Full wwPDB EM Validation Report ⓘ

Aug 28, 2024 – 04:42 pm BST

PDB ID	:	9F9Y
EMDB ID	:	EMD-50263
Title	:	SARS-CoV-2 BA-2.87.1 Spike ectodomain
Authors	:	Ren, J.; Stuart, D.I.; Duyvesteyn, H.M.E.
Deposited on	:	2024-05-09
Resolution	:	2.80 Å(reported)
Based on initial model	:	8R1C

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:

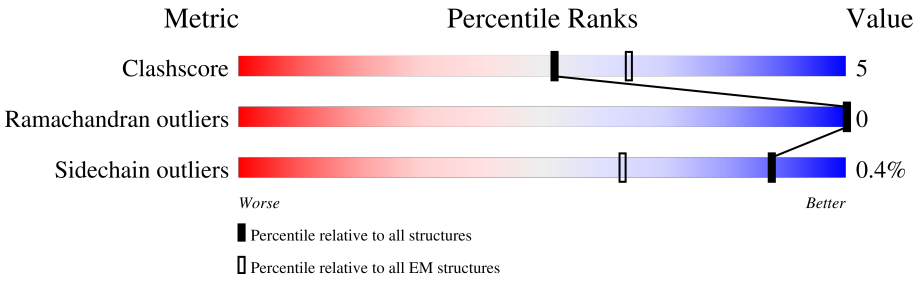
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 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	1263	70% 11% 19%
1	B	1263	69% 12% 19%
1	C	1263	69% 12% 19%
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24810 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1026	Total	C	N	O	S	0	0
			8004	5126	1331	1511	36		
1	B	1026	Total	C	N	O	S	0	0
			8004	5126	1331	1511	36		
1	C	1026	Total	C	N	O	S	0	0
			8004	5126	1331	1511	36		

There are 447 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	GLN	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	15	SER	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	61	ASP	GLY	conflict	UNP P0DTC2
A	84	PHE	SER	conflict	UNP P0DTC2
A	112	ALA	VAL	conflict	UNP P0DTC2
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	ASP	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	127	LEU	TRP	conflict	UNP P0DTC2
A	165	SER	ARG	variant	UNP P0DTC2
A	188	GLY	VAL	variant	UNP P0DTC2
A	190	GLY	ASP	variant	UNP P0DTC2
A	314	ASP	GLY	variant	UNP P0DTC2
A	346	PHE	SER	variant	UNP P0DTC2
A	348	PRO	SER	variant	UNP P0DTC2
A	350	PHE	SER	variant	UNP P0DTC2
A	351	ALA	THR	variant	UNP P0DTC2
A	380	ASN	ASP	variant	UNP P0DTC2
A	383	SER	ARG	variant	UNP P0DTC2
A	392	THR	LYS	variant	UNP P0DTC2
A	415	LYS	ASN	variant	UNP P0DTC2
A	419	ASN	LYS	conflict	UNP P0DTC2
A	420	GLY	VAL	conflict	UNP P0DTC2
A	427	MET	LEU	conflict	UNP P0DTC2
A	435	LYS	ASN	variant	UNP P0DTC2
A	452	ASN	SER	variant	UNP P0DTC2
A	456	LYS	ASN	conflict	UNP P0DTC2
A	459	ALA	GLU	variant	UNP P0DTC2
A	473	ARG	GLN	variant	UNP P0DTC2
A	476	TYR	ASN	variant	UNP P0DTC2
A	480	HIS	TYR	variant	UNP P0DTC2
A	589	GLY	ASP	variant	UNP P0DTC2
A	596	SER	PRO	conflict	UNP P0DTC2
A	617	GLY	VAL	conflict	UNP P0DTC2
A	630	TYR	HIS	conflict	UNP P0DTC2
A	654	ARG	ASN	conflict	UNP P0DTC2
A	656	HIS	PRO	conflict	UNP P0DTC2
A	657	GLY	ARG	conflict	UNP P0DTC2
A	658	SER	ARG	conflict	UNP P0DTC2
A	660	SER	ARG	conflict	UNP P0DTC2
A	666	PRO	SER	conflict	UNP P0DTC2
A	739	LYS	ASN	variant	UNP P0DTC2
A	766	ILE	THR	conflict	UNP P0DTC2
A	771	HIS	ASP	variant	UNP P0DTC2
A	911	GLY	ASP	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	929	HIS	GLN	variant	UNP P0DTC2
A	944	LYS	ASN	variant	UNP P0DTC2
A	961	PRO	LYS	engineered mutation	UNP P0DTC2
A	962	PRO	VAL	engineered mutation	UNP P0DTC2
A	1159	ASP	-	linker	UNP P0DTC2
A	1160	ARG	-	linker	UNP P0DTC2
A	1161	LEU	-	linker	UNP P0DTC2
A	1162	ASN	-	linker	UNP P0DTC2
A	1163	GLU	-	linker	UNP P0DTC2
A	1164	VAL	-	linker	UNP P0DTC2
A	1165	ALA	-	linker	UNP P0DTC2
A	1166	LYS	-	linker	UNP P0DTC2
A	1167	ASN	-	linker	UNP P0DTC2
A	1168	LEU	-	linker	UNP P0DTC2
A	1169	ASN	-	linker	UNP P0DTC2
A	1170	GLU	-	linker	UNP P0DTC2
A	1171	SER	-	linker	UNP P0DTC2
A	1172	LEU	-	linker	UNP P0DTC2
A	1173	ILE	-	linker	UNP P0DTC2
A	1174	ASP	-	linker	UNP P0DTC2
A	1175	LEU	-	linker	UNP P0DTC2
A	1176	GLN	-	linker	UNP P0DTC2
A	1177	GLU	-	linker	UNP P0DTC2
A	1178	LEU	-	linker	UNP P0DTC2
A	1179	GLY	-	linker	UNP P0DTC2
A	1180	LYS	-	linker	UNP P0DTC2
A	1181	TYR	-	linker	UNP P0DTC2
A	1182	GLU	-	linker	UNP P0DTC2
A	1183	GLN	-	linker	UNP P0DTC2
A	1184	GLY	-	linker	UNP P0DTC2
A	1185	SER	-	linker	UNP P0DTC2
A	1207	LEU	PHE	engineered mutation	UNP P10104
A	1213	GLY	-	expression tag	UNP P10104
A	1214	ARG	-	expression tag	UNP P10104
A	1215	SER	-	expression tag	UNP P10104
A	1216	LEU	-	expression tag	UNP P10104
A	1217	GLU	-	expression tag	UNP P10104
A	1218	VAL	-	expression tag	UNP P10104
A	1219	LEU	-	expression tag	UNP P10104
A	1220	PHE	-	expression tag	UNP P10104
A	1221	GLN	-	expression tag	UNP P10104
A	1222	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1223	PRO	-	expression tag	UNP P10104
A	1224	GLY	-	expression tag	UNP P10104
A	1225	HIS	-	expression tag	UNP P10104
A	1226	HIS	-	expression tag	UNP P10104
A	1227	HIS	-	expression tag	UNP P10104
A	1228	HIS	-	expression tag	UNP P10104
A	1229	HIS	-	expression tag	UNP P10104
A	1230	HIS	-	expression tag	UNP P10104
A	1231	HIS	-	expression tag	UNP P10104
A	1232	HIS	-	expression tag	UNP P10104
A	1233	GLY	-	expression tag	UNP P10104
A	1234	SER	-	expression tag	UNP P10104
A	1235	ALA	-	expression tag	UNP P10104
A	1236	TRP	-	expression tag	UNP P10104
A	1237	SER	-	expression tag	UNP P10104
A	1238	HIS	-	expression tag	UNP P10104
A	1239	PRO	-	expression tag	UNP P10104
A	1240	GLN	-	expression tag	UNP P10104
A	1241	PHE	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	LYS	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104
A	1245	GLY	-	expression tag	UNP P10104
A	1246	GLY	-	expression tag	UNP P10104
A	1247	SER	-	expression tag	UNP P10104
A	1248	GLY	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	GLY	-	expression tag	UNP P10104
A	1251	SER	-	expression tag	UNP P10104
A	1252	GLY	-	expression tag	UNP P10104
A	1253	GLY	-	expression tag	UNP P10104
A	1254	SER	-	expression tag	UNP P10104
A	1255	ALA	-	expression tag	UNP P10104
A	1256	TRP	-	expression tag	UNP P10104
A	1257	SER	-	expression tag	UNP P10104
A	1258	HIS	-	expression tag	UNP P10104
A	1259	PRO	-	expression tag	UNP P10104
A	1260	GLN	-	expression tag	UNP P10104
A	1261	PHE	-	expression tag	UNP P10104
A	1262	GLU	-	expression tag	UNP P10104
A	1263	LYS	-	expression tag	UNP P10104
B	?	-	CYS	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	GLN	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	15	SER	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	61	ASP	GLY	conflict	UNP P0DTC2
B	84	PHE	SER	conflict	UNP P0DTC2
B	112	ALA	VAL	conflict	UNP P0DTC2
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	ASP	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	127	LEU	TRP	conflict	UNP P0DTC2
B	165	SER	ARG	variant	UNP P0DTC2
B	188	GLY	VAL	variant	UNP P0DTC2
B	190	GLY	ASP	variant	UNP P0DTC2
B	314	ASP	GLY	variant	UNP P0DTC2
B	346	PHE	SER	variant	UNP P0DTC2
B	348	PRO	SER	variant	UNP P0DTC2
B	350	PHE	SER	variant	UNP P0DTC2
B	351	ALA	THR	variant	UNP P0DTC2
B	380	ASN	ASP	variant	UNP P0DTC2
B	383	SER	ARG	variant	UNP P0DTC2
B	392	THR	LYS	variant	UNP P0DTC2
B	415	LYS	ASN	variant	UNP P0DTC2
B	419	ASN	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	420	GLY	VAL	conflict	UNP P0DTC2
B	427	MET	LEU	conflict	UNP P0DTC2
B	435	LYS	ASN	variant	UNP P0DTC2
B	452	ASN	SER	variant	UNP P0DTC2
B	456	LYS	ASN	conflict	UNP P0DTC2
B	459	ALA	GLU	variant	UNP P0DTC2
B	473	ARG	GLN	variant	UNP P0DTC2
B	476	TYR	ASN	variant	UNP P0DTC2
B	480	HIS	TYR	variant	UNP P0DTC2
B	589	GLY	ASP	variant	UNP P0DTC2
B	596	SER	PRO	conflict	UNP P0DTC2
B	617	GLY	VAL	conflict	UNP P0DTC2
B	630	TYR	HIS	conflict	UNP P0DTC2
B	654	ARG	ASN	conflict	UNP P0DTC2
B	656	HIS	PRO	conflict	UNP P0DTC2
B	657	GLY	ARG	conflict	UNP P0DTC2
B	658	SER	ARG	conflict	UNP P0DTC2
B	660	SER	ARG	conflict	UNP P0DTC2
B	666	PRO	SER	conflict	UNP P0DTC2
B	739	LYS	ASN	variant	UNP P0DTC2
B	766	ILE	THR	conflict	UNP P0DTC2
B	771	HIS	ASP	variant	UNP P0DTC2
B	911	GLY	ASP	conflict	UNP P0DTC2
B	929	HIS	GLN	variant	UNP P0DTC2
B	944	LYS	ASN	variant	UNP P0DTC2
B	961	PRO	LYS	engineered mutation	UNP P0DTC2
B	962	PRO	VAL	engineered mutation	UNP P0DTC2
B	1159	ASP	-	linker	UNP P0DTC2
B	1160	ARG	-	linker	UNP P0DTC2
B	1161	LEU	-	linker	UNP P0DTC2
B	1162	ASN	-	linker	UNP P0DTC2
B	1163	GLU	-	linker	UNP P0DTC2
B	1164	VAL	-	linker	UNP P0DTC2
B	1165	ALA	-	linker	UNP P0DTC2
B	1166	LYS	-	linker	UNP P0DTC2
B	1167	ASN	-	linker	UNP P0DTC2
B	1168	LEU	-	linker	UNP P0DTC2
B	1169	ASN	-	linker	UNP P0DTC2
B	1170	GLU	-	linker	UNP P0DTC2
B	1171	SER	-	linker	UNP P0DTC2
B	1172	LEU	-	linker	UNP P0DTC2
B	1173	ILE	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1174	ASP	-	linker	UNP P0DTC2
B	1175	LEU	-	linker	UNP P0DTC2
B	1176	GLN	-	linker	UNP P0DTC2
B	1177	GLU	-	linker	UNP P0DTC2
B	1178	LEU	-	linker	UNP P0DTC2
B	1179	GLY	-	linker	UNP P0DTC2
B	1180	LYS	-	linker	UNP P0DTC2
B	1181	TYR	-	linker	UNP P0DTC2
B	1182	GLU	-	linker	UNP P0DTC2
B	1183	GLN	-	linker	UNP P0DTC2
B	1184	GLY	-	linker	UNP P0DTC2
B	1185	SER	-	linker	UNP P0DTC2
B	1207	LEU	PHE	engineered mutation	UNP P10104
B	1213	GLY	-	expression tag	UNP P10104
B	1214	ARG	-	expression tag	UNP P10104
B	1215	SER	-	expression tag	UNP P10104
B	1216	LEU	-	expression tag	UNP P10104
B	1217	GLU	-	expression tag	UNP P10104
B	1218	VAL	-	expression tag	UNP P10104
B	1219	LEU	-	expression tag	UNP P10104
B	1220	PHE	-	expression tag	UNP P10104
B	1221	GLN	-	expression tag	UNP P10104
B	1222	GLY	-	expression tag	UNP P10104
B	1223	PRO	-	expression tag	UNP P10104
B	1224	GLY	-	expression tag	UNP P10104
B	1225	HIS	-	expression tag	UNP P10104
B	1226	HIS	-	expression tag	UNP P10104
B	1227	HIS	-	expression tag	UNP P10104
B	1228	HIS	-	expression tag	UNP P10104
B	1229	HIS	-	expression tag	UNP P10104
B	1230	HIS	-	expression tag	UNP P10104
B	1231	HIS	-	expression tag	UNP P10104
B	1232	HIS	-	expression tag	UNP P10104
B	1233	GLY	-	expression tag	UNP P10104
B	1234	SER	-	expression tag	UNP P10104
B	1235	ALA	-	expression tag	UNP P10104
B	1236	TRP	-	expression tag	UNP P10104
B	1237	SER	-	expression tag	UNP P10104
B	1238	HIS	-	expression tag	UNP P10104
B	1239	PRO	-	expression tag	UNP P10104
B	1240	GLN	-	expression tag	UNP P10104
B	1241	PHE	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1242	GLU	-	expression tag	UNP P10104
B	1243	LYS	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	GLY	-	expression tag	UNP P10104
B	1246	GLY	-	expression tag	UNP P10104
B	1247	SER	-	expression tag	UNP P10104
B	1248	GLY	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	GLY	-	expression tag	UNP P10104
B	1251	SER	-	expression tag	UNP P10104
B	1252	GLY	-	expression tag	UNP P10104
B	1253	GLY	-	expression tag	UNP P10104
B	1254	SER	-	expression tag	UNP P10104
B	1255	ALA	-	expression tag	UNP P10104
B	1256	TRP	-	expression tag	UNP P10104
B	1257	SER	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	PRO	-	expression tag	UNP P10104
B	1260	GLN	-	expression tag	UNP P10104
B	1261	PHE	-	expression tag	UNP P10104
B	1262	GLU	-	expression tag	UNP P10104
B	1263	LYS	-	expression tag	UNP P10104
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	15	SER	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	61	ASP	GLY	conflict	UNP P0DTC2
C	84	PHE	SER	conflict	UNP P0DTC2
C	112	ALA	VAL	conflict	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	127	LEU	TRP	conflict	UNP P0DTC2
C	165	SER	ARG	variant	UNP P0DTC2
C	188	GLY	VAL	variant	UNP P0DTC2
C	190	GLY	ASP	variant	UNP P0DTC2
C	314	ASP	GLY	variant	UNP P0DTC2
C	346	PHE	SER	variant	UNP P0DTC2
C	348	PRO	SER	variant	UNP P0DTC2
C	350	PHE	SER	variant	UNP P0DTC2
C	351	ALA	THR	variant	UNP P0DTC2
C	380	ASN	ASP	variant	UNP P0DTC2
C	383	SER	ARG	variant	UNP P0DTC2
C	392	THR	LYS	variant	UNP P0DTC2
C	415	LYS	ASN	variant	UNP P0DTC2
C	419	ASN	LYS	conflict	UNP P0DTC2
C	420	GLY	VAL	conflict	UNP P0DTC2
C	427	MET	LEU	conflict	UNP P0DTC2
C	435	LYS	ASN	variant	UNP P0DTC2
C	452	ASN	SER	variant	UNP P0DTC2
C	456	LYS	ASN	conflict	UNP P0DTC2
C	459	ALA	GLU	variant	UNP P0DTC2
C	473	ARG	GLN	variant	UNP P0DTC2
C	476	TYR	ASN	variant	UNP P0DTC2
C	480	HIS	TYR	variant	UNP P0DTC2
C	589	GLY	ASP	variant	UNP P0DTC2
C	596	SER	PRO	conflict	UNP P0DTC2
C	617	GLY	VAL	conflict	UNP P0DTC2
C	630	TYR	HIS	conflict	UNP P0DTC2
C	654	ARG	ASN	conflict	UNP P0DTC2
C	656	HIS	PRO	conflict	UNP P0DTC2
C	657	GLY	ARG	conflict	UNP P0DTC2
C	658	SER	ARG	conflict	UNP P0DTC2
C	660	SER	ARG	conflict	UNP P0DTC2
C	666	PRO	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	739	LYS	ASN	variant	UNP P0DTC2
C	766	ILE	THR	conflict	UNP P0DTC2
C	771	HIS	ASP	variant	UNP P0DTC2
C	911	GLY	ASP	conflict	UNP P0DTC2
C	929	HIS	GLN	variant	UNP P0DTC2
C	944	LYS	ASN	variant	UNP P0DTC2
C	961	PRO	LYS	engineered mutation	UNP P0DTC2
C	962	PRO	VAL	engineered mutation	UNP P0DTC2
C	1159	ASP	-	linker	UNP P0DTC2
C	1160	ARG	-	linker	UNP P0DTC2
C	1161	LEU	-	linker	UNP P0DTC2
C	1162	ASN	-	linker	UNP P0DTC2
C	1163	GLU	-	linker	UNP P0DTC2
C	1164	VAL	-	linker	UNP P0DTC2
C	1165	ALA	-	linker	UNP P0DTC2
C	1166	LYS	-	linker	UNP P0DTC2
C	1167	ASN	-	linker	UNP P0DTC2
C	1168	LEU	-	linker	UNP P0DTC2
C	1169	ASN	-	linker	UNP P0DTC2
C	1170	GLU	-	linker	UNP P0DTC2
C	1171	SER	-	linker	UNP P0DTC2
C	1172	LEU	-	linker	UNP P0DTC2
C	1173	ILE	-	linker	UNP P0DTC2
C	1174	ASP	-	linker	UNP P0DTC2
C	1175	LEU	-	linker	UNP P0DTC2
C	1176	GLN	-	linker	UNP P0DTC2
C	1177	GLU	-	linker	UNP P0DTC2
C	1178	LEU	-	linker	UNP P0DTC2
C	1179	GLY	-	linker	UNP P0DTC2
C	1180	LYS	-	linker	UNP P0DTC2
C	1181	TYR	-	linker	UNP P0DTC2
C	1182	GLU	-	linker	UNP P0DTC2
C	1183	GLN	-	linker	UNP P0DTC2
C	1184	GLY	-	linker	UNP P0DTC2
C	1185	SER	-	linker	UNP P0DTC2
C	1207	LEU	PHE	engineered mutation	UNP P10104
C	1213	GLY	-	expression tag	UNP P10104
C	1214	ARG	-	expression tag	UNP P10104
C	1215	SER	-	expression tag	UNP P10104
C	1216	LEU	-	expression tag	UNP P10104
C	1217	GLU	-	expression tag	UNP P10104
C	1218	VAL	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1219	LEU	-	expression tag	UNP P10104
C	1220	PHE	-	expression tag	UNP P10104
C	1221	GLN	-	expression tag	UNP P10104
C	1222	GLY	-	expression tag	UNP P10104
C	1223	PRO	-	expression tag	UNP P10104
C	1224	GLY	-	expression tag	UNP P10104
C	1225	HIS	-	expression tag	UNP P10104
C	1226	HIS	-	expression tag	UNP P10104
C	1227	HIS	-	expression tag	UNP P10104
C	1228	HIS	-	expression tag	UNP P10104
C	1229	HIS	-	expression tag	UNP P10104
C	1230	HIS	-	expression tag	UNP P10104
C	1231	HIS	-	expression tag	UNP P10104
C	1232	HIS	-	expression tag	UNP P10104
C	1233	GLY	-	expression tag	UNP P10104
C	1234	SER	-	expression tag	UNP P10104
C	1235	ALA	-	expression tag	UNP P10104
C	1236	TRP	-	expression tag	UNP P10104
C	1237	SER	-	expression tag	UNP P10104
C	1238	HIS	-	expression tag	UNP P10104
C	1239	PRO	-	expression tag	UNP P10104
C	1240	GLN	-	expression tag	UNP P10104
C	1241	PHE	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	LYS	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	GLY	-	expression tag	UNP P10104
C	1246	GLY	-	expression tag	UNP P10104
C	1247	SER	-	expression tag	UNP P10104
C	1248	GLY	-	expression tag	UNP P10104
C	1249	GLY	-	expression tag	UNP P10104
C	1250	GLY	-	expression tag	UNP P10104
C	1251	SER	-	expression tag	UNP P10104
C	1252	GLY	-	expression tag	UNP P10104
C	1253	GLY	-	expression tag	UNP P10104
C	1254	SER	-	expression tag	UNP P10104
C	1255	ALA	-	expression tag	UNP P10104
C	1256	TRP	-	expression tag	UNP P10104
C	1257	SER	-	expression tag	UNP P10104
C	1258	HIS	-	expression tag	UNP P10104
C	1259	PRO	-	expression tag	UNP P10104
C	1260	GLN	-	expression tag	UNP P10104

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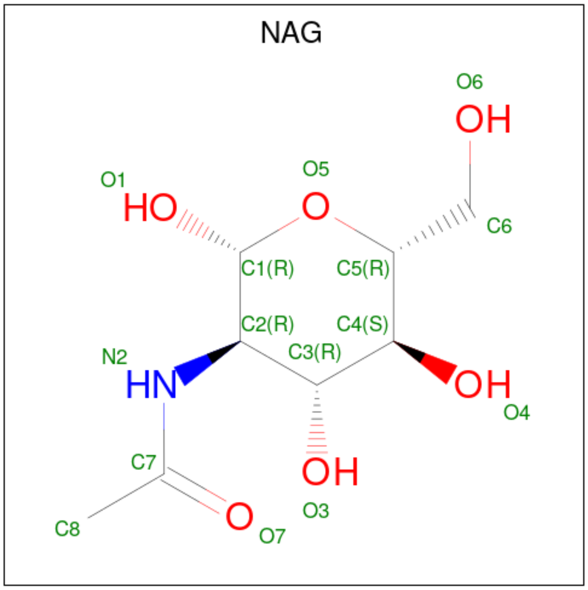
Chain	Residue	Modelled	Actual	Comment	Reference
C	1261	PHE	-	expression tag	UNP P10104
C	1262	GLU	-	expression tag	UNP P10104
C	1263	LYS	-	expression tag	UNP P10104

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

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

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



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

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

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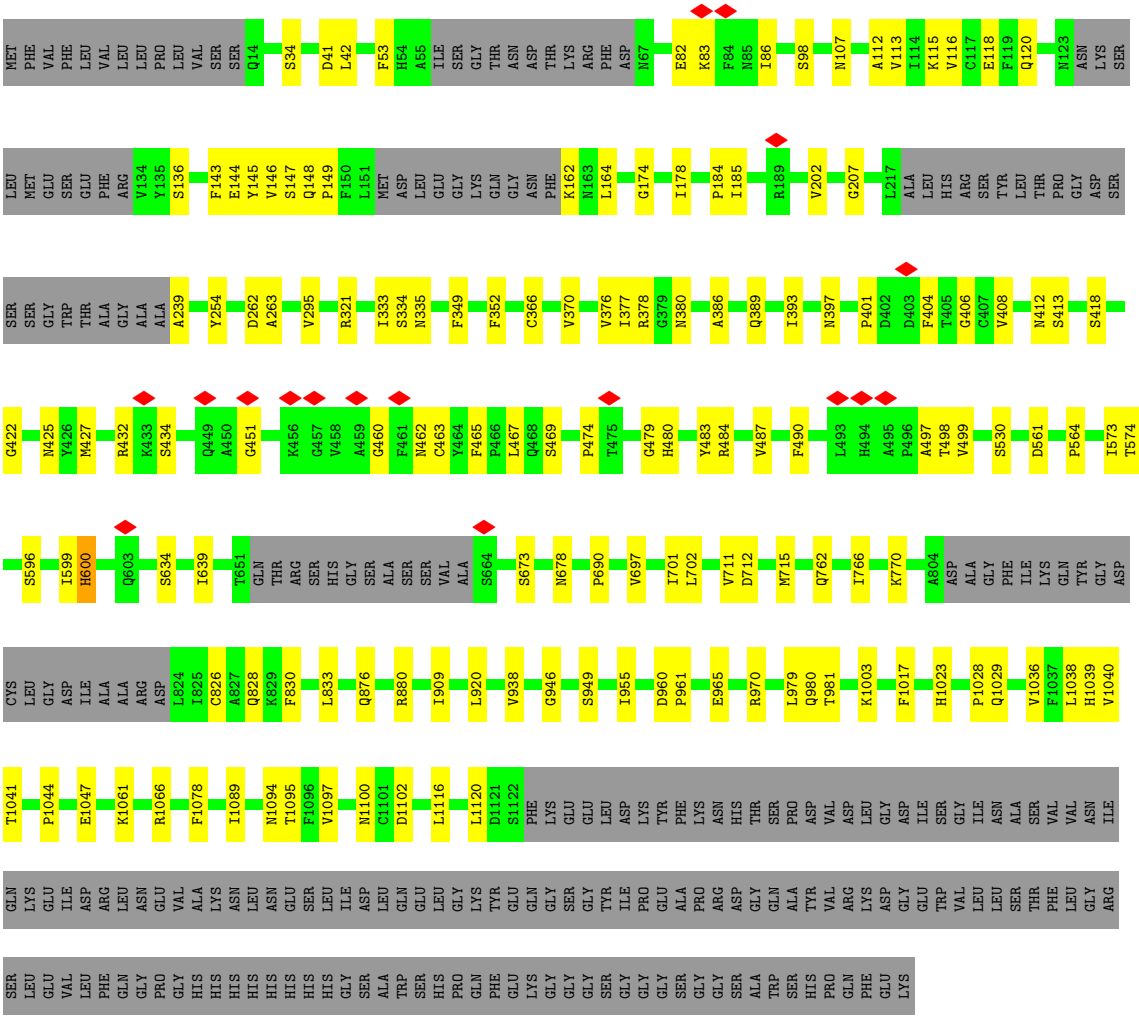
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 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.

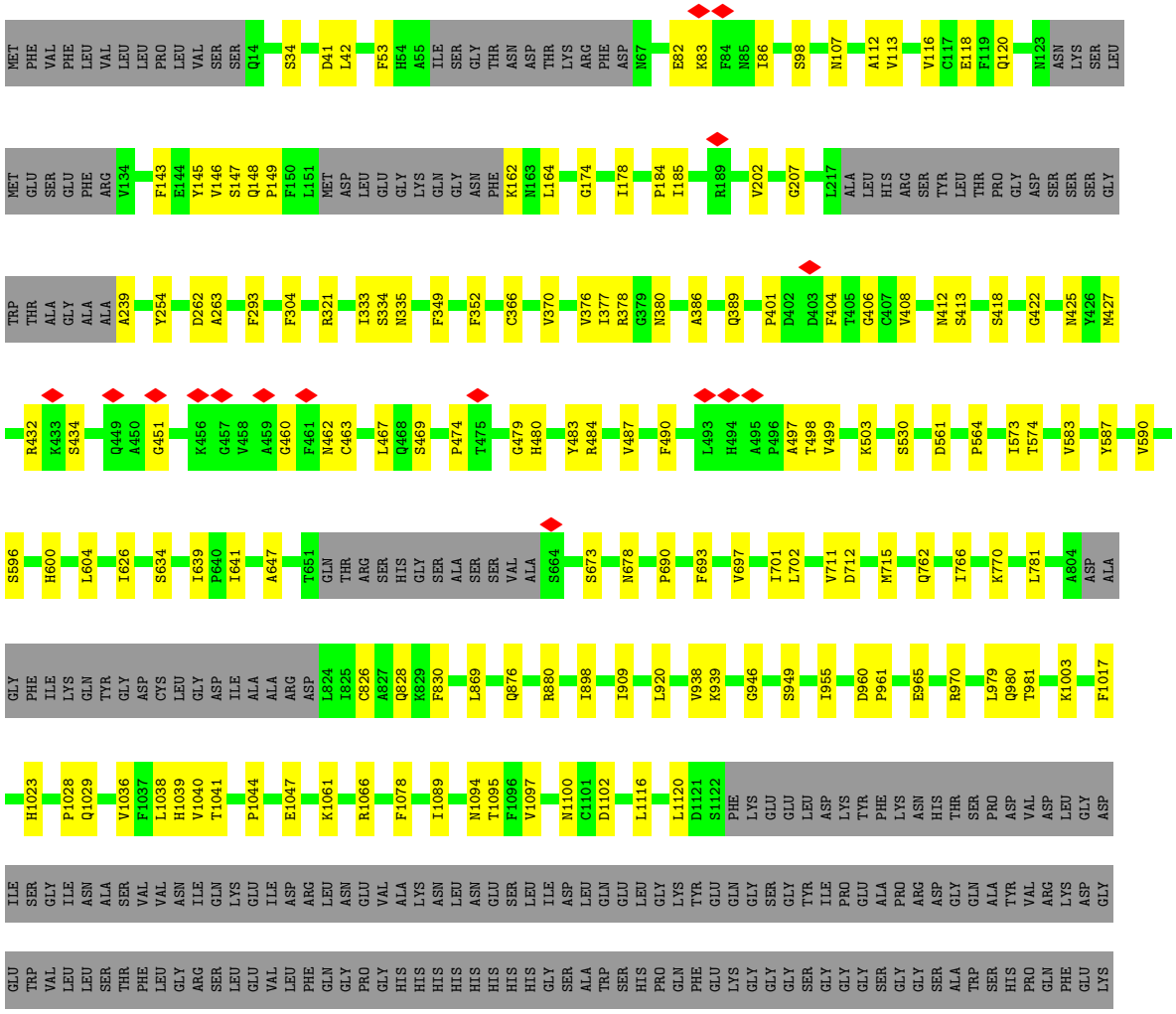
• Molecule 1: Spike glycoprotein,Fibritin

Chain A:



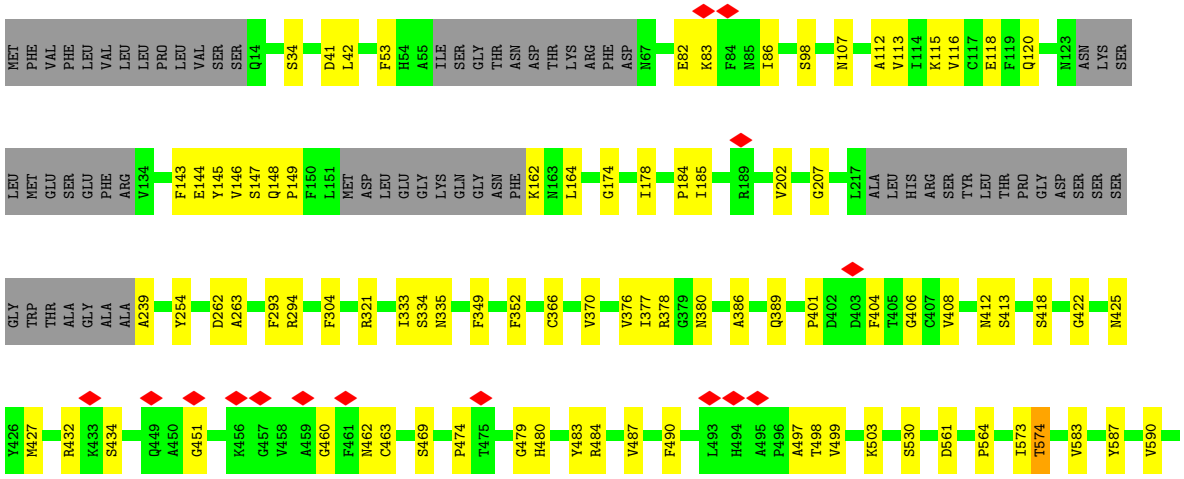
• Molecule 1: Spike glycoprotein,Fibritin

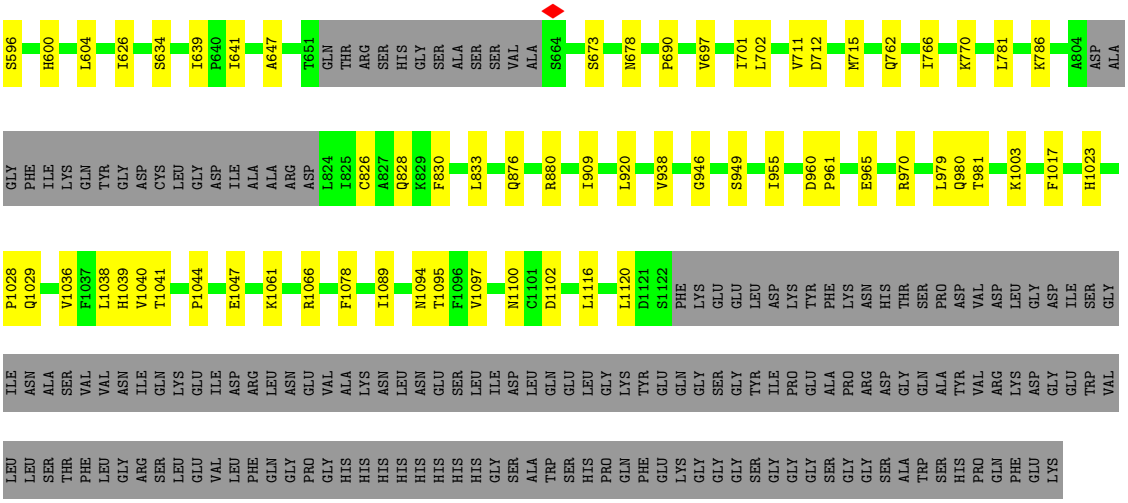
Chain B:



• Molecule 1: Spike glycoprotein,Fibritin

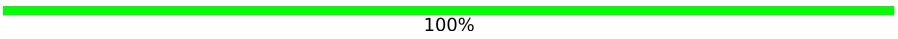
Chain C:





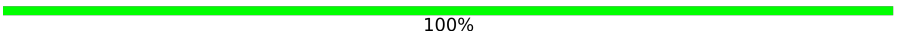
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:

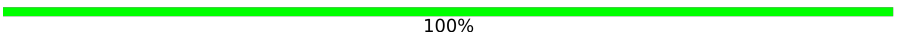


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

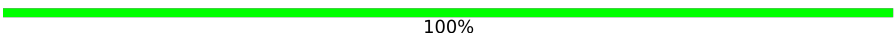
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

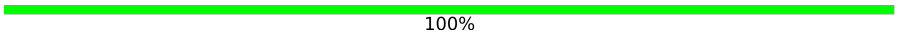


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

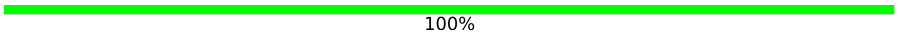
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	37441	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Determined using cryoSPARC live patch CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.492	Depositor
Minimum map value	-0.212	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0574	Depositor
Map size (Å)	255.605, 255.605, 255.605	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7303, 0.7303, 0.7303	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/8192	0.46	0/11146
1	B	0.28	0/8192	0.46	0/11146
1	C	0.28	0/8192	0.46	0/11146
All	All	0.28	0/24576	0.46	0/33438

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	8004	0	7826	86	0
1	B	8004	0	7826	91	0
1	C	8004	0	7826	91	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	1	0
3	A	182	0	169	1	0
3	B	182	0	169	1	0
3	C	182	0	169	1	0
All	All	24810	0	24210	257	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 5.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PHE:O	1:C:239:ALA:HA	1.80	0.80
1:B:53:PHE:O	1:B:239:ALA:HA	1.90	0.71
1:A:53:PHE:O	1:A:239:ALA:HA	1.95	0.67
1:A:711:VAL:HG11	1:A:979:LEU:HD21	1.77	0.66
1:B:711:VAL:HG11	1:B:979:LEU:HD21	1.77	0.65
1:C:711:VAL:HG11	1:C:979:LEU:HD21	1.78	0.63
1:C:41:ASP:OD1	1:C:42:LEU:N	2.33	0.60
1:B:1028:PRO:O	1:B:1029:GLN:NE2	2.31	0.60
1:A:1003:LYS:NZ	1:A:1017:PHE:O	2.35	0.59
1:B:34:SER:HA	1:B:254:TYR:O	2.02	0.59
1:B:41:ASP:OD1	1:B:42:LEU:N	2.34	0.59
1:A:34:SER:HA	1:A:254:TYR:O	2.03	0.58
1:B:1003:LYS:NZ	1:B:1017:PHE:O	2.36	0.58
1:A:1028:PRO:O	1:A:1029:GLN:NE2	2.31	0.58
1:C:1028:PRO:O	1:C:1029:GLN:NE2	2.31	0.58
1:A:401:PRO:HD2	1:A:404:PHE:HB2	1.87	0.57
1:B:401:PRO:HD2	1:B:404:PHE:HB2	1.86	0.57
1:A:946:GLY:HA3	1:A:970:ARG:HH21	1.69	0.57
1:B:946:GLY:HA3	1:B:970:ARG:HH21	1.70	0.57
1:C:113:VAL:HG12	1:C:146:VAL:HG22	1.86	0.57
1:A:1078:PHE:HZ	2:F:1:NAG:H62	1.70	0.57
1:C:34:SER:HA	1:C:254:TYR:O	2.04	0.57
1:C:1003:LYS:NZ	1:C:1017:PHE:O	2.37	0.57
1:B:113:VAL:HG12	1:B:146:VAL:HG22	1.87	0.56
1:C:401:PRO:HD2	1:C:404:PHE:HB2	1.87	0.56
1:A:113:VAL:HG12	1:A:146:VAL:HG22	1.87	0.56
1:A:1066:ARG:NH1	1:A:1095:THR:O	2.39	0.56
1:B:1078:PHE:HZ	2:I:1:NAG:H62	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:SER:H	1:A:600:HIS:HD2	1.54	0.55
1:A:41:ASP:OD1	1:A:42:LEU:N	2.34	0.55
1:C:1066:ARG:NH1	1:C:1095:THR:O	2.40	0.55
1:B:1066:ARG:NH1	1:B:1095:THR:O	2.40	0.54
1:C:1078:PHE:HZ	2:L:1:NAG:H62	1.70	0.54
1:A:530:SER:HB3	1:A:561:ASP:HB2	1.89	0.54
1:A:701:ILE:HD13	1:A:920:LEU:HD13	1.89	0.54
1:A:909:ILE:HD13	1:A:1038:LEU:HD22	1.90	0.54
1:C:376:VAL:HG22	1:C:484:ARG:HG2	1.90	0.54
1:C:909:ILE:HD13	1:C:1038:LEU:HD22	1.90	0.54
1:B:701:ILE:HD13	1:B:920:LEU:HD13	1.89	0.54
1:A:376:VAL:HG22	1:A:484:ARG:HG2	1.90	0.54
1:C:530:SER:HB3	1:C:561:ASP:HB2	1.89	0.54
1:C:946:GLY:HA3	1:C:970:ARG:HH21	1.72	0.54
1:B:530:SER:HB3	1:B:561:ASP:HB2	1.89	0.53
1:B:830:PHE:CG	1:C:564:PRO:HG2	2.44	0.53
1:C:83:LYS:HE3	1:C:162:LYS:HG2	1.89	0.53
1:A:83:LYS:HE3	1:A:162:LYS:HG2	1.89	0.53
1:B:83:LYS:HE3	1:B:162:LYS:HG2	1.89	0.53
1:A:564:PRO:HG2	1:C:830:PHE:CG	2.43	0.53
1:C:335:ASN:ND2	1:C:498:THR:OG1	2.42	0.53
1:B:1023:HIS:HA	1:B:1041:THR:HG22	1.91	0.53
1:C:701:ILE:HD13	1:C:920:LEU:HD13	1.89	0.53
1:A:460:GLY:H	1:A:463:CYS:HB2	1.74	0.53
1:B:762:GLN:OE1	1:C:678:ASN:ND2	2.36	0.53
1:C:178:ILE:HB	1:C:202:VAL:HG12	1.91	0.53
1:A:333:ILE:HB	1:A:370:VAL:HB	1.90	0.52
1:B:333:ILE:HB	1:B:370:VAL:HB	1.90	0.52
1:B:408:VAL:HG12	1:B:487:VAL:HG22	1.92	0.52
1:A:335:ASN:ND2	1:A:498:THR:OG1	2.42	0.52
1:B:909:ILE:HD13	1:B:1038:LEU:HD22	1.89	0.52
1:B:376:VAL:HG22	1:B:484:ARG:HG2	1.90	0.52
1:A:408:VAL:HG12	1:A:487:VAL:HG22	1.92	0.52
1:B:335:ASN:ND2	1:B:498:THR:OG1	2.42	0.52
1:B:697:VAL:HG22	1:B:1040:VAL:HG22	1.92	0.52
1:C:418:SER:HB2	1:C:474:PRO:HD3	1.92	0.52
1:B:178:ILE:HB	1:B:202:VAL:HG12	1.92	0.52
1:B:418:SER:HB2	1:B:474:PRO:HD3	1.92	0.52
1:C:333:ILE:HB	1:C:370:VAL:HB	1.91	0.52
1:C:1023:HIS:HA	1:C:1041:THR:HG22	1.91	0.52
1:A:830:PHE:CG	1:B:564:PRO:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:GLY:H	1:C:463:CYS:HB2	1.74	0.52
1:B:460:GLY:H	1:B:463:CYS:HB2	1.75	0.51
1:B:378:ARG:HD3	1:B:480:HIS:HD1	1.75	0.51
1:C:378:ARG:HD3	1:C:480:HIS:HD1	1.76	0.51
1:C:408:VAL:HG12	1:C:487:VAL:HG22	1.92	0.51
1:A:980:GLN:NE2	1:B:981:THR:OG1	2.43	0.51
1:A:178:ILE:HB	1:A:202:VAL:HG12	1.92	0.51
1:A:335:ASN:H	1:A:498:THR:HG23	1.76	0.51
1:B:116:VAL:HG22	1:B:143:PHE:H	1.76	0.51
1:A:184:PRO:HB3	3:A:1304:NAG:H82	1.93	0.51
1:A:981:THR:OG1	1:C:980:GLN:NE2	2.44	0.51
1:B:335:ASN:H	1:B:498:THR:HG23	1.76	0.51
1:C:335:ASN:H	1:C:498:THR:HG23	1.76	0.51
1:A:1023:HIS:HA	1:A:1041:THR:HG22	1.92	0.51
1:B:262:ASP:OD1	1:B:263:ALA:N	2.43	0.51
1:A:262:ASP:OD1	1:A:263:ALA:N	2.43	0.50
1:A:418:SER:HB2	1:A:474:PRO:HD3	1.92	0.50
1:B:980:GLN:NE2	1:C:981:THR:OG1	2.44	0.50
1:B:1061:LYS:HD2	1:B:1097:VAL:HG11	1.93	0.50
1:B:184:PRO:HB3	3:B:1304:NAG:H82	1.94	0.50
1:A:378:ARG:HD3	1:A:480:HIS:HD1	1.76	0.50
1:C:574:THR:HB	1:C:583:VAL:HG12	1.94	0.50
1:C:116:VAL:HG22	1:C:143:PHE:H	1.76	0.50
1:A:116:VAL:HG22	1:A:143:PHE:H	1.76	0.50
1:C:184:PRO:HB3	3:C:1304:NAG:H82	1.93	0.50
1:B:293:PHE:HZ	1:B:590:VAL:HG11	1.77	0.49
1:C:1061:LYS:HD2	1:C:1097:VAL:HG11	1.93	0.49
1:B:386:ALA:HB3	1:B:389:GLN:HG3	1.94	0.49
1:A:432:ARG:NH1	1:A:434:SER:O	2.37	0.49
1:A:574:THR:HB	1:A:583:VAL:HG12	1.94	0.49
1:A:961:PRO:O	1:A:965:GLU:HG2	2.12	0.49
1:C:828:GLN:HA	1:C:938:VAL:HG21	1.95	0.49
1:B:574:THR:HB	1:B:583:VAL:HG12	1.93	0.49
1:C:293:PHE:HZ	1:C:590:VAL:HG11	1.77	0.49
1:B:690:PRO:HA	1:B:1047:GLU:HA	1.94	0.49
1:A:412:ASN:HA	1:A:483:TYR:CD1	2.48	0.49
1:A:1061:LYS:HD2	1:A:1097:VAL:HG11	1.93	0.49
1:B:596:SER:O	1:B:600:HIS:HB2	2.12	0.49
1:A:386:ALA:HB3	1:A:389:GLN:HG3	1.95	0.49
1:C:596:SER:O	1:C:600:HIS:HB2	2.12	0.49
1:B:412:ASN:HA	1:B:483:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:PRO:O	1:B:965:GLU:HG2	2.12	0.49
1:A:690:PRO:HA	1:A:1047:GLU:HA	1.94	0.48
1:B:766:ILE:HD12	1:B:770:LYS:HE3	1.94	0.48
1:C:412:ASN:HA	1:C:483:TYR:CD1	2.48	0.48
1:B:148:GLN:HG2	1:B:149:PRO:HD2	1.95	0.48
1:C:262:ASP:OD1	1:C:263:ALA:N	2.43	0.48
1:C:690:PRO:HA	1:C:1047:GLU:HA	1.94	0.48
1:A:380:ASN:ND2	1:A:479:GLY:O	2.46	0.48
1:C:961:PRO:O	1:C:965:GLU:HG2	2.12	0.48
1:B:164:LEU:HB2	1:B:185:ILE:HD13	1.96	0.48
1:B:380:ASN:ND2	1:B:479:GLY:O	2.47	0.48
1:C:164:LEU:HB2	1:C:185:ILE:HD13	1.96	0.48
1:C:380:ASN:ND2	1:C:479:GLY:O	2.47	0.48
1:C:386:ALA:HB3	1:C:389:GLN:HG3	1.95	0.48
1:A:427:MET:HA	1:A:469:SER:HA	1.95	0.48
1:A:34:SER:CA	1:A:254:TYR:O	2.62	0.48
1:C:148:GLN:HG2	1:C:149:PRO:HD2	1.95	0.48
1:A:762:GLN:OE1	1:B:678:ASN:ND2	2.37	0.48
1:B:427:MET:HA	1:B:469:SER:HA	1.95	0.47
1:C:766:ILE:HD12	1:C:770:LYS:HE3	1.95	0.47
1:A:766:ILE:HD12	1:A:770:LYS:HE3	1.95	0.47
1:B:432:ARG:NH1	1:B:434:SER:O	2.37	0.47
1:C:366:CYS:HB3	1:C:497:ALA:HB1	1.96	0.47
1:C:432:ARG:NH1	1:C:434:SER:O	2.36	0.47
1:A:697:VAL:HG22	1:A:1040:VAL:HG22	1.95	0.47
1:C:451:GLY:H	1:C:462:ASN:HB3	1.79	0.47
1:A:451:GLY:H	1:A:462:ASN:HB3	1.79	0.47
1:B:451:GLY:H	1:B:462:ASN:HB3	1.79	0.47
1:C:145:TYR:HE1	1:C:147:SER:HB3	1.80	0.47
1:C:427:MET:HA	1:C:469:SER:HA	1.96	0.47
1:C:573:ILE:HG23	1:C:639:ILE:HG21	1.97	0.47
1:A:148:GLN:HG2	1:A:149:PRO:HD2	1.95	0.47
1:A:366:CYS:HB3	1:A:497:ALA:HB1	1.95	0.47
1:A:828:GLN:HA	1:A:938:VAL:HG21	1.95	0.47
1:B:828:GLN:HA	1:B:938:VAL:HG21	1.96	0.47
1:C:697:VAL:HG22	1:C:1040:VAL:HG22	1.95	0.47
1:C:960:ASP:OD1	1:C:960:ASP:N	2.45	0.47
1:A:164:LEU:HB2	1:A:185:ILE:HD13	1.95	0.47
1:B:366:CYS:HB3	1:B:497:ALA:HB1	1.96	0.47
1:C:604:LEU:HD23	1:C:604:LEU:H	1.79	0.47
1:A:573:ILE:HG23	1:A:639:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ARG:HH21	1:B:422:GLY:HA3	1.80	0.47
1:B:876:GLN:O	1:B:880:ARG:HG2	2.15	0.47
1:B:34:SER:CA	1:B:254:TYR:O	2.62	0.47
1:A:876:GLN:O	1:A:880:ARG:HG2	2.15	0.46
1:A:321:ARG:HH21	1:A:422:GLY:HA3	1.81	0.46
1:C:321:ARG:HH21	1:C:422:GLY:HA3	1.80	0.46
1:C:34:SER:CA	1:C:254:TYR:O	2.63	0.46
1:A:295:VAL:HG13	1:A:599:ILE:HD12	1.97	0.46
1:A:678:ASN:ND2	1:C:762:GLN:OE1	2.37	0.46
1:B:573:ILE:HG23	1:B:639:ILE:HG21	1.97	0.46
1:A:697:VAL:HA	1:A:1039:HIS:O	2.16	0.45
1:B:82:GLU:HG3	1:B:86:ILE:HG22	1.98	0.45
1:B:479:GLY:O	1:B:480:HIS:ND1	2.49	0.45
1:A:145:TYR:HE1	1:A:147:SER:HB3	1.80	0.45
1:B:145:TYR:HE1	1:B:147:SER:HB3	1.79	0.45
1:B:604:LEU:HD23	1:B:604:LEU:H	1.79	0.45
1:C:876:GLN:O	1:C:880:ARG:HG2	2.16	0.45
1:C:82:GLU:HG3	1:C:86:ILE:HG22	1.99	0.45
1:C:479:GLY:O	1:C:480:HIS:ND1	2.49	0.45
1:A:112:ALA:HB2	1:A:149:PRO:HA	1.99	0.45
1:A:377:ILE:HG12	1:A:378:ARG:H	1.82	0.45
1:A:98:SER:HA	1:A:118:GLU:HB3	1.99	0.45
1:A:479:GLY:O	1:A:480:HIS:ND1	2.49	0.44
1:B:98:SER:HA	1:B:118:GLU:HB3	1.99	0.44
1:B:377:ILE:HG12	1:B:378:ARG:H	1.82	0.44
1:B:422:GLY:HA2	1:B:425:ASN:HB3	1.99	0.44
1:C:712:ASP:HB3	1:C:715:MET:HB3	1.99	0.44
1:C:1100:ASN:ND2	1:C:1102:ASP:OD2	2.50	0.44
1:A:960:ASP:OD1	1:A:960:ASP:N	2.45	0.44
1:B:413:SER:HB3	1:B:484:ARG:HG3	1.99	0.44
1:C:112:ALA:HB2	1:C:149:PRO:HA	1.99	0.44
1:B:701:ILE:HG12	1:B:1036:VAL:HG22	1.99	0.44
1:B:960:ASP:OD1	1:B:960:ASP:N	2.45	0.44
1:C:98:SER:HA	1:C:118:GLU:HB3	2.00	0.44
1:B:112:ALA:HB2	1:B:149:PRO:HA	1.99	0.44
1:A:82:GLU:HG3	1:A:86:ILE:HG22	1.99	0.44
1:C:334:SER:HA	1:C:499:VAL:HG22	2.00	0.44
1:B:949:SER:HB3	1:B:955:ILE:HD11	1.99	0.44
1:A:120:GLN:O	1:A:136:SER:OG	2.26	0.44
1:A:334:SER:HA	1:A:499:VAL:HG22	2.00	0.43
1:C:1089:ILE:O	1:C:1094:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:VAL:HA	1:B:1039:HIS:O	2.18	0.43
1:A:1100:ASN:ND2	1:A:1102:ASP:OD2	2.51	0.43
1:A:422:GLY:HA2	1:A:425:ASN:HB3	1.99	0.43
1:A:1116:LEU:HG	1:A:1120:LEU:HD23	2.00	0.43
1:C:413:SER:HB3	1:C:484:ARG:HG3	1.99	0.43
1:C:422:GLY:HA2	1:C:425:ASN:HB3	2.00	0.43
1:C:377:ILE:HG12	1:C:378:ARG:H	1.82	0.43
1:C:786:LYS:HE2	1:C:786:LYS:HB3	1.91	0.43
1:C:697:VAL:HG12	1:C:909:ILE:HD11	2.01	0.43
1:C:949:SER:HB3	1:C:955:ILE:HD11	2.00	0.43
1:A:413:SER:HB3	1:A:484:ARG:HG3	2.00	0.43
1:A:949:SER:HB3	1:A:955:ILE:HD11	2.00	0.43
1:C:701:ILE:HG12	1:C:1036:VAL:HG22	2.00	0.43
1:A:697:VAL:HG12	1:A:909:ILE:HD11	2.00	0.43
1:B:1100:ASN:ND2	1:B:1102:ASP:OD2	2.52	0.43
1:C:697:VAL:HA	1:C:1039:HIS:O	2.19	0.43
1:B:712:ASP:HB3	1:B:715:MET:HB3	2.00	0.42
1:A:712:ASP:HB3	1:A:715:MET:HB3	2.00	0.42
1:A:1089:ILE:O	1:A:1094:ASN:ND2	2.53	0.42
1:B:334:SER:HA	1:B:499:VAL:HG22	2.00	0.42
1:B:587:TYR:HE1	1:B:626:ILE:HD12	1.83	0.42
1:B:1089:ILE:O	1:B:1094:ASN:ND2	2.52	0.42
1:B:174:GLY:HA2	1:B:207:GLY:HA2	2.01	0.42
1:B:1116:LEU:HG	1:B:1120:LEU:HD23	2.01	0.42
1:C:174:GLY:HA2	1:C:207:GLY:HA2	2.02	0.42
1:A:174:GLY:HA2	1:A:207:GLY:HA2	2.02	0.42
1:B:697:VAL:HG12	1:B:909:ILE:HD11	2.00	0.42
1:C:1116:LEU:HG	1:C:1120:LEU:HD23	2.01	0.42
1:B:693:PHE:HE1	1:B:898:ILE:HG12	1.85	0.42
1:B:702:LEU:HD11	1:B:1003:LYS:HD2	2.02	0.42
1:C:826:CYS:HB3	1:C:830:PHE:CZ	2.55	0.41
1:A:826:CYS:HB3	1:A:830:PHE:CZ	2.56	0.41
1:C:587:TYR:HE1	1:C:626:ILE:HD12	1.83	0.41
1:B:826:CYS:HB3	1:B:830:PHE:CZ	2.55	0.41
1:A:702:LEU:HD11	1:A:1003:LYS:HD2	2.01	0.41
1:B:98:SER:H	1:B:120:GLN:NE2	2.18	0.41
1:A:690:PRO:HG3	1:A:1044:PRO:HB3	2.03	0.41
1:A:406:GLY:HA2	1:A:490:PHE:CD2	2.56	0.41
1:B:304:PHE:CE2	1:B:503:LYS:HB3	2.55	0.41
1:B:715:MET:HE2	1:C:294:ARG:HH21	1.86	0.41
1:B:766:ILE:HD13	1:B:781:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:VAL:HG22	1:C:833:LEU:HD22	2.03	0.41
1:A:711:VAL:HG22	1:A:833:LEU:HD22	2.03	0.41
1:A:98:SER:H	1:A:120:GLN:NE2	2.18	0.41
1:A:115:LYS:HG2	1:A:144:GLU:HG2	2.03	0.41
1:A:634:SER:HB3	1:A:673:SER:HB2	2.03	0.41
1:A:701:ILE:HG12	1:A:1036:VAL:HG22	2.02	0.41
1:B:406:GLY:HA2	1:B:490:PHE:CD2	2.56	0.41
1:B:467:LEU:HD12	1:B:467:LEU:HA	1.93	0.41
1:B:869:LEU:HD13	1:C:690:PRO:HD3	2.03	0.41
1:B:939:LYS:HE3	1:B:939:LYS:HB3	1.89	0.41
1:C:690:PRO:HG3	1:C:1044:PRO:HB3	2.03	0.41
1:B:634:SER:HB3	1:B:673:SER:HB2	2.03	0.41
1:B:690:PRO:HG3	1:B:1044:PRO:HB3	2.03	0.41
1:C:641:ILE:HD11	1:C:647:ALA:HB2	2.02	0.41
1:C:406:GLY:HA2	1:C:490:PHE:CD2	2.56	0.40
1:C:766:ILE:HD13	1:C:781:LEU:HD22	2.02	0.40
1:C:115:LYS:HG2	1:C:144:GLU:HG2	2.03	0.40
1:C:304:PHE:CE2	1:C:503:LYS:HB3	2.56	0.40
1:C:702:LEU:HD11	1:C:1003:LYS:HD2	2.03	0.40
1:A:393:ILE:HA	1:A:397:ASN:HD22	1.87	0.40
1:C:98:SER:H	1:C:120:GLN:NE2	2.18	0.40
1:A:465:PHE:CE2	1:A:467:LEU:HB3	2.57	0.40
1:B:641:ILE:HD11	1:B:647:ALA:HB2	2.02	0.40
1:C:634:SER:HB3	1:C:673:SER:HB2	2.03	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	1012/1263 (80%)	990 (98%)	22 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1012/1263 (80%)	989 (98%)	23 (2%)	0	100	100
1	C	1012/1263 (80%)	988 (98%)	24 (2%)	0	100	100
All	All	3036/3789 (80%)	2967 (98%)	69 (2%)	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	890/1083 (82%)	886 (100%)	4 (0%)	89	96
1	B	890/1083 (82%)	887 (100%)	3 (0%)	91	97
1	C	890/1083 (82%)	886 (100%)	4 (0%)	89	96
All	All	2670/3249 (82%)	2659 (100%)	11 (0%)	88	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	349	PHE
1	A	352	PHE
1	A	600	HIS
1	B	107	ASN
1	B	349	PHE
1	B	352	PHE
1	C	107	ASN
1	C	349	PHE
1	C	352	PHE
1	C	574	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	335	ASN
1	A	494	HIS
1	A	600	HIS
1	A	665	GLN
1	A	730	GLN
1	A	932	GLN
1	A	980	GLN
1	B	120	GLN
1	B	335	ASN
1	B	494	HIS
1	B	665	GLN
1	B	730	GLN
1	B	932	GLN
1	B	980	GLN
1	B	985	GLN
1	C	120	GLN
1	C	335	ASN
1	C	494	HIS
1	C	665	GLN
1	C	730	GLN
1	C	932	GLN
1	C	980	GLN
1	C	985	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 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	0.20	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.18	0	17,19,21	0.39	0
2	NAG	E	1	2,1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	F	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	F	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	G	1	2,1	14,14,15	0.21	0	17,19,21	0.51	0
2	NAG	G	2	2	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	H	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	H	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	I	1	2,1	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	J	1	2,1	14,14,15	0.19	0	17,19,21	0.52	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	K	1	2,1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	K	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	L	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	L	2	2	14,14,15	0.20	0	17,19,21	0.42	0

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	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	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
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2

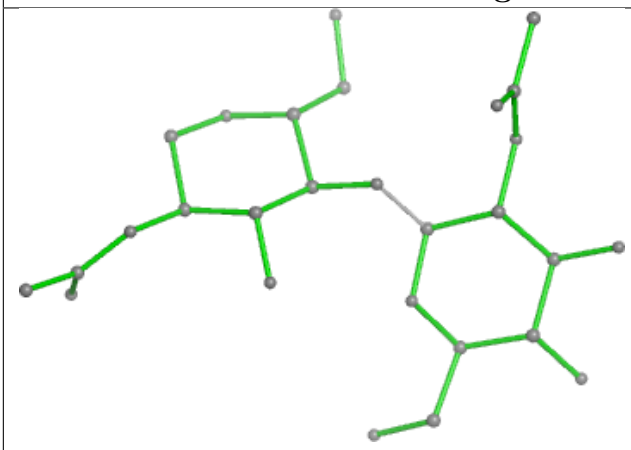
There are no ring outliers.

3 monomers are involved in 3 short contacts:

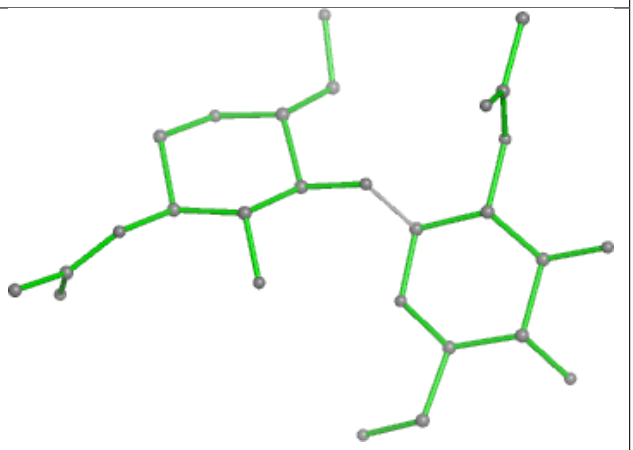
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	1	0
2	F	1	NAG	1	0
2	I	1	NAG	1	0

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

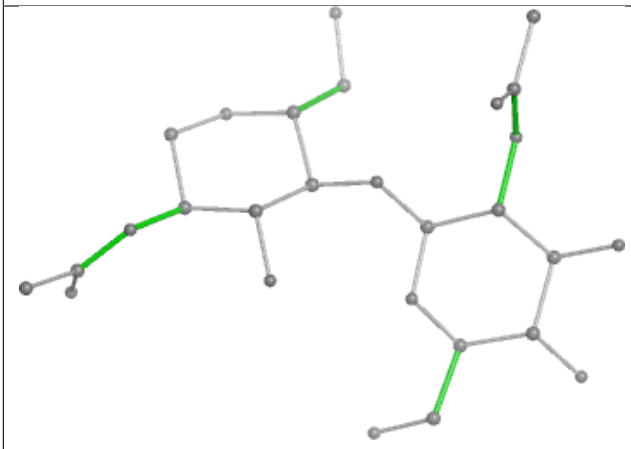
Oligosaccharide Chain D



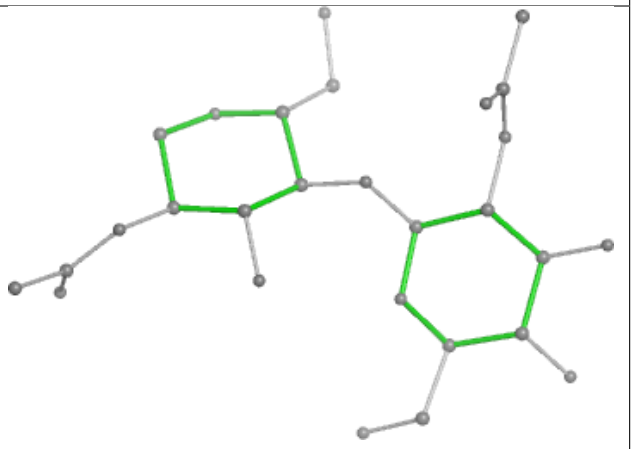
Bond lengths



Bond angles

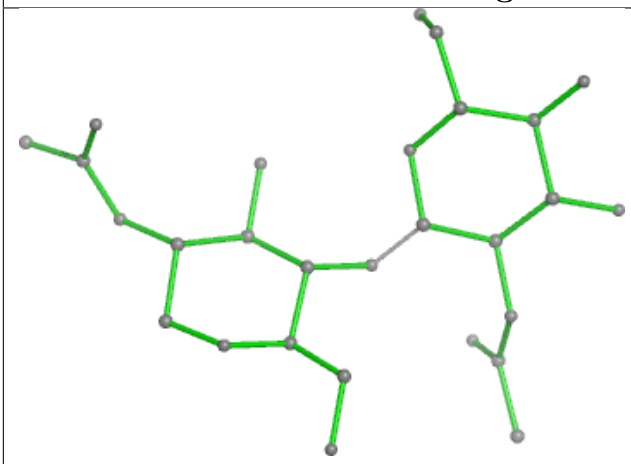


Torsions

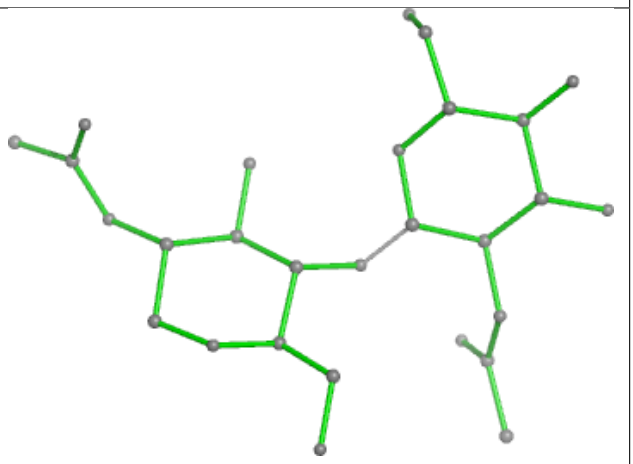


Rings

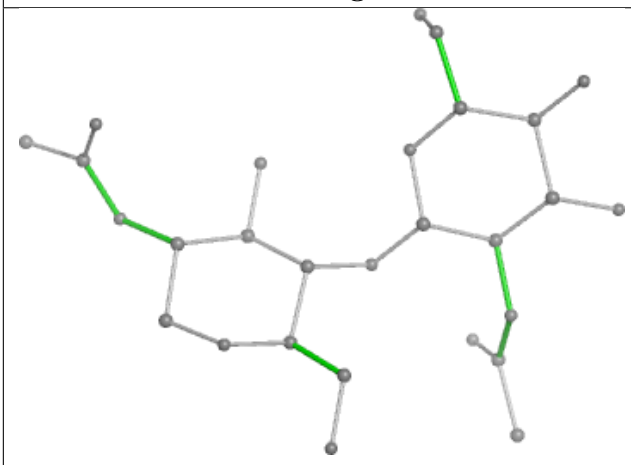
Oligosaccharide Chain E



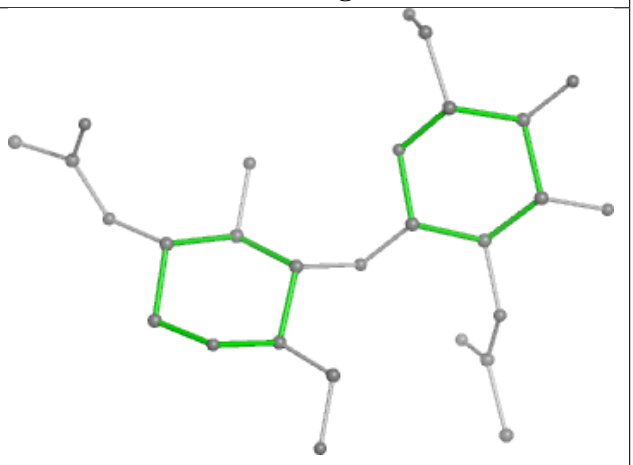
Bond lengths



Bond angles

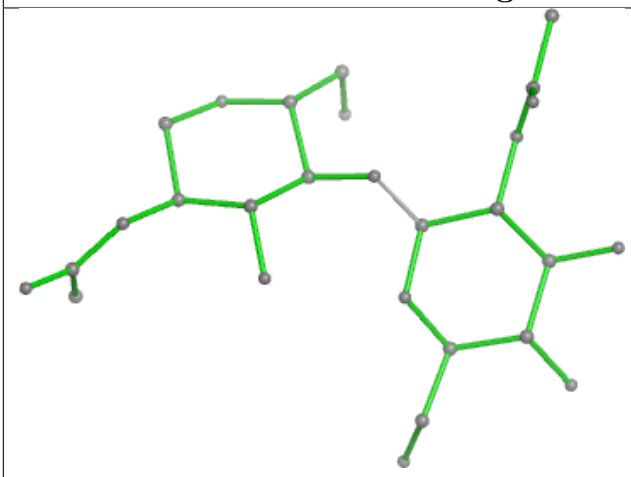


Torsions

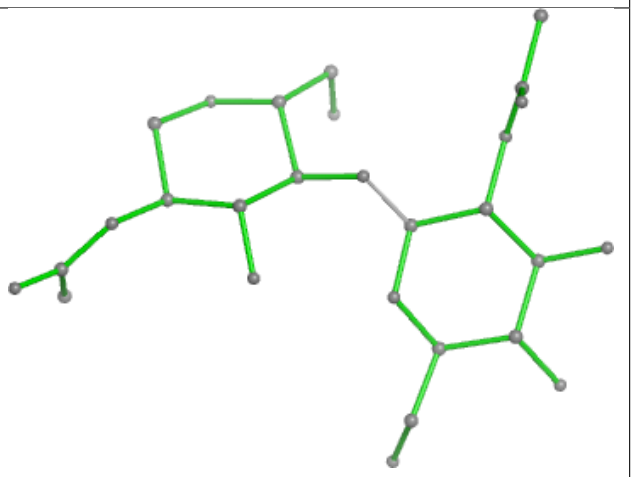


Rings

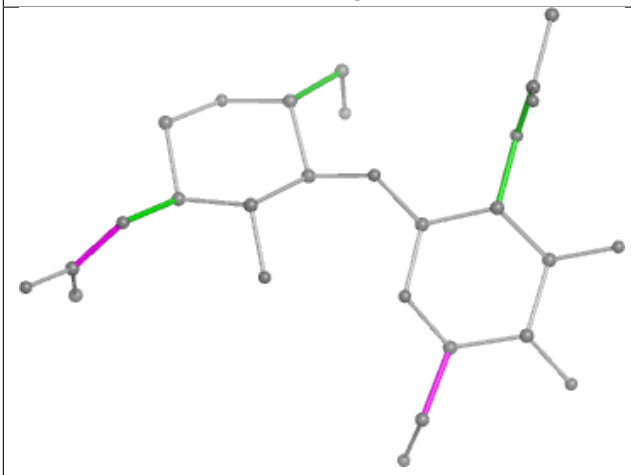
Oligosaccharide Chain F



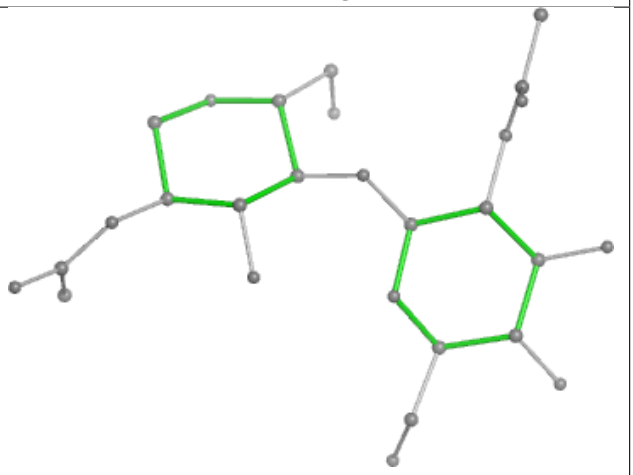
Bond lengths



Bond angles

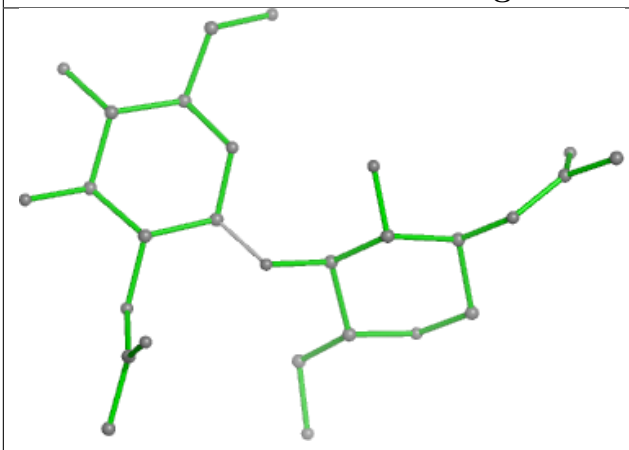


Torsions

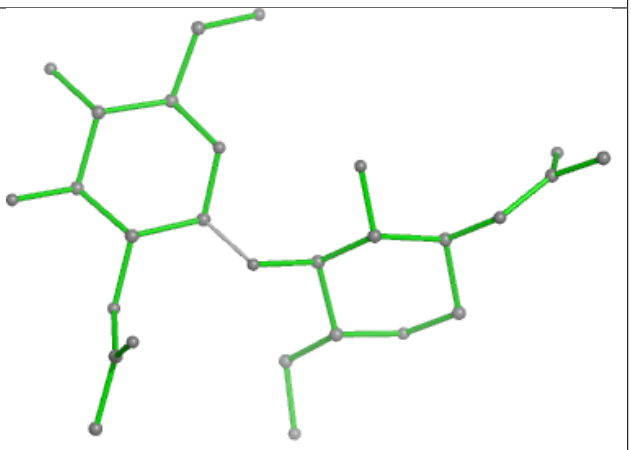


Rings

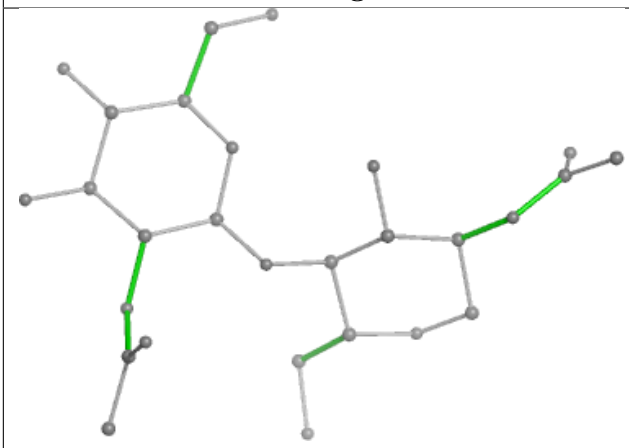
Oligosaccharide Chain G



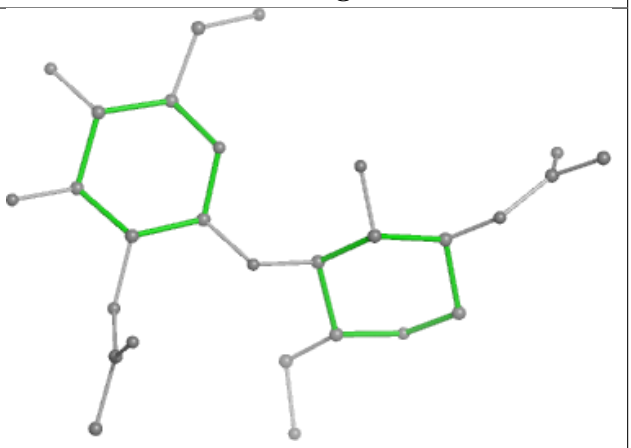
Bond lengths



Bond angles

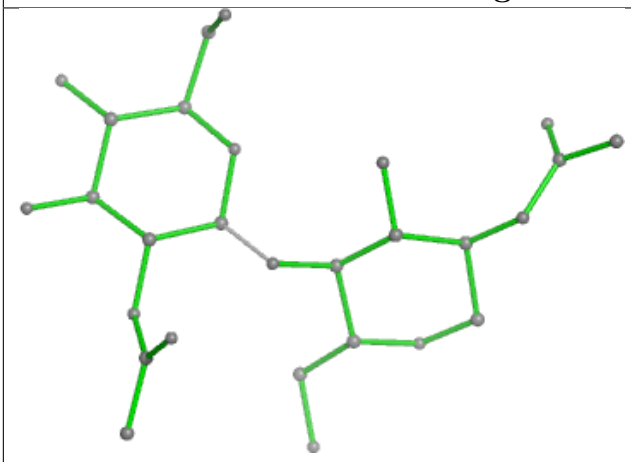


Torsions

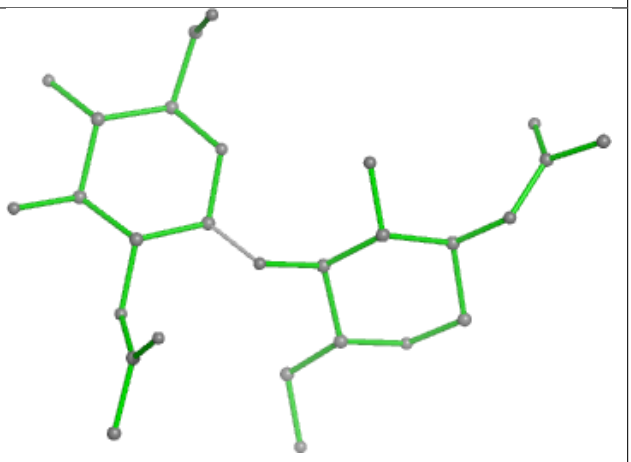


Rings

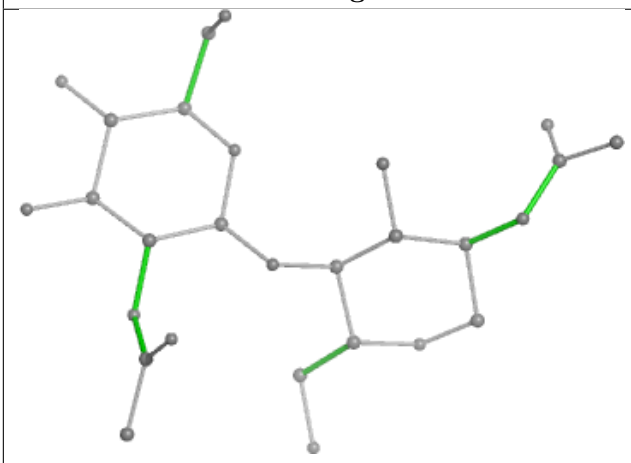
Oligosaccharide Chain H



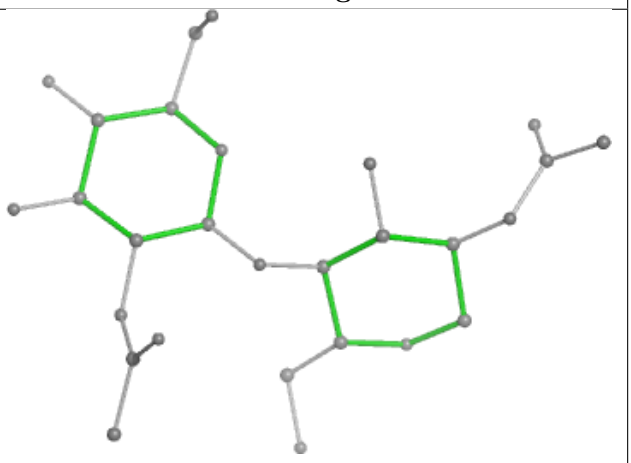
Bond lengths



Bond angles

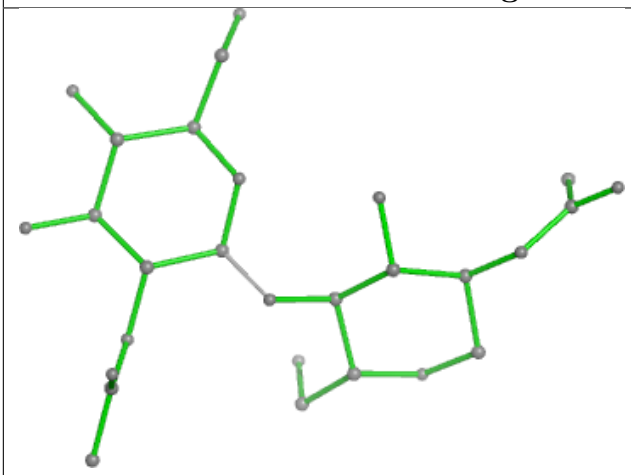


Torsions

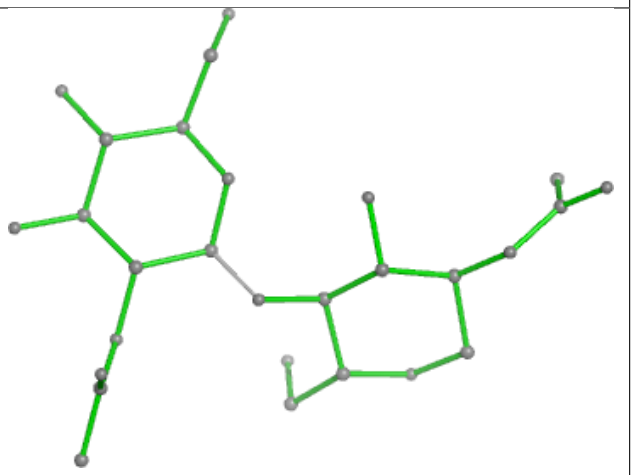


Rings

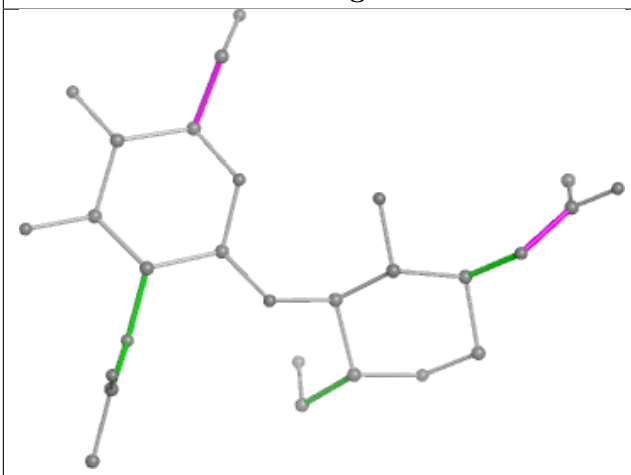
Oligosaccharide Chain I



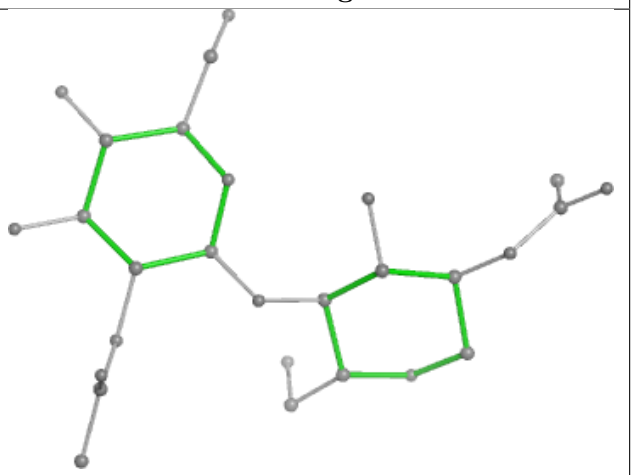
Bond lengths



Bond angles

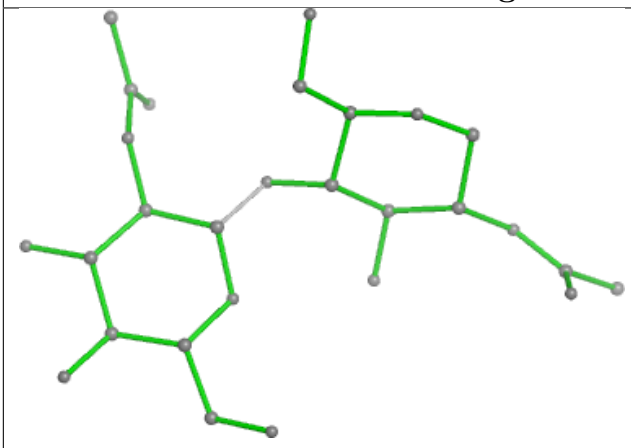


Torsions

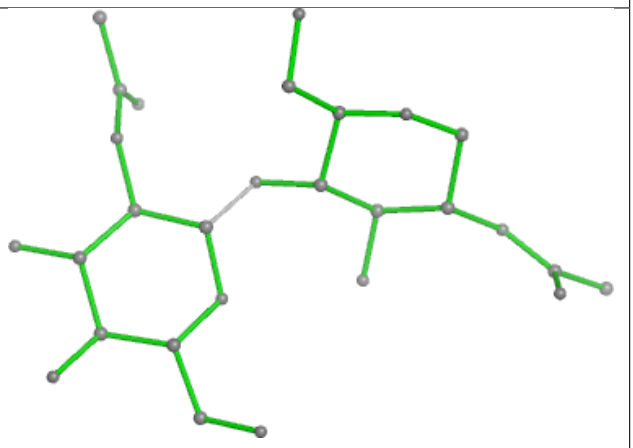


Rings

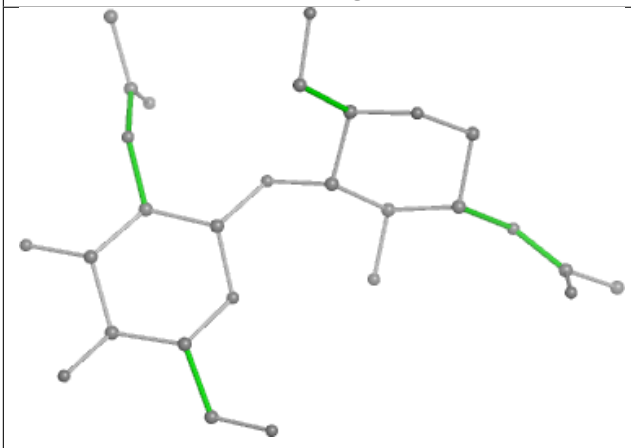
Oligosaccharide Chain J



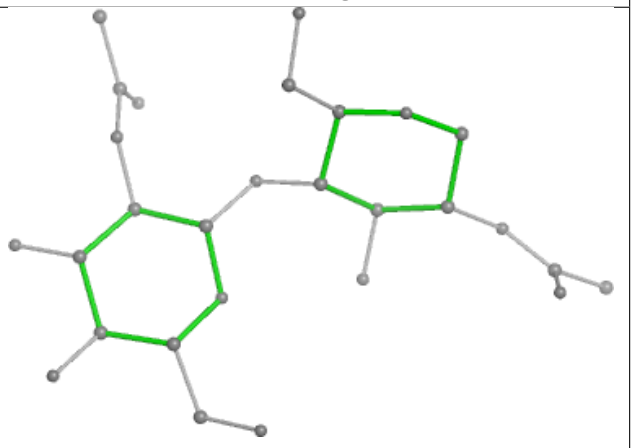
Bond lengths



Bond angles

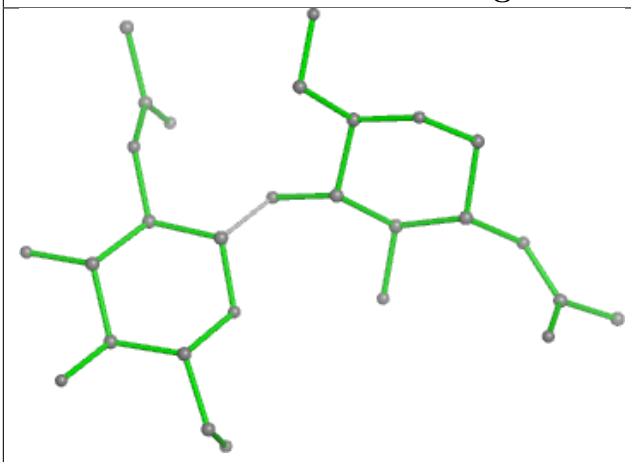


Torsions

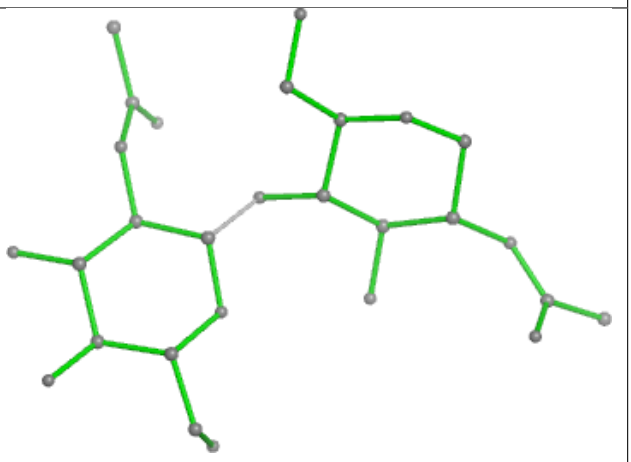


Rings

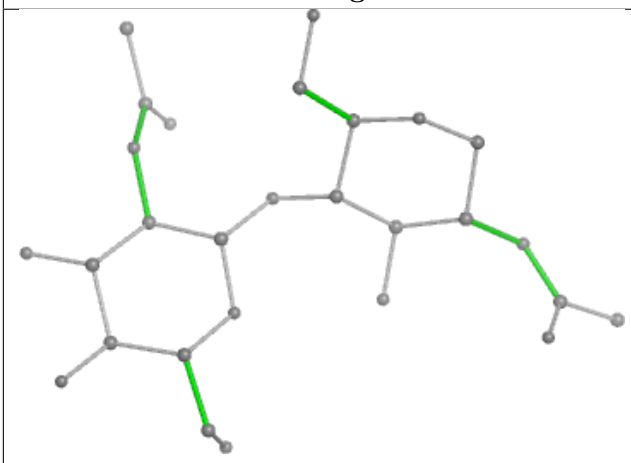
Oligosaccharide Chain K



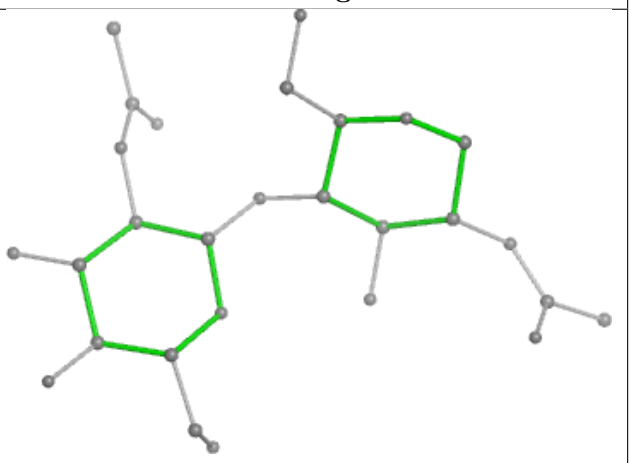
Bond lengths



Bond angles

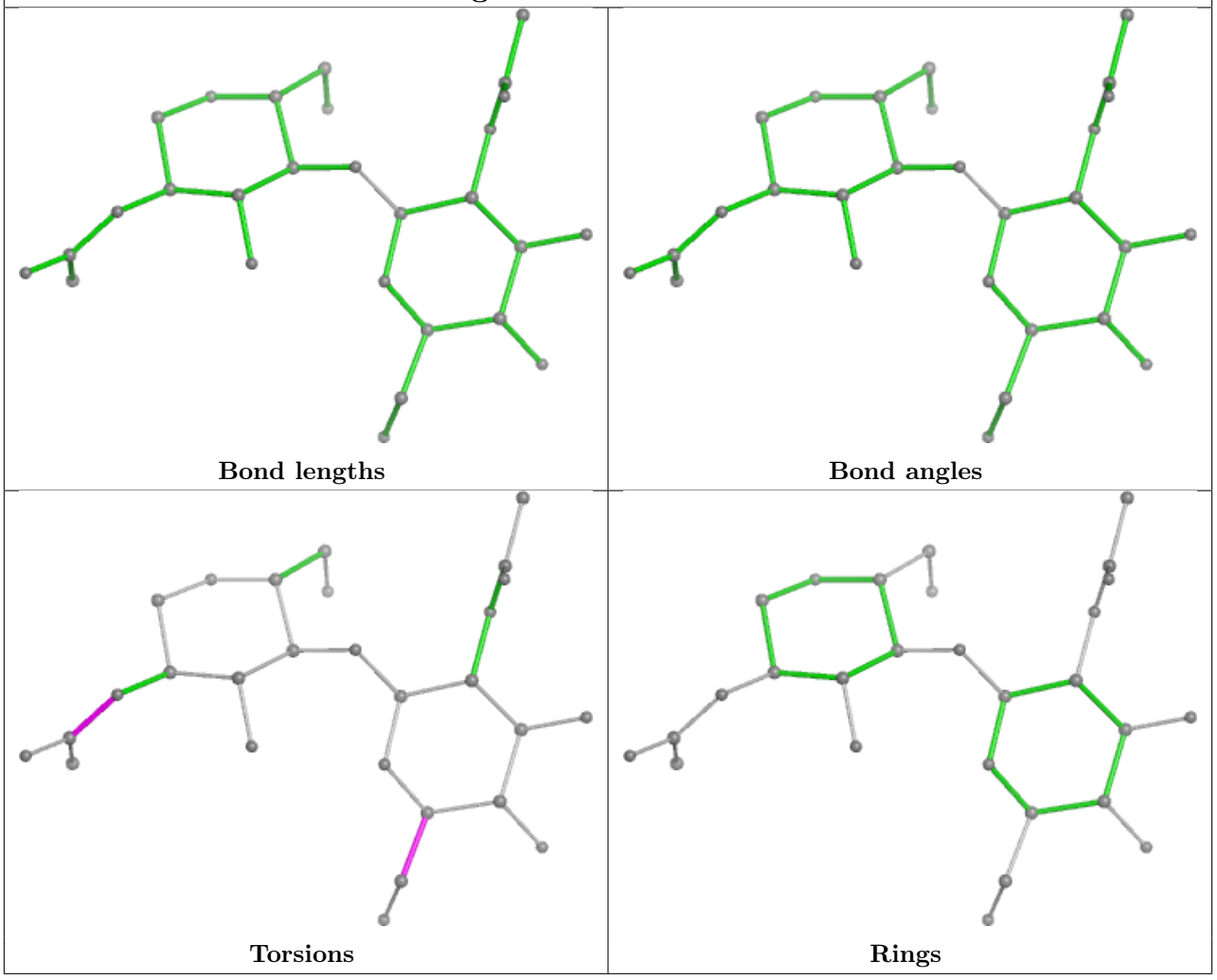


Torsions



Rings

Oligosaccharide Chain L



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	$\#\|Z\| > 2$
3	NAG	B	1311	1	14,14,15	0.18	0	17,19,21	0.40	0
3	NAG	C	1312	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	A	1309	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	C	1313	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	C	1302	1	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	A	1306	1	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	B	1312	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1307	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1312	1	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	B	1303	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1313	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	B	1305	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	C	1304	1	14,14,15	0.19	0	17,19,21	0.40	0
3	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	C	1309	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1306	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1311	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.40	0
3	NAG	C	1310	1	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	1313	1	14,14,15	0.18	0	17,19,21	0.51	0
3	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	1304	1	14,14,15	0.19	0	17,19,21	0.40	0
3	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	A	1311	1	14,14,15	0.18	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1312	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	C	1312	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1304	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	C	1312	NAG	O5-C5-C6-O6
3	A	1313	NAG	C4-C5-C6-O6
3	A	1313	NAG	O5-C5-C6-O6
3	C	1313	NAG	C4-C5-C6-O6
3	B	1313	NAG	C4-C5-C6-O6
3	C	1313	NAG	O5-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	1	0
3	B	1304	NAG	1	0
3	A	1304	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.

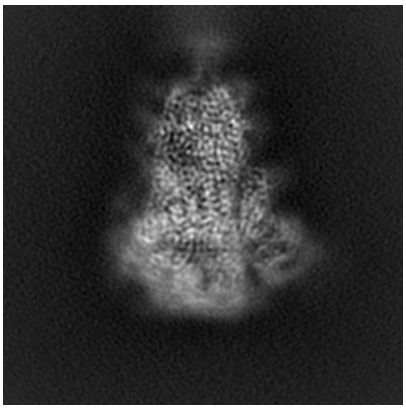
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50263. These allow visual inspection of the internal detail of the map and identification of artifacts.

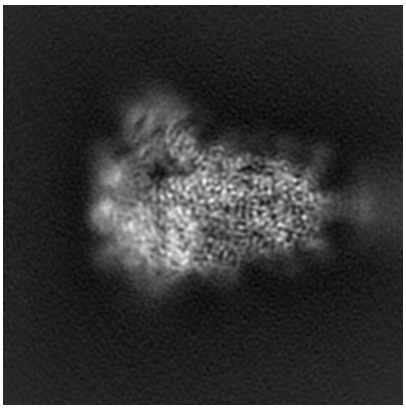
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

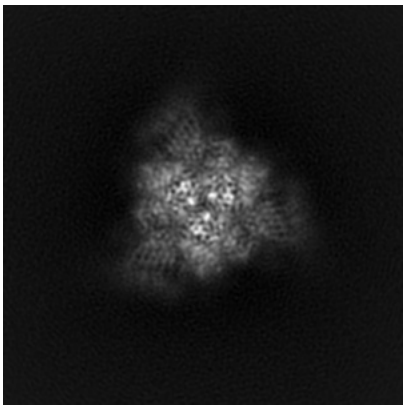
6.1.1 Primary map



X

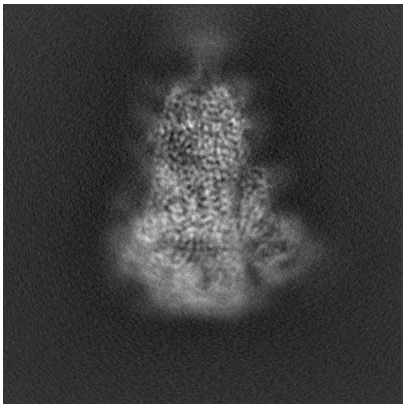


Y

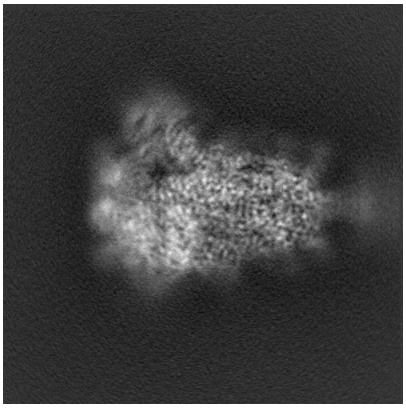


Z

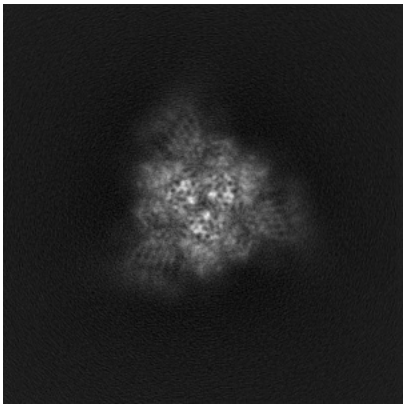
6.1.2 Raw map



X



Y

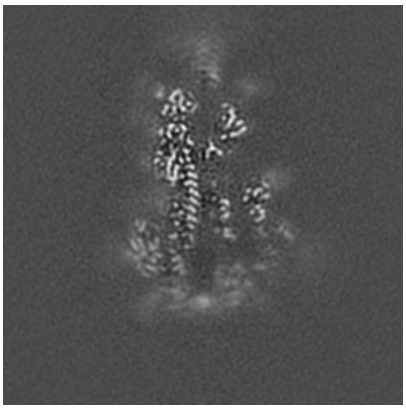


Z

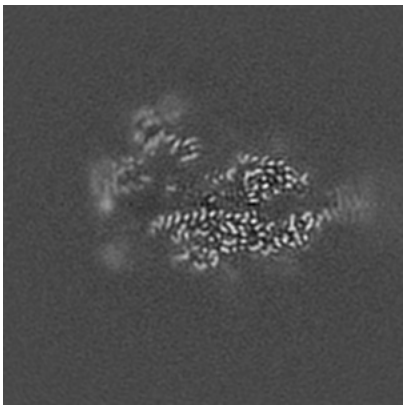
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

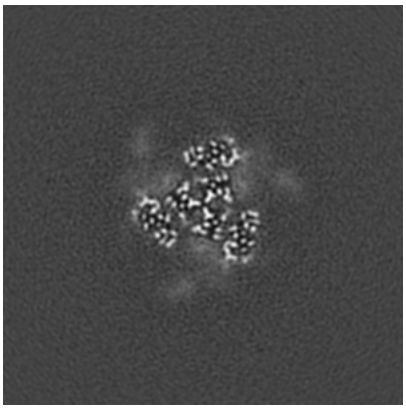
6.2.1 Primary map



X Index: 175

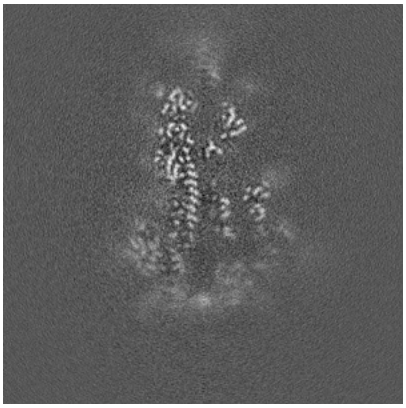


Y Index: 175

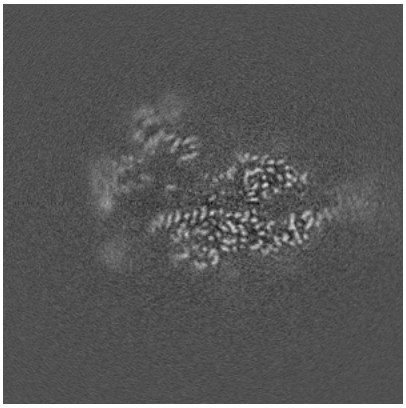


Z Index: 175

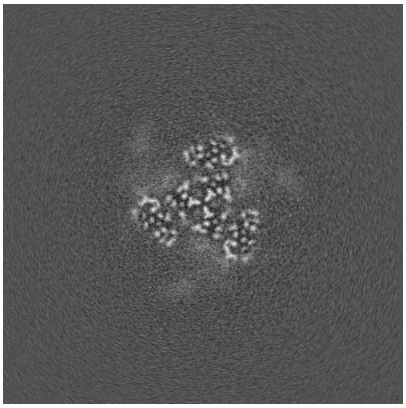
6.2.2 Raw map



X Index: 175



Y Index: 175

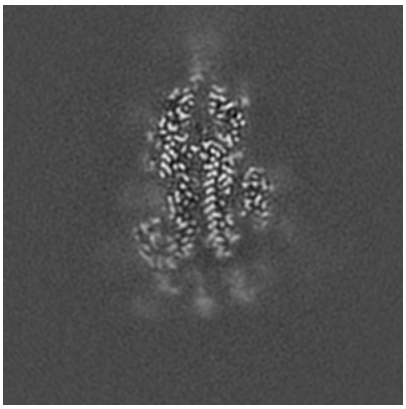


Z Index: 175

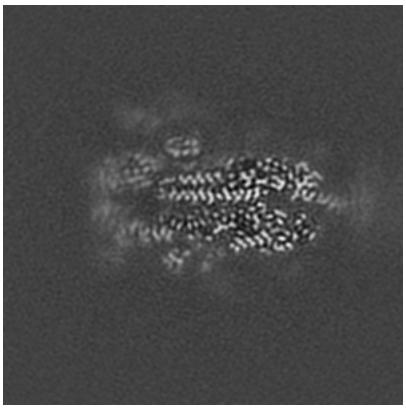
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

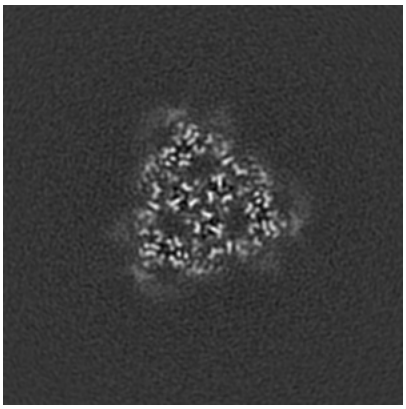
6.3.1 Primary map



X Index: 184

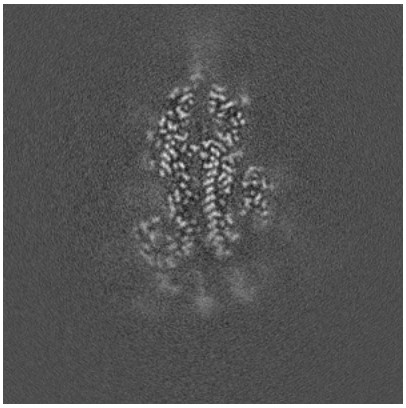


Y Index: 183

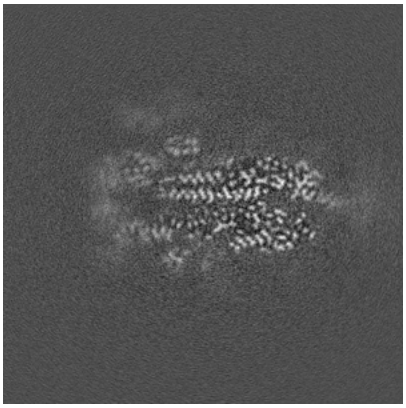


Z Index: 161

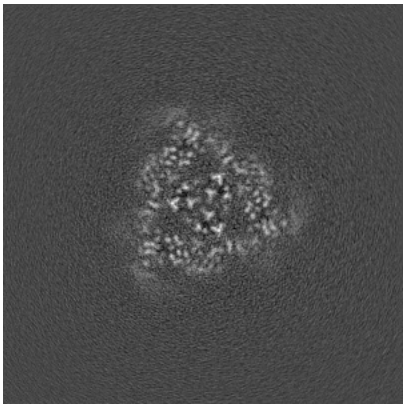
6.3.2 Raw map



X Index: 184



Y Index: 183

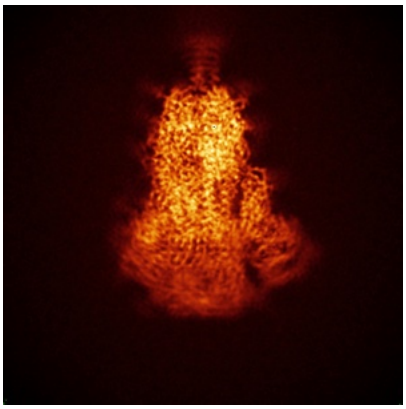


Z Index: 160

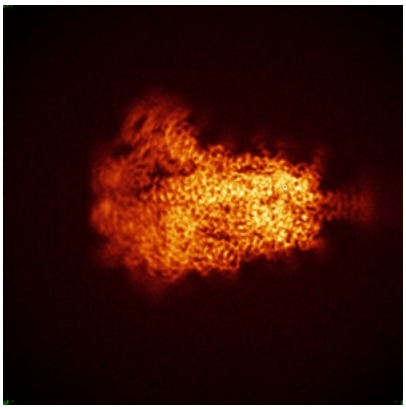
The images above show the largest variance slices of the map in three orthogonal directions.

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

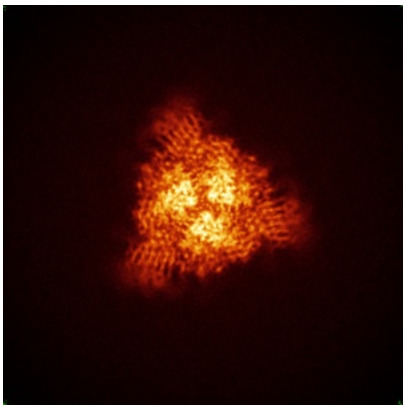
6.4.1 Primary map



X

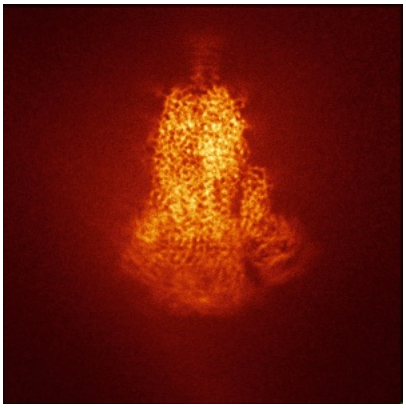


Y

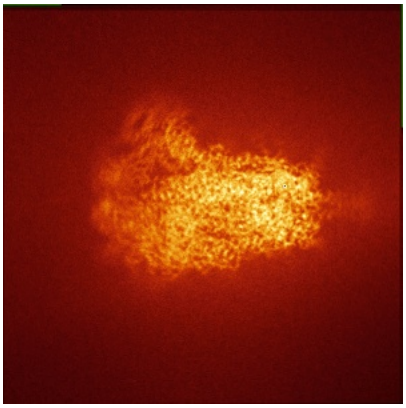


Z

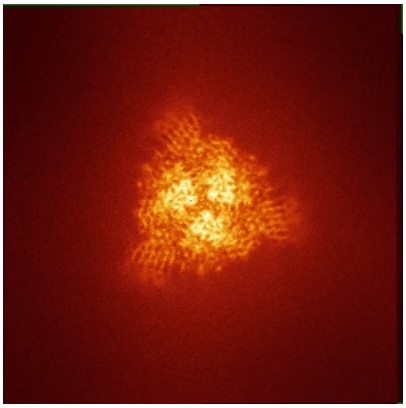
6.4.2 Raw map



X



Y

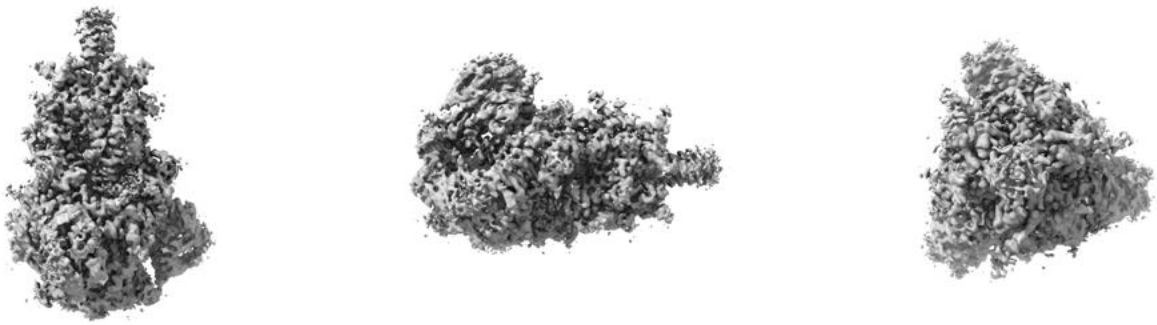


Z

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 0.0574. 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.

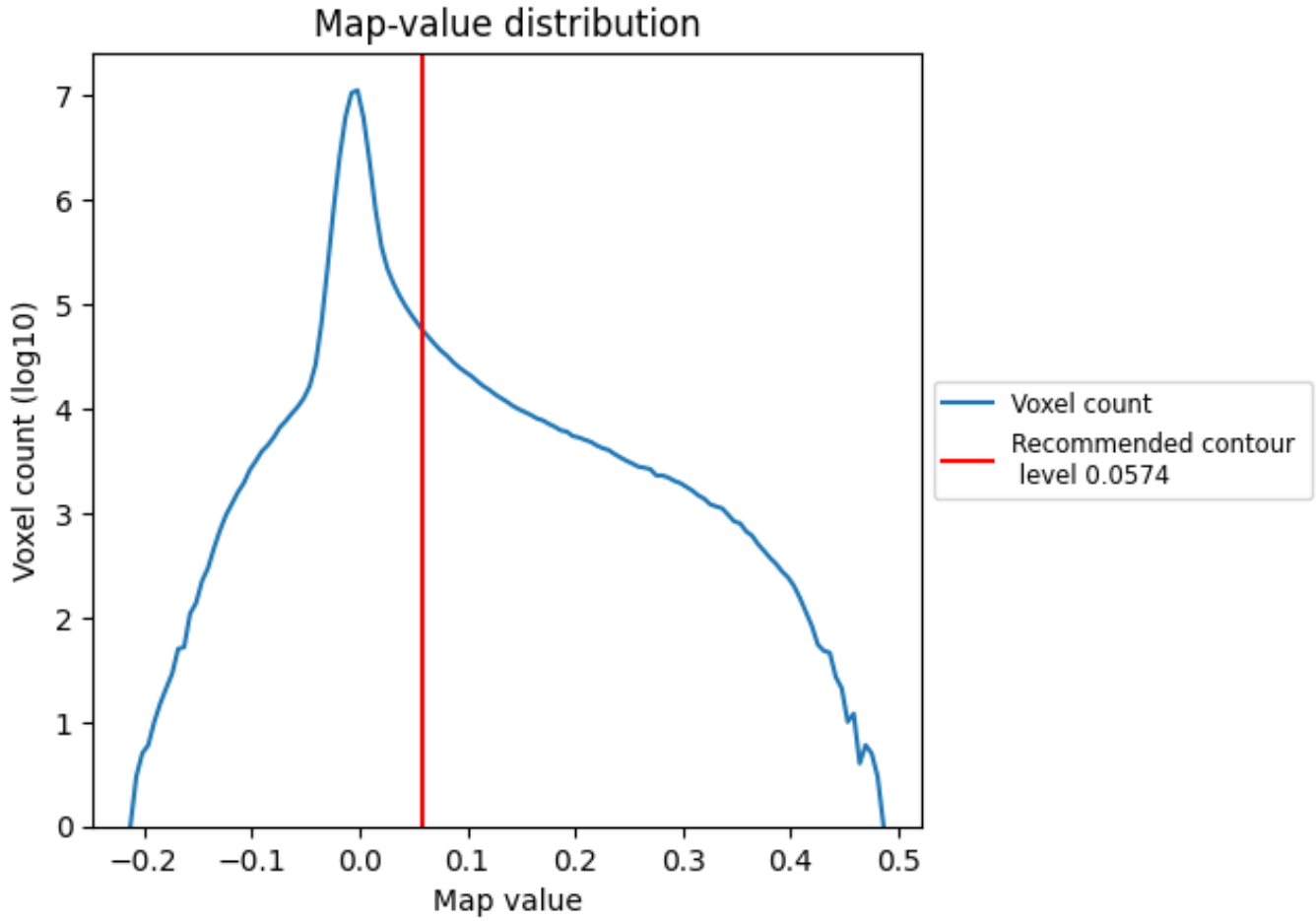
6.6 Mask visualisation (i)

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

7 Map analysis

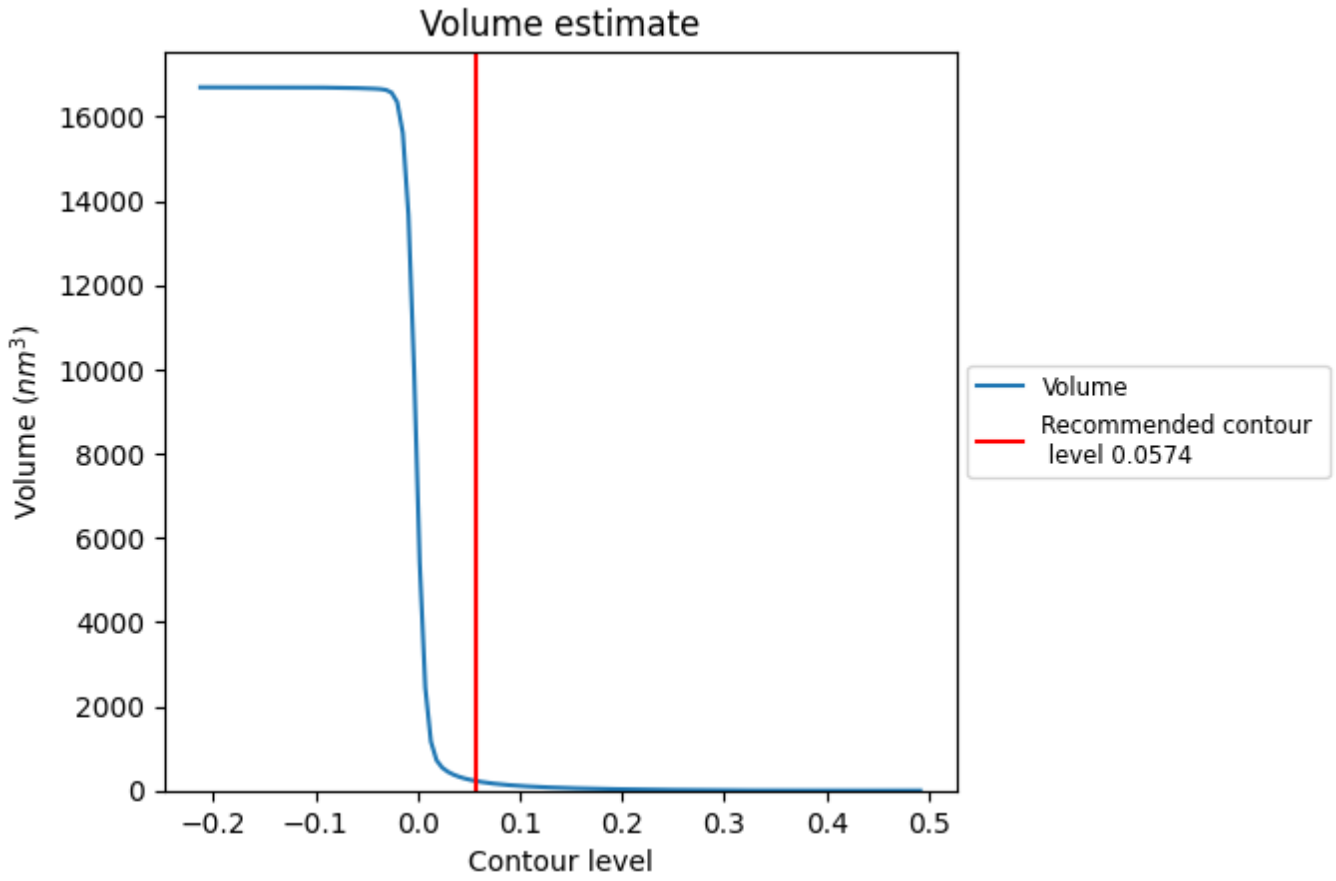
This section contains the results of statistical analysis of the map.

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.

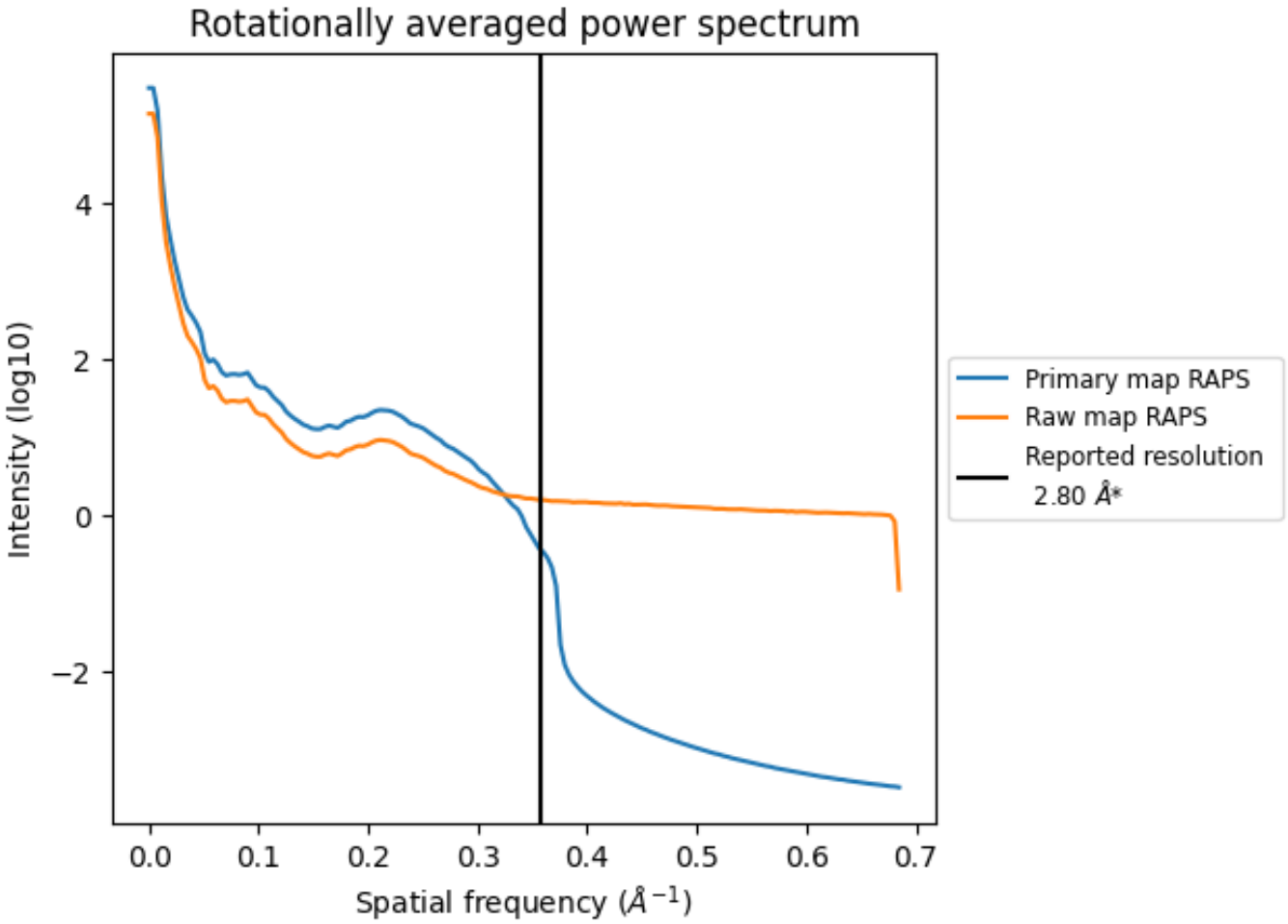
7.2 Volume estimate



The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 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)

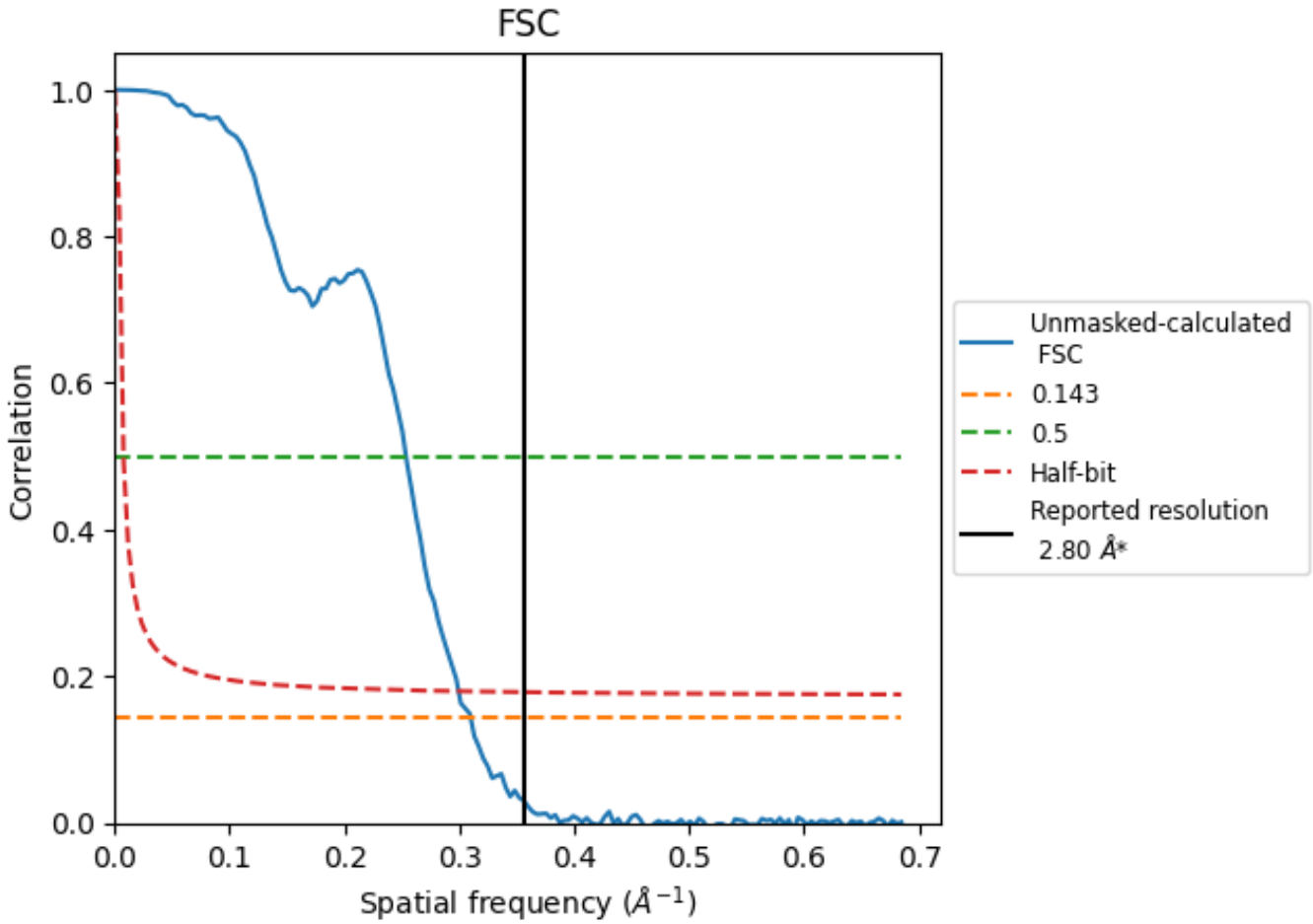


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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)

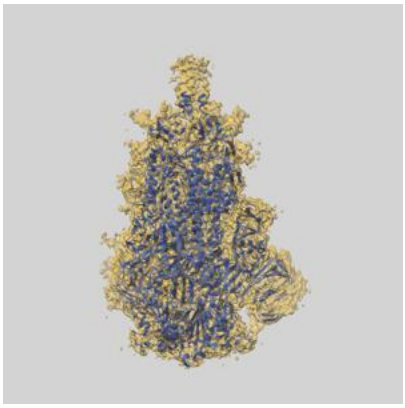
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.94	3.34

*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 3.23 differs from the reported value 2.8 by more than 10 %

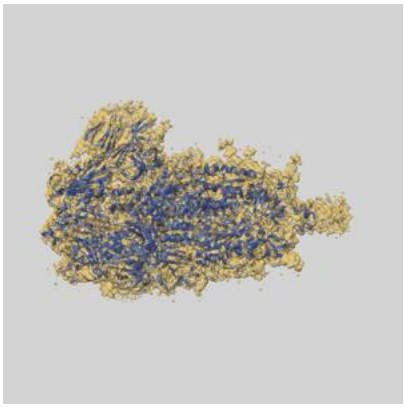
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50263 and PDB model 9F9Y. Per-residue inclusion information can be found in section 3 on page 19.

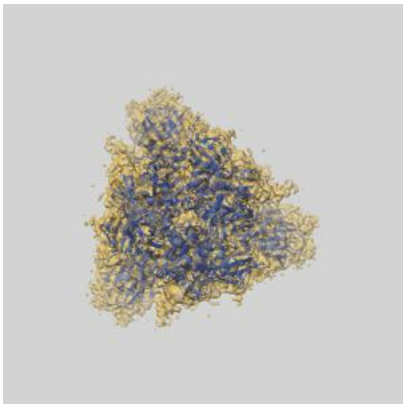
9.1 Map-model overlay



X



Y



Z

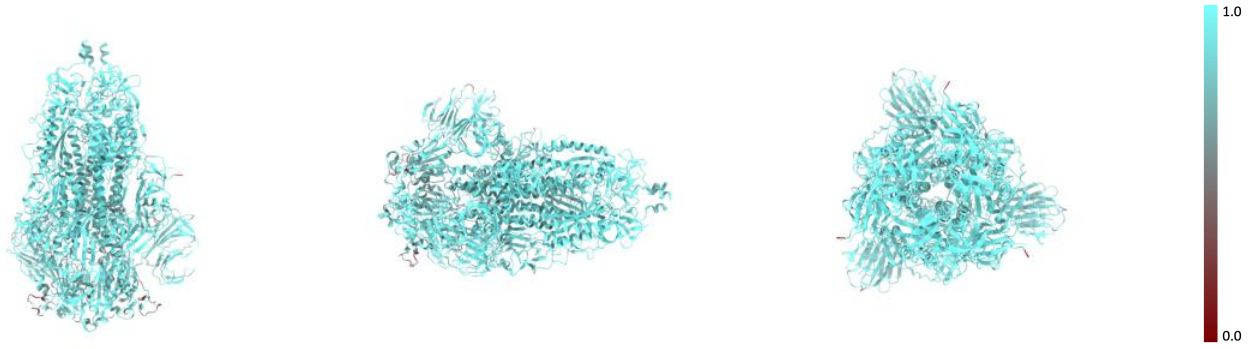
The images above show the 3D surface view of the map at the recommended contour level 0.0574 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

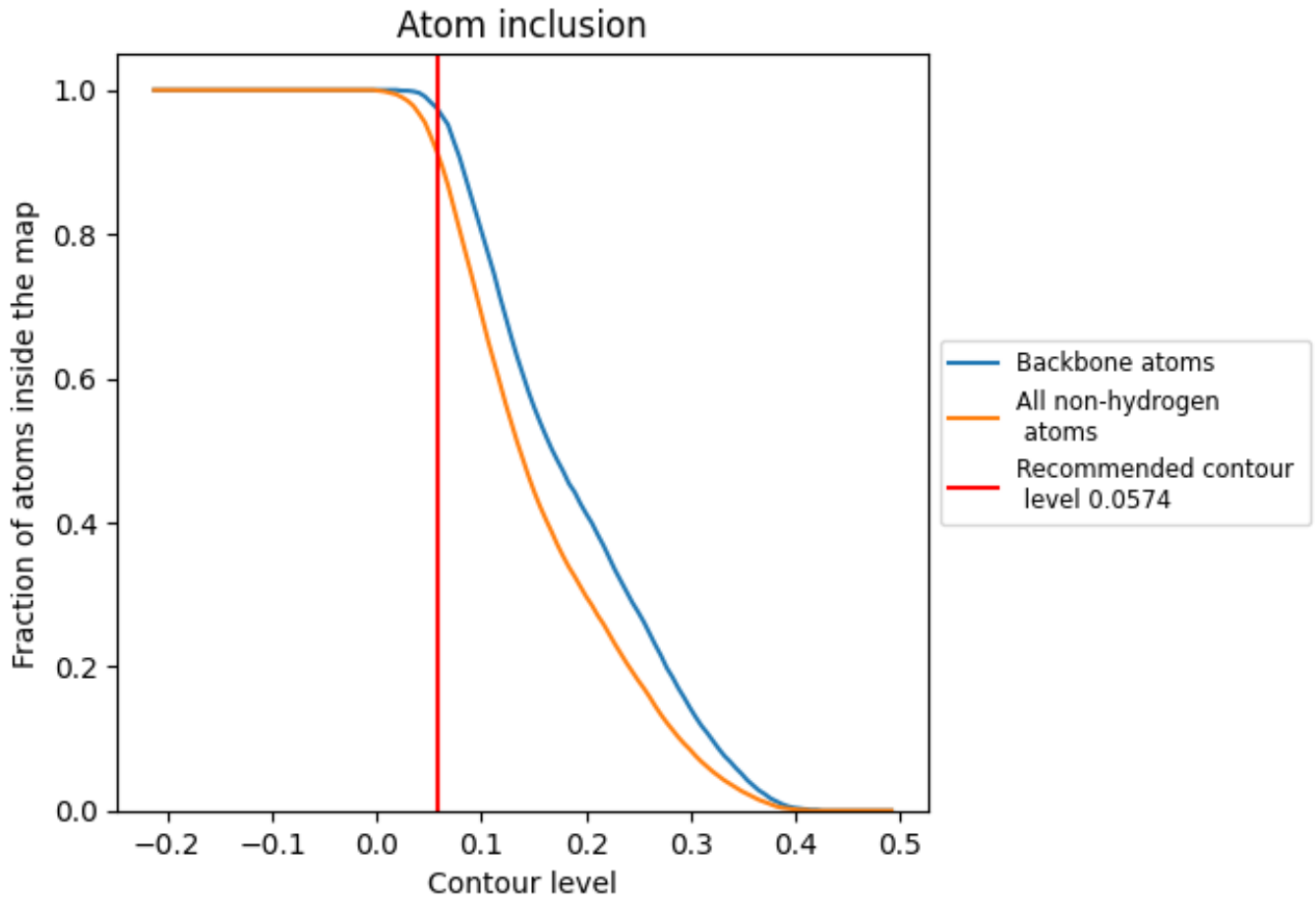
9.3 Atom inclusion mapped to coordinate model



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 (0.0574).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.0574) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.5220
A	0.9150	0.5220
B	0.9150	0.5230
C	0.9160	0.5220
D	0.9640	0.5140
E	0.9290	0.4960
F	0.9290	0.5410
G	0.9640	0.5180
H	0.9290	0.4840
I	0.9290	0.5390
J	0.9290	0.5250
K	0.9290	0.4920
L	0.9290	0.5390