



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 11:01 pm GMT

PDB ID : 8H3D  
EMDB ID : EMD-34464  
Title : Structure of apo SARS-CoV-2 spike protein with one RBD up  
Authors : Meng, F.; Wang, Q.; Xie, Y.; Ni, X.; Huang, N.  
Deposited on : 2022-10-08  
Resolution : 3.27 Å(reported)

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<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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.39

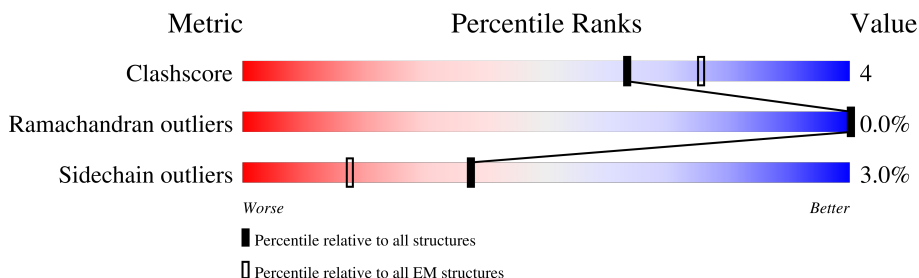
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.27 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1276	
1	B	1276	
1	C	1276	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24448 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	1023	Total	C	N	O	S	0	0
			8005	5119	1326	1524	36		
1	B	1041	Total	C	N	O	S	0	0
			8142	5205	1351	1548	38		
1	C	1039	Total	C	N	O	S	0	0
			8119	5187	1348	1546	38		

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	683	GLY	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	SER	-	linker	UNP P0DTC2
A	1213	GLY	-	linker	UNP P0DTC2
A	1214	ARG	-	linker	UNP P0DTC2
A	1215	GLU	-	linker	UNP P0DTC2
A	1216	ASN	-	linker	UNP P0DTC2
A	1217	LEU	-	linker	UNP P0DTC2
A	1218	TYR	-	linker	UNP P0DTC2
A	1219	PHE	-	linker	UNP P0DTC2
A	1220	GLN	-	linker	UNP P0DTC2
A	1221	GLY	-	linker	UNP P0DTC2
A	1222	GLY	-	linker	UNP P0DTC2
A	1223	GLY	-	linker	UNP P0DTC2
A	1224	GLY	-	linker	UNP P0DTC2
A	1225	SER	-	linker	UNP P0DTC2
A	1247	LEU	PHE	engineered mutation	UNP P10104
A	1254	GLY	-	expression tag	UNP P10104
A	1255	GLY	-	expression tag	UNP P10104
A	1256	GLY	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1258	HIS	-	expression tag	UNP P10104
A	1259	HIS	-	expression tag	UNP P10104
A	1260	HIS	-	expression tag	UNP P10104
A	1261	HIS	-	expression tag	UNP P10104
A	1262	HIS	-	expression tag	UNP P10104
A	1263	HIS	-	expression tag	UNP P10104
A	1264	HIS	-	expression tag	UNP P10104
A	1265	GLU	-	expression tag	UNP P10104
A	1266	ASP	-	expression tag	UNP P10104
A	1267	GLN	-	expression tag	UNP P10104
A	1268	VAL	-	expression tag	UNP P10104
A	1269	ASP	-	expression tag	UNP P10104
A	1270	PRO	-	expression tag	UNP P10104
A	1271	ARG	-	expression tag	UNP P10104
A	1272	LEU	-	expression tag	UNP P10104
A	1273	ILE	-	expression tag	UNP P10104
A	1274	ASP	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	LYS	-	expression tag	UNP P10104
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	683	GLY	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	SER	-	linker	UNP P0DTC2
B	1213	GLY	-	linker	UNP P0DTC2
B	1214	ARG	-	linker	UNP P0DTC2
B	1215	GLU	-	linker	UNP P0DTC2
B	1216	ASN	-	linker	UNP P0DTC2
B	1217	LEU	-	linker	UNP P0DTC2
B	1218	TYR	-	linker	UNP P0DTC2
B	1219	PHE	-	linker	UNP P0DTC2
B	1220	GLN	-	linker	UNP P0DTC2
B	1221	GLY	-	linker	UNP P0DTC2
B	1222	GLY	-	linker	UNP P0DTC2
B	1223	GLY	-	linker	UNP P0DTC2
B	1224	GLY	-	linker	UNP P0DTC2
B	1225	SER	-	linker	UNP P0DTC2
B	1247	LEU	PHE	engineered mutation	UNP P10104
B	1254	GLY	-	expression tag	UNP P10104
B	1255	GLY	-	expression tag	UNP P10104
B	1256	GLY	-	expression tag	UNP P10104

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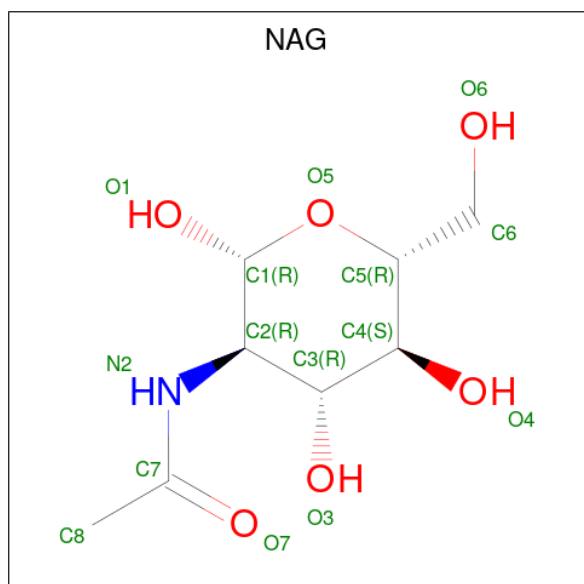
Chain	Residue	Modelled	Actual	Comment	Reference
B	1257	HIS	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	HIS	-	expression tag	UNP P10104
B	1260	HIS	-	expression tag	UNP P10104
B	1261	HIS	-	expression tag	UNP P10104
B	1262	HIS	-	expression tag	UNP P10104
B	1263	HIS	-	expression tag	UNP P10104
B	1264	HIS	-	expression tag	UNP P10104
B	1265	GLU	-	expression tag	UNP P10104
B	1266	ASP	-	expression tag	UNP P10104
B	1267	GLN	-	expression tag	UNP P10104
B	1268	VAL	-	expression tag	UNP P10104
B	1269	ASP	-	expression tag	UNP P10104
B	1270	PRO	-	expression tag	UNP P10104
B	1271	ARG	-	expression tag	UNP P10104
B	1272	LEU	-	expression tag	UNP P10104
B	1273	ILE	-	expression tag	UNP P10104
B	1274	ASP	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	LYS	-	expression tag	UNP P10104
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	683	GLY	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	SER	-	linker	UNP P0DTC2
C	1213	GLY	-	linker	UNP P0DTC2
C	1214	ARG	-	linker	UNP P0DTC2
C	1215	GLU	-	linker	UNP P0DTC2
C	1216	ASN	-	linker	UNP P0DTC2
C	1217	LEU	-	linker	UNP P0DTC2
C	1218	TYR	-	linker	UNP P0DTC2
C	1219	PHE	-	linker	UNP P0DTC2
C	1220	GLN	-	linker	UNP P0DTC2
C	1221	GLY	-	linker	UNP P0DTC2
C	1222	GLY	-	linker	UNP P0DTC2
C	1223	GLY	-	linker	UNP P0DTC2
C	1224	GLY	-	linker	UNP P0DTC2
C	1225	SER	-	linker	UNP P0DTC2
C	1247	LEU	PHE	engineered mutation	UNP P10104
C	1254	GLY	-	expression tag	UNP P10104
C	1255	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1256	GLY	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	HIS	-	expression tag	UNP P10104
C	1259	HIS	-	expression tag	UNP P10104
C	1260	HIS	-	expression tag	UNP P10104
C	1261	HIS	-	expression tag	UNP P10104
C	1262	HIS	-	expression tag	UNP P10104
C	1263	HIS	-	expression tag	UNP P10104
C	1264	HIS	-	expression tag	UNP P10104
C	1265	GLU	-	expression tag	UNP P10104
C	1266	ASP	-	expression tag	UNP P10104
C	1267	GLN	-	expression tag	UNP P10104
C	1268	VAL	-	expression tag	UNP P10104
C	1269	ASP	-	expression tag	UNP P10104
C	1270	PRO	-	expression tag	UNP P10104
C	1271	ARG	-	expression tag	UNP P10104
C	1272	LEU	-	expression tag	UNP P10104
C	1273	ILE	-	expression tag	UNP P10104
C	1274	ASP	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	LYS	-	expression tag	UNP P10104

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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





LEU	GLN	HIS	HIS	HIS	HIS	GLY	LYS	TVR	GLN	GLU	TVR	ILE	LYS	LYS	SER	GLY	ARG	GLU	ASN	LEU	TVR	PHE	GLN	GLY	GLY	GLY	GLY	SER	GLY	HIS
HIS	HIS	HIS	HIS	HIS	GLY	GLU	ASP	ASP	VAL	VAL	GLN	PRO	ARG	ARG	LEU	ILE	ASP	ASP	GLY	LYS										

● Molecule 1: Spike glycoprotein,Fibritin

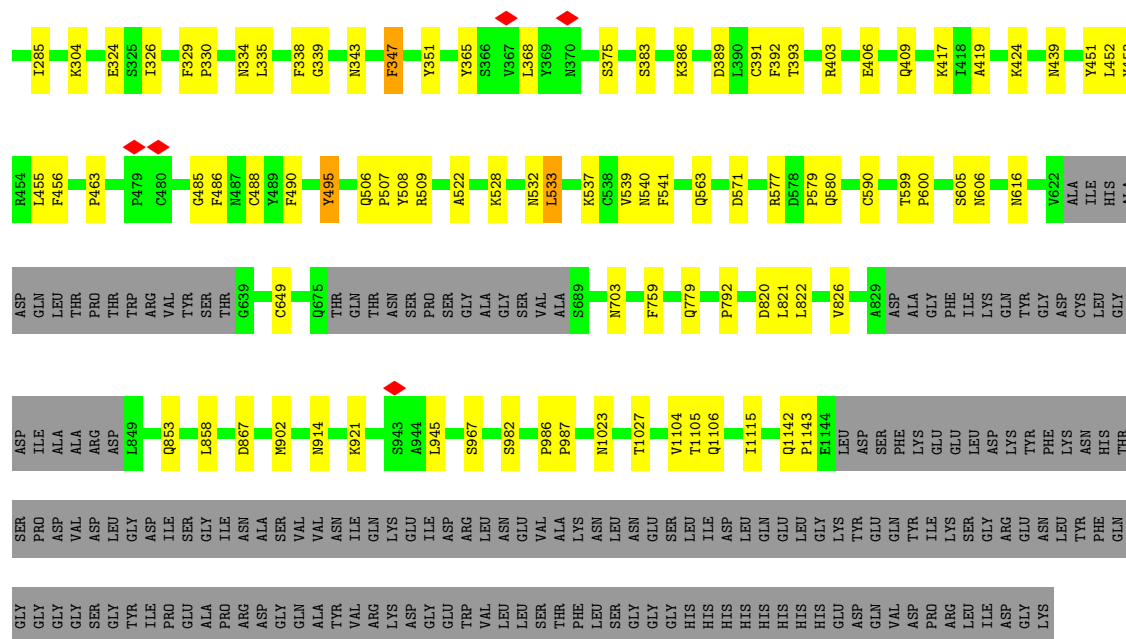


ASP	HIS	ASP	ASP	GLN	GLY	ASP	GLY	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: Spike glycoprotein,Fibritin



MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	PRO	VAL	SER	SER	GLN	CYS	VAL	ASN	LEU	THR	ARG	THR	GLN	LEU	PRO	PRO	PRO	GLY	GLY	SER	GLY	HIS
A27	V36	Q52	D53	L54	F55	A67	ILE	HIS	VAL	THR	GLY	GLY	THR	VAL	ASN	GLN	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
G142	Y145	HIS	LYS	ASN	ASN	LYS	S151	E156	F157	S172	G181	K182	E191	K202	V213	R214	F220	S221	A222	L229	P230	L231	R237	Y248	L249	THR	PRO	GLY	THR	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34118	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.177	Depositor
Minimum map value	-2.003	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.27	0/8188	0.49	0/11136
1	B	0.27	0/8329	0.49	0/11330
1	C	0.26	0/8305	0.49	0/11299
All	All	0.27	0/24822	0.49	0/33765

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	8005	0	7790	51	0
1	B	8142	0	7931	66	0
1	C	8119	0	7915	63	0
2	A	42	0	39	0	0
2	B	70	0	65	3	0
2	C	70	0	65	4	0
All	All	24448	0	23805	175	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.

The worst 5 of 175 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:339:GLY:HA3	2:C:1303:NAG:HN2	1.32	0.92
1:C:55:PHE:HB3	1:C:270:LEU:HB3	1.57	0.84
1:C:853:GLN:HB3	1:C:858:LEU:HD12	1.71	0.72
1:B:273:ARG:NH2	1:B:290:ASP:OD2	2.25	0.67
1:A:689:SER:OG	1:A:690:GLN:N	2.24	0.67

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	1001/1276 (78%)	946 (94%)	54 (5%)	1 (0%)	48	77
1	B	1023/1276 (80%)	950 (93%)	73 (7%)	0	100	100
1	C	1025/1276 (80%)	958 (94%)	67 (6%)	0	100	100
All	All	3049/3828 (80%)	2854 (94%)	194 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PRO

### 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	892/1106 (81%)	866 (97%)	26 (3%)	37	62
1	B	908/1106 (82%)	881 (97%)	27 (3%)	36	61
1	C	906/1106 (82%)	877 (97%)	29 (3%)	34	60
All	All	2706/3318 (82%)	2624 (97%)	82 (3%)	37	61

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	ARG
1	C	540	ASN
1	C	248	TYR
1	C	392	PHE
1	C	649	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 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
2	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.48	0
2	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.38	0
2	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.36	0
2	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.36	0
2	NAG	C	1303	1	14,14,15	0.57	0	17,19,21	1.27	1 (5%)
2	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	C	1304	1	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	B	1301	1	14,14,15	0.28	0	17,19,21	0.36	0
2	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	C	1301	1	14,14,15	0.34	0	17,19,21	0.40	0
2	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.52	0
2	NAG	A	1303	1	14,14,15	0.18	0	17,19,21	0.44	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	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1303	NAG	C2-N2-C7	4.33	129.07	122.90

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1305	NAG	O5-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	A	1303	NAG	O5-C5-C6-O6

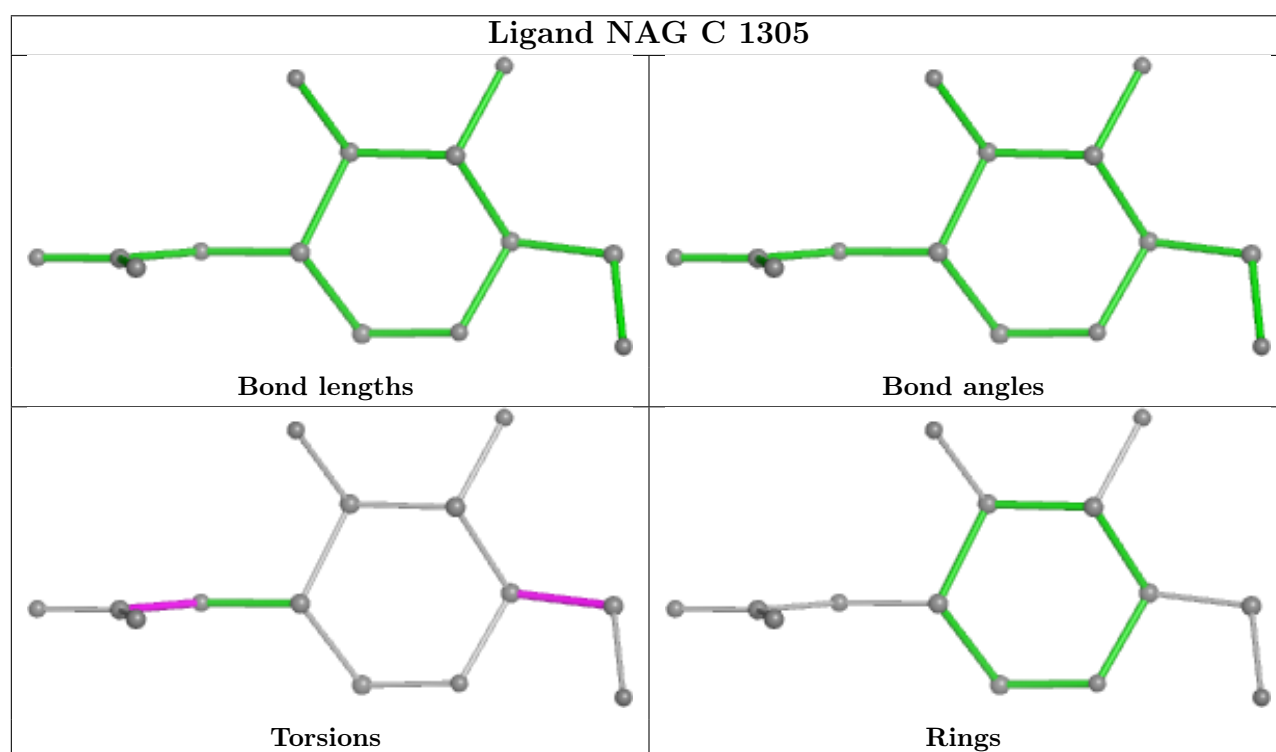
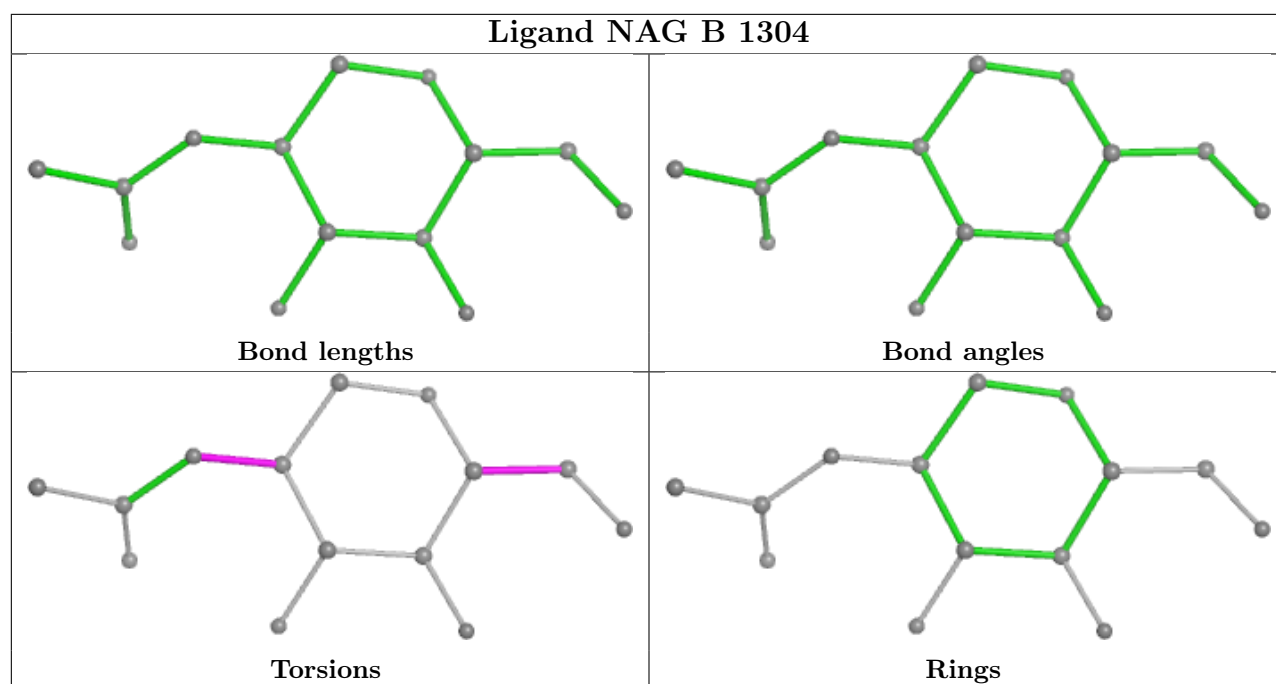
There are no ring outliers.

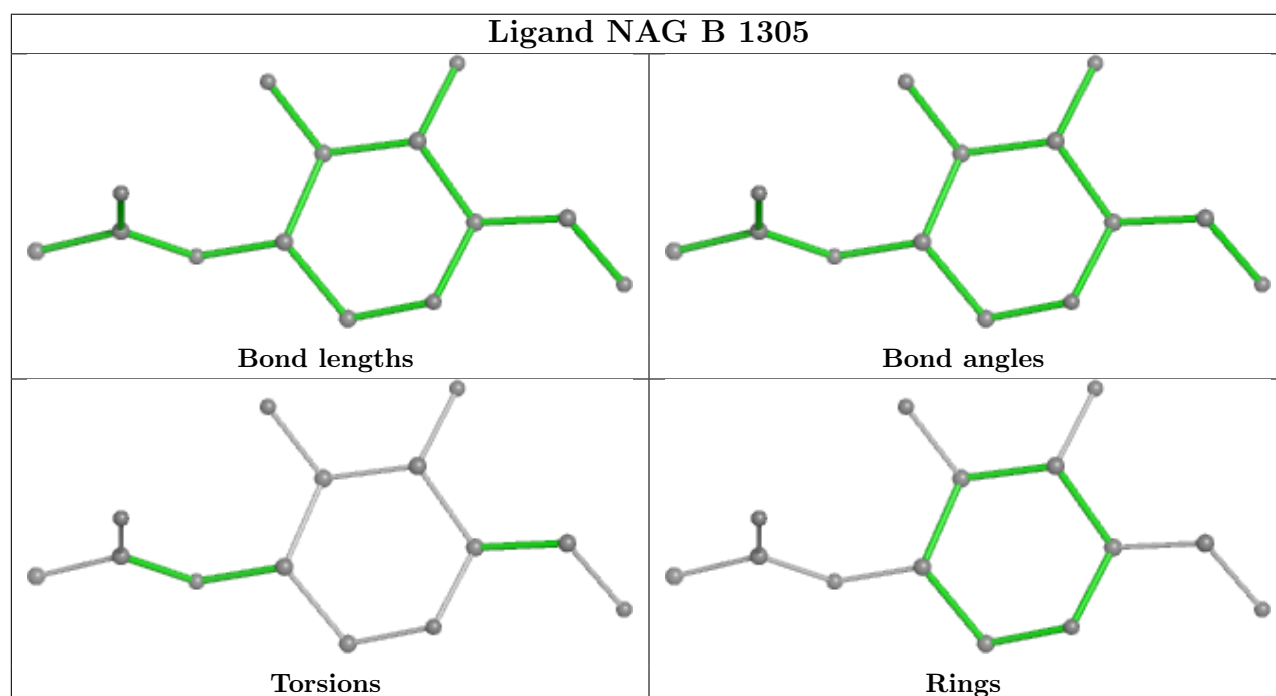
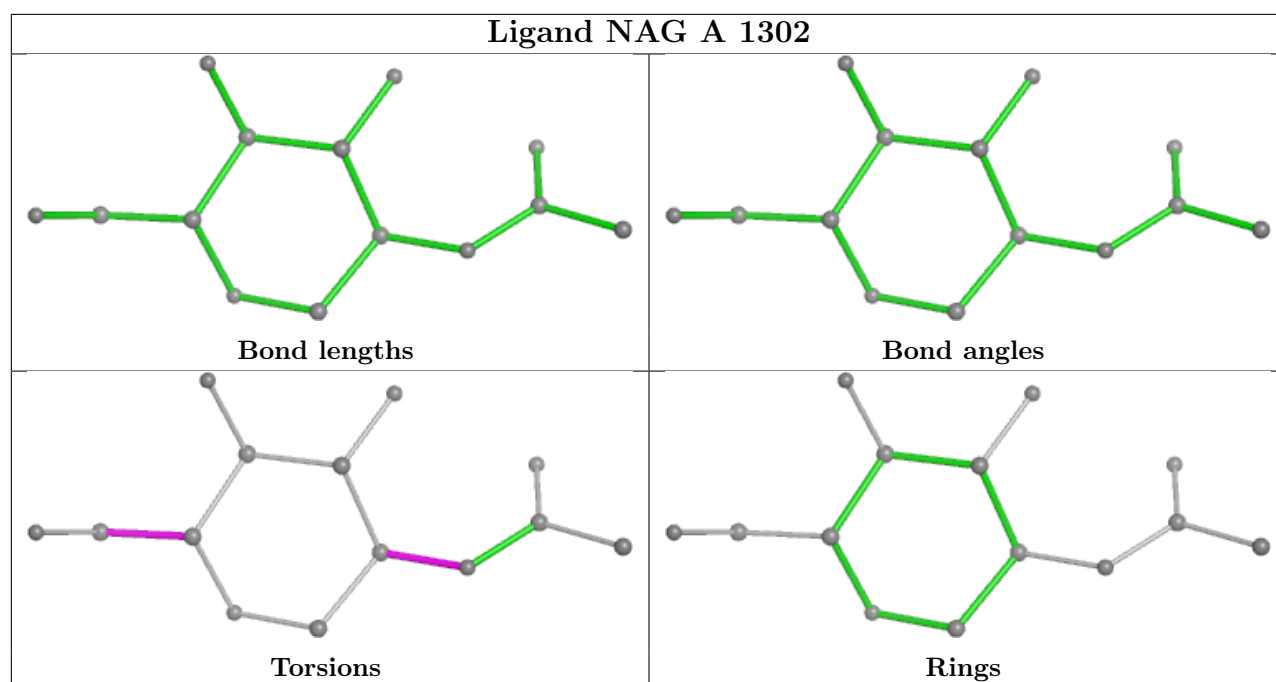
4 monomers are involved in 7 short contacts:

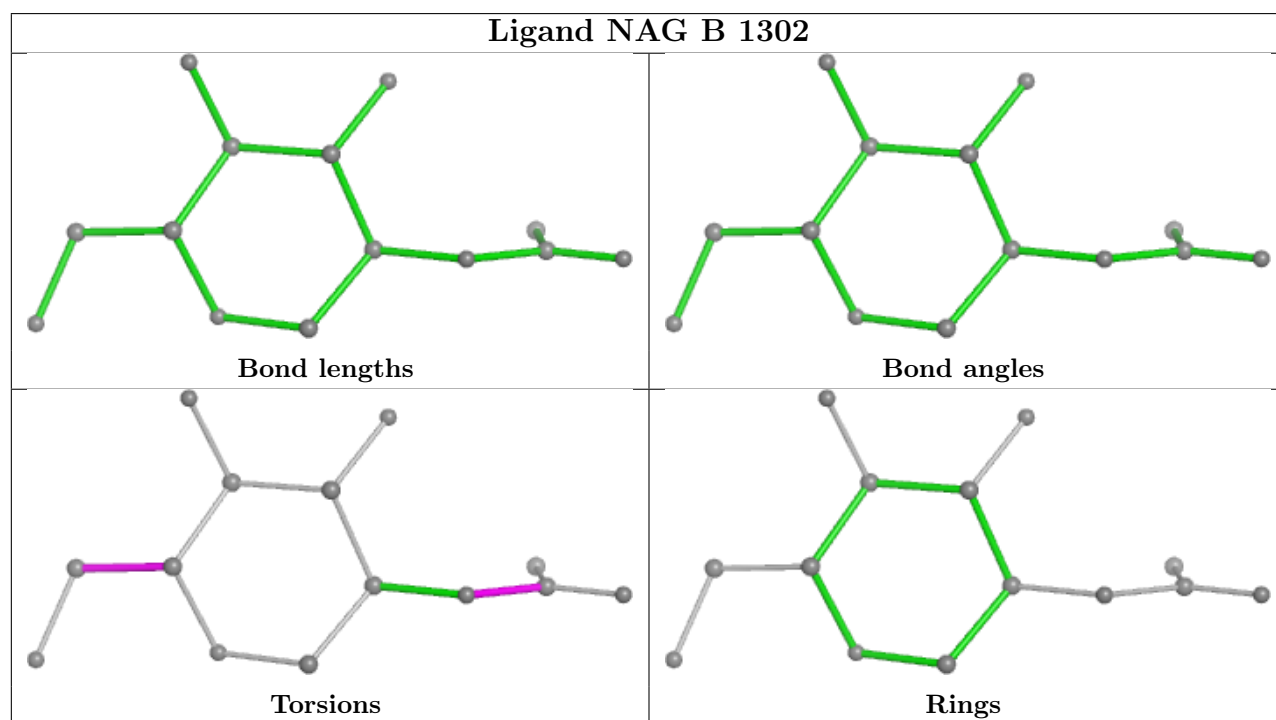
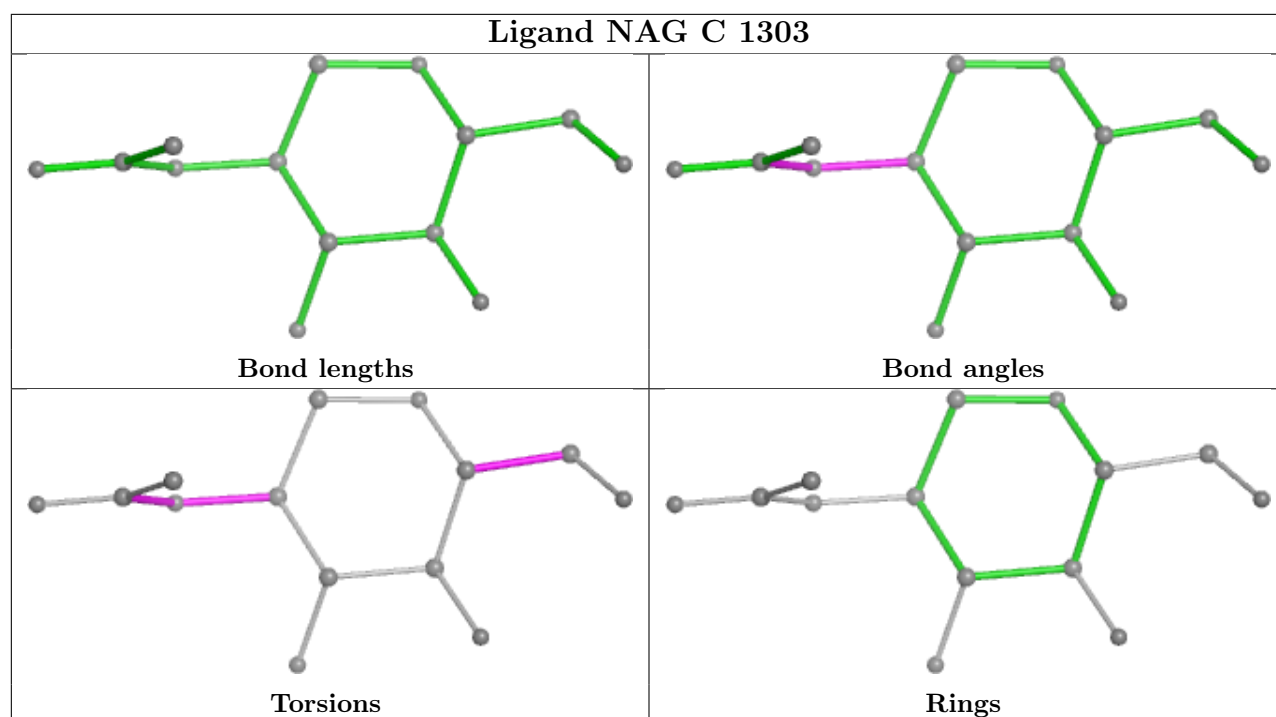
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1304	NAG	1	0
2	C	1303	NAG	4	0
2	B	1301	NAG	1	0
2	B	1303	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

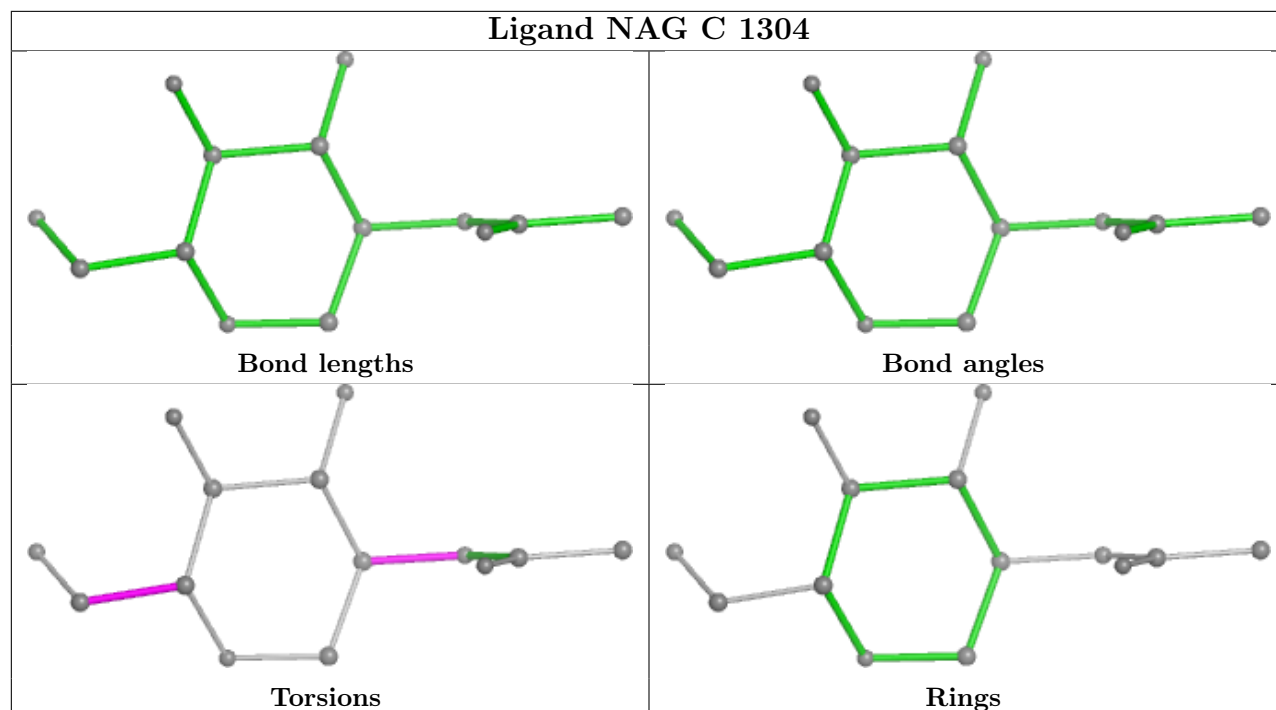




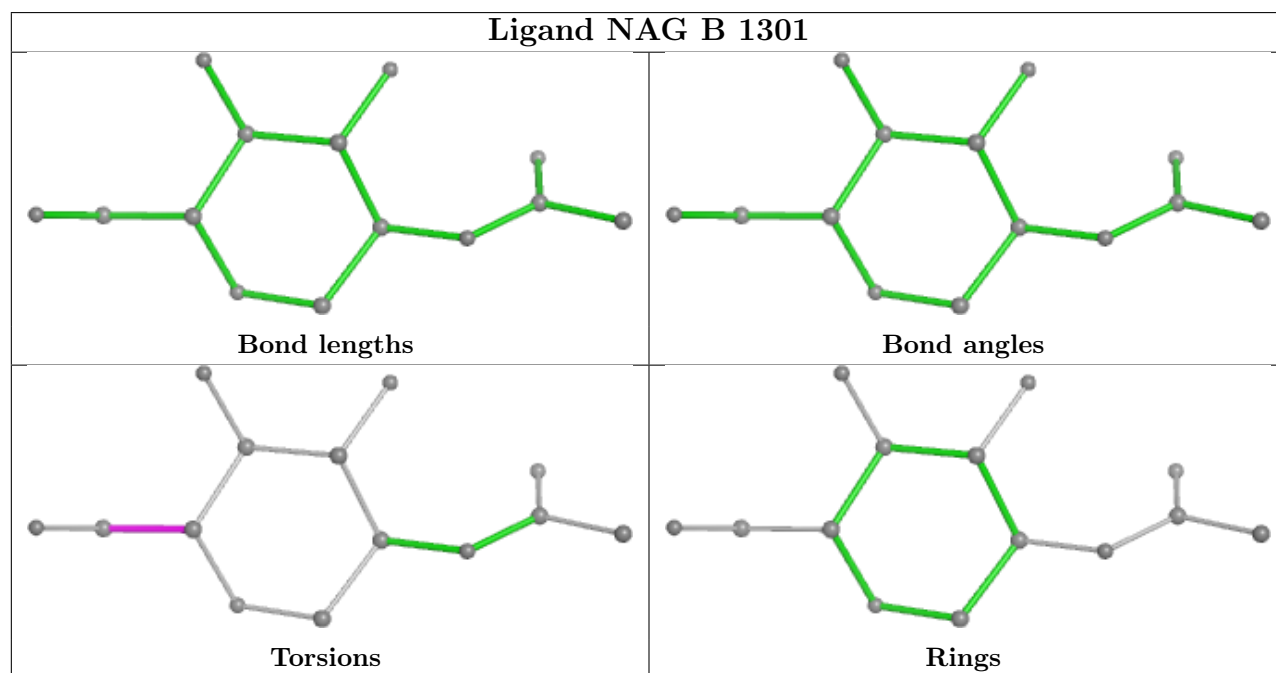


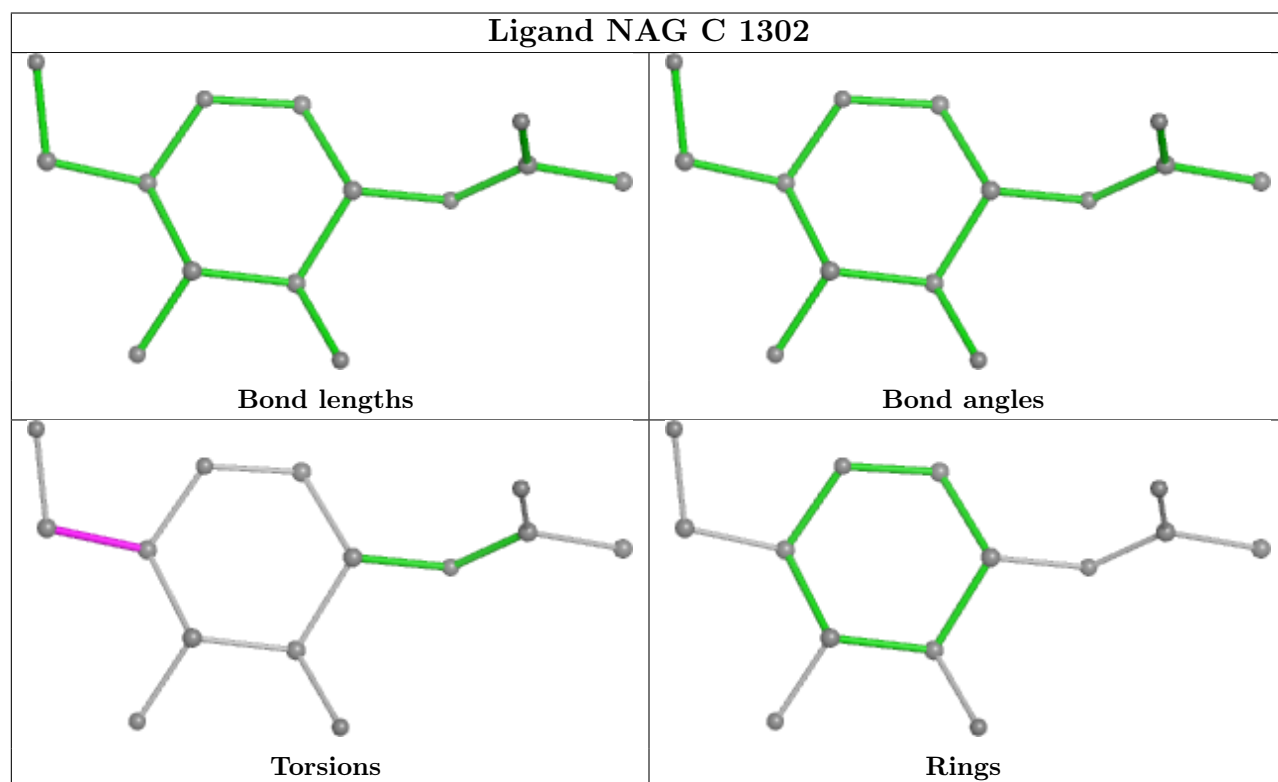
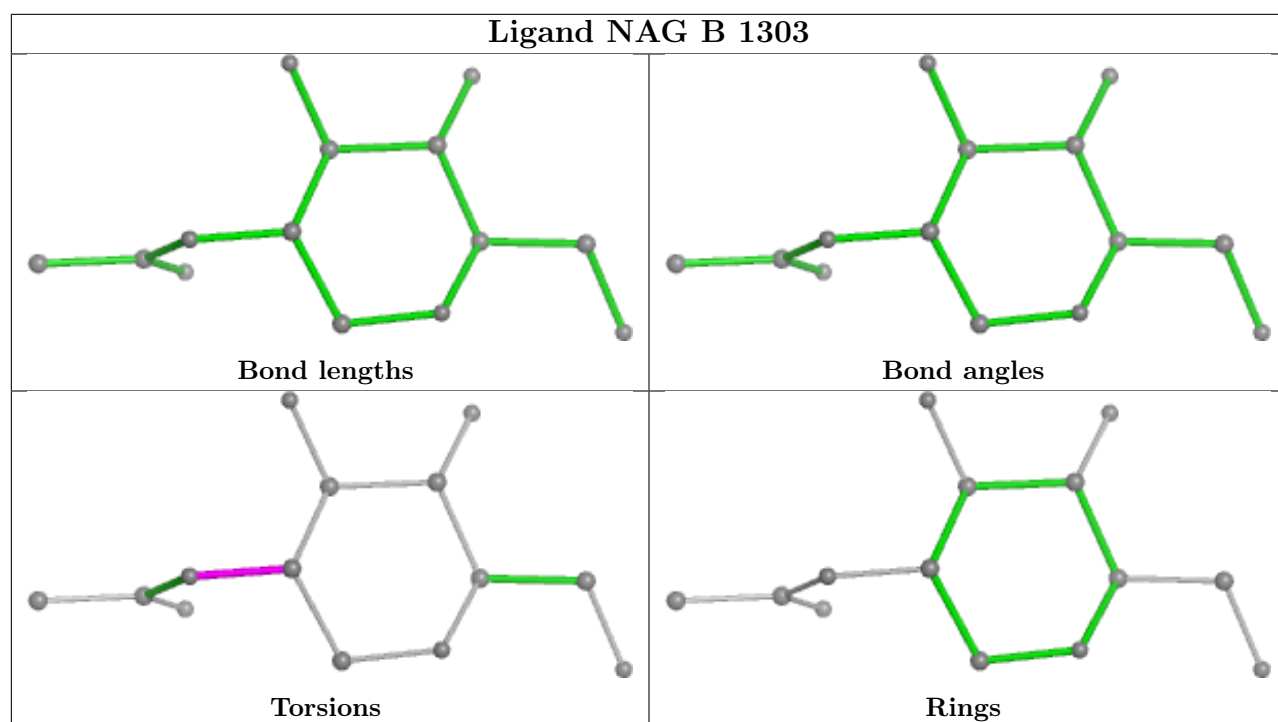


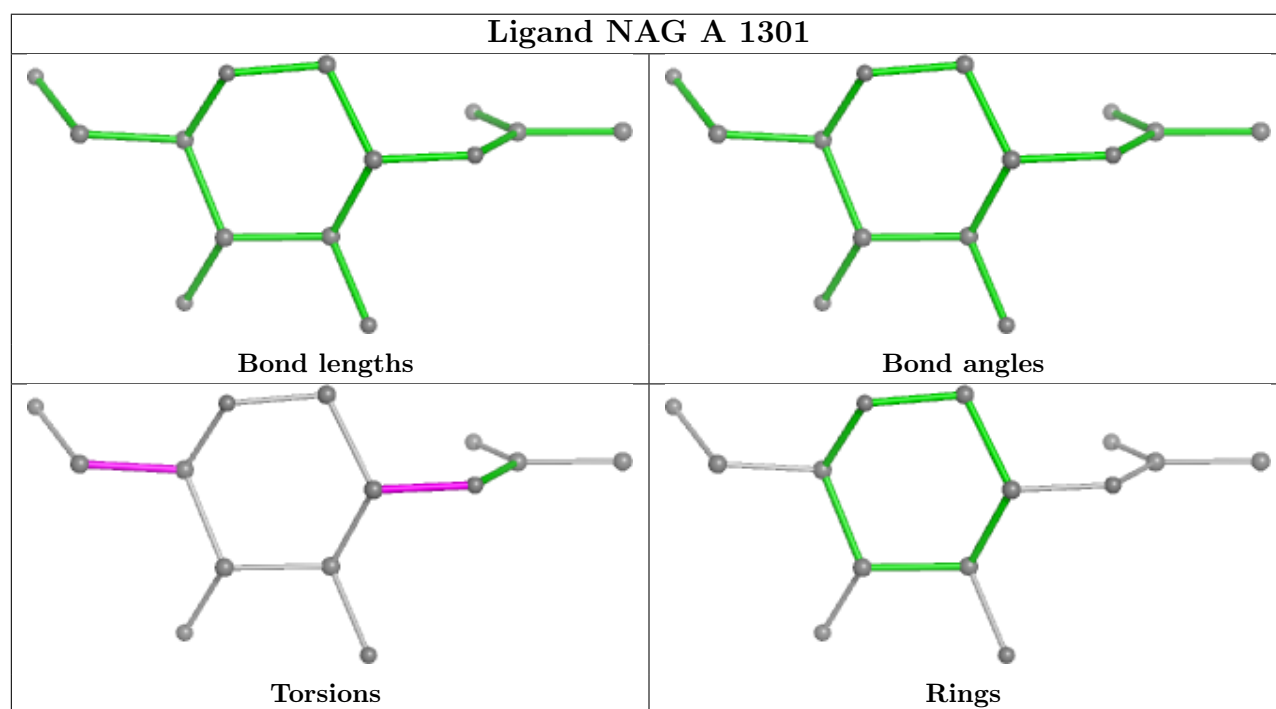
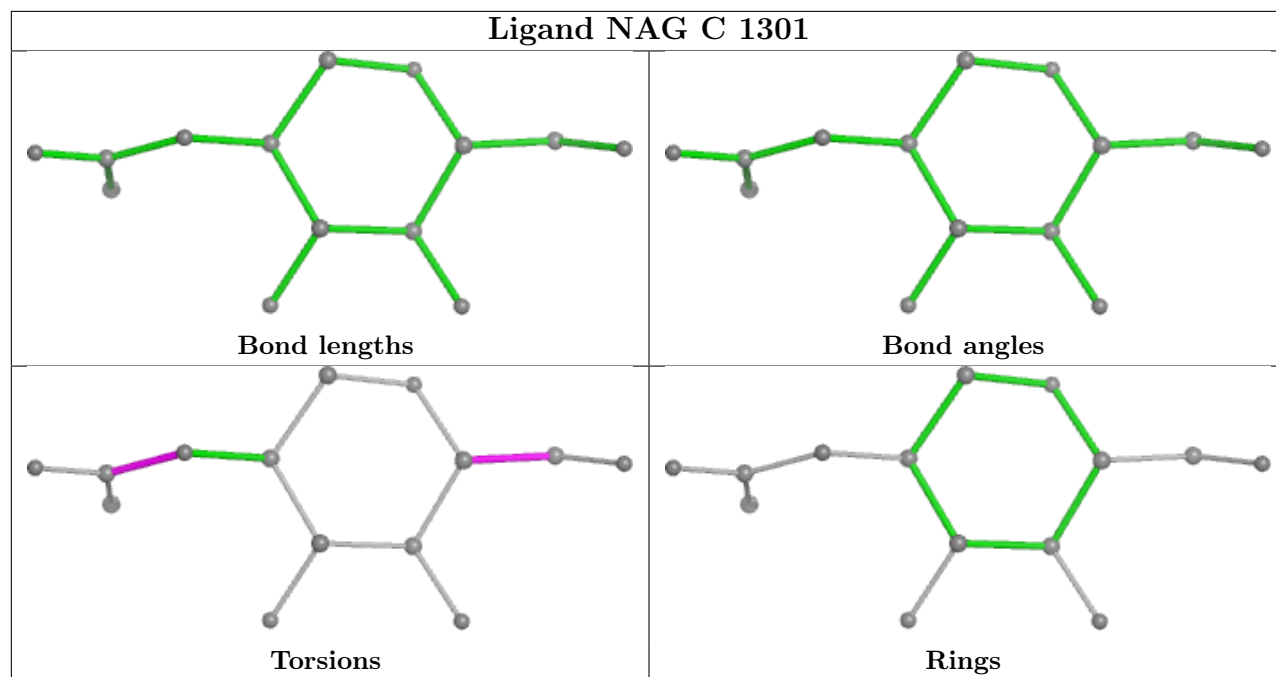
## Ligand NAG C 1304

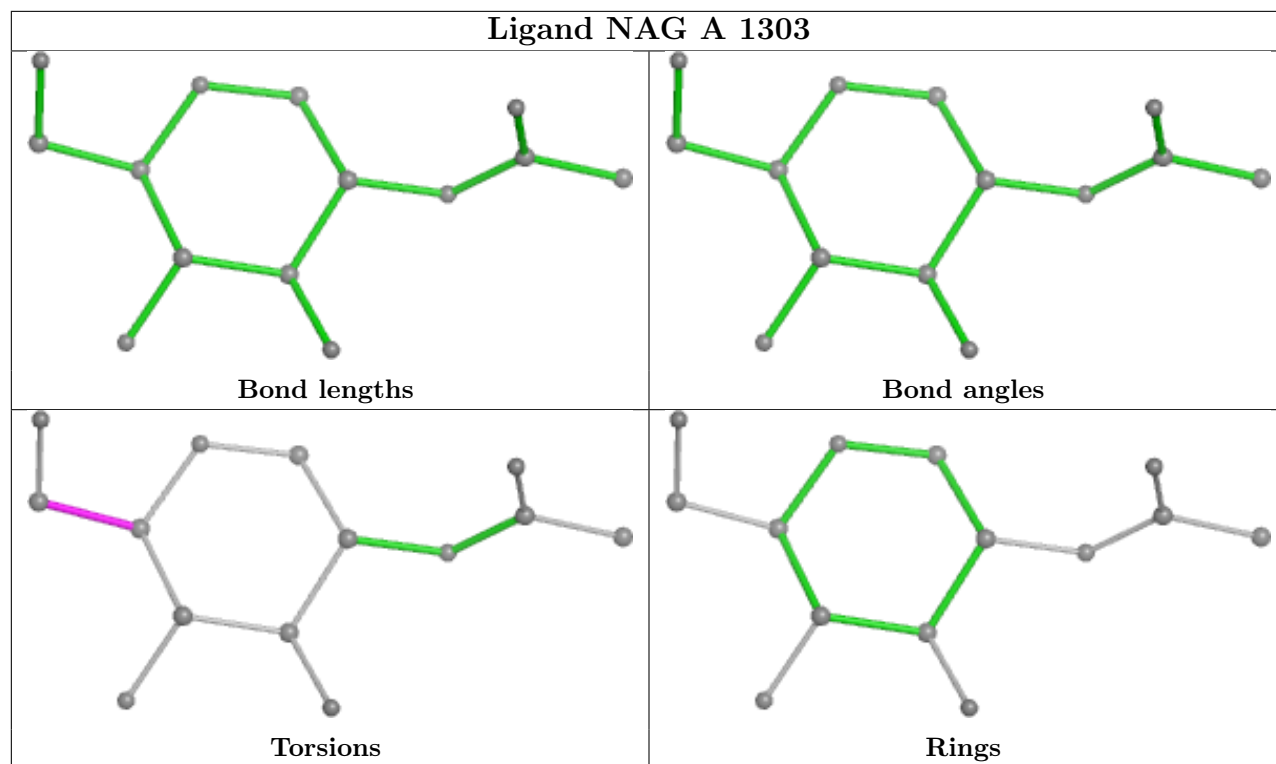


## Ligand NAG B 1301









## 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.

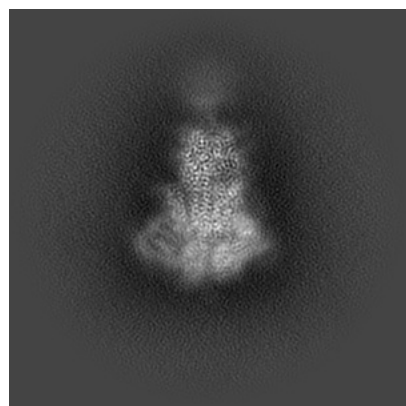
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34464. These allow visual inspection of the internal detail of the map and identification of artifacts.

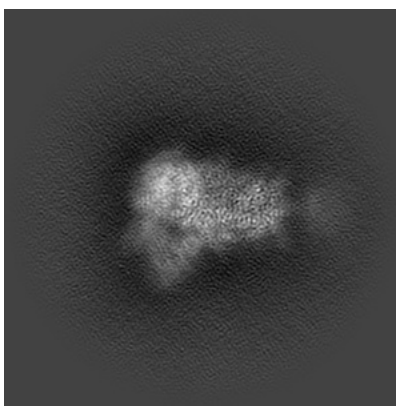
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

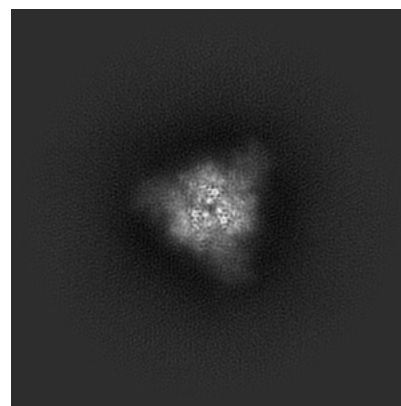
#### 6.1.1 Primary map



X

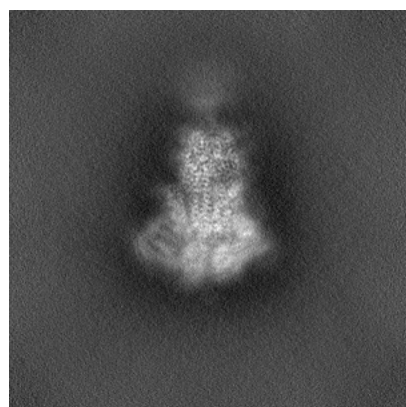


Y

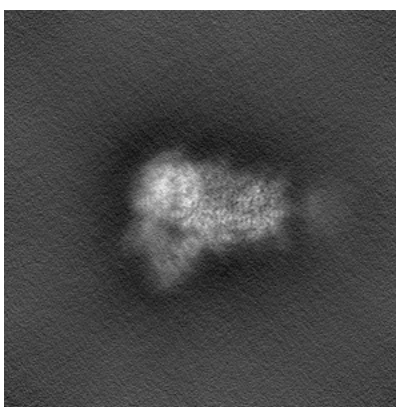


Z

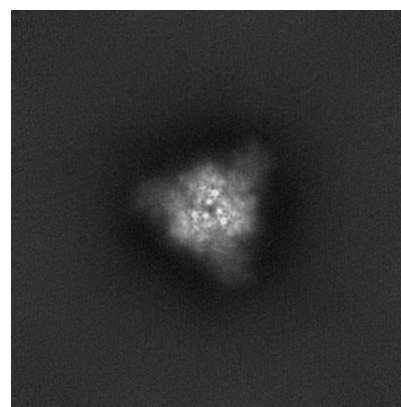
#### 6.1.2 Raw map



X



Y



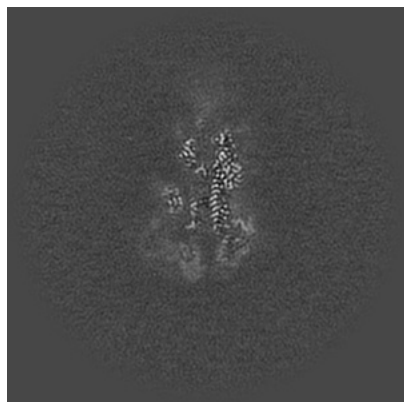
Z

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

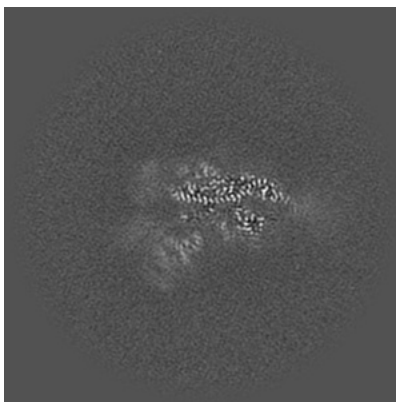


## 6.2 Central slices [i](#)

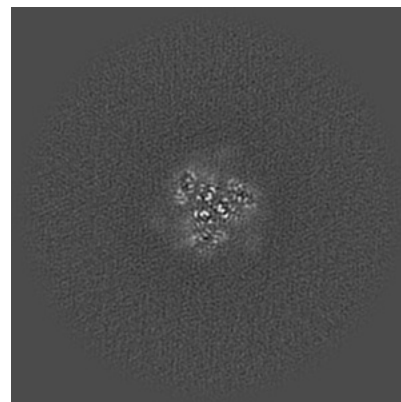
### 6.2.1 Primary map



X Index: 240

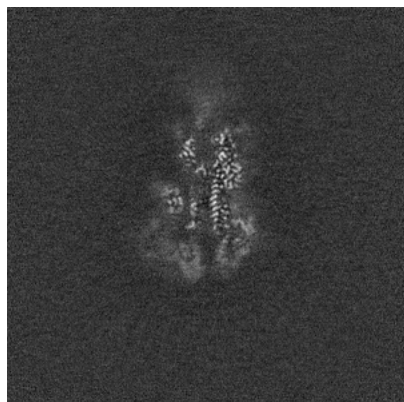


Y Index: 240

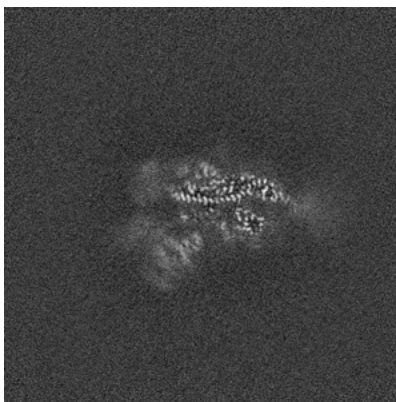


Z Index: 240

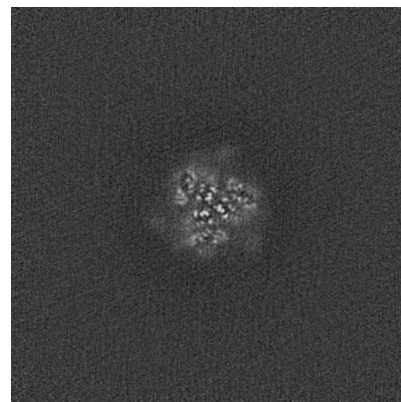
### 6.2.2 Raw map



X Index: 240



Y Index: 240

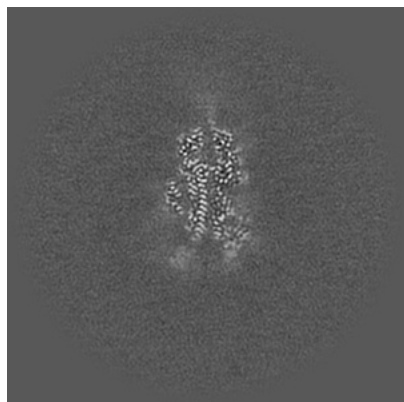


Z Index: 240

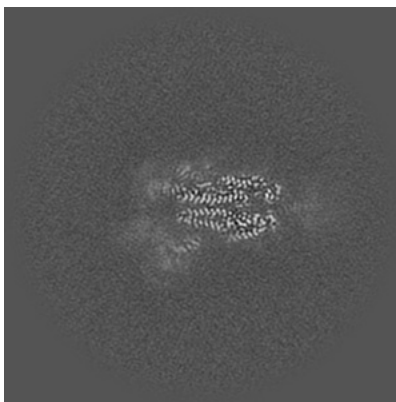
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

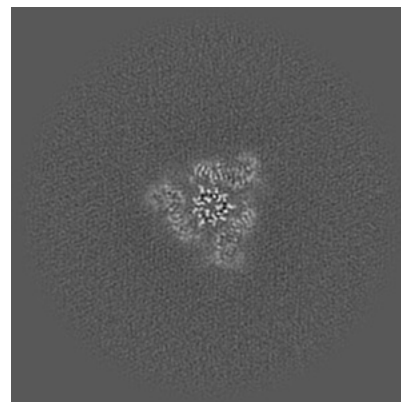
### 6.3.1 Primary map



X Index: 232

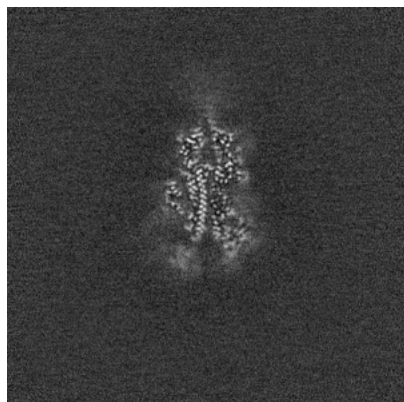


Y Index: 236

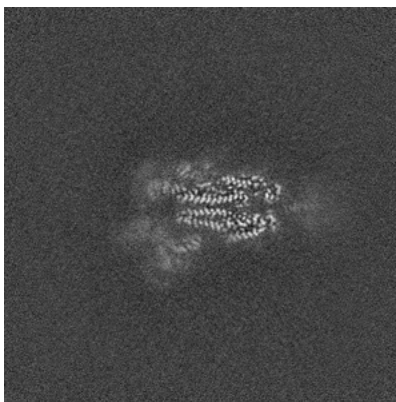


Z Index: 222

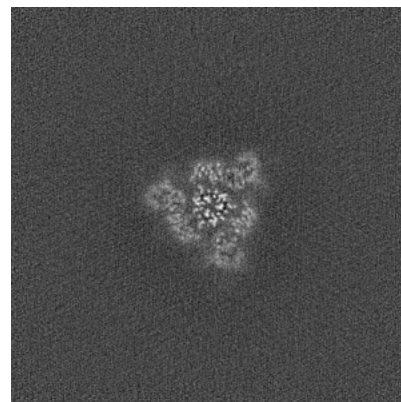
### 6.3.2 Raw map



X Index: 233



Y Index: 236

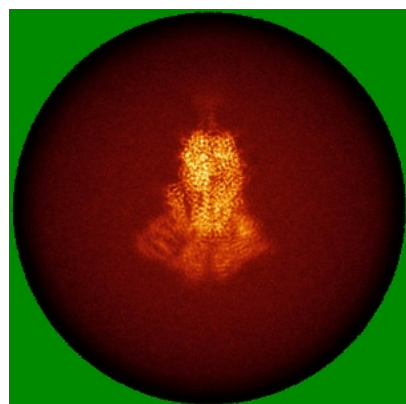


Z Index: 221

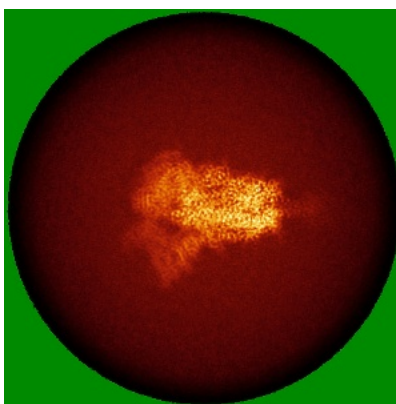
The images above show the largest variance slices of the map in three orthogonal directions.

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

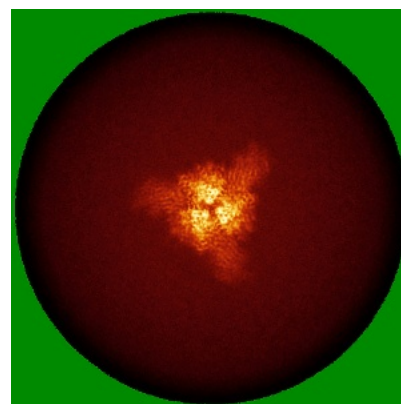
### 6.4.1 Primary map



X

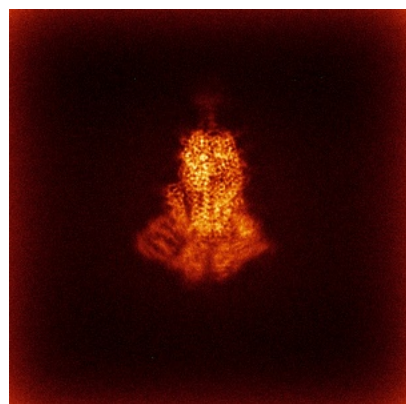


Y

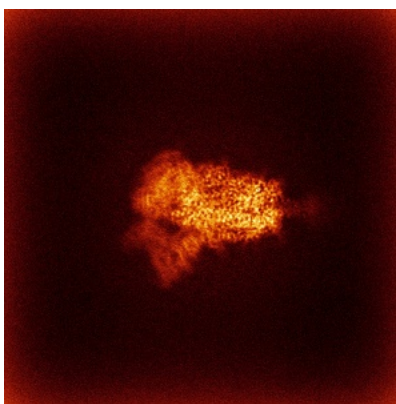


Z

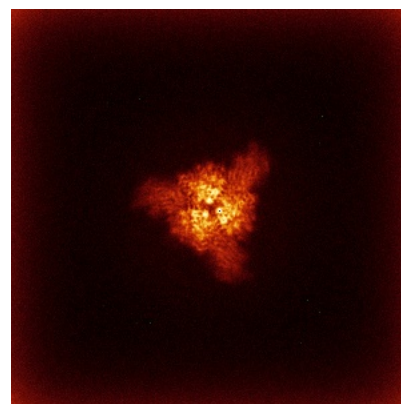
### 6.4.2 Raw map



X



Y

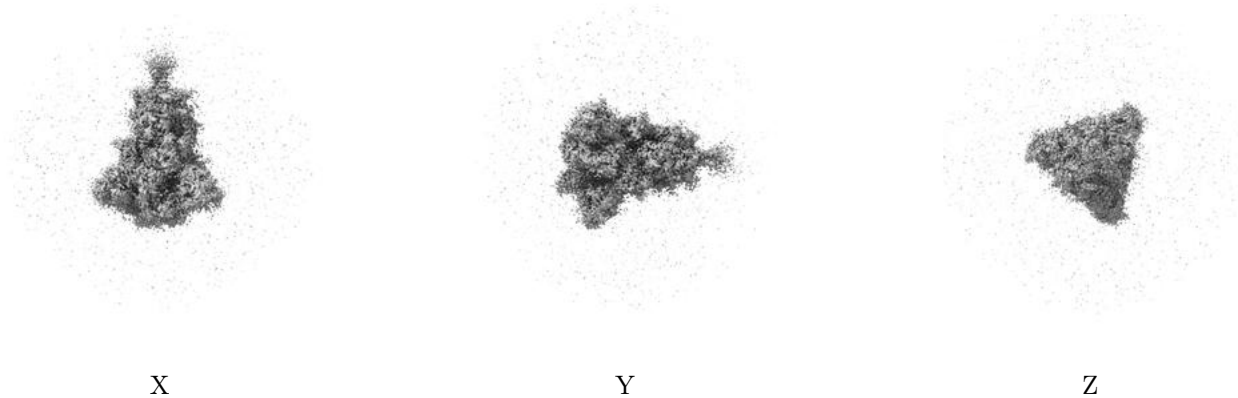


Z

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.

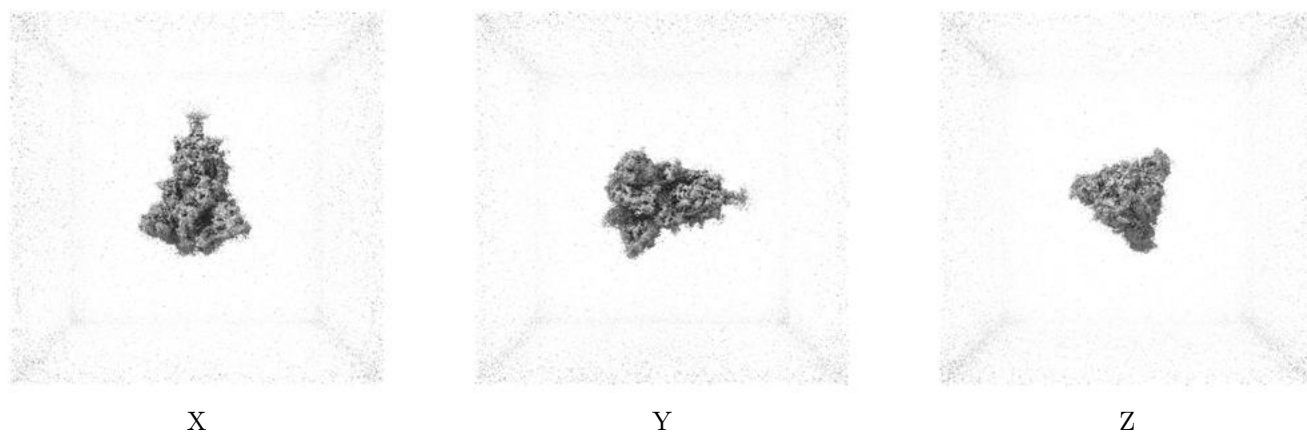
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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



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.

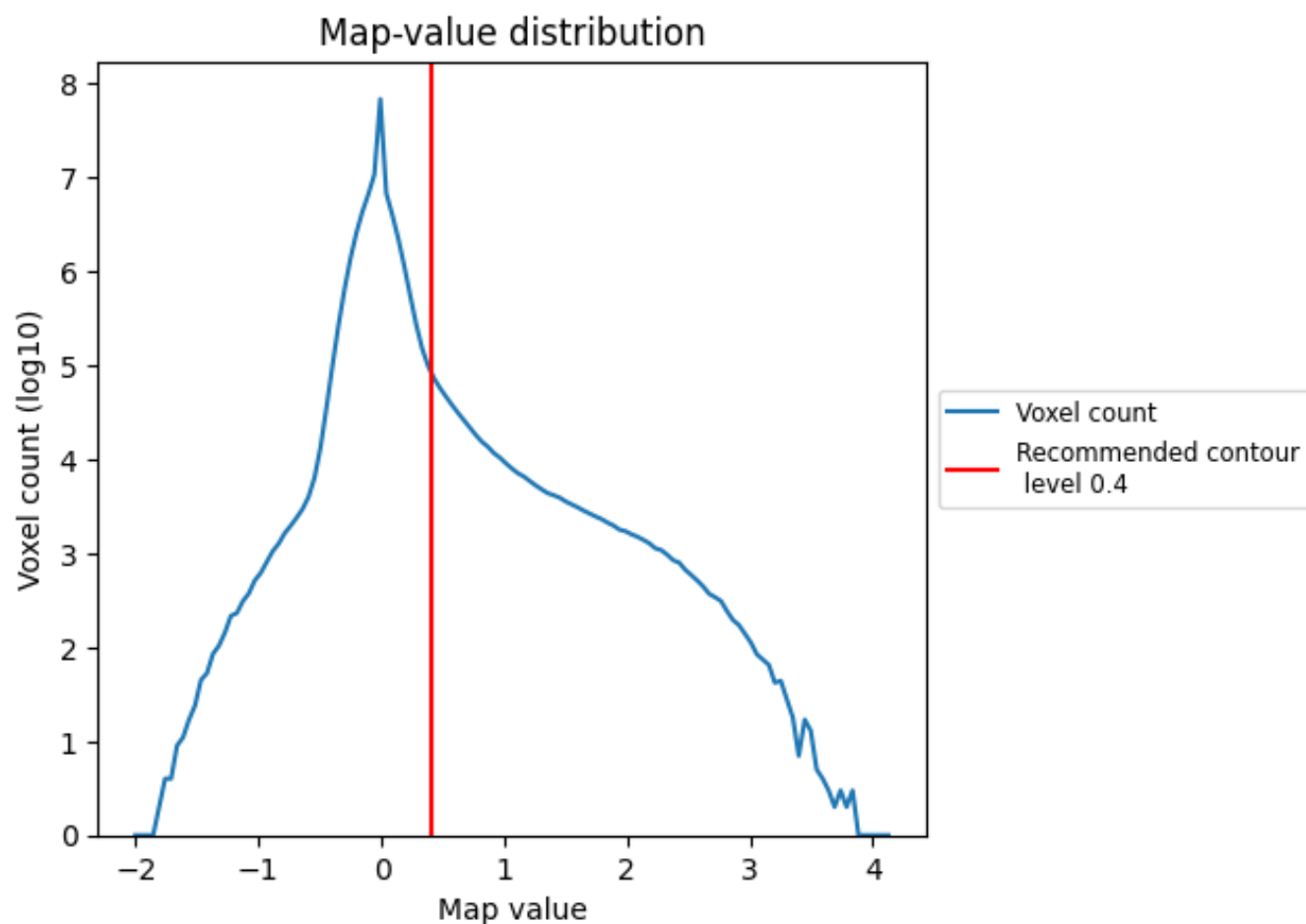
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

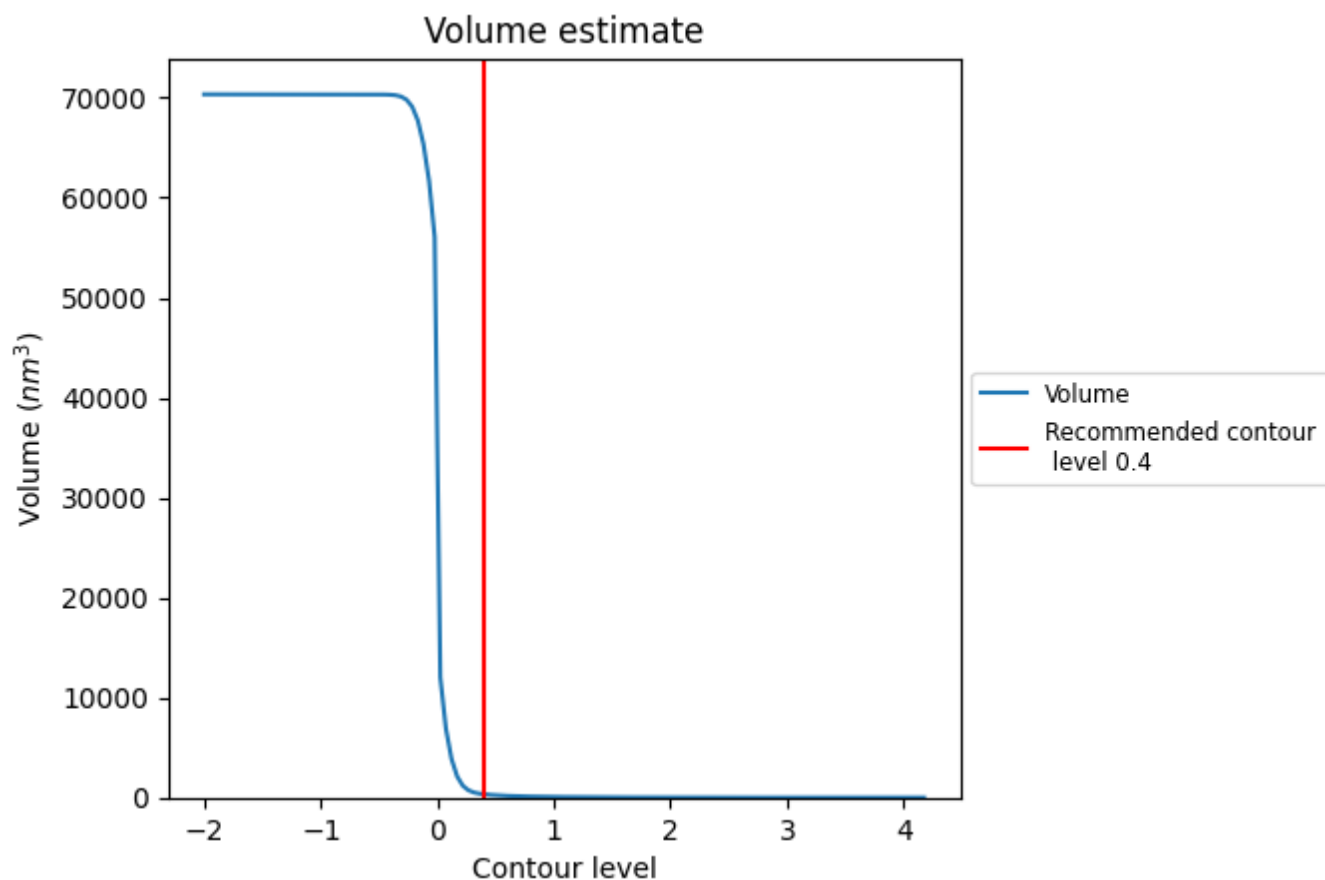
### 7.1 Map-value distribution [i](#)



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.



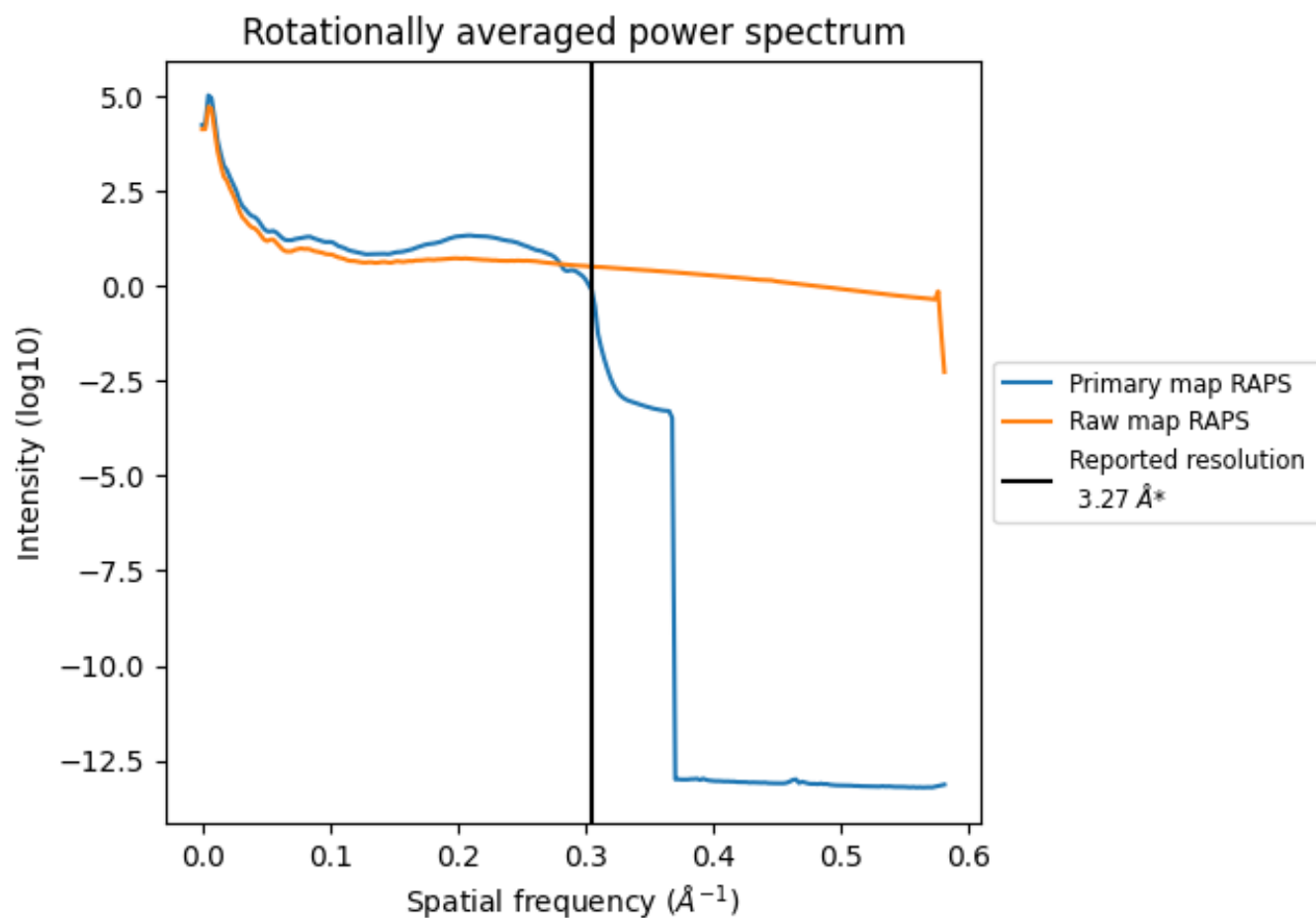
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm<sup>3</sup>; this corresponds to an approximate mass of 301 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

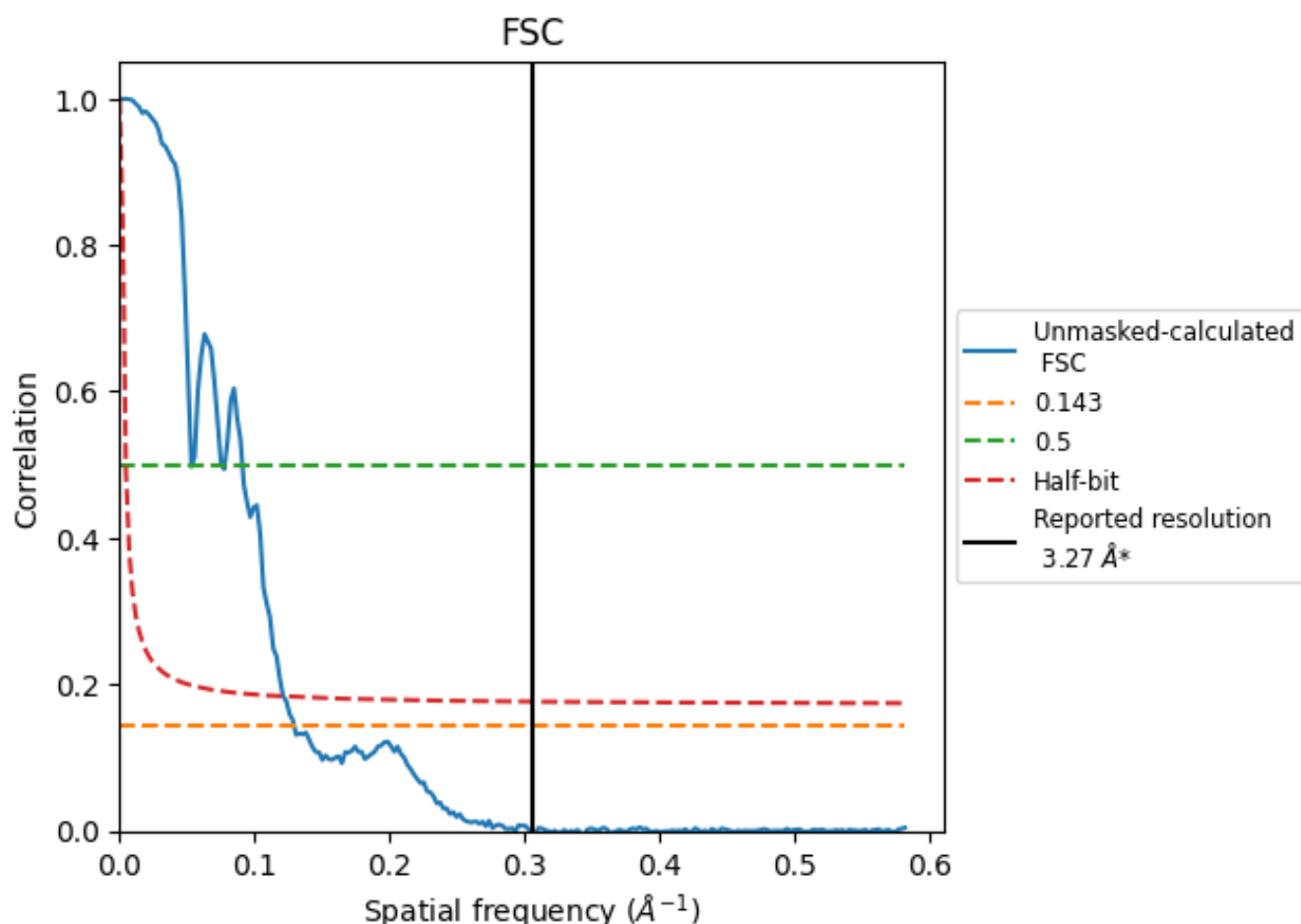


\*Reported resolution corresponds to spatial frequency of 0.306  $\text{\AA}^{-1}$

## 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 0.306 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

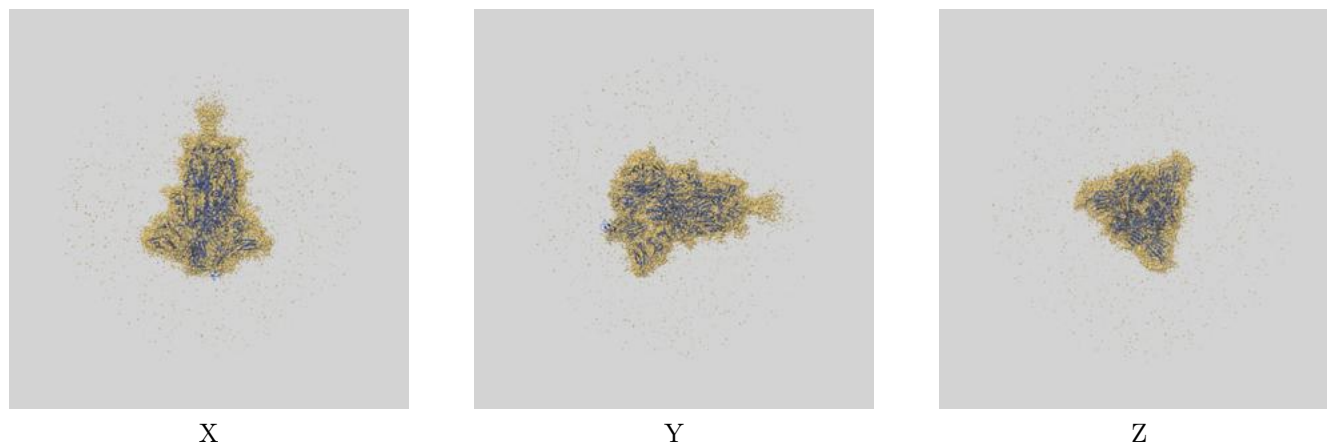
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.73	18.80	8.24

\*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 7.73 differs from the reported value 3.27 by more than 10 %

## 9 Map-model fit [i](#)

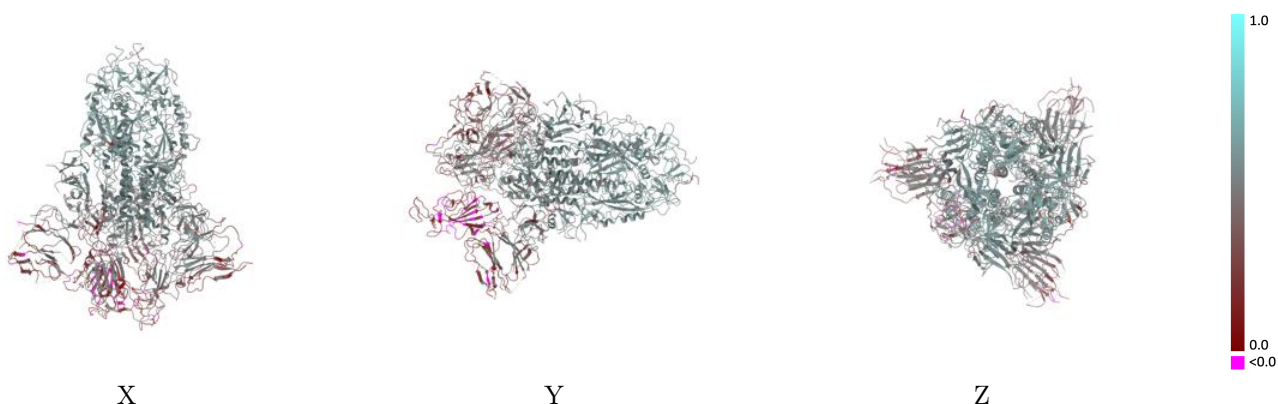
This section contains information regarding the fit between EMDB map EMD-34464 and PDB model 8H3D. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

### 9.1 Map-model overlay [i](#)



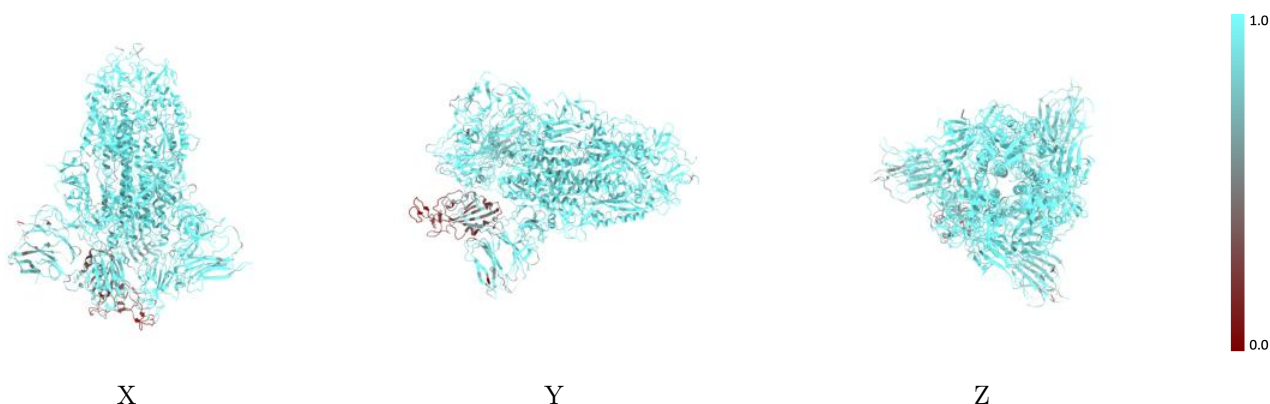
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



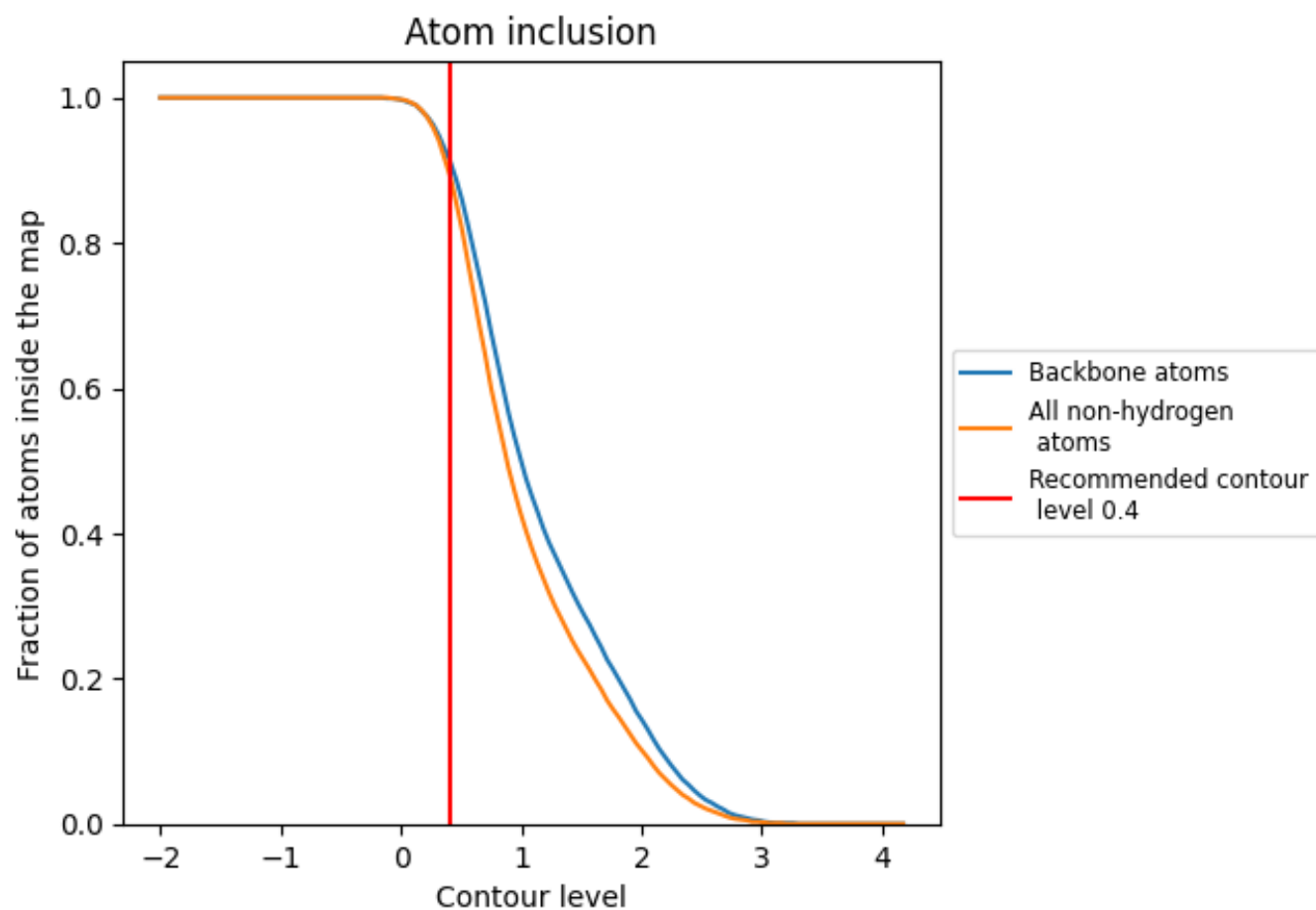
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8960	<div><div></div></div> 0.4480
A	<div><div></div></div> 0.8200	<div><div></div></div> 0.4150
B	<div><div></div></div> 0.9260	<div><div></div></div> 0.4640
C	<div><div></div></div> 0.9410	<div><div></div></div> 0.4650

