Full wwPDB EM Validation Report ⓘ

Aug 8, 2024 – 12:34 PM JST

PDB ID	:	8KEO
EMDB ID	:	EMD-37162
Title	:	Structure of SARS-CoV-2 Omicron BA.1 Spike complexed with antibody PW5-570
Authors	:	Sun, L.; Mao, Q.; Wang, Y.
Deposited on	:	2023-08-13
Resolution	:	2.78 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:

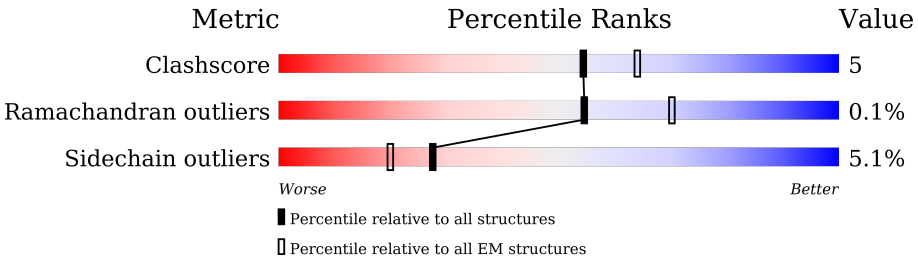
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.78 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	1285	69% 13% 17%
1	B	1285	67% 14% 17%
1	C	1285	67% 14% 17%
2	E	451	23% 39% 9% 52%
2	G	451	37% 38% 9% 52%
2	I	451	32% 38% 10% 52%
3	D	215	60% 83% 15%
3	F	215	87% 84% 13%

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Mol	Chain	Length	Quality of chain
3	H	215	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34788 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	B	1063	Total	C	N	O	S	0	0
			8336	5328	1391	1580	37		
1	A	1063	Total	C	N	O	S	0	0
			8336	5328	1391	1580	37		
1	C	1063	Total	C	N	O	S	0	0
			8336	5328	1391	1580	37		

There are 363 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	96	ILE	THR	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	variant	UNP P0DTC2
B	212	GLU	-	insertion	UNP P0DTC2
B	213	PRO	-	insertion	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	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	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
A	70	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	96	ILE	THR	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	variant	UNP P0DTC2
A	212	GLU	-	insertion	UNP P0DTC2
A	213	PRO	-	insertion	UNP P0DTC2
A	214	GLU	-	insertion	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	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	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
C	70	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	96	ILE	THR	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	ILE	LEU	variant	UNP P0DTC2
C	212	GLU	-	insertion	UNP P0DTC2
C	213	PRO	-	insertion	UNP P0DTC2
C	214	GLU	-	insertion	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	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called PW5-570 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	215	Total	C	N	O	S	0	0
			1615	1012	277	317	9		
2	G	215	Total	C	N	O	S	0	0
			1615	1012	277	317	9		
2	I	215	Total	C	N	O	S	0	0
			1615	1012	277	317	9		

- Molecule 3 is a protein called PW5-570 light chain.

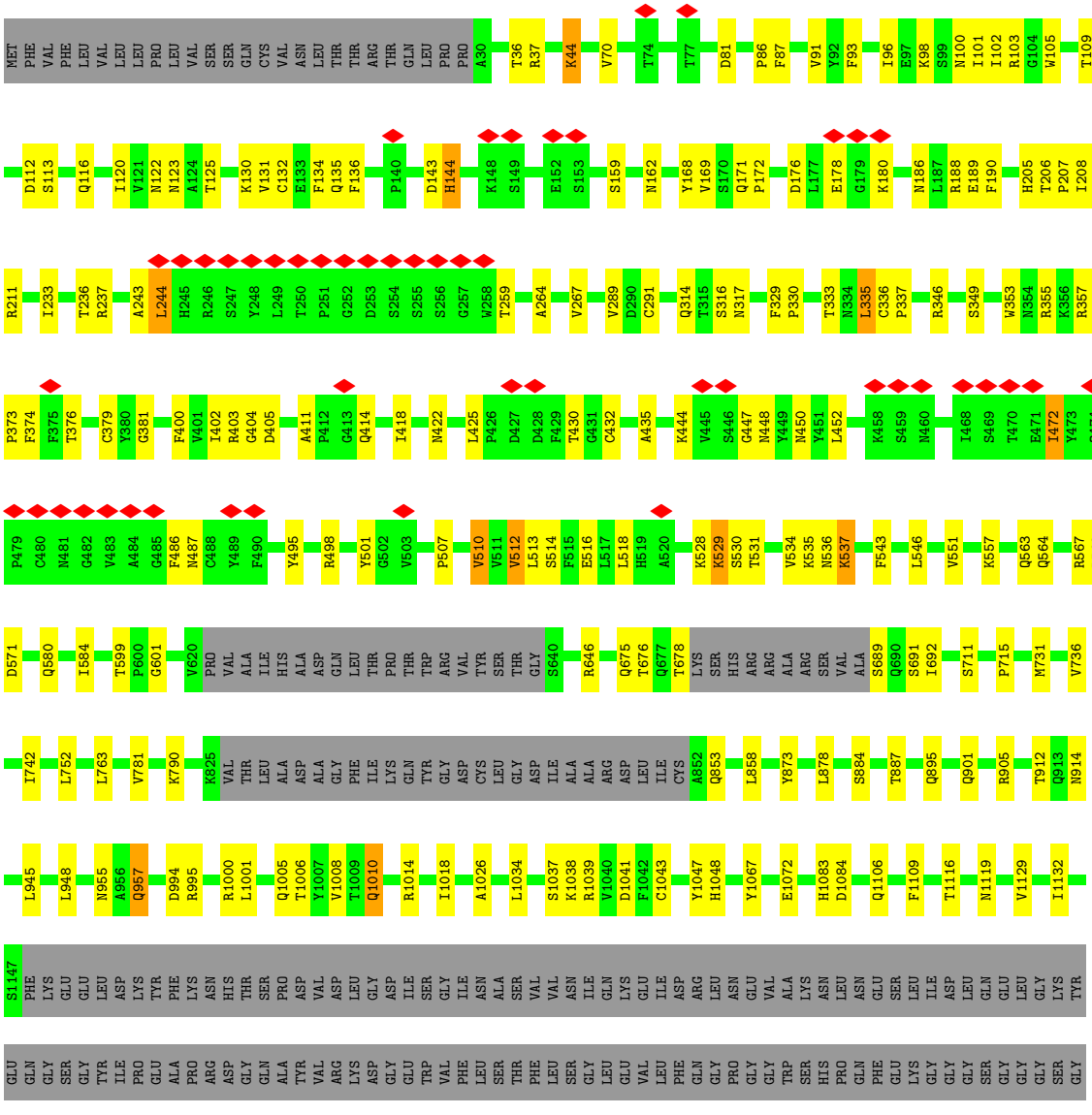
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	211	Total	C	N	O	S	0	0
			1645	1033	282	326	4		
3	F	211	Total	C	N	O	S	0	0
			1645	1033	282	326	4		
3	H	211	Total	C	N	O	S	0	0
			1645	1033	282	326	4		

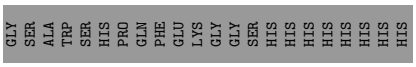
3 Residue-property plots (i)

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

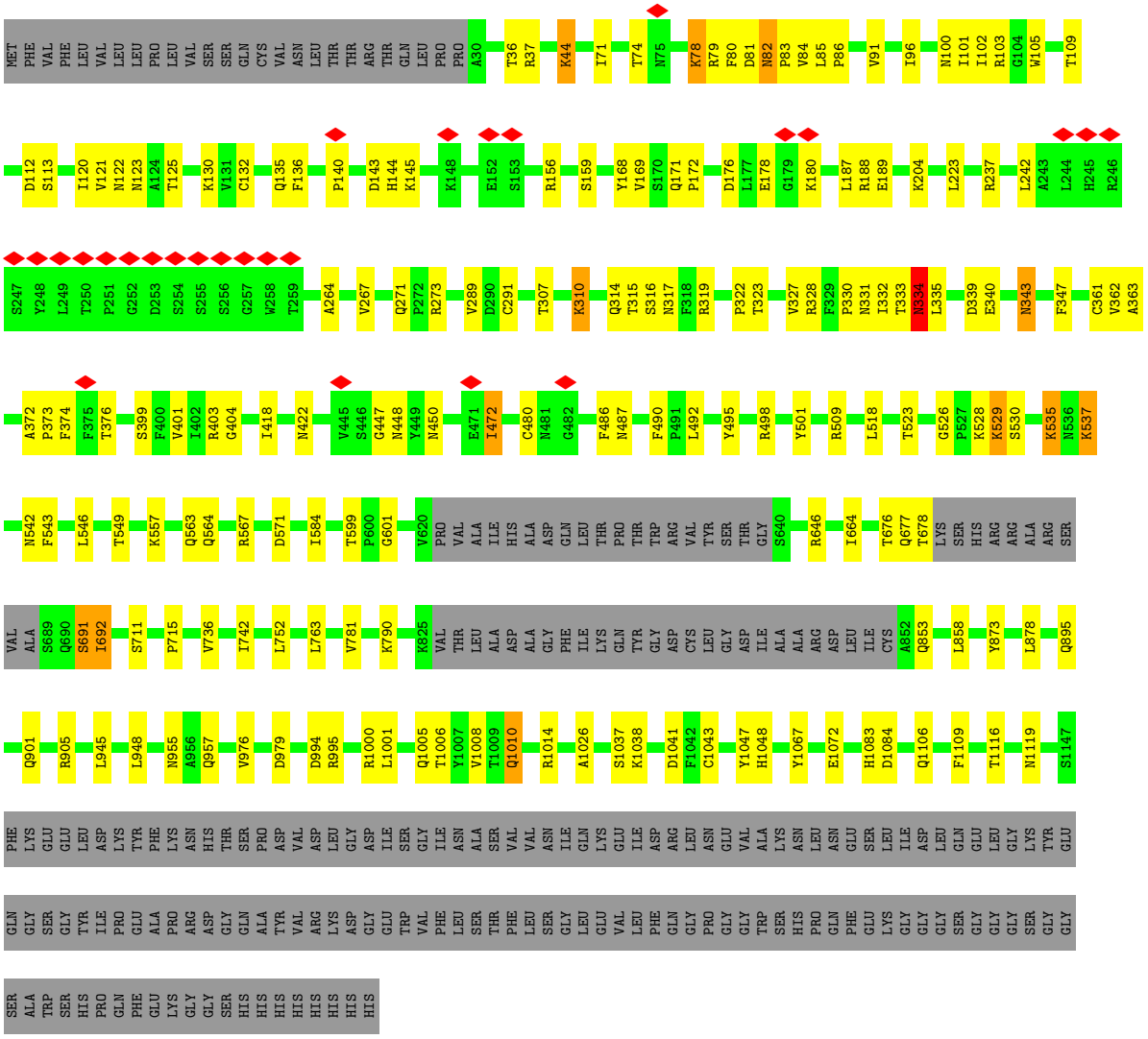
Chain B:





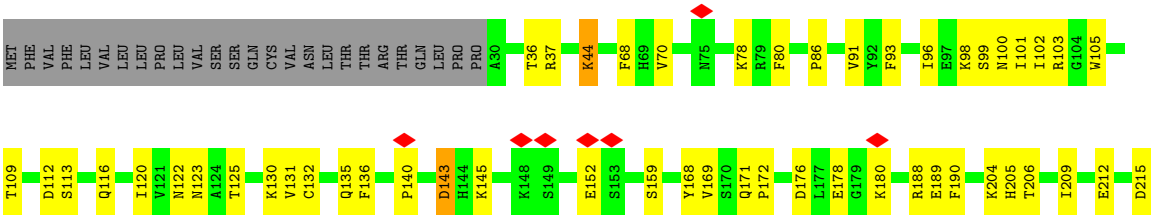
• Molecule 1: Spike glycoprotein

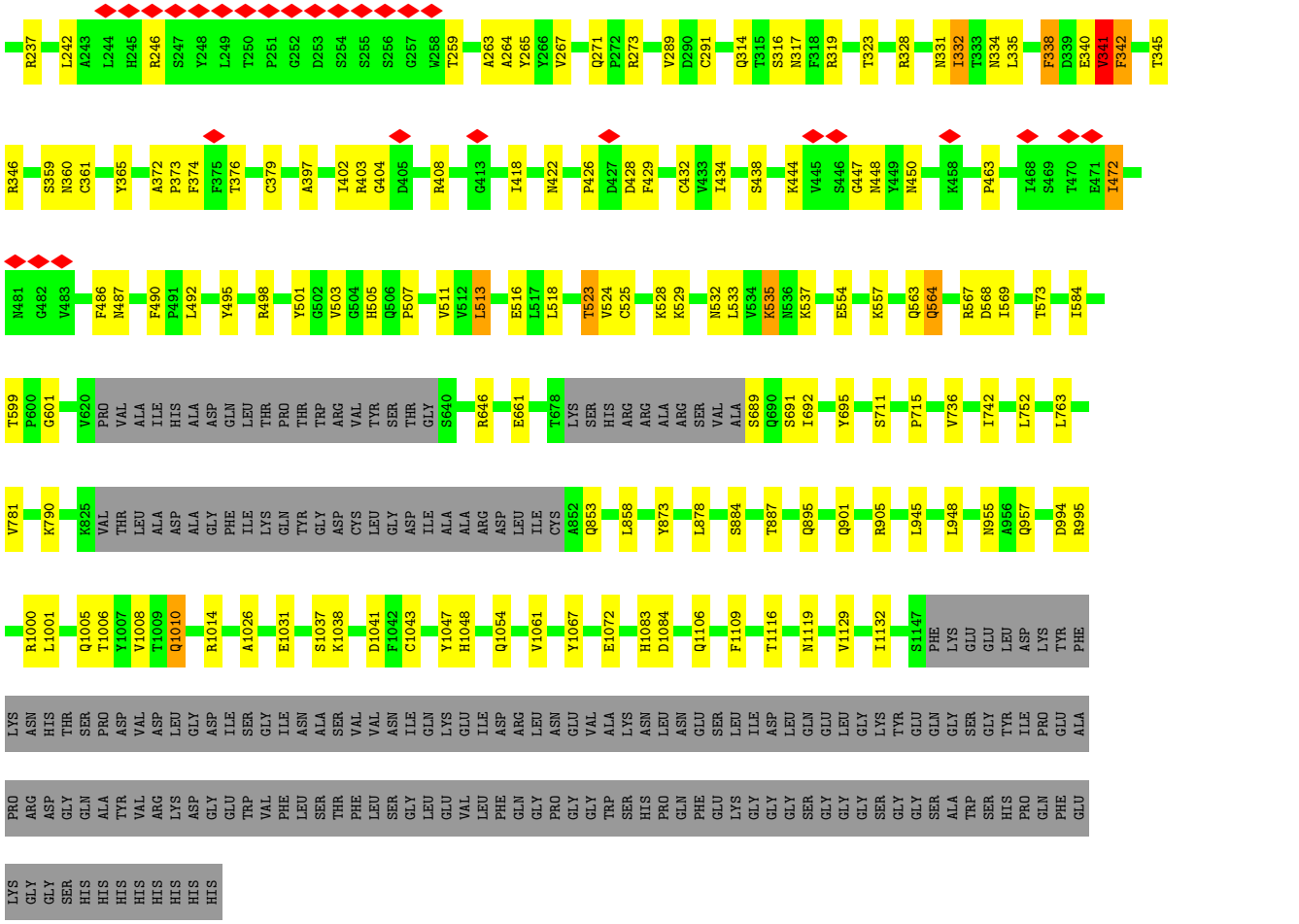
Chain A:



• Molecule 1: Spike glycoprotein

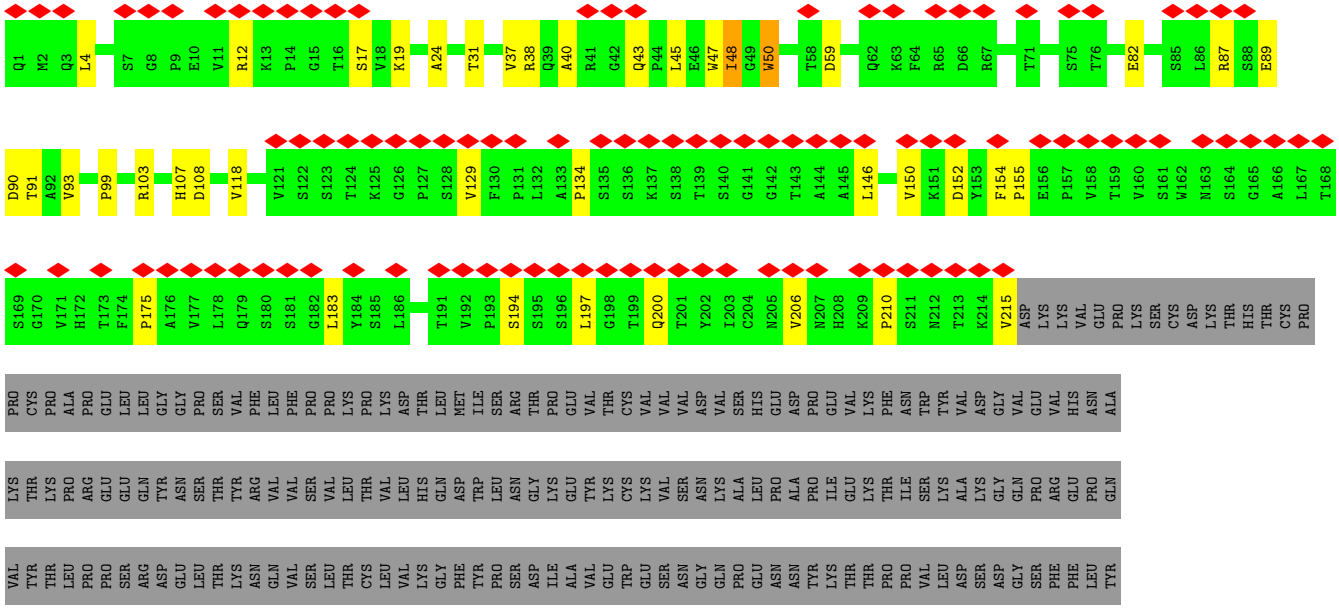
Chain C:





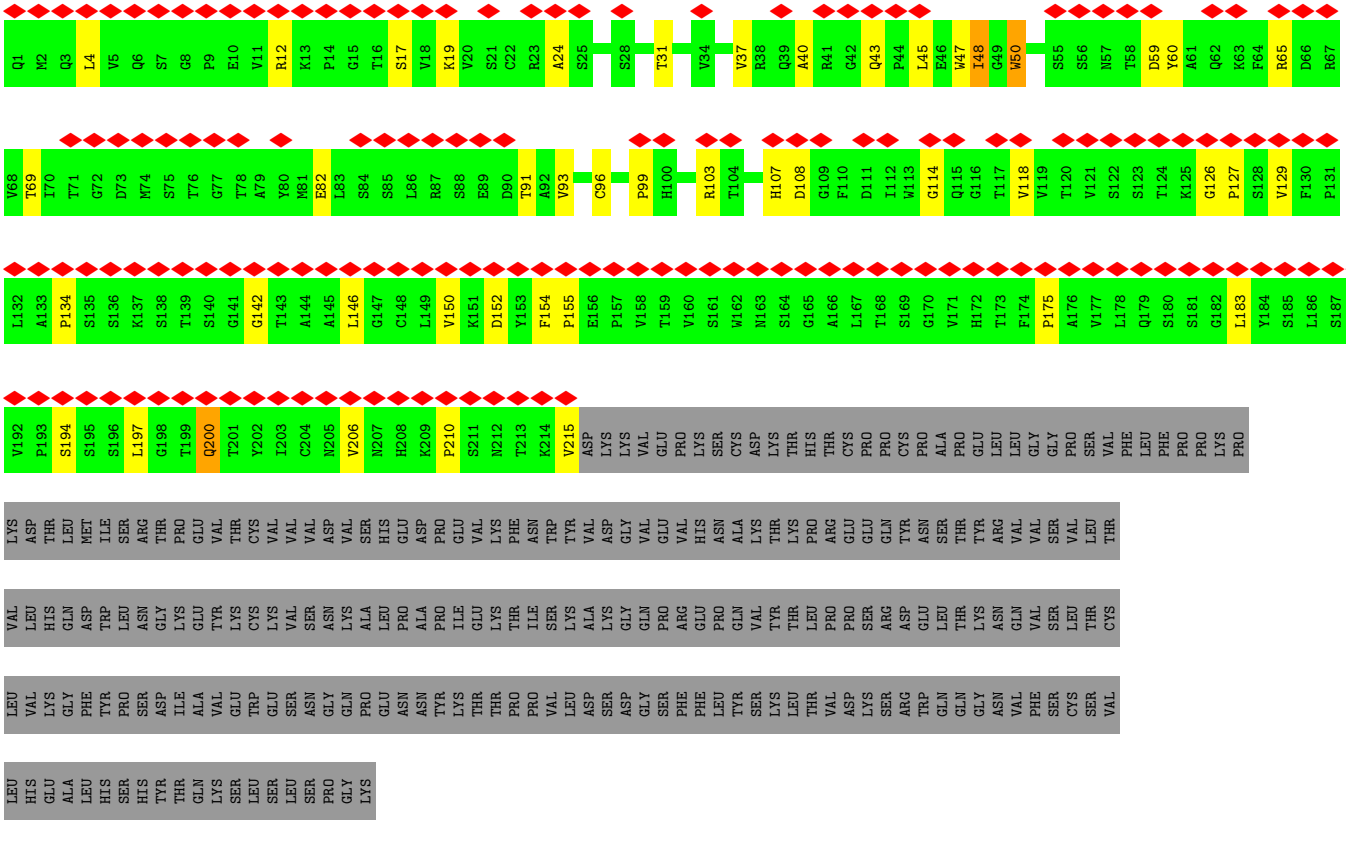
• Molecule 2: PW5-570 heavy chain

Chain E:



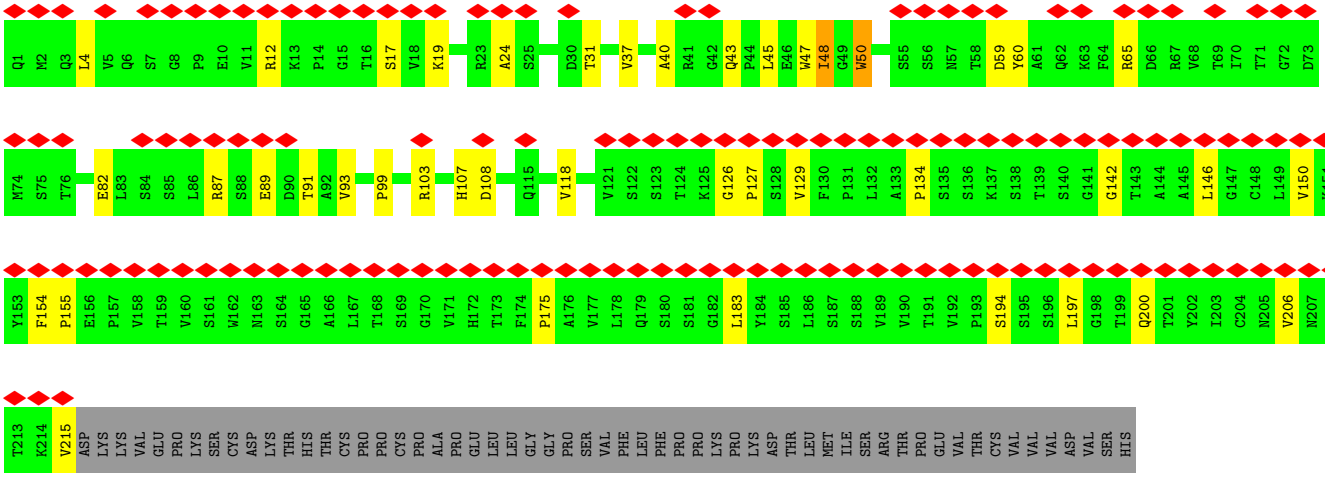
• Molecule 2: PW5-570 heavy chain

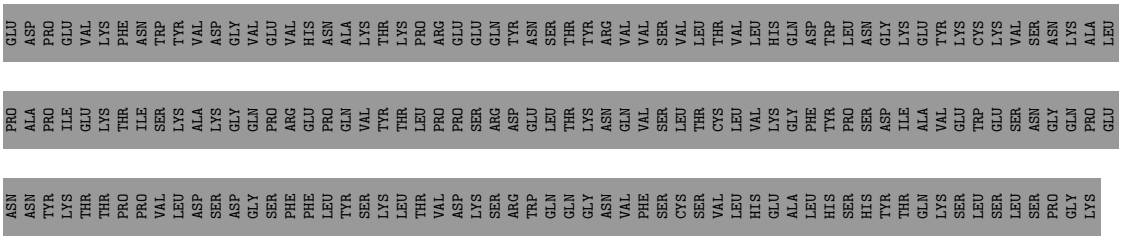
Chain G:



• Molecule 2: PW5-570 heavy chain

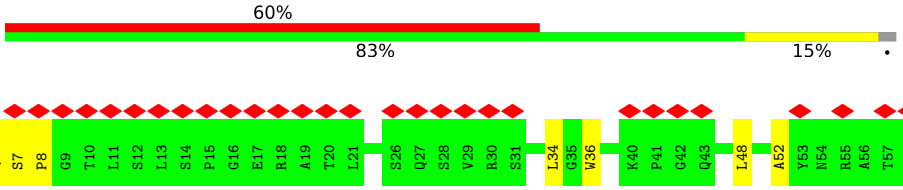
Chain I:

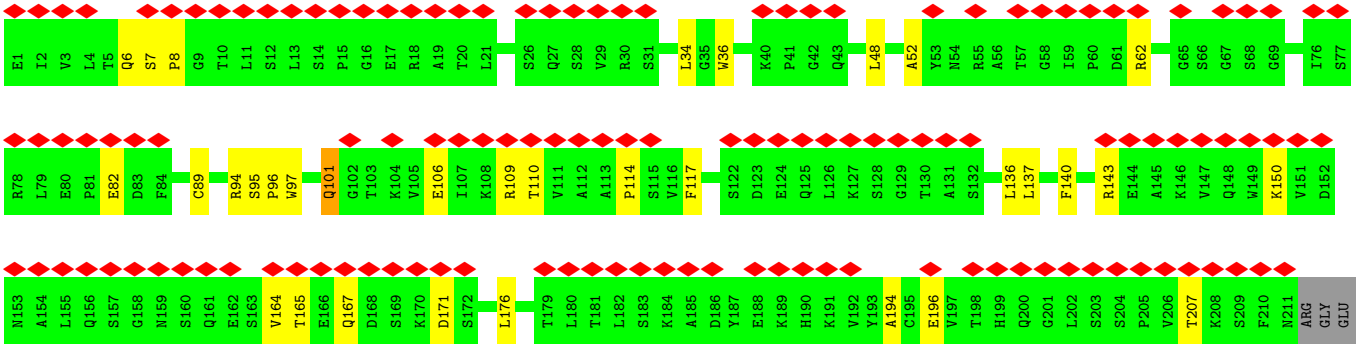




• Molecule 3: PW5-570 light chain

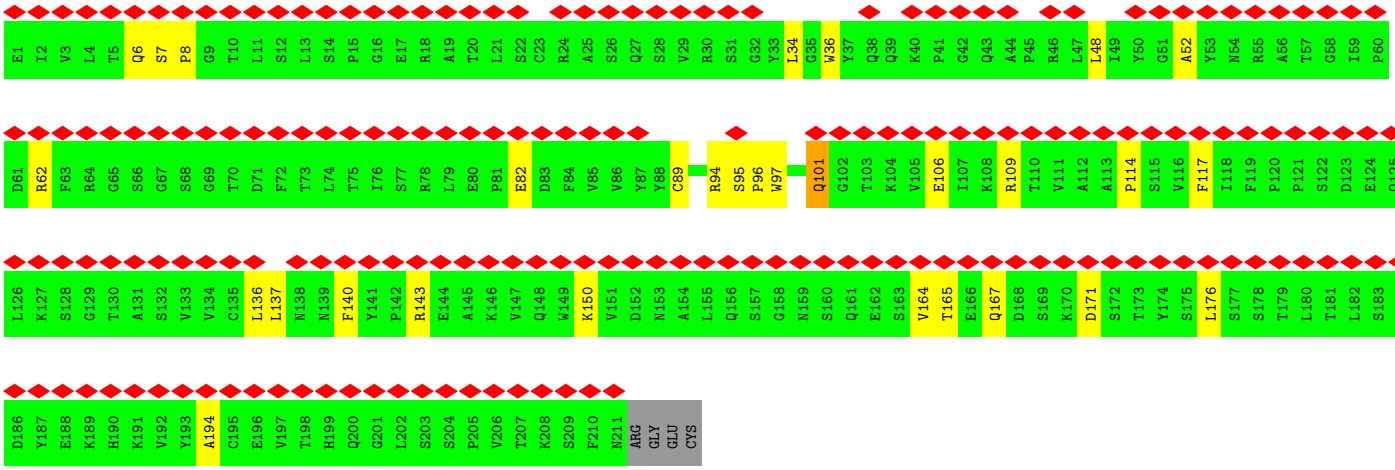
Chain D:





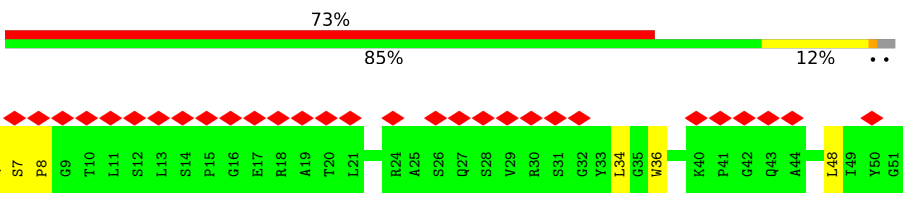
• Molecule 3: PW5-570 light chain

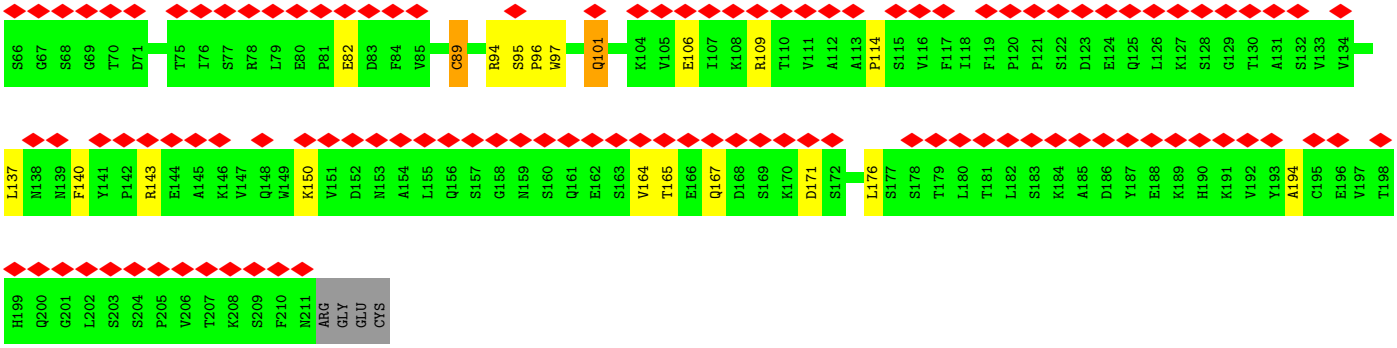
Chain F:



• Molecule 3: PW5-570 light chain

Chain H:




S66 G67 S68 G69 T70 D71 T75 I76 S77 R78 L79 E80 P81 E82 D83 F84 V85 C89 R94 S95 P96 W97 Q101 K104 V105 E106 I107 K108 R109 T110 V111 A112 A113 P114 S115 V116 F117 I118 F119 P120 P121 S122 D123 E124 Q125 L126 K127 S128 G129 T130 A131 S132 V133 V134
L137 N138 N139 F140 Y141 P142 R143 E144 A145 K146 V147 Q148 W149 K150 V151 D152 N153 A154 L155 Q156 S157 G158 N159 S160 Q161 E162 S163 V164 T165 E166 Q167 D168 S169 K170 D171 S172 L176 S177 S178 T179 L180 T181 L182 S183 K184 A185 D186 Y187 E188 K189 H190 K191 V192 Y193 A194 C195 E196 V197 T198
H199 Q200 G201 L202 S203 S204 P205 V206 T207 K208 S209 F210 N211 ARG GLY GLU CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439708	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	380.80002, 380.80002, 380.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/8534	0.44	0/11606
1	B	0.29	0/8534	0.44	0/11606
1	C	0.29	0/8534	0.45	0/11606
2	E	0.24	0/1655	0.44	0/2259
2	G	0.24	0/1655	0.44	0/2259
2	I	0.24	0/1655	0.44	0/2259
3	D	0.24	0/1683	0.43	0/2286
3	F	0.24	0/1683	0.43	0/2286
3	H	0.24	0/1683	0.43	0/2286
All	All	0.28	0/35616	0.44	0/48453

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8336	0	8153	84	0
1	B	8336	0	8155	93	0
1	C	8336	0	8153	95	0
2	E	1615	0	1566	22	0
2	G	1615	0	1566	26	0
2	I	1615	0	1566	25	0
3	D	1645	0	1600	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1645	0	1600	19	0
3	H	1645	0	1600	17	0
All	All	34788	0	33959	374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (374) 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:363:ALA:HB3	1:A:526:GLY:HA2	1.50	0.91
1:C:152:GLU:HA	1:C:246:ARG:HG2	1.74	0.70
1:C:338:PHE:HB2	1:C:365:TYR:CE1	2.29	0.67
3:F:143:ARG:HD3	3:F:164:VAL:HG11	1.77	0.67
2:E:134:PRO:HG3	2:E:146:LEU:HB3	1.77	0.66
1:A:96:ILE:H	1:A:264:ALA:HB3	1.60	0.66
2:I:134:PRO:HG3	2:I:146:LEU:HB3	1.77	0.66
3:D:143:ARG:HD3	3:D:164:VAL:HG11	1.78	0.65
2:G:134:PRO:HG3	2:G:146:LEU:HB3	1.77	0.65
1:B:435:ALA:HB2	1:B:510:VAL:HA	1.78	0.64
3:H:143:ARG:HD3	3:H:164:VAL:HG11	1.80	0.63
1:B:96:ILE:H	1:B:264:ALA:HB3	1.62	0.62
1:B:537:LYS:H	1:B:551:VAL:HG13	1.64	0.62
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.33	0.62
1:A:123:ASN:ND2	1:A:125:THR:OG1	2.33	0.62
1:C:96:ILE:H	1:C:264:ALA:HB3	1.65	0.62
1:B:123:ASN:ND2	1:B:125:THR:OG1	2.33	0.62
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.33	0.61
1:B:448:ASN:ND2	1:B:450:ASN:OD1	2.32	0.61
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.33	0.61
1:A:448:ASN:ND2	1:A:450:ASN:OD1	2.32	0.61
1:C:359:SER:HA	1:C:524:VAL:HG22	1.82	0.61
1:C:98:LYS:H	1:C:259:THR:HG21	1.66	0.61
2:E:50:TRP:HE1	2:E:59:ASP:HB3	1.65	0.61
1:A:102:ILE:HG12	1:A:242:LEU:HG	1.81	0.60
1:C:86:PRO:HA	1:C:237:ARG:HA	1.82	0.60
2:G:50:TRP:HE1	2:G:59:ASP:HB3	1.66	0.60
1:B:98:LYS:H	1:B:259:THR:HG21	1.66	0.60
1:C:123:ASN:ND2	1:C:125:THR:OG1	2.34	0.60
1:C:101:ILE:HG13	1:C:102:ILE:HG13	1.84	0.59
1:C:338:PHE:HB2	1:C:365:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HA	1:A:237:ARG:HA	1.84	0.59
1:B:381:GLY:HA3	1:B:430:THR:HA	1.85	0.59
1:B:543:PHE:HB2	1:B:546:LEU:HD12	1.85	0.59
2:I:50:TRP:HE1	2:I:59:ASP:HB3	1.67	0.59
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	1.85	0.58
1:B:37:ARG:NH1	1:B:189:GLU:OE2	2.37	0.58
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.85	0.58
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.85	0.58
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.86	0.58
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.86	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.86	0.57
1:A:487:ASN:ND2	2:E:108:ASP:OD1	2.37	0.57
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.86	0.57
1:A:37:ARG:NH1	1:A:189:GLU:OE2	2.38	0.57
2:I:12:ARG:NH2	2:I:17:SER:O	2.38	0.57
1:C:37:ARG:NH1	1:C:189:GLU:OE2	2.38	0.57
1:A:736:VAL:HG12	1:A:858:LEU:HG	1.86	0.57
1:C:736:VAL:HG12	1:C:858:LEU:HG	1.86	0.57
2:E:12:ARG:NH2	2:E:17:SER:O	2.37	0.57
1:B:86:PRO:HA	1:B:237:ARG:HA	1.87	0.57
3:H:114:PRO:HB3	3:H:140:PHE:HB3	1.87	0.57
1:B:400:PHE:HZ	1:B:510:VAL:HG22	1.70	0.57
1:A:101:ILE:HG13	1:A:102:ILE:HG13	1.86	0.57
1:B:736:VAL:HG12	1:B:858:LEU:HG	1.87	0.56
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.86	0.56
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.88	0.56
1:A:144:HIS:HB3	1:A:145:LYS:HE2	1.85	0.56
1:C:1006:THR:O	1:C:1010:GLN:NE2	2.39	0.56
3:D:114:PRO:HB3	3:D:140:PHE:HB3	1.86	0.56
2:I:108:ASP:OD1	1:C:487:ASN:ND2	2.39	0.56
1:B:116:GLN:NE2	1:B:131:VAL:O	2.35	0.56
1:B:120:ILE:O	1:B:122:ASN:ND2	2.39	0.56
1:B:487:ASN:ND2	2:G:108:ASP:OD1	2.39	0.56
1:A:123:ASN:HD22	1:A:125:THR:H	1.54	0.56
1:A:105:TRP:HB2	1:A:120:ILE:HD12	1.88	0.55
3:D:6:GLN:NE2	3:D:89:CYS:SG	2.74	0.55
1:B:70:VAL:HG22	1:B:81:ASP:HB2	1.87	0.55
1:B:329:PHE:HB3	1:B:528:LYS:HD3	1.89	0.55
3:F:114:PRO:HB3	3:F:140:PHE:HB3	1.87	0.55
1:A:955:ASN:OD1	1:A:1014:ARG:NH1	2.40	0.55
1:A:44:LYS:HB2	1:C:563:GLN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:HZ	2:E:99:PRO:HG3	1.71	0.55
1:C:116:GLN:NE2	1:C:131:VAL:O	2.35	0.55
2:I:99:PRO:HG3	1:C:486:PHE:HZ	1.71	0.55
1:C:123:ASN:HD22	1:C:125:THR:H	1.55	0.55
1:B:335:LEU:HG	1:B:364:ASP:HB3	1.89	0.55
1:B:955:ASN:OD1	1:B:1014:ARG:NH1	2.39	0.55
1:C:599:THR:HG22	1:C:601:GLY:H	1.71	0.55
1:B:1006:THR:OG1	1:C:1005:GLN:NE2	2.39	0.54
2:G:93:VAL:HG22	2:G:118:VAL:HG22	1.88	0.54
1:A:599:THR:HG22	1:A:601:GLY:H	1.72	0.54
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.90	0.54
1:A:1005:GLN:NE2	1:C:1006:THR:OG1	2.41	0.54
1:A:71:ILE:HB	1:A:78:LYS:HG3	1.90	0.54
1:C:1116:THR:H	1:C:1119:ASN:HD21	1.55	0.54
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.90	0.54
1:A:1006:THR:O	1:A:1010:GLN:NE2	2.39	0.54
1:B:123:ASN:HD22	1:B:125:THR:H	1.56	0.54
1:B:1005:GLN:NE2	1:A:1006:THR:OG1	2.41	0.54
1:A:143:ASP:HB2	1:A:156:ARG:HD3	1.89	0.54
3:F:6:GLN:NE2	3:F:89:CYS:SG	2.75	0.54
1:C:955:ASN:OD1	1:C:1014:ARG:NH1	2.41	0.54
1:B:178:GLU:HB3	1:B:180:LYS:HD3	1.90	0.53
1:B:472:ILE:HD13	1:B:472:ILE:H	1.73	0.53
1:C:472:ILE:HD13	1:C:472:ILE:H	1.74	0.53
1:B:1006:THR:O	1:B:1010:GLN:NE2	2.39	0.53
1:A:178:GLU:HB3	1:A:180:LYS:HD3	1.90	0.53
3:F:6:GLN:H	3:F:101:GLN:HE22	1.56	0.53
1:B:100:ASN:OD1	1:B:103:ARG:NE	2.40	0.53
1:B:599:THR:HG22	1:B:601:GLY:H	1.73	0.53
1:A:1037:SER:H	1:A:1048:HIS:HD2	1.56	0.53
2:E:19:LYS:NZ	2:E:82:GLU:OE2	2.42	0.53
1:C:178:GLU:HB3	1:C:180:LYS:HD3	1.91	0.53
2:I:93:VAL:HG22	2:I:118:VAL:HG22	1.90	0.53
2:E:93:VAL:HG22	2:E:118:VAL:HG22	1.91	0.52
1:C:143:ASP:OD1	1:C:143:ASP:N	2.41	0.52
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.90	0.52
1:A:472:ILE:HD13	1:A:472:ILE:H	1.74	0.52
1:C:176:ASP:O	1:C:188:ARG:NH2	2.42	0.52
1:B:884:SER:HG	1:B:887:THR:HG1	1.56	0.52
1:A:176:ASP:O	1:A:188:ARG:NH2	2.42	0.52
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLN:H	3:D:101:GLN:HE22	1.56	0.52
1:C:361:CYS:O	1:C:524:VAL:HA	2.09	0.52
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.91	0.52
3:H:6:GLN:H	3:H:101:GLN:HE22	1.58	0.52
1:C:379:CYS:HA	1:C:432:CYS:HA	1.91	0.52
1:C:448:ASN:ND2	1:C:450:ASN:OD1	2.32	0.52
1:B:144:HIS:H	1:B:243:ALA:HB1	1.75	0.52
1:B:349:SER:OG	1:B:452:LEU:O	2.28	0.52
1:B:486:PHE:HZ	2:G:99:PRO:HG3	1.75	0.52
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.92	0.52
1:A:135:GLN:HB3	1:A:159:SER:HB3	1.92	0.52
1:A:1116:THR:H	1:A:1119:ASN:HD21	1.58	0.52
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.91	0.52
2:G:12:ARG:NH2	2:G:17:SER:O	2.40	0.51
2:I:19:LYS:NZ	2:I:82:GLU:OE2	2.43	0.51
3:D:117:PHE:HB2	3:D:136:LEU:HB3	1.92	0.51
3:H:6:GLN:NE2	3:H:89:CYS:SG	2.75	0.51
1:C:91:VAL:HG23	1:C:267:VAL:HG13	1.92	0.51
1:C:120:ILE:O	1:C:122:ASN:ND2	2.43	0.51
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.93	0.51
1:B:130:LYS:HG2	1:B:132:CYS:H	1.76	0.51
2:I:175:PRO:HD3	3:H:165:THR:HG22	1.93	0.51
1:B:105:TRP:HB2	1:B:120:ILE:HD12	1.92	0.51
2:G:19:LYS:NZ	2:G:82:GLU:OE2	2.44	0.51
1:B:357:ARG:O	1:B:357:ARG:NH1	2.44	0.51
3:H:34:LEU:HD23	3:H:52:ALA:HB2	1.92	0.50
1:B:135:GLN:HB3	1:B:159:SER:HB3	1.92	0.50
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.92	0.50
1:A:310:LYS:HZ3	1:A:664:ILE:HG12	1.74	0.50
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.58	0.50
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.94	0.50
1:B:557:LYS:HB2	1:B:584:ILE:HG21	1.93	0.50
1:A:567:ARG:NH1	1:A:571:ASP:OD1	2.43	0.50
1:B:425:LEU:HD13	1:B:512:VAL:HG21	1.93	0.50
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.76	0.50
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.94	0.50
3:F:62:ARG:NH2	3:F:82:GLU:OE2	2.42	0.50
1:C:884:SER:OG	1:C:887:THR:OG1	2.29	0.50
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.77	0.50
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.57	0.50
1:A:752:LEU:HD23	1:A:752:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HG2	1:C:505:HIS:HA	1.94	0.49
1:C:204:LYS:NZ	1:C:205:HIS:O	2.45	0.49
1:B:895:GLN:NE2	1:A:711:SER:OG	2.45	0.49
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.59	0.49
1:C:752:LEU:HD23	1:C:752:LEU:H	1.77	0.49
1:B:112:ASP:OD1	1:B:113:SER:N	2.46	0.49
1:C:105:TRP:HB2	1:C:120:ILE:HD12	1.92	0.49
3:F:95:SER:HB3	3:F:96:PRO:HD3	1.94	0.49
1:B:752:LEU:H	1:B:752:LEU:HD23	1.77	0.49
1:A:895:GLN:NE2	1:C:711:SER:OG	2.46	0.49
2:E:175:PRO:HD3	3:D:165:THR:HG22	1.94	0.49
2:G:152:ASP:HA	2:G:183:LEU:HD13	1.95	0.49
2:E:206:VAL:HG22	2:E:215:VAL:HG22	1.95	0.48
1:A:100:ASN:OD1	1:A:103:ARG:NE	2.45	0.48
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.60	0.48
1:C:112:ASP:OD1	1:C:113:SER:N	2.45	0.48
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.78	0.48
1:B:711:SER:OG	1:C:895:GLN:NE2	2.46	0.48
1:A:130:LYS:HG2	1:A:132:CYS:H	1.77	0.48
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.77	0.48
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.94	0.48
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.78	0.48
1:C:130:LYS:HG2	1:C:132:CYS:H	1.77	0.48
2:G:40:ALA:HB3	2:G:43:GLN:HB2	1.95	0.48
2:I:152:ASP:HA	2:I:183:LEU:HD13	1.94	0.48
3:H:62:ARG:NH2	3:H:82:GLU:OE2	2.45	0.48
1:B:994:ASP:HB3	1:A:995:ARG:HH22	1.78	0.48
1:C:135:GLN:HB3	1:C:159:SER:HB3	1.96	0.48
1:B:529:LYS:HB3	1:B:529:LYS:HE3	1.47	0.48
1:A:103:ARG:HB3	1:A:121:VAL:HG13	1.95	0.48
2:G:60:TYR:HB2	2:G:65:ARG:HB2	1.95	0.48
2:E:4:LEU:HG	2:E:24:ALA:HB2	1.96	0.47
3:D:95:SER:HB3	3:D:96:PRO:HD3	1.94	0.47
1:C:426:PRO:HD3	1:C:463:PRO:HB3	1.95	0.47
1:B:995:ARG:HH22	1:C:994:ASP:HB3	1.79	0.47
1:A:91:VAL:HG23	1:A:267:VAL:HG13	1.96	0.47
2:G:154:PHE:HB3	2:G:155:PRO:HD3	1.97	0.47
2:E:129:VAL:HG22	2:E:150:VAL:HG22	1.95	0.47
1:C:1037:SER:H	1:C:1048:HIS:HD2	1.62	0.47
1:B:289:VAL:HG12	1:B:291:CYS:H	1.79	0.47
2:G:175:PRO:HD3	3:F:165:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:37:VAL:HG11	2:I:45:LEU:HD13	1.96	0.47
1:C:567:ARG:NH1	1:C:573:THR:OG1	2.47	0.47
1:A:78:LYS:HD2	1:A:78:LYS:HA	1.65	0.47
1:A:112:ASP:OD1	1:A:113:SER:N	2.46	0.47
3:F:137:LEU:HB2	3:F:176:LEU:HB3	1.95	0.47
3:H:95:SER:HB3	3:H:96:PRO:HD3	1.94	0.47
1:B:176:ASP:O	1:B:188:ARG:NH2	2.47	0.47
1:A:289:VAL:HG12	1:A:291:CYS:H	1.79	0.47
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.97	0.47
2:I:59:ASP:OD2	3:H:95:SER:OG	2.33	0.47
2:E:155:PRO:HG2	2:E:210:PRO:HG2	1.97	0.47
1:A:271:GLN:OE1	1:A:273:ARG:NH2	2.40	0.47
1:C:68:PHE:HB2	1:C:265:TYR:HD2	1.80	0.47
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.97	0.47
1:C:102:ILE:HG12	1:C:242:LEU:HG	1.97	0.46
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.81	0.46
1:A:120:ILE:O	1:A:122:ASN:ND2	2.48	0.46
2:I:4:LEU:HG	2:I:24:ALA:HB2	1.97	0.46
1:B:44:LYS:HB2	1:A:563:GLN:HA	1.97	0.46
1:B:372:ALA:HB3	1:B:373:PRO:HD3	1.97	0.46
2:E:37:VAL:HG11	2:E:45:LEU:HD13	1.97	0.46
3:F:106:GLU:HB2	3:F:167:GLN:HE22	1.80	0.46
1:A:143:ASP:OD1	1:A:143:ASP:N	2.48	0.46
2:G:4:LEU:HG	2:G:24:ALA:HB2	1.97	0.46
2:I:129:VAL:HG22	2:I:150:VAL:HG22	1.96	0.46
1:B:400:PHE:CZ	1:B:510:VAL:HG22	2.49	0.46
3:D:196:GLU:OE1	3:D:207:THR:OG1	2.34	0.46
2:E:152:ASP:HA	2:E:183:LEU:HD13	1.97	0.46
2:G:37:VAL:HG11	2:G:45:LEU:HD13	1.98	0.46
3:H:106:GLU:HB2	3:H:167:GLN:HE22	1.81	0.46
2:E:194:SER:HA	2:E:197:LEU:HD13	1.97	0.46
3:F:109:ARG:NH1	3:F:171:ASP:O	2.49	0.46
2:I:154:PHE:HB3	2:I:155:PRO:HD3	1.97	0.46
2:I:155:PRO:HG2	2:I:210:PRO:HG2	1.96	0.46
1:C:289:VAL:HG12	1:C:291:CYS:H	1.80	0.45
1:C:402:ILE:O	1:C:507:PRO:HA	2.16	0.45
2:I:206:VAL:HG22	2:I:215:VAL:HG22	1.99	0.45
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.97	0.45
1:A:105:TRP:HE3	1:A:120:ILE:HB	1.82	0.45
2:E:87:ARG:HH11	2:E:89:GLU:HG2	1.82	0.45
3:D:106:GLU:HB2	3:D:167:GLN:HE22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:SER:H	1:B:1048:HIS:HD2	1.65	0.45
3:F:34:LEU:HD23	3:F:52:ALA:HB2	1.98	0.45
1:C:271:GLN:OE1	1:C:273:ARG:NH2	2.40	0.45
1:B:87:PHE:N	1:B:236:THR:O	2.44	0.45
1:B:186:ASN:HD21	1:B:205:HIS:CD2	2.35	0.45
2:G:59:ASP:OD2	3:F:95:SER:OG	2.34	0.45
2:G:155:PRO:HG2	2:G:210:PRO:HG2	1.99	0.45
3:F:150:LYS:HB2	3:F:194:ALA:HB3	1.98	0.45
2:E:154:PHE:HB3	2:E:155:PRO:HD3	1.97	0.45
1:C:434:ILE:HD12	1:C:513:LEU:HD21	1.99	0.45
1:A:692:ILE:H	1:A:692:ILE:HG12	1.42	0.45
1:C:360:ASN:HA	1:C:523:THR:HB	1.98	0.45
2:I:194:SER:HA	2:I:197:LEU:HD13	1.98	0.45
2:E:38:ARG:NH1	2:E:90:ASP:OD1	2.49	0.44
2:G:206:VAL:HG22	2:G:215:VAL:HG22	1.98	0.44
1:A:83:PRO:HB2	1:A:85:LEU:HG	1.98	0.44
3:F:137:LEU:HD22	3:F:176:LEU:HD23	2.00	0.44
1:C:438:SER:OG	1:C:507:PRO:HB2	2.16	0.44
1:A:535:LYS:HE3	1:A:535:LYS:HB2	1.82	0.44
1:A:994:ASP:HB3	1:C:995:ARG:HH22	1.82	0.44
3:F:117:PHE:HB2	3:F:136:LEU:HB3	1.99	0.44
2:I:87:ARG:HH11	2:I:89:GLU:HG2	1.81	0.44
1:C:93:PHE:O	1:C:190:PHE:N	2.51	0.44
2:G:194:SER:HA	2:G:197:LEU:HD13	2.00	0.44
1:B:563:GLN:HA	1:C:44:LYS:HB2	1.99	0.44
1:C:568:ASP:OD1	1:C:569:ILE:N	2.45	0.44
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	2.00	0.44
1:B:143:ASP:N	1:B:143:ASP:OD1	2.50	0.44
1:A:343:ASN:O	1:A:343:ASN:ND2	2.47	0.44
3:D:137:LEU:HB2	3:D:176:LEU:HB3	1.99	0.44
3:H:137:LEU:HB2	3:H:176:LEU:HB3	1.99	0.44
1:B:134:PHE:HA	1:B:162:ASN:HD22	1.83	0.44
1:B:567:ARG:NH1	1:B:571:ASP:OD1	2.44	0.44
3:H:7:SER:HB2	3:H:8:PRO:HD3	2.00	0.44
2:E:59:ASP:OD2	3:D:95:SER:OG	2.35	0.44
3:D:34:LEU:HD23	3:D:52:ALA:HB2	2.00	0.44
3:D:150:LYS:HB2	3:D:194:ALA:HB3	1.99	0.44
1:A:334:ASN:HD22	1:A:361:CYS:HA	1.83	0.44
2:G:48:ILE:HD12	3:F:97:TRP:CD2	2.53	0.44
1:A:372:ALA:HB3	1:A:373:PRO:HD3	1.98	0.43
3:D:62:ARG:NH2	3:D:82:GLU:OE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLU:HB2	1:C:215:ASP:OD1	2.18	0.43
1:C:80:PHE:HE1	1:C:140:PRO:HB2	1.84	0.43
1:B:379:CYS:HA	1:B:432:CYS:HA	2.00	0.43
1:B:403:ARG:HG2	1:B:404:GLY:H	1.83	0.43
1:B:568:ASP:OD1	1:B:569:ILE:N	2.45	0.43
1:B:957:GLN:HE21	1:B:957:GLN:HB3	1.64	0.43
1:A:204:LYS:HB2	1:A:223:LEU:HA	1.99	0.43
3:F:7:SER:HB2	3:F:8:PRO:HD3	2.00	0.43
1:B:403:ARG:HH11	1:B:405:ASP:HB2	1.84	0.43
1:A:334:ASN:O	1:A:362:VAL:HG22	2.18	0.43
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.56	0.43
1:C:403:ARG:HG2	1:C:404:GLY:H	1.84	0.43
1:C:535:LYS:HG2	1:C:554:GLU:OE2	2.17	0.43
1:B:336:CYS:N	1:B:337:PRO:HD2	2.34	0.43
1:B:1129:VAL:HG13	1:B:1132:ILE:HB	2.01	0.43
2:G:126:GLY:HA2	2:G:127:PRO:HD3	1.93	0.43
1:B:91:VAL:HG23	1:B:267:VAL:HG13	2.00	0.43
1:B:209:ILE:HG22	1:B:210:VAL:HG22	1.99	0.43
1:A:543:PHE:HB2	1:A:546:LEU:HD11	2.01	0.43
1:A:322:PRO:HG3	1:A:549:THR:HG21	2.01	0.42
1:A:82:ASN:HD22	1:A:140:PRO:HB3	1.84	0.42
2:E:48:ILE:HD12	3:D:97:TRP:CD2	2.54	0.42
3:D:137:LEU:HD22	3:D:176:LEU:HD23	2.02	0.42
1:B:93:PHE:O	1:B:190:PHE:N	2.50	0.42
1:B:101:ILE:HG13	1:B:102:ILE:HG13	2.02	0.42
3:D:94:ARG:HG3	3:D:95:SER:H	1.84	0.42
3:H:171:ASP:N	3:H:171:ASP:OD1	2.52	0.42
1:B:444:LYS:HG2	1:B:448:ASN:HB2	2.02	0.42
1:B:912:THR:OG1	1:B:914:ASN:ND2	2.52	0.42
2:I:48:ILE:HD12	3:H:97:TRP:CD2	2.54	0.42
1:B:171:GLN:HB3	1:B:172:PRO:HD3	2.02	0.42
1:A:347:PHE:HD2	1:A:399:SER:HB2	1.84	0.42
3:D:7:SER:HB2	3:D:8:PRO:HD3	2.00	0.42
1:C:78:LYS:HD2	1:C:78:LYS:HA	1.82	0.42
1:C:428:ASP:OD1	1:C:428:ASP:N	2.47	0.42
1:C:99:SER:OG	1:C:259:THR:OG1	2.38	0.42
1:C:340:GLU:H	1:C:340:GLU:HG2	1.70	0.42
1:A:677:GLN:HE22	1:A:691:SER:H	1.67	0.42
1:A:1043:CYS:HB2	1:A:1048:HIS:HB2	2.02	0.42
3:D:109:ARG:HG2	3:D:110:THR:H	1.85	0.42
3:H:109:ARG:NH1	3:H:171:ASP:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LYS:H	1:C:44:LYS:HD2	1.85	0.42
1:B:186:ASN:HA	1:B:207:PRO:HA	2.01	0.42
1:B:330:PRO:HA	1:B:580:GLN:HB3	2.02	0.42
3:F:94:ARG:HG3	3:F:95:SER:H	1.85	0.42
1:A:171:GLN:HB3	1:A:172:PRO:HD3	2.01	0.41
3:H:94:ARG:HG3	3:H:95:SER:H	1.84	0.41
1:C:100:ASN:OD1	1:C:103:ARG:NE	2.53	0.41
1:C:372:ALA:HB3	1:C:373:PRO:HD3	2.01	0.41
1:B:116:GLN:HB3	1:B:233:ILE:HD12	2.03	0.41
1:B:1083:HIS:CG	1:B:1084:ASP:H	2.38	0.41
1:A:44:LYS:HD2	1:A:44:LYS:H	1.85	0.41
2:I:126:GLY:HA2	2:I:127:PRO:HD3	1.94	0.41
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.86	0.41
1:B:1039:ARG:NH2	1:C:1031:GLU:OE2	2.38	0.41
1:A:403:ARG:HG2	1:A:404:GLY:H	1.85	0.41
3:D:171:ASP:OD1	3:D:171:ASP:N	2.54	0.41
1:C:564:GLN:HE21	1:C:564:GLN:HB3	1.67	0.41
1:C:1043:CYS:HB2	1:C:1048:HIS:HB2	2.03	0.41
2:G:129:VAL:HG22	2:G:150:VAL:HG22	2.03	0.41
2:G:96:CYS:O	2:G:114:GLY:N	2.53	0.41
1:C:171:GLN:HB3	1:C:172:PRO:HD3	2.02	0.41
1:A:976:VAL:HG12	1:A:979:ASP:H	1.86	0.41
1:B:1043:CYS:HB2	1:B:1048:HIS:HB2	2.02	0.41
1:C:661:GLU:O	1:C:695:TYR:OH	2.30	0.41
1:B:44:LYS:H	1:B:44:LYS:HD2	1.85	0.41
1:A:96:ILE:HG12	1:A:187:LEU:HD13	2.03	0.41
3:F:171:ASP:N	3:F:171:ASP:OD1	2.53	0.41
3:H:150:LYS:HB2	3:H:194:ALA:HB3	2.02	0.41
1:A:472:ILE:HG13	1:A:480:CYS:SG	2.61	0.41
1:A:1083:HIS:CG	1:A:1084:ASP:H	2.38	0.41
1:C:340:GLU:O	1:C:341:VAL:C	2.59	0.41
1:C:360:ASN:H	1:C:523:THR:HB	1.86	0.41
1:C:444:LYS:HG2	1:C:448:ASN:HB2	2.02	0.41
1:C:1083:HIS:CG	1:C:1084:ASP:H	2.38	0.41
1:C:342:PHE:HD2	1:C:342:PHE:HA	1.69	0.40
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.56	0.40
1:C:1129:VAL:HG13	1:C:1132:ILE:HB	2.03	0.40
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.56	0.40
2:I:107:HIS:CG	2:I:108:ASP:H	2.39	0.40
2:I:142:GLY:H	2:I:194:SER:HB2	1.87	0.40
1:C:397:ALA:HB1	1:C:511:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.95	0.40
1:B:144:HIS:HA	1:B:244:LEU:H	1.87	0.40
1:B:402:ILE:O	1:B:507:PRO:HA	2.22	0.40
1:B:731:MET:HE3	1:B:1018:ILE:HG13	2.04	0.40
2:E:107:HIS:CG	2:E:108:ASP:H	2.39	0.40
2:I:60:TYR:HB2	2:I:65:ARG:HB2	2.04	0.40
2:I:209:LYS:HB2	2:I:210:PRO:HD3	2.04	0.40
1:A:537:LYS:HE2	1:A:537:LYS:HB2	1.82	0.40
3:D:109:ARG:NH1	3:D:171:ASP:O	2.55	0.40
2:G:200:GLN:HE21	2:G:200:GLN:HB3	1.71	0.40
1:A:327:VAL:HG12	1:A:542:ASN:HB3	2.04	0.40
2:G:69:THR:HG23	2:G:82:GLU:HB2	2.04	0.40
2:G:107:HIS:CG	2:G:108:ASP:H	2.40	0.40
2:G:142:GLY:H	2:G:194:SER:HB2	1.87	0.40
1:C:70:VAL:HB	1:C:263:ALA:HB3	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	1055/1285 (82%)	992 (94%)	61 (6%)	2 (0%)	47 76
1	B	1055/1285 (82%)	1001 (95%)	53 (5%)	1 (0%)	51 80
1	C	1055/1285 (82%)	991 (94%)	62 (6%)	2 (0%)	47 76
2	E	213/451 (47%)	202 (95%)	11 (5%)	0	100 100
2	G	213/451 (47%)	201 (94%)	12 (6%)	0	100 100
2	I	213/451 (47%)	201 (94%)	12 (6%)	0	100 100
3	D	209/215 (97%)	202 (97%)	7 (3%)	0	100 100
3	F	209/215 (97%)	202 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	H	209/215 (97%)	201 (96%)	8 (4%)	0	100 100
All	All	4431/5853 (76%)	4193 (95%)	233 (5%)	5 (0%)	54 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	PRO
1	C	332	ILE
1	C	341	VAL
1	B	209	ILE
1	A	334	ASN

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	929/1113 (84%)	872 (94%)	57 (6%)	18 45
1	B	929/1113 (84%)	875 (94%)	54 (6%)	20 47
1	C	929/1113 (84%)	872 (94%)	57 (6%)	18 45
2	E	184/403 (46%)	177 (96%)	7 (4%)	33 64
2	G	184/403 (46%)	177 (96%)	7 (4%)	33 64
2	I	184/403 (46%)	177 (96%)	7 (4%)	33 64
3	D	184/187 (98%)	181 (98%)	3 (2%)	62 86
3	F	184/187 (98%)	181 (98%)	3 (2%)	62 86
3	H	184/187 (98%)	180 (98%)	4 (2%)	52 80
All	All	3891/5109 (76%)	3692 (95%)	199 (5%)	27 53

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	THR
1	B	44	LYS

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Mol	Chain	Res	Type
1	B	109	THR
1	B	136	PHE
1	B	144	HIS
1	B	168	TYR
1	B	169	VAL
1	B	206	THR
1	B	208	ILE
1	B	210	VAL
1	B	211	ARG
1	B	244	LEU
1	B	314	GLN
1	B	316	SER
1	B	317	ASN
1	B	333	THR
1	B	335	LEU
1	B	346	ARG
1	B	374	PHE
1	B	376	THR
1	B	472	ILE
1	B	495	TYR
1	B	501	TYR
1	B	510	VAL
1	B	512	VAL
1	B	513	LEU
1	B	514	SER
1	B	516	GLU
1	B	518	LEU
1	B	529	LYS
1	B	530	SER
1	B	531	THR
1	B	534	VAL
1	B	535	LYS
1	B	536	ASN
1	B	537	LYS
1	B	564	GLN
1	B	646	ARG
1	B	675	GLN
1	B	676	THR
1	B	678	THR
1	B	689	SER
1	B	691	SER
1	B	692	ILE

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Mol	Chain	Res	Type
1	B	790	LYS
1	B	853	GLN
1	B	873	TYR
1	B	878	LEU
1	B	957	GLN
1	B	1001	LEU
1	B	1010	GLN
1	B	1034	LEU
1	B	1038	LYS
1	B	1041	ASP
1	A	36	THR
1	A	44	LYS
1	A	74	THR
1	A	78	LYS
1	A	79	ARG
1	A	80	PHE
1	A	81	ASP
1	A	82	ASN
1	A	84	VAL
1	A	109	THR
1	A	136	PHE
1	A	168	TYR
1	A	169	VAL
1	A	307	THR
1	A	310	LYS
1	A	314	GLN
1	A	315	THR
1	A	316	SER
1	A	317	ASN
1	A	319	ARG
1	A	323	THR
1	A	328	ARG
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	A	334	ASN
1	A	335	LEU
1	A	339	ASP
1	A	340	GLU
1	A	343	ASN
1	A	374	PHE
1	A	376	THR

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Mol	Chain	Res	Type
1	A	472	ILE
1	A	495	TYR
1	A	501	TYR
1	A	518	LEU
1	A	523	THR
1	A	528	LYS
1	A	529	LYS
1	A	530	SER
1	A	535	LYS
1	A	537	LYS
1	A	564	GLN
1	A	646	ARG
1	A	676	THR
1	A	678	THR
1	A	691	SER
1	A	692	ILE
1	A	790	LYS
1	A	853	GLN
1	A	873	TYR
1	A	878	LEU
1	A	957	GLN
1	A	1001	LEU
1	A	1010	GLN
1	A	1038	LYS
1	A	1041	ASP
2	E	31	THR
2	E	47	TRP
2	E	48	ILE
2	E	50	TRP
2	E	91	THR
2	E	103	ARG
2	E	200	GLN
3	D	36	TRP
3	D	48	LEU
3	D	101	GLN
2	G	31	THR
2	G	47	TRP
2	G	48	ILE
2	G	50	TRP
2	G	91	THR
2	G	103	ARG
2	G	200	GLN

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Mol	Chain	Res	Type
3	F	36	TRP
3	F	48	LEU
3	F	101	GLN
2	I	31	THR
2	I	47	TRP
2	I	48	ILE
2	I	50	TRP
2	I	91	THR
2	I	103	ARG
2	I	200	GLN
3	H	36	TRP
3	H	48	LEU
3	H	89	CYS
3	H	101	GLN
1	C	36	THR
1	C	44	LYS
1	C	109	THR
1	C	136	PHE
1	C	143	ASP
1	C	145	LYS
1	C	168	TYR
1	C	169	VAL
1	C	206	THR
1	C	209	ILE
1	C	314	GLN
1	C	316	SER
1	C	317	ASN
1	C	319	ARG
1	C	323	THR
1	C	328	ARG
1	C	331	ASN
1	C	332	ILE
1	C	334	ASN
1	C	335	LEU
1	C	338	PHE
1	C	341	VAL
1	C	342	PHE
1	C	345	THR
1	C	346	ARG
1	C	374	PHE
1	C	376	THR
1	C	408	ARG

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Mol	Chain	Res	Type
1	C	429	PHE
1	C	472	ILE
1	C	495	TYR
1	C	501	TYR
1	C	503	VAL
1	C	513	LEU
1	C	516	GLU
1	C	518	LEU
1	C	523	THR
1	C	525	CYS
1	C	528	LYS
1	C	529	LYS
1	C	532	ASN
1	C	535	LYS
1	C	537	LYS
1	C	564	GLN
1	C	646	ARG
1	C	689	SER
1	C	691	SER
1	C	692	ILE
1	C	790	LYS
1	C	853	GLN
1	C	873	TYR
1	C	878	LEU
1	C	957	GLN
1	C	1001	LEU
1	C	1010	GLN
1	C	1038	LYS
1	C	1041	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	ASN
1	B	123	ASN
1	B	126	ASN
1	B	162	ASN
1	B	183	ASN
1	B	186	ASN
1	B	205	HIS
1	B	218	GLN
1	B	245	HIS

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Mol	Chain	Res	Type
1	B	314	GLN
1	B	414	GLN
1	B	563	GLN
1	B	564	GLN
1	B	613	GLN
1	B	677	GLN
1	B	784	GLN
1	B	853	GLN
1	B	895	GLN
1	B	901	GLN
1	B	913	GLN
1	B	914	ASN
1	B	949	GLN
1	B	957	GLN
1	B	965	GLN
1	B	1005	GLN
1	B	1011	GLN
1	B	1048	HIS
1	B	1106	GLN
1	B	1119	ASN
1	B	1125	ASN
1	A	82	ASN
1	A	123	ASN
1	A	126	ASN
1	A	162	ASN
1	A	183	ASN
1	A	218	GLN
1	A	245	HIS
1	A	314	GLN
1	A	317	ASN
1	A	321	GLN
1	A	331	ASN
1	A	334	ASN
1	A	414	GLN
1	A	563	GLN
1	A	564	GLN
1	A	613	GLN
1	A	677	GLN
1	A	784	GLN
1	A	853	GLN
1	A	895	GLN
1	A	901	GLN

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Mol	Chain	Res	Type
1	A	913	GLN
1	A	914	ASN
1	A	949	GLN
1	A	957	GLN
1	A	965	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1048	HIS
1	A	1106	GLN
1	A	1119	ASN
1	A	1125	ASN
2	E	62	GLN
2	E	115	GLN
2	E	179	GLN
2	E	200	GLN
3	D	90	GLN
3	D	91	GLN
3	D	101	GLN
3	D	167	GLN
2	G	62	GLN
2	G	115	GLN
2	G	179	GLN
2	G	200	GLN
3	F	90	GLN
3	F	91	GLN
3	F	101	GLN
3	F	167	GLN
2	I	62	GLN
2	I	115	GLN
2	I	179	GLN
2	I	200	GLN
3	H	90	GLN
3	H	91	GLN
3	H	101	GLN
3	H	167	GLN
1	C	123	ASN
1	C	126	ASN
1	C	162	ASN
1	C	183	ASN
1	C	186	ASN
1	C	218	GLN
1	C	245	HIS

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Mol	Chain	Res	Type
1	C	314	GLN
1	C	317	ASN
1	C	331	ASN
1	C	414	GLN
1	C	563	GLN
1	C	564	GLN
1	C	613	GLN
1	C	690	GLN
1	C	784	GLN
1	C	853	GLN
1	C	895	GLN
1	C	901	GLN
1	C	913	GLN
1	C	914	ASN
1	C	949	GLN
1	C	957	GLN
1	C	965	GLN
1	C	1005	GLN
1	C	1011	GLN
1	C	1048	HIS
1	C	1106	GLN
1	C	1119	ASN
1	C	1125	ASN

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

There are no ligands in this entry.

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.

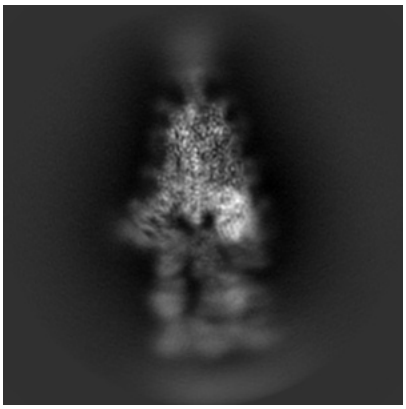
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37162. These allow visual inspection of the internal detail of the map and identification of artifacts.

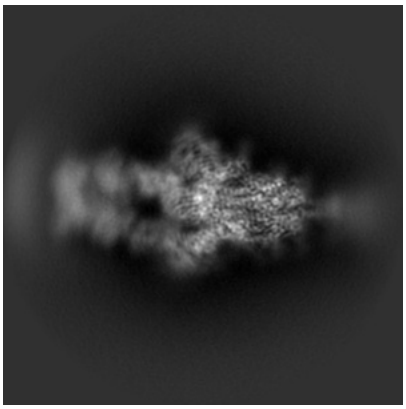
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

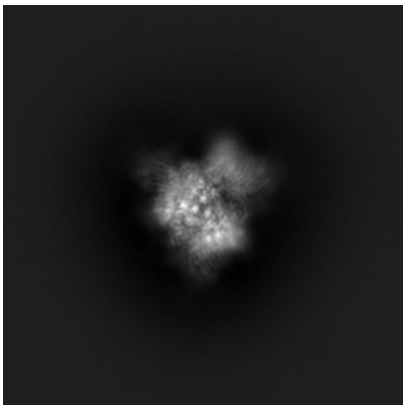
6.1.1 Primary map



X

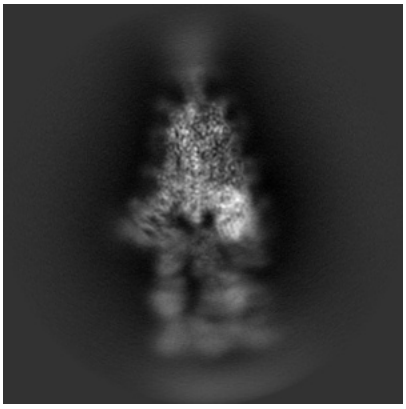


Y

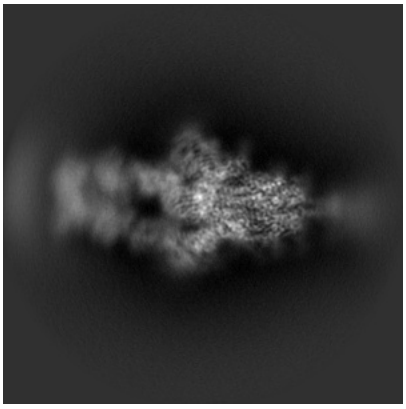


Z

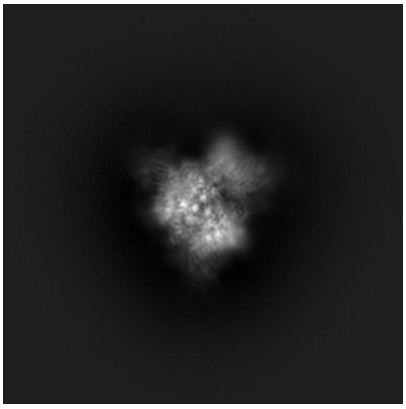
6.1.2 Raw map



X



Y

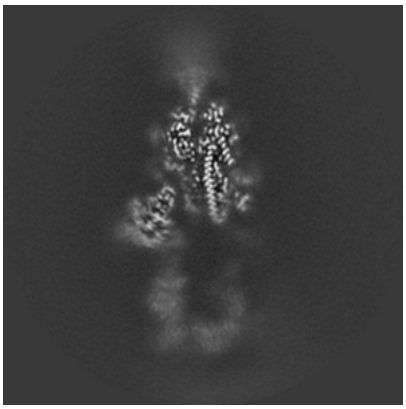


Z

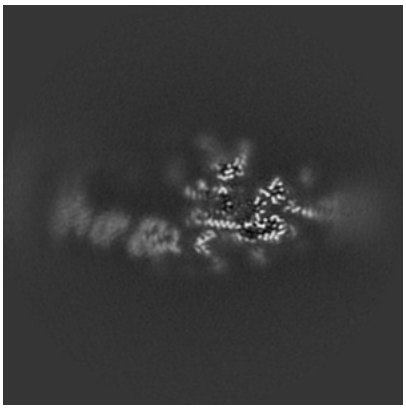
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

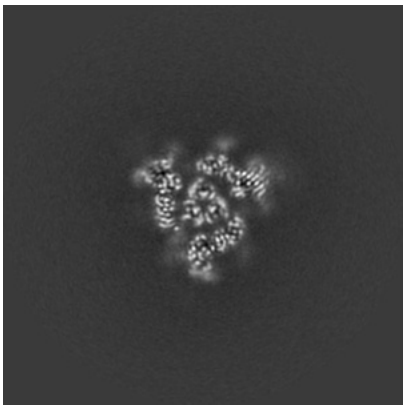
6.2.1 Primary map



X Index: 160

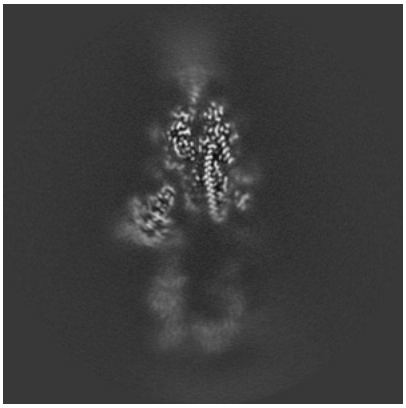


Y Index: 160

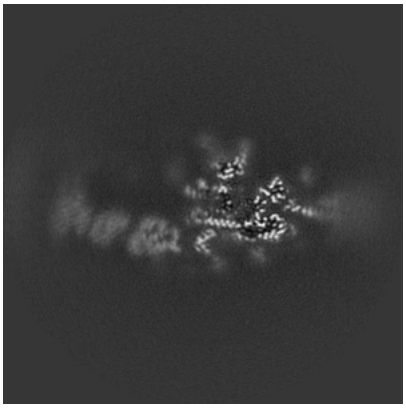


Z Index: 160

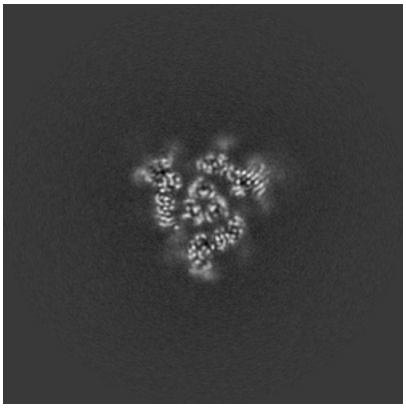
6.2.2 Raw map



X Index: 160



Y Index: 160

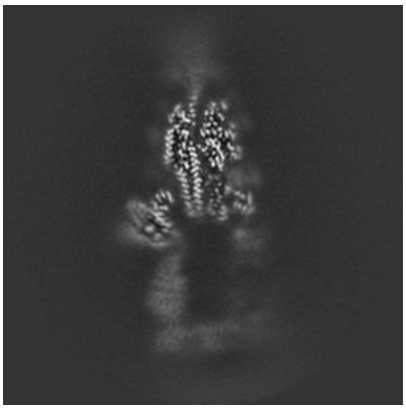


Z Index: 160

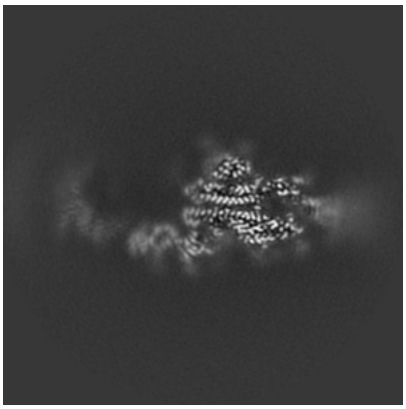
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

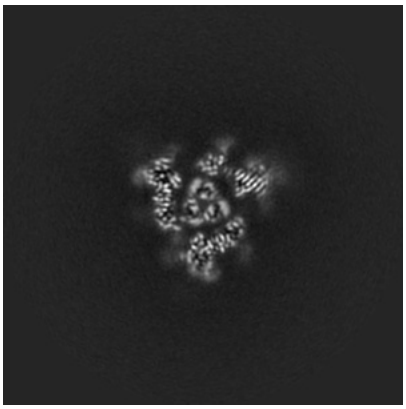
6.3.1 Primary map



X Index: 164

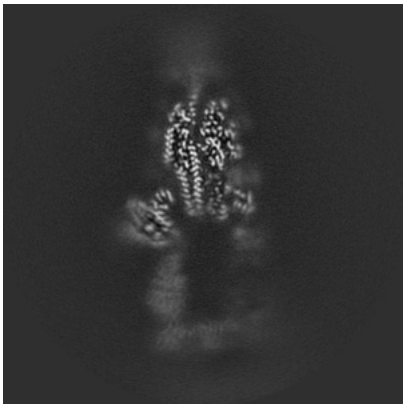


Y Index: 154

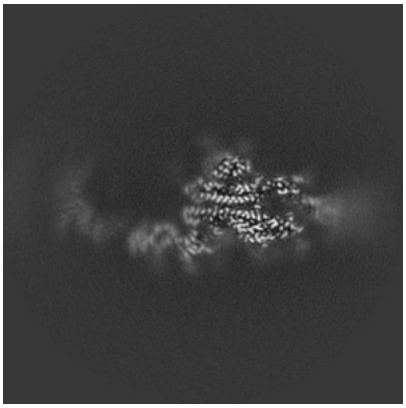


Z Index: 158

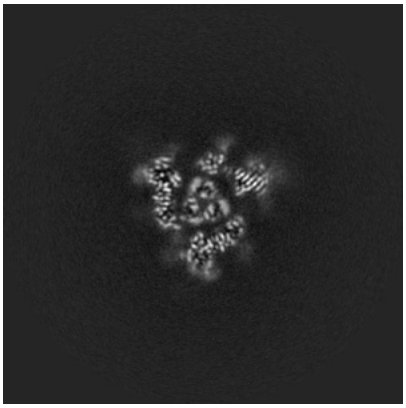
6.3.2 Raw map



X Index: 164



Y Index: 154

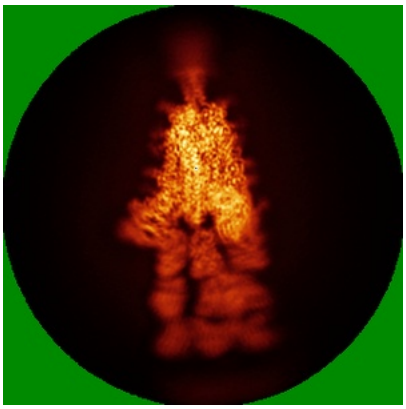


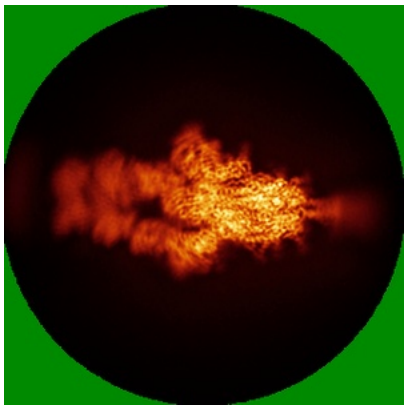
Z Index: 158

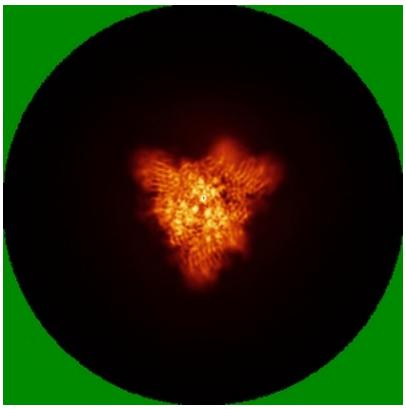
The images above show the largest variance slices of the map in three orthogonal directions.

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

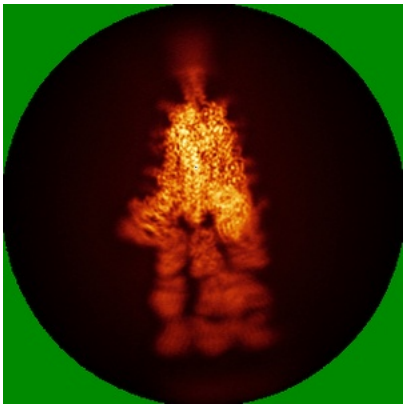
6.4.1 Primary map

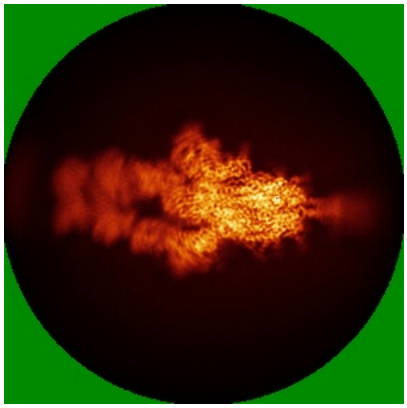

X

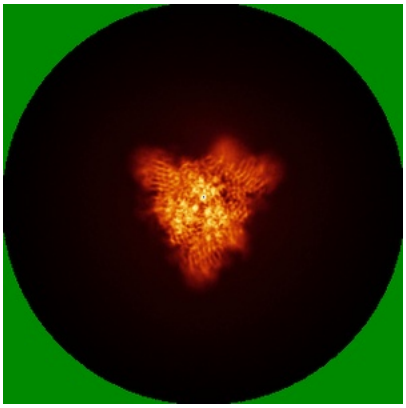

Y


Z

6.4.2 Raw map


X

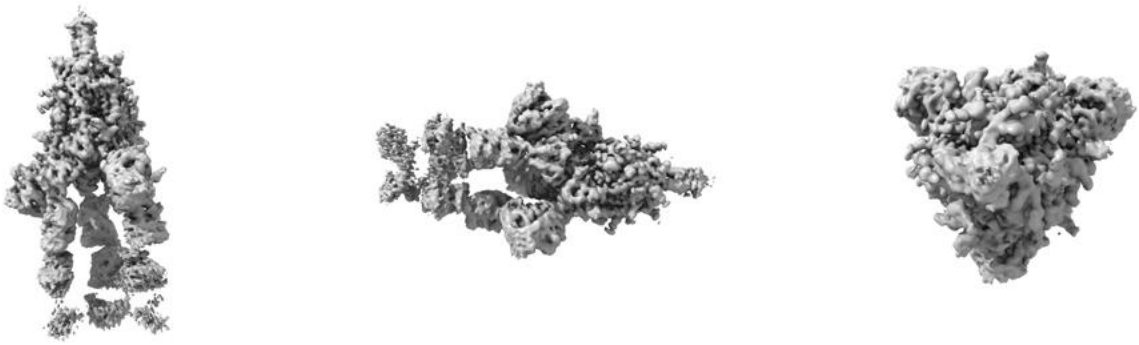

Y


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)

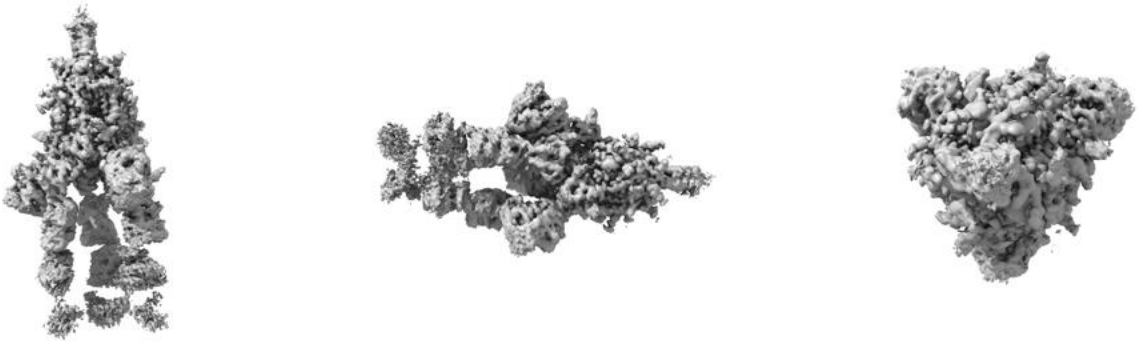
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

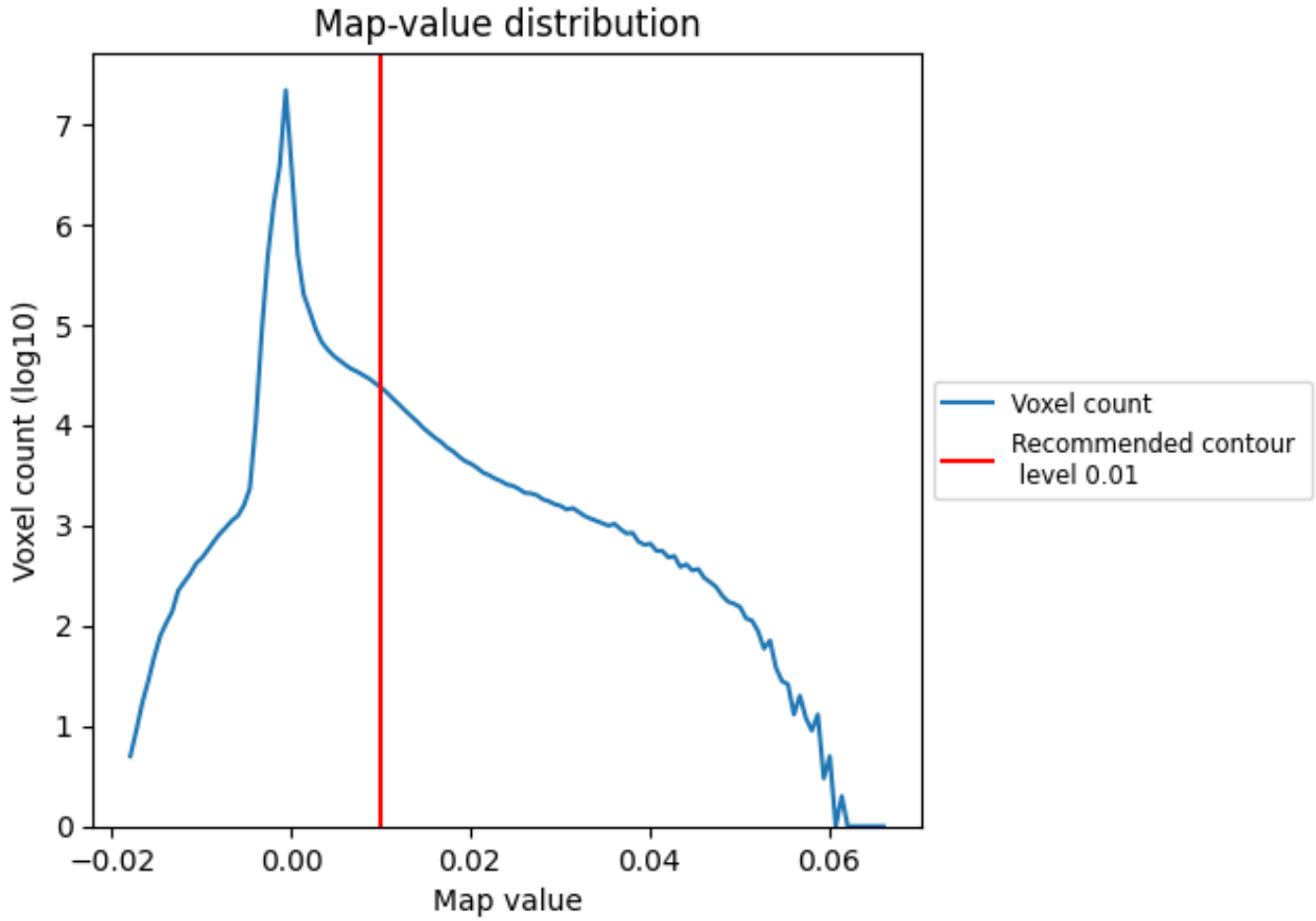
6.6 Mask visualisation (i)

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

7 Map analysis

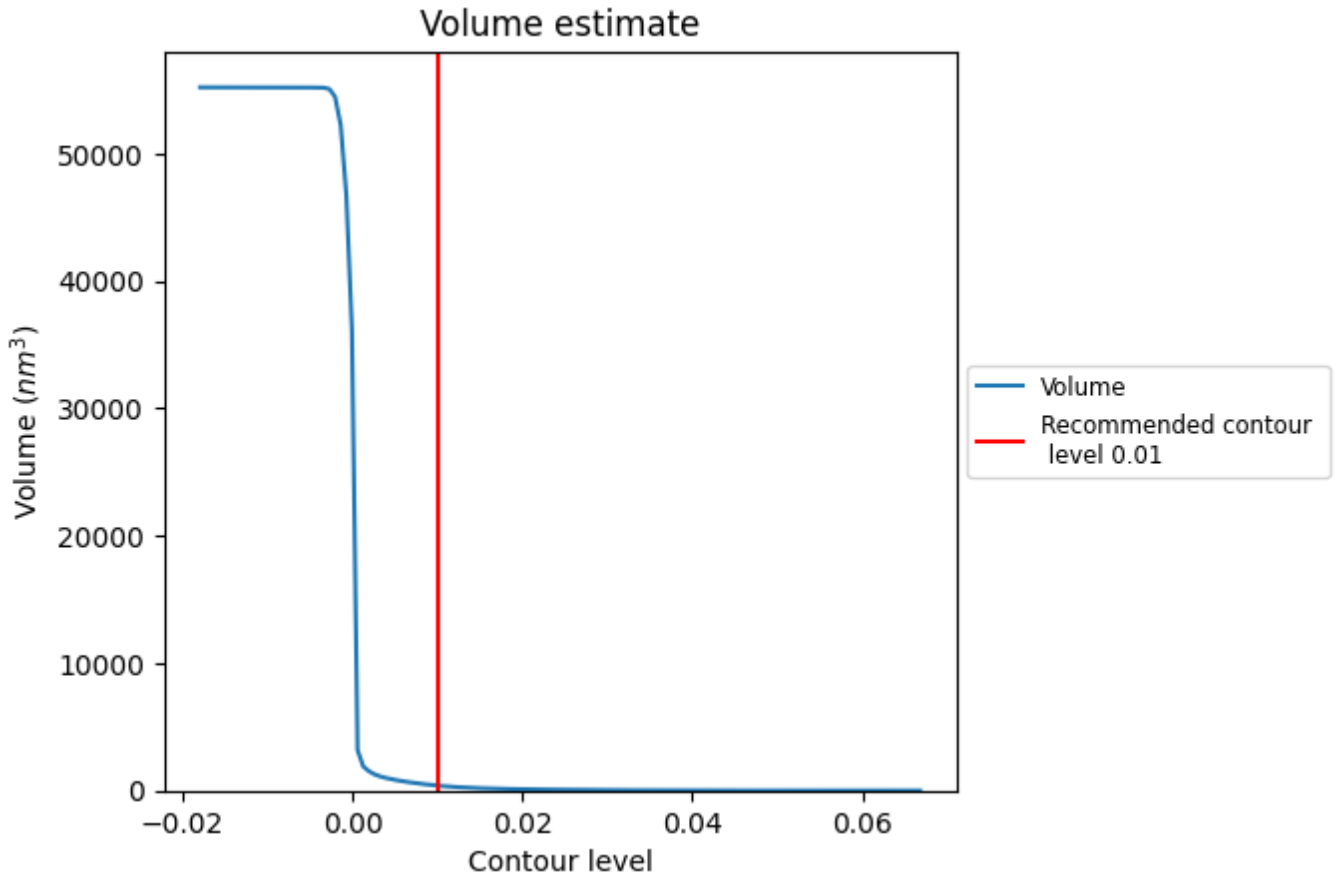
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

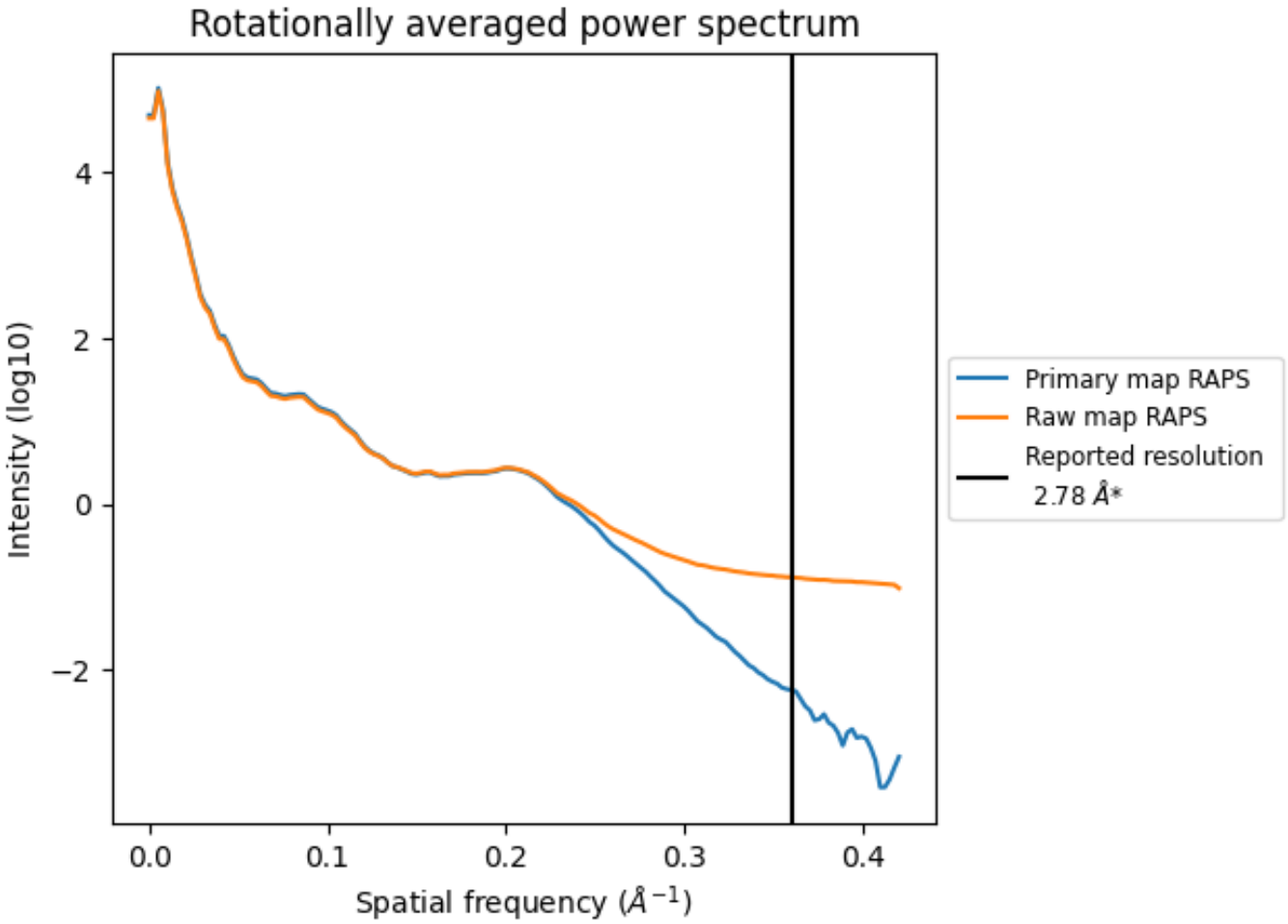
7.2 Volume estimate



The volume at the recommended contour level is 392 nm^3; this corresponds to an approximate mass of 354 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)

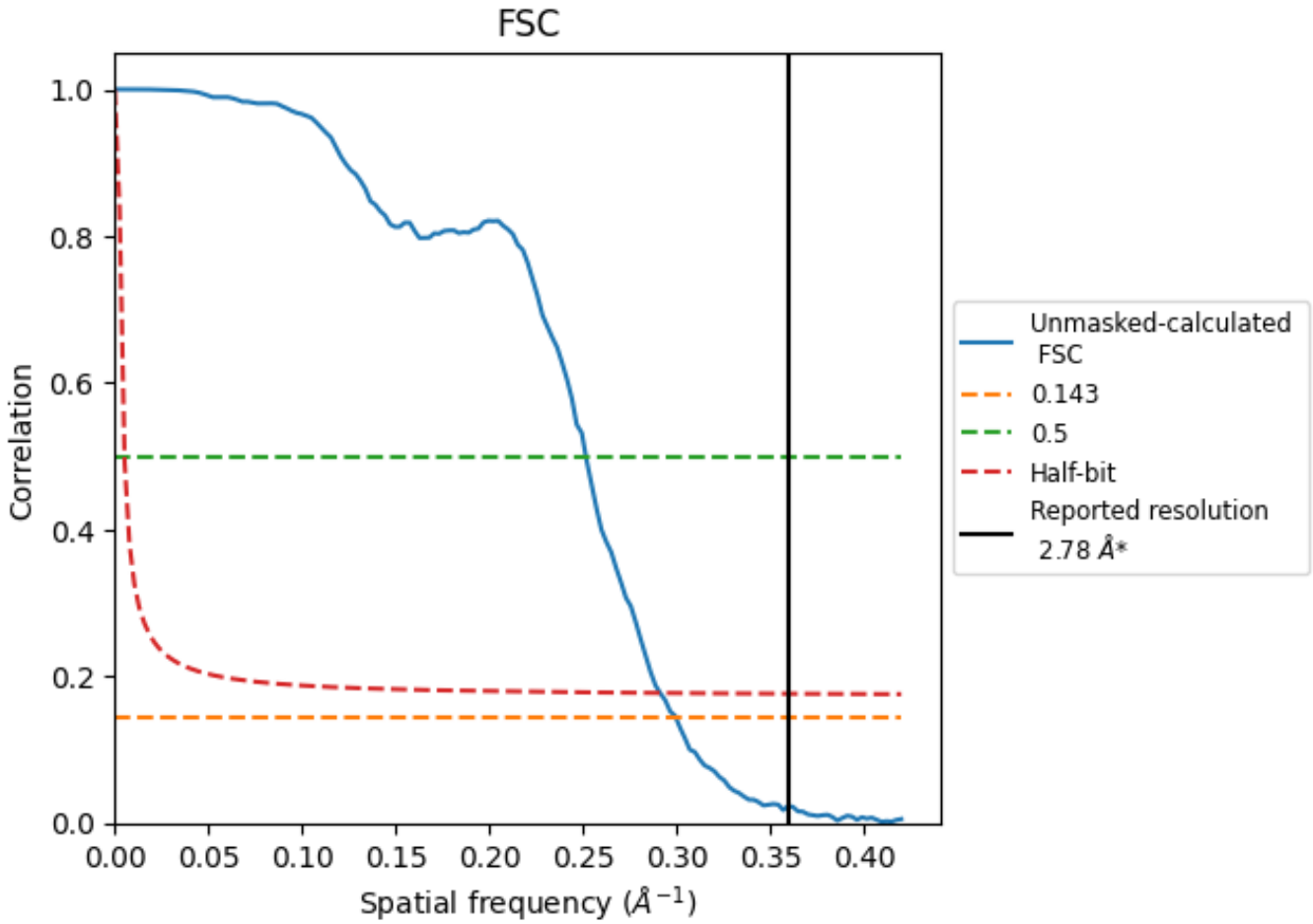


*Reported resolution corresponds to spatial frequency of 0.360 $Å^{-1}$

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 0.360 Å^{-1}

8.2 Resolution estimates (i)

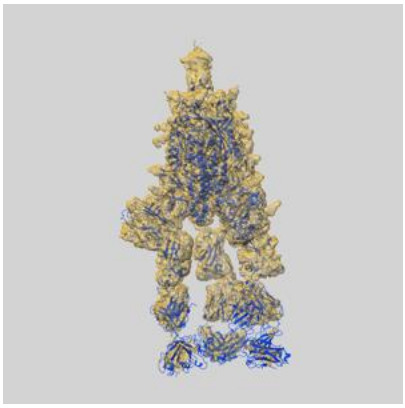
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.97	3.43

*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 3.34 differs from the reported value 2.78 by more than 10 %

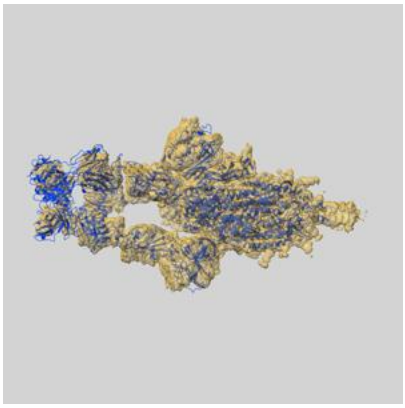
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37162 and PDB model 8KEO. Per-residue inclusion information can be found in section 3 on page 14.

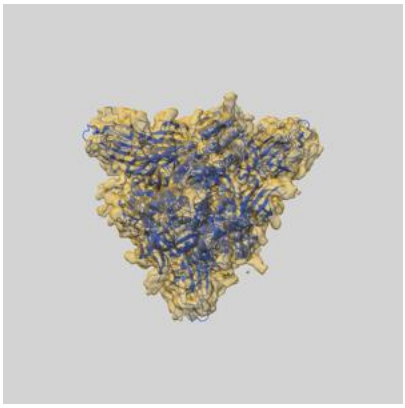
9.1 Map-model overlay



X



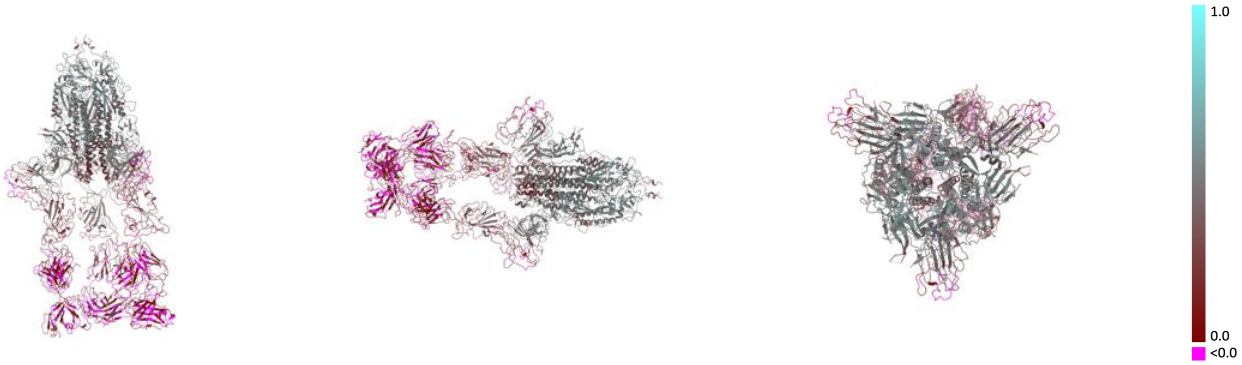
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

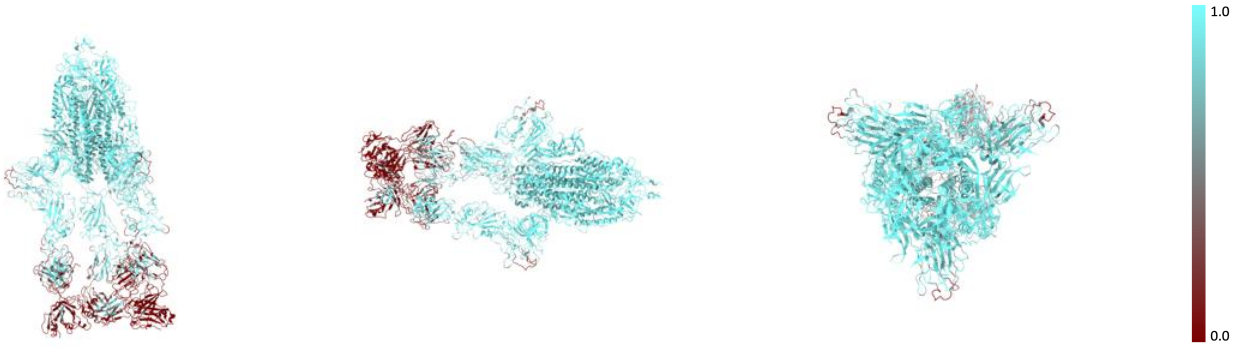
9.2 Q-score mapped to coordinate model (i)



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.

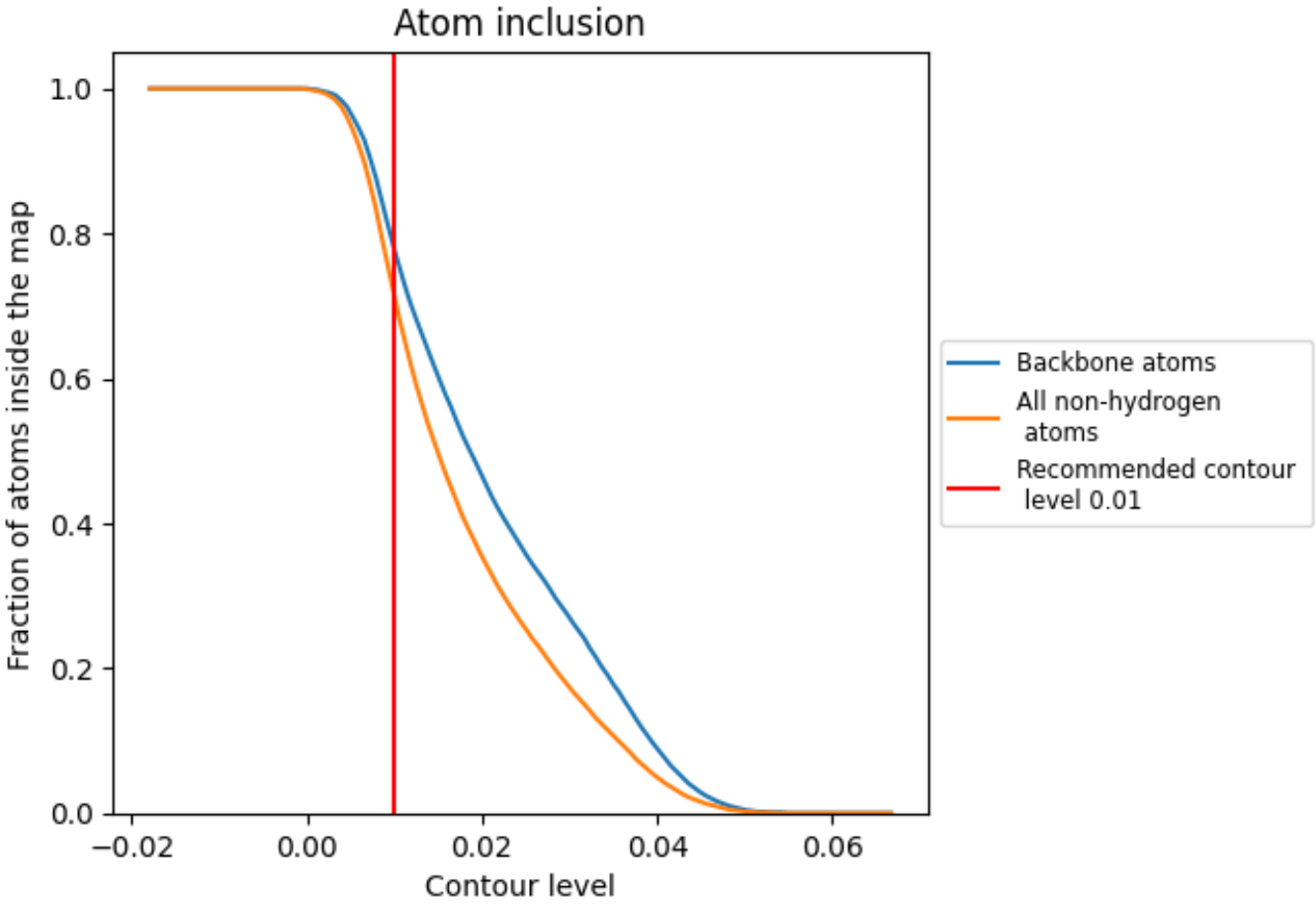
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.2940
A	0.8910	0.3900
B	0.8620	0.3750
C	0.8810	0.3780
D	0.3550	0.0720
E	0.4680	0.0870
F	0.1310	0.0500
G	0.2170	0.0680
H	0.2480	0.0820
I	0.3230	0.0700