Full wwPDB EM Validation Report

Nov 21, 2022 – 01:33 PM EST

PDB ID	:	7SG4
EMDB ID	:	EMD-25105
Title	:	Structure of SARS-CoV S protein in complex with Receptor Binding Domain antibody DH1047
Authors	:	Gobeil, S.; Acharya, P.
Deposited on	:	2021-10-04
Resolution	:	3.43 Å(reported)

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

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

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

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

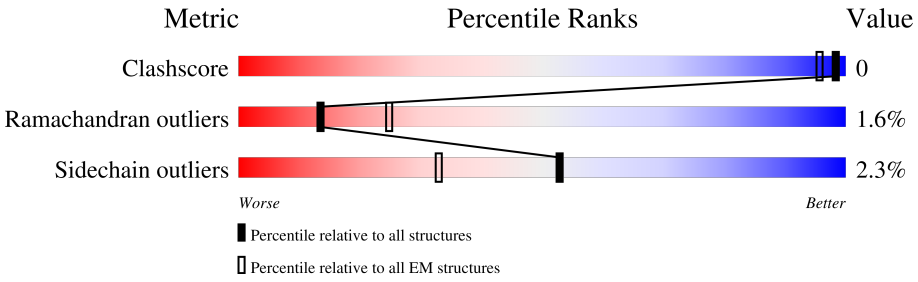
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.43 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	1270	6% 81% 5% · 14%
1	B	1270	11% 81% · 14%
1	C	1270	9% 82% · · 14%
2	H	232	29% 97% ·
3	L	220	25% 95% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0
			8525	5442	1410	1627	46		
1	B	1095	Total	C	N	O	S	0	0
			8525	5442	1410	1627	46		
1	C	1095	Total	C	N	O	S	0	0
			8525	5442	1410	1627	46		

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	968	PRO	LYS	engineered mutation	UNP P59594
A	969	PRO	VAL	engineered mutation	UNP P59594
A	1191	GLY	-	expression tag	UNP P59594
A	1192	SER	-	expression tag	UNP P59594
A	1193	GLY	-	expression tag	UNP P59594
A	1194	TYR	-	expression tag	UNP P59594
A	1195	ILE	-	expression tag	UNP P59594
A	1196	PRO	-	expression tag	UNP P59594
A	1197	GLU	-	expression tag	UNP P59594
A	1198	ALA	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	ARG	-	expression tag	UNP P59594
A	1201	ASP	-	expression tag	UNP P59594
A	1202	GLY	-	expression tag	UNP P59594
A	1203	GLN	-	expression tag	UNP P59594
A	1204	ALA	-	expression tag	UNP P59594
A	1205	TYR	-	expression tag	UNP P59594
A	1206	VAL	-	expression tag	UNP P59594
A	1207	ARG	-	expression tag	UNP P59594
A	1208	LYS	-	expression tag	UNP P59594
A	1209	ASP	-	expression tag	UNP P59594
A	1210	GLY	-	expression tag	UNP P59594
A	1211	GLU	-	expression tag	UNP P59594
A	1212	TRP	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1213	VAL	-	expression tag	UNP P59594
A	1214	LEU	-	expression tag	UNP P59594
A	1215	LEU	-	expression tag	UNP P59594
A	1216	SER	-	expression tag	UNP P59594
A	1217	THR	-	expression tag	UNP P59594
A	1218	PHE	-	expression tag	UNP P59594
A	1219	LEU	-	expression tag	UNP P59594
A	1220	GLY	-	expression tag	UNP P59594
A	1221	ARG	-	expression tag	UNP P59594
A	1222	SER	-	expression tag	UNP P59594
A	1223	LEU	-	expression tag	UNP P59594
A	1224	GLU	-	expression tag	UNP P59594
A	1225	VAL	-	expression tag	UNP P59594
A	1226	LEU	-	expression tag	UNP P59594
A	1227	PHE	-	expression tag	UNP P59594
A	1228	GLN	-	expression tag	UNP P59594
A	1229	GLY	-	expression tag	UNP P59594
A	1230	PRO	-	expression tag	UNP P59594
A	1231	GLY	-	expression tag	UNP P59594
A	1232	HIS	-	expression tag	UNP P59594
A	1233	HIS	-	expression tag	UNP P59594
A	1234	HIS	-	expression tag	UNP P59594
A	1235	HIS	-	expression tag	UNP P59594
A	1236	HIS	-	expression tag	UNP P59594
A	1237	HIS	-	expression tag	UNP P59594
A	1238	HIS	-	expression tag	UNP P59594
A	1239	HIS	-	expression tag	UNP P59594
A	1240	SER	-	expression tag	UNP P59594
A	1241	ALA	-	expression tag	UNP P59594
A	1242	TRP	-	expression tag	UNP P59594
A	1243	SER	-	expression tag	UNP P59594
A	1244	HIS	-	expression tag	UNP P59594
A	1245	PRO	-	expression tag	UNP P59594
A	1246	GLN	-	expression tag	UNP P59594
A	1247	PHE	-	expression tag	UNP P59594
A	1248	GLU	-	expression tag	UNP P59594
A	1249	LYS	-	expression tag	UNP P59594
A	1250	GLY	-	expression tag	UNP P59594
A	1251	GLY	-	expression tag	UNP P59594
A	1252	GLY	-	expression tag	UNP P59594
A	1253	SER	-	expression tag	UNP P59594
A	1254	GLY	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	GLY	-	expression tag	UNP P59594
A	1256	GLY	-	expression tag	UNP P59594
A	1257	GLY	-	expression tag	UNP P59594
A	1258	SER	-	expression tag	UNP P59594
A	1259	GLY	-	expression tag	UNP P59594
A	1260	GLY	-	expression tag	UNP P59594
A	1261	SER	-	expression tag	UNP P59594
A	1262	ALA	-	expression tag	UNP P59594
A	1263	TRP	-	expression tag	UNP P59594
A	1264	SER	-	expression tag	UNP P59594
A	1265	HIS	-	expression tag	UNP P59594
A	1266	PRO	-	expression tag	UNP P59594
A	1267	GLN	-	expression tag	UNP P59594
A	1268	PHE	-	expression tag	UNP P59594
A	1269	GLU	-	expression tag	UNP P59594
A	1270	LYS	-	expression tag	UNP P59594
B	968	PRO	LYS	engineered mutation	UNP P59594
B	969	PRO	VAL	engineered mutation	UNP P59594
B	1191	GLY	-	expression tag	UNP P59594
B	1192	SER	-	expression tag	UNP P59594
B	1193	GLY	-	expression tag	UNP P59594
B	1194	TYR	-	expression tag	UNP P59594
B	1195	ILE	-	expression tag	UNP P59594
B	1196	PRO	-	expression tag	UNP P59594
B	1197	GLU	-	expression tag	UNP P59594
B	1198	ALA	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	ARG	-	expression tag	UNP P59594
B	1201	ASP	-	expression tag	UNP P59594
B	1202	GLY	-	expression tag	UNP P59594
B	1203	GLN	-	expression tag	UNP P59594
B	1204	ALA	-	expression tag	UNP P59594
B	1205	TYR	-	expression tag	UNP P59594
B	1206	VAL	-	expression tag	UNP P59594
B	1207	ARG	-	expression tag	UNP P59594
B	1208	LYS	-	expression tag	UNP P59594
B	1209	ASP	-	expression tag	UNP P59594
B	1210	GLY	-	expression tag	UNP P59594
B	1211	GLU	-	expression tag	UNP P59594
B	1212	TRP	-	expression tag	UNP P59594
B	1213	VAL	-	expression tag	UNP P59594
B	1214	LEU	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1215	LEU	-	expression tag	UNP P59594
B	1216	SER	-	expression tag	UNP P59594
B	1217	THR	-	expression tag	UNP P59594
B	1218	PHE	-	expression tag	UNP P59594
B	1219	LEU	-	expression tag	UNP P59594
B	1220	GLY	-	expression tag	UNP P59594
B	1221	ARG	-	expression tag	UNP P59594
B	1222	SER	-	expression tag	UNP P59594
B	1223	LEU	-	expression tag	UNP P59594
B	1224	GLU	-	expression tag	UNP P59594
B	1225	VAL	-	expression tag	UNP P59594
B	1226	LEU	-	expression tag	UNP P59594
B	1227	PHE	-	expression tag	UNP P59594
B	1228	GLN	-	expression tag	UNP P59594
B	1229	GLY	-	expression tag	UNP P59594
B	1230	PRO	-	expression tag	UNP P59594
B	1231	GLY	-	expression tag	UNP P59594
B	1232	HIS	-	expression tag	UNP P59594
B	1233	HIS	-	expression tag	UNP P59594
B	1234	HIS	-	expression tag	UNP P59594
B	1235	HIS	-	expression tag	UNP P59594
B	1236	HIS	-	expression tag	UNP P59594
B	1237	HIS	-	expression tag	UNP P59594
B	1238	HIS	-	expression tag	UNP P59594
B	1239	HIS	-	expression tag	UNP P59594
B	1240	SER	-	expression tag	UNP P59594
B	1241	ALA	-	expression tag	UNP P59594
B	1242	TRP	-	expression tag	UNP P59594
B	1243	SER	-	expression tag	UNP P59594
B	1244	HIS	-	expression tag	UNP P59594
B	1245	PRO	-	expression tag	UNP P59594
B	1246	GLN	-	expression tag	UNP P59594
B	1247	PHE	-	expression tag	UNP P59594
B	1248	GLU	-	expression tag	UNP P59594
B	1249	LYS	-	expression tag	UNP P59594
B	1250	GLY	-	expression tag	UNP P59594
B	1251	GLY	-	expression tag	UNP P59594
B	1252	GLY	-	expression tag	UNP P59594
B	1253	SER	-	expression tag	UNP P59594
B	1254	GLY	-	expression tag	UNP P59594
B	1255	GLY	-	expression tag	UNP P59594
B	1256	GLY	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1257	GLY	-	expression tag	UNP P59594
B	1258	SER	-	expression tag	UNP P59594
B	1259	GLY	-	expression tag	UNP P59594
B	1260	GLY	-	expression tag	UNP P59594
B	1261	SER	-	expression tag	UNP P59594
B	1262	ALA	-	expression tag	UNP P59594
B	1263	TRP	-	expression tag	UNP P59594
B	1264	SER	-	expression tag	UNP P59594
B	1265	HIS	-	expression tag	UNP P59594
B	1266	PRO	-	expression tag	UNP P59594
B	1267	GLN	-	expression tag	UNP P59594
B	1268	PHE	-	expression tag	UNP P59594
B	1269	GLU	-	expression tag	UNP P59594
B	1270	LYS	-	expression tag	UNP P59594
C	968	PRO	LYS	engineered mutation	UNP P59594
C	969	PRO	VAL	engineered mutation	UNP P59594
C	1191	GLY	-	expression tag	UNP P59594
C	1192	SER	-	expression tag	UNP P59594
C	1193	GLY	-	expression tag	UNP P59594
C	1194	TYR	-	expression tag	UNP P59594
C	1195	ILE	-	expression tag	UNP P59594
C	1196	PRO	-	expression tag	UNP P59594
C	1197	GLU	-	expression tag	UNP P59594
C	1198	ALA	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	ARG	-	expression tag	UNP P59594
C	1201	ASP	-	expression tag	UNP P59594
C	1202	GLY	-	expression tag	UNP P59594
C	1203	GLN	-	expression tag	UNP P59594
C	1204	ALA	-	expression tag	UNP P59594
C	1205	TYR	-	expression tag	UNP P59594
C	1206	VAL	-	expression tag	UNP P59594
C	1207	ARG	-	expression tag	UNP P59594
C	1208	LYS	-	expression tag	UNP P59594
C	1209	ASP	-	expression tag	UNP P59594
C	1210	GLY	-	expression tag	UNP P59594
C	1211	GLU	-	expression tag	UNP P59594
C	1212	TRP	-	expression tag	UNP P59594
C	1213	VAL	-	expression tag	UNP P59594
C	1214	LEU	-	expression tag	UNP P59594
C	1215	LEU	-	expression tag	UNP P59594
C	1216	SER	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	THR	-	expression tag	UNP P59594
C	1218	PHE	-	expression tag	UNP P59594
C	1219	LEU	-	expression tag	UNP P59594
C	1220	GLY	-	expression tag	UNP P59594
C	1221	ARG	-	expression tag	UNP P59594
C	1222	SER	-	expression tag	UNP P59594
C	1223	LEU	-	expression tag	UNP P59594
C	1224	GLU	-	expression tag	UNP P59594
C	1225	VAL	-	expression tag	UNP P59594
C	1226	LEU	-	expression tag	UNP P59594
C	1227	PHE	-	expression tag	UNP P59594
C	1228	GLN	-	expression tag	UNP P59594
C	1229	GLY	-	expression tag	UNP P59594
C	1230	PRO	-	expression tag	UNP P59594
C	1231	GLY	-	expression tag	UNP P59594
C	1232	HIS	-	expression tag	UNP P59594
C	1233	HIS	-	expression tag	UNP P59594
C	1234	HIS	-	expression tag	UNP P59594
C	1235	HIS	-	expression tag	UNP P59594
C	1236	HIS	-	expression tag	UNP P59594
C	1237	HIS	-	expression tag	UNP P59594
C	1238	HIS	-	expression tag	UNP P59594
C	1239	HIS	-	expression tag	UNP P59594
C	1240	SER	-	expression tag	UNP P59594
C	1241	ALA	-	expression tag	UNP P59594
C	1242	TRP	-	expression tag	UNP P59594
C	1243	SER	-	expression tag	UNP P59594
C	1244	HIS	-	expression tag	UNP P59594
C	1245	PRO	-	expression tag	UNP P59594
C	1246	GLN	-	expression tag	UNP P59594
C	1247	PHE	-	expression tag	UNP P59594
C	1248	GLU	-	expression tag	UNP P59594
C	1249	LYS	-	expression tag	UNP P59594
C	1250	GLY	-	expression tag	UNP P59594
C	1251	GLY	-	expression tag	UNP P59594
C	1252	GLY	-	expression tag	UNP P59594
C	1253	SER	-	expression tag	UNP P59594
C	1254	GLY	-	expression tag	UNP P59594
C	1255	GLY	-	expression tag	UNP P59594
C	1256	GLY	-	expression tag	UNP P59594
C	1257	GLY	-	expression tag	UNP P59594
C	1258	SER	-	expression tag	UNP P59594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P59594
C	1260	GLY	-	expression tag	UNP P59594
C	1261	SER	-	expression tag	UNP P59594
C	1262	ALA	-	expression tag	UNP P59594
C	1263	TRP	-	expression tag	UNP P59594
C	1264	SER	-	expression tag	UNP P59594
C	1265	HIS	-	expression tag	UNP P59594
C	1266	PRO	-	expression tag	UNP P59594
C	1267	GLN	-	expression tag	UNP P59594
C	1268	PHE	-	expression tag	UNP P59594
C	1269	GLU	-	expression tag	UNP P59594
C	1270	LYS	-	expression tag	UNP P59594

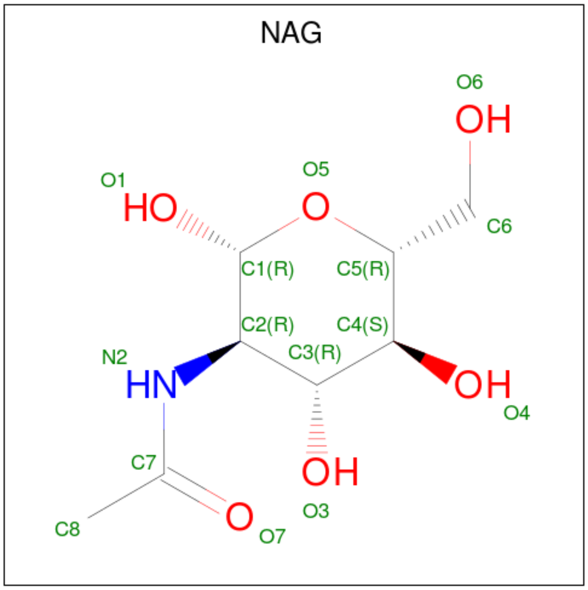
- Molecule 2 is a protein called DH1047 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	232	Total	C	N	O	S	0	0
			1239	755	236	242	6		

- Molecule 3 is a protein called DH1047 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	220	Total	C	N	O	S	0	0
			1237	753	230	249	5		

- 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
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 224 128 16 80	0
4	A	1	Total C N O 224 128 16 80	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	B	1	Total C N O 210 120 15 75	0
4	C	1	Total C N O 224 128 16 80	0
4	C	1	Total C N O 224 128 16 80	0
4	C	1	Total C N O 224 128 16 80	0
4	C	1	Total C N O 224 128 16 80	0

Continued on next page...

Continued from previous page...

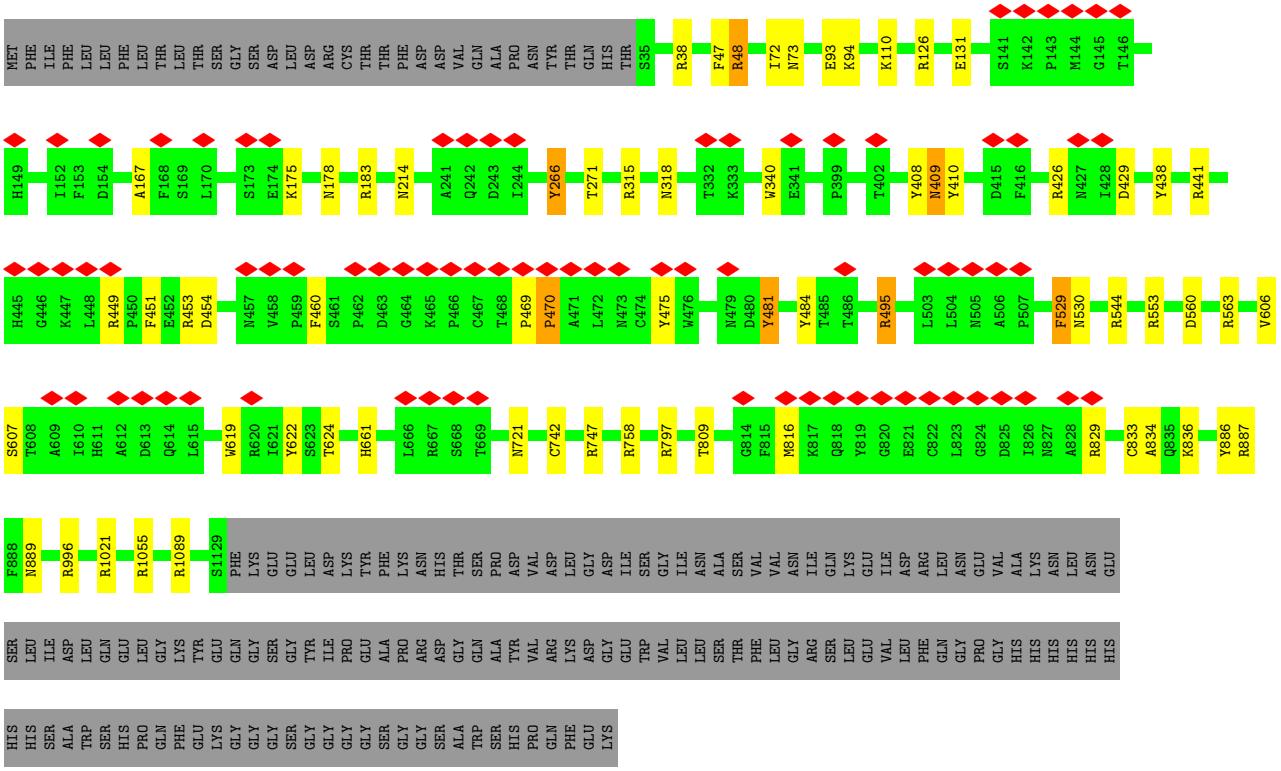
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	0
4	C	1	Total 224	C 128	N 16	O 80	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.

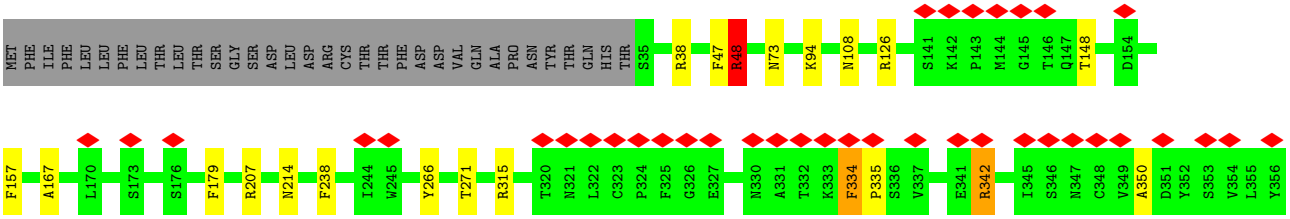
• Molecule 1: Spike glycoprotein

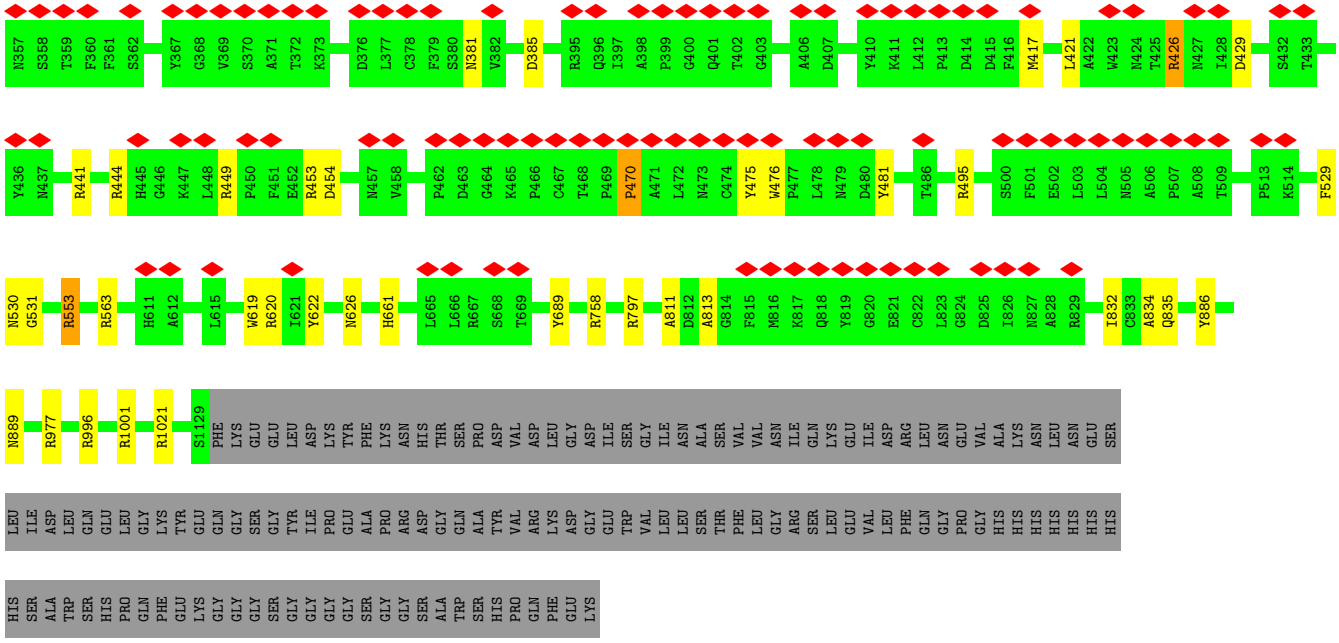
Chain A:



• Molecule 1: Spike glycoprotein

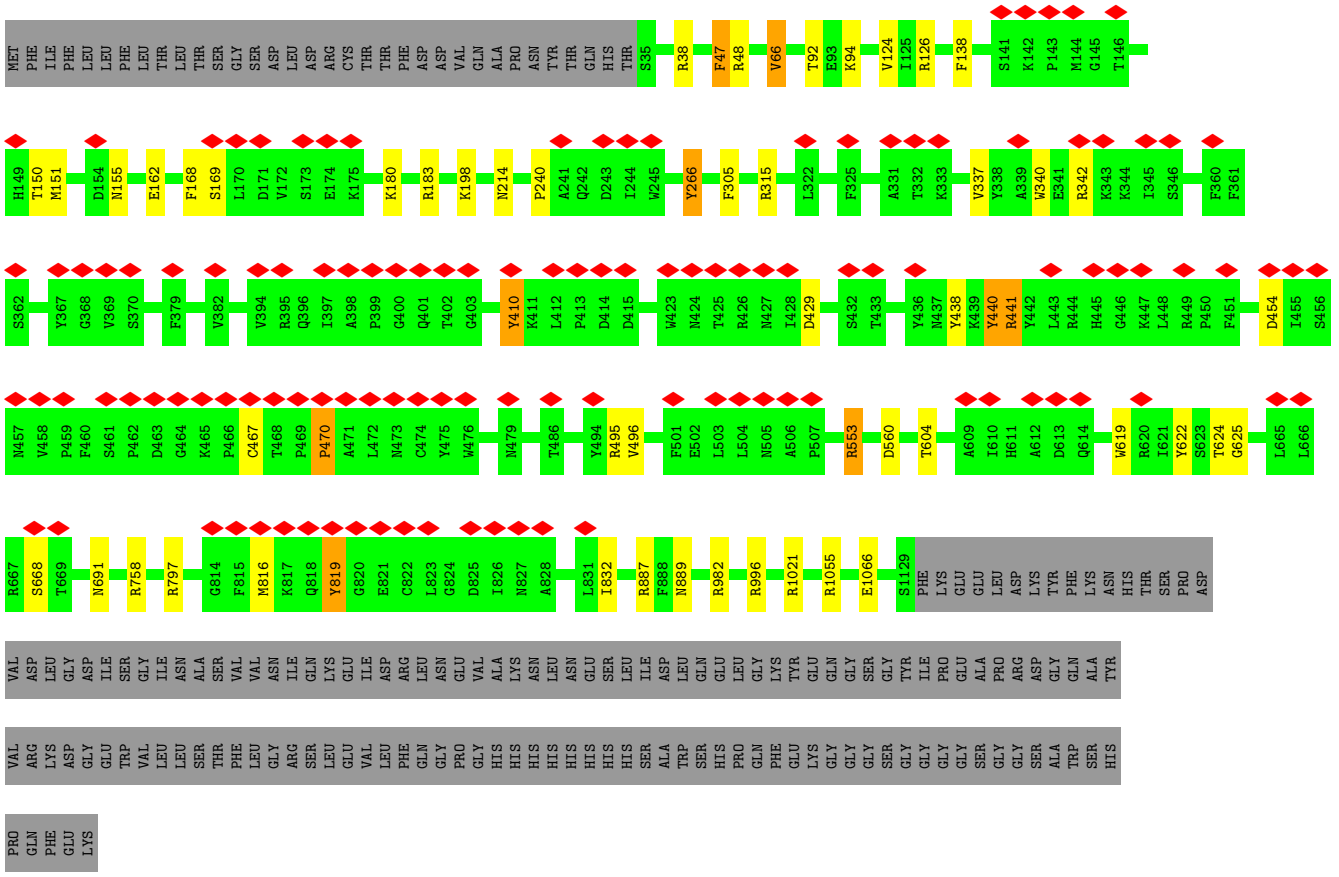
Chain B:





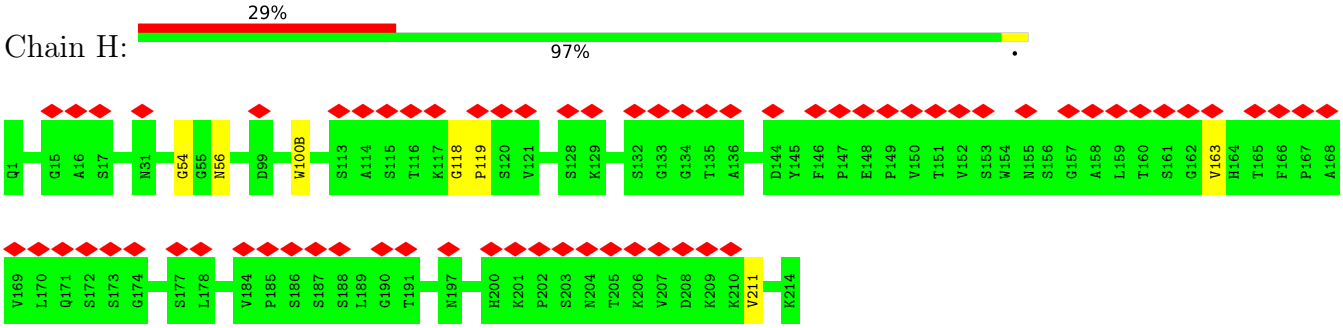
• Molecule 1: Spike glycoprotein

Chain C:



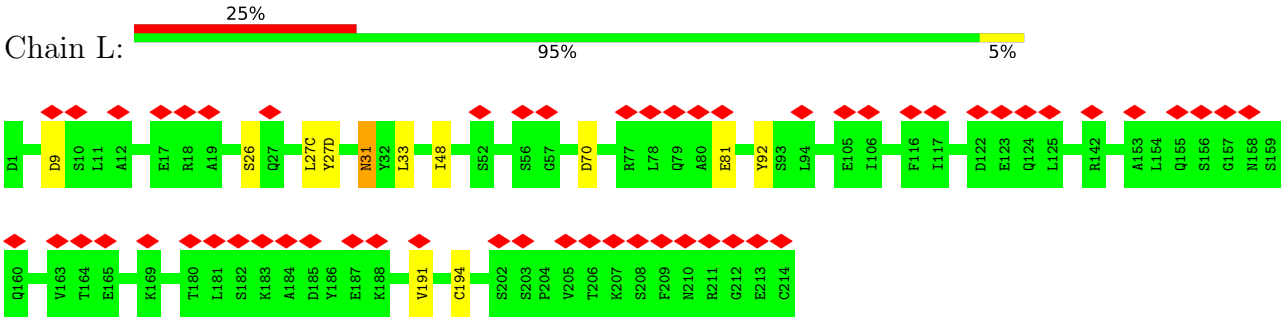
• Molecule 2: DH1047 Heavy chain

Chain H:



• Molecule 3: DH1047 light chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284619	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 ($e^-/Å^2$)	54.1	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	3.577	Depositor
Minimum map value	-0.895	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/8730	1.00	23/11886 (0.2%)
1	B	0.67	0/8730	0.99	22/11886 (0.2%)
1	C	0.67	0/8730	1.00	21/11886 (0.2%)
2	H	0.53	0/1256	0.94	0/1746
3	L	0.54	0/1253	0.97	0/1742
All	All	0.66	0/28699	0.99	66/39146 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	5
1	C	0	6
3	L	0	2
All	All	0	20

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	VAL	CA-CB-CG1	14.25	132.27	110.90
1	A	38	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	48	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	A	470	PRO	N-CA-C	8.37	133.86	112.10
1	A	126	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	996	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	449	ARG	NE-CZ-NH1	8.10	124.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	470	PRO	N-CA-C	7.89	132.61	112.10
1	A	48	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	495	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	470	PRO	N-CA-C	7.75	132.25	112.10
1	B	996	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	544	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	C	126	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	996	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	1021	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	758	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	797	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	126	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	495	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	829	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	797	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	C	887	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	441	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	38	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	315	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	342	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	342	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	553	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	797	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	38	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	481	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	A	495	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	758	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	441	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	48	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	426	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	438	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	1089	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	620	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	758	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	553	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	207	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	183	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	1001	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	747	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	1055	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	426	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	453	ARG	NE-CZ-NH1	5.39	122.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	977	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	887	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	1021	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	315	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	982	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	563	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	440	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	1055	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	449	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	183	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	444	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	1021	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	438	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	B	315	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	38	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	1021	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	563	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	TYR	Sidechain
1	A	408	TYR	Sidechain
1	A	441	ARG	Sidechain
1	A	475	TYR	Sidechain
1	A	495	ARG	Sidechain
1	A	622	TYR	Sidechain
1	A	886	TYR	Sidechain
1	B	475	TYR	Sidechain
1	B	48	ARG	Sidechain
1	B	481	TYR	Sidechain
1	B	689	TYR	Sidechain
1	B	886	TYR	Sidechain
1	C	150	THR	Peptide
1	C	266	TYR	Sidechain
1	C	410	TYR	Sidechain
1	C	47	PHE	Sidechain
1	C	622	TYR	Sidechain
1	C	819	TYR	Sidechain
3	L	27(D)	TYR	Sidechain
3	L	92	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8525	0	8283	5	0
1	B	8525	0	8284	3	0
1	C	8525	0	8283	2	0
2	H	1239	0	723	1	0
3	L	1237	0	781	0	0
4	A	224	0	208	1	0
4	B	210	0	195	0	0
4	C	224	0	208	0	0
All	All	28709	0	26965	11	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 0.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:VAL:HG12	1:A:607:SER:H	1.73	0.52
1:B:47:PHE:CD1	1:B:266:TYR:CZ	2.98	0.52
1:C:47:PHE:CD1	1:C:266:TYR:CZ	3.02	0.47
1:C:124:VAL:HG22	1:C:151:MET:SD	2.54	0.47
1:A:47:PHE:CD1	1:A:266:TYR:CZ	3.04	0.46
1:A:131:GLU:HG3	4:A:1302:NAG:H82	1.96	0.46
2:H:118:GLY:H	2:H:119:PRO:CD	2.28	0.46
1:A:529:PHE:CG	1:A:530:ASN:N	2.87	0.43
1:B:529:PHE:CG	1:B:530:ASN:N	2.87	0.42
1:A:606:VAL:CG1	1:A:607:SER:H	2.33	0.42
1:B:334:PHE:HA	1:B:335:PRO:HD3	1.95	0.42

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	1093/1270 (86%)	986 (90%)	89 (8%)	18 (2%)	9 42
1	B	1093/1270 (86%)	975 (89%)	101 (9%)	17 (2%)	9 42
1	C	1093/1270 (86%)	977 (89%)	101 (9%)	15 (1%)	11 44
2	H	230/232 (99%)	193 (84%)	34 (15%)	3 (1%)	12 46
3	L	218/220 (99%)	182 (84%)	30 (14%)	6 (3%)	5 31
All	All	3727/4262 (87%)	3313 (89%)	355 (10%)	59 (2%)	13 42

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ALA
1	A	470	PRO
1	B	470	PRO
1	B	832	ILE
1	C	470	PRO
1	C	832	ILE
2	H	211	VAL
3	L	31	ASN
1	A	453	ARG
1	A	836	LYS
1	B	73	ASN
1	B	108	ASN
1	B	811	ALA
1	C	340	TRP
1	C	691	ASN
3	L	26	SER
1	A	73	ASN
1	A	94	LYS
1	A	410	TYR
1	A	454	ASP
1	A	833	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	834	ALA
1	B	167	ALA
1	B	238	PHE
1	B	622	TYR
1	C	138	PHE
1	C	467	CYS
1	C	1066	GLU
2	H	163	VAL
3	L	48	ILE
3	L	191	VAL
1	A	110	LYS
1	A	340	TRP
1	A	529	PHE
1	A	624	THR
1	B	157	PHE
1	B	350	ALA
1	B	417	MET
1	B	454	ASP
1	B	834	ALA
1	C	94	LYS
1	C	168	PHE
1	C	410	TYR
1	C	668	SER
2	H	54	GLY
3	L	9	ASP
3	L	81	GLU
1	A	409	ASN
1	A	469	PRO
1	B	148	THR
1	B	179	PHE
1	C	180	LYS
1	C	454	ASP
1	A	451	PHE
1	B	813	ALA
1	B	531	GLY
1	C	240	PRO
1	A	72	ILE
1	C	625	GLY

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	947/1095 (86%)	926 (98%)	21 (2%)	52 77
1	B	947/1095 (86%)	929 (98%)	18 (2%)	57 80
1	C	947/1095 (86%)	926 (98%)	21 (2%)	52 77
2	H	35/196 (18%)	33 (94%)	2 (6%)	20 53
3	L	54/195 (28%)	49 (91%)	5 (9%)	9 34
All	All	2930/3676 (80%)	2863 (98%)	67 (2%)	53 77

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	93	GLU
1	A	175	LYS
1	A	178	ASN
1	A	214	ASN
1	A	271	THR
1	A	318	ASN
1	A	409	ASN
1	A	429	ASP
1	A	460	PHE
1	A	481	TYR
1	A	484	TYR
1	A	553	ARG
1	A	560	ASP
1	A	619	TRP
1	A	661	HIS
1	A	721	ASN
1	A	742	CYS
1	A	809	THR
1	A	816	MET
1	A	889	ASN
1	B	48	ARG
1	B	94	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	214	ASN
1	B	271	THR
1	B	334	PHE
1	B	342	ARG
1	B	381	ASN
1	B	385	ASP
1	B	421	LEU
1	B	426	ARG
1	B	429	ASP
1	B	476	TRP
1	B	553	ARG
1	B	619	TRP
1	B	626	ASN
1	B	661	HIS
1	B	835	GLN
1	B	889	ASN
1	C	66	VAL
1	C	92	THR
1	C	155	ASN
1	C	162	GLU
1	C	169	SER
1	C	198	LYS
1	C	214	ASN
1	C	305	PHE
1	C	337	VAL
1	C	429	ASP
1	C	440	TYR
1	C	441	ARG
1	C	496	VAL
1	C	553	ARG
1	C	560	ASP
1	C	604	THR
1	C	619	TRP
1	C	624	THR
1	C	816	MET
1	C	819	TYR
1	C	889	ASN
2	H	56	ASN
2	H	100(B)	TRP
3	L	27(C)	LEU
3	L	31	ASN
3	L	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	70	ASP
3	L	194	CYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

47 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1304	1	14,14,15	0.96	0	17,19,21	1.06	1 (5%)
4	NAG	B	1306	1	14,14,15	1.02	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	B	1310	1	14,14,15	1.35	3 (21%)	17,19,21	0.78	0
4	NAG	A	1308	1	14,14,15	1.14	1 (7%)	17,19,21	0.74	0
4	NAG	C	1310	1	14,14,15	1.25	2 (14%)	17,19,21	0.79	0
4	NAG	C	1312	1	14,14,15	1.39	3 (21%)	17,19,21	1.21	2 (11%)
4	NAG	B	1311	1	14,14,15	1.31	3 (21%)	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1303	1	14,14,15	1.31	3 (21%)	17,19,21	0.99	1 (5%)
4	NAG	A	1301	1	14,14,15	1.15	1 (7%)	17,19,21	0.74	0
4	NAG	A	1304	1	14,14,15	1.00	0	17,19,21	0.90	0
4	NAG	B	1315	1	14,14,15	1.24	3 (21%)	17,19,21	0.89	1 (5%)
4	NAG	B	1309	1	14,14,15	1.18	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	A	1316	1	14,14,15	1.25	2 (14%)	17,19,21	1.68	1 (5%)
4	NAG	A	1309	1	14,14,15	1.26	2 (14%)	17,19,21	0.94	0
4	NAG	A	1310	1	14,14,15	1.26	3 (21%)	17,19,21	0.76	0
4	NAG	C	1302	1	14,14,15	1.23	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	A	1312	1	14,14,15	1.43	3 (21%)	17,19,21	1.24	1 (5%)
4	NAG	C	1307	1	14,14,15	1.17	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	B	1301	1	14,14,15	1.14	2 (14%)	17,19,21	0.84	0
4	NAG	C	1314	1	14,14,15	1.18	1 (7%)	17,19,21	0.76	0
4	NAG	C	1301	1	14,14,15	1.27	3 (21%)	17,19,21	0.80	0
4	NAG	A	1313	1	14,14,15	1.16	2 (14%)	17,19,21	0.74	0
4	NAG	B	1305	1	14,14,15	1.29	3 (21%)	17,19,21	0.73	1 (5%)
4	NAG	C	1306	1	14,14,15	1.17	1 (7%)	17,19,21	0.78	0
4	NAG	C	1305	1	14,14,15	1.21	2 (14%)	17,19,21	0.71	0
4	NAG	A	1303	1	14,14,15	1.12	1 (7%)	17,19,21	0.97	0
4	NAG	A	1311	1	14,14,15	1.27	3 (21%)	17,19,21	0.97	1 (5%)
4	NAG	A	1302	1	14,14,15	1.29	3 (21%)	17,19,21	1.17	2 (11%)
4	NAG	A	1307	1	14,14,15	1.14	1 (7%)	17,19,21	0.87	0
4	NAG	C	1313	1	14,14,15	1.16	1 (7%)	17,19,21	0.61	0
4	NAG	A	1315	1	14,14,15	1.35	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	B	1313	1	14,14,15	1.28	3 (21%)	17,19,21	0.84	1 (5%)
4	NAG	B	1308	1	14,14,15	1.26	2 (14%)	17,19,21	0.88	1 (5%)
4	NAG	B	1302	1	14,14,15	1.32	2 (14%)	17,19,21	1.69	1 (5%)
4	NAG	A	1306	1	14,14,15	0.97	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	B	1314	1	14,14,15	1.21	2 (14%)	17,19,21	0.83	1 (5%)
4	NAG	B	1304	1	14,14,15	1.20	2 (14%)	17,19,21	1.17	2 (11%)
4	NAG	B	1307	1	14,14,15	1.16	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	A	1314	1	14,14,15	1.17	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	C	1308	1	14,14,15	1.23	1 (7%)	17,19,21	1.60	1 (5%)
4	NAG	C	1303	1	14,14,15	1.18	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	A	1305	1	14,14,15	1.25	2 (14%)	17,19,21	1.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1311	1	14,14,15	1.17	1 (7%)	17,19,21	1.56	1 (5%)
4	NAG	B	1312	1	14,14,15	1.30	3 (21%)	17,19,21	0.92	0
4	NAG	C	1316	1	14,14,15	1.30	3 (21%)	17,19,21	0.95	1 (5%)
4	NAG	C	1315	1	14,14,15	1.32	3 (21%)	17,19,21	1.06	1 (5%)
4	NAG	C	1309	1	14,14,15	1.25	1 (7%)	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	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	B	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1315	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1316	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1312	NAG	C1-C2	3.05	1.56	1.52
4	A	1309	NAG	O5-C5	2.88	1.49	1.43
4	A	1315	NAG	O5-C5	2.87	1.49	1.43
4	B	1302	NAG	C1-C2	2.85	1.56	1.52
4	C	1311	NAG	O5-C5	2.84	1.49	1.43
4	A	1312	NAG	C1-C2	2.84	1.56	1.52
4	C	1309	NAG	O5-C5	2.78	1.49	1.43
4	C	1315	NAG	O5-C5	2.77	1.49	1.43
4	A	1312	NAG	O5-C5	2.74	1.49	1.43
4	B	1312	NAG	C1-C2	2.74	1.56	1.52
4	B	1303	NAG	O5-C5	2.73	1.49	1.43
4	A	1316	NAG	O5-C5	2.72	1.49	1.43
4	B	1314	NAG	O5-C5	2.71	1.48	1.43
4	B	1302	NAG	O5-C5	2.71	1.48	1.43
4	C	1310	NAG	O5-C5	2.71	1.48	1.43
4	C	1306	NAG	O5-C5	2.69	1.48	1.43
4	B	1311	NAG	O5-C5	2.68	1.48	1.43
4	C	1308	NAG	O5-C5	2.68	1.48	1.43
4	B	1310	NAG	C1-C2	2.67	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1314	NAG	O5-C5	2.63	1.48	1.43
4	A	1305	NAG	C1-C2	2.62	1.56	1.52
4	B	1310	NAG	O5-C5	2.62	1.48	1.43
4	C	1307	NAG	O5-C5	2.59	1.48	1.43
4	C	1313	NAG	O5-C5	2.59	1.48	1.43
4	C	1312	NAG	O5-C5	2.57	1.48	1.43
4	C	1301	NAG	O5-C5	2.53	1.48	1.43
4	B	1305	NAG	O5-C5	2.52	1.48	1.43
4	A	1312	NAG	O5-C1	2.51	1.47	1.43
4	A	1302	NAG	O5-C5	2.50	1.48	1.43
4	A	1314	NAG	O5-C5	2.50	1.48	1.43
4	A	1301	NAG	O5-C5	2.47	1.48	1.43
4	C	1303	NAG	O5-C5	2.45	1.48	1.43
4	B	1313	NAG	O5-C5	2.45	1.48	1.43
4	A	1310	NAG	O5-C5	2.45	1.48	1.43
4	A	1311	NAG	O5-C5	2.45	1.48	1.43
4	C	1316	NAG	C1-C2	2.43	1.56	1.52
4	B	1304	NAG	O5-C5	2.43	1.48	1.43
4	C	1301	NAG	C1-C2	2.42	1.56	1.52
4	B	1308	NAG	O5-C5	2.42	1.48	1.43
4	B	1309	NAG	O5-C5	2.41	1.48	1.43
4	A	1315	NAG	O5-C1	2.40	1.47	1.43
4	A	1302	NAG	C1-C2	2.40	1.55	1.52
4	C	1316	NAG	O5-C1	2.39	1.47	1.43
4	C	1312	NAG	O5-C1	2.39	1.47	1.43
4	C	1305	NAG	O5-C5	2.38	1.48	1.43
4	B	1313	NAG	C1-C2	2.34	1.55	1.52
4	B	1312	NAG	O5-C5	2.32	1.48	1.43
4	B	1315	NAG	O5-C5	2.32	1.48	1.43
4	B	1301	NAG	O5-C5	2.29	1.48	1.43
4	C	1316	NAG	O5-C5	2.28	1.48	1.43
4	B	1306	NAG	O5-C5	2.27	1.48	1.43
4	B	1311	NAG	O5-C1	2.26	1.47	1.43
4	C	1315	NAG	C1-C2	2.26	1.55	1.52
4	B	1307	NAG	O5-C5	2.26	1.48	1.43
4	C	1310	NAG	C1-C2	2.23	1.55	1.52
4	B	1305	NAG	C1-C2	2.22	1.55	1.52
4	A	1308	NAG	O5-C5	2.22	1.47	1.43
4	A	1303	NAG	O5-C5	2.21	1.47	1.43
4	B	1308	NAG	C1-C2	2.21	1.55	1.52
4	A	1305	NAG	O5-C5	2.21	1.47	1.43
4	C	1315	NAG	O5-C1	2.19	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1307	NAG	O5-C5	2.18	1.47	1.43
4	A	1313	NAG	O5-C5	2.18	1.47	1.43
4	A	1316	NAG	C1-C2	2.17	1.55	1.52
4	B	1310	NAG	O5-C1	2.17	1.47	1.43
4	A	1311	NAG	C1-C2	2.16	1.55	1.52
4	B	1315	NAG	C1-C2	2.16	1.55	1.52
4	B	1304	NAG	C1-C2	2.14	1.55	1.52
4	C	1302	NAG	C1-C2	2.14	1.55	1.52
4	A	1313	NAG	C1-C2	2.12	1.55	1.52
4	C	1305	NAG	C1-C2	2.12	1.55	1.52
4	B	1303	NAG	C1-C2	2.11	1.55	1.52
4	B	1311	NAG	C1-C2	2.11	1.55	1.52
4	B	1312	NAG	O5-C1	2.11	1.47	1.43
4	A	1309	NAG	O5-C1	2.11	1.47	1.43
4	B	1301	NAG	C1-C2	2.10	1.55	1.52
4	A	1310	NAG	O5-C1	2.10	1.47	1.43
4	B	1314	NAG	O5-C1	2.09	1.47	1.43
4	B	1313	NAG	O5-C1	2.08	1.47	1.43
4	B	1303	NAG	O5-C1	2.07	1.47	1.43
4	B	1305	NAG	O5-C1	2.06	1.47	1.43
4	A	1310	NAG	C1-C2	2.03	1.55	1.52
4	A	1302	NAG	O5-C1	2.03	1.47	1.43
4	C	1301	NAG	O5-C1	2.02	1.46	1.43
4	A	1306	NAG	O5-C5	2.01	1.47	1.43
4	B	1315	NAG	O5-C1	2.01	1.46	1.43
4	A	1311	NAG	O5-C1	2.00	1.46	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1305	NAG	O5-C1-C2	6.78	122.00	111.29
4	A	1316	NAG	O5-C1-C2	6.19	121.07	111.29
4	C	1311	NAG	O5-C1-C2	5.88	120.58	111.29
4	B	1302	NAG	O5-C1-C2	5.87	120.56	111.29
4	C	1308	NAG	O5-C1-C2	5.62	120.17	111.29
4	A	1311	NAG	C1-O5-C5	3.34	116.72	112.19
4	C	1304	NAG	C1-O5-C5	3.24	116.58	112.19
4	B	1306	NAG	C1-O5-C5	3.23	116.56	112.19
4	C	1312	NAG	C1-O5-C5	3.17	116.49	112.19
4	C	1315	NAG	C1-O5-C5	3.16	116.47	112.19
4	A	1306	NAG	C1-O5-C5	3.03	116.30	112.19
4	C	1316	NAG	C1-O5-C5	2.98	116.23	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1302	NAG	C1-O5-C5	2.93	116.17	112.19
4	B	1309	NAG	C1-O5-C5	2.91	116.14	112.19
4	A	1302	NAG	C1-O5-C5	2.91	116.13	112.19
4	A	1314	NAG	C1-O5-C5	2.84	116.04	112.19
4	B	1308	NAG	C1-O5-C5	2.75	115.92	112.19
4	B	1315	NAG	C1-O5-C5	2.74	115.91	112.19
4	B	1303	NAG	C1-O5-C5	2.67	115.82	112.19
4	C	1312	NAG	C1-C2-N2	2.66	115.03	110.49
4	B	1304	NAG	C3-C4-C5	2.64	114.94	110.24
4	B	1314	NAG	C1-O5-C5	2.52	115.61	112.19
4	A	1302	NAG	C2-N2-C7	2.46	126.41	122.90
4	C	1309	NAG	C1-O5-C5	2.45	115.51	112.19
4	B	1313	NAG	C1-O5-C5	2.40	115.44	112.19
4	A	1315	NAG	C1-O5-C5	2.39	115.43	112.19
4	A	1312	NAG	O5-C5-C6	2.27	110.77	107.20
4	B	1311	NAG	C1-O5-C5	2.21	115.19	112.19
4	C	1307	NAG	C1-O5-C5	2.14	115.09	112.19
4	B	1304	NAG	C1-C2-N2	2.14	114.14	110.49
4	B	1307	NAG	C1-O5-C5	2.12	115.07	112.19
4	C	1303	NAG	C1-C2-N2	2.12	114.10	110.49
4	B	1305	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	C1-C2-N2-C7
4	B	1304	NAG	C8-C7-N2-C2
4	B	1315	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1314	NAG	O5-C5-C6-O6
4	A	1313	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	A	1303	NAG	C1-C2-N2-C7
4	A	1302	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1314	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1316	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	B	1304	NAG	O7-C7-N2-C2
4	A	1312	NAG	C1-C2-N2-C7
4	B	1302	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	A	1302	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	B	1312	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	C	1308	NAG	C3-C2-N2-C7
4	C	1312	NAG	C3-C2-N2-C7
4	C	1308	NAG	C1-C2-N2-C7
4	A	1302	NAG	C1-C2-N2-C7
4	A	1314	NAG	C3-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	B	1302	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

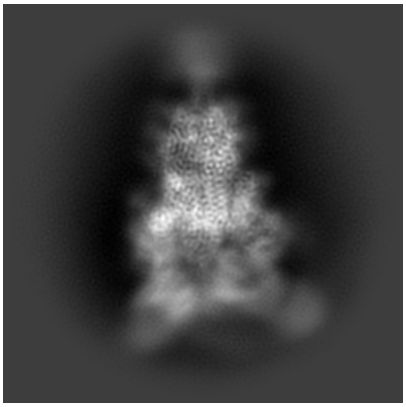
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25105. These allow visual inspection of the internal detail of the map and identification of artifacts.

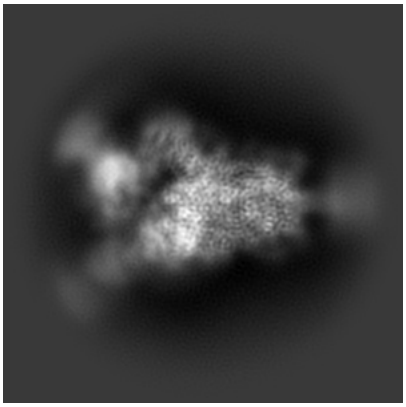
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

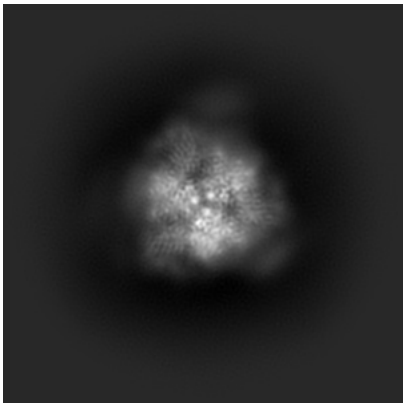
6.1.1 Primary map



X



Y

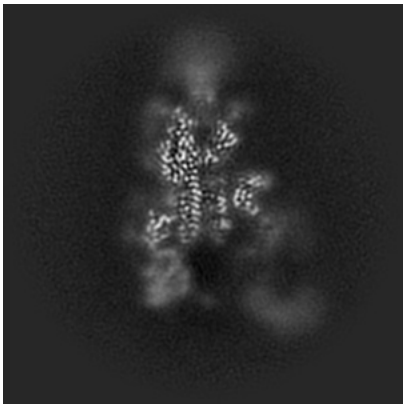


Z

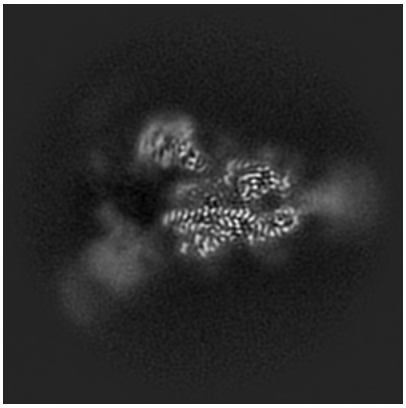
The images above show the map projected in three orthogonal directions.

6.2 Central slices

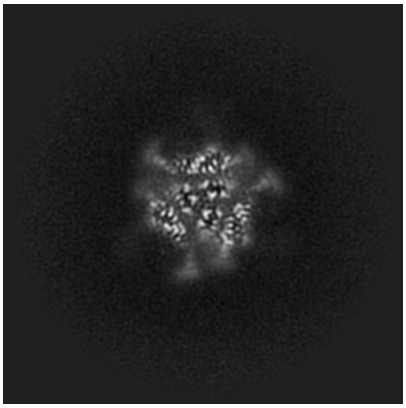
6.2.1 Primary map



X Index: 150



Y Index: 150

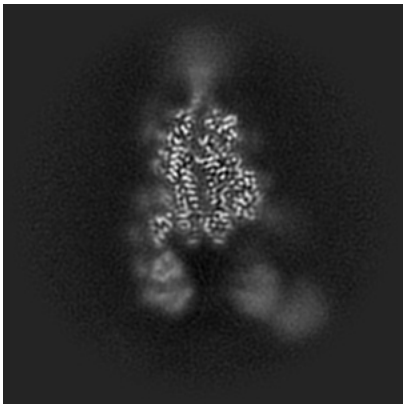


Z Index: 150

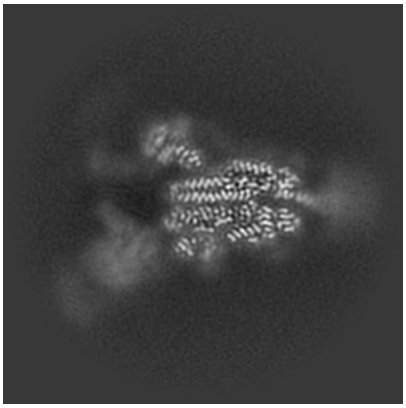
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

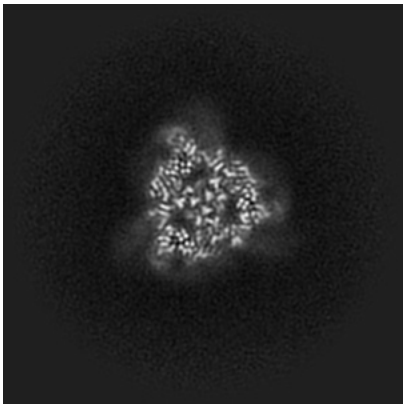
6.3.1 Primary map



X Index: 159



Y Index: 155



Z Index: 142

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 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

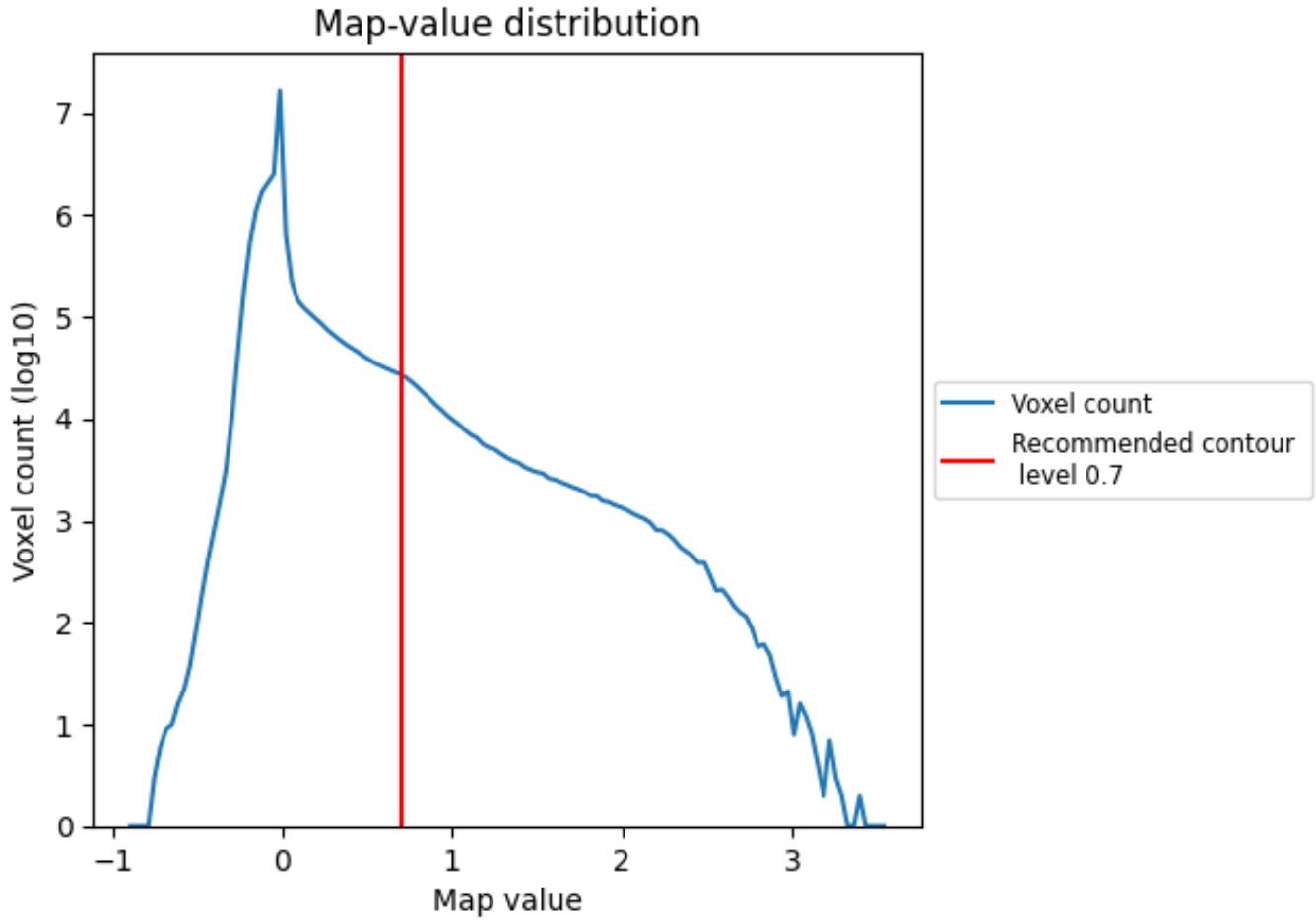
6.5 Mask visualisation (i)

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

7 Map analysis

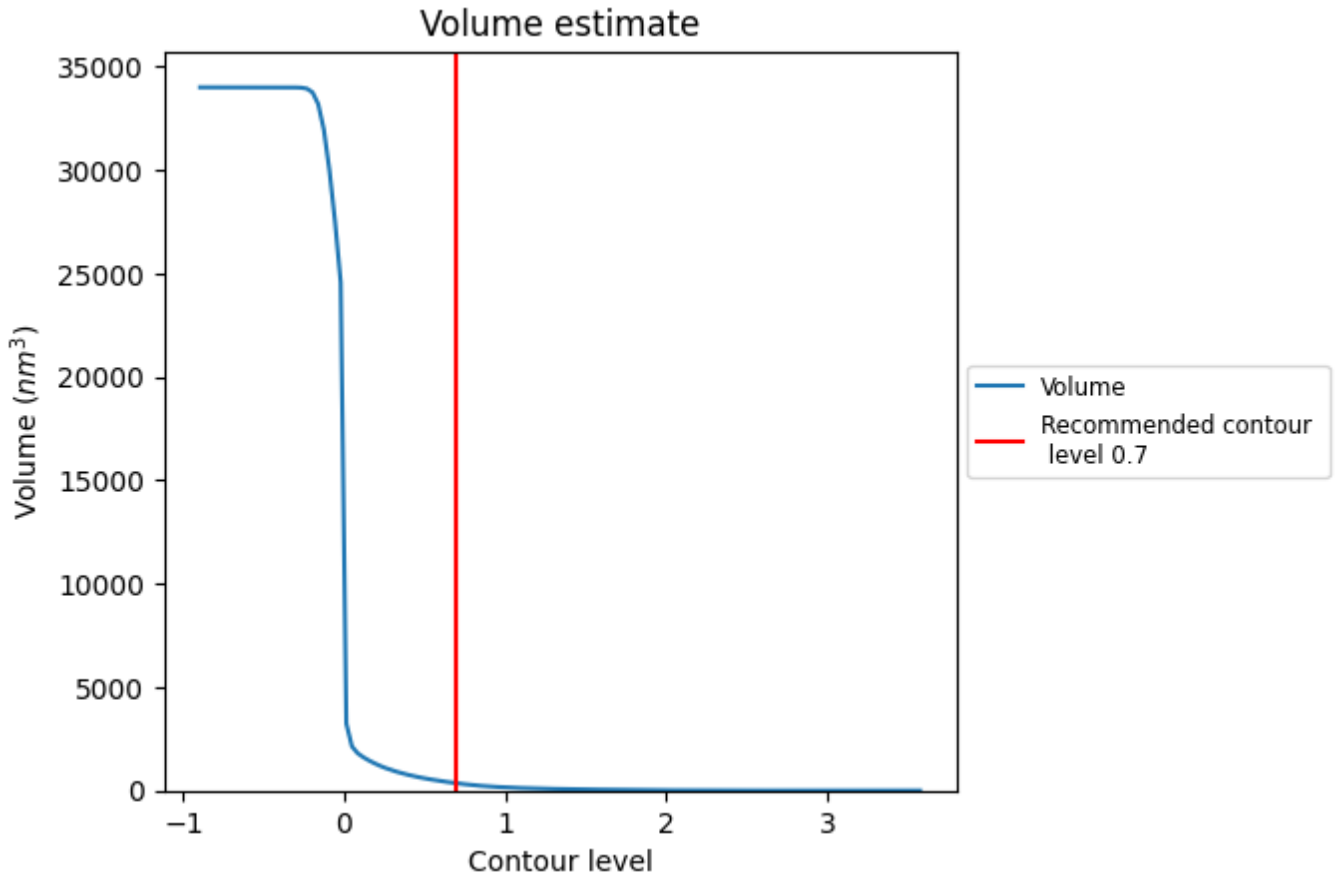
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

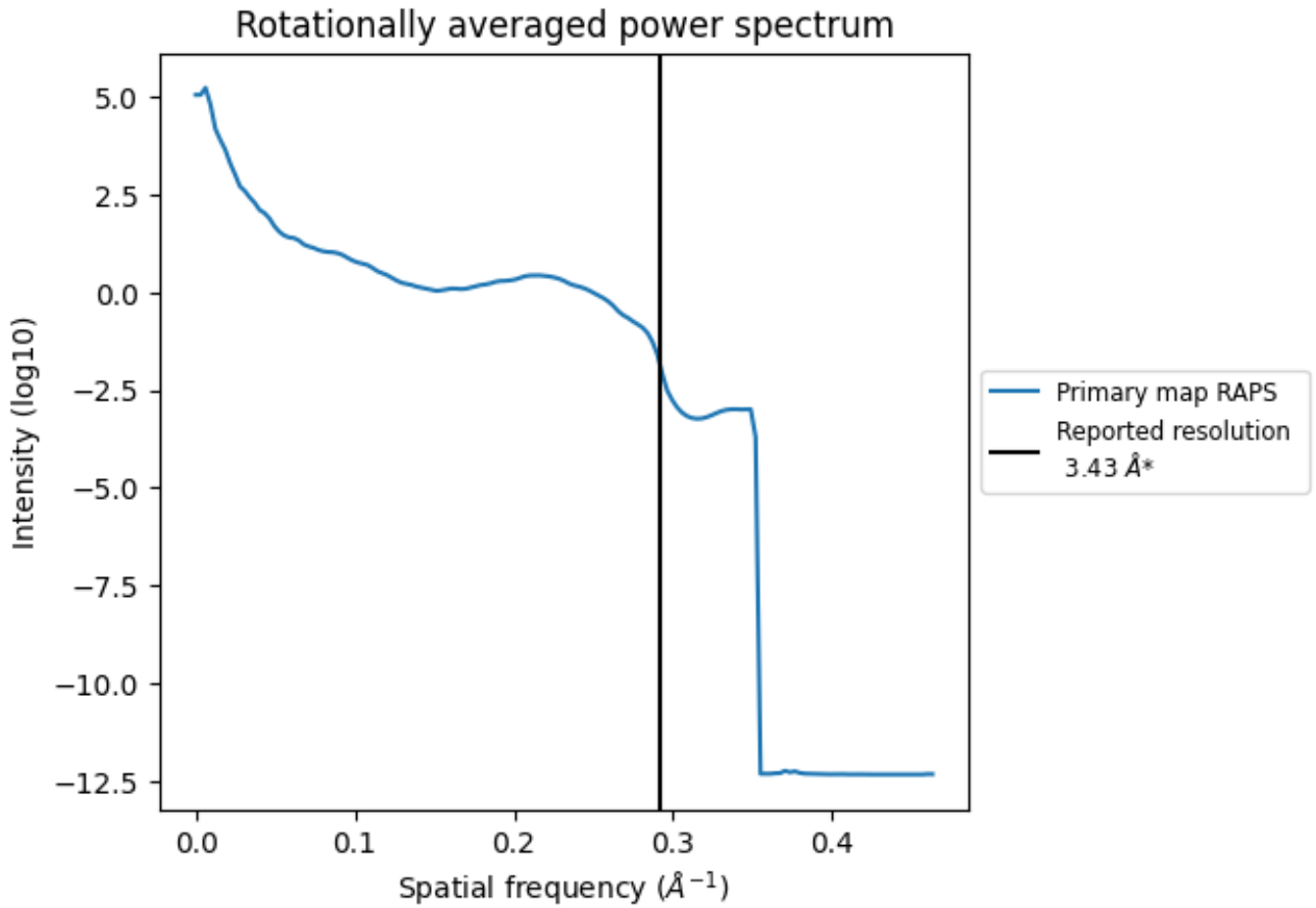
7.2 Volume estimate



The volume at the recommended contour level is 353 nm^3; this corresponds to an approximate mass of 319 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 0.292 $Å^{-1}$

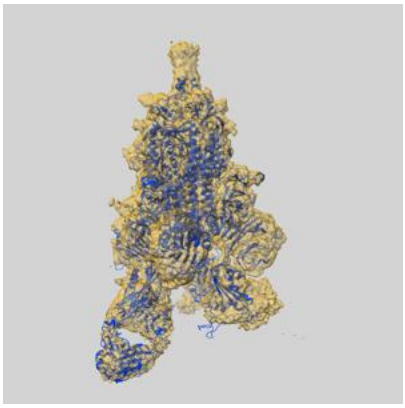
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

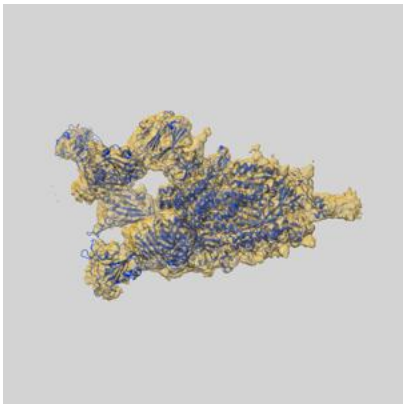
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25105 and PDB model 7SG4. Per-residue inclusion information can be found in section 3 on page 13.

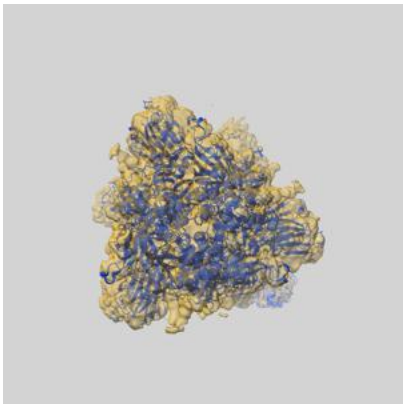
9.1 Map-model overlay



X



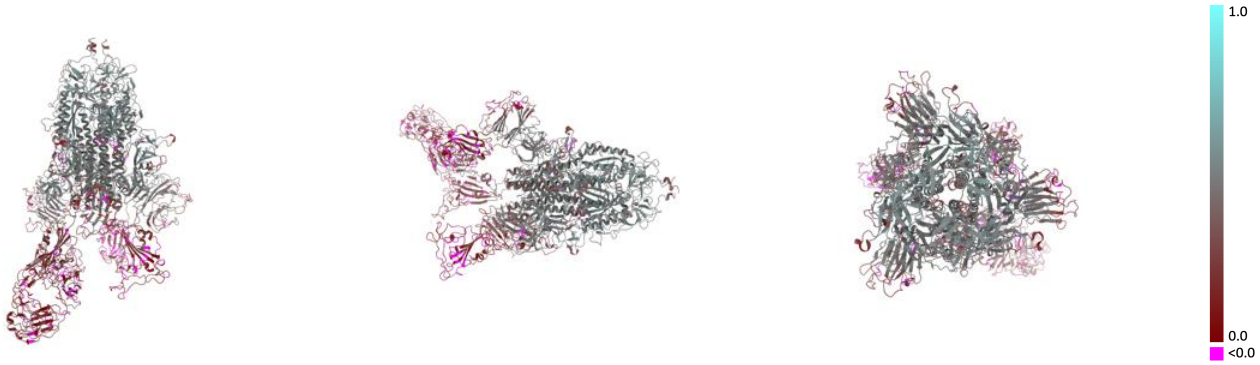
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

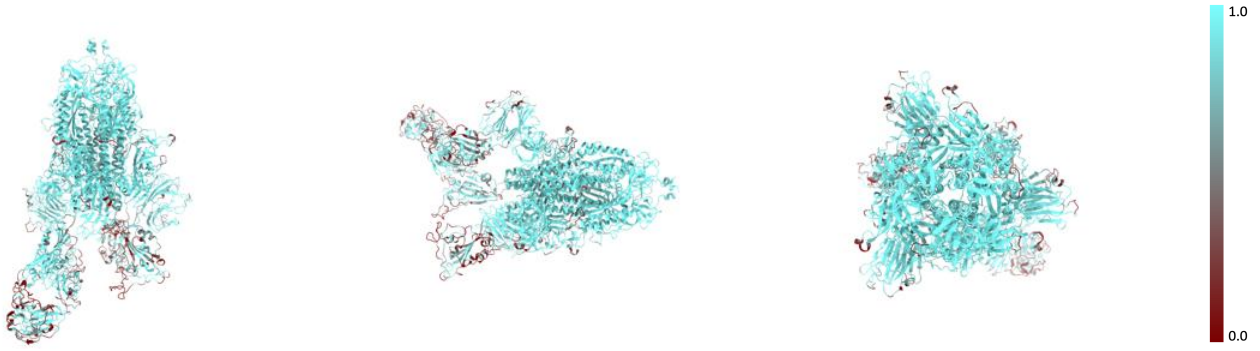
9.2 Q-score mapped to coordinate model (i)



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.

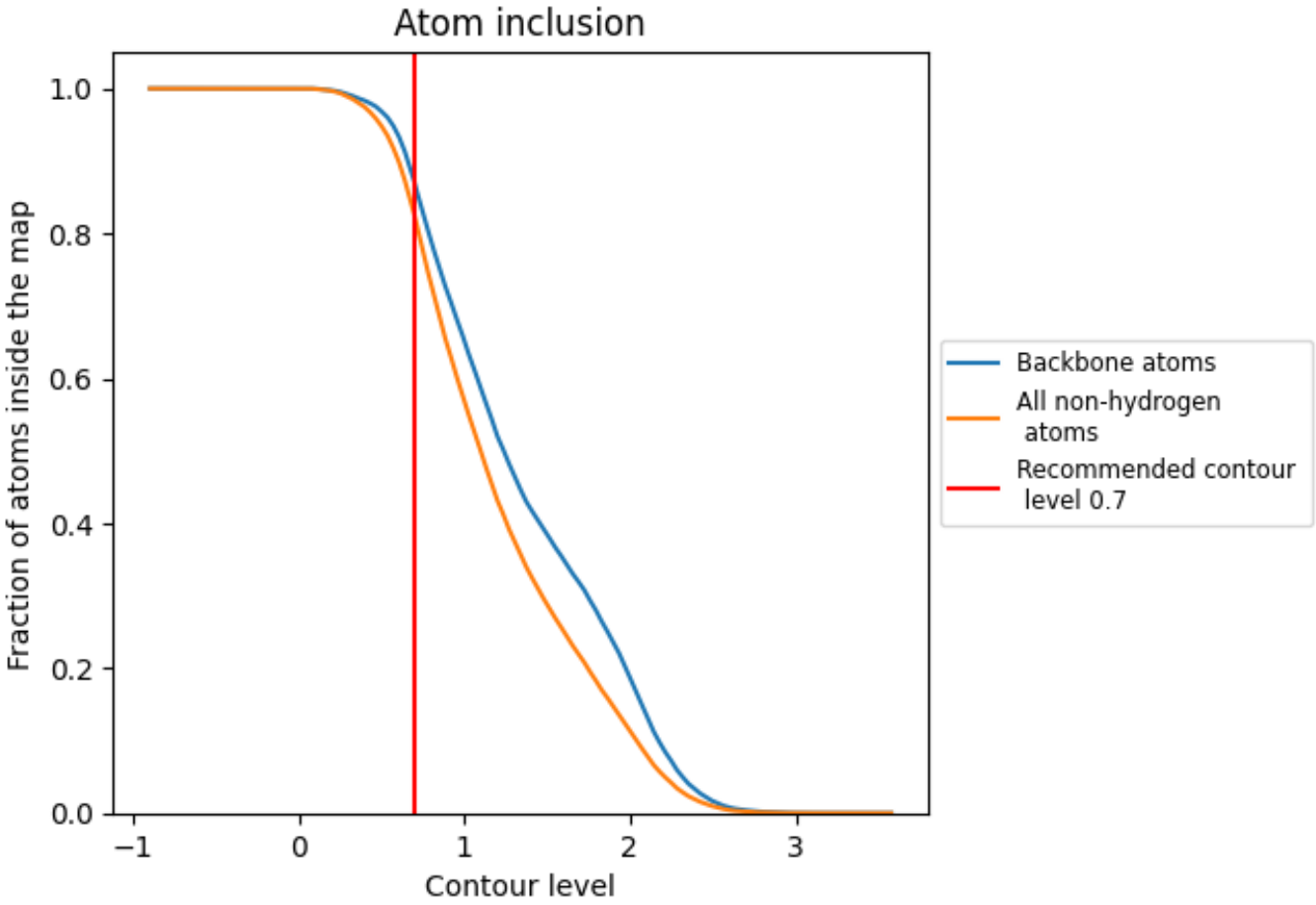
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8255	0.3550
A	0.8626	0.3770
B	0.8151	0.3690
C	0.8347	0.3750
H	0.6866	0.1740
L	0.7127	0.1350