Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 09:54 PM EST

PDB ID	:	7KNE
EMDB ID	:	EMD-22943
Title	:	Cryo-EM structure of single ACE2-bound SARS-CoV-2 trimer spike at pH 5.5
Authors	:	Gorman, J.; Rapp, M.; Kwong, P.D.; Shapiro, L.
Deposited on	:	2020-11-04
Resolution	:	3.85 Å(reported)
Based on initial model	:	6VXX

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

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

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

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

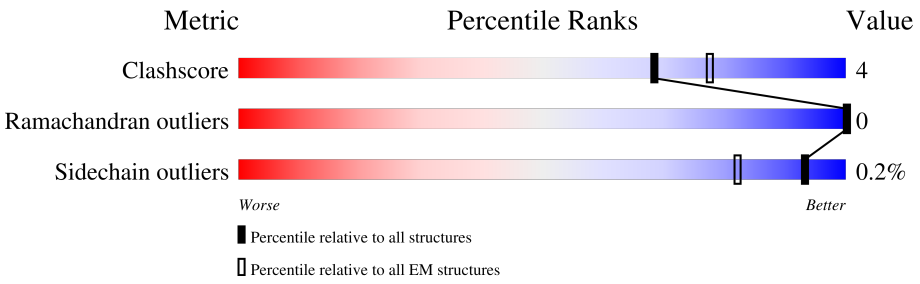
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	70% 8% 22%
1	B	1288	73% 7% 20%
1	C	1288	70% 8% 22%
2	D	597	46% 91% 9%
3	E	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	100% 100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29191 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	1006	7771	4960	1293	1483	35	0	0
1	A	1006	7771	4960	1293	1483	35	0	0
1	B	1029	8003	5118	1329	1519	37	0	0

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	596	4862	3111	805	917	29	0	0

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

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

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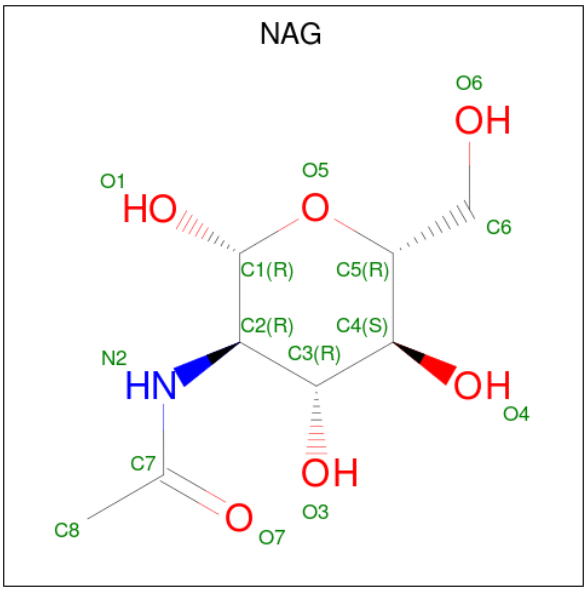
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	2	28	16	2	10	0	0
			Total	C	N	O		
3	I	2	28	16	2	10	0	0
			Total	C	N	O		
3	J	2	28	16	2	10	0	0

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



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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	182	104	13	65	0
			Total	C	N	O	
4	C	1	182	104	13	65	0
			Total	C	N	O	
4	C	1	182	104	13	65	0
			Total	C	N	O	
4	C	1	182	104	13	65	0
			Total	C	N	O	
4	C	1	182	104	13	65	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	A	1	168	96	12	60	0
			Total	C	N	O	
4	B	1	196	112	14	70	0
			Total	C	N	O	
4	B	1	196	112	14	70	0
			Total	C	N	O	
4	B	1	196	112	14	70	0
			Total	C	N	O	
4	B	1	196	112	14	70	0

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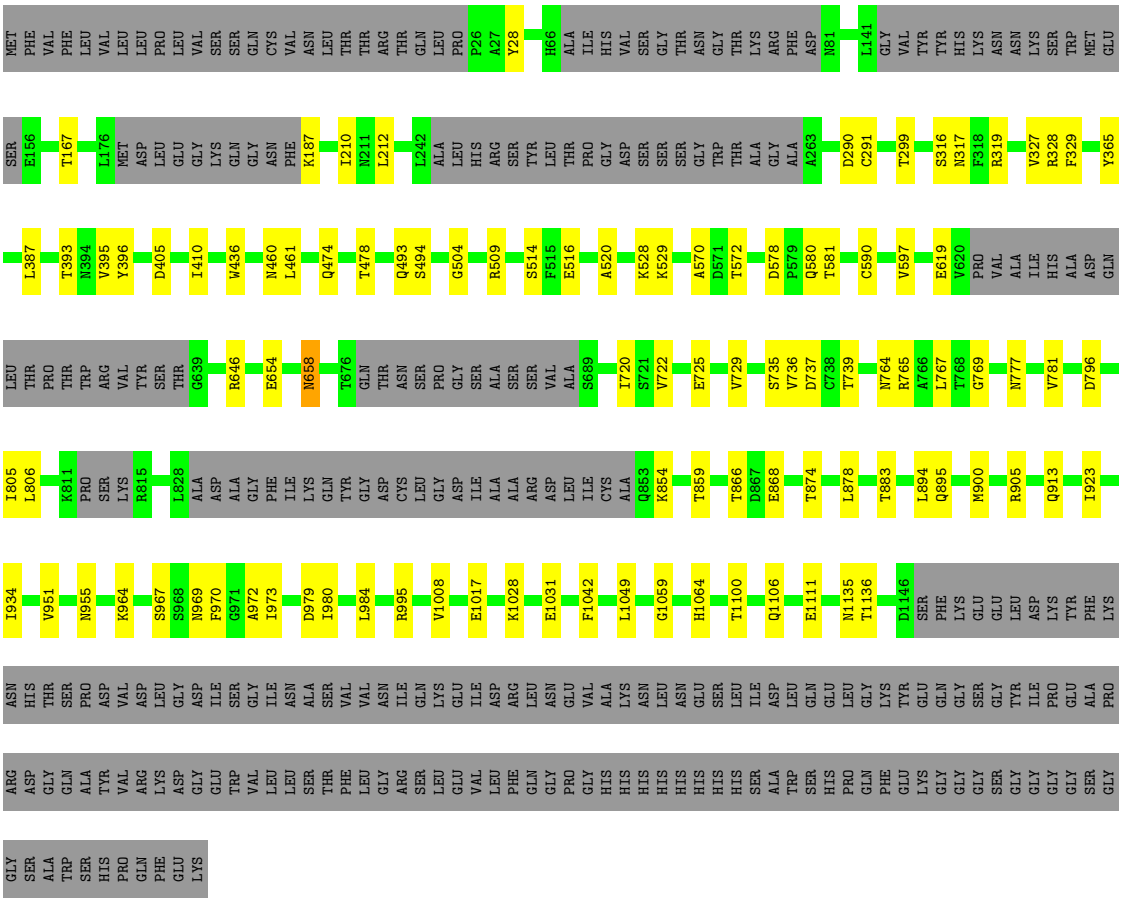
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	B	1	196	112	14	70	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0

3 Residue-property plots (i)

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

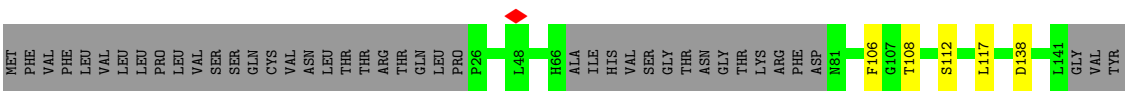
- Molecule 1: Spike glycoprotein

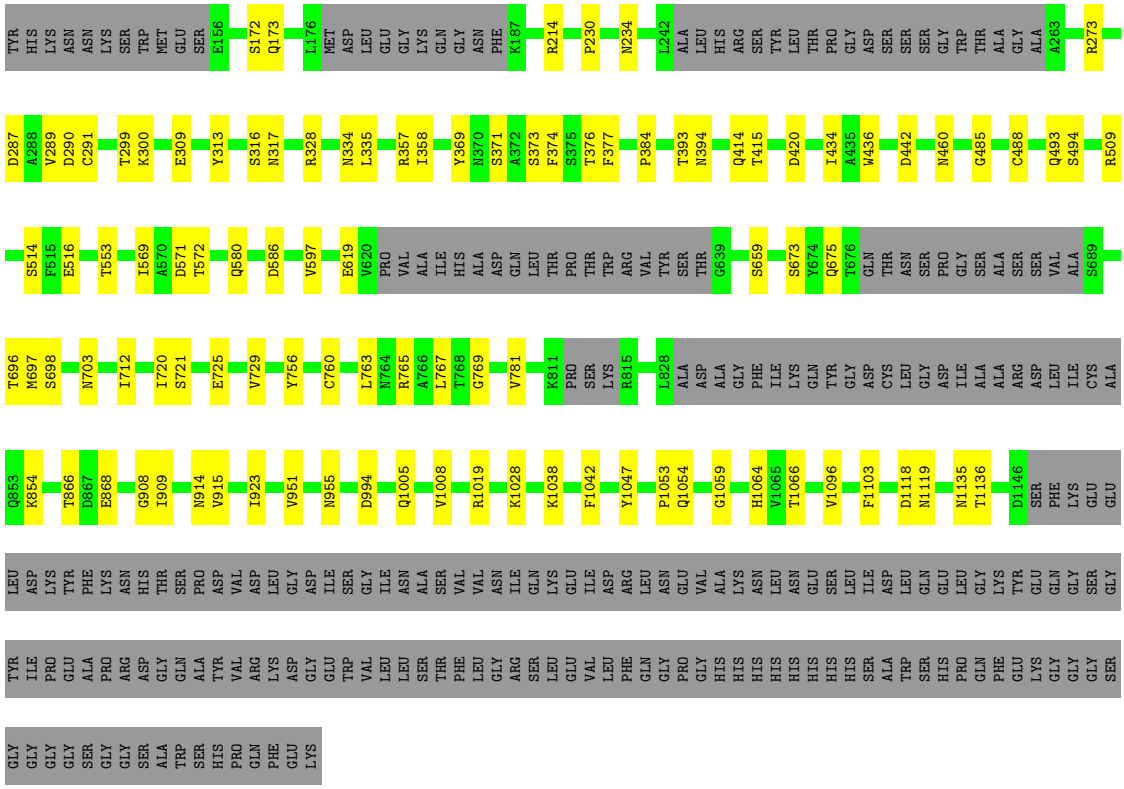
Chain C:



- Molecule 1: Spike glycoprotein

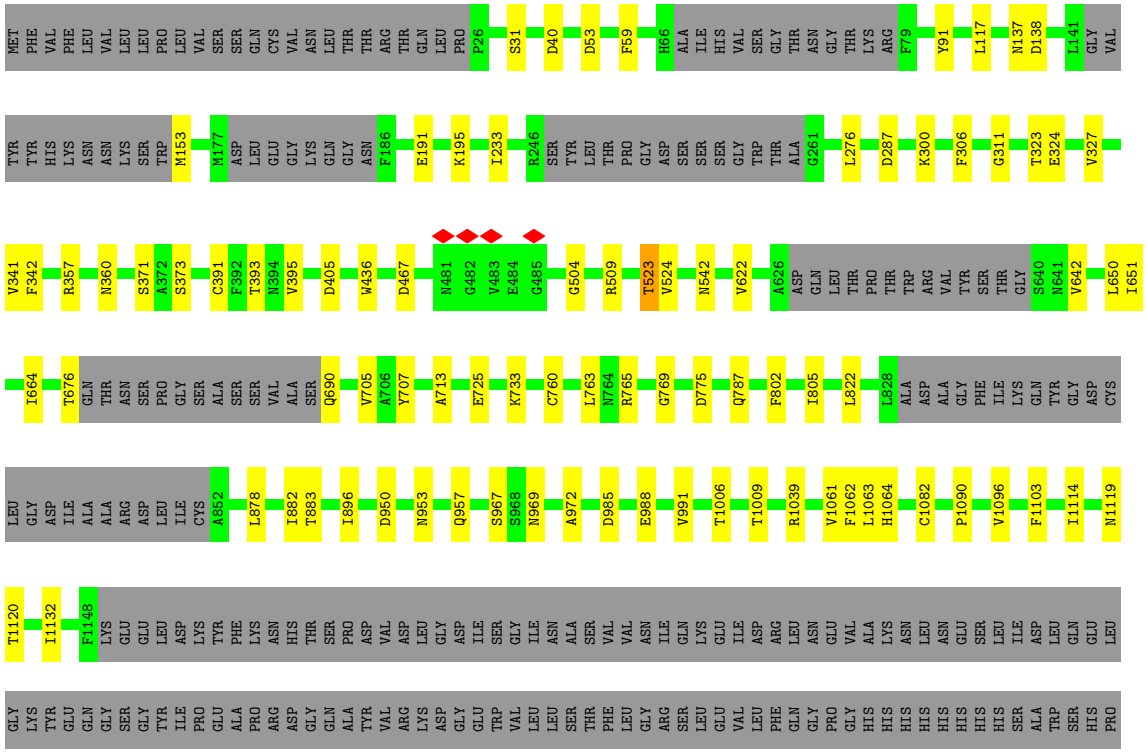
Chain A:





- Molecule 1: Spike glycoprotein

Chain B:



GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: Angiotensin-converting enzyme 2

Chain D: 46% 91% 9%

S19 E23 L45 A46 E56 Q60 N63 P84 L85 Q86 E87 I88 Q89 K94 A99 Q102 N103 G104 S105 S106 V107 L108 S109 E110 D111 K112 S113 K114 N117 T118 I119 L120 N121 T122 M123 S124 T125 I126 Y127 S128 T129 G130 K131 V132 C133 N134 P135 D136 N137 P138

Q139 E140 C141 L142 L143 L144 E145 P146 G147 L148 N149 E150 I151 M152 A153 N154 S155 L156 D157 Y158 N159 E160 R161 L162 W163 A164 W165 E166 S167 W168 R169 S170 E171 V172 G173 K174 R177 P178 L179 Y180 E181 V184 V185 L186 K187 N188 A193 D198 D206 Y207 E208 V209 N210 G211 V212

D213 G214 Y215 D216 Y217 S218 R219 G220 Q221 L222 I223 E224 D225 V226 E227 H228 T229 P230 E231 E232 I233 K234 P235 E238 H239 L240 H241 A242 Y243 V244 R245 A246 K247 L248 M249 N250 A251 Y252 P253 S254 Y255 I256 S257 P258 I259 G260 C261 L266 L267 G268 D269 F274 Y279 S280 L281 T282

V283 P284 F285 G286 Q287 K288 P289 N290 I291 D292 V293 T294 D295 A296 M297 V298 D299 Q300 A301 Q305 R306 I307 F308 K309 E310 A311 E312 K313 V316 S317 V318 G319 Q325 W328 E329 L333 T334 D335 N338 V364 M376 A386 A387 P415 K419 S420 I421 L424

S425 P426 D427 F428 Q429 E430 D431 N432 E433 T434 E435 I436 N437 F438 L439 L440 K441 Q442 A443 I446 V447 G448 T449 L450 T453 F464 K465 G466 E467 I468 P469 K470 D471 M474 K475 W478 E479 G486 E489 P490 V491 P492 H493 D494 E495 T496 S502 L503 F504 H505 N508

S511 F512 I513 R514 T519 L520 Y521 Q524 F525 L529 C530 Q531 A532 A533 K534 H535 E536 G537 P538 K541 I544 S545 N546 S547 T548 E549 A550 G551 Q552 K553 L554 F555 N556 M557 G561 L568 A569 L570 E571 N572 V573 V574 G575 A576 K577 N578 M579 N580 V581 R582 P583 L584

L585 N586 Y587 F588 E589 P590 L591 F592 T593 W594 L595 K596 D597 Q598 N599 K600 N601 S602 F603 V604 G605 W606 S607 T608 D609 W610 S611 P612 Y613 A614 ASP

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 100%

NAG1 NAG2

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

Chain G: 100%

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

Chain H: 100%

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

Chain I: 100%

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

Chain J: 100%
100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46714	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.693	Depositor
Minimum map value	-0.269	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	406.27197, 406.27197, 406.27197	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/7943	0.46	0/10816
1	B	0.26	0/8186	0.46	0/11141
1	C	0.26	0/7943	0.46	0/10816
2	D	0.28	0/4999	0.54	0/6792
All	All	0.26	0/29071	0.47	0/39565

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7771	0	7507	61	0
1	B	8003	0	7778	68	0
1	C	7771	0	7506	73	0
2	D	4862	0	4633	34	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
4	A	168	0	156	3	0
4	B	196	0	182	0	0
4	C	182	0	169	6	0
4	D	70	0	65	0	0
All	All	29191	0	28146	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (218) 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)
4:C:1302:NAG:H3	4:C:1302:NAG:H83	1.21	1.15
4:C:1302:NAG:H3	4:C:1302:NAG:C8	1.88	1.01
1:C:883:THR:HG23	1:B:707:TYR:HB2	1.41	1.00
1:C:883:THR:CG2	1:B:707:TYR:HB2	1.91	0.99
4:C:1302:NAG:H83	4:C:1302:NAG:C3	2.01	0.89
1:C:883:THR:HG21	1:B:705:VAL:CG2	2.09	0.82
1:C:883:THR:HG23	1:B:707:TYR:CB	2.10	0.80
2:D:108:LEU:HD23	2:D:112:LYS:HG3	1.68	0.76
1:C:319:ARG:NH1	1:C:590:CYS:SG	2.60	0.74
1:B:1006:THR:O	1:B:1009:THR:OG1	2.08	0.71
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.08	0.70
1:C:883:THR:HG23	1:B:707:TYR:CG	2.26	0.70
1:C:951:VAL:O	1:C:955:ASN:ND2	2.25	0.70
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.26	0.69
1:C:883:THR:CG2	1:B:705:VAL:HG21	2.23	0.69
2:D:503:LEU:HD23	2:D:505:HIS:H	1.58	0.68
2:D:508:ASN:ND2	2:D:508:ASN:O	2.25	0.68
2:D:107:VAL:HG23	2:D:108:LEU:HD12	1.75	0.67
1:C:1017:GLU:OE1	1:A:1019:ARG:NH1	2.27	0.67
1:A:420:ASP:OD2	1:A:460:ASN:ND2	2.28	0.66
1:B:676:THR:O	1:B:690:GLN:N	2.29	0.66
1:C:883:THR:HG21	1:B:705:VAL:HG23	1.78	0.65
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.29	0.65
1:C:964:LYS:O	1:C:967:SER:OG	2.14	0.65
2:D:544:ILE:O	2:D:547:SER:OG	2.15	0.65
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.30	0.64
2:D:177:ARG:NH2	2:D:181:GLU:OE1	2.31	0.64
1:C:28:TYR:HB2	4:C:1309:NAG:H82	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH2	1:A:358:ILE:O	2.31	0.63
1:C:736:VAL:O	1:C:764:ASN:ND2	2.31	0.63
1:A:299:THR:HG22	1:A:597:VAL:HG21	1.80	0.63
1:A:951:VAL:O	1:A:955:ASN:ND2	2.32	0.62
2:D:334:THR:HG22	2:D:335:ASP:H	1.64	0.62
1:C:493:GLN:NE2	1:C:494:SER:O	2.32	0.62
1:A:729:VAL:HG12	1:A:1059:GLY:HA2	1.82	0.61
1:C:570:ALA:O	1:C:572:THR:HG23	1.99	0.61
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.65	0.61
1:C:883:THR:CG2	1:B:705:VAL:CG2	2.77	0.61
1:B:642:VAL:HG12	1:B:651:ILE:HG22	1.83	0.61
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.35	0.60
4:A:1302:NAG:H82	4:A:1302:NAG:C1	2.32	0.60
1:C:619:GLU:OE2	1:C:619:GLU:N	2.34	0.60
1:C:765:ARG:NH1	1:B:957:GLN:OE1	2.34	0.60
2:D:208:GLU:OE2	2:D:210:ASN:ND2	2.35	0.60
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.34	0.59
1:B:153:MET:SD	1:B:153:MET:N	2.75	0.59
1:A:374:PHE:HB3	1:A:434:ILE:HD11	1.85	0.59
1:C:658:ASN:C	1:C:658:ASN:HD22	2.06	0.59
1:A:493:GLN:NE2	1:A:494:SER:O	2.35	0.59
1:B:985:ASP:N	1:B:988:GLU:OE2	2.36	0.58
1:C:405:ASP:N	1:C:504:GLY:O	2.36	0.58
1:A:1096:VAL:O	1:A:1103:PHE:N	2.36	0.58
1:B:371:SER:HG	1:B:373:SER:HG	1.49	0.58
1:C:395:VAL:HG12	1:C:395:VAL:O	2.04	0.58
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.36	0.57
1:A:371:SER:OG	1:A:373:SER:OG	2.17	0.57
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.36	0.57
2:D:574:VAL:HG23	2:D:576:ALA:H	1.68	0.57
1:A:763:LEU:HD11	1:A:1005:GLN:NE2	2.20	0.57
1:A:514:SER:OG	1:A:516:GLU:OE2	2.11	0.57
1:C:1031:GLU:OE2	1:B:1039:ARG:NH2	2.36	0.57
1:A:619:GLU:OE2	1:A:619:GLU:N	2.37	0.56
1:B:393:THR:HB	1:B:523:THR:HB	1.88	0.56
2:D:520:LEU:HD12	2:D:521:TYR:CD1	2.40	0.56
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.88	0.56
1:C:883:THR:HG23	1:B:707:TYR:CD1	2.41	0.55
1:A:414:GLN:NE2	1:A:415:THR:O	2.39	0.55
1:A:697:MET:SD	1:A:698:SER:N	2.79	0.55
1:C:290:ASP:OD1	1:C:291:CYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1302:NAG:C1	4:A:1302:NAG:C8	2.84	0.55
1:A:369:TYR:OH	1:A:384:PRO:O	2.20	0.55
1:A:377:PHE:HD1	1:A:434:ILE:HD13	1.72	0.55
1:A:1118:ASP:OD2	1:A:1119:ASN:N	2.39	0.55
1:A:309:GLU:O	1:A:313:TYR:OH	2.14	0.54
2:D:453:THR:HG23	2:D:512:PHE:CE2	2.43	0.54
1:C:474:GLN:NE2	1:C:478:THR:O	2.38	0.53
1:C:436:TRP:O	1:C:509:ARG:N	2.41	0.53
1:C:722:VAL:HG23	1:C:934:ILE:HD11	1.89	0.53
1:C:365:TYR:H	1:C:387:LEU:HD13	1.72	0.53
2:D:511:SER:OG	2:D:514:ARG:NH2	2.42	0.53
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.42	0.53
1:A:436:TRP:O	1:A:509:ARG:N	2.41	0.52
1:C:187:LYS:N	1:C:210:ILE:O	2.43	0.52
2:D:174:LYS:NZ	2:D:496:THR:OG1	2.42	0.52
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.39	0.52
1:B:31:SER:O	1:B:59:PHE:N	2.42	0.52
1:A:659:SER:OG	1:A:696:THR:O	2.21	0.52
1:B:395:VAL:O	1:B:395:VAL:HG12	2.09	0.52
1:C:796:ASP:OD1	1:C:796:ASP:N	2.42	0.52
1:B:300:LYS:NZ	1:B:306:PHE:O	2.43	0.52
2:D:453:THR:HG23	2:D:512:PHE:CD2	2.45	0.52
1:C:883:THR:HG21	1:B:707:TYR:HB2	1.85	0.51
1:B:405:ASP:N	1:B:504:GLY:O	2.43	0.51
1:C:735:SER:OG	1:C:859:THR:OG1	2.26	0.51
1:B:969:ASN:OD1	1:B:972:ALA:N	2.44	0.51
1:C:970:PHE:O	1:C:995:ARG:NE	2.44	0.51
1:A:765:ARG:O	1:A:769:GLY:N	2.42	0.50
2:D:553:LYS:HD2	2:D:573:VAL:HG12	1.93	0.50
1:A:106:PHE:O	1:A:117:LEU:N	2.43	0.50
1:A:290:ASP:OD1	1:A:291:CYS:N	2.44	0.50
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.19	0.50
1:C:913:GLN:NE2	1:B:1090:PRO:O	2.45	0.49
1:A:287:ASP:OD1	1:A:287:ASP:N	2.43	0.49
1:B:760:CYS:HA	1:B:763:LEU:HD12	1.94	0.49
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.45	0.49
1:A:442:ASP:OD2	1:A:509:ARG:NH2	2.46	0.49
2:D:108:LEU:HD23	2:D:112:LYS:CG	2.41	0.49
1:C:514:SER:OG	1:C:516:GLU:OE2	2.25	0.48
4:C:1302:NAG:C8	4:C:1302:NAG:C3	2.59	0.48
1:A:112:SER:O	4:A:1311:NAG:O3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:TYR:OH	1:A:230:PRO:O	2.31	0.48
1:C:410:ILE:HG23	1:C:410:ILE:O	2.13	0.48
1:B:1082:CYS:SG	1:B:1132:ILE:HG21	2.54	0.48
1:C:883:THR:HG22	1:B:705:VAL:HG21	1.95	0.48
1:A:334:ASN:OD1	1:A:335:LEU:N	2.44	0.48
1:A:866:THR:HG23	1:A:868:GLU:H	1.79	0.47
1:C:299:THR:HG22	1:C:597:VAL:HG21	1.95	0.47
1:C:805:ILE:HG23	1:C:806:LEU:HD22	1.96	0.47
1:A:571:ASP:OD2	1:B:967:SER:OG	2.28	0.47
1:A:720:ILE:HD11	1:A:923:ILE:HD11	1.96	0.47
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.47	0.47
2:D:556:ASN:OD1	2:D:557:MET:N	2.46	0.47
1:C:327:VAL:HG11	1:C:528:LYS:HD2	1.97	0.47
1:A:214:ARG:NE	1:A:214:ARG:O	2.47	0.47
1:C:210:ILE:HG22	1:C:212:LEU:H	1.78	0.47
1:C:883:THR:CG2	1:B:707:TYR:CB	2.77	0.47
1:A:569:ILE:O	1:A:572:THR:HG22	2.13	0.47
2:D:188:ASN:ND2	2:D:464:PHE:O	2.47	0.47
1:A:553:THR:O	1:A:586:ASP:N	2.45	0.47
1:A:138:ASP:N	1:A:138:ASP:OD1	2.46	0.47
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.48	0.47
1:B:40:ASP:OD1	1:B:40:ASP:N	2.48	0.46
1:C:1106:GLN:NE2	1:C:1111:GLU:OE2	2.44	0.46
1:A:909:ILE:HD12	1:A:1047:TYR:HB3	1.97	0.46
1:C:883:THR:HG21	1:B:705:VAL:HG21	1.83	0.46
1:A:712:ILE:HD13	1:B:896:ILE:HD12	1.97	0.46
1:C:316:SER:OG	1:C:317:ASN:N	2.48	0.46
1:B:117:LEU:HD23	1:B:233:ILE:HD11	1.98	0.46
2:D:334:THR:HG22	2:D:335:ASP:N	2.28	0.46
1:B:341:VAL:HG13	1:B:342:PHE:HD2	1.80	0.46
2:D:112:LYS:HE2	2:D:186:LEU:HD13	1.97	0.46
1:C:578:ASP:OD2	1:C:581:THR:OG1	2.25	0.46
1:C:725:GLU:OE2	1:C:1064:HIS:NE2	2.48	0.45
1:C:1100:THR:HG22	4:C:1303:NAG:H81	1.98	0.45
1:B:276:LEU:HD23	1:B:306:PHE:HE1	1.81	0.45
1:B:1096:VAL:O	1:B:1103:PHE:N	2.47	0.45
1:A:376:THR:O	1:A:376:THR:HG22	2.16	0.45
1:C:167:THR:OG1	1:B:357:ARG:NH2	2.50	0.45
1:B:137:ASN:OD1	1:B:138:ASP:N	2.50	0.45
1:B:765:ARG:O	1:B:769:GLY:N	2.47	0.44
2:D:436:ILE:HD11	2:D:594:TRP:CE3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:ASN:HD22	2:D:508:ASN:C	2.16	0.44
1:C:777:ASN:O	1:C:781:VAL:HG12	2.17	0.44
1:B:327:VAL:HG13	1:B:542:ASN:O	2.18	0.44
1:B:360:ASN:N	1:B:524:VAL:HG11	2.32	0.44
1:C:894:LEU:HB3	1:B:713:ALA:HB3	1.99	0.44
1:A:767:LEU:HD21	1:A:1008:VAL:HG22	2.00	0.44
2:D:520:LEU:HD12	2:D:521:TYR:HD1	1.79	0.44
1:A:721:SER:O	1:A:1066:THR:OG1	2.35	0.44
1:B:436:TRP:O	1:B:509:ARG:N	2.49	0.44
1:C:973:ILE:HD11	1:C:984:LEU:HD11	2.00	0.44
2:D:168:TRP:O	2:D:172:VAL:HG12	2.17	0.43
1:C:658:ASN:C	1:C:658:ASN:ND2	2.70	0.43
1:B:311:GLY:C	1:B:664:ILE:HD11	2.37	0.43
1:A:760:CYS:HA	1:A:763:LEU:HD12	2.00	0.43
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.30	0.43
1:A:289:VAL:HG11	1:A:300:LYS:HE3	2.01	0.43
1:A:316:SER:OG	1:A:317:ASN:N	2.51	0.43
2:D:525:PHE:O	2:D:529:LEU:HD13	2.18	0.43
1:B:53:ASP:OD2	1:B:195:LYS:NZ	2.52	0.43
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.52	0.43
1:B:1114:ILE:HD12	1:B:1114:ILE:H	1.84	0.43
1:B:650:LEU:HD23	1:B:650:LEU:H	1.84	0.42
1:C:979:ASP:OD2	1:C:980:ILE:N	2.52	0.42
1:B:642:VAL:CG1	1:B:651:ILE:HG22	2.49	0.42
1:B:822:LEU:HD21	1:B:1061:VAL:HG21	2.01	0.42
2:D:166:GLU:OE1	2:D:166:GLU:N	2.52	0.42
2:D:311:ALA:HB1	2:D:376:MET:SD	2.59	0.42
1:C:393:THR:HG21	1:C:520:ALA:HB3	2.02	0.42
1:C:866:THR:HG23	1:C:868:GLU:H	1.85	0.42
2:D:19:SER:N	2:D:23:GLU:OE2	2.52	0.42
2:D:144:LEU:HA	2:D:148:LEU:HD23	2.01	0.42
1:A:108:THR:OG1	1:A:234:ASN:O	2.37	0.42
1:A:374:PHE:CB	1:A:434:ILE:HD11	2.50	0.42
1:A:729:VAL:HG21	1:A:781:VAL:HG11	2.02	0.42
1:B:988:GLU:O	1:B:991:VAL:HG12	2.19	0.42
1:C:654:GLU:N	1:C:654:GLU:OE1	2.52	0.42
1:A:172:SER:OG	1:A:173:GLN:N	2.53	0.42
1:C:329:PHE:O	1:C:580:GLN:NE2	2.52	0.42
1:C:460:ASN:OD1	1:C:461:LEU:N	2.53	0.42
1:A:273:ARG:NH2	1:A:290:ASP:OD2	2.53	0.41
1:A:673:SER:OG	1:A:675:GLN:NE2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:N	1:B:287:ASP:OD2	2.53	0.41
1:B:805:ILE:HD12	1:B:878:LEU:HD11	2.02	0.41
1:C:720:ILE:HD12	1:C:923:ILE:HG13	2.02	0.41
1:C:874:THR:O	1:C:878:LEU:HD23	2.20	0.41
2:D:259:ILE:HD12	2:D:612:PRO:CG	2.51	0.41
1:C:900:MET:SD	1:C:900:MET:N	2.94	0.41
1:A:485:GLY:N	1:A:488:CYS:SG	2.93	0.41
2:D:291:ILE:HG23	2:D:424:LEU:HD13	2.02	0.41
1:B:391:CYS:SG	1:B:524:VAL:O	2.78	0.41
1:B:950:ASP:O	1:B:953:ASN:N	2.53	0.41
1:C:895:GLN:CD	1:B:713:ALA:HB2	2.41	0.41
1:A:914:ASN:OD1	1:A:915:VAL:N	2.53	0.41
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.49	0.41
1:A:393:THR:OG1	1:A:394:ASN:N	2.54	0.41
1:B:882:ILE:HG13	1:B:883:THR:HG23	2.03	0.41
2:D:308:PHE:CE2	2:D:333:LEU:HD11	2.55	0.41
1:C:737:ASP:OD1	1:C:739:THR:HG22	2.21	0.41
1:B:1062:PHE:O	1:B:1063:LEU:HD22	2.20	0.41
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	2.02	0.40
2:D:433:GLU:HA	2:D:436:ILE:HG22	2.03	0.40
1:B:1119:ASN:OD1	1:B:1120:THR:HG23	2.21	0.40
2:D:583:PRO:O	2:D:584:LEU:HD12	2.21	0.40
1:C:765:ARG:O	1:C:769:GLY:N	2.52	0.40
1:C:969:ASN:ND2	1:C:972:ALA:O	2.54	0.40
1:B:467:ASP:OD1	1:B:467:ASP:N	2.51	0.40
1:B:622:VAL:O	1:B:622:VAL:HG22	2.21	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	988/1288 (77%)	950 (96%)	38 (4%)	0	100	100
1	B	1013/1288 (79%)	978 (96%)	35 (4%)	0	100	100
1	C	988/1288 (77%)	956 (97%)	32 (3%)	0	100	100
2	D	594/597 (100%)	570 (96%)	24 (4%)	0	100	100
All	All	3583/4461 (80%)	3454 (96%)	129 (4%)	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	857/1113 (77%)	856 (100%)	1 (0%)	93	97
1	B	888/1113 (80%)	887 (100%)	1 (0%)	93	97
1	C	857/1113 (77%)	853 (100%)	4 (0%)	88	93
2	D	526/527 (100%)	525 (100%)	1 (0%)	93	96
All	All	3128/3866 (81%)	3121 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	529	LYS
1	C	646	ARG
1	C	658	ASN
1	C	854	LYS
1	A	854	LYS
1	B	523	THR
2	D	508	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	508	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)

12 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.17	0	17,19,21	0.41	0
3	NAG	F	1	1,3	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	G	1	1,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	H	1	1,3	14,14,15	0.33	0	17,19,21	0.50	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	I	1	1,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	J	1	2,3	14,14,15	0.41	0	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.23	0	17,19,21	0.46	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	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.

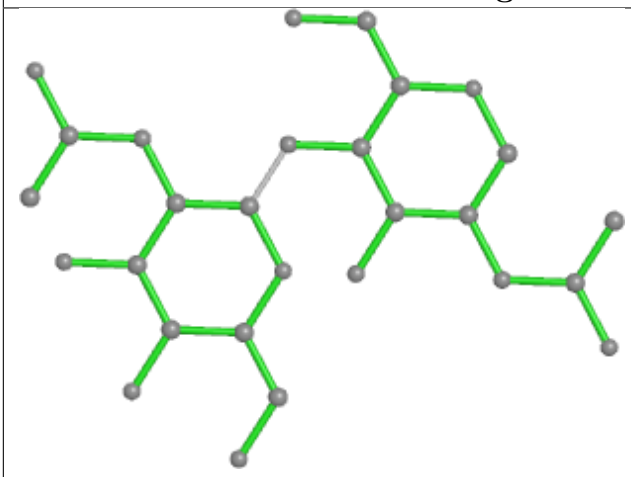
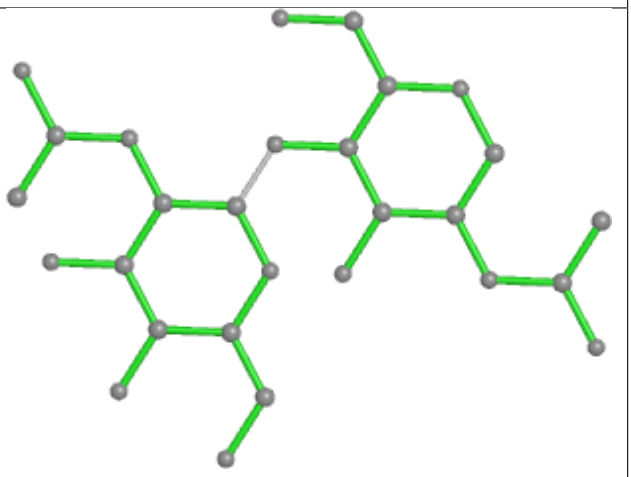
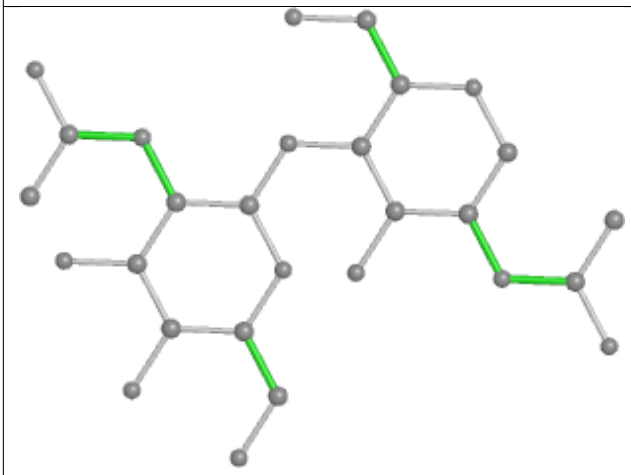
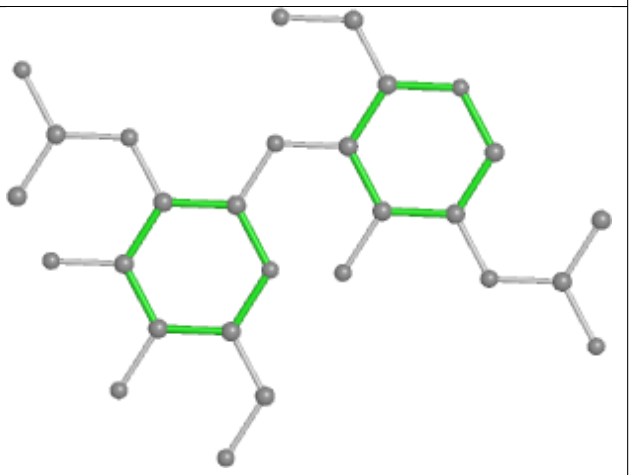
All (10) torsion outliers are listed below:

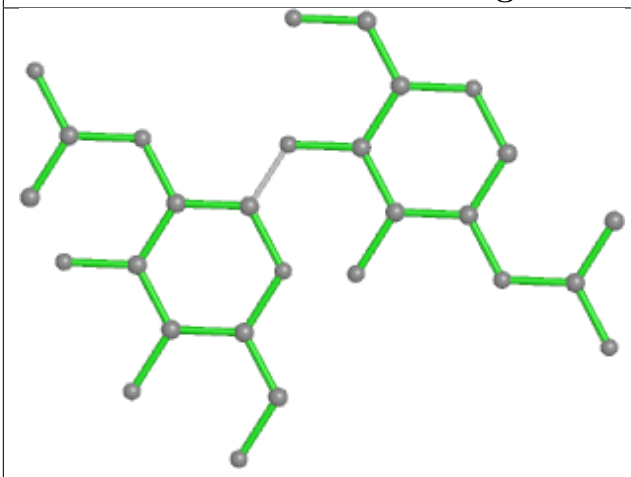
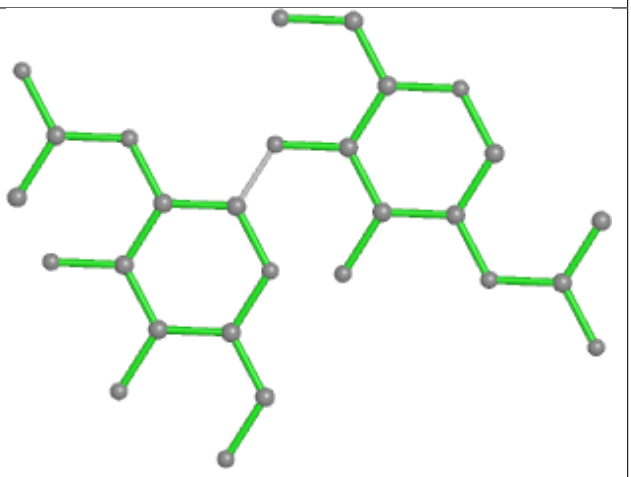
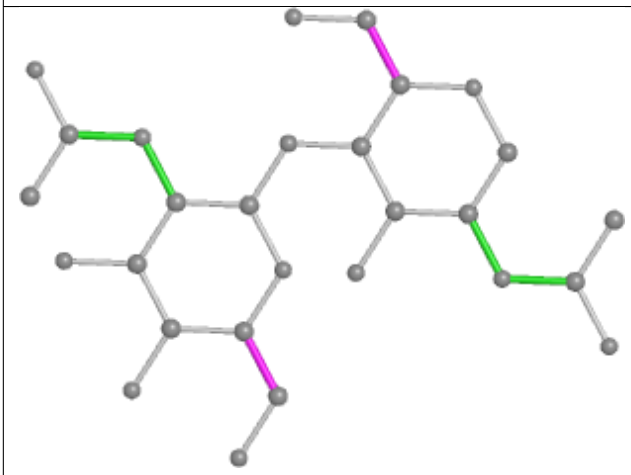
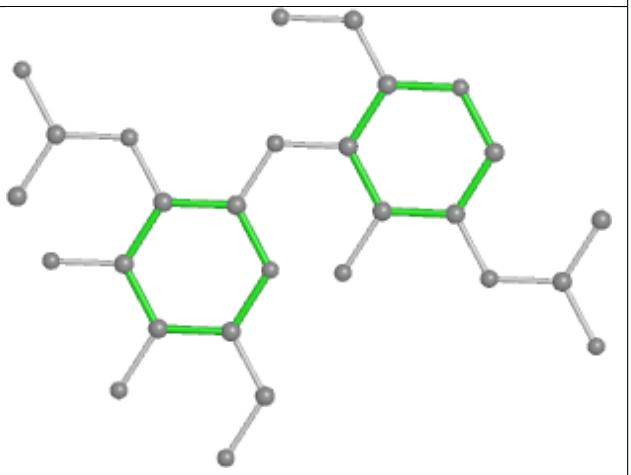
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

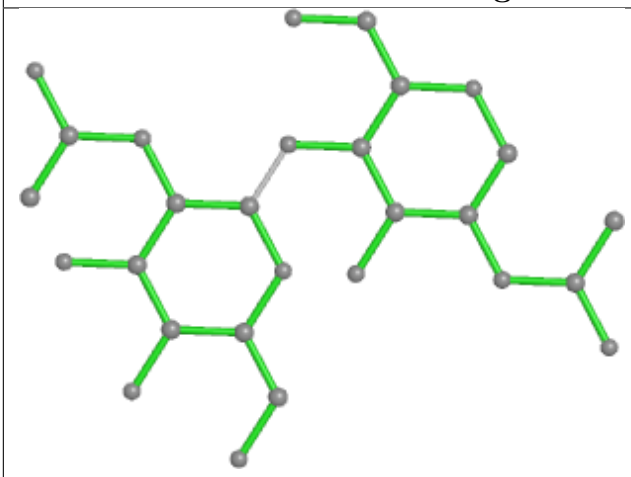
No monomer is involved in short contacts.

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

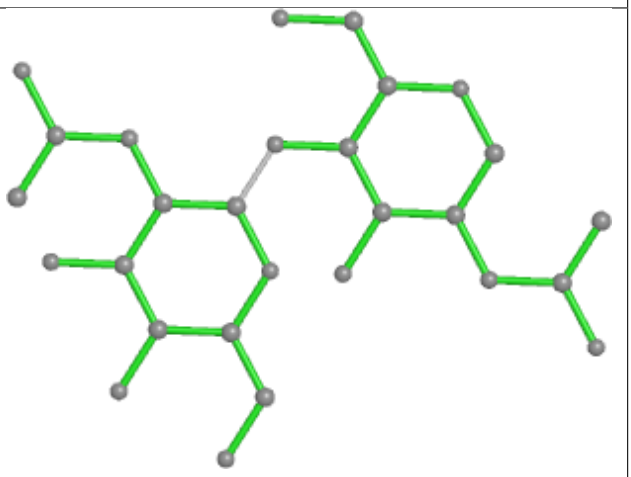
Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

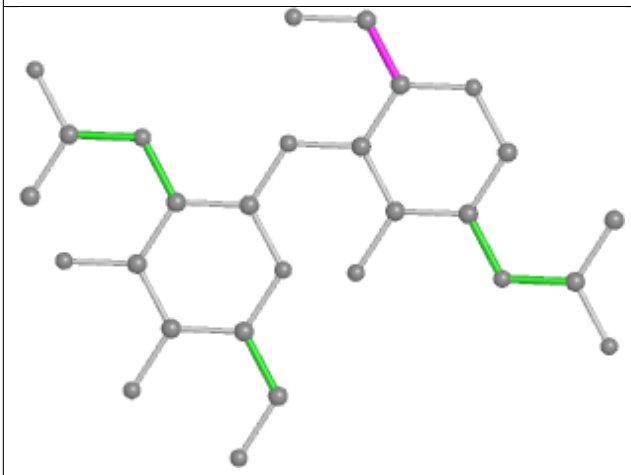
Oligosaccharide Chain G



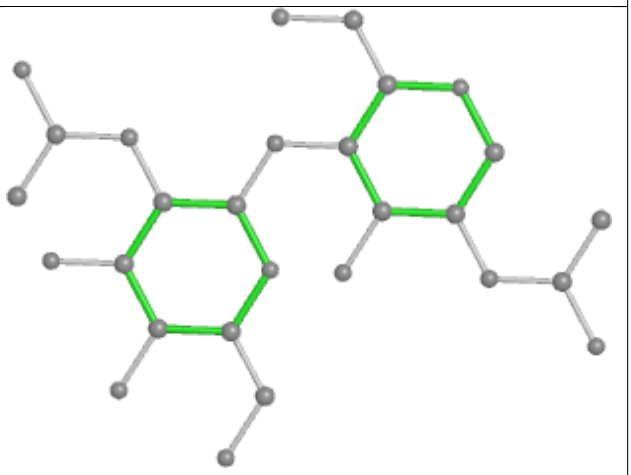
Bond lengths



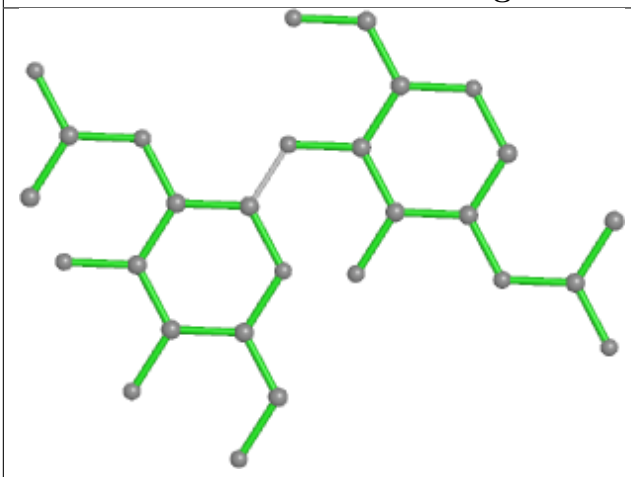
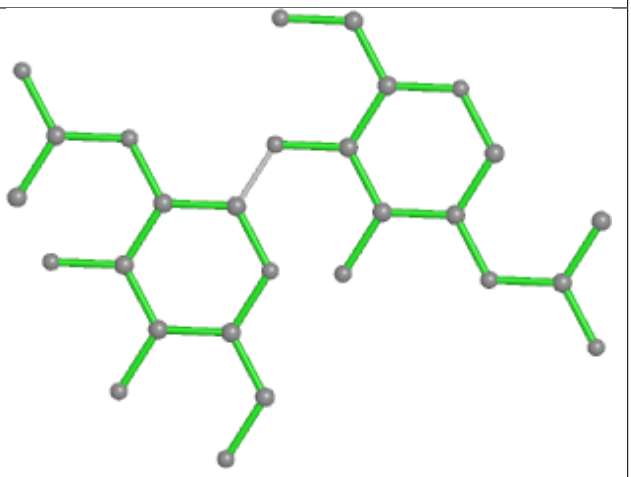
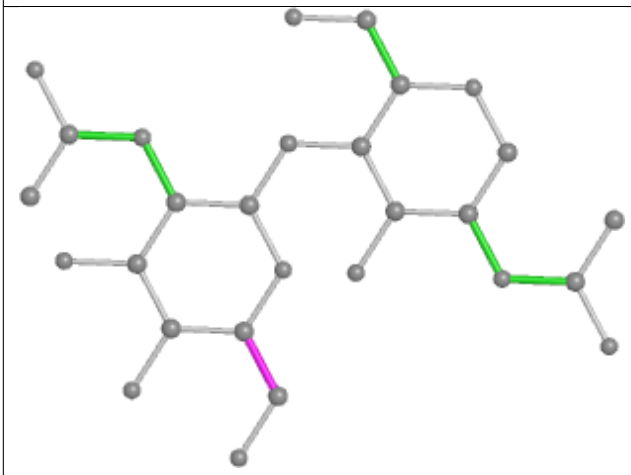
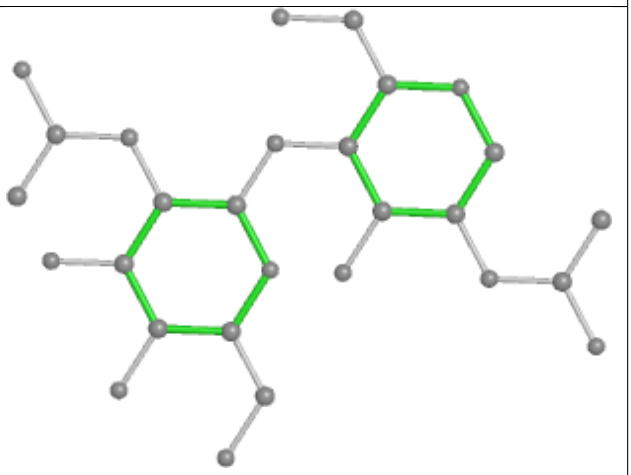
Bond angles



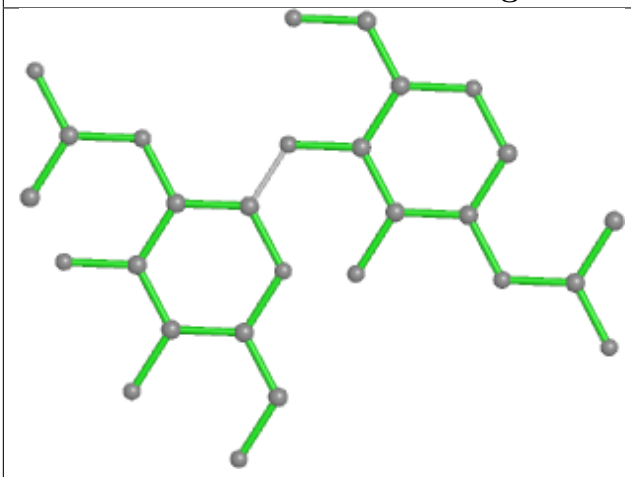
Torsions



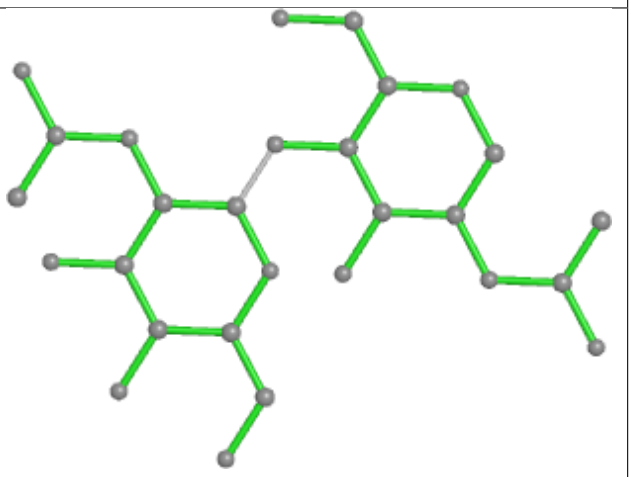
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

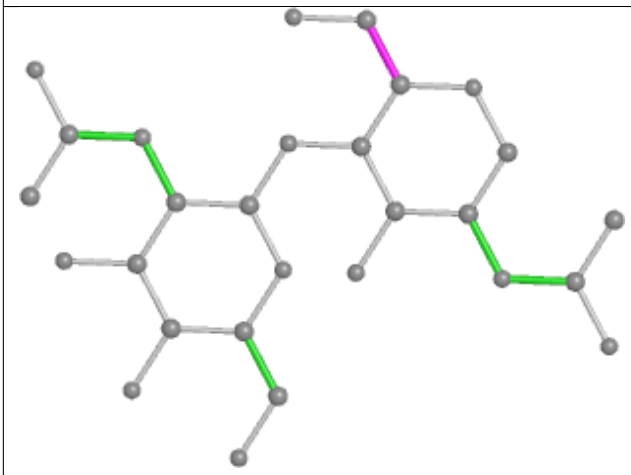
Oligosaccharide Chain I



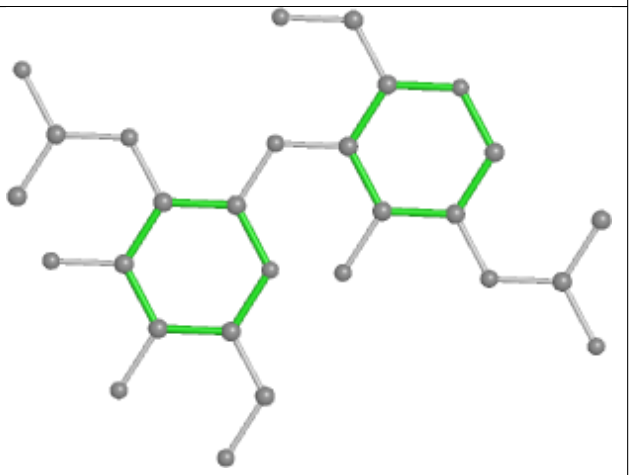
Bond lengths



Bond angles

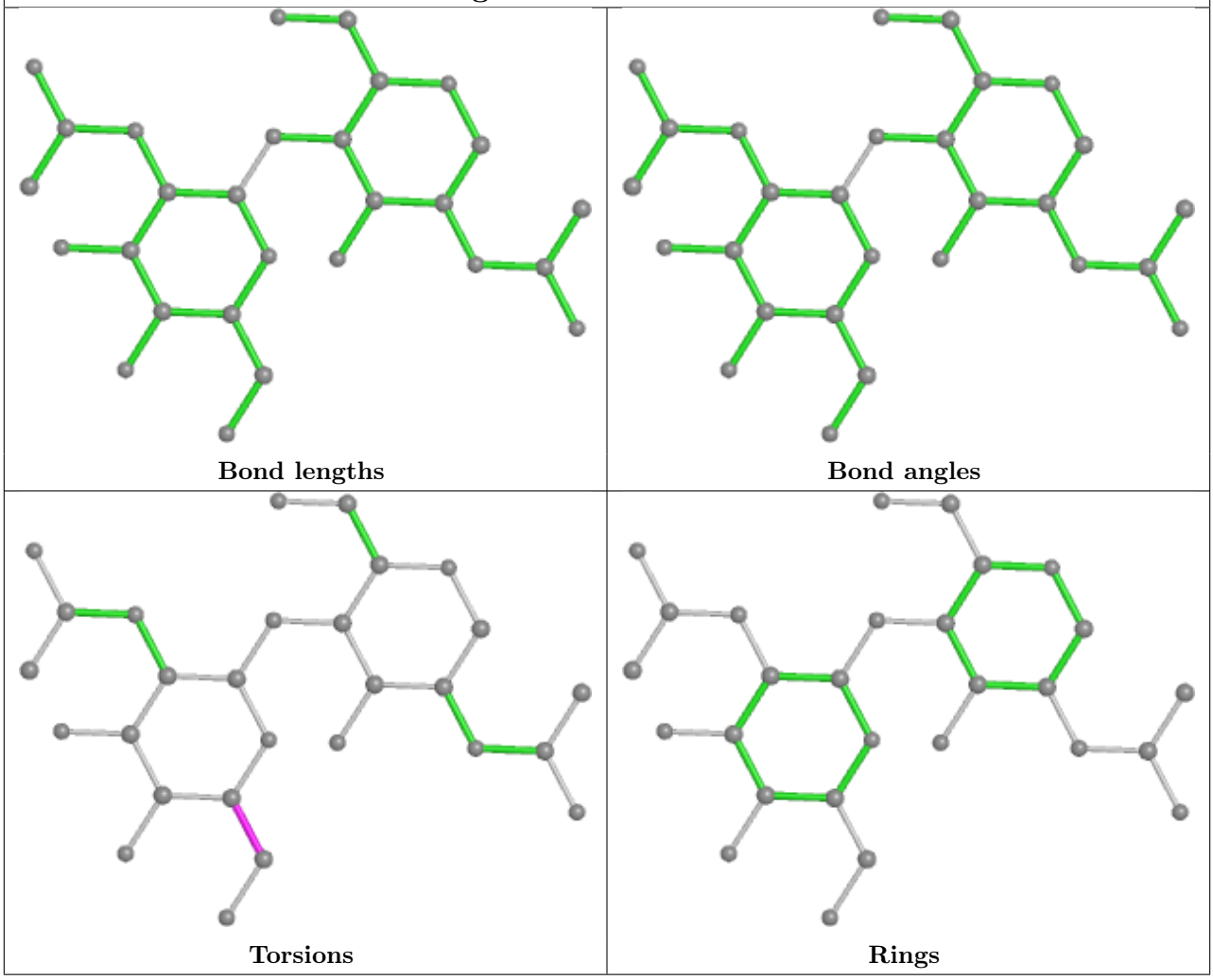


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

44 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	B	1305	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	D	705	2	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	C	1306	1	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	A	1306	1	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	B	1310	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1312	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1312	1	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	A	1309	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.46	0
4	NAG	B	1314	1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	0.81	0
4	NAG	D	704	2	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	C	1304	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	1.20	2 (11%)
4	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.63	0
4	NAG	C	1309	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1311	1	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	D	703	2	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	A	1305	1	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.67	1 (5%)
4	NAG	A	1303	1	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	B	1306	1	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	C	1310	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	C	1312	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	D	701	2	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	B	1313	1	14,14,15	0.30	0	17,19,21	0.73	0
4	NAG	D	702	2	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	1313	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	A	1311	1	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	B	1303	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1308	1	14,14,15	0.27	0	17,19,21	0.73	0
4	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.71	0
4	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.41	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
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	D	705	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	D	704	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	D	703	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	D	701	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	D	702	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1302	NAG	C2-N2-C7	2.34	126.24	122.90
4	A	1302	NAG	C8-C7-N2	2.21	119.84	116.10
4	B	1304	NAG	C2-N2-C7	2.13	125.94	122.90

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	D	704	NAG	O5-C5-C6-O6
4	B	1313	NAG	C8-C7-N2-C2
4	A	1309	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1306	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	B	1314	NAG	C4-C5-C6-O6
4	B	1313	NAG	O7-C7-N2-C2
4	B	1311	NAG	O5-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	D	704	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	D	705	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1314	NAG	O5-C5-C6-O6
4	A	1302	NAG	C1-C2-N2-C7
4	C	1311	NAG	O5-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	D	705	NAG	C4-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	O5-C5-C6-O6
4	C	1302	NAG	C3-C2-N2-C7
4	A	1306	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	C	1303	NAG	C3-C2-N2-C7
4	C	1313	NAG	C3-C2-N2-C7
4	A	1312	NAG	C3-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7
4	C	1313	NAG	C1-C2-N2-C7
4	A	1312	NAG	C1-C2-N2-C7
4	B	1305	NAG	C1-C2-N2-C7
4	B	1303	NAG	C1-C2-N2-C7
4	C	1309	NAG	C4-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	A	1303	NAG	C1-C2-N2-C7
4	A	1303	NAG	C3-C2-N2-C7
4	C	1309	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1303	NAG	1	0
4	C	1302	NAG	4	0
4	A	1302	NAG	2	0
4	C	1309	NAG	1	0
4	A	1311	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.

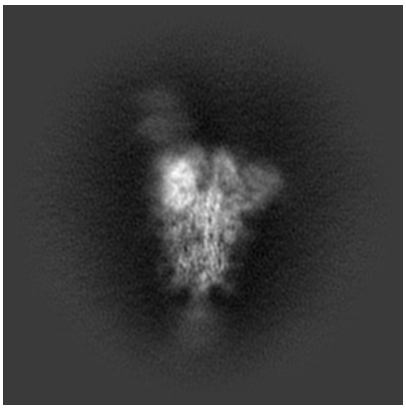
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22943. These allow visual inspection of the internal detail of the map and identification of artifacts.

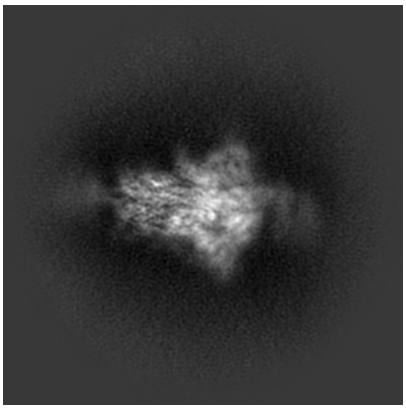
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

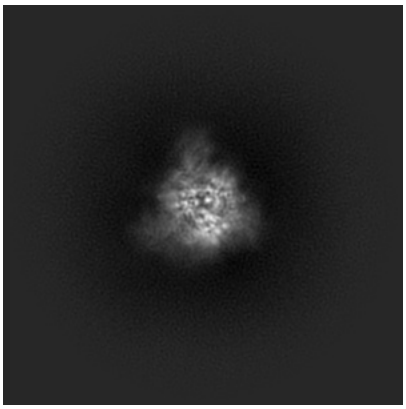
6.1.1 Primary map



X

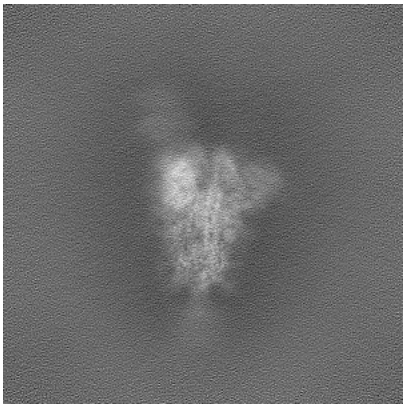


Y

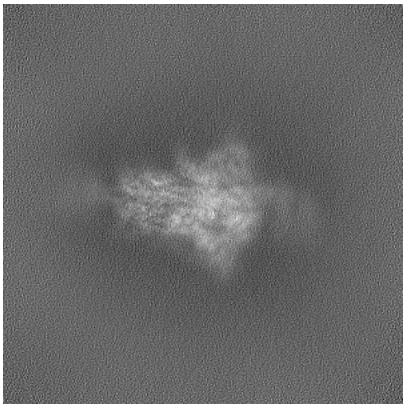


Z

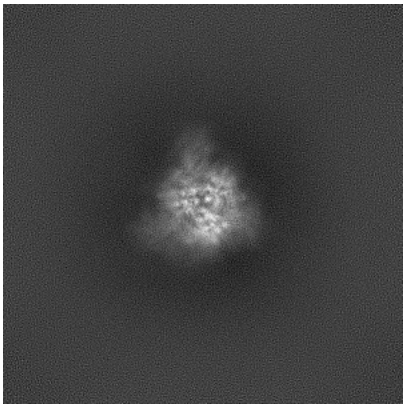
6.1.2 Raw map



X



Y

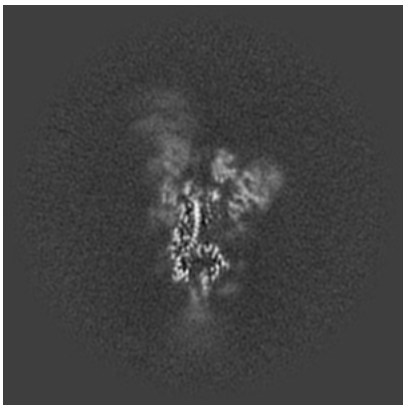


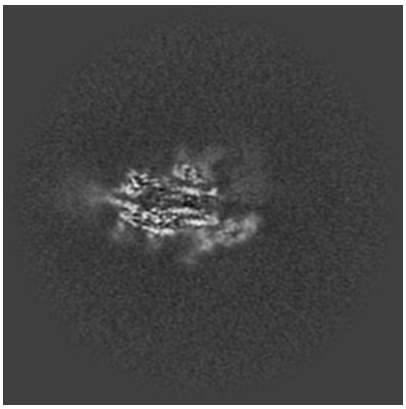
Z

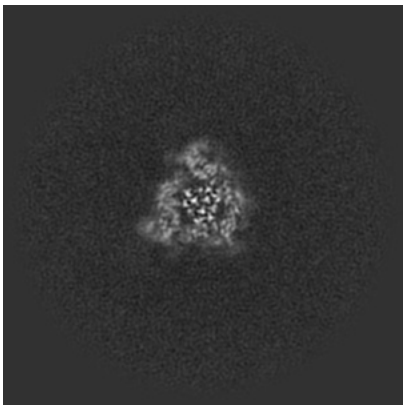
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

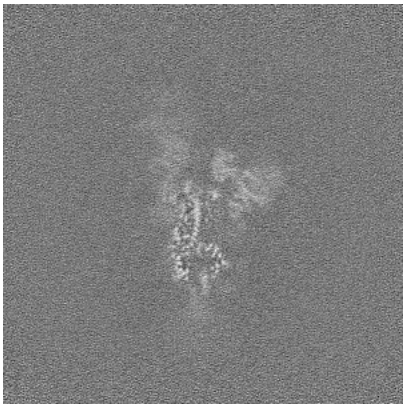
6.2.1 Primary map

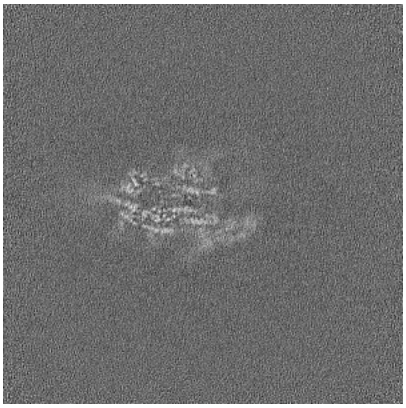

X Index: 192

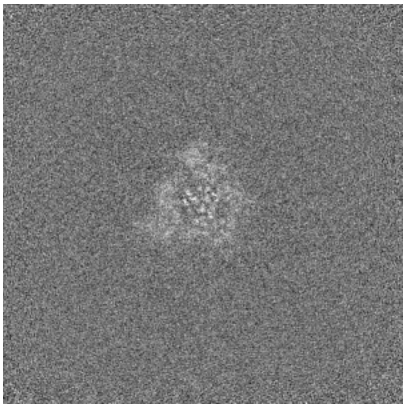

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

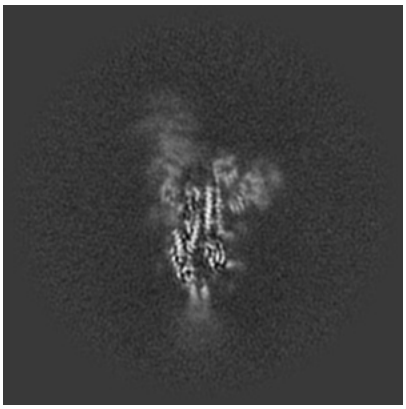

Y Index: 192


Z Index: 192

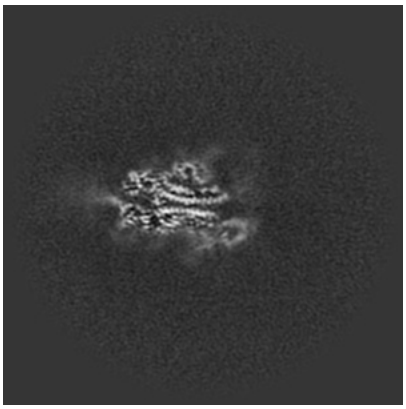
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

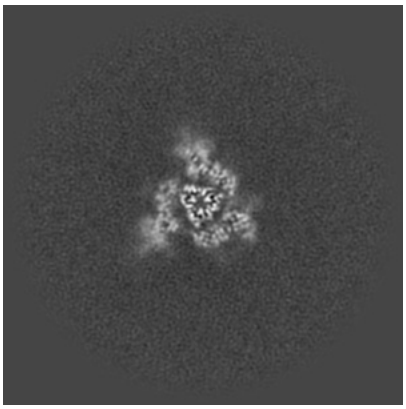
6.3.1 Primary map



X Index: 195

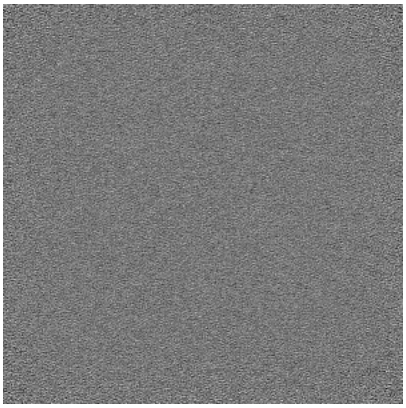


Y Index: 195

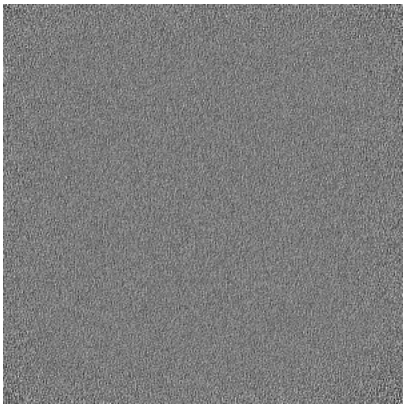


Z Index: 199

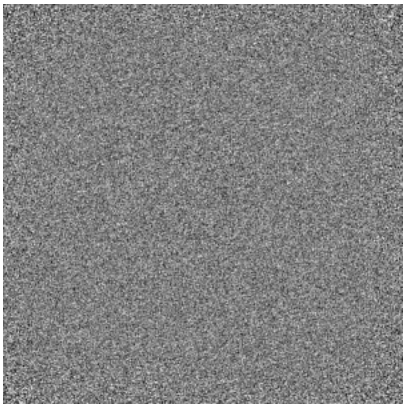
6.3.2 Raw map



X Index: 0



Y Index: 0

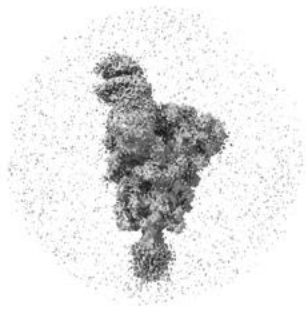


Z Index: 0

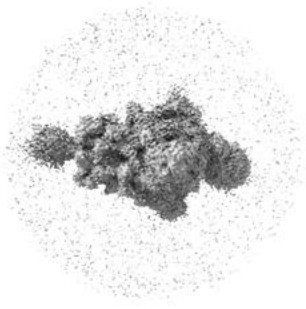
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

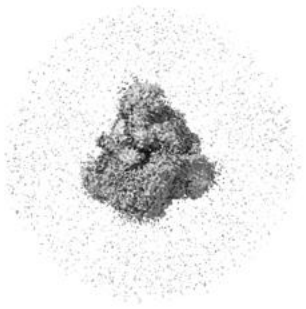
6.4.1 Primary map



X



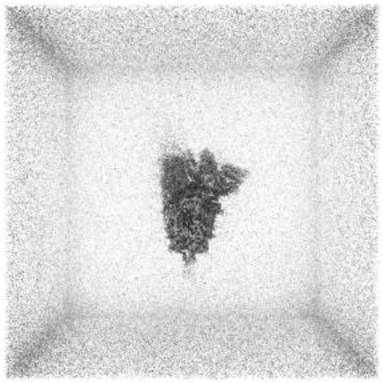
Y



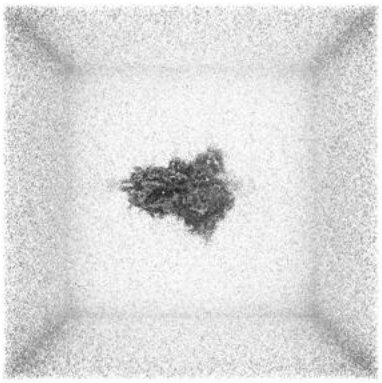
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

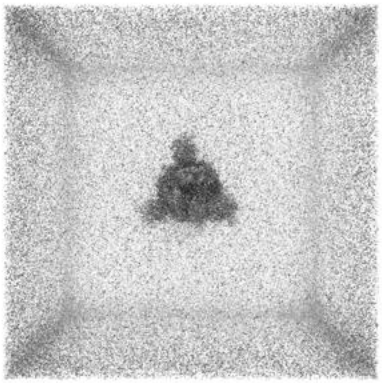
6.4.2 Raw map



X



Y



Z

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

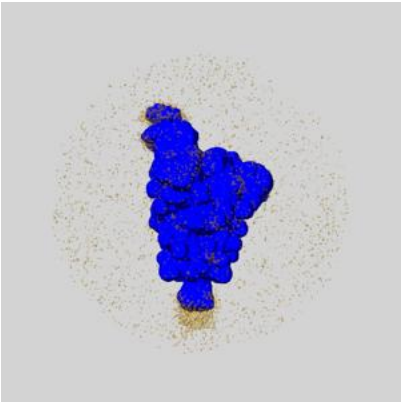
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

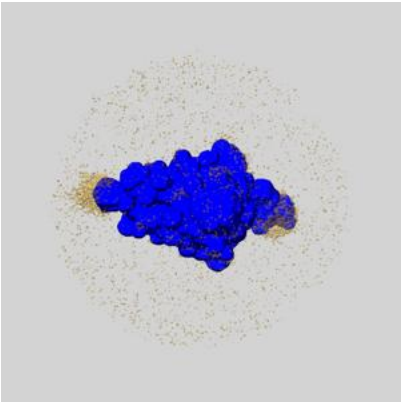
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

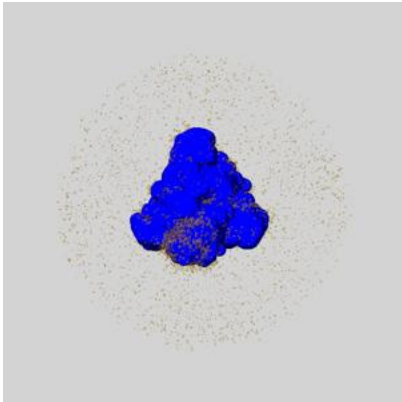
6.5.1 emd_22943_msk_1.map (i)



X



Y

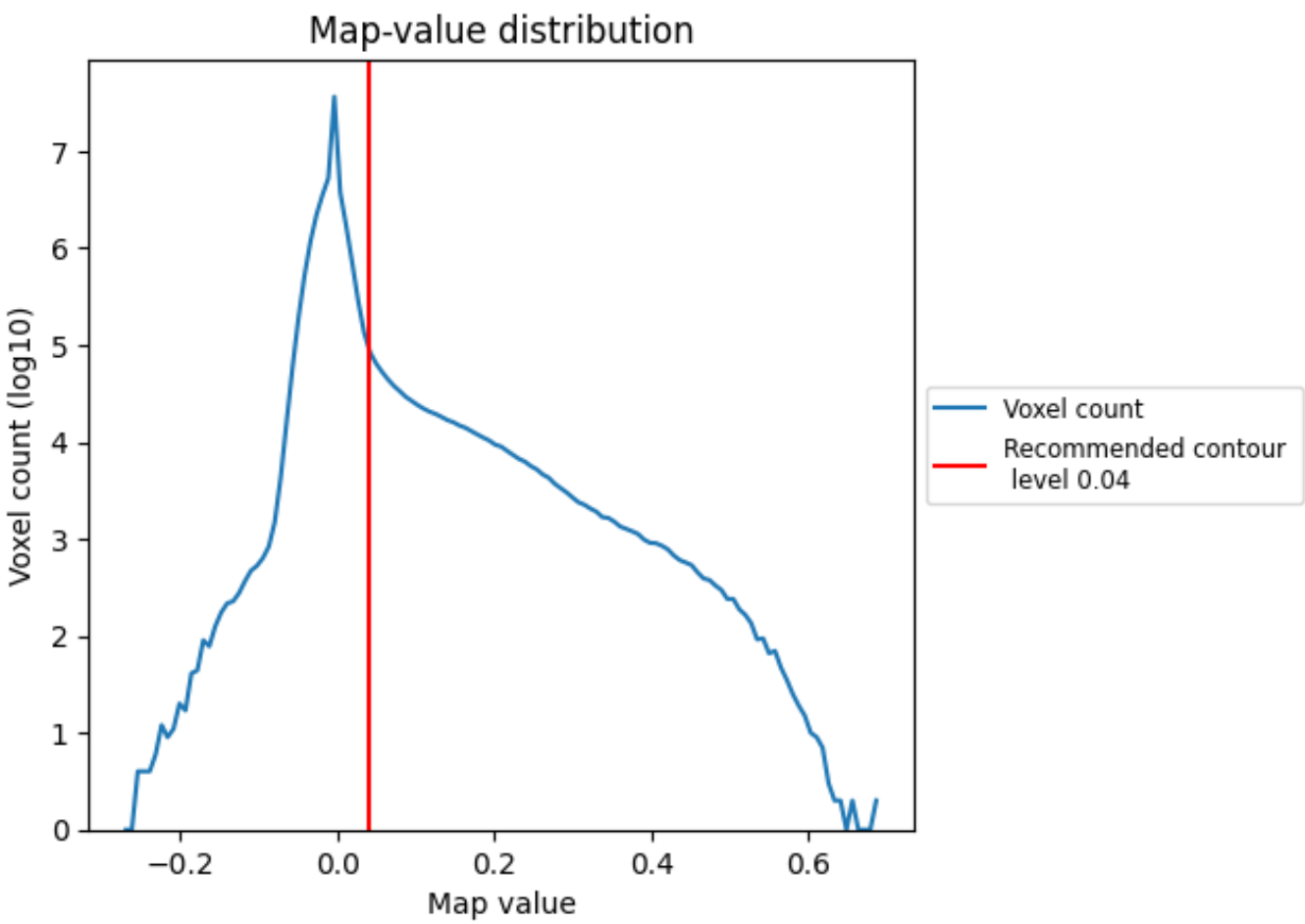


Z

7 Map analysis (i)

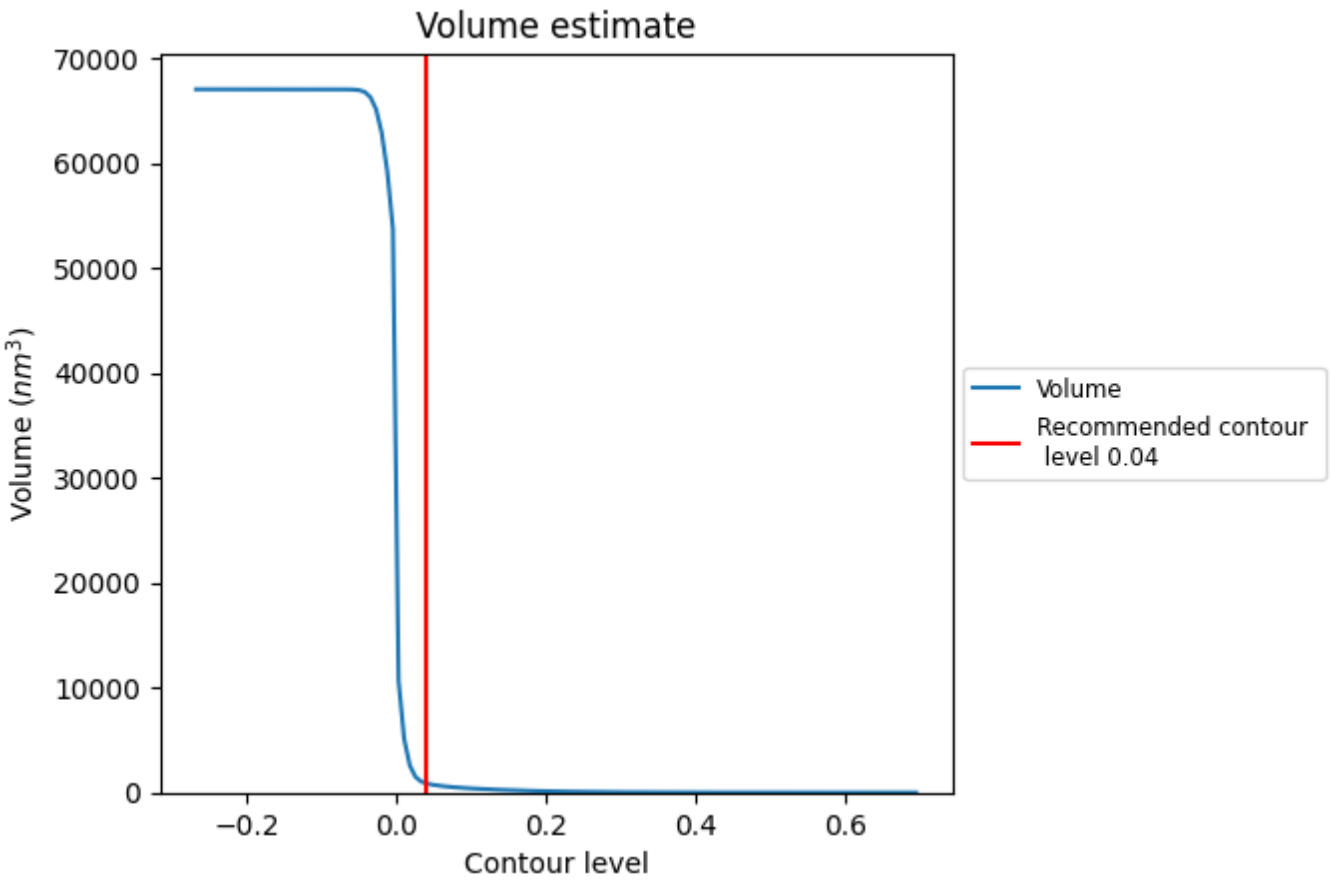
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

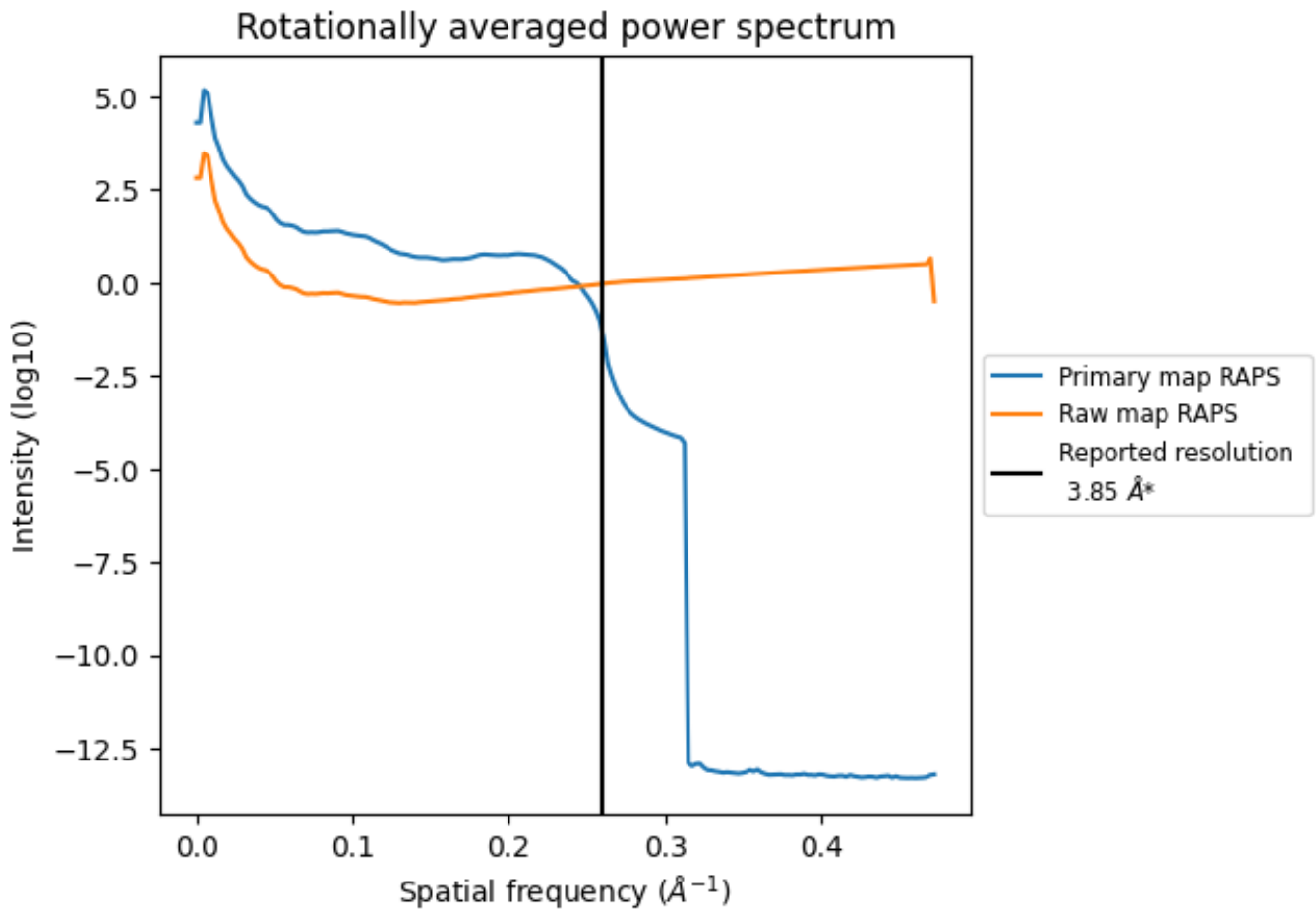
7.2 Volume estimate (i)



The volume at the recommended contour level is 856 nm^3; this corresponds to an approximate mass of 773 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)

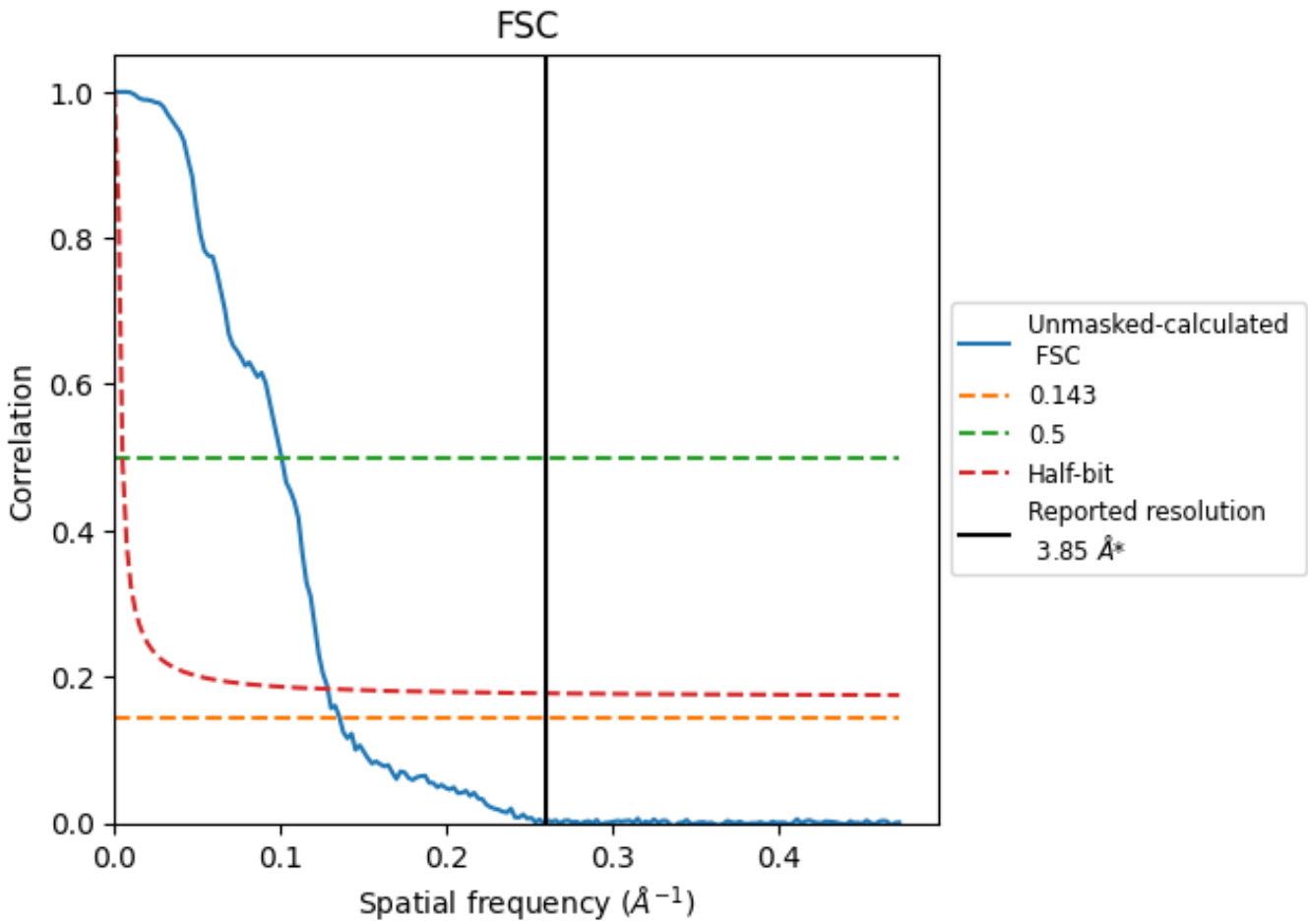


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8.2 Resolution estimates (i)

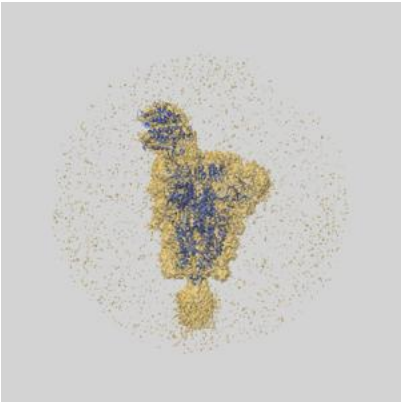
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.37	9.94	7.79

*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 7.37 differs from the reported value 3.85 by more than 10 %

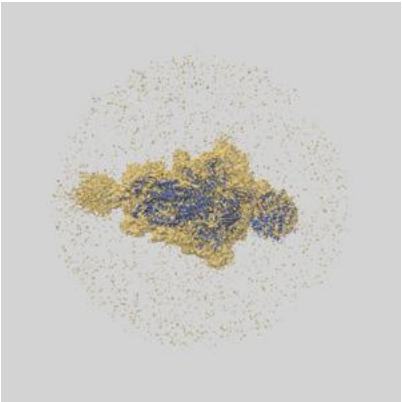
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22943 and PDB model 7KNE. Per-residue inclusion information can be found in section 3 on page 14.

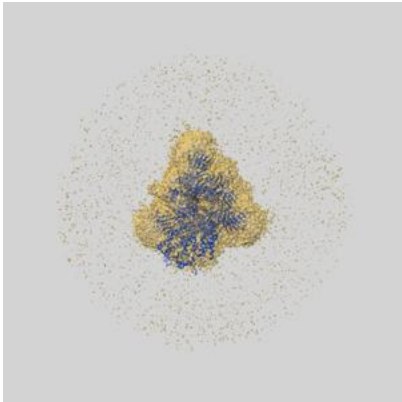
9.1 Map-model overlay (i)



X



Y



Z

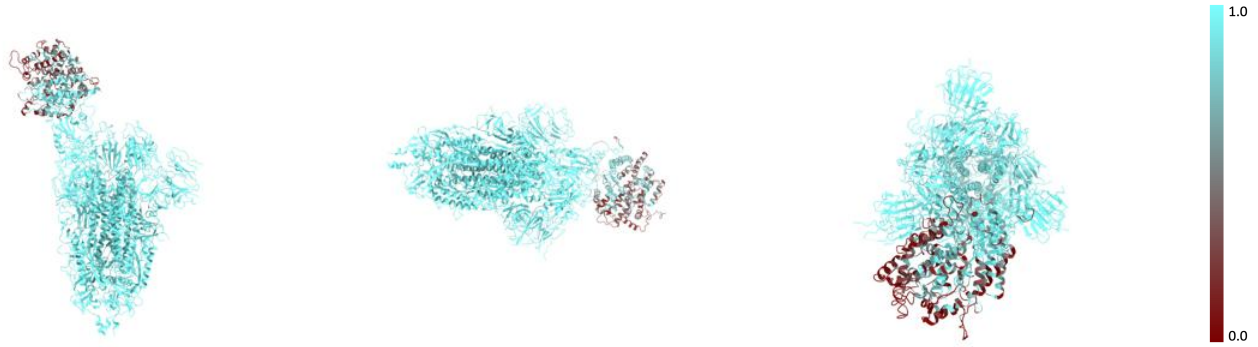
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

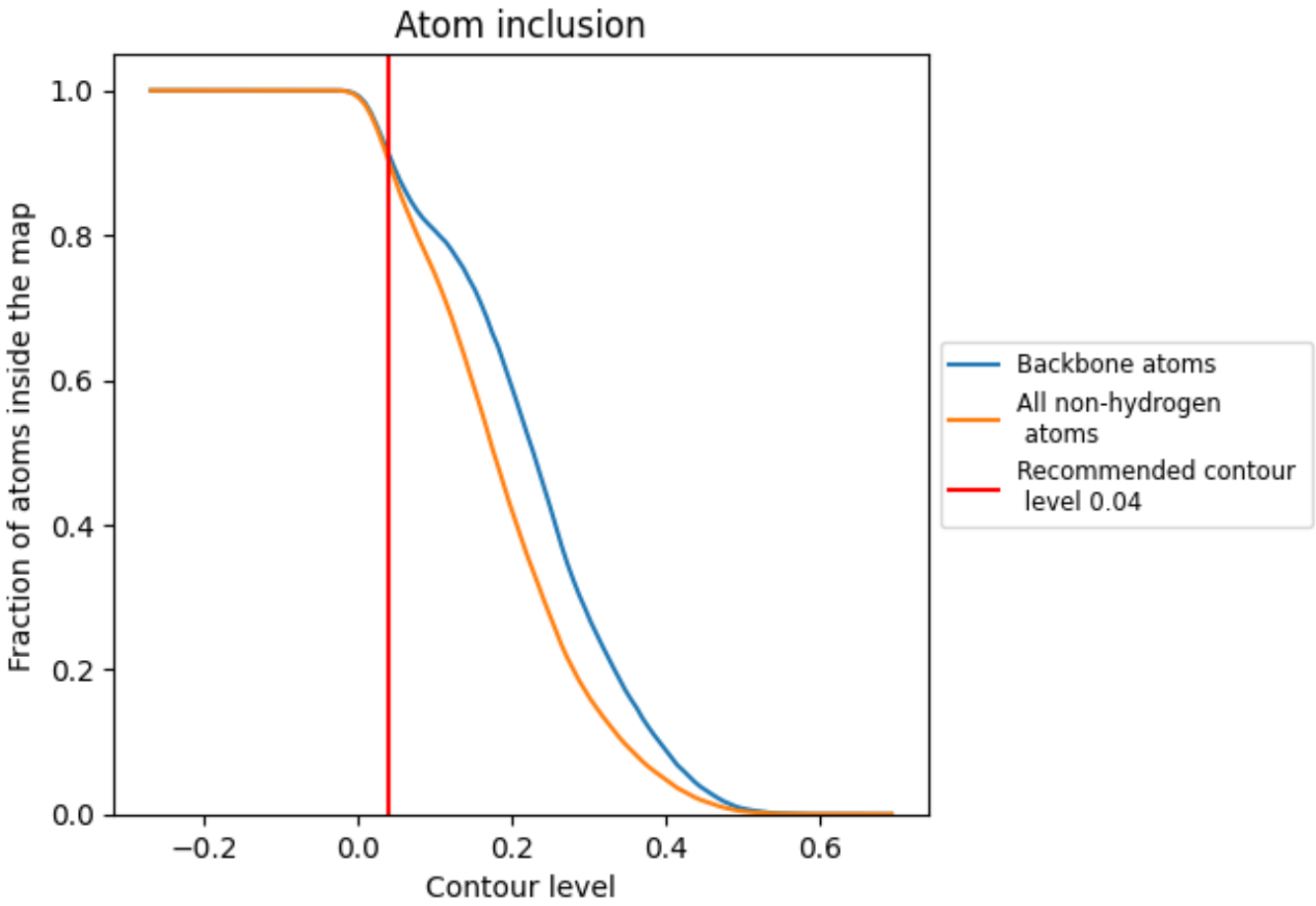
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9037	0.2530
A	0.9925	0.2970
B	0.9881	0.2790
C	0.9964	0.3130
D	0.4724	0.0370
E	1.0000	0.4430
F	1.0000	0.1870
G	1.0000	0.4330
H	1.0000	0.2310
I	1.0000	0.4830
J	0.0000	0.1960