Full wwPDB EM Validation Report ⓘ

Jul 25, 2023 – 12:42 PM JST

PDB ID	:	8H3M
EMDB ID	:	EMD-34469
Title	:	Conformation 1 of SARS-CoV-2 Omicron BA.1 Variant Spike protein complexed with MO1 Fab
Authors	:	Ishimaru, H.; Nishimura, M.; Sutandhio, S.; Shigematsu, H.; Kato, K.; Hasegawa, N.; Mori, Y.
Deposited on	:	2022-10-09
Resolution	:	2.48 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:

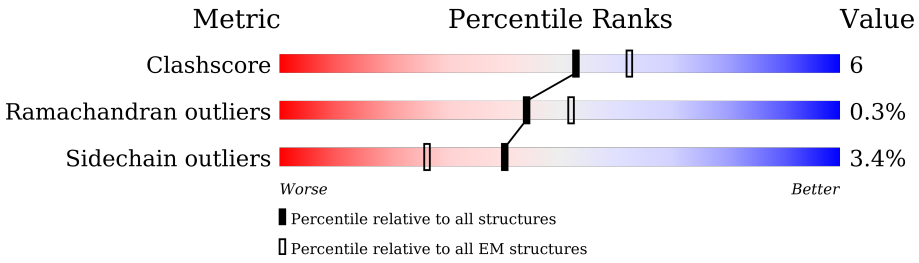
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.48 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	1249	63% 9% 27%
1	B	1249	50% 10% 39%
1	C	1249	62% 12% 26%
2	D	449	5% 93%
2	H	449	94%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20936 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	910	Total	C	N	O	S	0	0
			7039	4521	1173	1314	31		
1	B	763	Total	C	N	O	S	0	0
			5883	3777	979	1102	25		
1	C	930	Total	C	N	O	S	0	0
			7213	4633	1208	1341	31		

There are 279 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	145	ASP	TYR	variant	UNP P0DTC2
A	209B	ILE	-	insertion	UNP P0DTC2
A	209C	VAL	-	insertion	UNP P0DTC2
A	209D	ARG	ASN	variant	UNP P0DTC2
A	209E	GLU	LEU	variant	UNP P0DTC2
A	209F	PRO	VAL	variant	UNP P0DTC2
A	209G	GLU	ARG	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	682	LYS	ASN	variant	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	684	HIS	ALA	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1213	PRO	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	VAL	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	PHE	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	PHE	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	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
B	69	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	145	ASP	TYR	variant	UNP P0DTC2
B	207D	ILE	-	insertion	UNP P0DTC2
B	207E	VAL	-	insertion	UNP P0DTC2
B	207F	ARG	ASN	variant	UNP P0DTC2
B	207G	GLU	LEU	variant	UNP P0DTC2
B	207H	PRO	VAL	variant	UNP P0DTC2
B	207I	GLU	ARG	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	682	LYS	ASN	variant	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	684	HIS	ALA	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1213	PRO	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	VAL	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	PHE	-	expression tag	UNP P0DTC2
B	1219	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	ILE	-	expression tag	UNP P0DTC2
B	1225	PRO	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	ALA	-	expression tag	UNP P0DTC2
B	1228	PRO	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLN	-	expression tag	UNP P0DTC2
B	1233	ALA	-	expression tag	UNP P0DTC2
B	1234	TYR	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	LYS	-	expression tag	UNP P0DTC2
B	1238	ASP	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLU	-	expression tag	UNP P0DTC2
B	1241	TRP	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	PHE	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	SER	-	expression tag	UNP P0DTC2
B	1246	THR	-	expression tag	UNP P0DTC2
B	1247	PHE	-	expression tag	UNP P0DTC2
B	1248	LEU	-	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
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	TYR	deletion	UNP P0DTC2
C	145	ASP	TYR	variant	UNP P0DTC2
C	209B	ILE	-	insertion	UNP P0DTC2
C	209C	VAL	-	insertion	UNP P0DTC2
C	209D	ARG	ASN	variant	UNP P0DTC2
C	209E	GLU	LEU	variant	UNP P0DTC2
C	209F	PRO	VAL	variant	UNP P0DTC2
C	209G	GLU	ARG	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	682	LYS	ASN	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	684	HIS	ALA	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1213	PRO	-	expression tag	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	VAL	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	PHE	-	expression tag	UNP P0DTC2
C	1219	GLN	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	ALA	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLN	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TYR	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	LYS	-	expression tag	UNP P0DTC2
C	1238	ASP	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	TRP	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	PHE	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	THR	-	expression tag	UNP P0DTC2
C	1247	PHE	-	expression tag	UNP P0DTC2
C	1248	LEU	-	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

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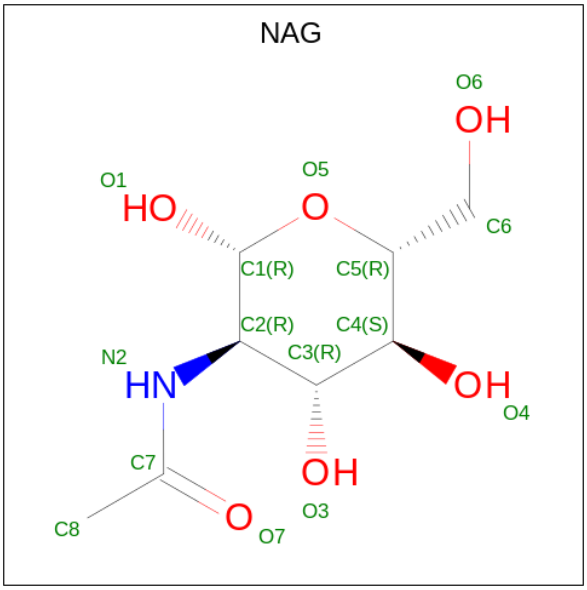
Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called MO1 heavy chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	30	Total C N O 255 164 38 53	0	0
2	H	29	Total C N O S 238 149 38 50 1	0	0

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



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

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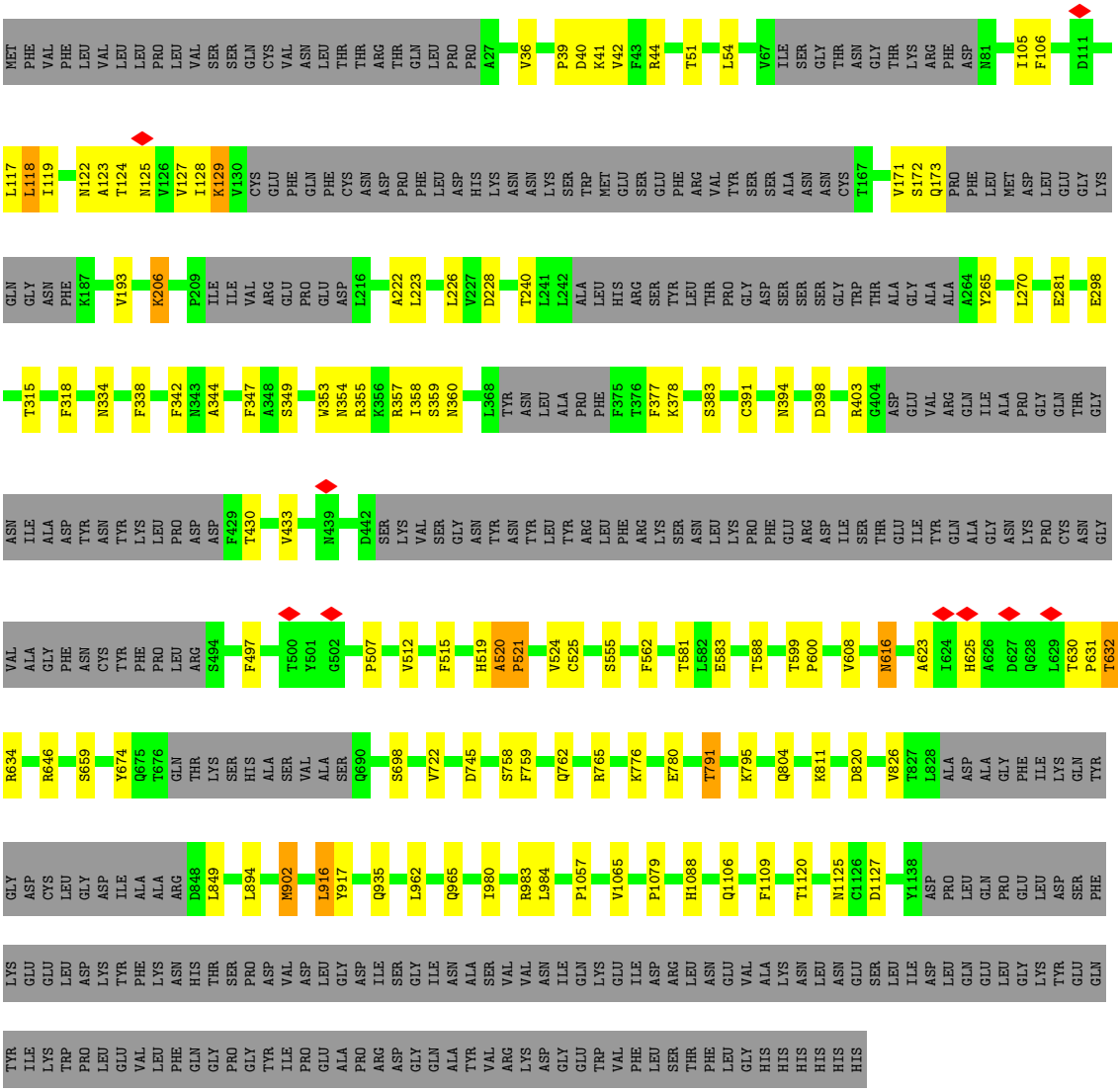
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B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

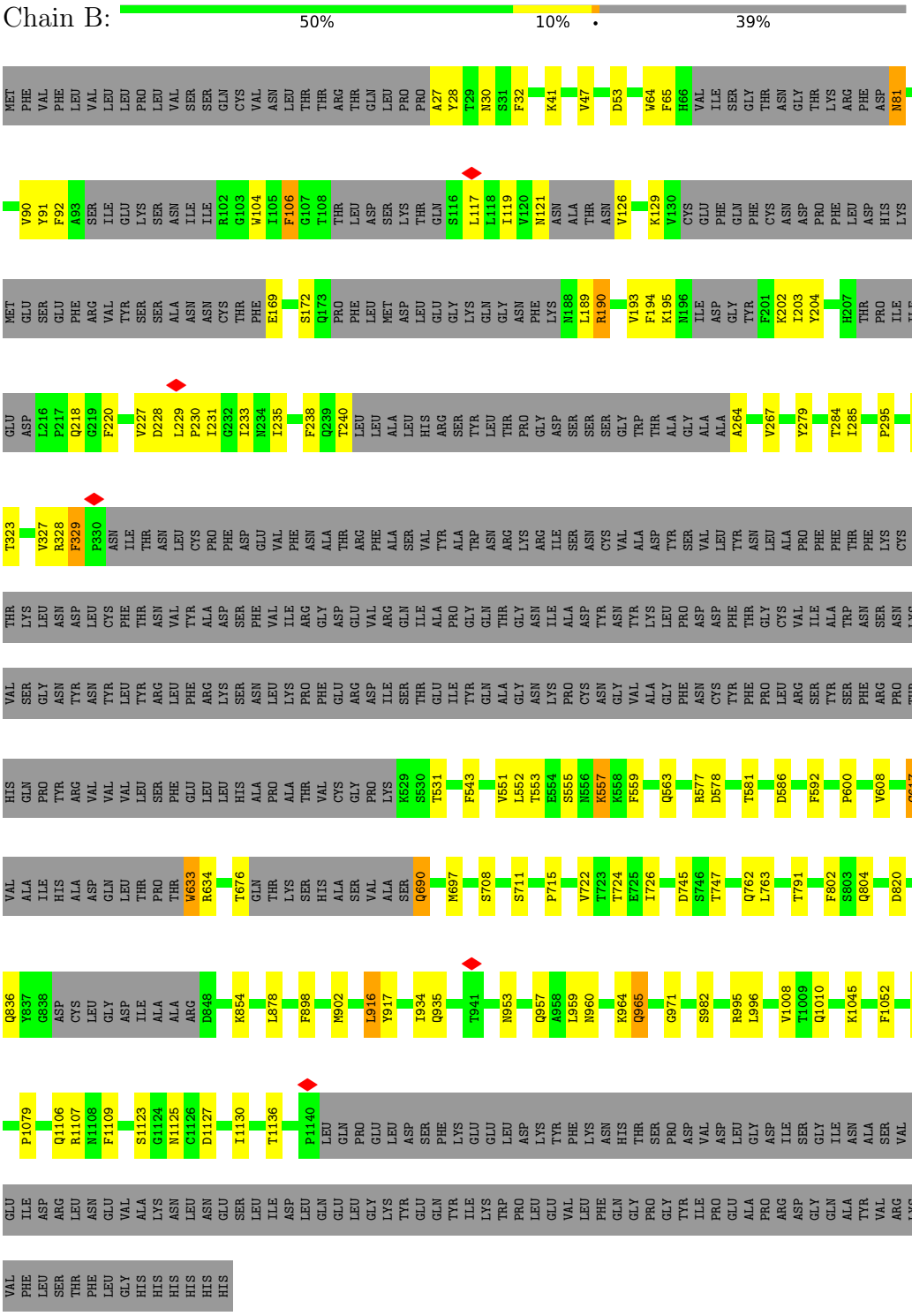
- Molecule 1: Spike glycoprotein

Chain A:



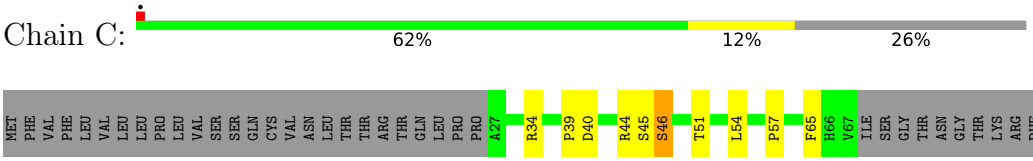
- Molecule 1: Spike glycoprotein

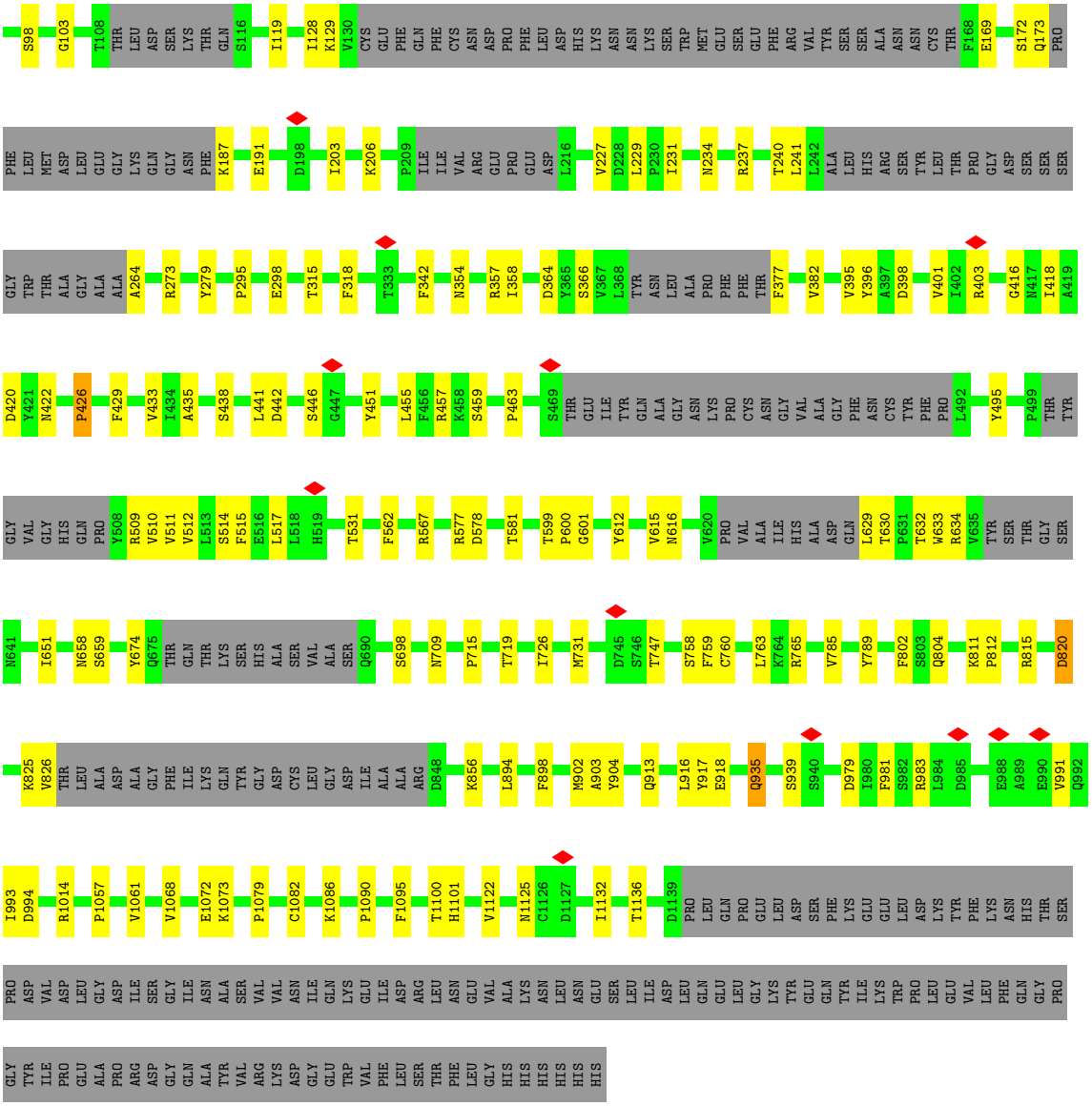
Chain B:



• Molecule 1: Spike glycoprotein

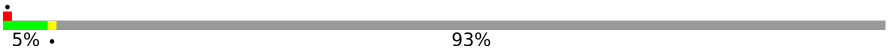
Chain C:

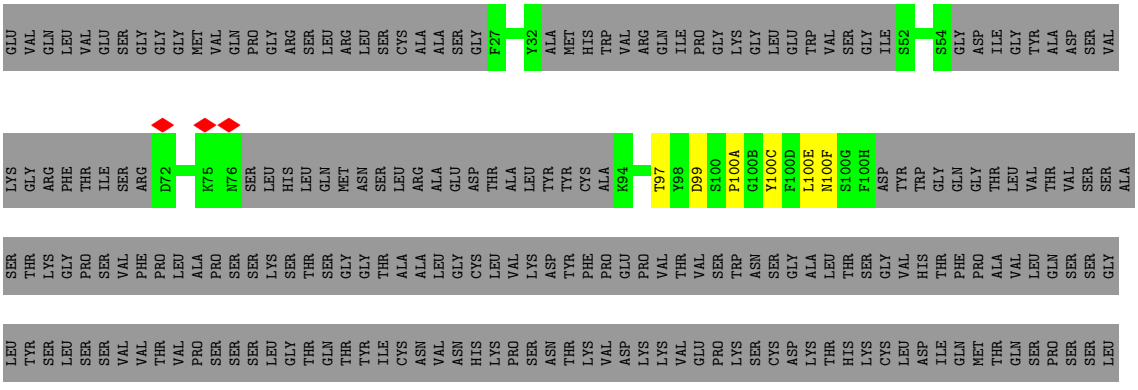


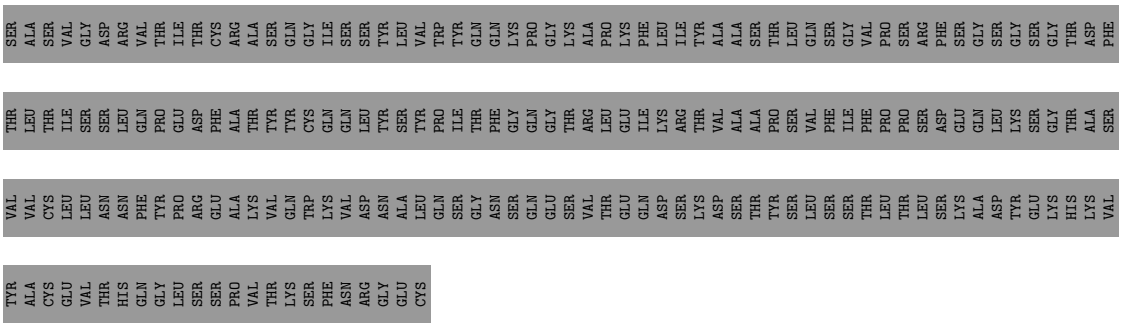


• Molecule 2: MO1 heavy chain

Chain D:

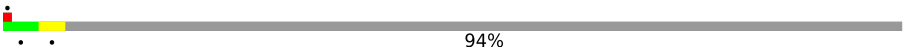


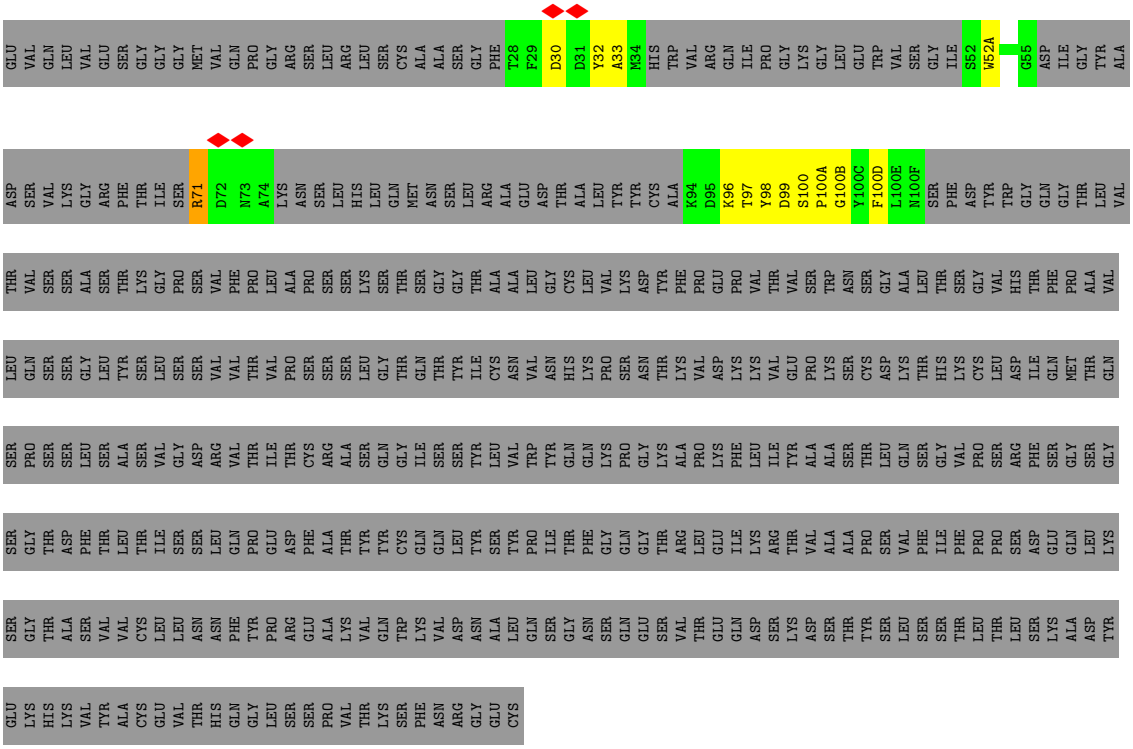




- Molecule 2: MO1 heavy chain

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	533315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	385.024, 385.024, 385.024	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	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	0.27	0/7199	0.50	2/9807 (0.0%)
1	B	0.27	0/6009	0.50	1/8172 (0.0%)
1	C	0.27	0/7372	0.49	1/10028 (0.0%)
2	D	0.26	0/261	0.46	0/348
2	H	0.26	0/242	0.48	0/322
All	All	0.27	0/21083	0.49	4/28677 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	426	PRO	N-CD-CG	-6.73	93.11	103.20
1	A	521	PRO	CA-N-CD	-6.22	102.79	111.50
1	B	745	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	745	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7039	0	6874	70	0
1	B	5883	0	5744	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7213	0	7048	79	0
2	D	255	0	212	4	0
2	H	238	0	200	7	0
3	A	126	0	117	3	0
3	B	84	0	78	0	0
3	C	98	0	91	1	0
All	All	20936	0	20364	230	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 6.

All (230) 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:391:CYS:HA	1:A:525:CYS:HB3	1.38	1.05
1:C:65:PHE:O	1:C:264:ALA:HA	1.77	0.85
2:H:97:THR:HG21	2:H:100(B):GLY:HA3	1.59	0.84
2:H:99:ASP:HB2	2:H:100(A):PRO:HD2	1.66	0.77
1:A:358:ILE:HG22	1:A:524:VAL:HG21	1.70	0.74
1:C:815:ARG:NH1	1:C:820:ASP:OD1	2.24	0.71
1:C:902:MET:HB3	1:C:916:LEU:HD11	1.73	0.70
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.75	0.69
1:A:119:ILE:HG12	1:A:128:ILE:HG13	1.76	0.68
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.60	0.67
1:B:231:ILE:HG12	1:B:233:ILE:HG12	1.77	0.66
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.78	0.66
1:C:395:VAL:HA	1:C:514:SER:O	1.97	0.65
1:C:95:ILE:HG22	1:C:187:LYS:HE2	1.78	0.65
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.79	0.63
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.80	0.63
1:B:30:ASN:HB3	1:B:32:PHE:CE1	2.35	0.62
1:B:229:LEU:HD22	1:B:230:PRO:HD2	1.82	0.62
1:B:30:ASN:HB3	1:B:32:PHE:HE1	1.65	0.61
1:B:555:SER:HB2	1:B:586:ASP:HB2	1.82	0.61
1:C:825:LYS:HE2	1:C:939:SER:HA	1.82	0.61
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.83	0.61
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.23	0.60
1:C:81:ASN:ND2	1:C:240:THR:O	2.33	0.60
1:A:342:PHE:HB2	3:A:1308:NAG:H82	1.83	0.60
1:C:457:ARG:NH1	1:C:459:SER:O	2.34	0.59
1:B:971:GLY:O	1:B:995:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:THR:HG22	1:C:601:GLY:H	1.67	0.59
1:A:122:ASN:OD1	1:A:123:ALA:N	2.36	0.59
1:A:520:ALA:HB1	1:A:521:PRO:HD3	1.85	0.59
1:B:563:GLN:O	1:B:577:ARG:NH1	2.36	0.58
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.67	0.58
1:C:719:THR:HG23	1:C:1068:VAL:HB	1.86	0.58
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.30	0.58
1:B:64:TRP:HD1	1:B:65:PHE:H	1.50	0.58
1:B:190:ARG:NH2	1:B:264:ALA:O	2.35	0.57
1:B:84:LEU:HD13	1:B:267:VAL:HG21	1.86	0.57
1:B:322:PRO:O	1:B:323:THR:HG22	2.03	0.57
1:A:125:ASN:ND2	1:A:172:SER:O	2.38	0.57
1:A:616:ASN:OD1	1:A:616:ASN:N	2.28	0.57
1:B:104:TRP:HB3	1:B:238:PHE:HE1	1.69	0.57
1:C:46:SER:HA	1:C:279:TYR:O	2.04	0.56
1:A:983:ARG:HD2	1:C:517:LEU:HD13	1.86	0.56
1:B:327:VAL:HG12	1:B:329:PHE:H	1.71	0.55
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.70	0.55
1:C:435:ALA:HB2	1:C:510:VAL:HG13	1.88	0.55
1:C:902:MET:HB3	1:C:916:LEU:CD1	2.36	0.55
2:D:97:THR:HG22	2:D:100(E):LEU:HD23	1.87	0.55
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.88	0.55
1:A:616:ASN:HB3	3:A:1304:NAG:HN2	1.72	0.54
1:A:40:ASP:OD2	1:A:44:ARG:NH2	2.41	0.54
1:B:81:ASN:HD22	1:B:81:ASN:N	2.04	0.54
1:B:298:GLU:OE1	1:B:633:TRP:NE1	2.39	0.54
1:B:957:GLN:NE2	1:C:765:ARG:HD3	2.23	0.54
1:A:562:PHE:HD2	1:B:41:LYS:HD3	1.73	0.54
1:B:126:VAL:HG22	1:B:172:SER:HB3	1.89	0.54
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.90	0.53
1:C:203:ILE:HB	1:C:227:VAL:HG22	1.89	0.53
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.90	0.53
1:A:616:ASN:ND2	1:B:836:GLN:HG2	2.23	0.53
1:B:620:VAL:HG13	1:B:621:PRO:HD3	1.91	0.53
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.90	0.53
1:A:391:CYS:HA	1:A:525:CYS:CB	2.25	0.53
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.90	0.53
1:B:995:ARG:HH22	1:C:991:VAL:HG22	1.73	0.53
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.89	0.53
1:C:357:ARG:HD3	1:C:396:TYR:CE1	2.43	0.53
1:A:980:ILE:HG23	1:A:984:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:LEU:HB2	1:C:634:ARG:NH1	2.25	0.52
1:A:659:SER:HB3	1:A:698:SER:HB3	1.91	0.52
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.91	0.52
1:A:354:ASN:O	1:A:398:ASP:HA	2.10	0.52
1:A:616:ASN:HD21	1:B:836:GLN:HG2	1.75	0.52
1:C:811:LYS:HD2	1:C:812:PRO:HD2	1.92	0.52
1:A:581:THR:HG23	1:A:583:GLU:HG2	1.91	0.51
1:B:1123:SER:OG	1:C:918:GLU:OE2	2.28	0.51
1:C:981:PHE:CZ	1:C:993:ILE:HG13	2.45	0.51
1:B:1127:ASP:OD1	1:B:1127:ASP:N	2.37	0.51
1:C:578:ASP:OD2	1:C:581:THR:OG1	2.23	0.51
1:A:646:ARG:HG3	1:A:646:ARG:HH11	1.75	0.51
2:H:30:ASP:O	2:H:52(A):TRP:HB2	2.11	0.51
1:B:202:LYS:HD2	1:B:202:LYS:H	1.76	0.50
1:B:32:PHE:CD2	1:B:218:GLN:HG2	2.46	0.50
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.45	0.50
1:B:557:LYS:HD2	1:B:559:PHE:HE1	1.77	0.50
1:B:64:TRP:HD1	1:B:65:PHE:N	2.10	0.49
2:D:99:ASP:HB3	2:D:100(C):TYR:CE2	2.48	0.49
2:H:33:ALA:HB2	2:H:99:ASP:HA	1.94	0.49
1:B:676:THR:HG1	1:B:690:GLN:N	2.10	0.49
2:H:32:TYR:O	2:H:71:ARG:NH2	2.45	0.49
1:B:1107:ARG:HD3	1:C:904:TYR:CZ	2.47	0.49
1:B:91:TYR:CG	1:B:91:TYR:O	2.66	0.49
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.48	0.48
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.78	0.48
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.96	0.48
1:C:760:CYS:HA	1:C:763:LEU:HD12	1.95	0.48
1:C:354:ASN:O	1:C:398:ASP:HA	2.14	0.48
1:C:364:ASP:OD1	1:C:366:SER:OG	2.22	0.48
1:A:334:ASN:OD1	1:A:334:ASN:N	2.47	0.48
1:A:776:LYS:O	1:A:780:GLU:HG3	2.14	0.48
1:B:960:ASN:HB3	1:B:964:LYS:NZ	2.28	0.48
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.96	0.48
1:A:127:VAL:HG22	1:A:171:VAL:HG22	1.95	0.48
1:C:342:PHE:CE2	1:C:511:VAL:HG11	2.49	0.47
1:C:600:PRO:HB3	1:C:674:TYR:HB2	1.95	0.47
1:A:1079:PRO:HB3	1:B:917:TYR:CE1	2.49	0.47
1:B:65:PHE:CZ	1:B:84:LEU:HD21	2.50	0.47
1:B:90:VAL:HG23	1:B:92:PHE:H	1.79	0.47
1:B:117:LEU:HD21	1:B:119:ILE:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.95	0.47
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.96	0.47
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.96	0.47
1:B:965:GLN:HE22	1:C:759:PHE:HE2	1.62	0.47
1:A:646:ARG:HG3	1:A:646:ARG:NH1	2.30	0.47
1:A:902:MET:HB3	1:A:916:LEU:HD11	1.96	0.47
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.96	0.47
1:B:328:ARG:NH1	1:B:531:THR:O	2.47	0.47
1:C:98:SER:O	1:C:98:SER:OG	2.31	0.47
1:C:438:SER:HB2	1:C:441:LEU:HB2	1.96	0.47
2:H:97:THR:HG22	2:H:98:TYR:CD1	2.49	0.47
1:A:122:ASN:ND2	1:A:124:THR:OG1	2.47	0.47
1:B:902:MET:HB3	1:B:916:LEU:HD11	1.95	0.47
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.97	0.46
1:A:298:GLU:HG2	1:A:315:THR:HB	1.97	0.46
1:C:34:ARG:HH21	1:C:191:GLU:CD	2.19	0.46
1:C:616:ASN:HB3	3:C:1304:NAG:HN2	1.80	0.46
1:A:791:THR:HB	1:A:795:LYS:HE2	1.98	0.46
1:B:1045:LYS:HB3	1:B:1045:LYS:HE3	1.65	0.46
2:H:100:SER:N	2:H:100(A):PRO:HD2	2.30	0.46
1:C:172:SER:OG	1:C:173:GLN:N	2.49	0.46
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.98	0.45
1:C:630:THR:O	1:C:632:THR:HG23	2.16	0.45
1:A:758:SER:O	1:A:762:GLN:HG3	2.16	0.45
1:B:227:VAL:HG22	1:B:228:ASP:H	1.82	0.45
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.98	0.45
1:B:555:SER:HB2	1:B:586:ASP:CB	2.46	0.45
1:B:953:ASN:O	1:B:957:GLN:HB3	2.17	0.45
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.52	0.45
1:B:555:SER:OG	1:B:557:LYS:HG3	2.17	0.45
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.49	0.45
1:B:551:VAL:HG12	1:B:553:THR:HG23	1.98	0.45
1:C:785:VAL:HG21	1:C:789:TYR:HE2	1.81	0.45
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.52	0.45
1:B:620:VAL:N	1:B:621:PRO:HD2	2.32	0.45
1:B:825:LYS:HD2	1:B:825:LYS:HA	1.88	0.45
1:A:1106:GLN:HG3	1:A:1109:PHE:O	2.17	0.44
1:A:105:ILE:HG22	1:A:118:LEU:HD23	1.98	0.44
1:A:599:THR:HG22	1:A:608:VAL:HG12	1.99	0.44
1:C:295:PRO:HG3	1:C:633:TRP:CZ3	2.53	0.44
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.99	0.44
1:B:190:ARG:O	1:B:190:ARG:HG2	2.17	0.44
1:A:42:VAL:HG21	1:C:567:ARG:HH21	1.81	0.44
1:B:552:LEU:HA	1:B:586:ASP:O	2.18	0.44
1:C:119:ILE:HG12	1:C:128:ILE:HG12	2.00	0.44
1:B:119:ILE:HG22	1:B:121:ASN:OD1	2.18	0.44
1:C:731:MET:HE1	1:C:1014:ARG:HB3	2.00	0.44
1:A:172:SER:OG	1:A:173:GLN:N	2.49	0.44
1:B:64:TRP:CD1	1:B:65:PHE:N	2.86	0.43
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.36	0.43
1:C:103:GLY:O	1:C:241:LEU:N	2.44	0.43
1:A:521:PRO:HD2	1:A:521:PRO:O	2.18	0.43
1:C:659:SER:HB3	1:C:698:SER:HB3	2.00	0.43
2:D:99:ASP:HB3	2:D:100(C):TYR:HE2	1.82	0.43
1:B:708:SER:HB3	1:B:711:SER:HB3	2.00	0.43
1:B:32:PHE:N	1:B:32:PHE:CD1	2.86	0.43
1:B:328:ARG:HG3	1:B:543:PHE:CE2	2.53	0.43
1:B:555:SER:H	1:B:586:ASP:H	1.66	0.43
1:A:623:ALA:HB3	1:A:634:ARG:HH12	1.83	0.43
1:B:81:ASN:N	1:B:81:ASN:ND2	2.66	0.43
1:B:117:LEU:HD13	1:B:231:ILE:HD12	2.01	0.43
1:A:281:GLU:N	1:A:281:GLU:OE1	2.51	0.43
1:A:36:VAL:O	1:A:222:ALA:HA	2.19	0.43
3:A:1304:NAG:H82	1:B:834:ILE:HG21	2.00	0.43
1:A:631:PRO:O	1:A:632:THR:HG22	2.19	0.42
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.39	0.42
1:A:1088:HIS:HB3	1:A:1120:THR:HG21	2.01	0.42
1:B:715:PRO:HD3	1:C:894:LEU:HD13	2.01	0.42
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.01	0.42
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.00	0.42
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.99	0.42
1:A:1088:HIS:HB3	1:A:1120:THR:CG2	2.48	0.42
1:A:983:ARG:O	1:C:382:VAL:HA	2.19	0.42
1:B:129:LYS:HG2	1:B:169:GLU:HG2	2.01	0.42
1:C:612:TYR:HE2	1:C:651:ILE:HD12	1.85	0.42
1:A:240:THR:HG21	1:A:265:TYR:CZ	2.55	0.42
1:B:195:LYS:HD3	1:B:204:TYR:HE1	1.85	0.42
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.92	0.42
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.51	0.42
2:D:100(A):PRO:HA	2:D:100(F):ASN:ND2	2.35	0.42
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.02	0.42
1:A:318:PHE:HA	1:A:631:PRO:HD3	2.02	0.41
1:A:894:LEU:HD13	1:C:715:PRO:HD3	2.01	0.41
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.92	0.41
1:B:1106:GLN:HG3	1:B:1109:PHE:O	2.19	0.41
1:A:623:ALA:HB3	1:A:634:ARG:NH1	2.35	0.41
1:B:617:CYS:C	1:B:619:GLU:H	2.24	0.41
1:C:577:ARG:HG3	1:C:577:ARG:HH11	1.83	0.41
1:C:979:ASP:O	1:C:983:ARG:HB2	2.21	0.41
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.03	0.41
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.21	0.41
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.56	0.41
1:C:616:ASN:OD1	1:C:616:ASN:N	2.52	0.41
1:A:41:LYS:HD2	1:C:562:PHE:HD1	1.85	0.41
1:A:962:LEU:HD12	1:A:962:LEU:HA	1.94	0.41
1:C:129:LYS:HG2	1:C:169:GLU:HG2	2.03	0.41
1:A:902:MET:HB3	1:A:916:LEU:CD1	2.51	0.41
1:B:804:GLN:OE1	1:B:935:GLN:HG2	2.21	0.41
1:C:403:ARG:HB2	1:C:495:TYR:CD1	2.56	0.41
1:B:106:PHE:HB3	1:B:235:ILE:HG23	2.03	0.41
1:B:1079:PRO:HG2	1:B:1130:ILE:O	2.21	0.41
1:B:1125:ASN:HB2	1:B:1127:ASP:OD1	2.20	0.41
1:C:442:ASP:OD1	1:C:451:TYR:OH	2.27	0.41
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	2.03	0.41
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.47	0.40
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.96	0.40
1:C:416:GLY:O	1:C:420:ASP:HB2	2.21	0.40
1:C:1082:CYS:HB2	1:C:1132:ILE:HG12	2.03	0.40
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.95	0.40
1:A:965:GLN:HE22	1:B:762:GLN:HE22	1.68	0.40
1:B:27:ALA:O	1:B:64:TRP:N	2.52	0.40
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.39	0.40
1:B:633:TRP:HE3	1:B:633:TRP:O	2.03	0.40
1:C:298:GLU:HB3	1:C:315:THR:HG21	2.03	0.40
1:A:118:LEU:HB3	1:A:129:LYS:HG3	2.03	0.40
1:B:32:PHE:N	1:B:32:PHE:HD1	2.18	0.40
1:B:47:VAL:HG12	1:B:279:TYR:HB2	2.04	0.40
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	2.04	0.40
1:C:128:ILE:HD13	1:C:229:LEU:HD11	2.04	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	888/1249 (71%)	862 (97%)	24 (3%)	2 (0%)	47	66
1	B	735/1249 (59%)	703 (96%)	29 (4%)	3 (0%)	34	52
1	C	902/1249 (72%)	866 (96%)	34 (4%)	2 (0%)	47	66
2	D	22/449 (5%)	21 (96%)	1 (4%)	0	100	100
2	H	21/449 (5%)	17 (81%)	4 (19%)	0	100	100
All	All	2568/4645 (55%)	2469 (96%)	92 (4%)	7 (0%)	44	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	LYS
1	C	231	ILE
1	C	446	SER
1	A	519	HIS
1	B	592	PHE
1	B	189	LEU
1	A	520	ALA

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	776/1094 (71%)	747 (96%)	29 (4%)	34	57
1	B	645/1094 (59%)	621 (96%)	24 (4%)	34	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	792/1094 (72%)	771 (97%)	21 (3%)	44 69
2	D	28/387 (7%)	28 (100%)	0	100 100
2	H	25/387 (6%)	22 (88%)	3 (12%)	5 8
All	All	2266/4056 (56%)	2189 (97%)	77 (3%)	40 61

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	118	LEU
1	A	129	LYS
1	A	206	LYS
1	A	228	ASP
1	A	338	PHE
1	A	349	SER
1	A	357	ARG
1	A	359	SER
1	A	360	ASN
1	A	377	PHE
1	A	378	LYS
1	A	383	SER
1	A	394	ASN
1	A	403	ARG
1	A	430	THR
1	A	515	PHE
1	A	555	SER
1	A	588	THR
1	A	616	ASN
1	A	625	HIS
1	A	630	THR
1	A	632	THR
1	A	759	PHE
1	A	765	ARG
1	A	791	THR
1	A	902	MET
1	A	916	LEU
1	A	1125	ASN
1	B	28	TYR
1	B	53	ASP
1	B	81	ASN
1	B	86	PHE

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Mol	Chain	Res	Type
1	B	87	ASN
1	B	106	PHE
1	B	190	ARG
1	B	240	THR
1	B	284	THR
1	B	329	PHE
1	B	617	CYS
1	B	633	TRP
1	B	634	ARG
1	B	690	GLN
1	B	697	MET
1	B	747	THR
1	B	791	THR
1	B	820	ASP
1	B	854	LYS
1	B	916	LEU
1	B	965	GLN
1	B	982	SER
1	B	1010	GLN
1	B	1136	THR
1	C	45	SER
1	C	46	SER
1	C	54	LEU
1	C	206	LYS
1	C	234	ASN
1	C	237	ARG
1	C	377	PHE
1	C	455	LEU
1	C	515	PHE
1	C	531	THR
1	C	658	ASN
1	C	709	ASN
1	C	747	THR
1	C	758	SER
1	C	820	ASP
1	C	856	LYS
1	C	935	GLN
1	C	994	ASP
1	C	1073	LYS
1	C	1125	ASN
1	C	1136	THR
2	H	71	ARG

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Mol	Chain	Res	Type
2	H	96	LYS
2	H	100(D)	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	762	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	A	1306	1	14,14,15	0.27	0	17,19,21	0.51	0
3	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.42	0
3	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1305	1	14,14,15	0.27	0	17,19,21	0.34	0
3	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	C	1307	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1304	1	14,14,15	0.34	0	17,19,21	0.49	0
3	NAG	A	1307	1	14,14,15	0.51	0	17,19,21	0.70	1 (5%)
3	NAG	B	1304	1	14,14,15	0.18	0	17,19,21	0.51	0
3	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.41	0
3	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	C	1303	1	14,14,15	0.56	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	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(^{o})	Ideal(^{o})
3	A	1307	NAG	C1-O5-C5	2.33	115.35	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1307	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1307	NAG	C8-C7-N2-C2
3	A	1307	NAG	O7-C7-N2-C2
3	C	1305	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1305	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1305	NAG	C1-C2-N2-C7
3	B	1302	NAG	C4-C5-C6-O6
3	C	1305	NAG	C1-C2-N2-C7
3	A	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7
3	A	1304	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	1	0
3	A	1304	NAG	2	0
3	A	1308	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.

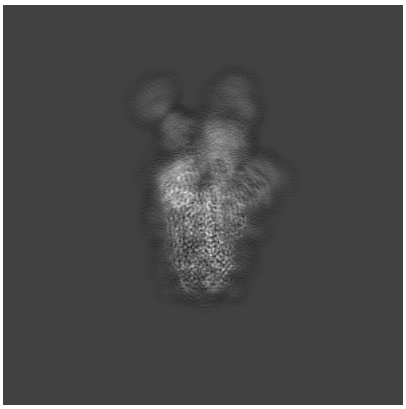
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34469. These allow visual inspection of the internal detail of the map and identification of artifacts.

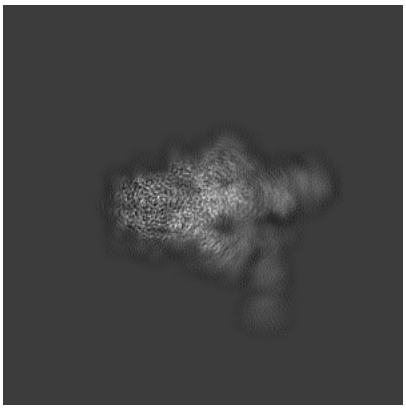
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

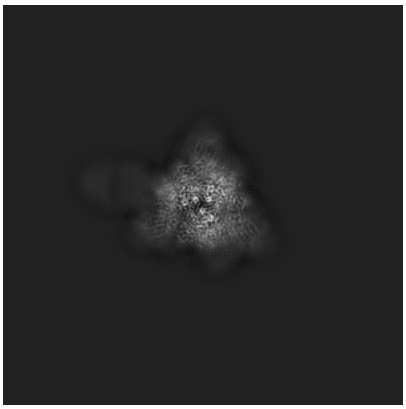
6.1.1 Primary map



X

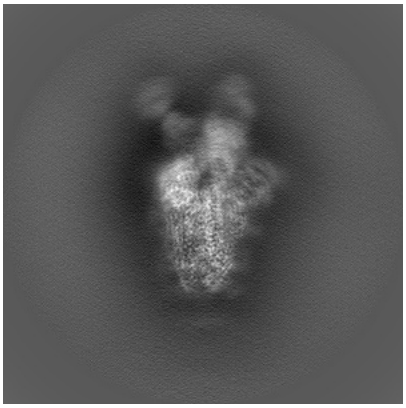


Y

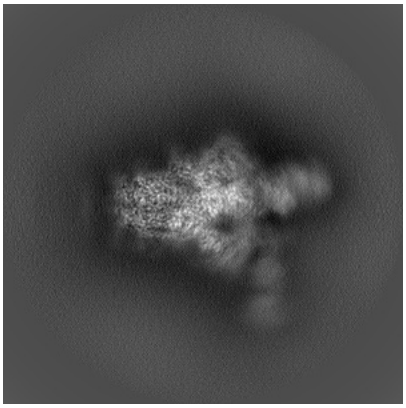


Z

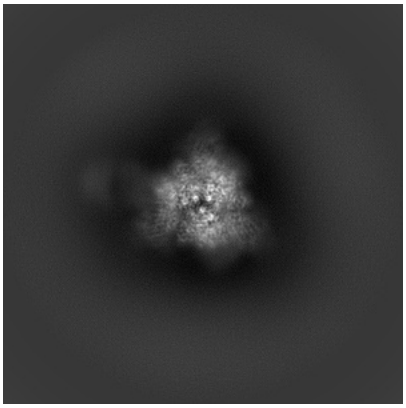
6.1.2 Raw map



X



Y

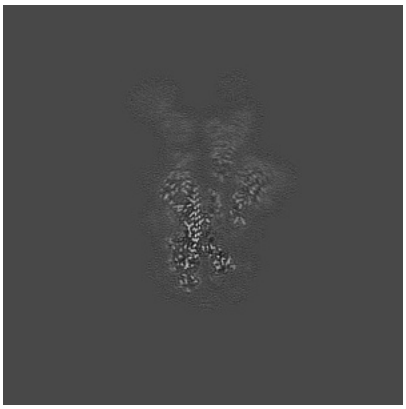


Z

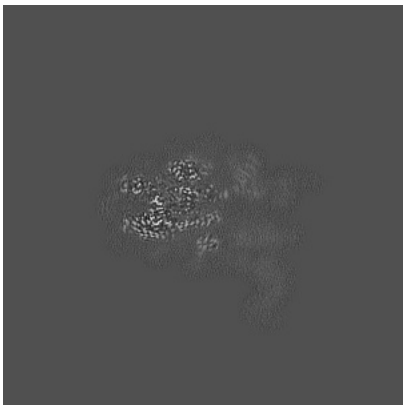
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

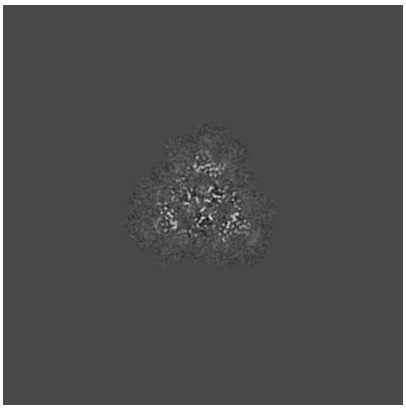
6.2.1 Primary map



X Index: 256

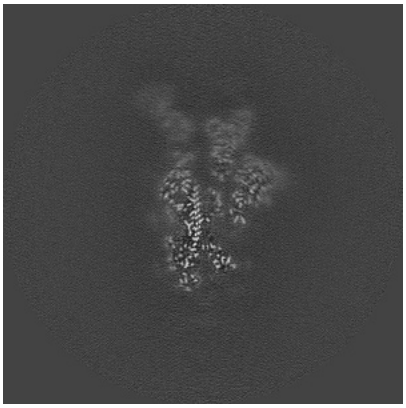


Y Index: 256

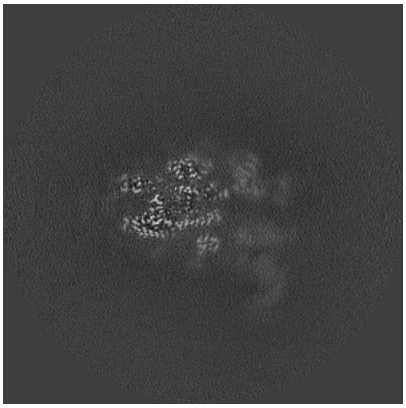


Z Index: 256

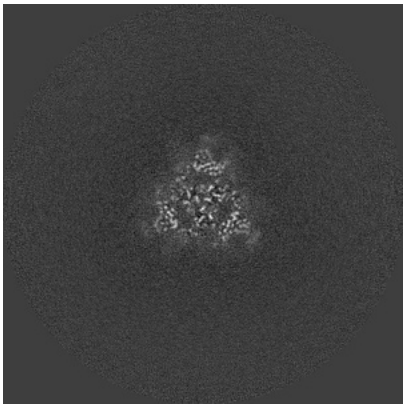
6.2.2 Raw map



X Index: 256



Y Index: 256

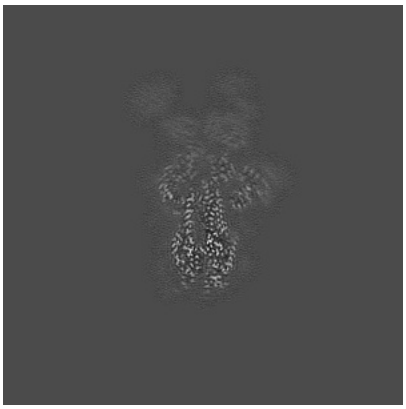


Z Index: 256

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

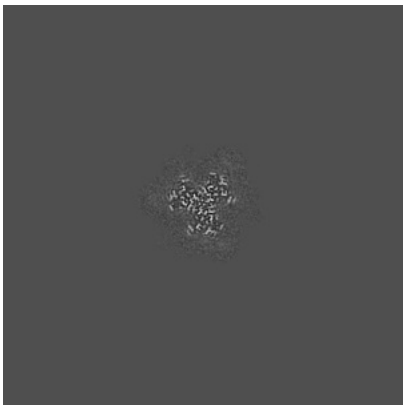
6.3 Largest variance slices (i)

6.3.1 Primary map



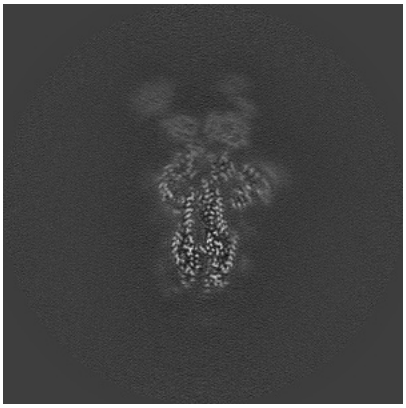
X Index: 267

Y Index: 265

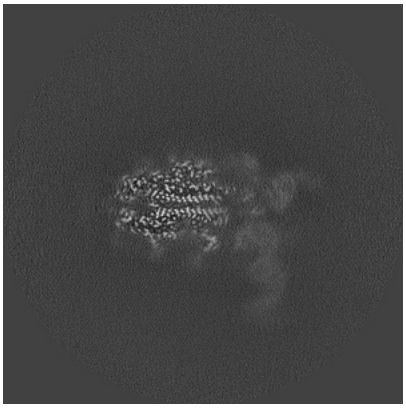


Z Index: 199

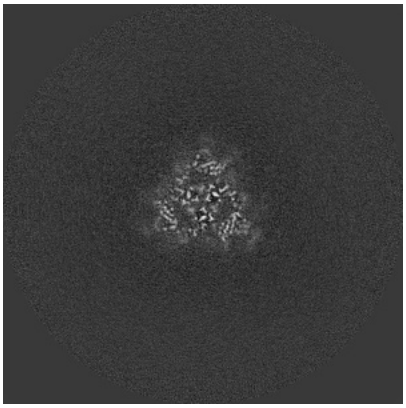
6.3.2 Raw map



X Index: 267



Y Index: 264

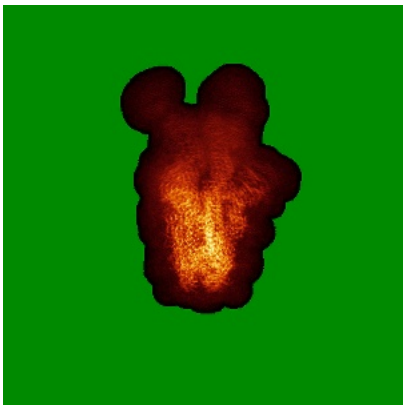


Z Index: 255

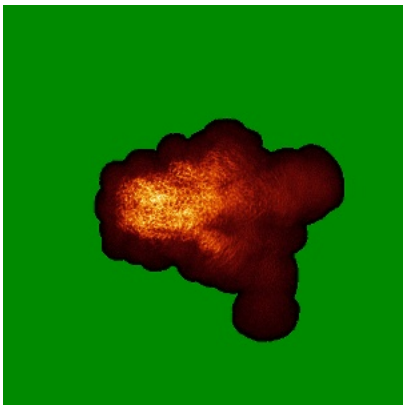
The images above show the largest variance slices of the map in three orthogonal directions.

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

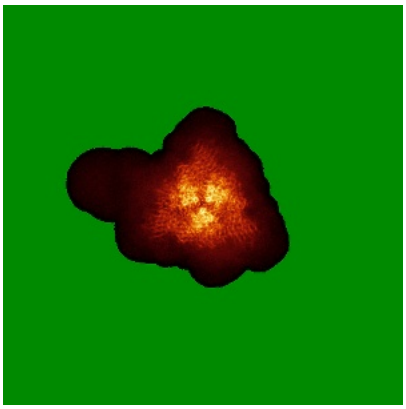
6.4.1 Primary map



X

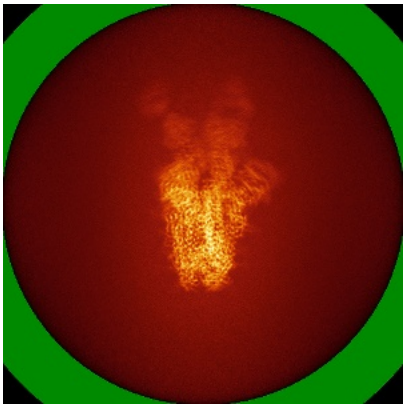


Y

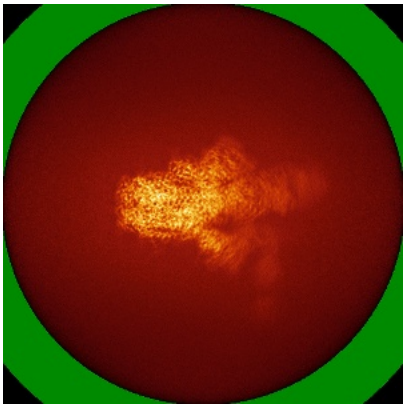


Z

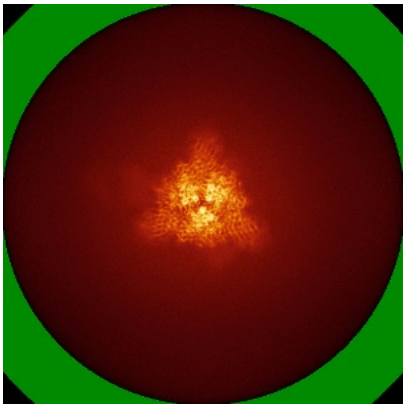
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

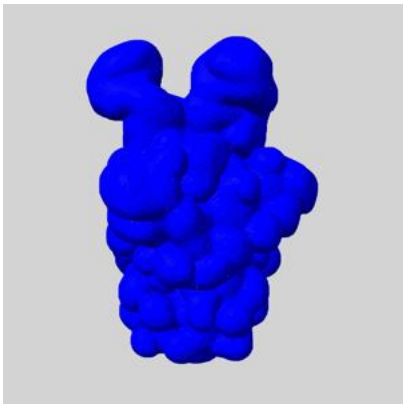
6.6 Mask visualisation (i)

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

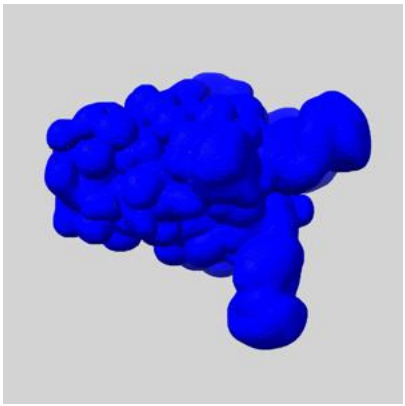
A mask typically either:

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

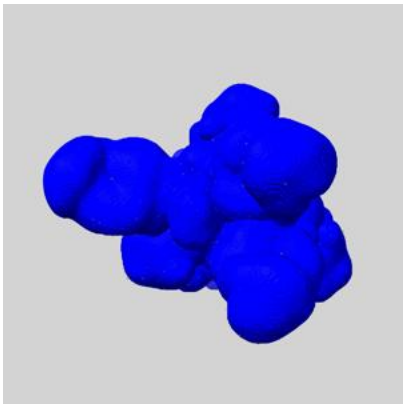
6.6.1 emd_34469_msk_1.map (i)



X



Y

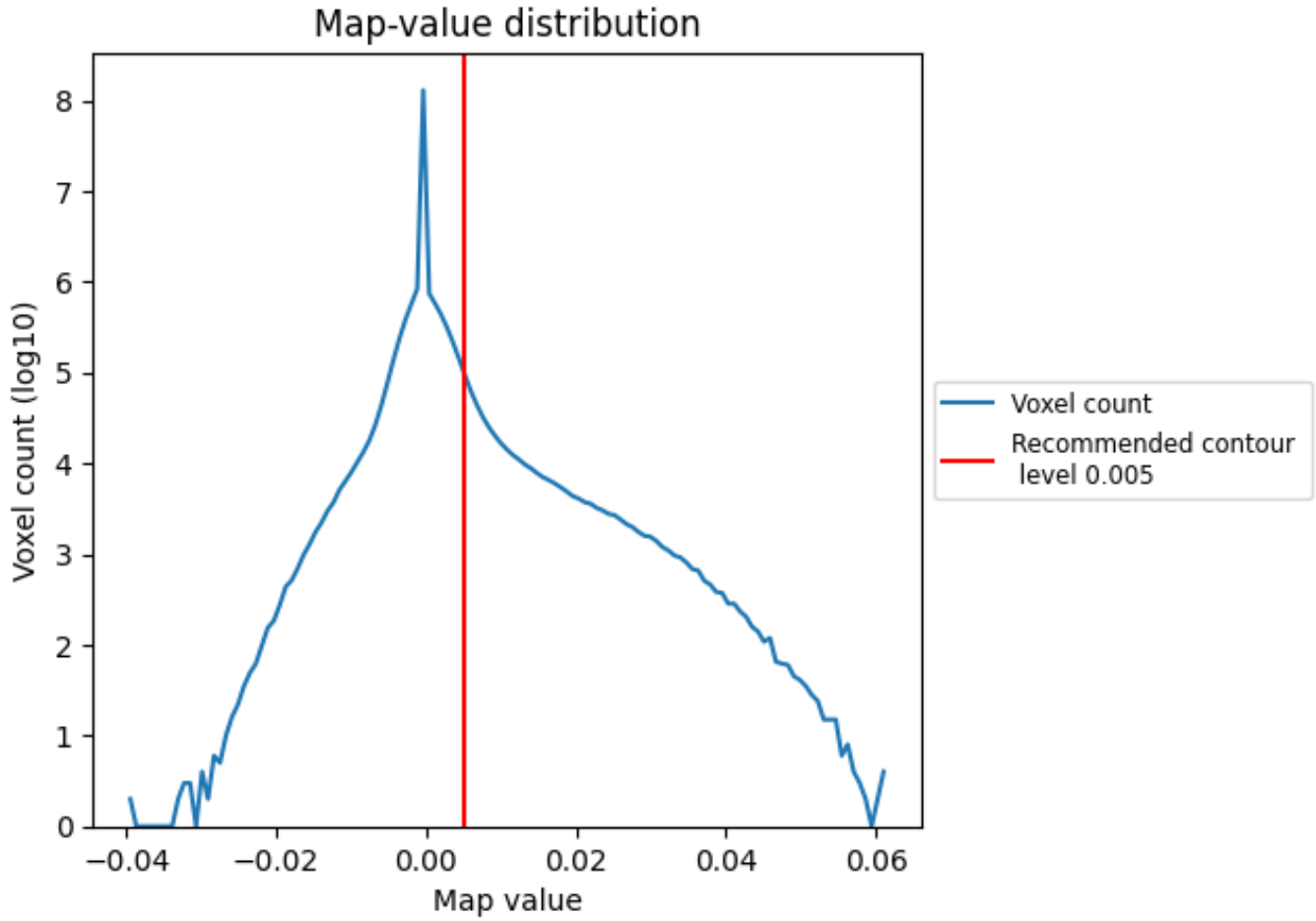


Z

7 Map analysis

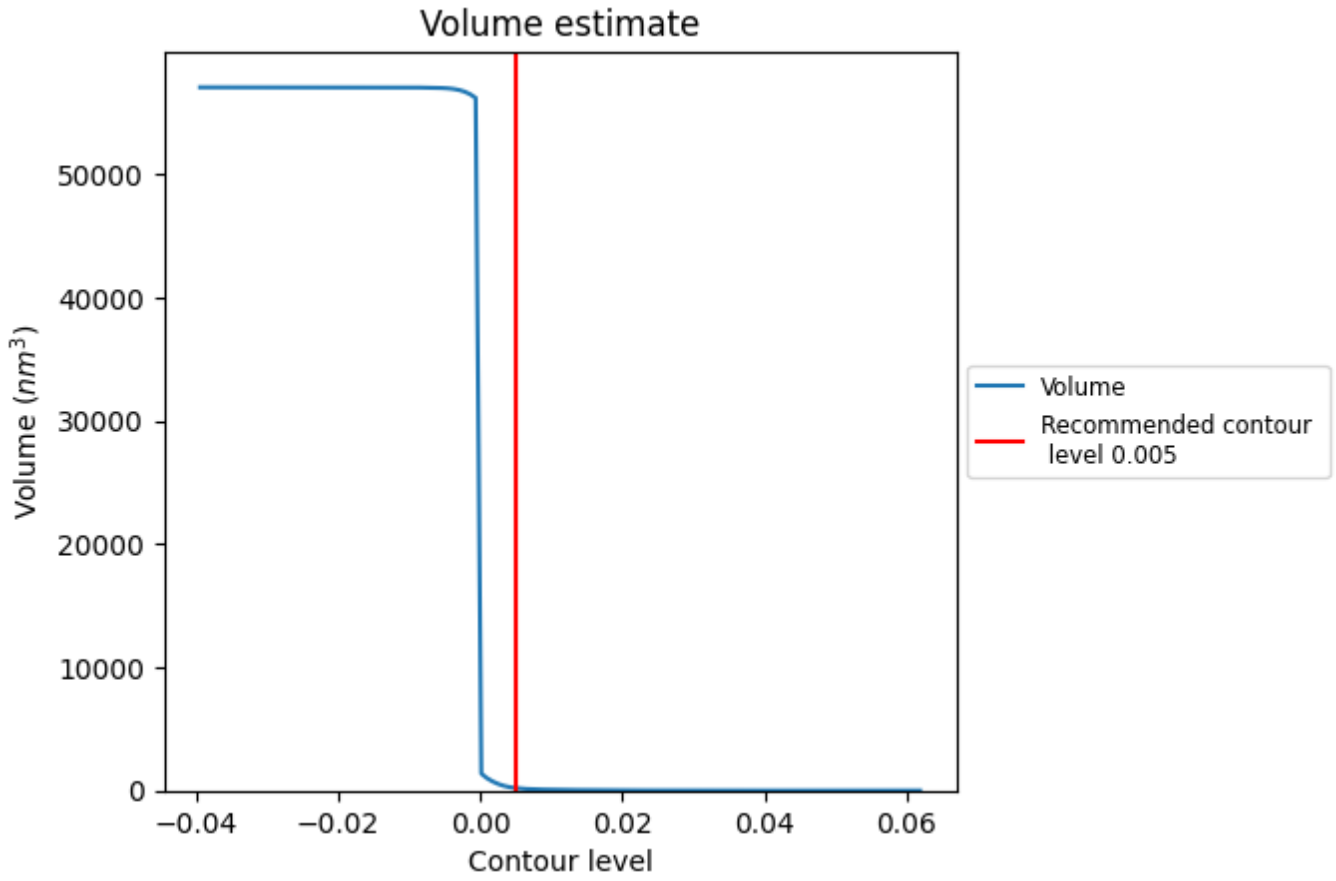
This section contains the results of statistical analysis of the map.

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.

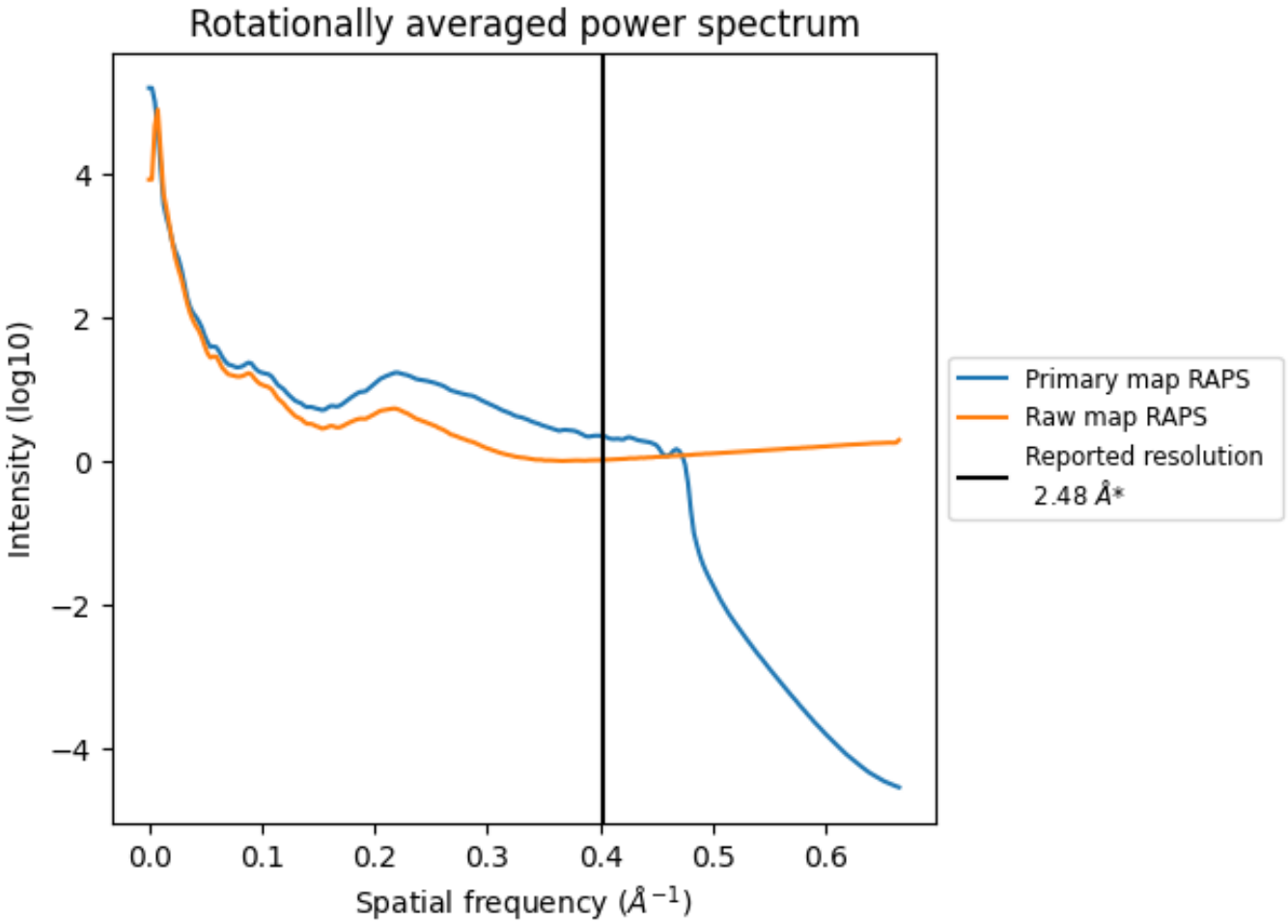
7.2 Volume estimate



The volume at the recommended contour level is 201 nm^3; this corresponds to an approximate mass of 181 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)

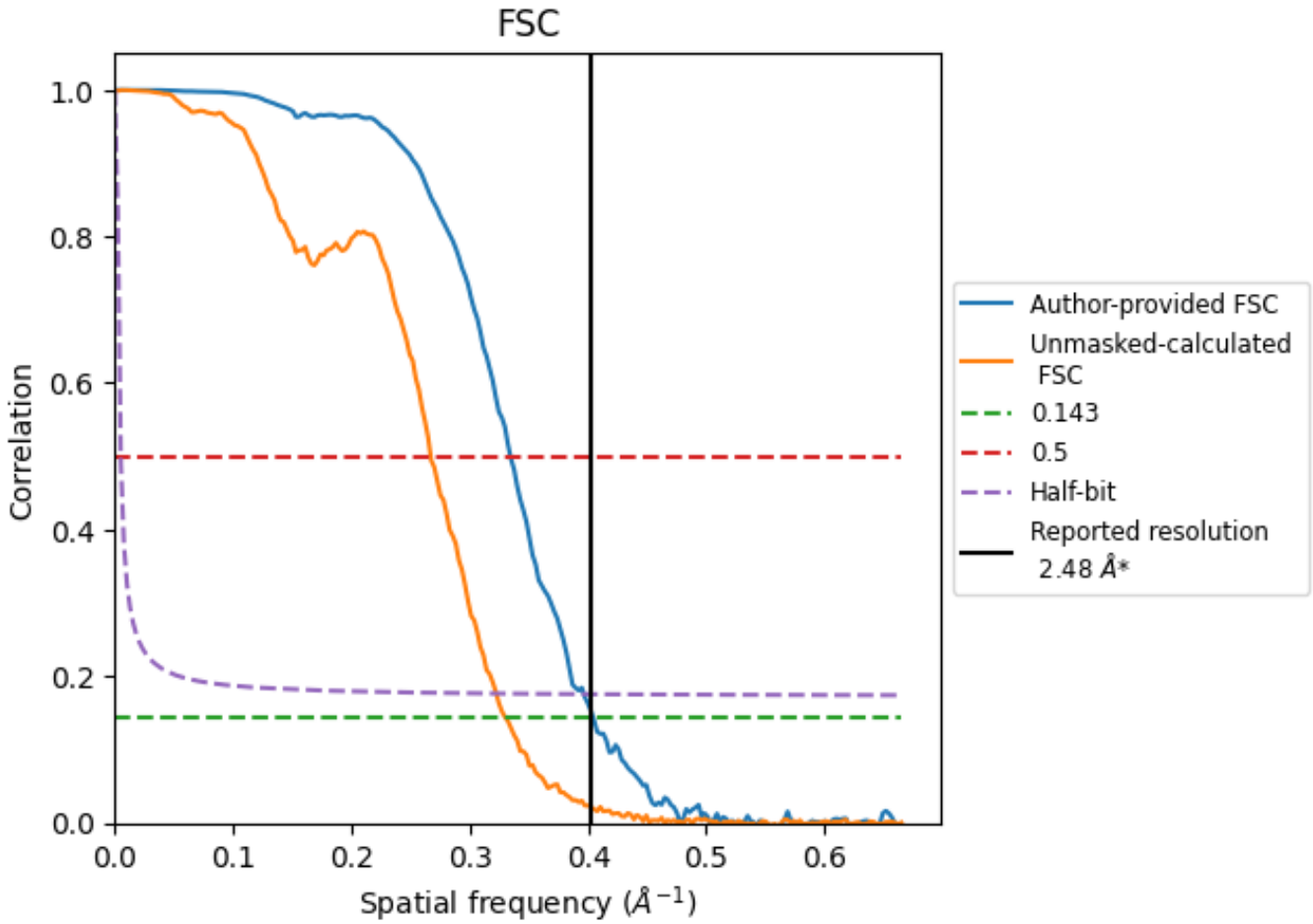


*Reported resolution corresponds to spatial frequency of 0.403 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.403 Å^{-1}

8.2 Resolution estimates (i)

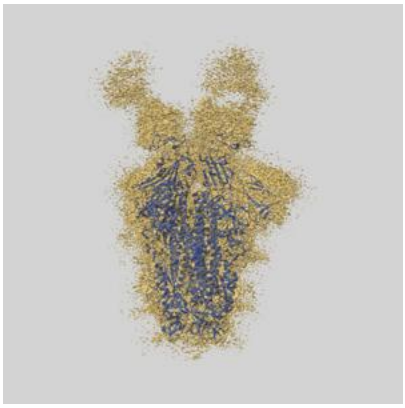
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.47	2.99	2.52
Unmasked-calculated*	3.03	3.74	3.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.48 by more than 10 %

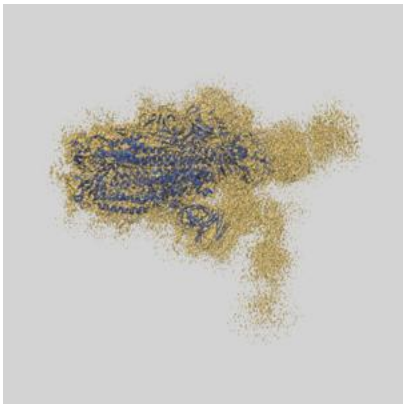
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34469 and PDB model 8H3M. Per-residue inclusion information can be found in section 3 on page 12.

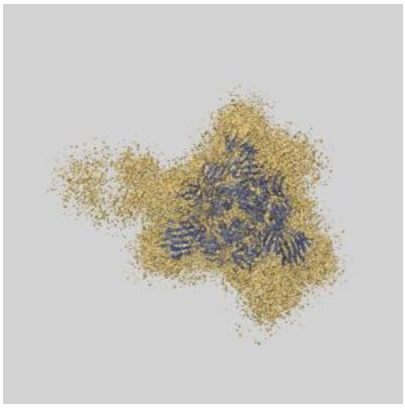
9.1 Map-model overlay



X



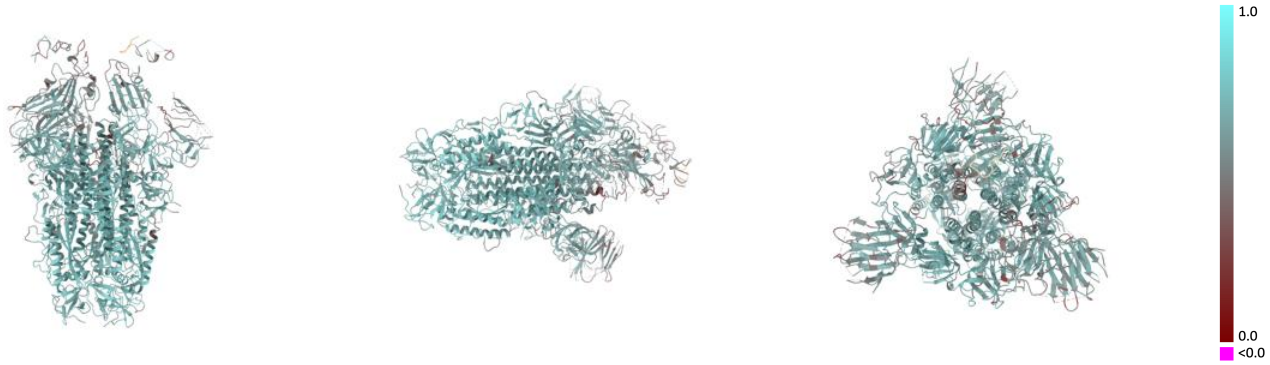
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

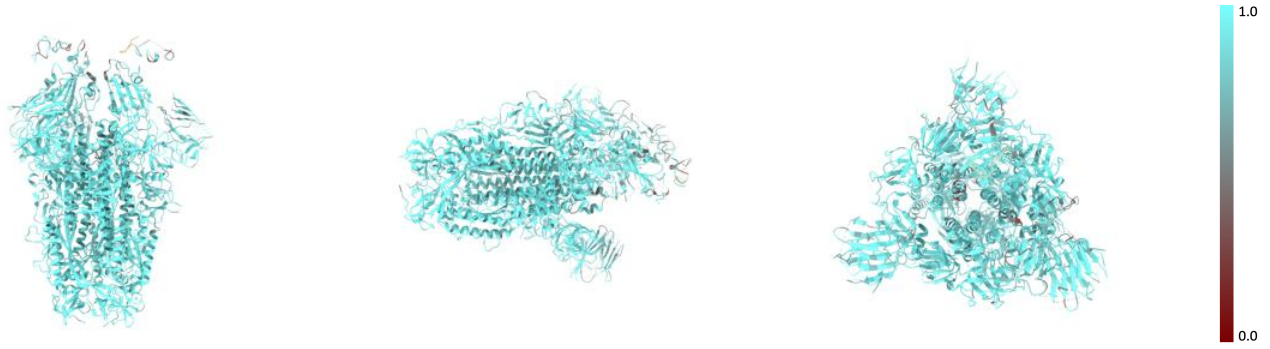
9.2 Q-score mapped to coordinate model (i)



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.

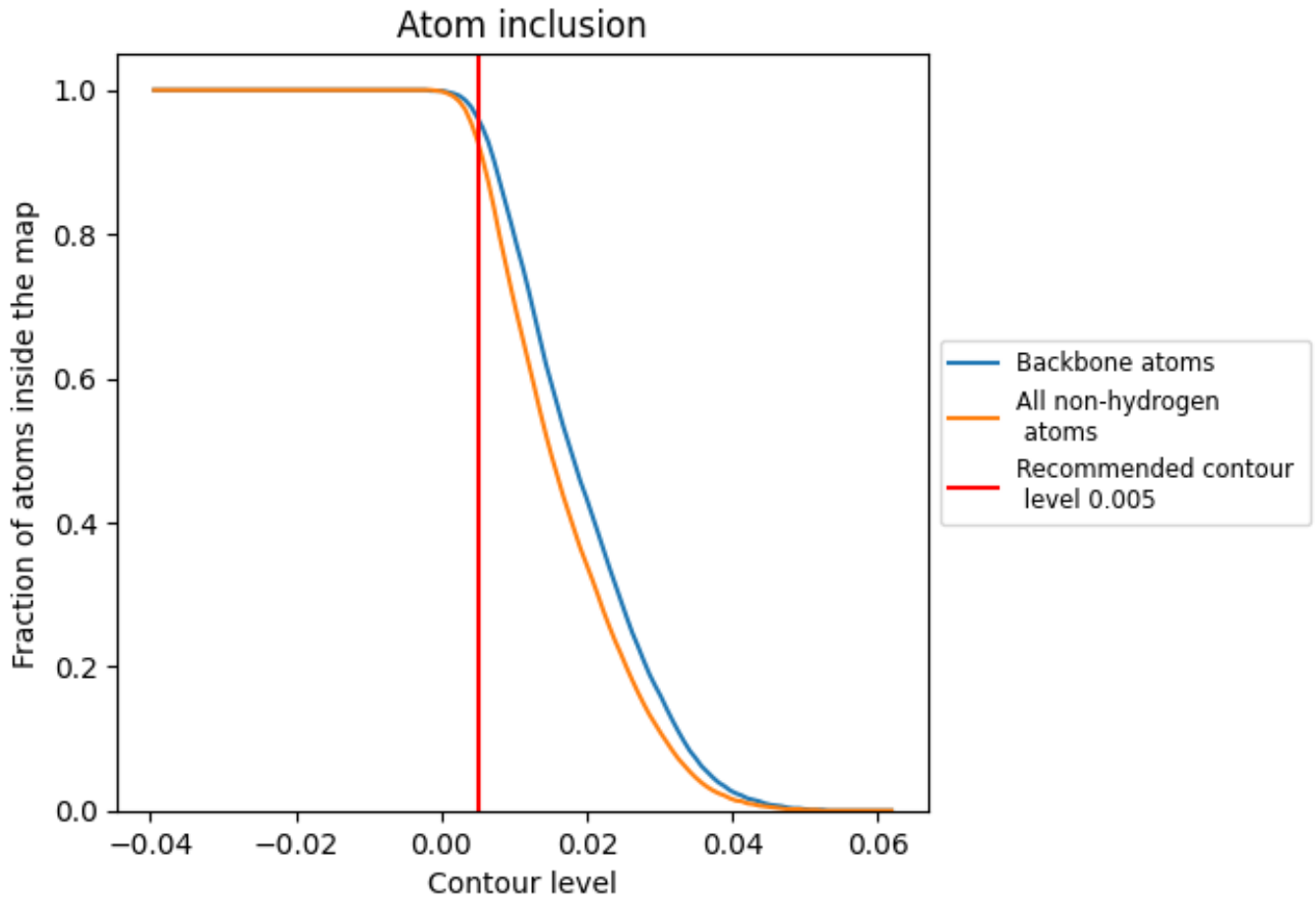
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9290	0.6350
A	0.9390	0.6430
B	0.9430	0.6470
C	0.9250	0.6300
D	0.6810	0.4580
H	0.6720	0.4540