	NAG	B	1407	1	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
4	NAG	A	1411	1	14,14,15	0.70	0	17,19,21	0.83	0
4	NAG	A	1403	1	14,14,15	0.71	0	17,19,21	1.23	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1409	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1408	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1413	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1411	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1412	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1412	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1411	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1405	NAG	C2-N2-C7	8.30	134.02	122.90
4	B	1405	NAG	C2-N2-C7	8.29	134.01	122.90
4	C	1405	NAG	C2-N2-C7	8.22	133.92	122.90
4	C	1408	NAG	C2-N2-C7	8.17	133.84	122.90
4	A	1408	NAG	C2-N2-C7	8.16	133.83	122.90
4	B	1408	NAG	C2-N2-C7	8.11	133.77	122.90
4	B	1403	NAG	C2-N2-C7	3.61	127.74	122.90
4	C	1403	NAG	C2-N2-C7	3.45	127.53	122.90
4	B	1406	NAG	C2-N2-C7	3.37	127.42	122.90
4	C	1406	NAG	C2-N2-C7	3.33	127.36	122.90
4	B	1409	NAG	C2-N2-C7	3.32	127.34	122.90
4	A	1403	NAG	C2-N2-C7	3.31	127.34	122.90
4	A	1413	NAG	C2-N2-C7	3.30	127.33	122.90
4	A	1409	NAG	C2-N2-C7	3.30	127.32	122.90
4	A	1406	NAG	C2-N2-C7	3.25	127.25	122.90
4	B	1408	NAG	C1-O5-C5	3.02	116.23	112.19
4	C	1408	NAG	C1-O5-C5	2.71	115.81	112.19
4	B	1408	NAG	C1-C2-N2	2.68	114.65	110.43
4	B	1408	NAG	C8-C7-N2	2.65	120.52	116.12
4	A	1408	NAG	C8-C7-N2	2.62	120.46	116.12
4	A	1405	NAG	C8-C7-N2	2.57	120.38	116.12
4	C	1408	NAG	C8-C7-N2	2.57	120.37	116.12
4	B	1405	NAG	C8-C7-N2	2.56	120.36	116.12
4	C	1405	NAG	C8-C7-N2	2.54	120.33	116.12
4	A	1408	NAG	C1-O5-C5	2.54	115.58	112.19
4	A	1408	NAG	C1-C2-N2	2.36	114.15	110.43
4	B	1407	NAG	C2-N2-C7	2.27	125.94	122.90
4	A	1407	NAG	C2-N2-C7	2.23	125.89	122.90
4	C	1408	NAG	C1-C2-N2	2.22	113.94	110.43
4	C	1407	NAG	C2-N2-C7	2.08	125.68	122.90
4	C	1409	NAG	C2-N2-C7	2.04	125.63	122.90
4	B	1405	NAG	C1-C2-N2	2.04	113.64	110.43
4	A	1405	NAG	C1-C2-N2	2.03	113.63	110.43
4	B	1401	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1402	NAG	C8-C7-N2-C2
4	A	1402	NAG	O7-C7-N2-C2
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1407	NAG	C8-C7-N2-C2
4	A	1407	NAG	O7-C7-N2-C2
4	A	1408	NAG	C8-C7-N2-C2
4	A	1408	NAG	O7-C7-N2-C2
4	A	1410	NAG	C8-C7-N2-C2
4	A	1410	NAG	O7-C7-N2-C2
4	A	1411	NAG	C8-C7-N2-C2
4	A	1411	NAG	O7-C7-N2-C2
4	B	1401	NAG	C8-C7-N2-C2
4	B	1401	NAG	O7-C7-N2-C2
4	B	1402	NAG	C8-C7-N2-C2
4	B	1402	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	B	1407	NAG	C8-C7-N2-C2
4	B	1407	NAG	O7-C7-N2-C2
4	B	1408	NAG	C8-C7-N2-C2
4	B	1408	NAG	O7-C7-N2-C2
4	B	1410	NAG	C8-C7-N2-C2
4	B	1410	NAG	O7-C7-N2-C2
4	B	1411	NAG	C8-C7-N2-C2
4	B	1411	NAG	O7-C7-N2-C2
4	C	1402	NAG	C8-C7-N2-C2
4	C	1402	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	C	1407	NAG	C8-C7-N2-C2
4	C	1407	NAG	O7-C7-N2-C2
4	C	1408	NAG	C8-C7-N2-C2
4	C	1408	NAG	O7-C7-N2-C2
4	C	1409	NAG	C8-C7-N2-C2
4	C	1409	NAG	O7-C7-N2-C2
4	C	1410	NAG	C8-C7-N2-C2
4	C	1410	NAG	O7-C7-N2-C2
4	B	1412	NAG	O5-C5-C6-O6
4	C	1411	NAG	O5-C5-C6-O6
4	A	1412	NAG	O5-C5-C6-O6
4	A	1413	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1404	NAG	O5-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1403	NAG	C1-C2-N2-C7
4	A	1406	NAG	C1-C2-N2-C7
4	A	1409	NAG	C1-C2-N2-C7
4	A	1413	NAG	C1-C2-N2-C7
4	B	1403	NAG	C1-C2-N2-C7
4	B	1406	NAG	C1-C2-N2-C7
4	C	1406	NAG	C1-C2-N2-C7
4	A	1403	NAG	C3-C2-N2-C7
4	A	1408	NAG	C3-C2-N2-C7
4	A	1409	NAG	C3-C2-N2-C7
4	B	1403	NAG	C3-C2-N2-C7
4	B	1408	NAG	C3-C2-N2-C7
4	B	1409	NAG	C3-C2-N2-C7
4	C	1403	NAG	C3-C2-N2-C7
4	A	1405	NAG	C1-C2-N2-C7
4	A	1408	NAG	C1-C2-N2-C7
4	B	1405	NAG	C1-C2-N2-C7
4	B	1408	NAG	C1-C2-N2-C7
4	B	1409	NAG	C1-C2-N2-C7
4	C	1403	NAG	C1-C2-N2-C7
4	C	1405	NAG	C1-C2-N2-C7
4	C	1408	NAG	C1-C2-N2-C7
4	A	1405	NAG	C3-C2-N2-C7
4	A	1406	NAG	C3-C2-N2-C7
4	A	1413	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	B	1406	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7
4	C	1406	NAG	C3-C2-N2-C7
4	C	1408	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1409	NAG	1	0
4	A	1413	NAG	1	0
4	B	1401	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1412	NAG	2	0
4	A	1412	NAG	2	0
4	C	1411	NAG	2	0
4	C	1401	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

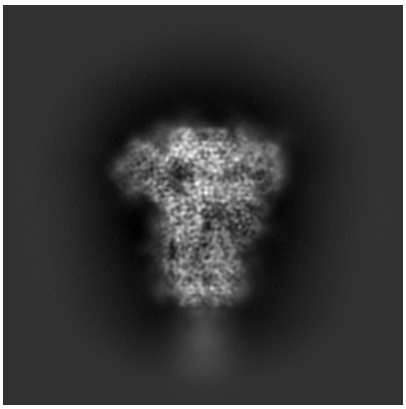
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46569. These allow visual inspection of the internal detail of the map and identification of artifacts.

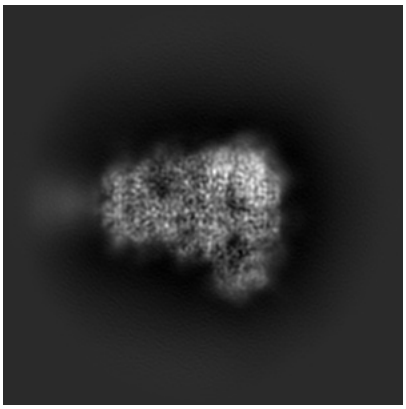
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

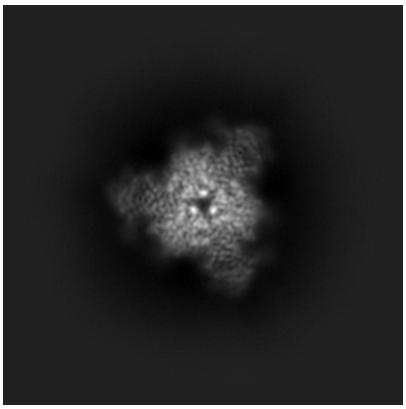
6.1.1 Primary map



X

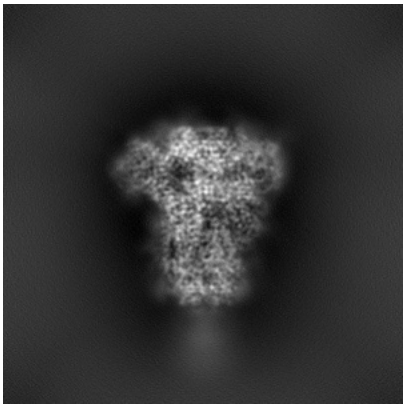


Y

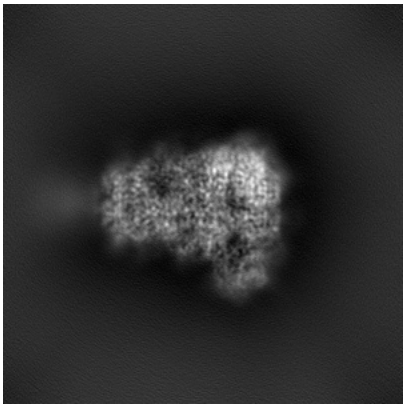


Z

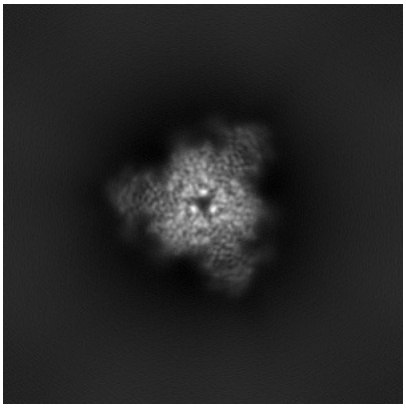
6.1.2 Raw map



X



Y

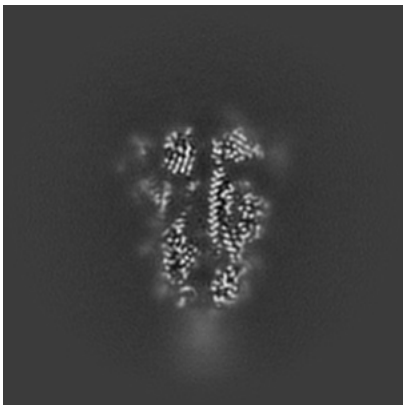


Z

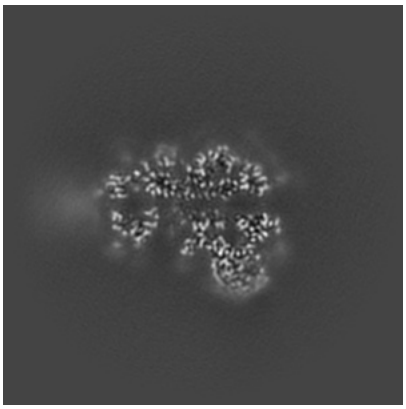
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

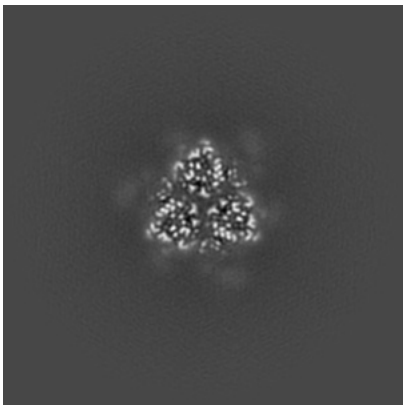
6.2.1 Primary map



X Index: 180

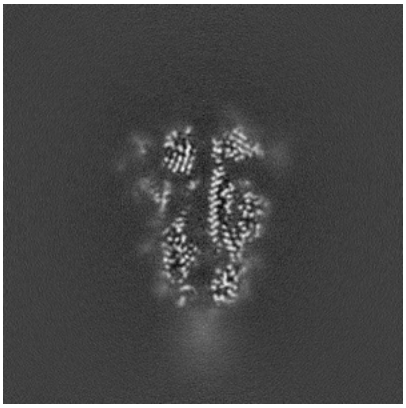


Y Index: 180

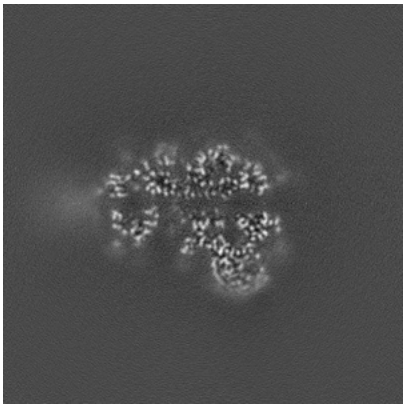


Z Index: 180

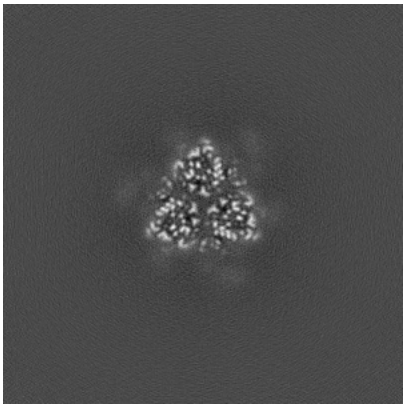
6.2.2 Raw map



X Index: 180



Y Index: 180

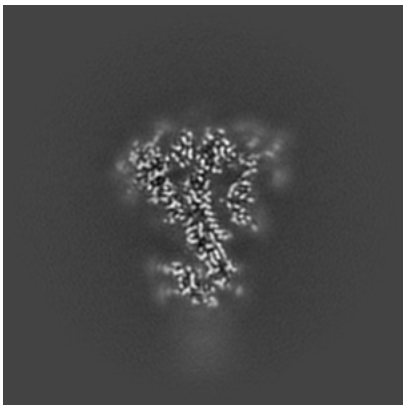


Z Index: 180

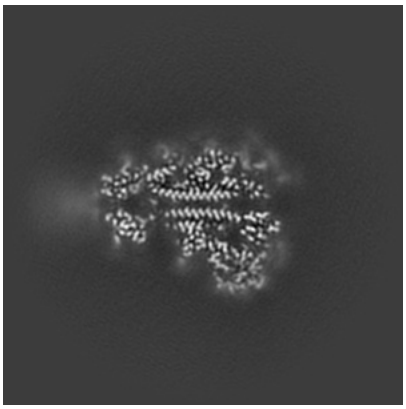
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

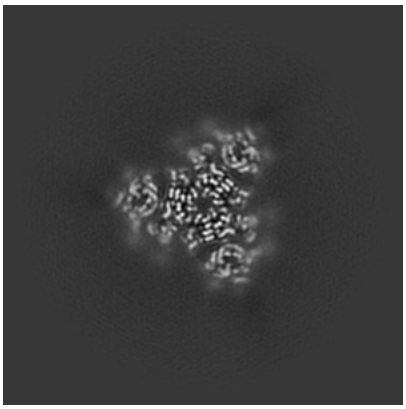
6.3.1 Primary map



X Index: 197

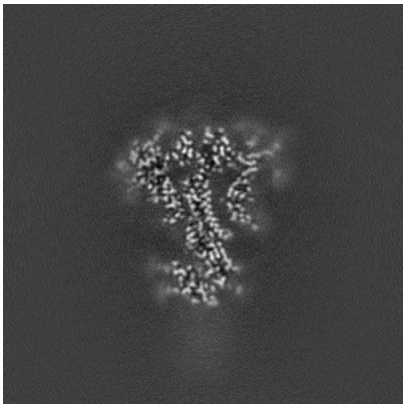


Y Index: 176

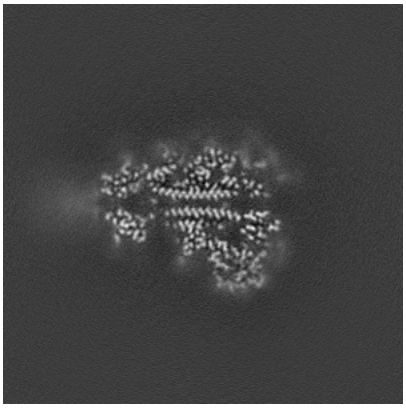


Z Index: 224

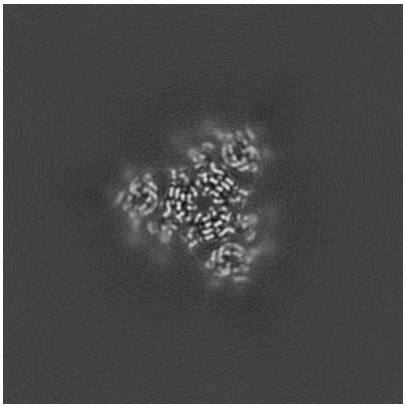
6.3.2 Raw map



X Index: 198



Y Index: 176

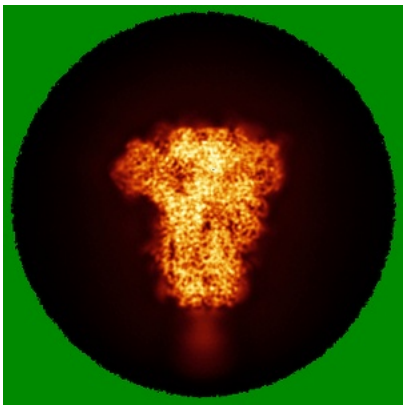


Z Index: 224

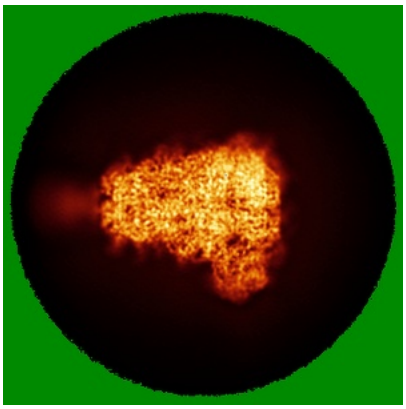
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

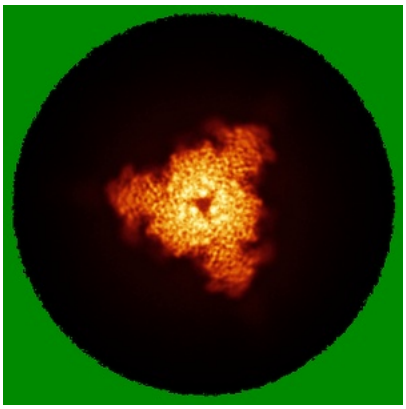
6.4.1 Primary map



X

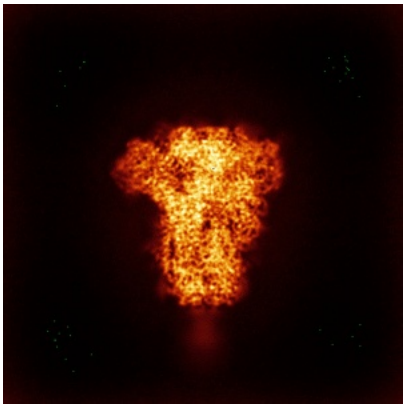


Y

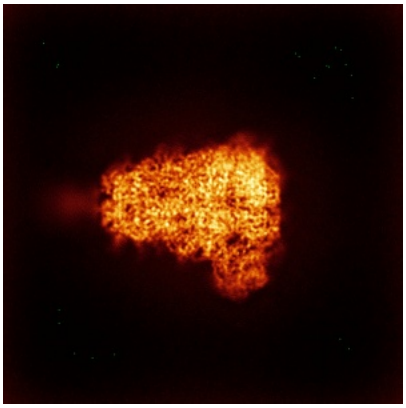


Z

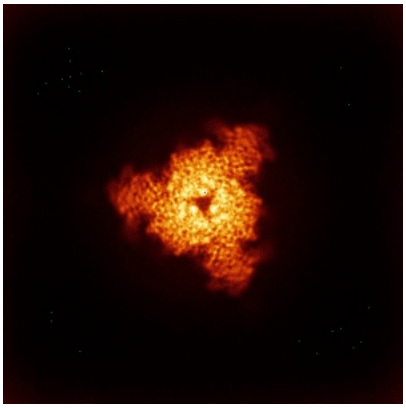
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0649. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

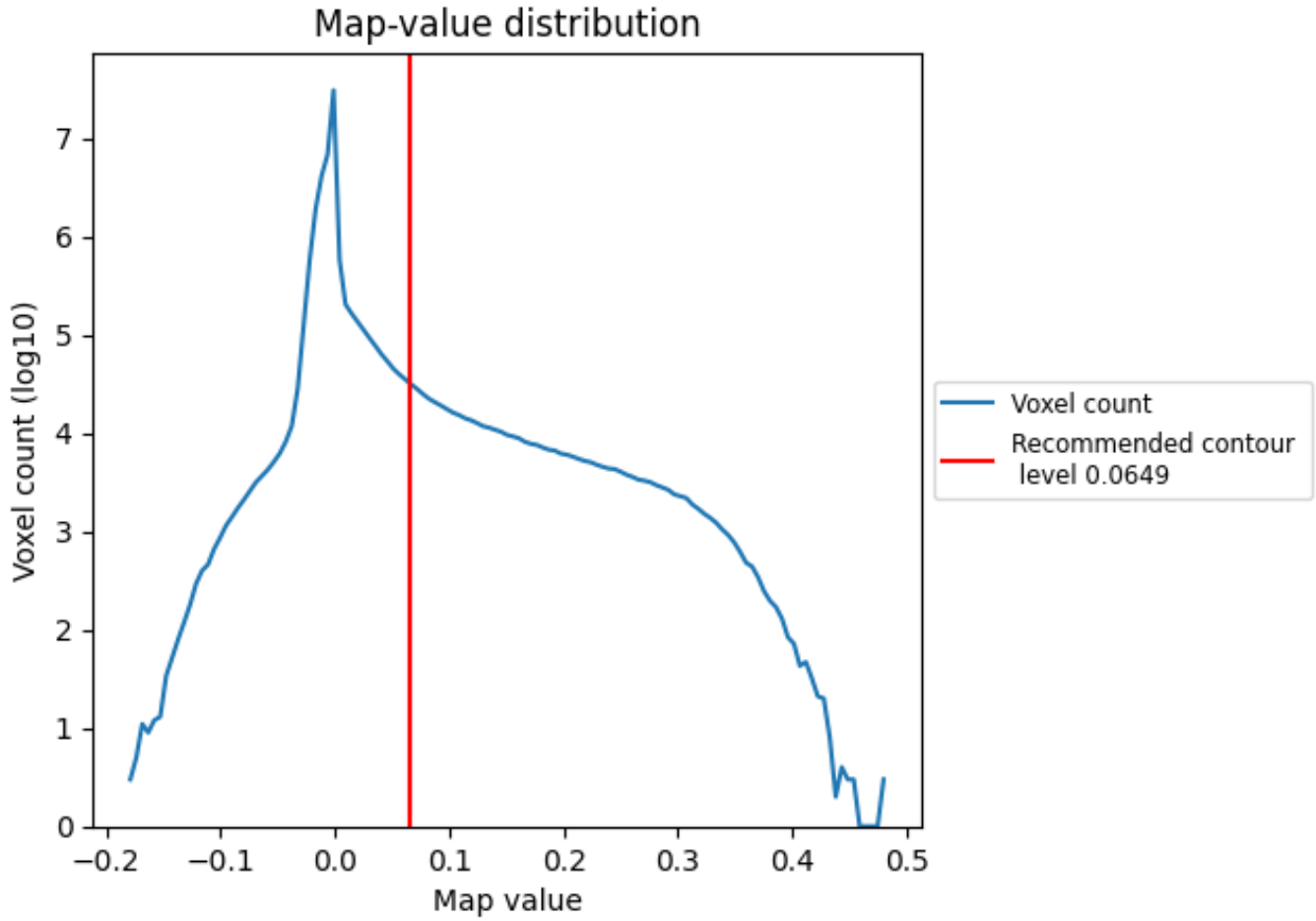
6.6 Mask visualisation (i)

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

7 Map analysis

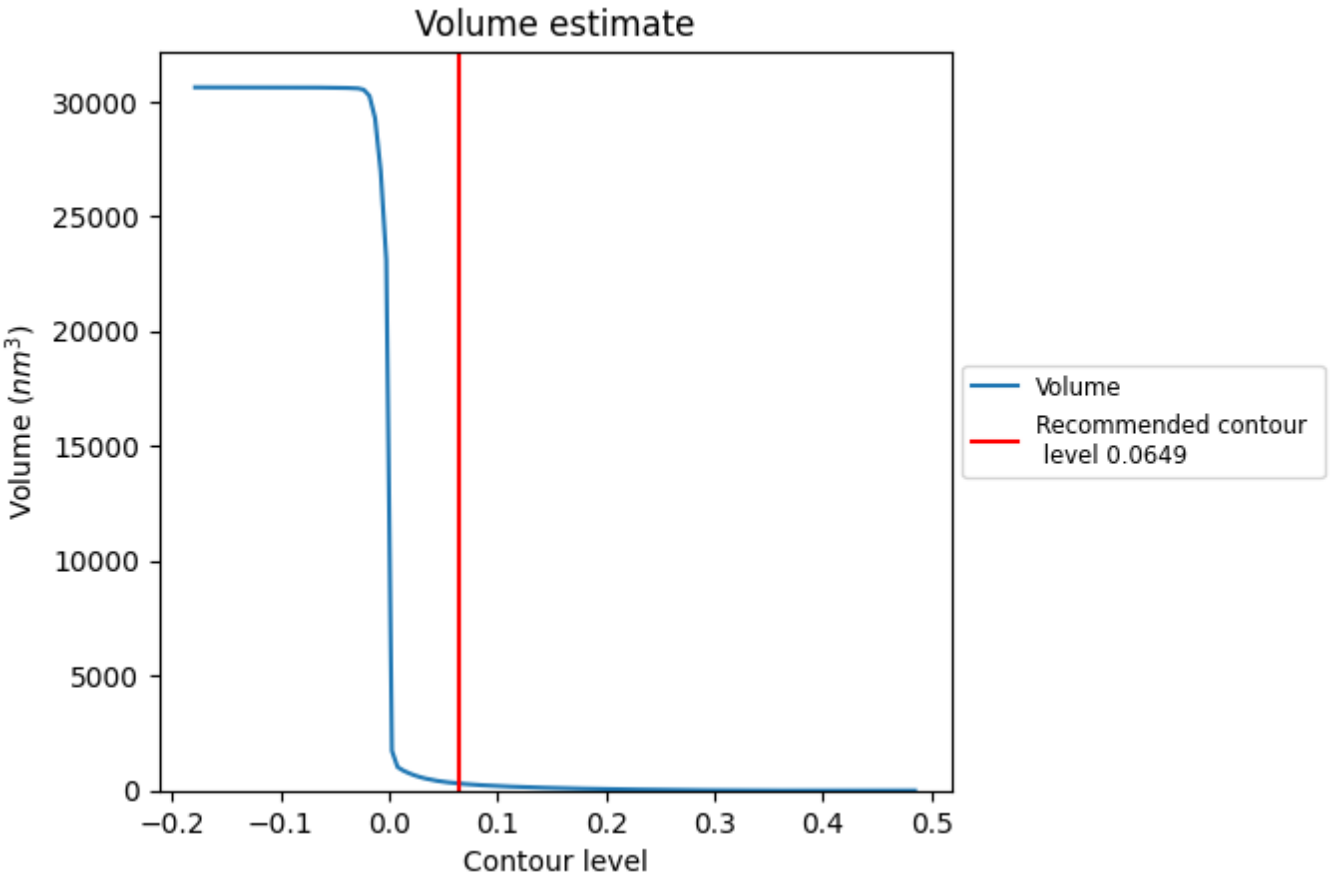
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

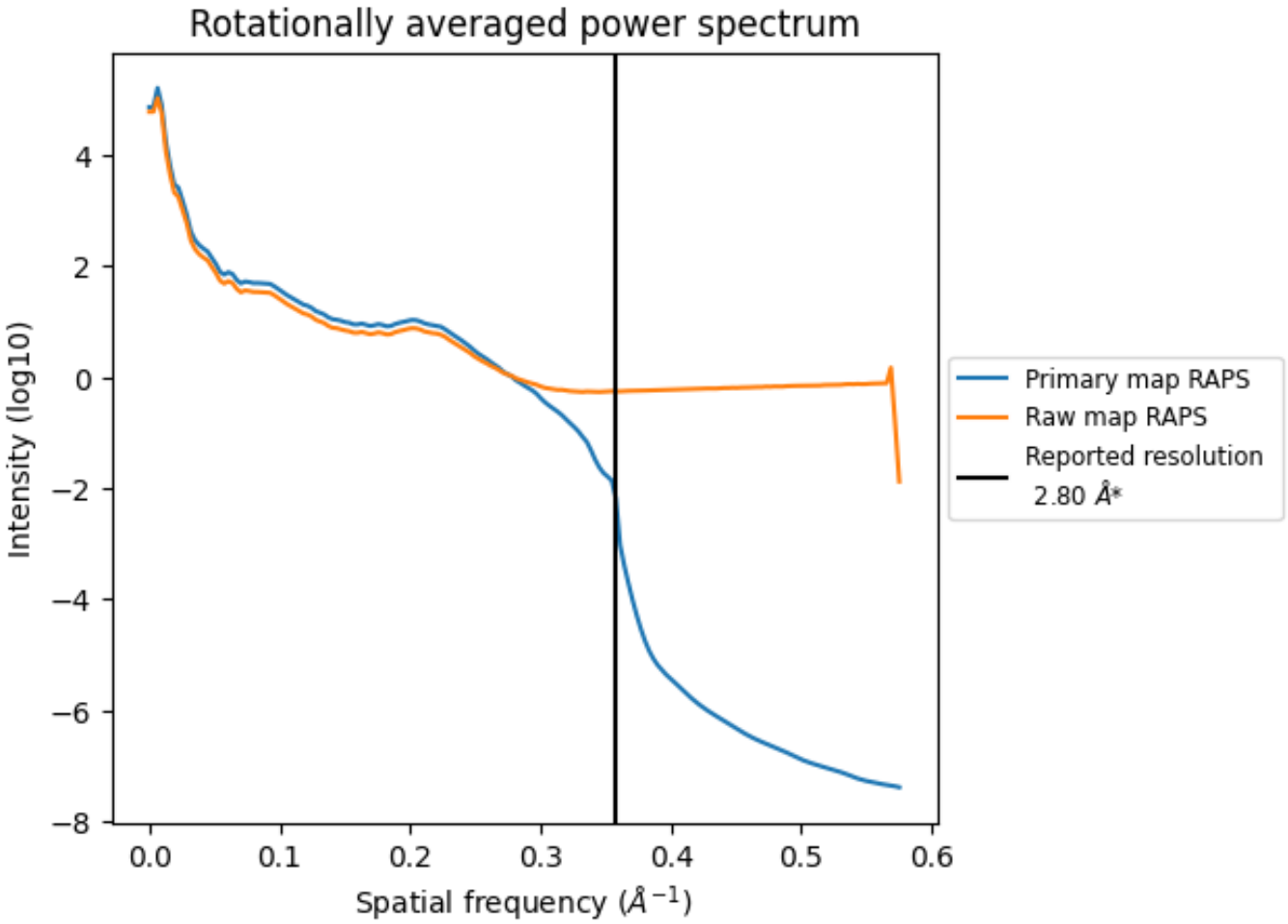
7.2 Volume estimate



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 276 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)

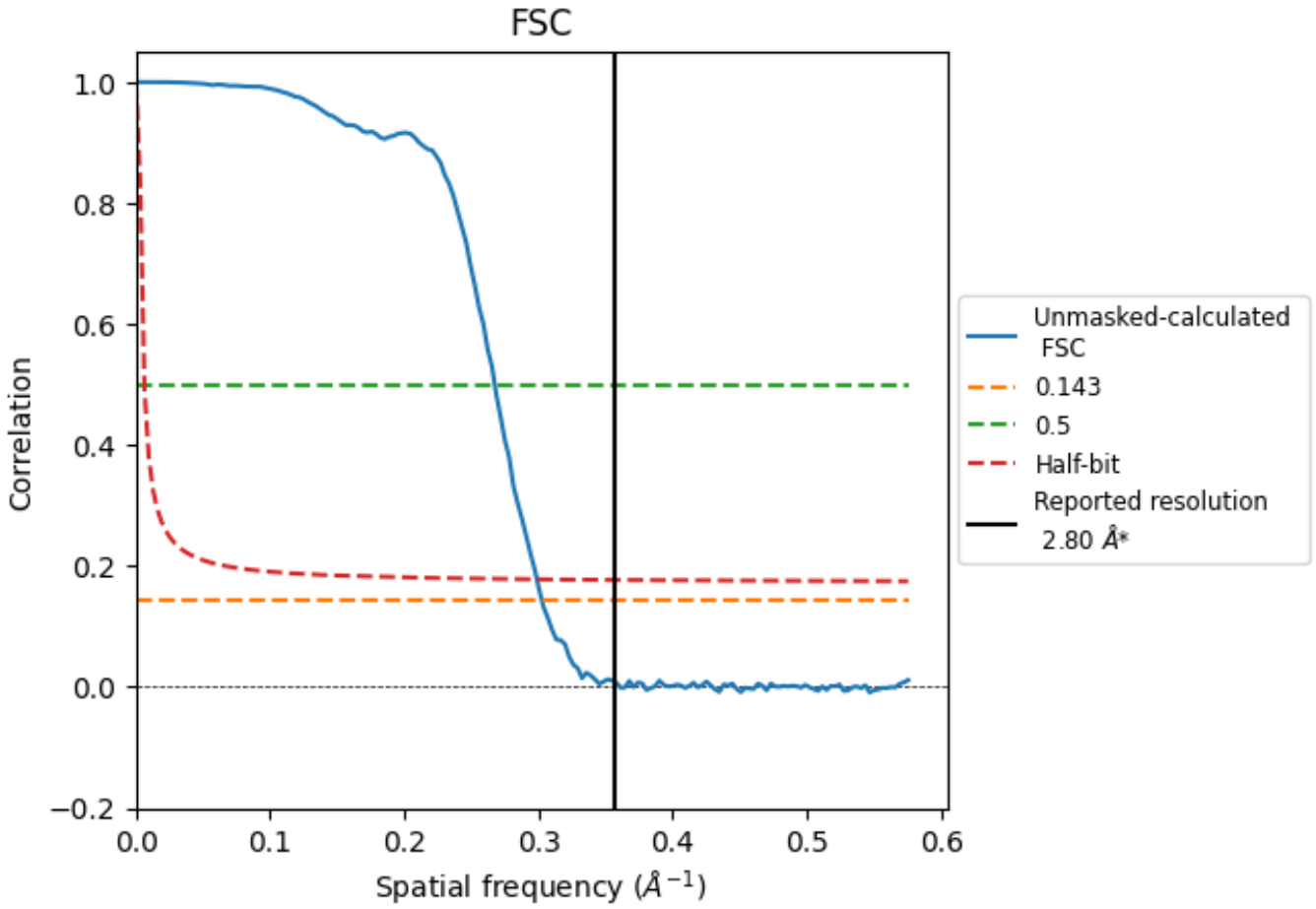


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

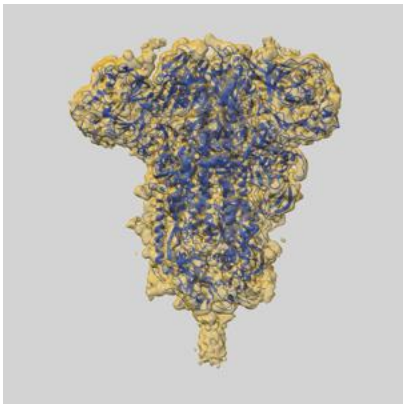
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	3.74	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.8 by more than 10 %

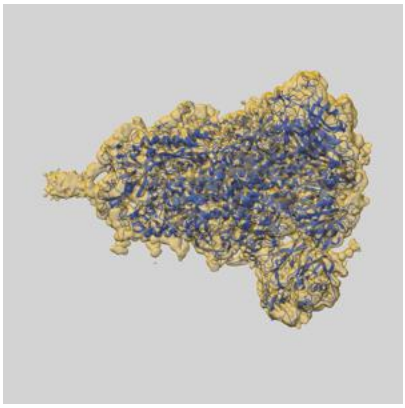
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46569 and PDB model 9D4T. Per-residue inclusion information can be found in section 3 on page 14.

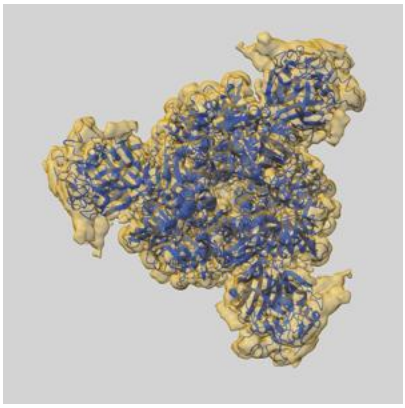
9.1 Map-model overlay



X



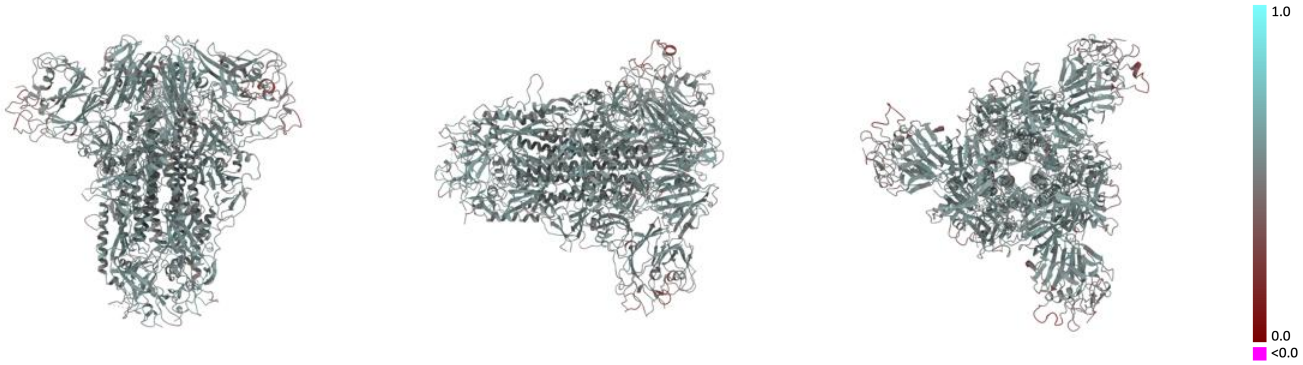
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0649 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.

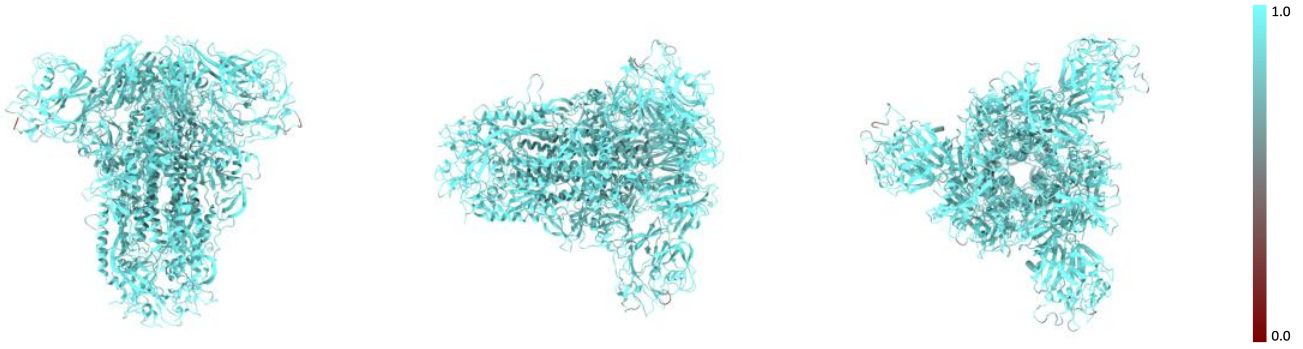
9.2 Q-score mapped to coordinate model (i)



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.

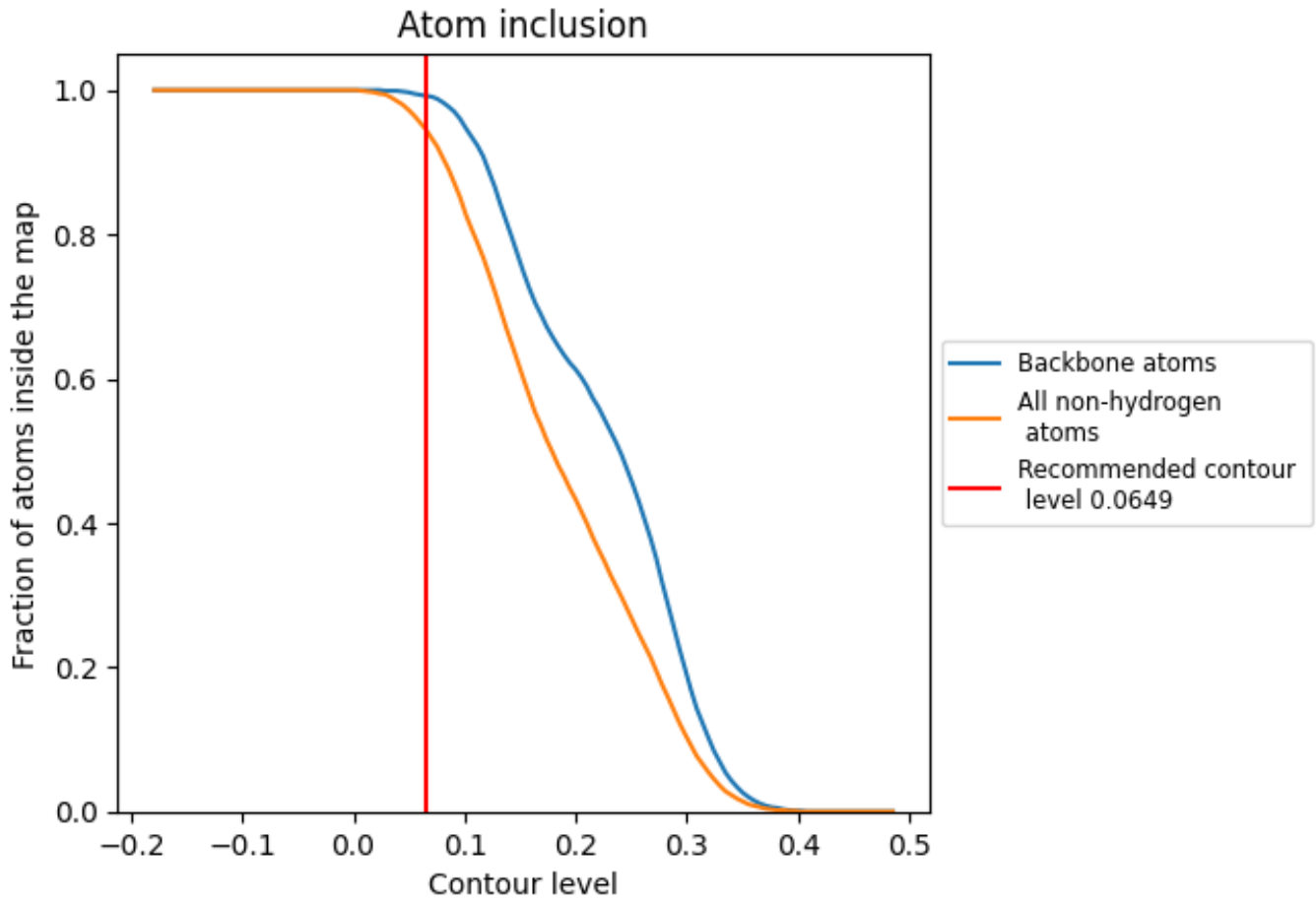
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0649).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0649) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.5220
A	0.9460	0.5240
B	0.9470	0.5230
C	0.9460	0.5220
D	0.9640	0.4720
E	0.8460	0.4160
F	0.9290	0.4560
G	1.0000	0.4710
H	0.9640	0.4660
I	0.8460	0.4280
J	0.8930	0.4490
K	1.0000	0.4760
L	0.9640	0.4540
M	0.8720	0.4420
N	0.8930	0.4470
O	1.0000	0.4670