



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:37 PM UTC

PDB ID : 8Q5Y / pdb_00008q5y
EMDB ID : EMD-18180
Title : cryoEM structure of SARS-CoV2 Spike trimer in complex with Fab23
Authors : Hallberg, M.; Das, H.
Deposited on : 2023-08-10
Resolution : 2.60 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

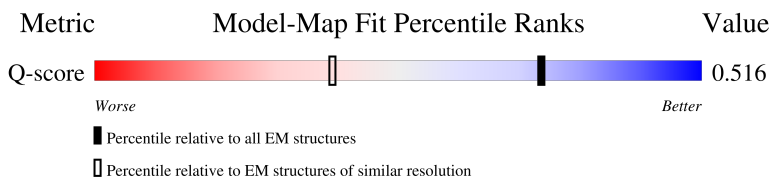
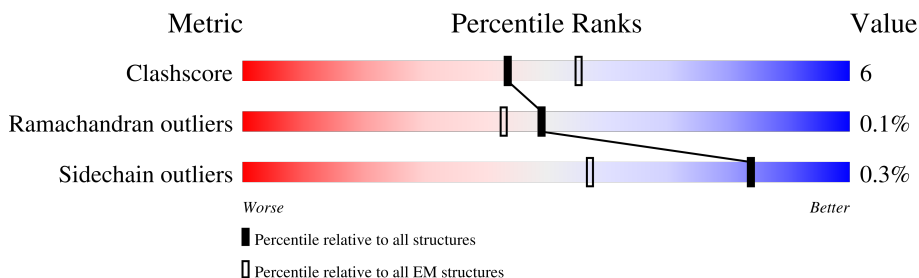
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	
1	H	214	
1	L	214	
2	B	447	

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Mol	Chain	Length	Quality of chain
2	G	447	26%23%74%
2	R	447	26%24%74%
3	C	1288	74%68%11%21%
3	D	1288	73%69%8%22%
3	E	1288	72%67%10%22%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 28689 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 Monoclonal antibody Mab 23 (Light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	106	Total	C	N	O	S	0	0
			798	505	133	157	3		
1	H	104	Total	C	N	O	S	0	0
			778	491	131	153	3		
1	A	106	Total	C	N	O	S	0	0
			798	505	133	157	3		

- Molecule 2 is a protein called Monoclonal antibody Mab 23 (Heavy Chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	115	Total	C	N	O	S	0	0
			896	567	151	174	4		
2	G	115	Total	C	N	O	S	0	0
			896	567	151	174	4		
2	B	116	Total	C	N	O	S	0	0
			902	570	152	176	4		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		
3	E	1001	Total	C	N	O	S	0	0
			7818	4993	1299	1491	35		
3	C	1022	Total	C	N	O	S	0	0
			7978	5095	1327	1521	35		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	682	GLY	ARG	conflict	UNP P0DTC2
D	683	SER	ARG	conflict	UNP P0DTC2
D	685	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	817	PRO	PHE	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	944	PRO	ALA	conflict	UNP P0DTC2
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
E	682	GLY	ARG	conflict	UNP P0DTC2
E	683	SER	ARG	conflict	UNP P0DTC2
E	685	SER	ARG	conflict	UNP P0DTC2
E	817	PRO	PHE	conflict	UNP P0DTC2
E	899	PRO	ALA	conflict	UNP P0DTC2
E	942	PRO	ALA	conflict	UNP P0DTC2
E	944	PRO	ALA	conflict	UNP P0DTC2
E	986	PRO	LYS	conflict	UNP P0DTC2
E	987	PRO	VAL	conflict	UNP P0DTC2
E	1209	GLY	-	expression tag	UNP P0DTC2
E	1210	SER	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	TYR	-	expression tag	UNP P0DTC2
E	1213	ILE	-	expression tag	UNP P0DTC2
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	GLU	-	expression tag	UNP P0DTC2
E	1216	ALA	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	ARG	-	expression tag	UNP P0DTC2
E	1219	ASP	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	ALA	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	VAL	-	expression tag	UNP P0DTC2
E	1225	ARG	-	expression tag	UNP P0DTC2
E	1226	LYS	-	expression tag	UNP P0DTC2
E	1227	ASP	-	expression tag	UNP P0DTC2
E	1228	GLY	-	expression tag	UNP P0DTC2
E	1229	GLU	-	expression tag	UNP P0DTC2
E	1230	TRP	-	expression tag	UNP P0DTC2
E	1231	VAL	-	expression tag	UNP P0DTC2
E	1232	LEU	-	expression tag	UNP P0DTC2
E	1233	LEU	-	expression tag	UNP P0DTC2
E	1234	SER	-	expression tag	UNP P0DTC2
E	1235	THR	-	expression tag	UNP P0DTC2
E	1236	PHE	-	expression tag	UNP P0DTC2
E	1237	LEU	-	expression tag	UNP P0DTC2
E	1238	GLY	-	expression tag	UNP P0DTC2
E	1239	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1240	SER	-	expression tag	UNP P0DTC2
E	1241	LEU	-	expression tag	UNP P0DTC2
E	1242	GLU	-	expression tag	UNP P0DTC2
E	1243	VAL	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	PHE	-	expression tag	UNP P0DTC2
E	1246	GLN	-	expression tag	UNP P0DTC2
E	1247	GLY	-	expression tag	UNP P0DTC2
E	1248	PRO	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2
E	1256	HIS	-	expression tag	UNP P0DTC2
E	1257	HIS	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2
E	1259	ALA	-	expression tag	UNP P0DTC2
E	1260	TRP	-	expression tag	UNP P0DTC2
E	1261	SER	-	expression tag	UNP P0DTC2
E	1262	HIS	-	expression tag	UNP P0DTC2
E	1263	PRO	-	expression tag	UNP P0DTC2
E	1264	GLN	-	expression tag	UNP P0DTC2
E	1265	PHE	-	expression tag	UNP P0DTC2
E	1266	GLU	-	expression tag	UNP P0DTC2
E	1267	LYS	-	expression tag	UNP P0DTC2
E	1268	GLY	-	expression tag	UNP P0DTC2
E	1269	GLY	-	expression tag	UNP P0DTC2
E	1270	GLY	-	expression tag	UNP P0DTC2
E	1271	SER	-	expression tag	UNP P0DTC2
E	1272	GLY	-	expression tag	UNP P0DTC2
E	1273	GLY	-	expression tag	UNP P0DTC2
E	1274	GLY	-	expression tag	UNP P0DTC2
E	1275	GLY	-	expression tag	UNP P0DTC2
E	1276	SER	-	expression tag	UNP P0DTC2
E	1277	GLY	-	expression tag	UNP P0DTC2
E	1278	GLY	-	expression tag	UNP P0DTC2
E	1279	SER	-	expression tag	UNP P0DTC2
E	1280	ALA	-	expression tag	UNP P0DTC2
E	1281	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1282	SER	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
E	1284	PRO	-	expression tag	UNP P0DTC2
E	1285	GLN	-	expression tag	UNP P0DTC2
E	1286	PHE	-	expression tag	UNP P0DTC2
E	1287	GLU	-	expression tag	UNP P0DTC2
E	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	944	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2

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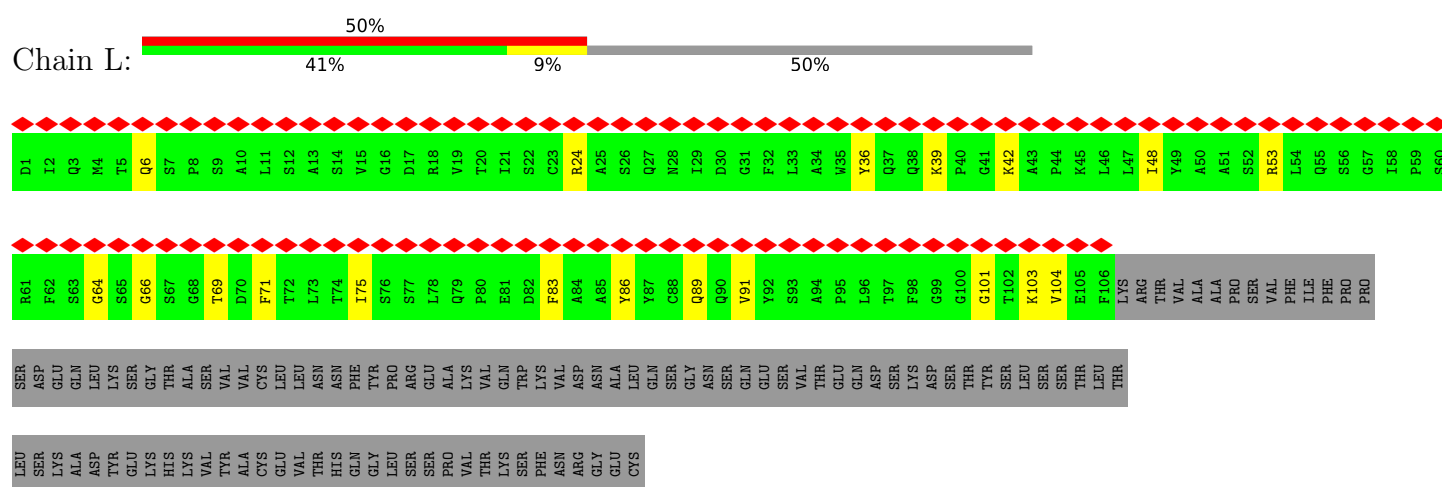
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

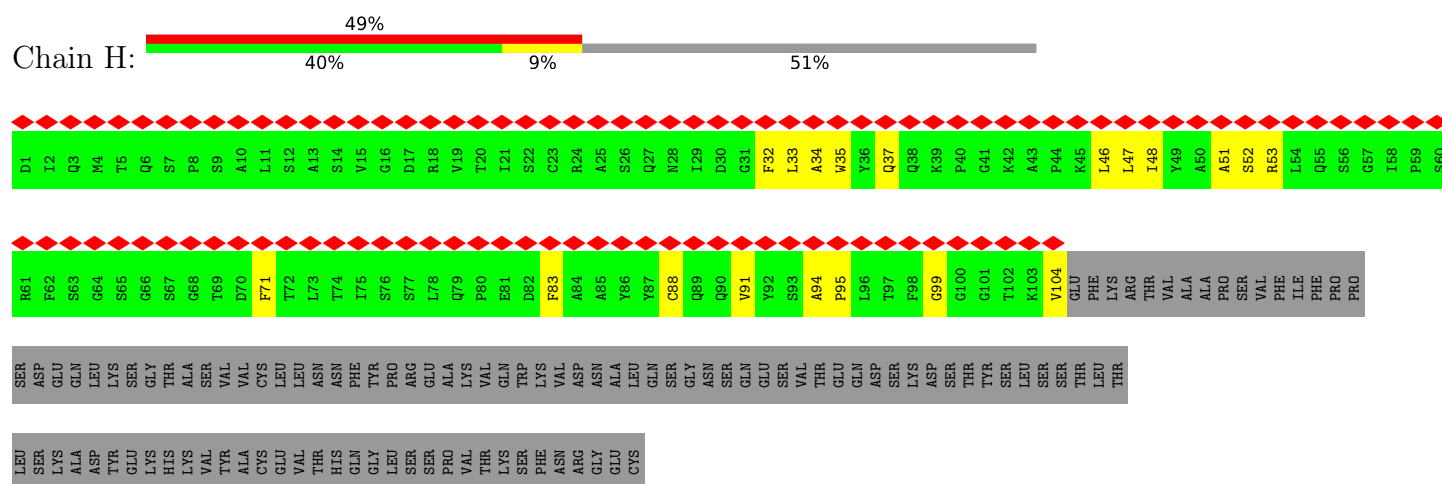
3 Residue-property plots

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: Monoclonal antibody Mab 23 (Light chain)

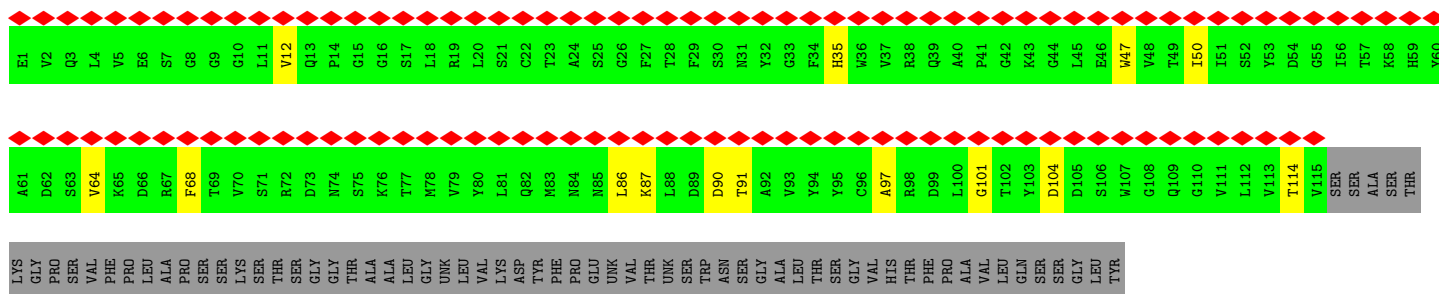


- Molecule 1: Monoclonal antibody Mab 23 (Light chain)



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R905	F906	I909	G910	V911	T912	N913	N914	V915	L916	V917	E918	N919	Q920	K921	L922	I923	A924	N925	Q926	F927	N928	S929	A930	I931	G932	K933	I934	Q935	D936	S937	L938	S939	S940	T941	P942	S943	P944	L945	G946	K947	L948	Q949	D950	A951	V952	K953	L954	P955	P956	A957	P958	A959	M900	Q957	Q901	A958	M902	L959	N960	T961	L962	V963	K964	Q965				
LEU	GLY	ASP	ILE	ALA	ALA	ARG	ASP	LEU	ILE	ALA	CYS	ALA	GLN	K854	F855	N856	G857	L858	T859	V860	G798	G799	F800	P801	L802	S803	T866	D867	L806	E868	M869	I870	D808	A871	Q872	Y873	T874	L877	L878	I882	G885	W886	T887	F888	G889	A890	G891	A892	A893	L894	V895	T896	L896	P897	F898	P899	A956	Q957	Q901	A958	M902	L959	N960	T961	L962	V963	K964	Q965
S721	V722	T723	T724	E725	T726	L727	F728	V729	S730	M731	T732	K733	T734	S735	V736	D737	C738	T739	M740	T741	I742	C743	G744	D745	S746	T747	E748	C749	S750	M751	L752	L753	L754	Q755	V756	G757	S758	F759	C760	T761	Q762	L763	N764	R765	A766	L767	T768	G769	I770	A771	V772	E773	Q774	D775	K776	N777	T778	Q779	E780									
E661	C662	D663	T664	P665	T666	G667	A668	G669	L670	C671	A672	S673	V674	Q675	T676	GLN	THR	ASN	PRO	GLY	ALA	VAL	ALA	S689	P690	T691	L692	A694	V695	T696	M697	S698	L699	G700	A701	E702	N703	S704	Q705	A706	V707	S708	N709	M710	S711	I712	A713	I714	P715	T716	N717	F718	T719	I720														
G601	T602	M603	T604	S605	N606	Q607	V608	A609	V610	L611	V612	Q613	D614	V615	N616	C617	T618	E619	P620	PRO	VAL	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	F643	Q644	T645	R646	A647	G648	C649	L650	I651	G652	T598	P589	C590	S591	F592	G593	G594	V595	S596	V597	L598	T599	P600					
M481	G482	V483	E484	G485	F486	M487	C488	V489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	M501	L502	G503	V504	G505	Y506	Q506	P507	Y508	R509	V510	V511	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	V538	N540									
C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	S371	A372	V333	L434	A435	N436	M437	S438	M439	N440	L441	D442	S443	K444	V445	G446	G447	N448	Y449	N450	Y451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	K462	P463	F464	E465	R466	D467	T468	S469	T470	E471	L472	Y473	Q474	A475	G476	S477	T478	P479	C480									
C301	T302	L303	K304	S305	F306	T307	V308	E309	K310	G311	T312	Q313	Q314	T315	S316	N317	F318	R319	V320	Q321	P322	S383	E324	S325	T326	V327	R328	F329	P330	N331	T332	T333	N334	L335	C336	P337	F338	Q339	S399	F400	V401	E340	V341	F342	N343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	L353	N354	R355	T356	F357	L358	N360							
L241	L242	A243	L244	H245	ARG	SER	THR	THR	PRO	GLY	ASP	SER	SER	GLY	THR	ALA	GLY	ALA	A263	A264	Y265	Y266	V267	G268	K206	H207	T208	P209	L210	N211	L212	F275	L276	T277	K278	Y279	N280	E281	N282	A288	V289	D290	C291	A292	L293	D294	P295	L296	S297	E298	T299	K300																
GLY	LYS	GLN	GLY	ASN	F186	K187	N188	L189	R190	E191	F192	SER	F194	K195	I197	N198	G199	Y200	F201	K202	T203	S204	S205	K206	H207	T208	P209	L210	N211	L212	F275	L276	T277	K278	Y279	N280	E281	N282	A288	V289	D290	C291	A292	L293	D294	P295	L296	S297	E298	T299	K300																	
N121	N122	A123	T124	N125	V126	V127	L128	K129	V130	C131	E132	F133	Q134	F135	C136	N137	G138	P139	F140	G142	V143	T143	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	MET	GLU	SER	R214	D215	L216	P217	Q218	G219	F220	G283	T284	A222	N165	C166	T167	F168	E169	Y170	V171	S172	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU									

F782	A783	Q784	V785	K786	Q787	I788	V789	K790	T791	F792	P793	I794	K795	D796	F797	Q798	G799	F800	N801	F802	S803	Q804	I805	L806	P807	D808	P809	K811	P812	S813	K814	R815	S816	P817	I818	E819	D820	L821	L822	F823	N824	K825	V826	T827	LEU	ALA	ASP	ALA	ALA	GLY	PHE	ILE	GLN	THR	GLY	ASP	CYS	LEU				
S721	V722	T723	T724	E725	I726	L727	S730	M731	T732	Y733	T734	S735	V736	D737	C738	T739	M740	Y741	I742	C743	G744	D745	S746	T747	E748	C749	S750	N751	L752	L753	K754	Q755	Y756	G757	S758	F759	D760	T761	Q762	L763	N764	T765	A766	L767	T768	G769	I770	A771	V772	E773	Q774	D775	K776	N777	T778	Q779	E780	V781				
E661	C662	D663	I664	P665	I666	G667	A668	G669	I670	C671	A672	S673	Y674	Q675	T676	GLN	THR	ASN	SER	PRO	GLY	SER	ALA	SER	VAL	ALA	S689	Q690	S691	I692	I693	A694	Y695	T696	M697	S698	L699	G700	A701	E702	N703	S704	V705	A706	Y707	S708	N709	N710	S711	I712	A713	I651	G652	A653	E654	N717	F718	T719	I720			
G601	T602	N603	T604	S605	N606	Q607	V608	A609	V610	L611	Y612	Q613	D614	V615	N616	C617	T618	E619	V620	P621	V622	A623	I624	H625	A626	D627	Q628	L629	N630	P631	T632	W633	R634	V635	Y636	S637	T638	G639	S640	N641	V642	F643	Q644	T645	R646	A647	G648	C649	L650	I651	G652	A653	E654	H655	V656	N657	N658	S659	Y660			
F541	N542	F543	N544	G545	L546	T547	G548	T549	G550	V551	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	G566	R567	D568	I569	L570	A571	D572	T573	D574	A575	V576	R577	D578	P579	Q580	T581	A582	L582	F583	Q584	T585	D586	I587	T588	P589	C589	L590	I591	F592	G593	E594	V595	S596	V597	I598	T599	P600	
N481	Q482	V483	E484	G485	F486	N487	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505	Q506	P507	Y508	S509	V510	Y511	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	S529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540			
Y421	N422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	A432	V433	A434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447	N448	Y449	N450	Y451	L452	Y453	N454	L455	F456	R457	K458	S459	N460	L461	K462	P463	V464	E465	R466	D467	I468	S469	T470	S471	I472	Q474	A475	K476	S477	T478	P479	C480				
C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F374	S375	T376	F377	K378	C379	Y380	G381	V382	S383	P384	T385	K386	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	A397	D398	S399	F400	V401	L402	R403	G404	D405	E406	V407	R408	Q409	S409	I410	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420		
L241	L242	A243	L244	H245	ARG	SER	TYR	LEU	THR	PRO	K310	ASP	SER	SER	SER	Q314	T315	S316	N317	F318	R319	V320	Q321	T322	T323	E324	S325	L326	V327	R328	P329	N330	N331	I332	T333	N334	L335	C336	P337	F338	G339	E340	V341	F342	N343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	W353	N354	R355	K356	R357	Y358	S359	N360
GLY	LYS	GLN	ASN	F186	K187	N188	L189	R190	E191	GLY	F192	V193	F194	K195	H196	I197	D198	Y200	F201	K202	I203	Y204	S205	K206	H207	T208	P209	I210	N211	L212	V213	R214	D215	L216	P217	Q218	G219	F220	S221	A222	L223	E224	P225	L226	V227	D228	L229	P230	I231	G232	I233	N234	I235	T236	R237	F238	Q239	T240				
M121	N122	T123	A123	T124	N125	V126	V127	I128	K129	W130	C131	E132	F133	Q134	F135	C136	M137	D138	P139	F140	L141	G142	V143	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	MET	GLU	SER	GLU	PHE	ARG	VAL	TYR	SER	SER	ALA	ASN	N165	C166	T167	F168	E169	Y170	V171	S172	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU			
N61	V62	T63	N64	F65	H66	A67	H68	VAL	SER	SER	GLN	GLY	THR	ASN	THR	ARG	PHE	D80	N81	P82	V83	L84	P85	F86	N87	D88	G89	V90	L91	F92	A93	S94	T95	E96	K97	S98	N99	I100	I101	R102	G103	W104	I105	F106	G107	T108	T109	L110	D111	S112	K113	Q114	Q115	S116	L117	L118	I119	V120				
MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	VAL	SER	SER	GLN	CYS	ASN	VAL	ASN	THR	THR	THR	ARG	THR	GLN	LEU	PRO	PRO	A27	Y28	T29	N30	S31	F32	T33	R34	G35	V36	V37	V38	P39	D40	K41	V42	F43	R44	S45	S46	V47	L48	H49	S50	T51	Q52	D53	L54	F55	L56	P57	F58	F59	S60			

GLU LYS	ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU LEU GLY ARG SER LEU GLU VAL PHE GLN GLY PRO HIS HIS HIS HIS HIS HIS HIS SER ALA TRP HIS PRO GLN PHE		GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN		R1107 N1108 F1109 Y1110 E1111 P1112 Q1113 I1114 I1115 T1116 T1117 D1118 N1119 T1120 F1121 V1122 S1123 G1124 N1125 C1126 D1127 V1128 V1129 I1130 G1131 I1132 V1133 N1134 M1135 T1136 V1137 Y1138 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 S1147 PHE LYS GLU LEU LEU ASP LYS TYR VAL ARG LYS		R905 F906 N907 G908 I909 Q910 V911 T912 Q913 N914 V915 L916 Y917 E918 N919 Q920 K921 L922 I923 A924 N925 Q926 F927 N928 S929 A930 I931 Q932 K933 I934 Q935 D936 S937 L938 S939 S940 T941 P942 S943 P944 L945 Q946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A956 Q957 A958 L959 N960 T961 L962 V963 K964		Q965 L966 S967 S968 N969 F970 G971 A972 I973 S974 S975 V976 L977 N978 D979 I980 L981 S982 R983 L984 D985 P986 P987 E988 A989 E990 V991 Q992 I993 D994 R995 L996 I997 T998 G999 R1000 L1001 Q1002 S1003 L1004 Q1005 T1006 Y1007 V1008 T1009 Q1010 Q1011 L1012 I1013 R1014 A1015 A1016 E1017 I1018 R1019 A1020 H1023 T1027		L1034 G1035 K1038 D1041 F1042 K1045 S1051 S1055 A1056 P1057 H1058 V1061 V1065 P1069 A1070 Q1071 E1072 K1073 N1074 F1075 T1076 T1077 A1078 P1079 I1081 C1082 H1083 D1084 G1085 K1086 A1087 H1088 F1089 P1090 I1091 E1092 G1093 V1094 F1095 V1096 S1097 N1098 G1099 T1100 H1101 W1102 F1103 V1104 T1105 Q1106		K854 F855 N856 G857 L858 T859 V860 L861 P862 P863 L864 L865 T866 D867 E868 M869 I870 Q872 Y873 L877 L878 T881 I882 T883 S884 G885 W886 T887 F888 G889 A890 G891 A892 A893 L894 Q895 I896 P897 F898 P899 M900 Q901 M902 A903 Y904	
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.808	Depositor
Minimum map value	-3.324	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	517.12, 517.12, 517.12	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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	0/816	0.65	0/1106
1	H	0.44	0/795	0.71	0/1078
1	L	0.38	0/816	0.71	0/1106
2	B	0.24	0/922	0.55	0/1251
2	G	0.29	0/916	0.62	0/1243
2	R	0.26	0/916	0.55	0/1243
3	C	0.31	0/8163	0.67	6/11118 (0.1%)
3	D	0.35	0/8004	0.67	5/10896 (0.0%)
3	E	0.33	0/7995	0.67	6/10881 (0.1%)
All	All	0.33	0/29343	0.67	17/39922 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	942	PRO	CA-N-CD	-9.39	98.85	112.00
3	E	944	PRO	CA-N-CD	-9.36	98.90	112.00
3	E	899	PRO	CA-N-CD	-9.34	98.93	112.00
3	C	944	PRO	CA-N-CD	-9.16	99.17	112.00
3	C	942	PRO	CA-N-CD	-9.14	99.21	112.00
3	D	817	PRO	CA-N-CD	-9.12	99.23	112.00
3	D	944	PRO	CA-N-CD	-9.09	99.28	112.00
3	E	817	PRO	CA-N-CD	-9.09	99.28	112.00
3	C	817	PRO	CA-N-CD	-9.06	99.31	112.00
3	D	899	PRO	CA-N-CD	-9.04	99.34	112.00
3	D	942	PRO	CA-N-CD	-9.02	99.38	112.00
3	C	899	PRO	CA-N-CD	-8.92	99.51	112.00
3	C	636	TYR	CA-CB-CG	5.62	124.01	113.90
3	C	527	PRO	N-CA-CB	5.55	110.31	103.15
3	D	913	GLN	N-CA-CB	-5.17	102.25	110.22
3	E	87	ASN	CA-C-N	5.02	131.12	121.54
3	E	87	ASN	C-N-CA	5.02	131.12	121.54

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	798	0	778	9	0
1	H	778	0	763	13	0
1	L	798	0	778	11	0
2	B	902	0	866	10	0
2	G	896	0	861	9	0
2	R	896	0	861	5	0
3	C	7978	0	7788	116	0
3	D	7825	0	7644	99	0
3	E	7818	0	7636	111	0
All	All	28689	0	27975	366	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 (366) 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)
3:E:804:GLN:O	3:E:817:PRO:CD	1.82	1.26
3:C:804:GLN:O	3:C:817:PRO:CD	1.92	1.16
3:C:899:PRO:HD2	3:C:900:MET:H	1.10	1.15
3:D:944:PRO:HD2	3:D:945:LEU:H	1.10	1.15
3:E:899:PRO:HD2	3:E:900:MET:H	1.11	1.15
3:E:817:PRO:HD2	3:E:818:ILE:H	1.12	1.14
3:D:804:GLN:O	3:D:817:PRO:CD	1.95	1.13
3:D:817:PRO:HD2	3:D:818:ILE:H	1.13	1.13
3:E:944:PRO:HD2	3:E:945:LEU:H	1.12	1.13
3:D:899:PRO:HD2	3:D:900:MET:H	1.12	1.09
3:C:944:PRO:HD2	3:C:945:LEU:H	1.14	1.08
3:C:817:PRO:HD2	3:C:818:ILE:H	1.14	1.08
3:E:804:GLN:O	3:E:817:PRO:HD3	1.54	1.04
3:E:942:PRO:C	3:E:944:PRO:HD3	1.85	1.02

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:942:PRO:C	3:C:944:PRO:HD3	1.87	1.00
3:E:804:GLN:O	3:E:817:PRO:HD2	1.63	0.99
3:D:942:PRO:C	3:D:944:PRO:HD3	1.88	0.98
3:D:804:GLN:O	3:D:817:PRO:HD3	1.64	0.95
3:C:804:GLN:O	3:C:817:PRO:HD2	1.68	0.92
3:C:804:GLN:O	3:C:817:PRO:HD3	1.69	0.91
3:D:804:GLN:HA	3:D:817:PRO:HG2	1.53	0.91
3:E:897:PRO:C	3:E:899:PRO:HD3	1.98	0.89
3:D:899:PRO:HD2	3:D:900:MET:N	1.88	0.88
3:C:899:PRO:HD2	3:C:900:MET:N	1.87	0.87
3:D:804:GLN:O	3:D:817:PRO:HD2	1.75	0.87
3:D:944:PRO:HD2	3:D:945:LEU:N	1.88	0.86
3:E:804:GLN:HA	3:E:817:PRO:HG2	1.56	0.86
3:E:817:PRO:HD2	3:E:818:ILE:N	1.88	0.86
3:D:942:PRO:C	3:D:944:PRO:CD	2.48	0.86
3:E:899:PRO:HD2	3:E:900:MET:N	1.87	0.85
3:E:897:PRO:C	3:E:899:PRO:CD	2.50	0.85
3:C:816:SER:HB2	3:C:817:PRO:HD3	1.58	0.84
3:D:943:SER:N	3:D:944:PRO:HD3	1.92	0.84
3:E:944:PRO:HD2	3:E:945:LEU:N	1.90	0.83
3:C:817:PRO:HD2	3:C:818:ILE:N	1.90	0.83
3:E:804:GLN:HA	3:E:817:PRO:CG	2.10	0.81
3:D:898:PHE:N	3:D:899:PRO:HD3	1.96	0.80
3:C:942:PRO:C	3:C:944:PRO:CD	2.55	0.80
3:D:897:PRO:C	3:D:899:PRO:HD3	2.06	0.80
3:C:899:PRO:CD	3:C:900:MET:H	1.93	0.79
3:C:944:PRO:HD2	3:C:945:LEU:N	1.90	0.79
3:E:899:PRO:CD	3:E:900:MET:H	1.95	0.79
3:C:902:MET:HG3	3:C:916:LEU:HD11	1.65	0.78
3:E:898:PHE:N	3:E:899:PRO:HD3	1.97	0.78
3:E:942:PRO:C	3:E:944:PRO:CD	2.55	0.78
3:D:897:PRO:C	3:D:899:PRO:CD	2.57	0.77
3:D:899:PRO:CD	3:D:900:MET:H	1.95	0.77
3:E:817:PRO:CD	3:E:818:ILE:H	1.95	0.77
3:C:64:TRP:HE1	3:C:264:ALA:HB1	1.49	0.77
3:D:944:PRO:CD	3:D:945:LEU:H	1.94	0.77
3:C:944:PRO:CD	3:C:945:LEU:H	1.98	0.77
3:C:897:PRO:C	3:C:899:PRO:HD3	2.10	0.77
3:C:898:PHE:N	3:C:899:PRO:HD3	2.00	0.77
3:D:817:PRO:CD	3:D:818:ILE:H	1.96	0.76
3:D:804:GLN:HA	3:D:817:PRO:CG	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:943:SER:N	3:C:944:PRO:HD3	1.99	0.76
3:E:943:SER:N	3:E:944:PRO:HD3	2.00	0.76
3:C:817:PRO:CD	3:C:818:ILE:H	1.97	0.75
3:C:897:PRO:C	3:C:899:PRO:CD	2.60	0.75
3:E:944:PRO:CD	3:E:945:LEU:H	1.96	0.74
3:D:817:PRO:HD2	3:D:818:ILE:N	1.89	0.73
3:C:804:GLN:HA	3:C:817:PRO:HG2	1.70	0.72
3:E:1076:THR:HB	3:E:1097:SER:HB3	1.74	0.70
3:D:816:SER:HB2	3:D:817:PRO:HD3	1.73	0.69
3:C:816:SER:HB2	3:C:817:PRO:CD	2.23	0.69
3:E:825:LYS:HZ3	3:E:944:PRO:HG2	1.58	0.68
3:E:816:SER:HB2	3:E:817:PRO:HD3	1.75	0.67
3:D:944:PRO:CD	3:D:945:LEU:N	2.57	0.67
3:C:804:GLN:HA	3:C:817:PRO:CG	2.24	0.67
2:G:47:TRP:HZ2	2:G:50:ILE:HG22	1.60	0.66
3:D:899:PRO:CD	3:D:900:MET:N	2.56	0.66
3:E:899:PRO:CD	3:E:900:MET:N	2.56	0.66
1:H:33:LEU:HD11	1:H:88:CYS:HB2	1.76	0.66
1:H:94:ALA:HA	3:E:445:VAL:HG11	1.78	0.66
3:D:354:ASN:HB3	3:D:399:SER:HB2	1.78	0.66
3:C:944:PRO:CD	3:C:945:LEU:N	2.59	0.66
2:G:104:ASP:OD1	3:E:346:ARG:NH2	2.28	0.65
3:C:117:LEU:HD11	3:C:128:ILE:HD12	1.78	0.65
3:D:943:SER:N	3:D:944:PRO:CD	2.59	0.65
3:C:899:PRO:CD	3:C:900:MET:N	2.55	0.65
3:C:817:PRO:CD	3:C:818:ILE:N	2.59	0.65
3:E:817:PRO:CD	3:E:818:ILE:N	2.57	0.64
3:C:126:VAL:H	3:C:172:SER:HB3	1.62	0.64
3:D:898:PHE:N	3:D:899:PRO:CD	2.60	0.64
3:C:103:GLY:HA3	3:C:241:LEU:HB2	1.80	0.64
3:D:817:PRO:CD	3:D:818:ILE:N	2.58	0.64
3:E:804:GLN:CA	3:E:817:PRO:HG2	2.26	0.63
3:E:396:TYR:HB2	3:E:514:SER:HB2	1.79	0.63
3:E:93:ALA:HB3	3:E:266:TYR:HB2	1.80	0.63
3:E:825:LYS:NZ	3:E:944:PRO:HG2	2.14	0.62
3:E:804:GLN:O	3:E:817:PRO:CG	2.45	0.62
3:C:89:GLY:HA3	3:C:270:LEU:HD12	1.82	0.61
3:C:898:PHE:N	3:C:899:PRO:CD	2.63	0.61
3:D:32:PHE:HB3	3:D:218:GLN:HA	1.82	0.60
3:D:280:ASN:HD21	3:D:284:THR:HB	1.67	0.59
3:C:742:ILE:HA	3:C:1000:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:804:GLN:O	3:C:817:PRO:CG	2.50	0.59
3:D:1076:THR:HB	3:D:1097:SER:HB3	1.83	0.59
3:D:132:GLU:OE1	3:D:165:ASN:ND2	2.35	0.59
3:E:376:THR:HG23	3:E:378:LYS:HD3	1.84	0.59
3:E:944:PRO:CD	3:E:945:LEU:N	2.59	0.58
3:C:393:THR:HA	3:C:522:ALA:HA	1.84	0.58
2:B:35:HIS:CD2	2:B:100:LEU:H	2.22	0.58
2:G:35:HIS:HB2	2:G:97:ALA:HB3	1.85	0.58
3:E:297:SER:HA	3:E:300:LYS:HD2	1.85	0.58
3:C:733:LYS:HG2	3:C:771:ALA:HA	1.86	0.58
3:E:102:ARG:HG3	3:E:121:ASN:H	1.67	0.58
3:C:100:ILE:HD11	3:C:263:ALA:HB2	1.84	0.58
1:A:6:GLN:HG3	1:A:101:GLY:H	1.68	0.58
3:C:130:VAL:HG21	3:C:168:PHE:HB3	1.85	0.58
2:G:101:GLY:HA2	1:H:34:ALA:HB2	1.85	0.57
3:D:804:GLN:CA	3:D:817:PRO:HG2	2.31	0.57
3:C:131:CYS:HB3	3:C:166:CYS:HA	1.86	0.57
1:L:36:TYR:OH	1:L:89:GLN:NE2	2.38	0.57
3:C:620:VAL:HG11	3:C:651:ILE:HD11	1.87	0.57
3:C:943:SER:N	3:C:944:PRO:CD	2.67	0.56
3:E:34:ARG:HE	3:E:216:LEU:HD13	1.71	0.56
3:E:37:TYR:HA	3:E:223:LEU:H	1.70	0.56
3:D:412:PRO:HB3	3:D:427:ASP:HA	1.87	0.55
1:A:8:PRO:HG2	1:A:102:THR:HG21	1.89	0.55
2:B:61:ALA:HB3	2:B:64:VAL:HG22	1.88	0.55
3:C:93:ALA:HB3	3:C:266:TYR:HB2	1.88	0.55
3:E:193:VAL:HG13	3:E:270:LEU:HD11	1.88	0.55
3:C:382:VAL:HG13	3:C:430:THR:HB	1.89	0.55
3:E:357:ARG:NH2	3:E:396:TYR:OH	2.40	0.54
3:E:362:VAL:HG13	3:E:526:GLY:HA2	1.89	0.54
1:L:6:GLN:HG3	1:L:101:GLY:H	1.71	0.54
3:D:930:ALA:HA	3:D:933:LYS:HE2	1.89	0.54
3:C:403:ARG:NH2	3:C:406:GLU:OE2	2.40	0.54
3:D:398:ASP:HB2	3:D:512:VAL:HB	1.89	0.54
3:E:376:THR:HB	3:E:435:ALA:HB3	1.89	0.54
3:D:350:VAL:HG11	3:D:418:ILE:HD11	1.89	0.54
3:E:666:ILE:HD11	3:E:672:ALA:HB2	1.89	0.54
1:L:53:ARG:NH1	3:D:343:ASN:O	2.41	0.54
3:C:412:PRO:HB3	3:C:427:ASP:HA	1.89	0.53
3:E:930:ALA:HA	3:E:933:LYS:HE2	1.90	0.53
3:E:897:PRO:C	3:E:899:PRO:HD2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:722:VAL:HG22	3:C:1065:VAL:HG22	1.91	0.53
1:H:52:SER:OG	1:H:53:ARG:NH1	2.42	0.53
3:D:310:LYS:HG3	3:D:600:PRO:HA	1.89	0.53
3:E:731:MET:HB2	3:E:955:ASN:HD21	1.72	0.53
3:E:897:PRO:HB2	3:E:899:PRO:CD	2.38	0.53
3:C:97:LYS:HB3	3:C:187:LYS:H	1.72	0.52
3:D:206:LYS:HB2	3:D:223:LEU:HA	1.91	0.52
3:E:898:PHE:N	3:E:899:PRO:CD	2.61	0.52
3:C:106:PHE:HB3	3:C:235:ILE:HG12	1.92	0.52
3:C:193:VAL:HG13	3:C:270:LEU:HD11	1.91	0.52
3:D:393:THR:HA	3:D:522:ALA:HA	1.91	0.52
3:C:379:CYS:HB3	3:C:382:VAL:HG23	1.91	0.52
3:D:214:ARG:NH1	3:D:215:ASP:OD2	2.43	0.52
3:E:444:LYS:HE2	3:E:448:ASN:HA	1.90	0.52
3:E:722:VAL:HG22	3:E:1065:VAL:HG22	1.91	0.52
3:D:722:VAL:HG22	3:D:1065:VAL:HG22	1.90	0.52
3:C:212:LEU:HG	3:C:215:ASP:H	1.74	0.52
3:E:1048:HIS:HA	3:E:1066:THR:HG22	1.91	0.52
3:C:376:THR:HG22	3:C:435:ALA:HB3	1.91	0.52
2:R:102:THR:HG21	3:D:444:LYS:HE2	1.91	0.52
3:E:101:ILE:O	3:E:190:ARG:NH2	2.42	0.52
3:E:37:TYR:OH	3:E:195:LYS:NZ	2.39	0.51
3:C:1076:THR:HB	3:C:1097:SER:HB3	1.92	0.51
2:R:12:VAL:HG11	2:R:86:LEU:HD13	1.90	0.51
3:E:943:SER:N	3:E:944:PRO:CD	2.68	0.51
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.92	0.51
3:C:806:LEU:HD23	3:C:878:LEU:HD23	1.93	0.51
2:B:91:THR:HG23	2:B:114:THR:HA	1.92	0.51
3:D:424:LYS:HB3	3:D:463:PRO:HA	1.93	0.51
3:C:498:GLN:HB3	3:C:501:ASN:HB2	1.93	0.51
3:C:598:ILE:HG23	3:C:664:ILE:HG21	1.92	0.51
3:C:1086:LYS:HA	3:C:1125:ASN:HA	1.93	0.51
3:E:616:ASN:HB3	3:E:619:GLU:HG2	1.93	0.51
3:E:560:LEU:HB2	3:E:563:GLN:HG3	1.93	0.51
3:C:101:ILE:HG12	3:C:242:LEU:HG	1.93	0.51
3:C:115:GLN:HA	3:C:132:GLU:HB3	1.91	0.51
3:C:954:GLN:OE1	3:C:1014:ARG:NH1	2.43	0.51
3:D:140:PHE:HD1	3:D:244:LEU:HB2	1.75	0.50
3:C:816:SER:CB	3:C:817:PRO:CD	2.88	0.50
3:D:562:PHE:HD2	3:E:41:LYS:HD2	1.76	0.50
3:E:1116:THR:HG22	3:E:1138:TYR:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:ARG:NH2	2:B:104:ASP:OD1	2.42	0.50
2:G:64:VAL:HG13	2:G:68:PHE:HB2	1.93	0.50
3:E:96:GLU:HG3	3:E:99:ASN:HA	1.92	0.50
3:E:204:TYR:HA	3:E:225:PRO:HA	1.93	0.50
2:R:91:THR:HG23	2:R:114:THR:HA	1.93	0.50
3:D:44:ARG:HE	3:C:567:ARG:HD2	1.75	0.50
3:E:902:MET:HG3	3:E:916:LEU:HD11	1.94	0.50
1:H:33:LEU:HD22	1:H:71:PHE:CG	2.47	0.49
3:E:39:PRO:HB3	3:E:51:THR:HG21	1.94	0.49
3:D:742:ILE:HA	3:D:1000:ARG:HD3	1.94	0.49
3:D:804:GLN:O	3:D:817:PRO:CG	2.56	0.49
2:B:38:ARG:NE	2:B:46:GLU:OE1	2.43	0.49
3:E:347:PHE:HB2	3:E:401:VAL:HG23	1.95	0.49
3:C:186:PHE:HB2	3:C:213:VAL:HG13	1.94	0.49
3:C:231:ILE:HD12	3:C:233:ILE:HG12	1.94	0.49
3:E:962:LEU:HD11	3:E:1004:LEU:HD23	1.95	0.49
3:C:108:THR:HA	3:C:236:THR:H	1.77	0.49
3:D:347:PHE:CD1	3:D:399:SER:HB3	2.47	0.49
3:E:942:PRO:CA	3:E:944:PRO:HD3	2.43	0.49
2:R:98:ARG:NH2	2:R:104:ASP:O	2.44	0.49
3:D:319:ARG:HH11	3:D:592:PHE:HB2	1.76	0.49
3:C:1116:THR:HG22	3:C:1138:TYR:HD2	1.78	0.49
3:D:816:SER:CB	3:D:817:PRO:HD3	2.41	0.48
3:E:426:PRO:HG2	3:E:429:PHE:HB2	1.94	0.48
3:C:280:ASN:ND2	3:C:286:THR:OG1	2.46	0.48
3:C:316:SER:HB3	3:C:595:VAL:HB	1.96	0.48
3:D:666:ILE:HD11	3:D:672:ALA:HB2	1.94	0.48
3:D:897:PRO:C	3:D:899:PRO:HD2	2.38	0.48
3:D:906:PHE:CD2	3:D:916:LEU:HB2	2.48	0.48
3:C:941:THR:OG1	3:C:942:PRO:CD	2.61	0.48
3:E:310:LYS:HG3	3:E:600:PRO:HA	1.95	0.48
2:G:91:THR:HG23	2:G:114:THR:HA	1.96	0.48
3:D:379:CYS:HB2	3:D:384:PRO:HD3	1.96	0.48
3:E:567:ARG:HD2	3:C:42:VAL:HG11	1.96	0.48
3:E:417:LYS:HE2	3:E:417:LYS:HB2	1.67	0.48
1:A:93:SER:OG	1:A:95:PRO:O	2.30	0.48
3:E:1040:VAL:HG21	3:C:1035:GLY:HA3	1.95	0.48
3:C:552:LEU:HB3	3:C:585:LEU:HD23	1.95	0.48
3:D:942:PRO:CA	3:D:944:PRO:HD3	2.43	0.47
3:D:379:CYS:HB3	3:D:382:VAL:HG13	1.96	0.47
3:E:102:ARG:HH21	3:E:120:VAL:HG13	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:902:MET:HG3	3:D:916:LEU:HD11	1.96	0.47
3:D:901:GLN:O	3:D:905:ARG:HG2	2.15	0.47
3:D:816:SER:CB	3:D:817:PRO:CD	2.93	0.47
1:L:89:GLN:HE22	2:R:100:LEU:HB3	1.79	0.47
3:E:88:ASP:OD1	3:E:89:GLY:N	2.48	0.47
3:D:776:LYS:NZ	3:D:780:GLU:OE2	2.46	0.47
3:E:143:VAL:HB	3:E:245:HIS:HA	1.96	0.47
3:C:433:VAL:HG22	3:C:512:VAL:HG22	1.96	0.47
1:L:103:LYS:HD2	1:L:103:LYS:HA	1.76	0.46
1:H:35:TRP:HB2	1:H:48:ILE:HB	1.97	0.46
3:C:529:LYS:HD2	3:C:531:THR:H	1.80	0.46
1:A:46:LEU:HD22	1:A:55:GLN:HE21	1.80	0.46
3:D:1049:LEU:HD11	3:D:1067:TYR:HB2	1.97	0.46
3:E:825:LYS:HE3	3:E:942:PRO:HA	1.98	0.46
3:D:362:VAL:HG13	3:D:526:GLY:HA2	1.98	0.46
1:L:75:ILE:HD11	1:L:86:TYR:HE2	1.81	0.46
3:D:406:GLU:HB3	3:D:418:ILE:HG21	1.96	0.46
3:E:391:CYS:HA	3:E:525:CYS:HA	1.98	0.46
3:C:27:ALA:HB3	3:C:64:TRP:HB3	1.98	0.46
1:H:83:PHE:HD1	1:H:104:VAL:HG12	1.80	0.46
3:D:932:GLY:O	3:D:935:GLN:HG2	2.16	0.46
3:E:897:PRO:CB	3:E:899:PRO:HD3	2.46	0.46
3:C:1082:CYS:HB2	3:C:1126:CYS:HB3	1.56	0.46
3:C:395:VAL:HG22	3:C:515:PHE:HD1	1.80	0.45
3:E:804:GLN:CA	3:E:817:PRO:CG	2.89	0.45
3:E:102:ARG:HA	3:E:190:ARG:HH22	1.80	0.45
3:D:106:PHE:HB2	3:D:117:LEU:HB3	1.97	0.45
3:D:379:CYS:HA	3:D:432:CYS:HA	1.99	0.45
3:E:119:ILE:HG13	3:E:128:ILE:HG23	1.97	0.45
1:A:28:ASN:ND2	1:A:30:ASP:OD1	2.49	0.45
1:L:83:PHE:HD1	1:L:104:VAL:HG12	1.82	0.45
3:C:350:VAL:HG11	3:C:418:ILE:HD11	1.99	0.45
3:C:945:LEU:HD12	3:C:948:LEU:HD12	1.99	0.45
3:D:139:PRO:HG2	3:D:241:LEU:HA	1.98	0.45
3:D:942:PRO:C	3:D:944:PRO:HD2	2.38	0.45
3:E:350:VAL:HG22	3:E:422:ASN:HB3	1.99	0.45
3:E:804:GLN:HA	3:E:817:PRO:HG3	1.92	0.45
3:C:402:ILE:HB	3:C:406:GLU:HB2	1.99	0.45
2:G:12:VAL:HG11	2:G:86:LEU:HD13	1.98	0.45
2:G:87:LYS:N	2:G:90:ASP:OD2	2.45	0.45
3:C:897:PRO:HB2	3:C:900:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ARG:HE	1:L:69:THR:HB	1.82	0.45
3:E:411:ALA:HB3	3:E:414:GLN:HG3	1.98	0.45
3:D:44:ARG:HH21	3:C:567:ARG:HH11	1.64	0.45
3:D:193:VAL:HG13	3:D:270:LEU:HD11	1.99	0.45
3:D:903:ALA:HB1	3:D:913:GLN:HG3	1.98	0.45
3:E:647:ALA:HA	3:C:862:PRO:HG3	1.99	0.45
3:D:411:ALA:HB3	3:D:414:GLN:HG3	1.98	0.44
3:D:902:MET:HE1	3:D:1049:LEU:HD13	1.99	0.44
3:C:763:LEU:HD22	3:C:1008:VAL:HG21	1.99	0.44
1:H:34:ALA:HB1	1:H:46:LEU:HD11	1.98	0.44
3:E:129:LYS:HB2	3:E:129:LYS:HE2	1.58	0.44
3:E:106:PHE:HA	3:E:238:PHE:HA	1.99	0.44
3:D:996:LEU:HD13	3:D:1000:ARG:HH12	1.83	0.44
2:B:98:ARG:NH2	2:B:104:ASP:O	2.45	0.44
3:D:129:LYS:HD3	3:D:131:CYS:SG	2.58	0.44
3:D:903:ALA:HB2	3:D:916:LEU:HD22	1.99	0.44
3:D:1090:PRO:HD3	3:D:1095:PHE:CE2	2.53	0.44
3:C:529:LYS:HZ2	3:C:531:THR:HG22	1.82	0.44
3:D:362:VAL:HG22	3:D:527:PRO:HD2	2.00	0.44
3:E:816:SER:HB2	3:E:817:PRO:CD	2.46	0.44
3:C:189:LEU:HD22	3:C:210:ILE:HD12	2.00	0.44
3:C:297:SER:HA	3:C:300:LYS:HD2	2.00	0.44
3:C:897:PRO:HB2	3:C:899:PRO:HD2	1.99	0.44
1:A:2:ILE:HG23	1:A:27:GLN:H	1.82	0.44
3:D:516:GLU:HG2	3:D:518:LEU:HG	2.00	0.44
3:C:897:PRO:C	3:C:899:PRO:HD2	2.41	0.44
1:H:32:PHE:HB3	1:H:91:VAL:HG23	2.00	0.43
3:D:239:GLN:HG2	3:D:240:THR:H	1.83	0.43
3:D:947:LYS:HB3	3:D:947:LYS:HE2	1.80	0.43
3:E:103:GLY:HA3	3:E:241:LEU:HD12	1.99	0.43
3:E:816:SER:CB	3:E:817:PRO:CD	2.97	0.43
3:C:204:TYR:HB3	3:C:223:LEU:HB3	2.00	0.43
3:C:278:LYS:HB2	3:C:278:LYS:HE3	1.83	0.43
2:G:47:TRP:CZ2	2:G:50:ILE:HG22	2.48	0.43
1:H:37:GLN:HB2	1:H:47:LEU:HD11	2.00	0.43
1:H:88:CYS:O	1:H:99:GLY:N	2.51	0.43
3:D:826:VAL:HG23	3:D:945:LEU:HD13	2.01	0.43
3:E:897:PRO:HB2	3:E:899:PRO:HD2	1.99	0.43
3:C:358:ILE:HD13	3:C:395:VAL:HG12	2.01	0.43
3:C:455:LEU:HG	3:C:493:GLN:HB3	2.01	0.43
3:C:992:GLN:HA	3:C:995:ARG:HD2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:819:GLU:HA	3:C:822:LEU:HD12	2.01	0.43
3:D:576:VAL:HG22	3:D:587:ILE:HD11	2.00	0.43
3:D:790:LYS:HE3	3:C:704:SER:HB2	2.00	0.43
3:C:94:SER:OG	3:C:96:GLU:OE1	2.35	0.43
3:E:37:TYR:H	3:E:55:PHE:HE1	1.66	0.43
3:E:100:ILE:HB	3:E:243:ALA:HB3	2.00	0.43
3:E:393:THR:HA	3:E:522:ALA:HA	2.01	0.43
3:C:642:VAL:HG22	3:C:651:ILE:HG12	2.00	0.43
3:C:1073:LYS:HA	3:C:1073:LYS:HD3	1.82	0.43
3:D:350:VAL:HG22	3:D:422:ASN:HB3	2.01	0.43
3:C:662:CYS:HB2	3:C:697:MET:HE3	2.01	0.42
3:C:347:PHE:CD1	3:C:399:SER:HB3	2.54	0.42
3:C:897:PRO:HB2	3:C:899:PRO:CD	2.49	0.42
3:E:105:ILE:HG23	3:E:241:LEU:HD11	2.02	0.42
3:C:804:GLN:CA	3:C:817:PRO:HG2	2.44	0.42
3:E:576:VAL:HG13	3:E:587:ILE:HD11	2.02	0.42
3:C:295:PRO:HG2	3:C:608:VAL:HG21	2.01	0.42
3:E:35:GLY:HA3	3:E:56:LEU:HB3	2.01	0.42
3:C:906:PHE:CD2	3:C:916:LEU:HB2	2.53	0.42
3:D:310:LYS:HE3	3:D:310:LYS:HB3	1.83	0.42
3:D:396:TYR:HB2	3:D:514:SER:HB3	2.02	0.42
3:E:366:SER:H	3:E:388:ASN:HD21	1.66	0.42
3:E:790:LYS:HE3	3:E:790:LYS:HB3	1.83	0.42
3:C:942:PRO:CA	3:C:944:PRO:HD3	2.47	0.42
3:E:105:ILE:HD12	3:E:110:LEU:HD22	2.02	0.41
3:D:403:ARG:HG3	3:D:505:TYR:HA	2.02	0.41
3:E:319:ARG:NH2	3:C:745:ASP:OD2	2.52	0.41
3:C:350:VAL:HG22	3:C:422:ASN:HB3	2.01	0.41
3:C:733:LYS:HE3	3:C:863:PRO:HA	2.02	0.41
3:E:901:GLN:O	3:E:905:ARG:HG2	2.20	0.41
3:D:898:PHE:HZ	3:D:1050:MET:HE1	1.85	0.41
3:D:980:ILE:HD13	3:D:992:GLN:HB3	2.02	0.41
2:B:37:VAL:HG11	2:B:45:LEU:HD23	2.03	0.41
3:D:966:LEU:HD23	3:D:1000:ARG:HE	1.85	0.41
3:C:293:LEU:O	3:C:632:THR:HA	2.21	0.41
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.75	0.41
1:L:39:LYS:HB3	1:L:42:LYS:HB2	2.02	0.41
3:D:110:LEU:HD23	3:D:116:SER:HB3	2.02	0.41
3:E:54:LEU:HA	3:E:272:PRO:HA	2.02	0.41
1:H:33:LEU:HB3	1:H:51:ALA:HB2	2.03	0.41
3:E:897:PRO:CB	3:E:899:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:984:LEU:HD23	3:E:984:LEU:HA	1.95	0.41
1:L:48:ILE:HG21	1:L:64:GLY:HA3	2.03	0.41
3:D:106:PHE:O	3:D:117:LEU:N	2.54	0.41
3:D:195:LYS:HB2	3:D:195:LYS:HE3	1.80	0.41
3:C:296:LEU:HG	3:C:300:LYS:HE2	2.01	0.41
1:A:96:LEU:HD12	2:B:47:TRP:CD2	2.56	0.41
1:H:94:ALA:HB3	1:H:95:PRO:HD3	2.03	0.40
3:D:897:PRO:O	3:D:899:PRO:HD2	2.21	0.40
3:E:773:GLU:HA	3:E:776:LYS:HE2	2.03	0.40
3:E:942:PRO:HD2	3:E:943:SER:N	2.36	0.40
3:C:878:LEU:HA	3:C:878:LEU:HD12	1.88	0.40
3:D:347:PHE:HD1	3:D:399:SER:HB3	1.85	0.40
3:E:104:TRP:HE3	3:E:119:ILE:HD13	1.86	0.40
3:E:743:CYS:HB3	3:E:749:CYS:HB3	1.84	0.40
3:E:905:ARG:HD2	3:E:1049:LEU:O	2.22	0.40
3:E:1084:ASP:HB2	3:E:1086:LYS:HE3	2.03	0.40
3:C:104:TRP:HH2	3:C:190:ARG:HH21	1.69	0.40
3:D:984:LEU:HD13	3:D:988:GLU:HB3	2.03	0.40
3:C:576:VAL:HG13	3:C:587:ILE:HD11	2.03	0.40
3:C:726:ILE:HG13	3:C:1061:VAL:HG22	2.03	0.40
1:A:96:LEU:HD12	2:B:47:TRP:CE2	2.57	0.40
3:E:108:THR:OG1	3:E:234:ASN:O	2.39	0.40
3:E:319:ARG:NH1	3:E:590:CYS:HB2	2.36	0.40
1:L:66:GLY:HA3	1:L:71:PHE:HA	2.02	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	104/214 (49%)	100 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	102/214 (48%)	93 (91%)	9 (9%)	0	100	100
1	L	104/214 (49%)	96 (92%)	8 (8%)	0	100	100
2	B	114/447 (26%)	114 (100%)	0	0	100	100
2	G	113/447 (25%)	110 (97%)	3 (3%)	0	100	100
2	R	113/447 (25%)	113 (100%)	0	0	100	100
3	C	1008/1288 (78%)	983 (98%)	25 (2%)	0	100	100
3	D	986/1288 (77%)	964 (98%)	21 (2%)	1 (0%)	48	70
3	E	983/1288 (76%)	962 (98%)	20 (2%)	1 (0%)	48	70
All	All	3627/5847 (62%)	3535 (98%)	90 (2%)	2 (0%)	49	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	942	PRO
3	E	942	PRO

5.3.2 Protein sidechains ⓘ

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	86/183 (47%)	86 (100%)	0	100	100
1	H	84/183 (46%)	84 (100%)	0	100	100
1	L	86/183 (47%)	85 (99%)	1 (1%)	63	83
2	B	98/393 (25%)	98 (100%)	0	100	100
2	G	97/393 (25%)	97 (100%)	0	100	100
2	R	97/393 (25%)	97 (100%)	0	100	100
3	C	895/1116 (80%)	892 (100%)	3 (0%)	86	94
3	D	879/1116 (79%)	877 (100%)	2 (0%)	87	95
3	E	878/1116 (79%)	873 (99%)	5 (1%)	78	91
All	All	3200/5076 (63%)	3189 (100%)	11 (0%)	84	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	91	VAL
3	D	495	TYR
3	D	498	GLN
3	E	129	LYS
3	E	130	VAL
3	E	131	CYS
3	E	166	CYS
3	E	167	THR
3	C	130	VAL
3	C	166	CYS
3	C	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	55	GLN
1	L	79	GLN
1	L	89	GLN
2	R	84	ASN
2	G	84	ASN
1	H	79	GLN
3	D	87	ASN
3	D	99	ASN
3	D	196	ASN
3	D	314	GLN
3	D	388	ASN
3	D	448	ASN
3	D	498	GLN
3	D	540	ASN
3	D	641	ASN
3	D	784	GLN
3	D	872	GLN
3	D	1002	GLN
3	D	1125	ASN
3	D	1142	GLN
3	E	121	ASN
3	E	125	ASN
3	E	207	HIS
3	E	245	HIS
3	E	360	ASN

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Mol	Chain	Res	Type
3	E	414	GLN
3	E	481	ASN
3	E	487	ASN
3	E	536	ASN
3	E	542	ASN
3	E	675	GLN
3	E	751	ASN
3	E	901	GLN
3	E	907	ASN
3	E	926	GLN
3	E	1011	GLN
3	E	1064	HIS
3	E	1125	ASN
3	C	99	ASN
3	C	188	ASN
3	C	196	ASN
3	C	282	ASN
3	C	481	ASN
3	C	487	ASN
3	C	540	ASN
3	C	628	GLN
3	C	703	ASN
3	C	787	GLN
3	C	919	ASN
3	C	926	GLN
2	B	84	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

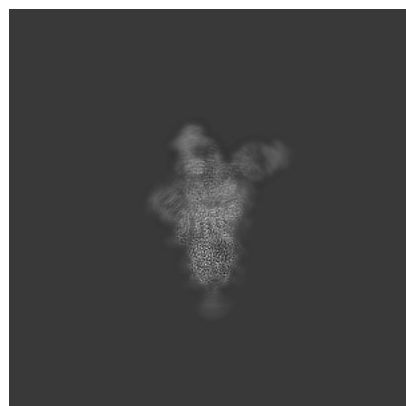
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18180. These allow visual inspection of the internal detail of the map and identification of artifacts.

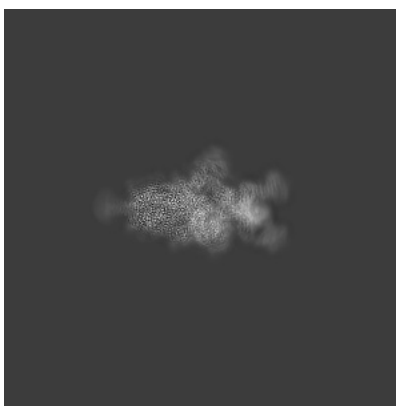
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

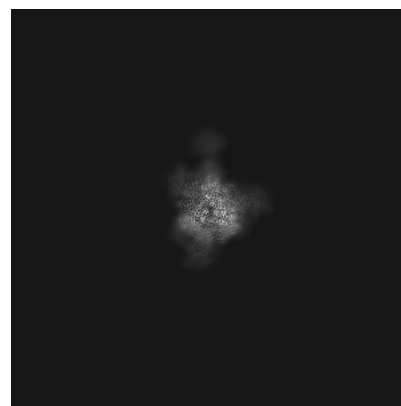
6.1.1 Primary map



X

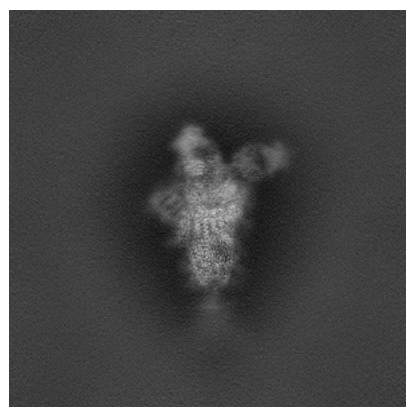


Y

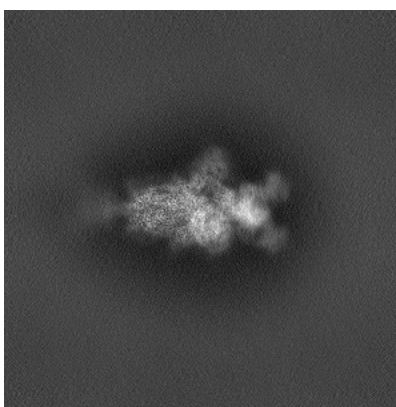


Z

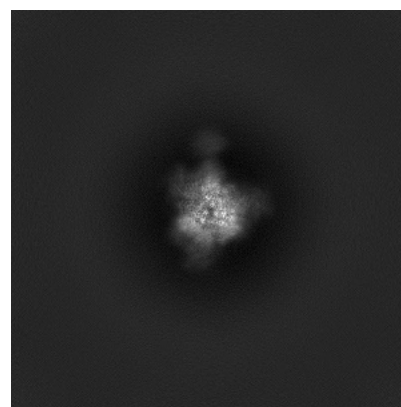
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

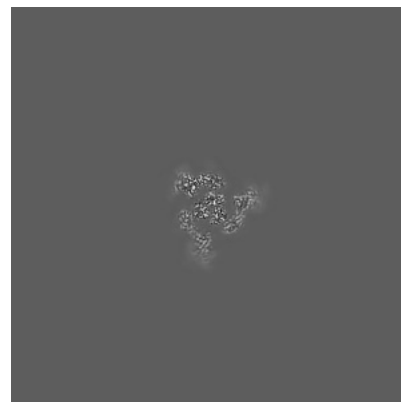
6.2.1 Primary map



X Index: 256

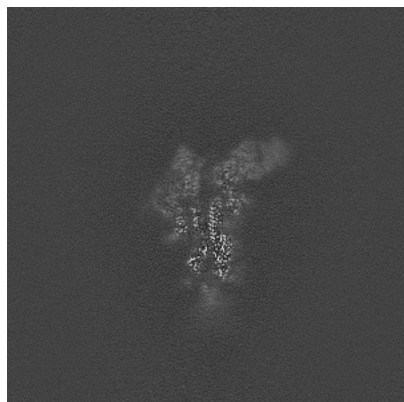


Y Index: 256

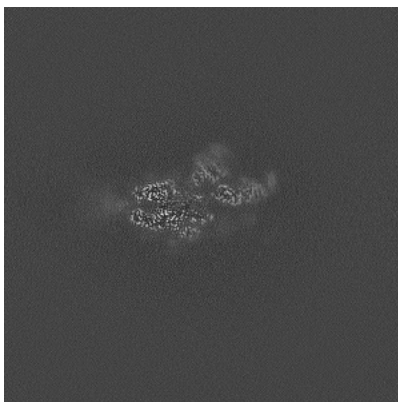


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

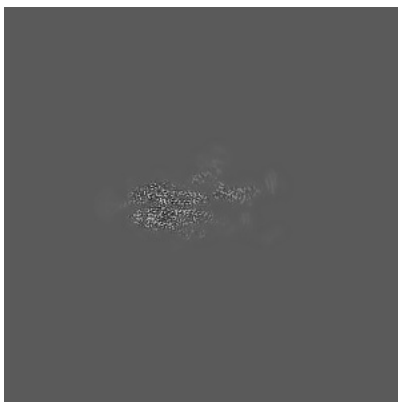
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

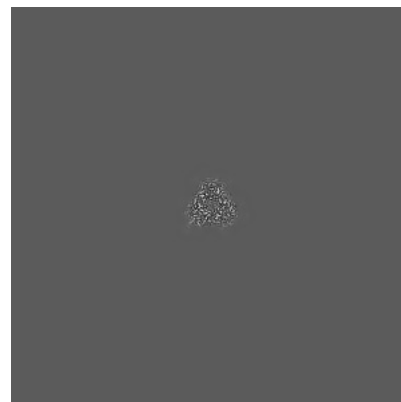
6.3.1 Primary map



X Index: 263

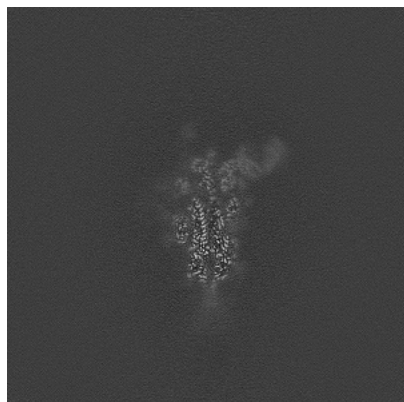


Y Index: 251

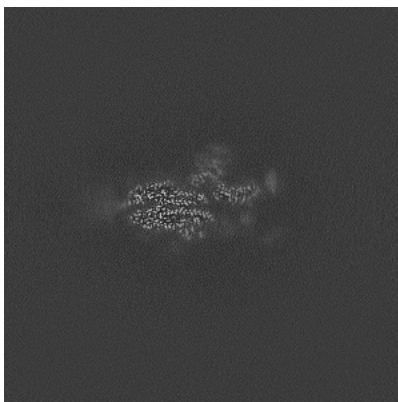


Z Index: 193

6.3.2 Raw map



X Index: 263



Y Index: 252

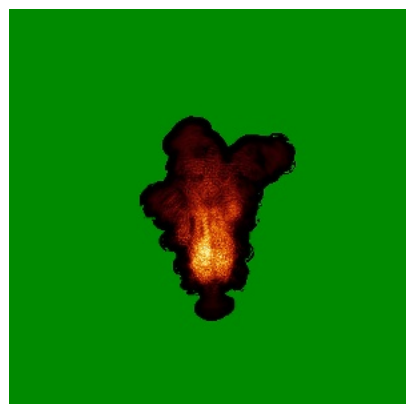


Z Index: 201

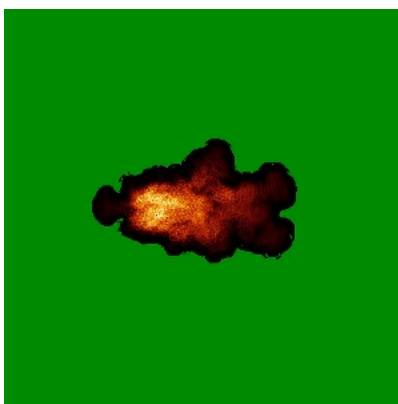
The images above show the largest variance slices of the map in three orthogonal directions.

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

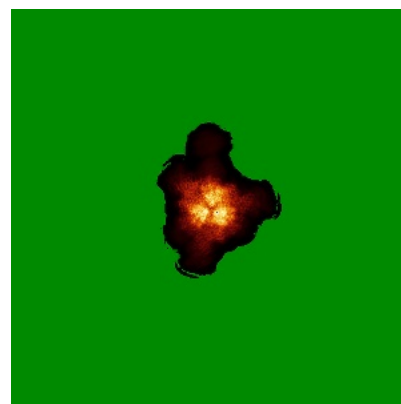
6.4.1 Primary map



X

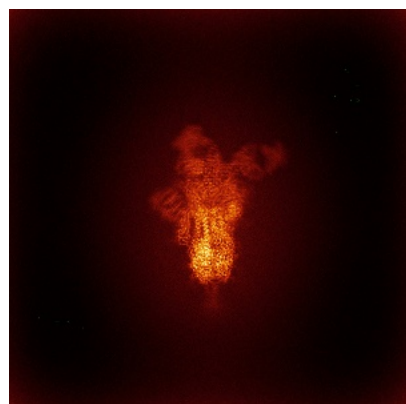


Y

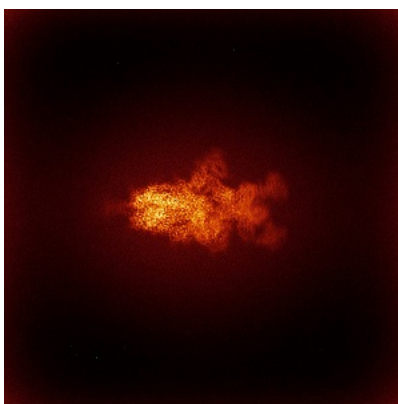


Z

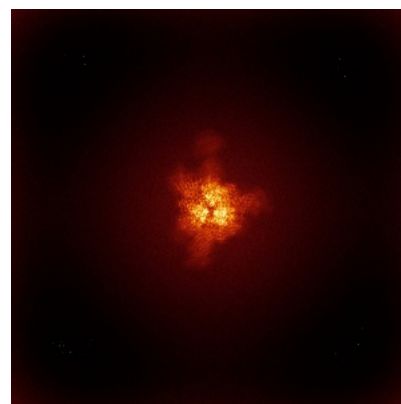
6.4.2 Raw map



X



Y

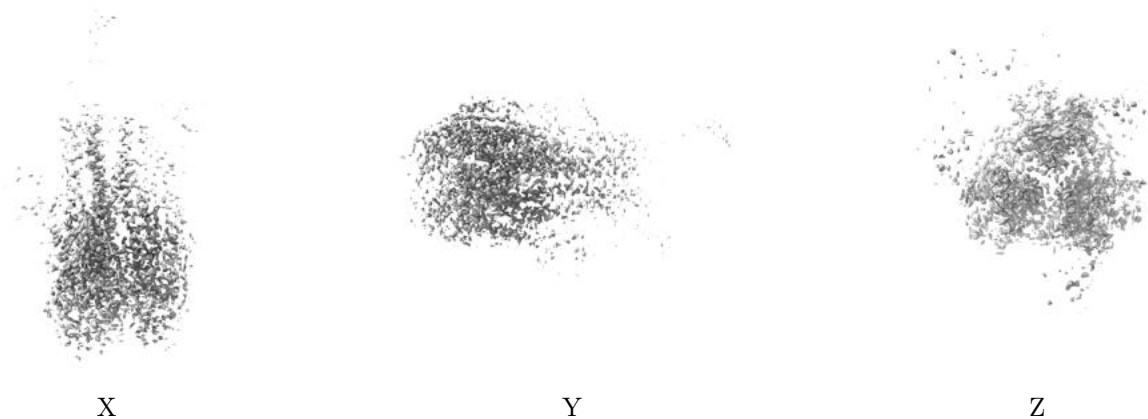


Z

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

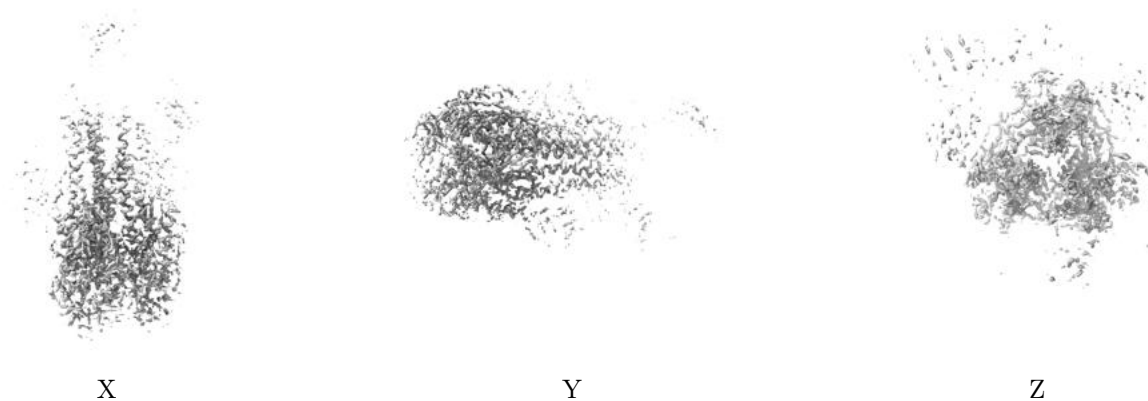
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

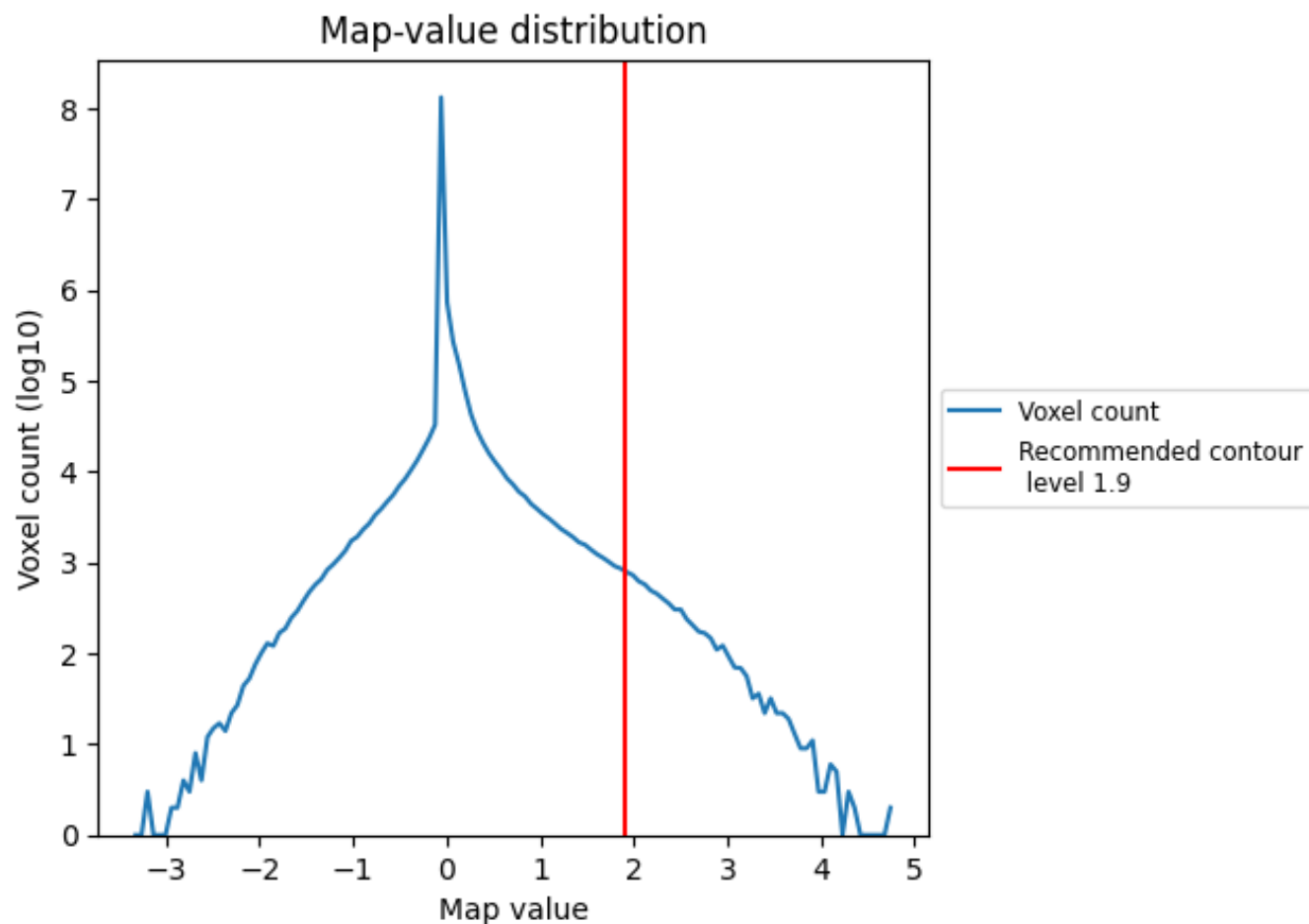
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

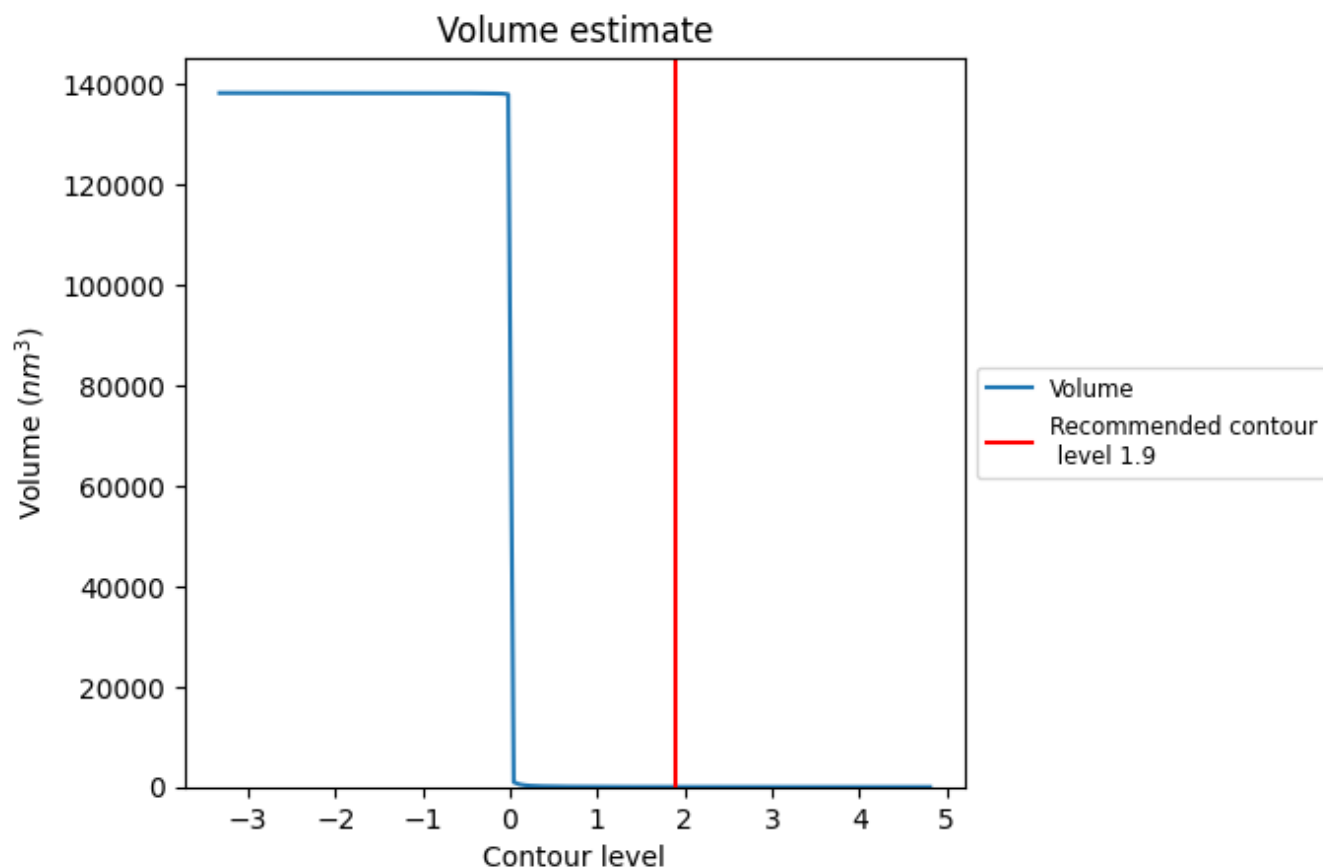
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

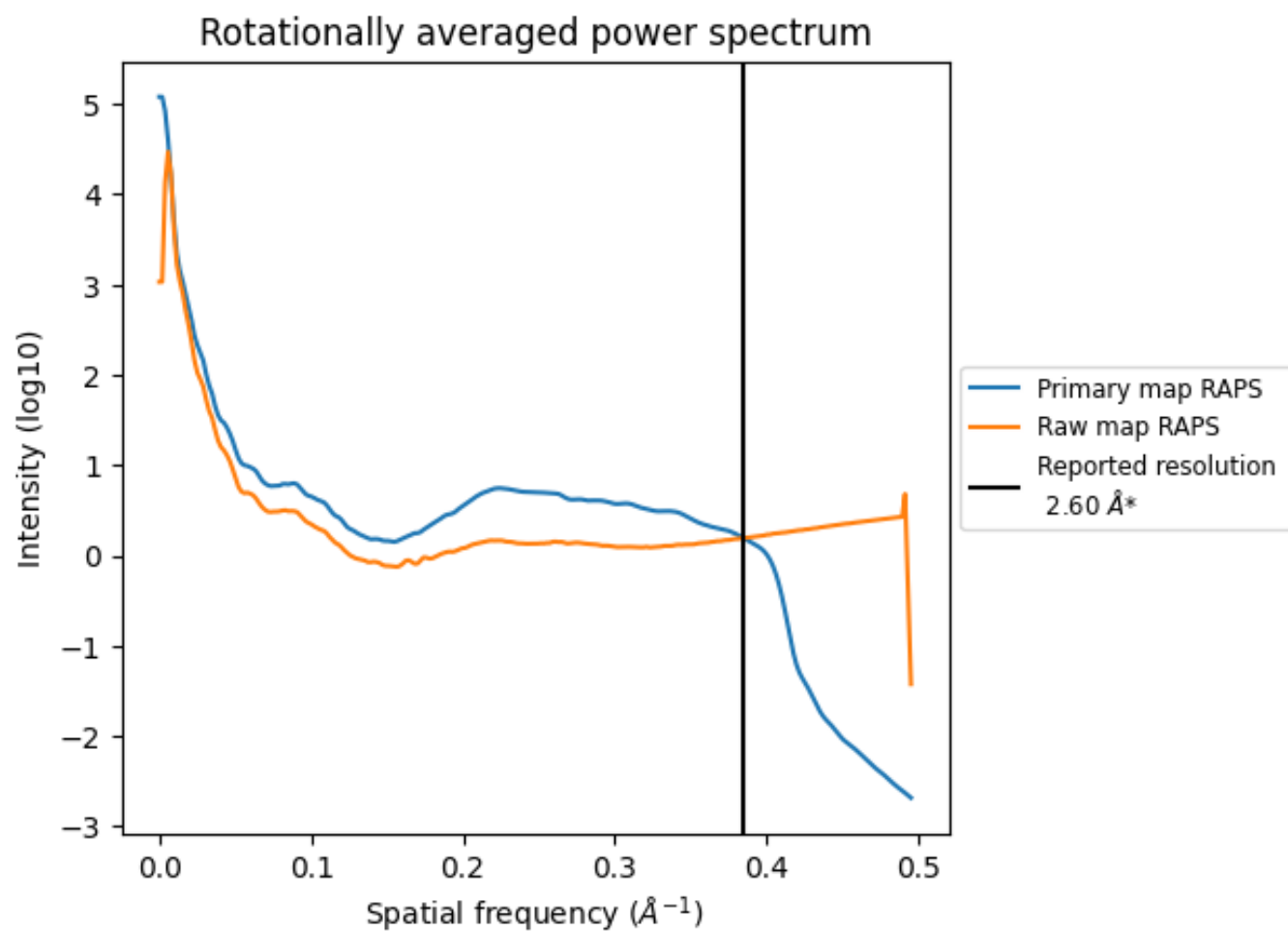
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7 nm^3 ; this corresponds to an approximate mass of 7 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

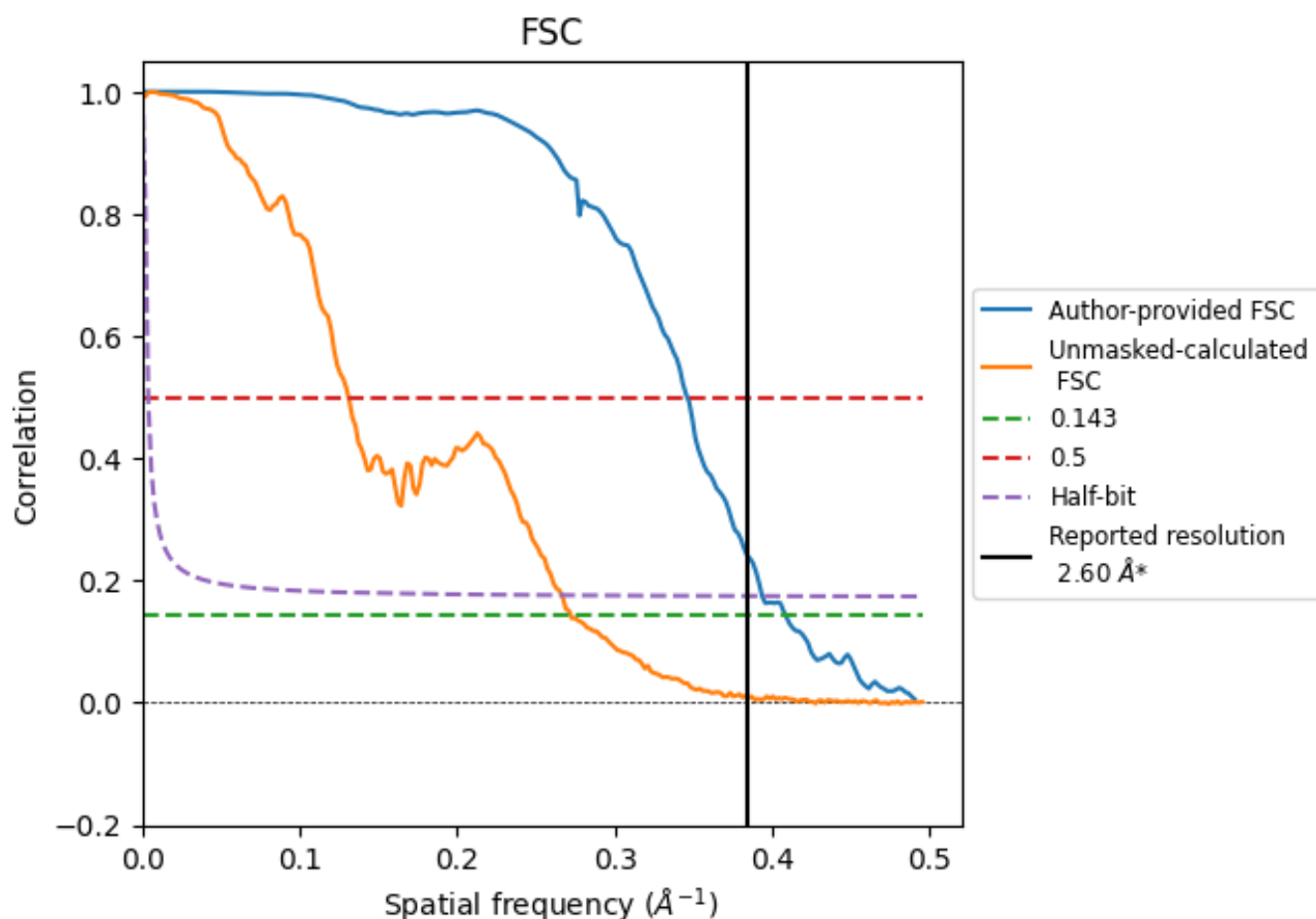


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

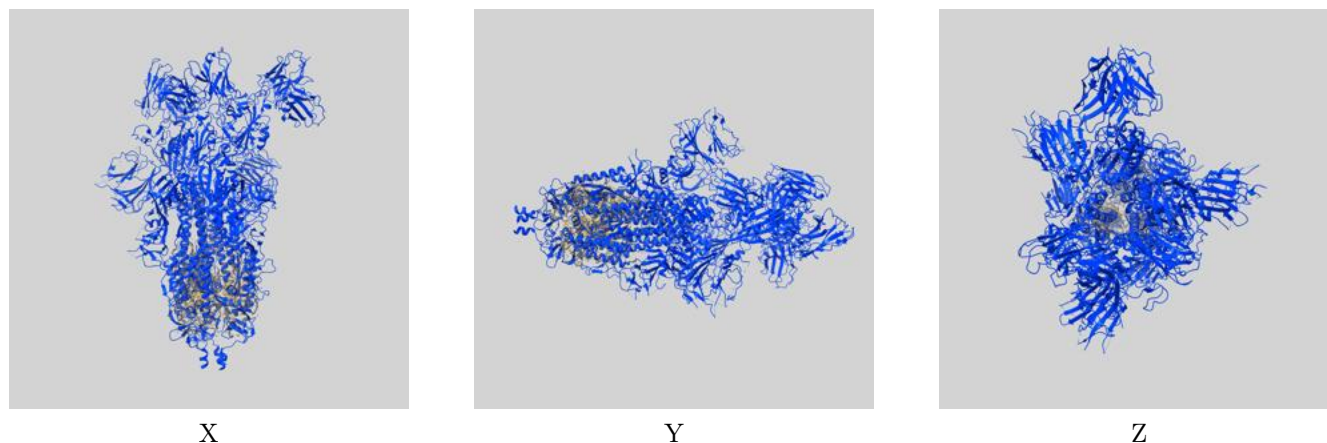
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.45	2.89	2.54
Unmasked-calculated*	3.68	7.64	3.76

*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 3.68 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

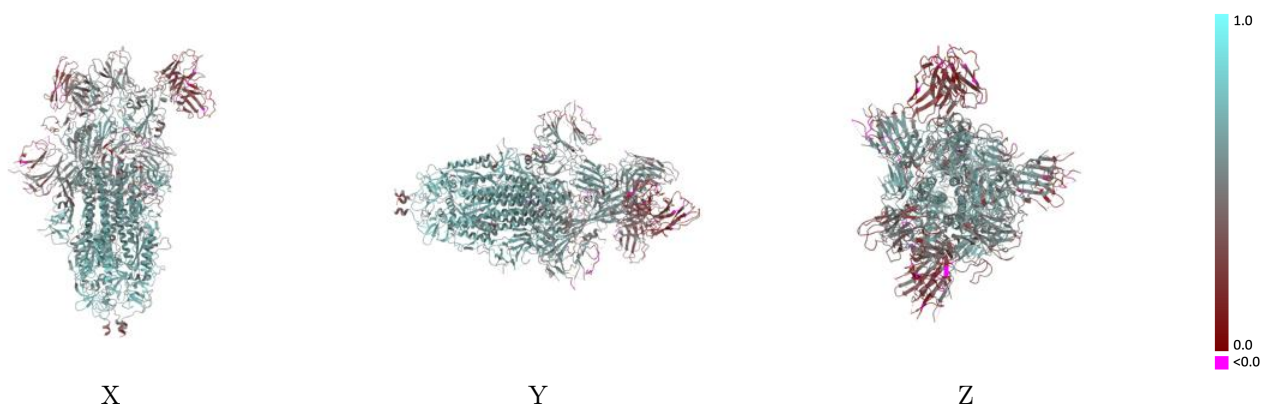
This section contains information regarding the fit between EMDB map EMD-18180 and PDB model 8Q5Y. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



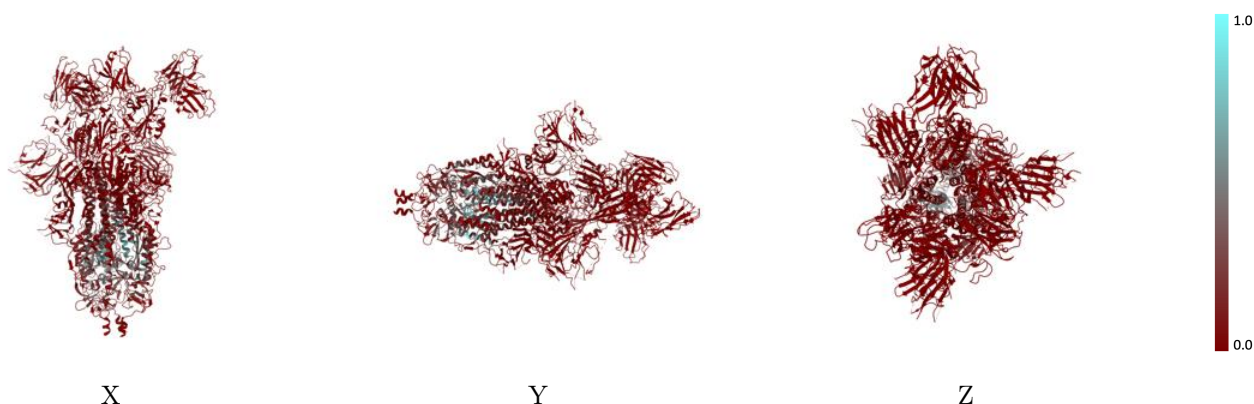
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



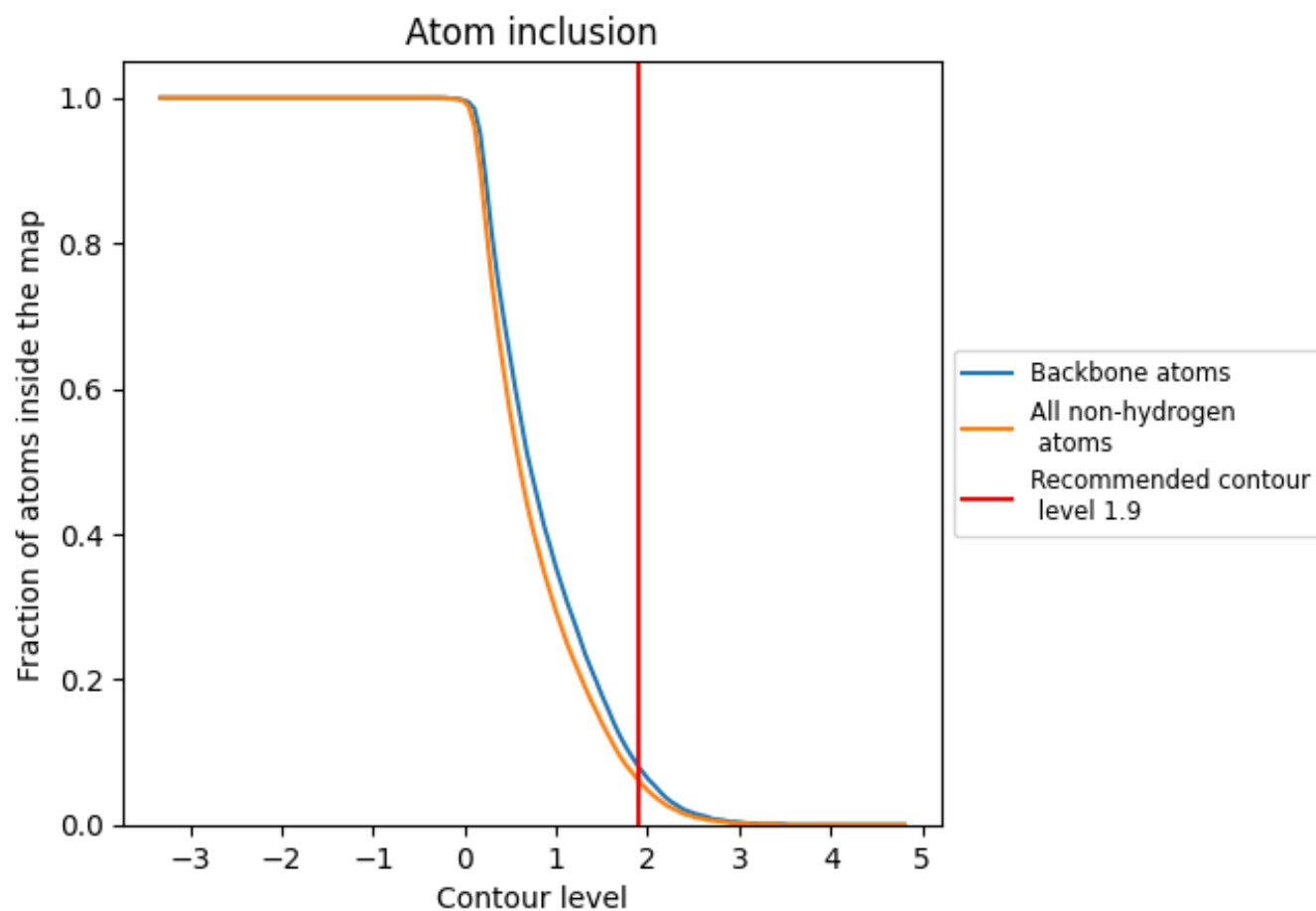
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 8% of all backbone atoms, 6% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0610	0.5160
A	0.0000	0.2410
B	0.0000	0.2370
C	0.0730	0.5490
D	0.0700	0.5660
E	0.0790	0.5510
G	0.0000	0.4750
H	0.0000	0.4750
L	0.0000	0.3510
R	0.0000	0.2370

1.0

0.0

<0.0