



Full wwPDB EM Validation Report ⓘ

Nov 18, 2024 – 01:34 PM JST

PDB ID : 8XEA
EMDB ID : EMD-38284
Title : XBB.1.5 spike protein in complex with BD55-1205
Authors : Feng, L.L.
Deposited on : 2023-12-11
Resolution : 3.42 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

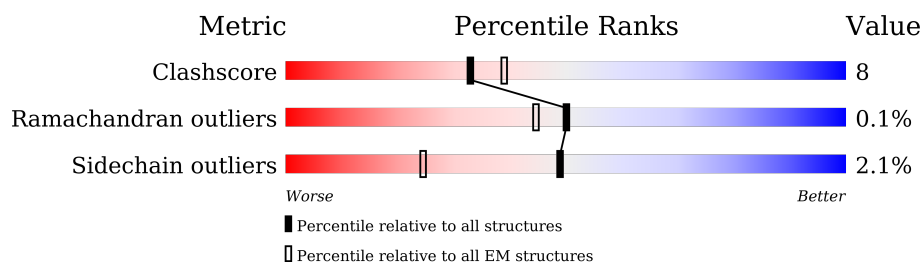
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	117	<div> <div>57%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
1	G	117	<div> <div>57%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	H	117	<div> <div>56%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	B	107	<div> <div>54%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
2	I	107	<div> <div>53%</div> <div>66%</div> <div>34%</div> </div>
2	J	107	<div> <div>52%</div> <div>79%</div> <div>21%</div> </div>
3	D	1221	<div> <div>.</div> <div>69%</div> <div>17%</div> <div>.</div> <div>13%</div> </div>
3	E	1221	<div> <div>5%</div> <div>68%</div> <div>19%</div> <div>.</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	1221	 <div> <div></div> <div>69%</div> <div>18%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 30213 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 BD55-1205 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	117	Total	C	N	O	S	0	0
			888	557	155	172	4		
1	G	117	Total	C	N	O	S	0	0
			888	557	155	172	4		
1	H	117	Total	C	N	O	S	0	0
			888	557	155	172	4		

- Molecule 2 is a protein called BD55-1205 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			821	518	137	163	3		
2	I	107	Total	C	N	O	S	0	0
			821	518	137	163	3		
2	J	107	Total	C	N	O	S	0	0
			821	518	137	163	3		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1066	Total	C	N	O	S	0	0
			8360	5346	1396	1579	39		
3	E	1066	Total	C	N	O	S	0	0
			8359	5344	1396	1580	39		
3	F	1067	Total	C	N	O	S	0	0
			8367	5350	1397	1581	39		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	19	ILE	THR	variant	UNP P0DTC2
D	26	GLN	PRO	variant	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	83	ALA	VAL	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	146	GLN	HIS	variant	UNP P0DTC2
D	183	GLU	GLN	variant	UNP P0DTC2
D	213	GLU	VAL	variant	UNP P0DTC2
D	252	VAL	GLY	variant	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	368	ILE	LEU	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	PRO	VAL	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	490	SER	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	variant	UNP P0DTC2
D	892	PRO	ALA	variant	UNP P0DTC2
D	899	PRO	ALA	variant	UNP P0DTC2
D	942	PRO	ALA	variant	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1141	GLY	-	expression tag	UNP P0DTC2
D	1142	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1143	SER	-	expression tag	UNP P0DTC2
D	1144	GLY	-	expression tag	UNP P0DTC2
D	1145	GLY	-	expression tag	UNP P0DTC2
D	1146	SER	-	expression tag	UNP P0DTC2
D	1147	TYR	-	expression tag	UNP P0DTC2
D	1148	ILE	-	expression tag	UNP P0DTC2
D	1149	PRO	-	expression tag	UNP P0DTC2
D	1150	GLU	-	expression tag	UNP P0DTC2
D	1151	ALA	-	expression tag	UNP P0DTC2
D	1152	PRO	-	expression tag	UNP P0DTC2
D	1153	ARG	-	expression tag	UNP P0DTC2
D	1154	ASP	-	expression tag	UNP P0DTC2
D	1155	GLY	-	expression tag	UNP P0DTC2
D	1156	GLN	-	expression tag	UNP P0DTC2
D	1157	ALA	-	expression tag	UNP P0DTC2
D	1158	TYR	-	expression tag	UNP P0DTC2
D	1159	VAL	-	expression tag	UNP P0DTC2
D	1160	ARG	-	expression tag	UNP P0DTC2
D	1161	LYS	-	expression tag	UNP P0DTC2
D	1162	ASP	-	expression tag	UNP P0DTC2
D	1163	GLY	-	expression tag	UNP P0DTC2
D	1164	GLU	-	expression tag	UNP P0DTC2
D	1165	TRP	-	expression tag	UNP P0DTC2
D	1166	VAL	-	expression tag	UNP P0DTC2
D	1167	LEU	-	expression tag	UNP P0DTC2
D	1168	LEU	-	expression tag	UNP P0DTC2
D	1169	SER	-	expression tag	UNP P0DTC2
D	1170	THR	-	expression tag	UNP P0DTC2
D	1171	PHE	-	expression tag	UNP P0DTC2
D	1172	LEU	-	expression tag	UNP P0DTC2
D	1173	GLY	-	expression tag	UNP P0DTC2
D	1174	ARG	-	expression tag	UNP P0DTC2
D	1175	SER	-	expression tag	UNP P0DTC2
D	1176	LEU	-	expression tag	UNP P0DTC2
D	1177	GLU	-	expression tag	UNP P0DTC2
D	1178	VAL	-	expression tag	UNP P0DTC2
D	1179	LEU	-	expression tag	UNP P0DTC2
D	1180	PHE	-	expression tag	UNP P0DTC2
D	1181	GLN	-	expression tag	UNP P0DTC2
D	1182	GLY	-	expression tag	UNP P0DTC2
D	1183	PRO	-	expression tag	UNP P0DTC2
D	1184	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1185	TRP	-	expression tag	UNP P0DTC2
D	1186	SER	-	expression tag	UNP P0DTC2
D	1187	HIS	-	expression tag	UNP P0DTC2
D	1188	PRO	-	expression tag	UNP P0DTC2
D	1189	GLN	-	expression tag	UNP P0DTC2
D	1190	PHE	-	expression tag	UNP P0DTC2
D	1191	GLU	-	expression tag	UNP P0DTC2
D	1192	LYS	-	expression tag	UNP P0DTC2
D	1193	GLY	-	expression tag	UNP P0DTC2
D	1194	GLY	-	expression tag	UNP P0DTC2
D	1195	GLY	-	expression tag	UNP P0DTC2
D	1196	SER	-	expression tag	UNP P0DTC2
D	1197	GLY	-	expression tag	UNP P0DTC2
D	1198	GLY	-	expression tag	UNP P0DTC2
D	1199	GLY	-	expression tag	UNP P0DTC2
D	1200	SER	-	expression tag	UNP P0DTC2
D	1201	GLY	-	expression tag	UNP P0DTC2
D	1202	GLY	-	expression tag	UNP P0DTC2
D	1203	SER	-	expression tag	UNP P0DTC2
D	1204	SER	-	expression tag	UNP P0DTC2
D	1205	ALA	-	expression tag	UNP P0DTC2
D	1206	TRP	-	expression tag	UNP P0DTC2
D	1207	SER	-	expression tag	UNP P0DTC2
D	1208	HIS	-	expression tag	UNP P0DTC2
D	1209	PRO	-	expression tag	UNP P0DTC2
D	1210	GLN	-	expression tag	UNP P0DTC2
D	1211	PHE	-	expression tag	UNP P0DTC2
D	1212	GLU	-	expression tag	UNP P0DTC2
D	1213	LYS	-	expression tag	UNP P0DTC2
D	1214	HIS	-	expression tag	UNP P0DTC2
D	1215	HIS	-	expression tag	UNP P0DTC2
D	1216	HIS	-	expression tag	UNP P0DTC2
D	1217	HIS	-	expression tag	UNP P0DTC2
D	1218	HIS	-	expression tag	UNP P0DTC2
D	1219	HIS	-	expression tag	UNP P0DTC2
D	1220	HIS	-	expression tag	UNP P0DTC2
D	1221	HIS	-	expression tag	UNP P0DTC2
E	19	ILE	THR	variant	UNP P0DTC2
E	26	GLN	PRO	variant	UNP P0DTC2
E	27	SER	ALA	variant	UNP P0DTC2
E	83	ALA	VAL	variant	UNP P0DTC2
E	142	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	146	GLN	HIS	variant	UNP P0DTC2
E	183	GLU	GLN	variant	UNP P0DTC2
E	213	GLU	VAL	variant	UNP P0DTC2
E	252	VAL	GLY	variant	UNP P0DTC2
E	339	HIS	GLY	variant	UNP P0DTC2
E	346	THR	ARG	variant	UNP P0DTC2
E	368	ILE	LEU	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	445	PRO	VAL	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	460	LYS	ASN	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	486	PRO	PHE	variant	UNP P0DTC2
E	490	SER	PHE	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	655	TYR	HIS	variant	UNP P0DTC2
E	764	LYS	ASN	variant	UNP P0DTC2
E	796	TYR	ASP	variant	UNP P0DTC2
E	817	PRO	PHE	variant	UNP P0DTC2
E	892	PRO	ALA	variant	UNP P0DTC2
E	899	PRO	ALA	variant	UNP P0DTC2
E	942	PRO	ALA	variant	UNP P0DTC2
E	954	HIS	GLN	variant	UNP P0DTC2
E	969	LYS	ASN	variant	UNP P0DTC2
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1141	GLY	-	expression tag	UNP P0DTC2
E	1142	GLY	-	expression tag	UNP P0DTC2
E	1143	SER	-	expression tag	UNP P0DTC2
E	1144	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1145	GLY	-	expression tag	UNP P0DTC2
E	1146	SER	-	expression tag	UNP P0DTC2
E	1147	TYR	-	expression tag	UNP P0DTC2
E	1148	ILE	-	expression tag	UNP P0DTC2
E	1149	PRO	-	expression tag	UNP P0DTC2
E	1150	GLU	-	expression tag	UNP P0DTC2
E	1151	ALA	-	expression tag	UNP P0DTC2
E	1152	PRO	-	expression tag	UNP P0DTC2
E	1153	ARG	-	expression tag	UNP P0DTC2
E	1154	ASP	-	expression tag	UNP P0DTC2
E	1155	GLY	-	expression tag	UNP P0DTC2
E	1156	GLN	-	expression tag	UNP P0DTC2
E	1157	ALA	-	expression tag	UNP P0DTC2
E	1158	TYR	-	expression tag	UNP P0DTC2
E	1159	VAL	-	expression tag	UNP P0DTC2
E	1160	ARG	-	expression tag	UNP P0DTC2
E	1161	LYS	-	expression tag	UNP P0DTC2
E	1162	ASP	-	expression tag	UNP P0DTC2
E	1163	GLY	-	expression tag	UNP P0DTC2
E	1164	GLU	-	expression tag	UNP P0DTC2
E	1165	TRP	-	expression tag	UNP P0DTC2
E	1166	VAL	-	expression tag	UNP P0DTC2
E	1167	LEU	-	expression tag	UNP P0DTC2
E	1168	LEU	-	expression tag	UNP P0DTC2
E	1169	SER	-	expression tag	UNP P0DTC2
E	1170	THR	-	expression tag	UNP P0DTC2
E	1171	PHE	-	expression tag	UNP P0DTC2
E	1172	LEU	-	expression tag	UNP P0DTC2
E	1173	GLY	-	expression tag	UNP P0DTC2
E	1174	ARG	-	expression tag	UNP P0DTC2
E	1175	SER	-	expression tag	UNP P0DTC2
E	1176	LEU	-	expression tag	UNP P0DTC2
E	1177	GLU	-	expression tag	UNP P0DTC2
E	1178	VAL	-	expression tag	UNP P0DTC2
E	1179	LEU	-	expression tag	UNP P0DTC2
E	1180	PHE	-	expression tag	UNP P0DTC2
E	1181	GLN	-	expression tag	UNP P0DTC2
E	1182	GLY	-	expression tag	UNP P0DTC2
E	1183	PRO	-	expression tag	UNP P0DTC2
E	1184	GLY	-	expression tag	UNP P0DTC2
E	1185	TRP	-	expression tag	UNP P0DTC2
E	1186	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1187	HIS	-	expression tag	UNP P0DTC2
E	1188	PRO	-	expression tag	UNP P0DTC2
E	1189	GLN	-	expression tag	UNP P0DTC2
E	1190	PHE	-	expression tag	UNP P0DTC2
E	1191	GLU	-	expression tag	UNP P0DTC2
E	1192	LYS	-	expression tag	UNP P0DTC2
E	1193	GLY	-	expression tag	UNP P0DTC2
E	1194	GLY	-	expression tag	UNP P0DTC2
E	1195	GLY	-	expression tag	UNP P0DTC2
E	1196	SER	-	expression tag	UNP P0DTC2
E	1197	GLY	-	expression tag	UNP P0DTC2
E	1198	GLY	-	expression tag	UNP P0DTC2
E	1199	GLY	-	expression tag	UNP P0DTC2
E	1200	SER	-	expression tag	UNP P0DTC2
E	1201	GLY	-	expression tag	UNP P0DTC2
E	1202	GLY	-	expression tag	UNP P0DTC2
E	1203	SER	-	expression tag	UNP P0DTC2
E	1204	SER	-	expression tag	UNP P0DTC2
E	1205	ALA	-	expression tag	UNP P0DTC2
E	1206	TRP	-	expression tag	UNP P0DTC2
E	1207	SER	-	expression tag	UNP P0DTC2
E	1208	HIS	-	expression tag	UNP P0DTC2
E	1209	PRO	-	expression tag	UNP P0DTC2
E	1210	GLN	-	expression tag	UNP P0DTC2
E	1211	PHE	-	expression tag	UNP P0DTC2
E	1212	GLU	-	expression tag	UNP P0DTC2
E	1213	LYS	-	expression tag	UNP P0DTC2
E	1214	HIS	-	expression tag	UNP P0DTC2
E	1215	HIS	-	expression tag	UNP P0DTC2
E	1216	HIS	-	expression tag	UNP P0DTC2
E	1217	HIS	-	expression tag	UNP P0DTC2
E	1218	HIS	-	expression tag	UNP P0DTC2
E	1219	HIS	-	expression tag	UNP P0DTC2
E	1220	HIS	-	expression tag	UNP P0DTC2
E	1221	HIS	-	expression tag	UNP P0DTC2
F	19	ILE	THR	variant	UNP P0DTC2
F	26	GLN	PRO	variant	UNP P0DTC2
F	27	SER	ALA	variant	UNP P0DTC2
F	83	ALA	VAL	variant	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	146	GLN	HIS	variant	UNP P0DTC2
F	183	GLU	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	213	GLU	VAL	variant	UNP P0DTC2
F	252	VAL	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	variant	UNP P0DTC2
F	892	PRO	ALA	variant	UNP P0DTC2
F	899	PRO	ALA	variant	UNP P0DTC2
F	942	PRO	ALA	variant	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	variant	UNP P0DTC2
F	987	PRO	VAL	variant	UNP P0DTC2
F	1141	GLY	-	expression tag	UNP P0DTC2
F	1142	GLY	-	expression tag	UNP P0DTC2
F	1143	SER	-	expression tag	UNP P0DTC2
F	1144	GLY	-	expression tag	UNP P0DTC2
F	1145	GLY	-	expression tag	UNP P0DTC2
F	1146	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1147	TYR	-	expression tag	UNP P0DTC2
F	1148	ILE	-	expression tag	UNP P0DTC2
F	1149	PRO	-	expression tag	UNP P0DTC2
F	1150	GLU	-	expression tag	UNP P0DTC2
F	1151	ALA	-	expression tag	UNP P0DTC2
F	1152	PRO	-	expression tag	UNP P0DTC2
F	1153	ARG	-	expression tag	UNP P0DTC2
F	1154	ASP	-	expression tag	UNP P0DTC2
F	1155	GLY	-	expression tag	UNP P0DTC2
F	1156	GLN	-	expression tag	UNP P0DTC2
F	1157	ALA	-	expression tag	UNP P0DTC2
F	1158	TYR	-	expression tag	UNP P0DTC2
F	1159	VAL	-	expression tag	UNP P0DTC2
F	1160	ARG	-	expression tag	UNP P0DTC2
F	1161	LYS	-	expression tag	UNP P0DTC2
F	1162	ASP	-	expression tag	UNP P0DTC2
F	1163	GLY	-	expression tag	UNP P0DTC2
F	1164	GLU	-	expression tag	UNP P0DTC2
F	1165	TRP	-	expression tag	UNP P0DTC2
F	1166	VAL	-	expression tag	UNP P0DTC2
F	1167	LEU	-	expression tag	UNP P0DTC2
F	1168	LEU	-	expression tag	UNP P0DTC2
F	1169	SER	-	expression tag	UNP P0DTC2
F	1170	THR	-	expression tag	UNP P0DTC2
F	1171	PHE	-	expression tag	UNP P0DTC2
F	1172	LEU	-	expression tag	UNP P0DTC2
F	1173	GLY	-	expression tag	UNP P0DTC2
F	1174	ARG	-	expression tag	UNP P0DTC2
F	1175	SER	-	expression tag	UNP P0DTC2
F	1176	LEU	-	expression tag	UNP P0DTC2
F	1177	GLU	-	expression tag	UNP P0DTC2
F	1178	VAL	-	expression tag	UNP P0DTC2
F	1179	LEU	-	expression tag	UNP P0DTC2
F	1180	PHE	-	expression tag	UNP P0DTC2
F	1181	GLN	-	expression tag	UNP P0DTC2
F	1182	GLY	-	expression tag	UNP P0DTC2
F	1183	PRO	-	expression tag	UNP P0DTC2
F	1184	GLY	-	expression tag	UNP P0DTC2
F	1185	TRP	-	expression tag	UNP P0DTC2
F	1186	SER	-	expression tag	UNP P0DTC2
F	1187	HIS	-	expression tag	UNP P0DTC2
F	1188	PRO	-	expression tag	UNP P0DTC2

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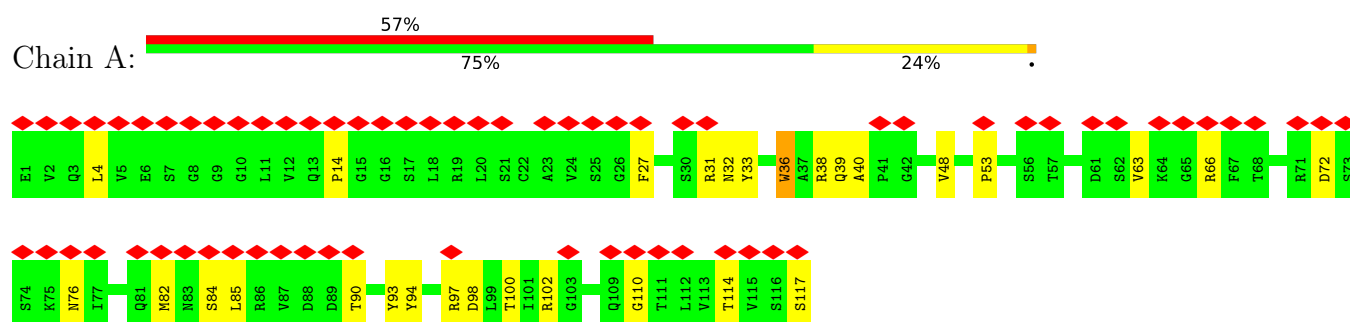
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1189	GLN	-	expression tag	UNP P0DTC2
F	1190	PHE	-	expression tag	UNP P0DTC2
F	1191	GLU	-	expression tag	UNP P0DTC2
F	1192	LYS	-	expression tag	UNP P0DTC2
F	1193	GLY	-	expression tag	UNP P0DTC2
F	1194	GLY	-	expression tag	UNP P0DTC2
F	1195	GLY	-	expression tag	UNP P0DTC2
F	1196	SER	-	expression tag	UNP P0DTC2
F	1197	GLY	-	expression tag	UNP P0DTC2
F	1198	GLY	-	expression tag	UNP P0DTC2
F	1199	GLY	-	expression tag	UNP P0DTC2
F	1200	SER	-	expression tag	UNP P0DTC2
F	1201	GLY	-	expression tag	UNP P0DTC2
F	1202	GLY	-	expression tag	UNP P0DTC2
F	1203	SER	-	expression tag	UNP P0DTC2
F	1204	SER	-	expression tag	UNP P0DTC2
F	1205	ALA	-	expression tag	UNP P0DTC2
F	1206	TRP	-	expression tag	UNP P0DTC2
F	1207	SER	-	expression tag	UNP P0DTC2
F	1208	HIS	-	expression tag	UNP P0DTC2
F	1209	PRO	-	expression tag	UNP P0DTC2
F	1210	GLN	-	expression tag	UNP P0DTC2
F	1211	PHE	-	expression tag	UNP P0DTC2
F	1212	GLU	-	expression tag	UNP P0DTC2
F	1213	LYS	-	expression tag	UNP P0DTC2
F	1214	HIS	-	expression tag	UNP P0DTC2
F	1215	HIS	-	expression tag	UNP P0DTC2
F	1216	HIS	-	expression tag	UNP P0DTC2
F	1217	HIS	-	expression tag	UNP P0DTC2
F	1218	HIS	-	expression tag	UNP P0DTC2
F	1219	HIS	-	expression tag	UNP P0DTC2
F	1220	HIS	-	expression tag	UNP P0DTC2
F	1221	HIS	-	expression tag	UNP P0DTC2

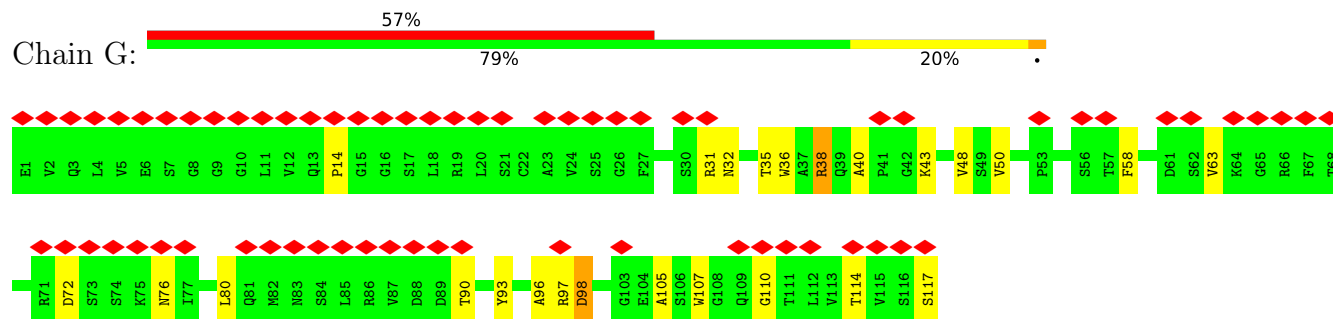
3 Residue-property plots [i](#)

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.

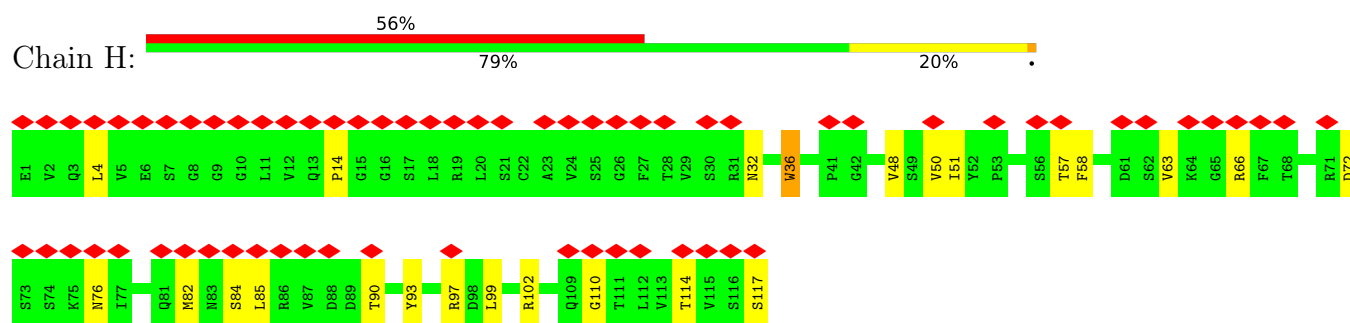
- Molecule 1: BD55-1205 heavy chain



- Molecule 1: BD55-1205 heavy chain

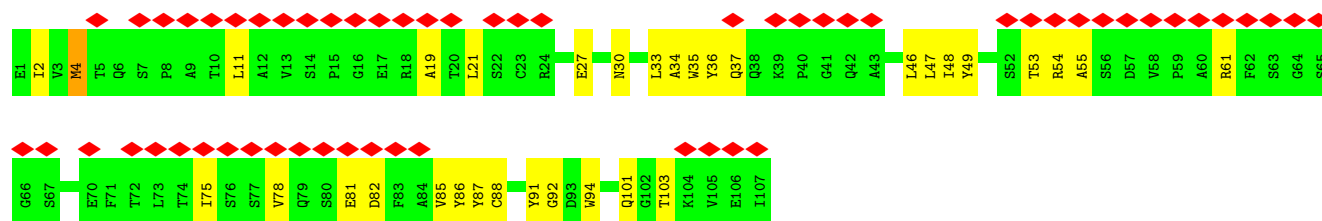


- Molecule 1: BD55-1205 heavy chain

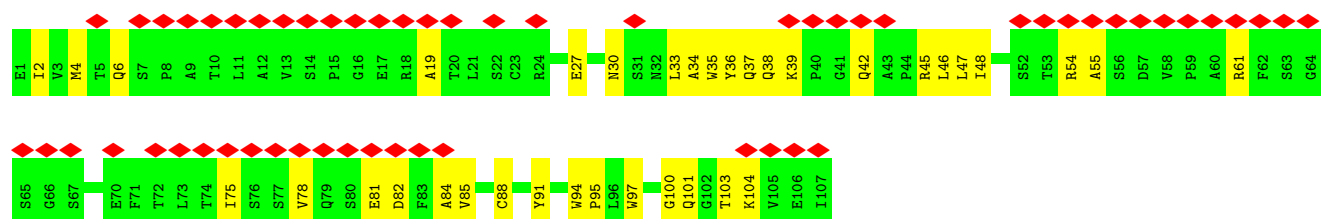


- Molecule 2: BD55-1205 light chain

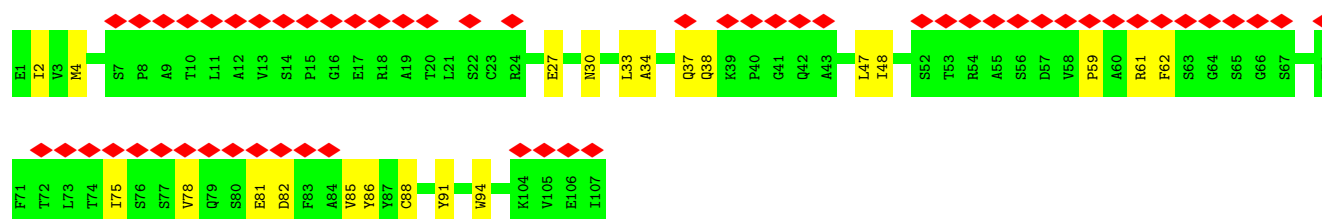
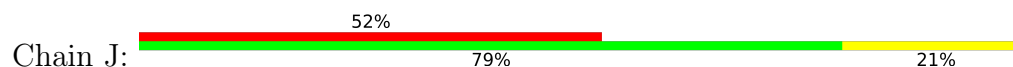




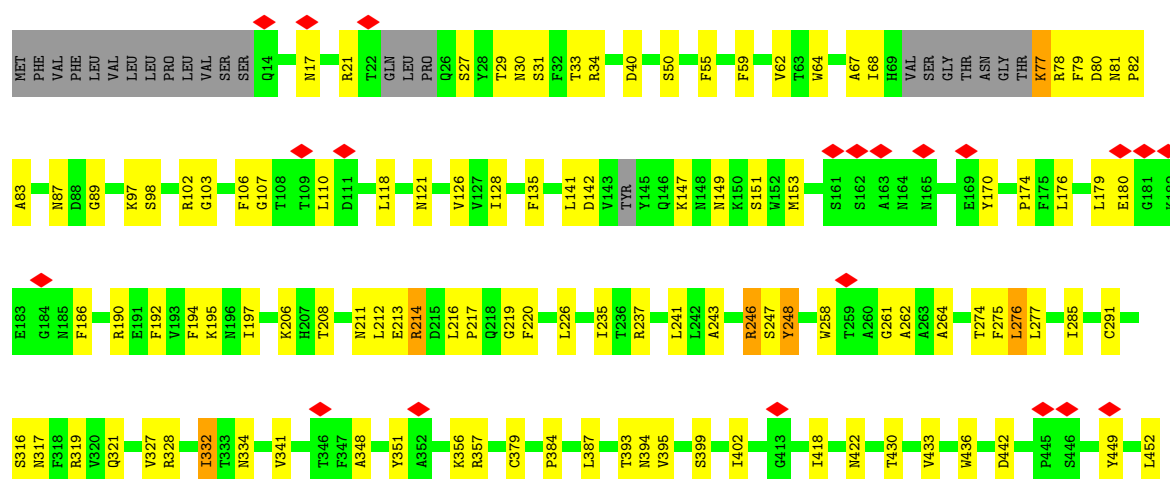
• Molecule 2: BD55-1205 light chain

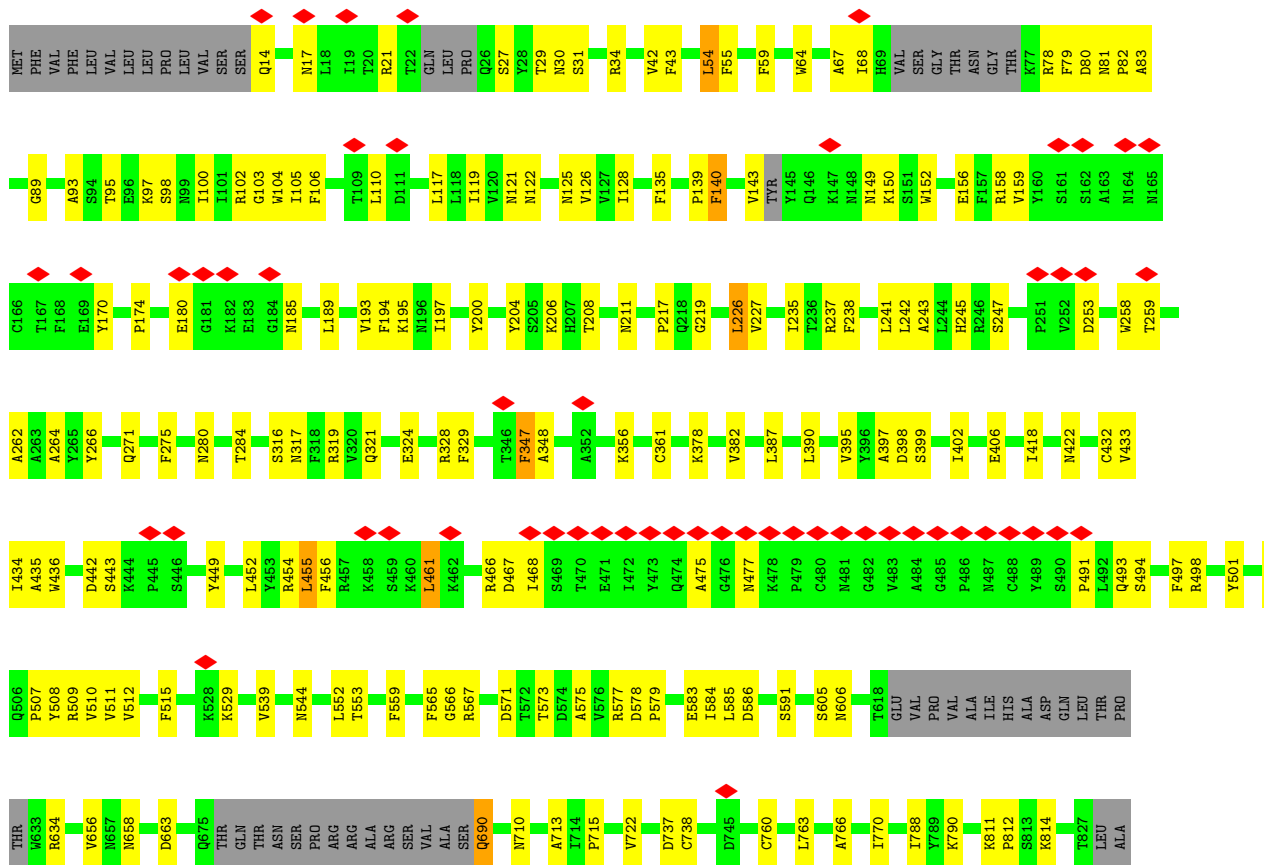


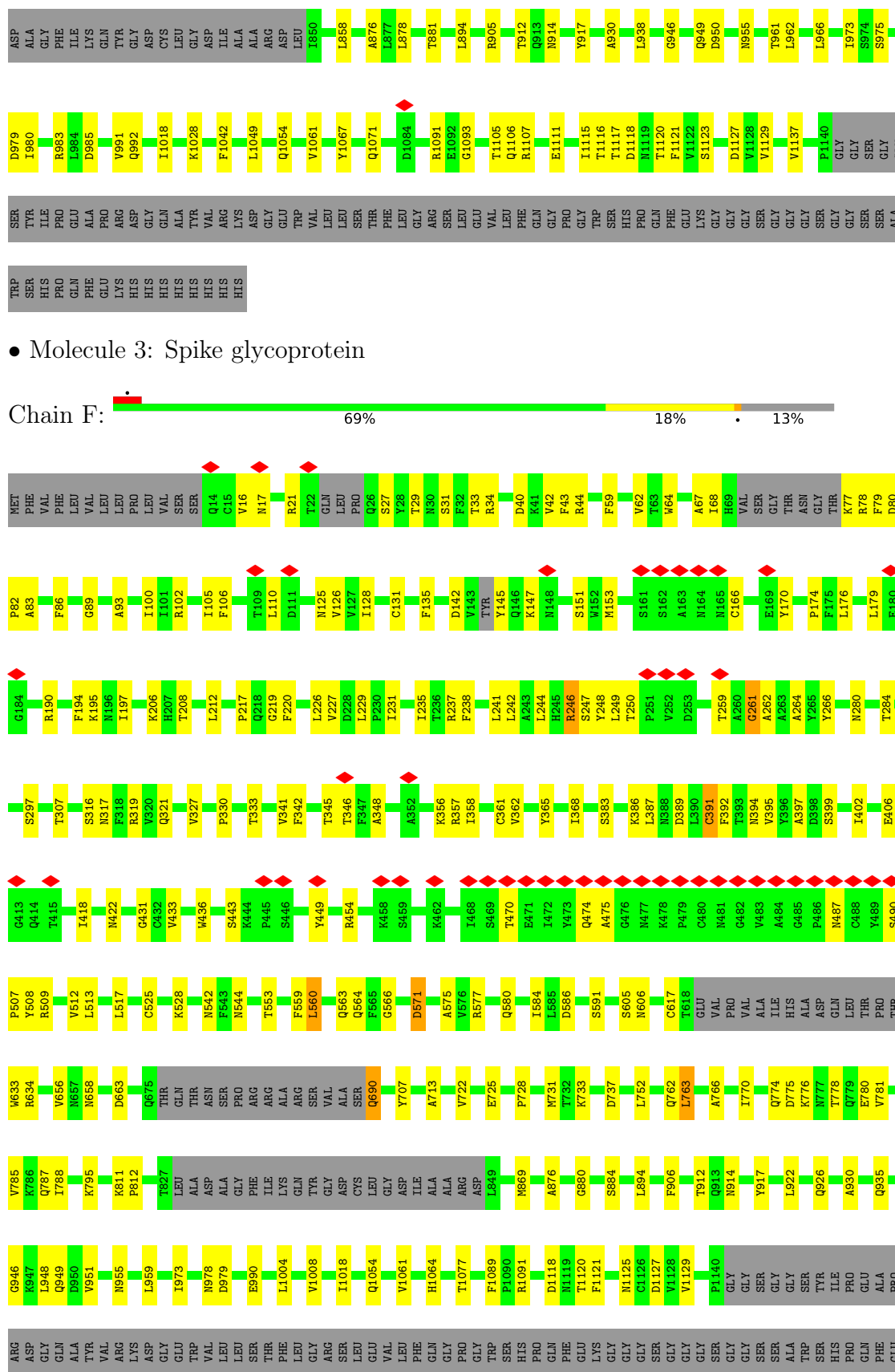
• Molecule 2: BD55-1205 light chain



• Molecule 3: Spike glycoprotein







• Molecule 3: Spike glycoprotein

Chain F:

LYS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	238788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.953	Depositor
Minimum map value	-0.253	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.26	0/906	0.56	0/1229
1	G	0.26	0/906	0.59	0/1229
1	H	0.25	0/906	0.55	0/1229
2	B	0.26	0/842	0.55	0/1147
2	I	0.27	0/842	0.62	0/1147
2	J	0.27	0/842	0.56	0/1147
3	D	0.27	0/8561	0.56	6/11648 (0.1%)
3	E	0.27	0/8560	0.55	3/11647 (0.0%)
3	F	0.28	0/8568	0.56	3/11658 (0.0%)
All	All	0.27	0/30933	0.56	12/42081 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	40	ASP	CB-CG-OD2	7.97	125.48	118.30
3	E	985	ASP	CB-CG-OD1	6.90	124.51	118.30
3	D	985	ASP	CB-CG-OD1	6.80	124.42	118.30
3	D	40	ASP	CB-CG-OD2	6.70	124.33	118.30
3	D	546	LEU	CA-CB-CG	6.00	129.10	115.30
3	D	650	LEU	CA-CB-CG	5.65	128.29	115.30
3	E	455	LEU	CA-CB-CG	5.50	127.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	54	LEU	CA-CB-CG	5.42	127.77	115.30
3	D	276	LEU	CA-CB-CG	5.22	127.32	115.30
3	D	118	LEU	CA-CB-CG	5.17	127.18	115.30
3	F	242	LEU	CA-CB-CG	5.10	127.02	115.30
3	F	560	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	261	GLY	Peptide
3	F	261	GLY	Peptide

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	888	0	871	19	0
1	G	888	0	871	19	0
1	H	888	0	871	14	0
2	B	821	0	781	20	0
2	I	821	0	781	21	0
2	J	821	0	781	11	0
3	D	8360	0	8170	136	0
3	E	8359	0	8166	148	0
3	F	8367	0	8177	137	0
All	All	30213	0	29469	492	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 8.

All (492) 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:690:GLN:N	3:E:690:GLN:HE21	1.42	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:690:GLN:HE21	3:F:690:GLN:N	1.42	1.15
3:F:402:ILE:O	3:F:508:TYR:HB2	1.80	0.82
3:D:402:ILE:O	3:D:508:TYR:HB2	1.78	0.82
3:D:89:GLY:HA2	3:D:194:PHE:O	1.82	0.80
3:E:690:GLN:N	3:E:690:GLN:NE2	2.28	0.80
3:F:690:GLN:N	3:F:690:GLN:NE2	2.27	0.76
3:E:402:ILE:O	3:E:508:TYR:HB2	1.89	0.72
3:E:98:SER:HA	3:E:180:GLU:H	1.56	0.69
3:F:89:GLY:HA2	3:F:194:PHE:O	1.94	0.68
2:I:36:TYR:HA	2:I:46:LEU:HA	1.74	0.68
2:I:34:ALA:HA	2:I:48:ILE:O	1.94	0.67
3:E:80:ASP:HB2	3:E:262:ALA:H	1.59	0.67
2:I:85:VAL:HB	2:I:104:LYS:HG2	1.76	0.66
2:I:85:VAL:HG23	2:I:103:THR:H	1.61	0.65
3:E:89:GLY:HA2	3:E:194:PHE:O	1.95	0.65
3:F:392:PHE:HA	3:F:517:LEU:HD12	1.79	0.64
3:F:475:ALA:O	1:G:32:ASN:ND2	2.30	0.64
3:D:731:MET:HG2	3:D:774:GLN:HE22	1.63	0.64
3:D:179:LEU:HD12	3:D:180:GLU:HG2	1.81	0.63
2:I:33:LEU:HD11	2:I:88:CYS:HB2	1.80	0.63
2:I:35:TRP:O	2:I:47:LEU:N	2.30	0.62
3:D:332:ILE:HG22	3:D:334:ASN:H	1.65	0.62
3:D:106:PHE:HB3	3:D:235:ILE:HG12	1.82	0.61
3:E:80:ASP:H	3:E:262:ALA:HB2	1.65	0.61
1:A:27:PHE:HA	3:E:477:ASN:HB2	1.83	0.61
2:B:91:TYR:HB2	2:B:94:TRP:HB2	1.83	0.61
2:J:78:VAL:HG13	2:J:82:ASP:HB2	1.81	0.61
3:F:564:GLN:HB2	3:F:577:ARG:HB2	1.83	0.61
3:E:553:THR:HB	3:E:586:ASP:HB2	1.82	0.61
3:F:176:LEU:HD12	3:F:190:ARG:HH11	1.66	0.60
2:J:33:LEU:HD11	2:J:88:CYS:HB2	1.83	0.60
3:D:98:SER:HA	3:D:180:GLU:HA	1.84	0.60
1:A:32:ASN:ND2	3:E:475:ALA:O	2.34	0.60
3:E:103:GLY:HA3	3:E:241:LEU:HB2	1.83	0.60
3:D:433:VAL:HA	3:D:512:VAL:HG12	1.82	0.60
3:D:475:ALA:O	1:H:32:ASN:ND2	2.33	0.60
3:F:80:ASP:H	3:F:262:ALA:HB2	1.67	0.59
3:F:433:VAL:HA	3:F:512:VAL:HG12	1.83	0.59
3:E:991:VAL:HG23	3:E:992:GLN:HE21	1.68	0.59
3:D:553:THR:HB	3:D:586:ASP:HB2	1.84	0.59
3:E:961:THR:OG1	3:F:762:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:566:GLY:HA3	3:D:575:ALA:HB3	1.84	0.58
3:D:567:ARG:HH11	3:D:571:ASP:HA	1.67	0.58
3:F:27:SER:OG	3:F:64:TRP:O	2.20	0.58
3:F:80:ASP:HB2	3:F:262:ALA:H	1.68	0.58
2:B:34:ALA:HB1	2:B:46:LEU:HD11	1.86	0.58
3:F:102:ARG:HH12	3:F:179:LEU:HD13	1.66	0.58
3:F:422:ASN:OD1	3:F:454:ARG:NH1	2.37	0.58
1:G:72:ASP:O	1:G:76:ASN:N	2.37	0.58
1:G:93:TYR:O	1:G:110:GLY:HA2	2.04	0.58
3:F:206:LYS:HE3	3:F:208:THR:HB	1.86	0.58
3:F:728:PRO:HB2	3:F:1018:ILE:HD11	1.86	0.57
2:B:33:LEU:HD11	2:B:88:CYS:HB2	1.86	0.57
3:F:566:GLY:HA3	3:F:575:ALA:HB3	1.86	0.57
1:H:90:THR:HG23	1:H:114:THR:HA	1.85	0.57
1:A:36:TRP:HZ3	1:A:93:TYR:HB3	1.69	0.57
2:I:6:GLN:HE22	2:I:100:GLY:HA3	1.68	0.57
1:H:97:ARG:HG2	1:H:99:LEU:HD23	1.87	0.57
3:D:50:SER:HB2	3:D:276:LEU:HB2	1.86	0.57
3:D:466:ARG:HD2	3:D:468:ILE:HD11	1.87	0.57
3:F:389:ASP:OD1	3:F:528:LYS:NZ	2.37	0.57
3:E:905:ARG:NH1	3:E:1049:LEU:O	2.36	0.57
3:E:1115:ILE:HG22	3:E:1137:VAL:HG23	1.86	0.57
1:A:72:ASP:O	1:A:76:ASN:N	2.38	0.57
1:H:72:ASP:O	1:H:76:ASN:N	2.38	0.57
1:A:90:THR:HG23	1:A:114:THR:HA	1.86	0.56
3:F:82:PRO:O	3:F:237:ARG:NH2	2.37	0.56
3:E:328:ARG:HG2	3:E:579:PRO:HD2	1.87	0.56
3:D:27:SER:OG	3:D:64:TRP:O	2.22	0.56
3:D:663:ASP:OD1	3:D:663:ASP:N	2.39	0.56
3:E:79:PHE:HB3	3:E:258:TRP:HB3	1.88	0.56
3:F:383:SER:HB2	3:F:386:LYS:HB2	1.86	0.56
3:E:34:ARG:HH21	3:E:217:PRO:HG2	1.70	0.56
2:B:78:VAL:HG13	2:B:82:ASP:HB2	1.88	0.56
3:D:126:VAL:HG13	3:D:174:PRO:HA	1.87	0.56
3:E:27:SER:OG	3:E:64:TRP:O	2.24	0.56
3:F:67:ALA:HA	3:F:264:ALA:HB2	1.86	0.56
1:H:93:TYR:O	1:H:110:GLY:HA2	2.06	0.56
3:D:737:ASP:OD2	3:F:317:ASN:ND2	2.39	0.55
2:B:36:TYR:HB2	2:B:87:TYR:HB2	1.88	0.55
3:D:147:LYS:HB3	3:D:248:TYR:HD2	1.71	0.55
3:E:454:ARG:NH1	3:E:467:ASP:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.88	0.55
2:B:54:ARG:NH1	2:B:55:ALA:O	2.39	0.55
3:D:128:ILE:HB	3:D:170:TYR:HB3	1.89	0.55
3:D:151:SER:OG	3:D:153:MET:SD	2.65	0.55
2:I:54:ARG:HD2	2:I:55:ALA:HB3	1.89	0.55
1:A:32:ASN:OD1	1:A:97:ARG:NH2	2.40	0.55
3:F:559:PHE:HD2	3:F:563:GLN:HB3	1.71	0.55
1:G:35:THR:HG23	1:G:96:ALA:HB3	1.88	0.55
1:H:36:TRP:HZ3	1:H:93:TYR:HB3	1.72	0.55
1:A:48:VAL:HG13	1:A:63:VAL:HG21	1.89	0.55
3:F:195:LYS:HG2	3:F:197:ILE:HG12	1.89	0.55
3:D:110:LEU:HB3	3:D:135:PHE:HD2	1.70	0.55
3:D:726:ILE:HG13	3:D:1061:VAL:HG23	1.89	0.55
3:E:544:ASN:HD21	3:E:579:PRO:HB3	1.72	0.55
3:D:82:PRO:O	3:D:237:ARG:NH2	2.40	0.54
3:D:1091:ARG:NH1	3:D:1118:ASP:O	2.40	0.54
3:D:103:GLY:HA3	3:D:241:LEU:HB3	1.89	0.54
1:H:93:TYR:O	1:H:110:GLY:CA	2.56	0.54
3:F:365:TYR:HA	3:F:368:ILE:HD12	1.88	0.54
3:D:781:VAL:HG22	3:D:1026:ALA:HB2	1.90	0.54
3:D:206:LYS:HE3	3:D:208:THR:HB	1.89	0.54
3:E:34:ARG:NH1	3:E:219:GLY:O	2.40	0.54
3:E:663:ASP:OD1	3:E:663:ASP:N	2.40	0.54
2:I:91:TYR:HB2	2:I:94:TRP:HB2	1.89	0.54
3:F:348:ALA:HB3	3:F:399:SER:HB2	1.88	0.54
3:F:731:MET:H	3:F:774:GLN:HE22	1.55	0.54
3:E:1093:GLY:HA3	3:E:1105:THR:O	2.07	0.54
2:J:61:ARG:NH2	2:J:81:GLU:OE2	2.40	0.54
1:A:38:ARG:HH12	1:A:40:ALA:HB2	1.73	0.54
3:E:68:ILE:O	3:E:78:ARG:NH1	2.41	0.54
2:I:78:VAL:HG13	2:I:82:ASP:HB2	1.90	0.54
3:D:917:TYR:HB3	3:F:1129:VAL:HG23	1.89	0.54
3:D:591:SER:O	3:D:634:ARG:NH2	2.41	0.53
3:E:912:THR:OG1	3:E:914:ASN:OD1	2.27	0.53
3:E:110:LEU:HB3	3:E:135:PHE:HD2	1.72	0.53
3:E:760:CYS:HA	3:E:763:LEU:HB2	1.91	0.53
3:F:327:VAL:HG23	3:F:542:ASN:HB3	1.91	0.53
3:E:193:VAL:HB	3:E:204:TYR:HB2	1.91	0.53
3:E:1093:GLY:CA	3:E:1105:THR:O	2.57	0.53
3:F:605:SER:OG	3:F:606:ASN:N	2.42	0.53
1:G:48:VAL:HG13	1:G:63:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1129:VAL:HG23	3:F:917:TYR:HB3	1.91	0.53
3:D:725:GLU:OE1	3:D:1064:HIS:NE2	2.43	0.52
2:I:61:ARG:NH2	2:I:81:GLU:OE2	2.42	0.52
2:B:61:ARG:NH2	2:B:81:GLU:OE2	2.42	0.52
3:D:107:GLY:H	3:D:235:ILE:HG23	1.74	0.52
3:F:788:ILE:HG13	3:F:876:ALA:HB2	1.91	0.52
1:G:90:THR:HG23	1:G:114:THR:HA	1.92	0.52
3:D:449:TYR:OH	3:D:498:ARG:NH2	2.42	0.52
3:E:82:PRO:O	3:E:237:ARG:NH2	2.42	0.52
3:E:195:LYS:HG2	3:E:197:ILE:HG12	1.90	0.52
3:D:605:SER:OG	3:D:606:ASN:N	2.42	0.52
3:E:466:ARG:HD2	3:E:468:ILE:HD11	1.91	0.52
3:F:406:GLU:HB3	3:F:418:ILE:HG13	1.90	0.52
3:F:785:VAL:HG22	3:F:787:GLN:H	1.75	0.52
3:D:34:ARG:NH1	3:D:219:GLY:O	2.42	0.52
3:D:67:ALA:HA	3:D:264:ALA:HB2	1.91	0.52
3:F:34:ARG:HH21	3:F:217:PRO:HG2	1.73	0.52
3:D:34:ARG:HH21	3:D:217:PRO:HG2	1.75	0.52
3:E:1127:ASP:OD1	3:E:1127:ASP:N	2.42	0.52
3:D:77:LYS:HG3	3:D:78:ARG:HG2	1.92	0.52
2:I:37:GLN:HB2	2:I:47:LEU:HD21	1.92	0.52
3:E:605:SER:OG	3:E:606:ASN:N	2.42	0.52
3:F:979:ASP:OD1	3:F:979:ASP:N	2.43	0.52
3:F:93:ALA:O	3:F:266:TYR:HB2	2.10	0.51
3:F:34:ARG:NH1	3:F:219:GLY:O	2.43	0.51
3:D:422:ASN:O	3:D:454:ARG:NH2	2.44	0.51
3:F:449:TYR:OH	3:F:498:ARG:NH2	2.43	0.51
3:D:319:ARG:O	3:D:321:GLN:NE2	2.42	0.51
3:E:435:ALA:HA	3:E:510:VAL:HA	1.91	0.51
3:F:1125:ASN:N	3:F:1125:ASN:OD1	2.43	0.51
3:F:733:LYS:NZ	3:F:775:ASP:OD2	2.41	0.51
3:D:948:LEU:O	3:D:951:VAL:HB	2.11	0.51
3:E:128:ILE:HB	3:E:170:TYR:HB3	1.92	0.51
3:E:1106:GLN:NE2	3:E:1111:GLU:OE2	2.43	0.51
3:D:936:ASP:OD2	3:D:936:ASP:N	2.43	0.51
3:D:912:THR:OG1	3:D:914:ASN:OD1	2.27	0.51
3:D:1127:ASP:N	3:D:1127:ASP:OD1	2.44	0.51
3:E:126:VAL:HG13	3:E:174:PRO:HA	1.93	0.51
3:F:42:VAL:HG11	3:F:44:ARG:HE	1.76	0.51
3:F:663:ASP:OD1	3:F:663:ASP:N	2.37	0.51
3:F:1127:ASP:N	3:F:1127:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HD3	3:E:456:PHE:HZ	1.75	0.51
2:J:91:TYR:HB2	2:J:94:TRP:HB2	1.93	0.50
3:F:341:VAL:HG13	3:F:356:LYS:HZ1	1.76	0.50
3:E:14:GLN:HB2	3:E:158:ARG:HD3	1.94	0.50
3:F:68:ILE:HB	3:F:78:ARG:HE	1.76	0.50
3:D:1118:ASP:N	3:D:1118:ASP:OD1	2.44	0.50
1:A:82:MET:HB2	1:A:85:LEU:HD21	1.94	0.50
3:F:151:SER:OG	3:F:153:MET:SD	2.70	0.50
3:E:567:ARG:HH11	3:E:571:ASP:HA	1.77	0.50
3:F:752:LEU:HD21	3:F:990:GLU:HB2	1.93	0.50
3:D:357:ARG:HH21	3:D:394:ASN:HD21	1.57	0.50
3:E:31:SER:O	3:E:59:PHE:HA	2.12	0.50
3:E:565:PHE:HE1	3:E:573:THR:HG23	1.77	0.50
3:E:591:SER:H	3:E:634:ARG:HH12	1.58	0.50
3:F:505:HIS:HB3	2:I:30:ASN:HB3	1.94	0.50
1:G:105:ALA:O	2:I:45:ARG:NH2	2.44	0.50
3:E:139:PRO:HB2	3:E:241:LEU:HD11	1.94	0.50
3:E:316:SER:OG	3:E:317:ASN:N	2.45	0.50
3:E:348:ALA:HB3	3:E:399:SER:HB2	1.94	0.50
3:D:316:SER:OG	3:D:317:ASN:N	2.44	0.50
3:F:81:ASN:OD1	3:F:81:ASN:N	2.45	0.49
3:D:214:ARG:NH2	3:D:216:LEU:O	2.46	0.49
3:E:591:SER:O	3:E:634:ARG:NH2	2.43	0.49
3:E:788:ILE:HG13	3:E:876:ALA:HB2	1.94	0.49
3:F:86:PHE:HB2	3:F:238:PHE:HB3	1.93	0.49
3:D:83:ALA:HA	3:D:237:ARG:HH21	1.77	0.49
3:E:185:ASN:ND2	3:E:211:ASN:OD1	2.46	0.49
3:E:493:GLN:NE2	3:E:494:SER:O	2.45	0.49
3:F:474:GLN:HB3	1:G:31:ARG:HH21	1.77	0.49
3:F:591:SER:O	3:F:634:ARG:NH2	2.45	0.49
3:D:317:ASN:ND2	3:E:737:ASP:OD2	2.43	0.49
3:F:358:ILE:HB	3:F:395:VAL:HB	1.95	0.49
1:G:38:ARG:HH12	1:G:40:ALA:HB2	1.77	0.49
1:G:93:TYR:O	1:G:110:GLY:CA	2.60	0.49
3:D:556:ASN:O	3:D:558:LYS:NZ	2.45	0.49
3:E:422:ASN:O	3:E:454:ARG:NH2	2.46	0.49
3:E:1091:ARG:NH1	3:E:1118:ASP:O	2.45	0.49
3:D:328:ARG:NH1	3:D:531:THR:O	2.45	0.49
3:D:710:ASN:HD22	3:D:1076:THR:HG23	1.78	0.49
1:A:33:TYR:OH	3:E:455:LEU:O	2.31	0.49
3:E:247:SER:OG	3:E:253:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:345:THR:HG22	3:F:346:THR:HG23	1.95	0.48
3:F:778:THR:HA	3:F:781:VAL:HG12	1.93	0.48
1:H:48:VAL:HG13	1:H:63:VAL:HG21	1.95	0.48
2:B:11:LEU:HD22	2:B:21:LEU:HD13	1.94	0.48
2:B:86:TYR:O	2:B:103:THR:OG1	2.30	0.48
3:E:722:VAL:HG22	3:E:930:ALA:HB1	1.94	0.48
3:D:1077:THR:OG1	3:D:1078:ALA:N	2.46	0.48
3:D:341:VAL:HG13	3:D:356:LYS:HZ1	1.79	0.48
3:D:1125:ASN:OD1	3:D:1125:ASN:N	2.46	0.48
3:D:81:ASN:N	3:D:81:ASN:OD1	2.46	0.48
3:E:67:ALA:HA	3:E:264:ALA:HB2	1.94	0.48
3:E:21:ARG:NH2	3:E:81:ASN:O	2.47	0.48
3:E:578:ASP:N	3:E:583:GLU:O	2.47	0.48
3:E:1054:GLN:HB2	3:E:1061:VAL:HG13	1.96	0.48
3:D:186:PHE:HD2	3:D:213:GLU:HG3	1.78	0.48
1:H:50:VAL:HG12	1:H:58:PHE:HB2	1.95	0.48
3:D:712:ILE:O	3:D:1074:ASN:HA	2.14	0.48
3:E:347:PHE:HZ	3:E:511:VAL:HG22	1.78	0.48
1:G:35:THR:HG21	2:I:97:TRP:HZ2	1.79	0.48
3:D:1093:GLY:CA	3:D:1105:THR:O	2.62	0.48
3:E:83:ALA:HA	3:E:237:ARG:HH21	1.78	0.48
3:F:110:LEU:HB3	3:F:135:PHE:HD2	1.78	0.48
2:J:34:ALA:HA	2:J:48:ILE:O	2.14	0.48
2:B:2:ILE:HG23	2:B:27:GLU:H	1.79	0.48
3:D:29:THR:HG23	3:D:62:VAL:HG13	1.95	0.48
3:E:100:ILE:O	3:E:243:ALA:N	2.43	0.48
3:F:319:ARG:O	3:F:321:GLN:NE2	2.46	0.48
1:G:36:TRP:HE1	1:G:80:LEU:HD22	1.78	0.48
1:G:98:ASP:OD1	1:G:107:TRP:NE1	2.43	0.48
1:A:14:PRO:HD2	1:A:117:SER:HB2	1.96	0.47
3:D:966:LEU:O	3:D:975:SER:OG	2.27	0.47
3:D:141:LEU:HD23	3:D:241:LEU:HD21	1.95	0.47
3:E:422:ASN:ND2	3:E:454:ARG:O	2.47	0.47
2:J:2:ILE:HG23	2:J:27:GLU:H	1.80	0.47
3:E:14:GLN:NE2	3:E:156:GLU:OE2	2.47	0.47
3:E:143:VAL:HG13	3:E:152:TRP:HB3	1.96	0.47
3:E:432:CYS:HB3	3:E:434:ILE:HG13	1.95	0.47
3:E:433:VAL:HA	3:E:512:VAL:HG12	1.96	0.47
3:D:452:LEU:HD22	3:D:492:LEU:HB3	1.96	0.47
3:E:356:LYS:HB3	3:E:397:ALA:HB3	1.96	0.47
3:F:431:GLY:HA3	3:F:513:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:21:ARG:NH2	3:D:81:ASN:O	2.46	0.47
3:F:16:VAL:HG21	3:F:142:ASP:HB3	1.95	0.47
1:G:14:PRO:HD2	1:G:117:SER:HB2	1.97	0.47
3:D:715:PRO:HA	3:D:1071:GLN:O	2.15	0.47
3:D:979:ASP:OD2	3:D:983:ARG:NH2	2.38	0.47
3:F:316:SER:OG	3:F:317:ASN:N	2.47	0.47
3:F:422:ASN:ND2	3:F:454:ARG:O	2.48	0.47
3:F:497:PHE:CG	3:F:507:PRO:HG3	2.50	0.47
1:G:32:ASN:OD1	1:G:97:ARG:NH1	2.42	0.47
1:H:99:LEU:HD12	1:H:102:ARG:HH12	1.79	0.47
3:D:277:LEU:HD22	3:D:285:ILE:HD13	1.97	0.47
3:D:1093:GLY:HA3	3:D:1105:THR:O	2.14	0.47
3:F:912:THR:OG1	3:F:914:ASN:OD1	2.27	0.47
3:E:449:TYR:OH	3:E:498:ARG:NH2	2.48	0.47
3:F:591:SER:H	3:F:634:ARG:HH12	1.63	0.47
2:B:30:ASN:HB3	3:E:505:HIS:HB3	1.97	0.46
3:D:902:MET:HA	3:D:902:MET:HE2	1.96	0.46
3:E:78:ARG:HA	3:E:259:THR:H	1.80	0.46
1:H:82:MET:HB2	1:H:85:LEU:HD21	1.97	0.46
3:D:656:VAL:HG23	3:D:658:ASN:H	1.80	0.46
3:E:442:ASP:OD1	3:E:509:ARG:NH2	2.45	0.46
3:F:29:THR:HG23	3:F:62:VAL:HG13	1.97	0.46
3:D:68:ILE:HB	3:D:78:ARG:HE	1.80	0.46
3:F:21:ARG:NH2	3:F:81:ASN:O	2.48	0.46
3:D:80:ASP:HB2	3:D:262:ALA:H	1.80	0.46
3:E:578:ASP:HB2	3:E:583:GLU:HB2	1.97	0.46
1:H:14:PRO:HD2	1:H:117:SER:HB2	1.96	0.46
1:A:39:GLN:HB3	1:A:94:TYR:HE2	1.81	0.46
3:E:973:ILE:HD11	3:E:980:ILE:HG23	1.98	0.46
3:F:106:PHE:HB3	3:F:235:ILE:HD12	1.98	0.46
3:E:1118:ASP:OD1	3:E:1118:ASP:N	2.44	0.46
1:H:66:ARG:NH1	1:H:84:SER:O	2.48	0.46
3:D:176:LEU:HD12	3:D:190:ARG:HD3	1.96	0.46
3:E:319:ARG:O	3:E:321:GLN:NE2	2.46	0.46
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.97	0.46
3:E:979:ASP:OD2	3:E:983:ARG:NH2	2.38	0.46
3:E:1028:LYS:NZ	3:E:1042:PHE:O	2.45	0.46
3:F:725:GLU:OE1	3:F:1064:HIS:NE2	2.47	0.46
3:F:869:MET:H	3:F:869:MET:HG2	1.56	0.46
3:E:139:PRO:HB3	3:E:159:VAL:HA	1.98	0.46
3:E:140:PHE:HE2	3:E:242:LEU:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:811:LYS:HZ3	3:E:812:PRO:HD2	1.81	0.46
3:F:246:ARG:HA	3:F:246:ARG:HD3	1.77	0.46
3:E:280:ASN:OD1	3:E:284:THR:N	2.49	0.45
3:D:1054:GLN:HB2	3:D:1061:VAL:HG12	1.97	0.45
3:E:81:ASN:OD1	3:E:81:ASN:N	2.50	0.45
3:E:497:PHE:CG	3:E:507:PRO:HG3	2.52	0.45
3:E:656:VAL:HG23	3:E:658:ASN:H	1.82	0.45
3:F:77:LYS:HB2	3:F:246:ARG:HH22	1.81	0.45
1:A:100:THR:HA	2:B:49:TYR:HE1	1.81	0.45
3:D:1129:VAL:HG23	3:E:917:TYR:HB3	1.99	0.45
3:F:1054:GLN:HB2	3:F:1061:VAL:HG13	1.98	0.45
3:D:430:THR:OG1	3:D:515:PHE:O	2.35	0.45
3:F:946:GLY:HA2	3:F:949:GLN:HB2	1.99	0.45
3:E:387:LEU:HD23	3:E:390:LEU:HD12	1.98	0.45
3:E:566:GLY:HA3	3:E:575:ALA:HB3	1.98	0.45
3:D:565:PHE:O	3:E:43:PHE:N	2.50	0.45
3:D:722:VAL:HG22	3:D:930:ALA:HB1	1.97	0.45
3:D:935:GLN:HE21	3:D:935:GLN:HB3	1.54	0.45
3:E:577:ARG:HA	3:E:584:ILE:HA	1.98	0.45
3:D:274:THR:OG1	3:D:291:CYS:SG	2.72	0.45
3:E:226:LEU:HG	3:E:227:VAL:HG23	1.98	0.45
3:F:501:TYR:HB3	3:F:505:HIS:HB2	1.99	0.45
3:F:722:VAL:HG22	3:F:930:ALA:HB1	1.98	0.45
1:A:98:ASP:HB3	1:A:100:THR:HG23	1.99	0.45
3:F:105:ILE:HG12	3:F:241:LEU:HD11	1.99	0.45
3:D:894:LEU:HB3	3:F:713:ALA:HB3	1.99	0.45
3:E:105:ILE:O	3:E:238:PHE:HA	2.16	0.45
3:F:553:THR:HB	3:F:586:ASP:HB2	1.98	0.45
3:F:656:VAL:HG23	3:F:658:ASN:H	1.82	0.45
2:B:19:ALA:HB3	2:B:75:ILE:HB	1.99	0.45
3:E:206:LYS:HE3	3:E:208:THR:HB	1.99	0.45
3:F:391:CYS:HB2	3:F:525:CYS:HA	1.99	0.45
3:E:54:LEU:HA	3:E:271:GLN:O	2.17	0.44
3:F:342:PHE:HD2	3:F:436:TRP:HE1	1.65	0.44
3:F:811:LYS:HZ3	3:F:812:PRO:HD2	1.81	0.44
3:F:330:PRO:HA	3:F:580:GLN:HB3	2.00	0.44
3:D:27:SER:OG	3:D:27:SER:O	2.35	0.44
3:E:378:LYS:HB2	3:E:433:VAL:HB	1.99	0.44
3:E:456:PHE:HB2	3:E:491:PRO:HA	2.00	0.44
3:E:577:ARG:HG2	3:E:584:ILE:HG12	2.00	0.44
3:F:617:CYS:O	3:F:633:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:SER:HB3	3:E:790:LYS:HZ2	1.82	0.44
3:E:710:ASN:N	3:E:710:ASN:OD1	2.51	0.44
3:D:722:VAL:HG12	3:D:1065:VAL:HG22	1.99	0.44
3:E:715:PRO:HA	3:E:1071:GLN:O	2.17	0.44
3:F:436:TRP:HB2	3:F:509:ARG:HB2	2.00	0.44
1:G:50:VAL:HG12	1:G:58:PHE:HB2	1.98	0.44
3:D:418:ILE:HA	3:D:422:ASN:HD22	1.83	0.44
3:D:811:LYS:HZ3	3:D:812:PRO:HD2	1.83	0.44
3:D:880:GLY:O	3:D:884:SER:OG	2.29	0.44
3:F:294:ASP:O	3:F:297:SER:OG	2.27	0.44
3:D:79:PHE:HB3	3:D:258:TRP:HB3	2.00	0.44
3:F:280:ASN:OD1	3:F:284:THR:N	2.51	0.44
3:D:327:VAL:HG12	3:D:542:ASN:HB3	1.99	0.43
3:D:591:SER:H	3:D:634:ARG:HH12	1.66	0.43
3:D:897:PRO:HA	3:F:707:TYR:HE1	1.83	0.43
3:E:34:ARG:HA	3:E:34:ARG:HD3	1.78	0.43
1:G:36:TRP:NE1	1:G:80:LEU:HD22	2.33	0.43
2:B:49:TYR:N	2:B:53:THR:O	2.44	0.43
3:F:79:PHE:N	3:F:259:THR:O	2.35	0.43
3:F:126:VAL:HG13	3:F:174:PRO:HA	2.00	0.43
3:D:436:TRP:HB2	3:D:509:ARG:HB2	2.00	0.43
3:F:356:LYS:HB2	3:F:397:ALA:HB3	2.00	0.43
2:B:30:ASN:ND2	2:B:92:GLY:O	2.42	0.43
3:F:487:ASN:OD1	1:G:97:ARG:NH2	2.49	0.43
3:F:387:LEU:HD23	3:F:387:LEU:HA	1.88	0.43
3:D:348:ALA:HB3	3:D:399:SER:HB2	1.99	0.43
3:D:505:HIS:HB3	2:J:30:ASN:HB3	1.99	0.43
3:E:121:ASN:HA	3:E:126:VAL:HG12	2.00	0.43
2:I:38:GLN:O	2:I:84:ALA:HB1	2.19	0.43
3:E:185:ASN:OD1	3:E:185:ASN:N	2.52	0.43
3:F:147:LYS:HE3	3:F:247:SER:HB2	2.00	0.43
3:D:33:THR:OG1	3:D:219:GLY:O	2.37	0.43
3:D:436:TRP:N	3:D:509:ARG:O	2.47	0.43
3:E:443:SER:HB3	3:E:507:PRO:HG2	2.01	0.43
3:F:1091:ARG:NH1	3:F:1118:ASP:O	2.39	0.43
3:D:80:ASP:H	3:D:262:ALA:HB2	1.84	0.43
3:F:131:CYS:HA	3:F:166:CYS:HB3	2.01	0.43
3:F:470:THR:O	3:F:470:THR:OG1	2.37	0.43
3:F:722:VAL:HA	3:F:1064:HIS:O	2.19	0.43
3:F:1120:THR:OG1	3:F:1121:PHE:N	2.52	0.43
1:H:51:ILE:HG13	1:H:57:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:PHE:HD2	3:D:235:ILE:HG21	1.83	0.42
3:D:246:ARG:HB2	3:D:247:SER:H	1.68	0.42
3:E:565:PHE:O	3:F:43:PHE:N	2.52	0.42
3:D:195:LYS:HG2	3:D:197:ILE:HG12	2.02	0.42
3:D:900:MET:HE1	3:F:1077:THR:HG21	2.00	0.42
3:D:917:TYR:HD2	3:F:1089:PHE:HE2	1.66	0.42
3:E:95:THR:HB	3:E:189:LEU:HD12	2.01	0.42
3:F:766:ALA:O	3:F:770:ILE:HG12	2.19	0.42
3:D:387:LEU:HD23	3:D:387:LEU:HA	1.89	0.42
3:E:122:ASN:ND2	3:E:125:ASN:O	2.52	0.42
3:E:966:LEU:O	3:E:975:SER:OG	2.27	0.42
3:F:31:SER:O	3:F:59:PHE:HA	2.19	0.42
3:F:226:LEU:HG	3:F:227:VAL:HG23	2.01	0.42
3:F:443:SER:HB3	3:F:507:PRO:HG2	2.01	0.42
3:F:948:LEU:O	3:F:951:VAL:HB	2.18	0.42
1:A:93:TYR:O	1:A:110:GLY:CA	2.67	0.42
2:B:4:MET:HE3	2:B:4:MET:H	1.85	0.42
3:D:461:LEU:HD23	3:D:461:LEU:HA	1.93	0.42
3:D:650:LEU:HD21	3:D:653:ALA:HB3	2.01	0.42
3:E:29:THR:OG1	3:E:30:ASN:N	2.51	0.42
3:E:398:ASP:HB2	3:E:512:VAL:HG23	2.00	0.42
3:F:577:ARG:HG2	3:F:584:ILE:HG12	2.01	0.42
3:E:382:VAL:HG11	3:E:390:LEU:HD11	2.01	0.42
3:E:436:TRP:HB2	3:E:509:ARG:HB2	2.02	0.42
3:E:80:ASP:OD1	3:E:81:ASN:N	2.52	0.42
3:E:552:LEU:HD12	3:E:585:LEU:HB3	2.01	0.42
3:F:307:THR:O	3:F:307:THR:OG1	2.33	0.42
3:F:342:PHE:HB3	3:F:436:TRP:HZ2	1.84	0.42
3:F:357:ARG:HH21	3:F:394:ASN:HD21	1.67	0.42
3:D:55:PHE:HB2	3:D:275:PHE:CE2	2.54	0.42
3:D:485:GLY:H	3:D:488:CYS:HB2	1.84	0.42
3:D:493:GLN:NE2	3:D:494:SER:O	2.53	0.42
3:E:93:ALA:O	3:E:266:TYR:HB2	2.20	0.42
3:E:814:LYS:HA	3:E:814:LYS:HD3	1.96	0.42
3:E:1123:SER:O	3:E:1123:SER:OG	2.37	0.42
3:F:34:ARG:HA	3:F:34:ARG:HD3	1.77	0.42
2:J:38:GLN:HB3	2:J:85:VAL:HG12	2.01	0.42
2:I:2:ILE:HG23	2:I:27:GLU:H	1.84	0.42
1:A:31:ARG:HA	1:A:53:PRO:HB3	2.02	0.42
2:B:85:VAL:HG13	2:B:103:THR:H	1.85	0.42
3:D:31:SER:O	3:D:59:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:GLN:NE2	3:D:935:GLN:OE1	2.43	0.42
3:E:501:TYR:HB3	3:E:505:HIS:HB2	2.02	0.42
3:F:978:ASN:N	3:F:978:ASN:OD1	2.52	0.42
2:J:59:PRO:HD2	2:J:62:PHE:HE2	1.83	0.42
1:A:66:ARG:NH1	1:A:84:SER:O	2.53	0.42
3:D:743:CYS:HB3	3:D:749:CYS:HB3	1.90	0.42
3:F:763:LEU:HD23	3:F:1008:VAL:HG21	2.00	0.42
3:F:973:ILE:H	3:F:973:ILE:HG12	1.72	0.42
2:B:21:LEU:HD12	2:B:21:LEU:HA	1.87	0.41
3:D:393:THR:HA	3:D:522:ALA:HA	2.01	0.41
3:D:558:LYS:HA	3:D:558:LYS:HD3	1.88	0.41
3:D:722:VAL:HA	3:D:1064:HIS:O	2.19	0.41
3:E:119:ILE:HG23	3:E:128:ILE:HG13	2.01	0.41
3:E:766:ALA:O	3:E:770:ILE:HG12	2.20	0.41
2:B:35:TRP:HB2	2:B:48:ILE:HB	2.02	0.41
3:E:317:ASN:ND2	3:F:737:ASP:OD2	2.51	0.41
3:E:452:LEU:HG	3:E:494:SER:HA	2.02	0.41
3:F:145:TYR:HA	3:F:248:TYR:H	1.84	0.41
3:F:212:LEU:HD21	3:F:217:PRO:HB3	2.01	0.41
3:F:776:LYS:NZ	3:F:780:GLU:OE1	2.53	0.41
2:I:39:LYS:HB2	2:I:42:GLN:HB2	2.01	0.41
3:D:29:THR:OG1	3:D:30:ASN:N	2.53	0.41
3:E:436:TRP:N	3:E:509:ARG:O	2.46	0.41
2:J:75:ILE:HD11	2:J:86:TYR:HE2	1.85	0.41
3:D:328:ARG:HB3	3:D:579:PRO:HD2	2.01	0.41
3:D:497:PHE:CG	3:D:507:PRO:HG3	2.55	0.41
3:D:869:MET:H	3:D:869:MET:HG2	1.55	0.41
3:F:78:ARG:CZ	3:F:261:GLY:HA3	2.50	0.41
3:F:83:ALA:HA	3:F:237:ARG:HE	1.84	0.41
3:F:229:LEU:HG	3:F:231:ILE:HG23	2.02	0.41
3:F:571:ASP:N	3:F:571:ASP:OD1	2.54	0.41
3:F:880:GLY:O	3:F:884:SER:OG	2.30	0.41
3:D:560:LEU:HB2	3:D:563:GLN:HG2	2.02	0.41
3:D:1049:LEU:HD23	3:D:1049:LEU:HA	1.91	0.41
1:A:93:TYR:O	1:A:110:GLY:HA2	2.20	0.41
3:D:102:ARG:HH21	3:D:243:ALA:HB3	1.86	0.41
3:D:492:LEU:HD13	3:D:492:LEU:HA	1.92	0.41
3:D:713:ALA:HB3	3:E:894:LEU:HB3	2.02	0.41
3:D:906:PHE:HE1	3:D:1049:LEU:HD11	1.84	0.41
3:E:55:PHE:HB2	3:E:275:PHE:CE2	2.56	0.41
3:E:713:ALA:HB3	3:F:894:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:100:ILE:HG23	3:F:244:LEU:HB2	2.01	0.41
3:F:147:LYS:HB2	3:F:249:LEU:HD21	2.02	0.41
3:F:560:LEU:HB3	3:F:563:GLN:HB2	2.03	0.41
3:E:106:PHE:HB3	3:E:235:ILE:HD12	2.01	0.41
3:E:395:VAL:HG22	3:E:515:PHE:HD1	1.86	0.41
3:F:280:ASN:ND2	3:F:284:THR:OG1	2.54	0.41
1:G:50:VAL:HG21	2:I:95:PRO:HG2	2.02	0.41
3:E:156:GLU:HB2	3:E:245:HIS:CE1	2.56	0.41
3:E:566:GLY:HA2	3:F:43:PHE:HB3	2.02	0.41
3:E:1116:THR:HG22	3:E:1117:THR:H	1.86	0.41
2:I:38:GLN:HB3	2:I:85:VAL:HG13	2.01	0.41
3:D:33:THR:OG1	3:D:33:THR:O	2.36	0.41
3:D:121:ASN:HA	3:D:126:VAL:HG12	2.02	0.41
3:E:68:ILE:HB	3:E:78:ARG:CZ	2.51	0.41
3:E:406:GLU:HB3	3:E:418:ILE:HG13	2.02	0.41
3:E:950:ASP:OD1	3:E:950:ASP:N	2.54	0.41
2:I:19:ALA:HB3	2:I:75:ILE:HB	2.03	0.41
3:E:461:LEU:HD23	3:E:461:LEU:HA	1.90	0.41
3:E:1018:ILE:HD13	3:E:1018:ILE:HA	1.98	0.41
3:E:1120:THR:OG1	3:E:1121:PHE:N	2.54	0.41
3:F:128:ILE:HB	3:F:170:TYR:HB3	2.03	0.41
3:F:333:THR:HB	3:F:362:VAL:HG11	2.01	0.41
3:D:212:LEU:HD21	3:D:217:PRO:HB3	2.02	0.40
3:D:563:GLN:NE2	3:E:42:VAL:O	2.52	0.40
3:E:878:LEU:HA	3:E:881:THR:HG22	2.02	0.40
3:D:379:CYS:HB2	3:D:384:PRO:HD3	2.03	0.40
3:D:442:ASP:OD1	3:D:509:ARG:NH2	2.43	0.40
3:D:745:ASP:N	3:D:745:ASP:OD1	2.54	0.40
3:E:324:GLU:HG2	3:E:539:VAL:HG23	2.03	0.40
3:D:395:VAL:HG22	3:D:515:PHE:HD1	1.86	0.40
3:D:456:PHE:HB2	3:D:491:PRO:HA	2.03	0.40
3:E:329:PHE:HB2	3:E:529:LYS:HB3	2.03	0.40
3:E:938:LEU:HD23	3:E:938:LEU:HA	1.93	0.40
3:E:946:GLY:HA2	3:E:949:GLN:HB2	2.03	0.40
3:F:33:THR:OG1	3:F:219:GLY:O	2.39	0.40
3:F:922:LEU:HD23	3:F:926:GLN:HG3	2.03	0.40
3:D:89:GLY:CA	3:D:194:PHE:O	2.60	0.40
3:D:814:LYS:HA	3:D:814:LYS:HD3	1.94	0.40
3:E:102:ARG:HE	3:E:243:ALA:HB2	1.87	0.40
3:F:1004:LEU:HD23	3:F:1004:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	G	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	H	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
2	B	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	I	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	J	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
3	D	1052/1221 (86%)	965 (92%)	84 (8%)	3 (0%)	37	67
3	E	1052/1221 (86%)	965 (92%)	87 (8%)	0	100	100
3	F	1053/1221 (86%)	978 (93%)	74 (7%)	1 (0%)	48	78
All	All	3817/4335 (88%)	3530 (92%)	283 (7%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	142	ASP
3	F	250	THR
3	D	246	ARG
3	D	332	ILE

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	96/96 (100%)	94 (98%)	2 (2%)	48	69
1	G	96/96 (100%)	93 (97%)	3 (3%)	35	60
1	H	96/96 (100%)	94 (98%)	2 (2%)	48	69
2	B	88/88 (100%)	86 (98%)	2 (2%)	45	67
2	I	88/88 (100%)	86 (98%)	2 (2%)	45	67
2	J	88/88 (100%)	87 (99%)	1 (1%)	70	81
3	D	934/1056 (88%)	913 (98%)	21 (2%)	47	68
3	E	934/1056 (88%)	914 (98%)	20 (2%)	48	69
3	F	935/1056 (88%)	919 (98%)	16 (2%)	56	74
All	All	3355/3720 (90%)	3286 (98%)	69 (2%)	49	69

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	36	TRP
2	B	4	MET
2	B	101	GLN
3	D	17	ASN
3	D	77	LYS
3	D	87	ASN
3	D	97	LYS
3	D	149	ASN
3	D	192	PHE
3	D	211	ASN
3	D	214	ARG
3	D	220	PHE
3	D	226	LEU
3	D	248	TYR
3	D	351	TYR
3	D	493	GLN
3	D	565	PHE
3	D	571	ASP
3	D	580	GLN
3	D	775	ASP
3	D	780	GLU
3	D	906	PHE
3	D	955	ASN
3	D	1067	TYR
3	E	17	ASN

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Mol	Chain	Res	Type
3	E	97	LYS
3	E	104	TRP
3	E	117	LEU
3	E	140	PHE
3	E	149	ASN
3	E	150	LYS
3	E	200	TYR
3	E	226	LEU
3	E	347	PHE
3	E	361	CYS
3	E	461	LEU
3	E	559	PHE
3	E	690	GLN
3	E	738	CYS
3	E	858	LEU
3	E	955	ASN
3	E	962	LEU
3	E	1067	TYR
3	E	1107	ARG
3	F	17	ASN
3	F	125	ASN
3	F	220	PHE
3	F	246	ARG
3	F	361	CYS
3	F	391	CYS
3	F	490	SER
3	F	544	ASN
3	F	571	ASP
3	F	690	GLN
3	F	763	LEU
3	F	795	LYS
3	F	906	PHE
3	F	935	GLN
3	F	955	ASN
3	F	959	LEU
1	G	38	ARG
1	G	43	LYS
1	G	98	ASP
2	I	4	MET
2	I	101	GLN
1	H	4	LEU
1	H	36	TRP

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Mol	Chain	Res	Type
2	J	4	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	185	ASN
3	E	211	ASN
3	E	1106	GLN
2	I	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

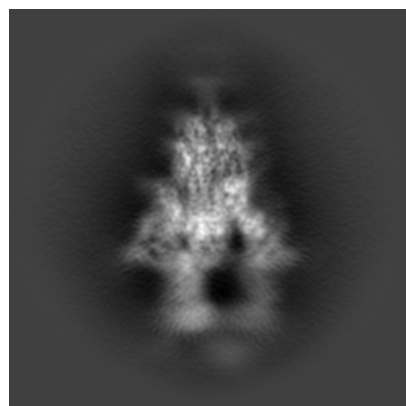
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38284. These allow visual inspection of the internal detail of the map and identification of artifacts.

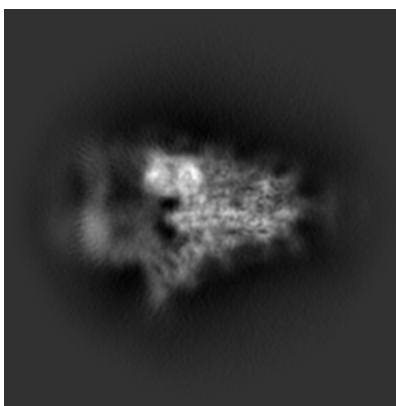
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

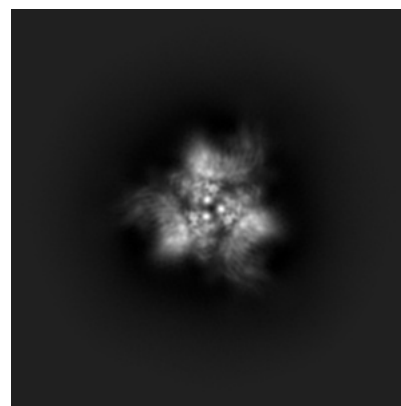
6.1.1 Primary map



X

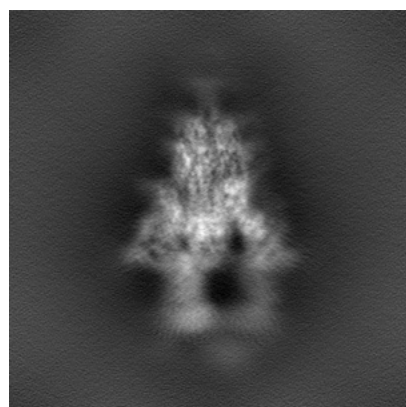


Y

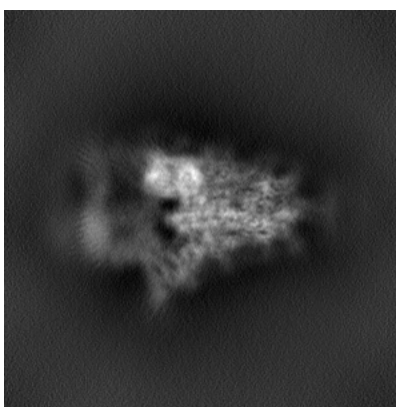


Z

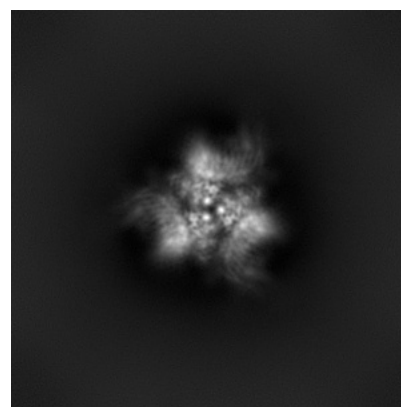
6.1.2 Raw map



X



Y

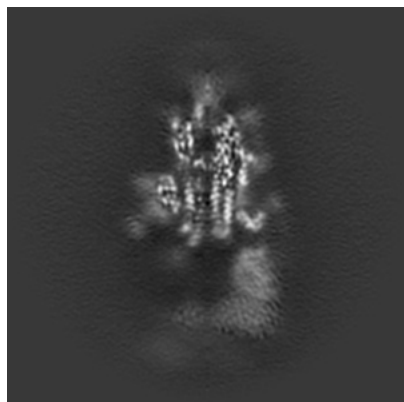


Z

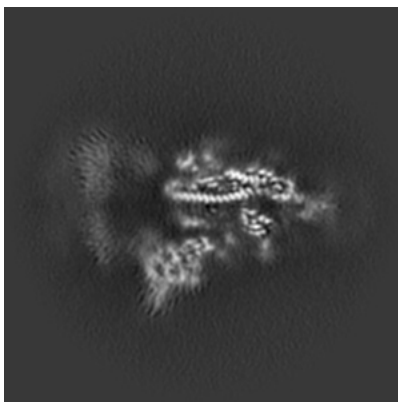
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

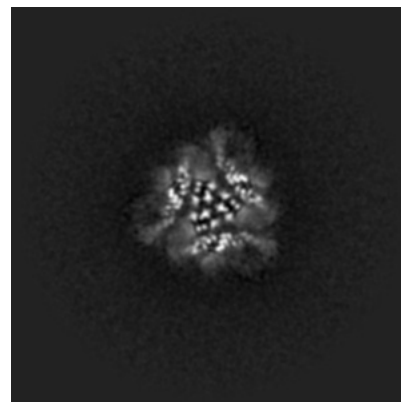
6.2.1 Primary map



X Index: 160

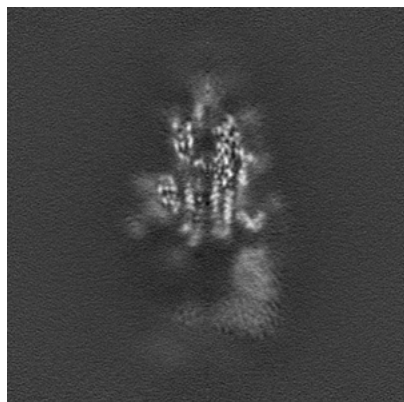


Y Index: 160

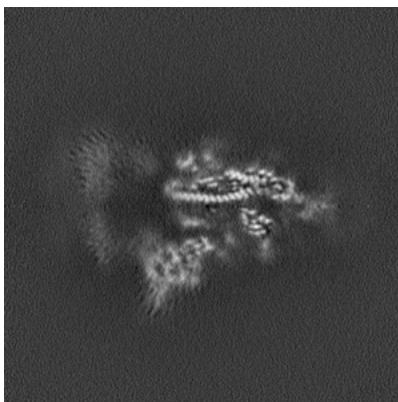


Z Index: 160

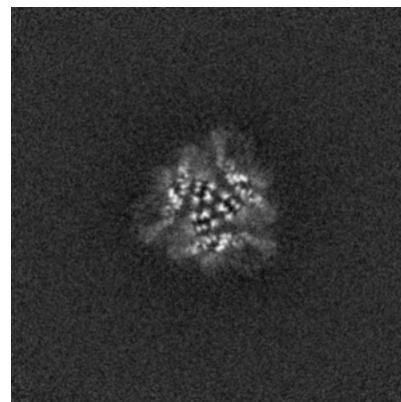
6.2.2 Raw map



X Index: 160



Y Index: 160

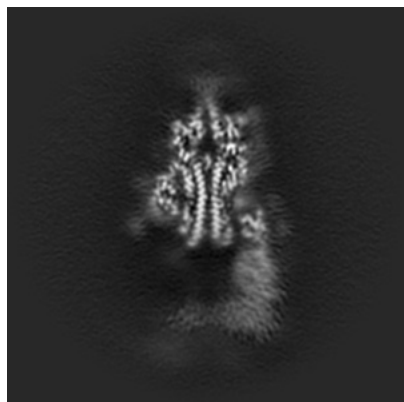


Z Index: 160

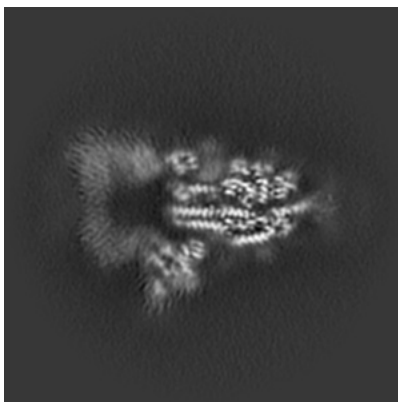
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

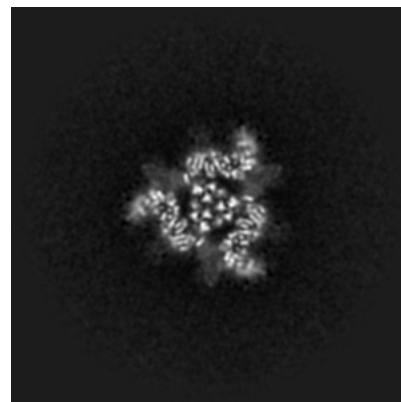
6.3.1 Primary map



X Index: 156

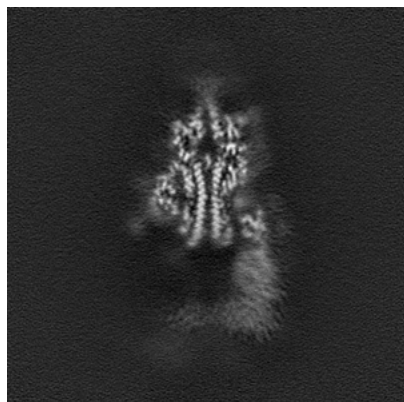


Y Index: 153

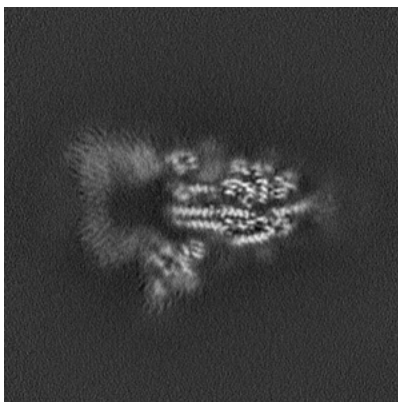


Z Index: 151

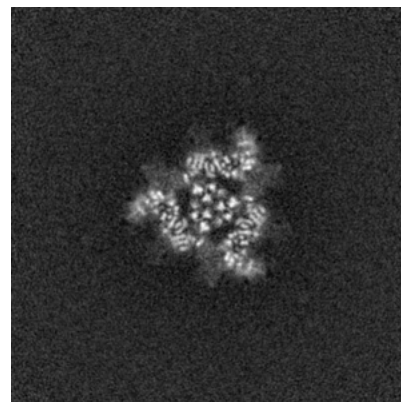
6.3.2 Raw map



X Index: 156



Y Index: 153

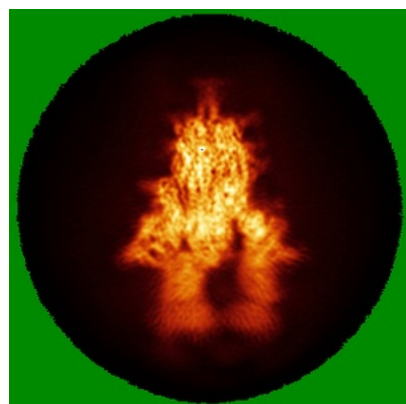


Z Index: 151

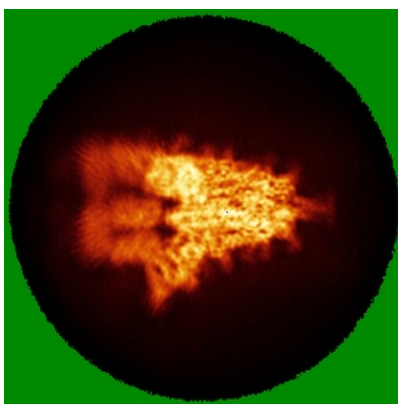
The images above show the largest variance slices of the map in three orthogonal directions.

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

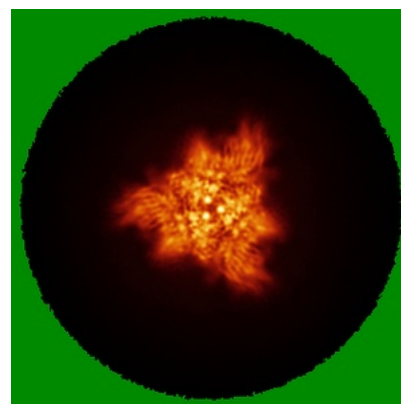
6.4.1 Primary map



X

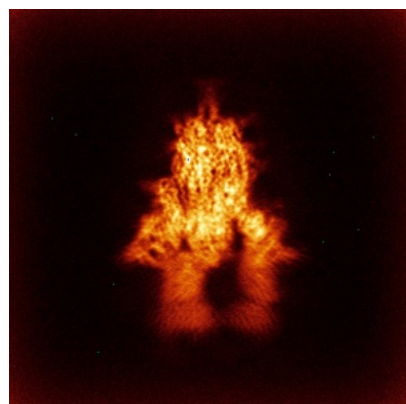


Y

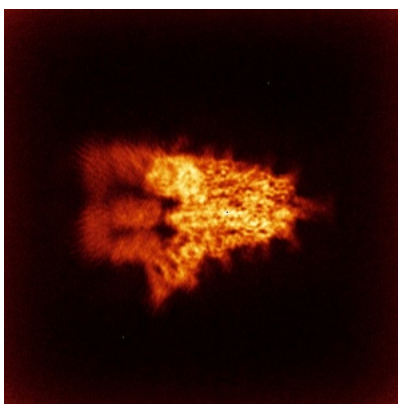


Z

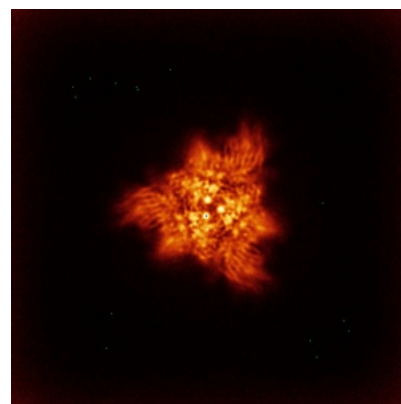
6.4.2 Raw map



X



Y

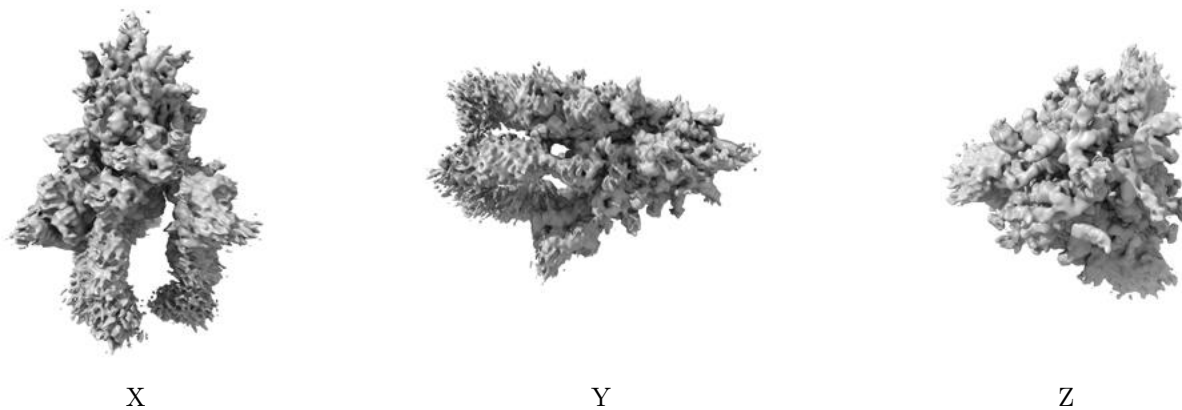


Z

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

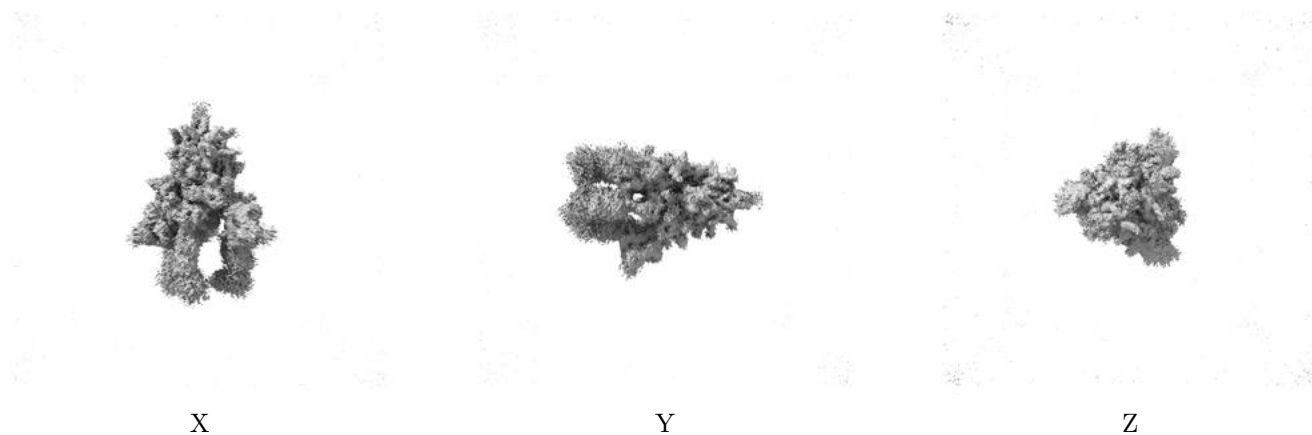
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

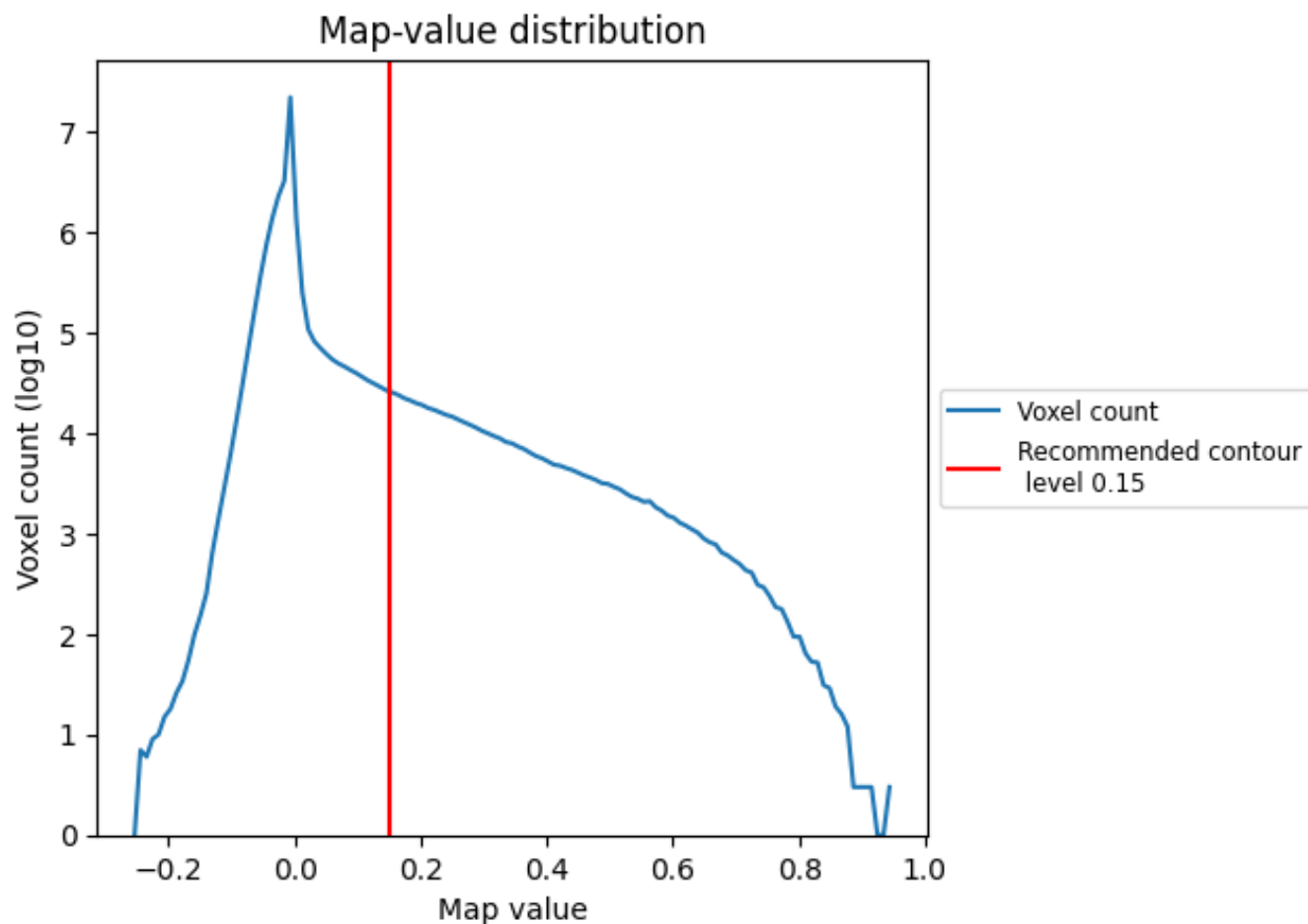
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

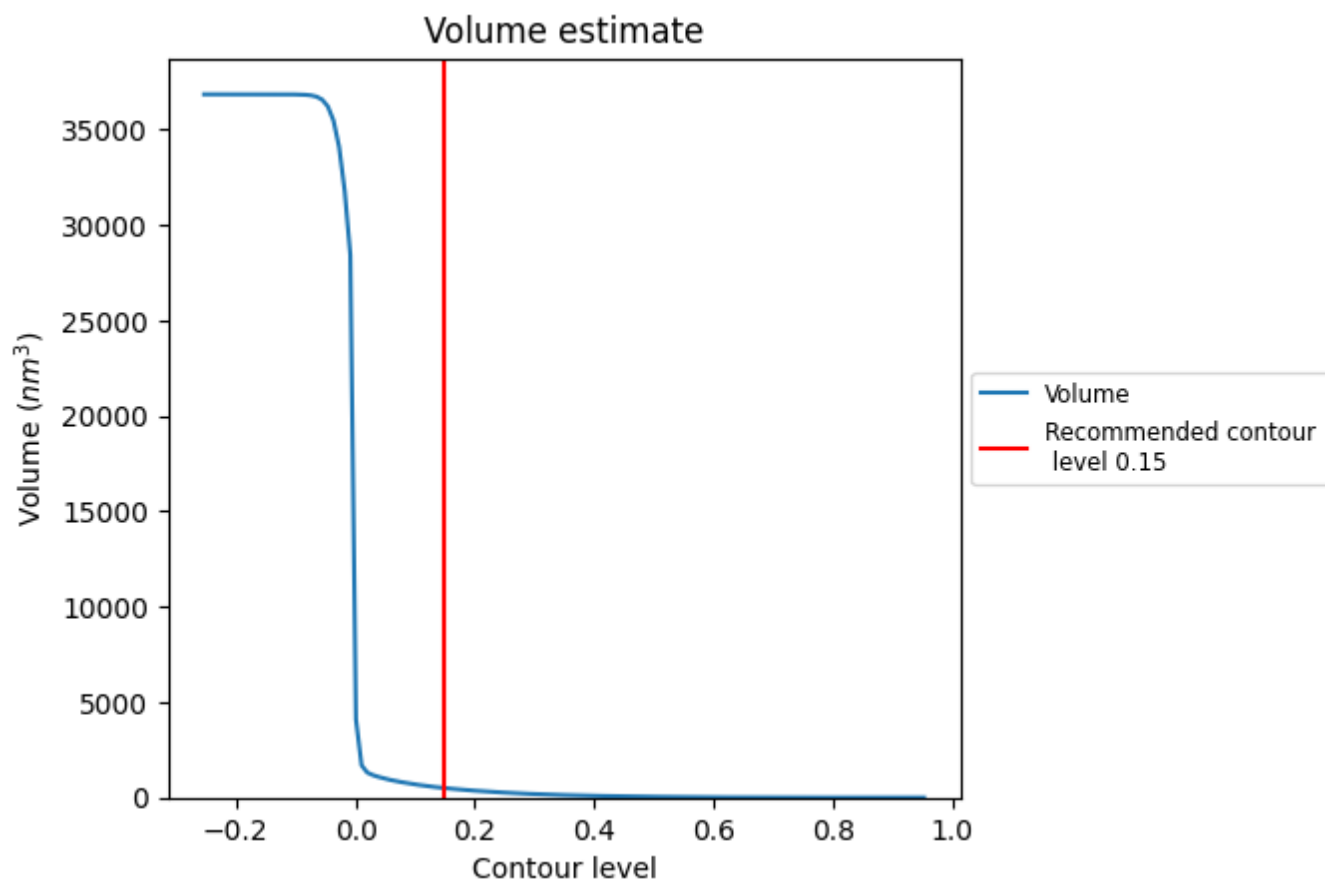
This section contains the results of statistical analysis of the map.

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.

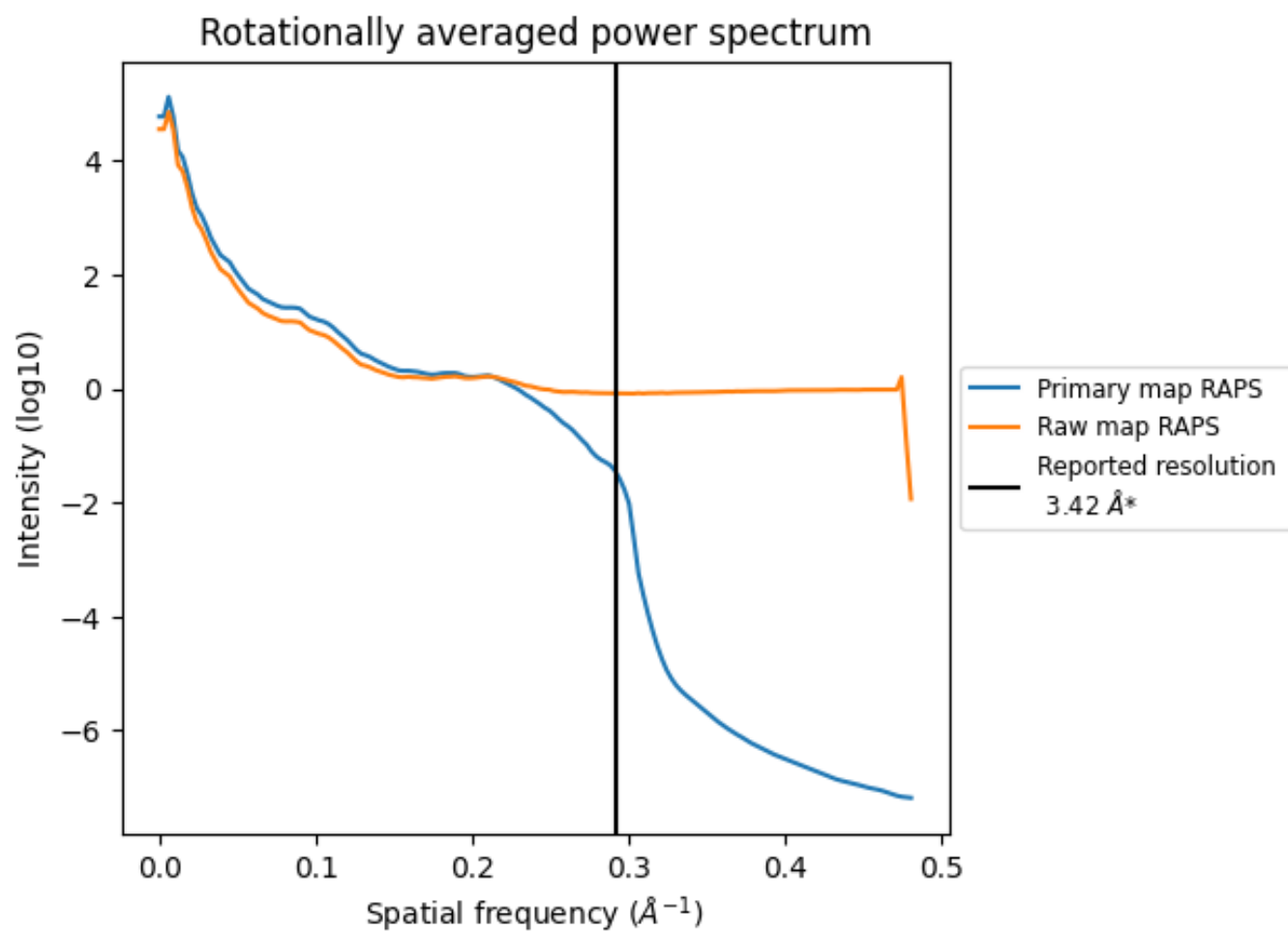
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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 ⓘ

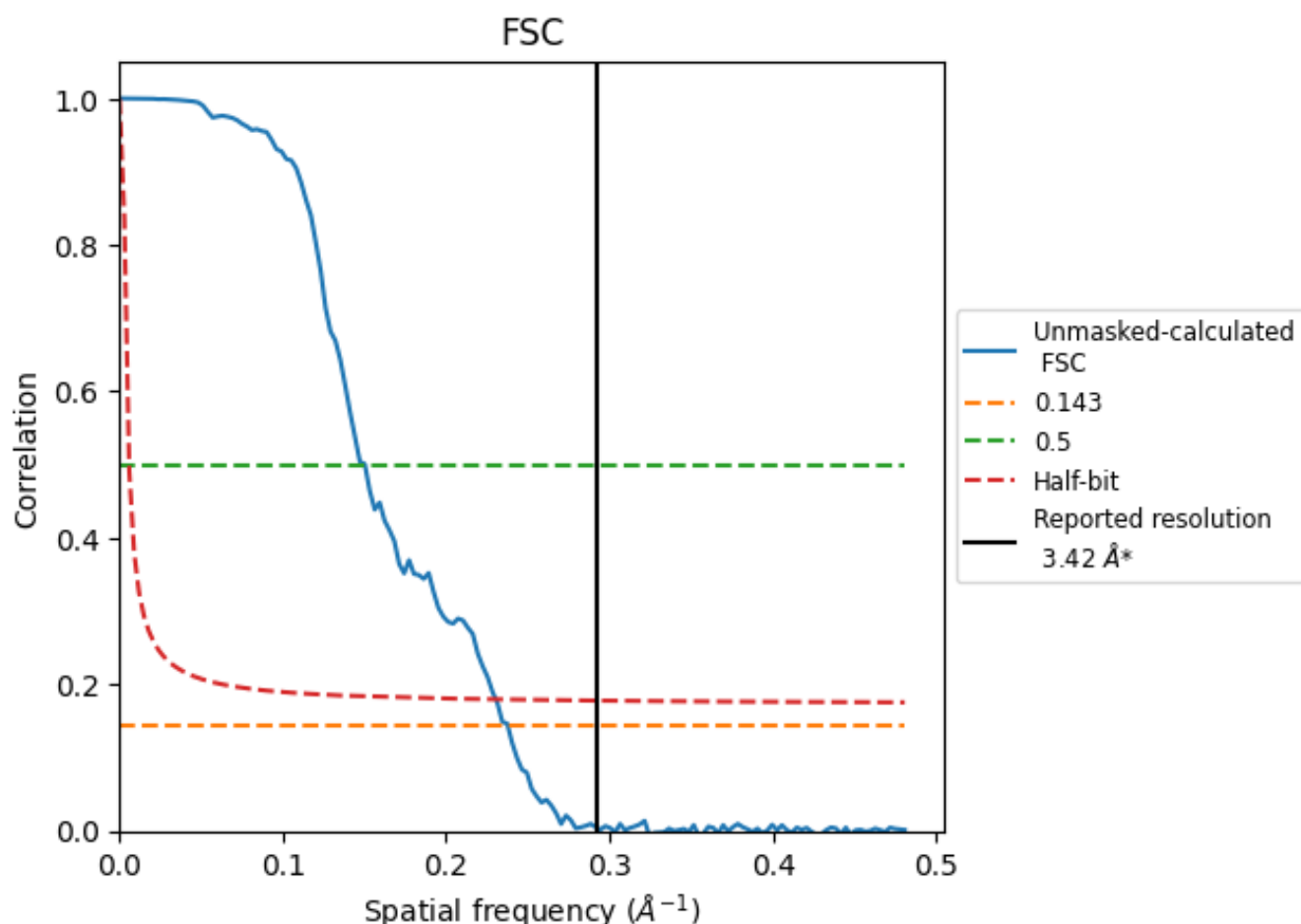


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

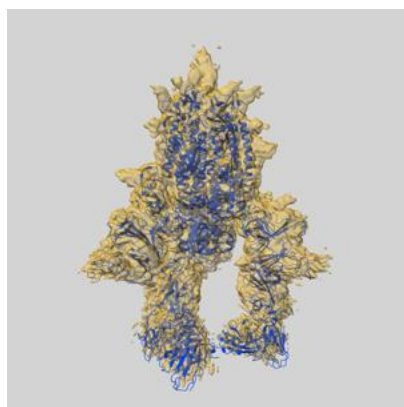
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	6.65	4.34

*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 4.21 differs from the reported value 3.42 by more than 10 %

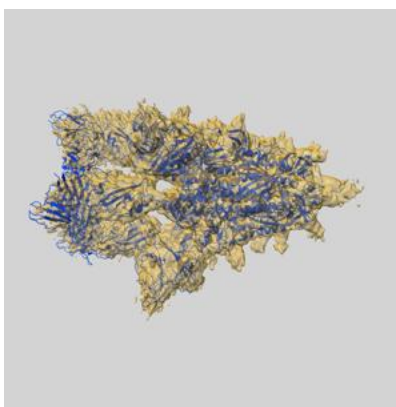
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38284 and PDB model 8XEA. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

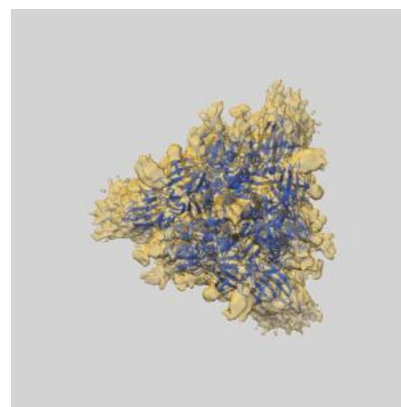
9.1 Map-model overlay [i](#)



X



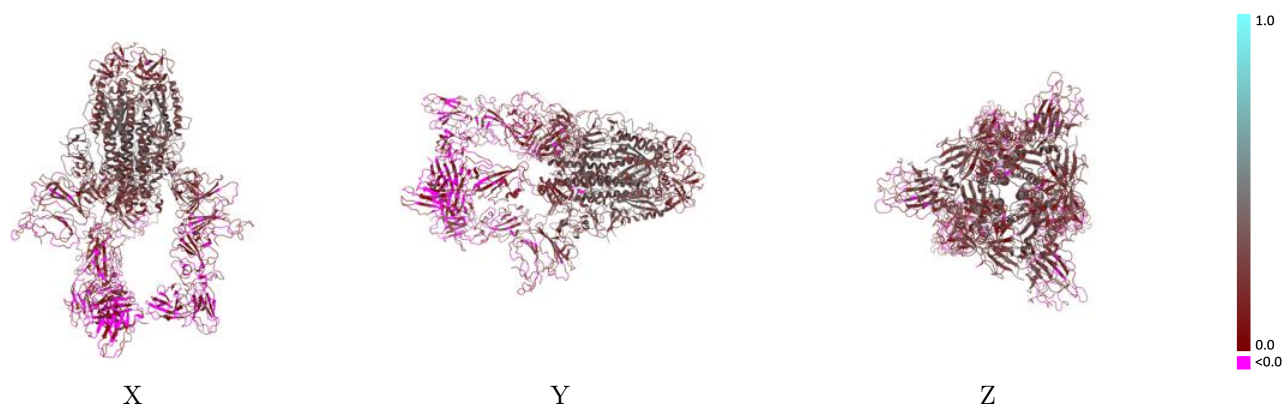
Y



Z

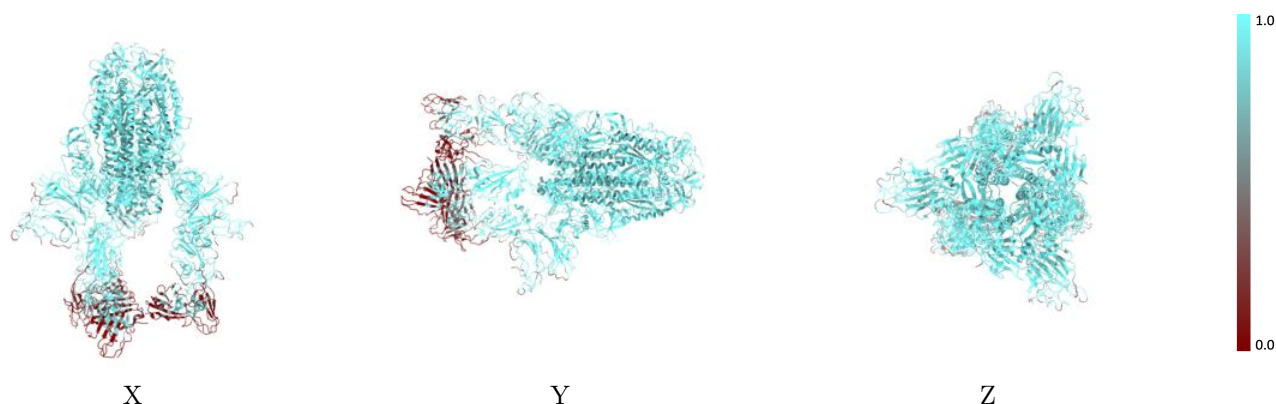
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



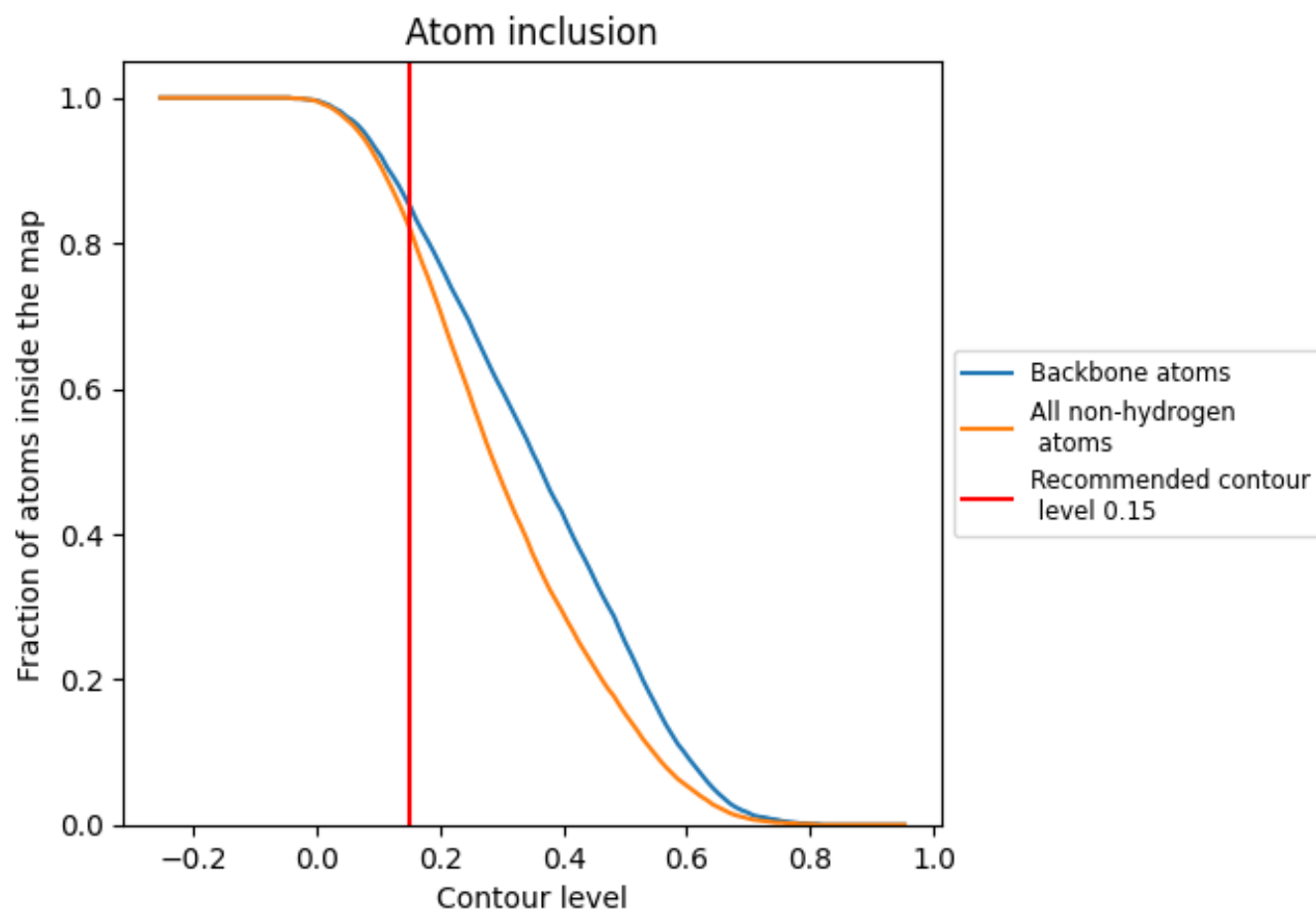
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8210	<div></div> 0.1920
A	<div></div> 0.3980	<div></div> 0.0110
B	<div></div> 0.4530	<div></div> 0.0360
D	<div></div> 0.9030	<div></div> 0.2260
E	<div></div> 0.8990	<div></div> 0.2280
F	<div></div> 0.8990	<div></div> 0.2250
G	<div></div> 0.4070	<div></div> 0.0210
H	<div></div> 0.4060	<div></div> 0.0110
I	<div></div> 0.4580	<div></div> 0.0300
J	<div></div> 0.4610	<div></div> 0.0270

1.0

0.0

<0.0