



wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 03:40 AM EDT

PDB ID : 7KL9 / pdb_00007kl9
EMDB ID : EMD-22916
Title : Structure of the SARS-CoV-2 S 6P trimer in complex with the ACE2 protein decoy, CTC-445.2 (State 4)
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2020-10-29
Resolution : 4.10 Å(reported)

This is a wwPDB EM Validation Summary 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

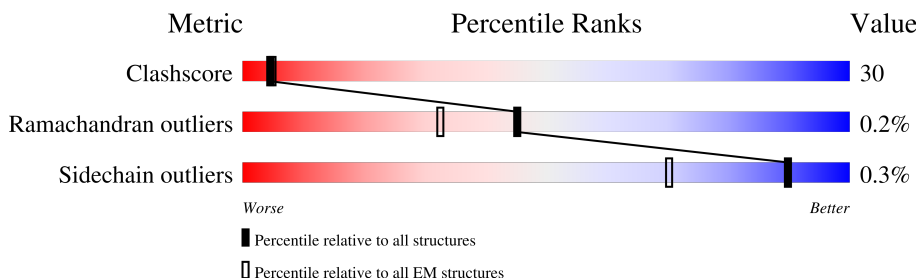
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	1257	
1	B	1257	
1	C	1257	
2	D	160	
2	E	160	
2	F	160	
3	G	2	
3	H	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1308	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	995	Total	C	N	O	S	0	0
			7433	4780	1250	1369	34		
1	B	998	Total	C	N	O	S	0	0
			7435	4779	1256	1367	33		
1	C	995	Total	C	N	O	S	0	0
			7435	4779	1251	1371	34		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	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	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	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

- Molecule 2 is a protein called CTC-445.2 inhibitor.

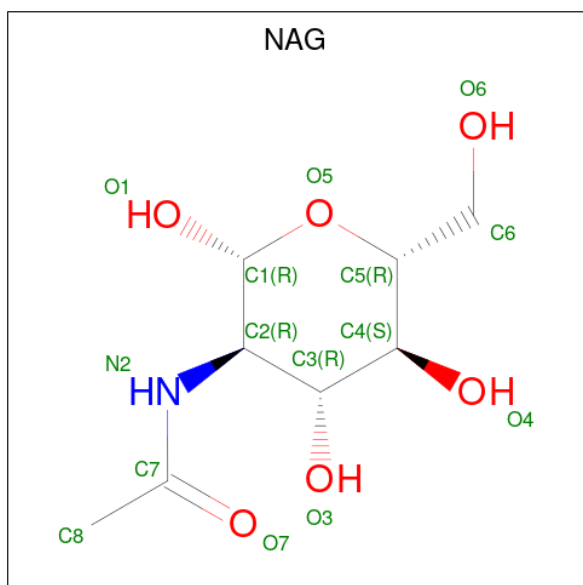
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	160	Total	C	N	O	S	0	0
			1207	739	222	243	3		
2	D	160	Total	C	N	O	S	0	0
			1207	739	222	243	3		
2	F	160	Total	C	N	O	S	0	0
			1207	739	222	243	3		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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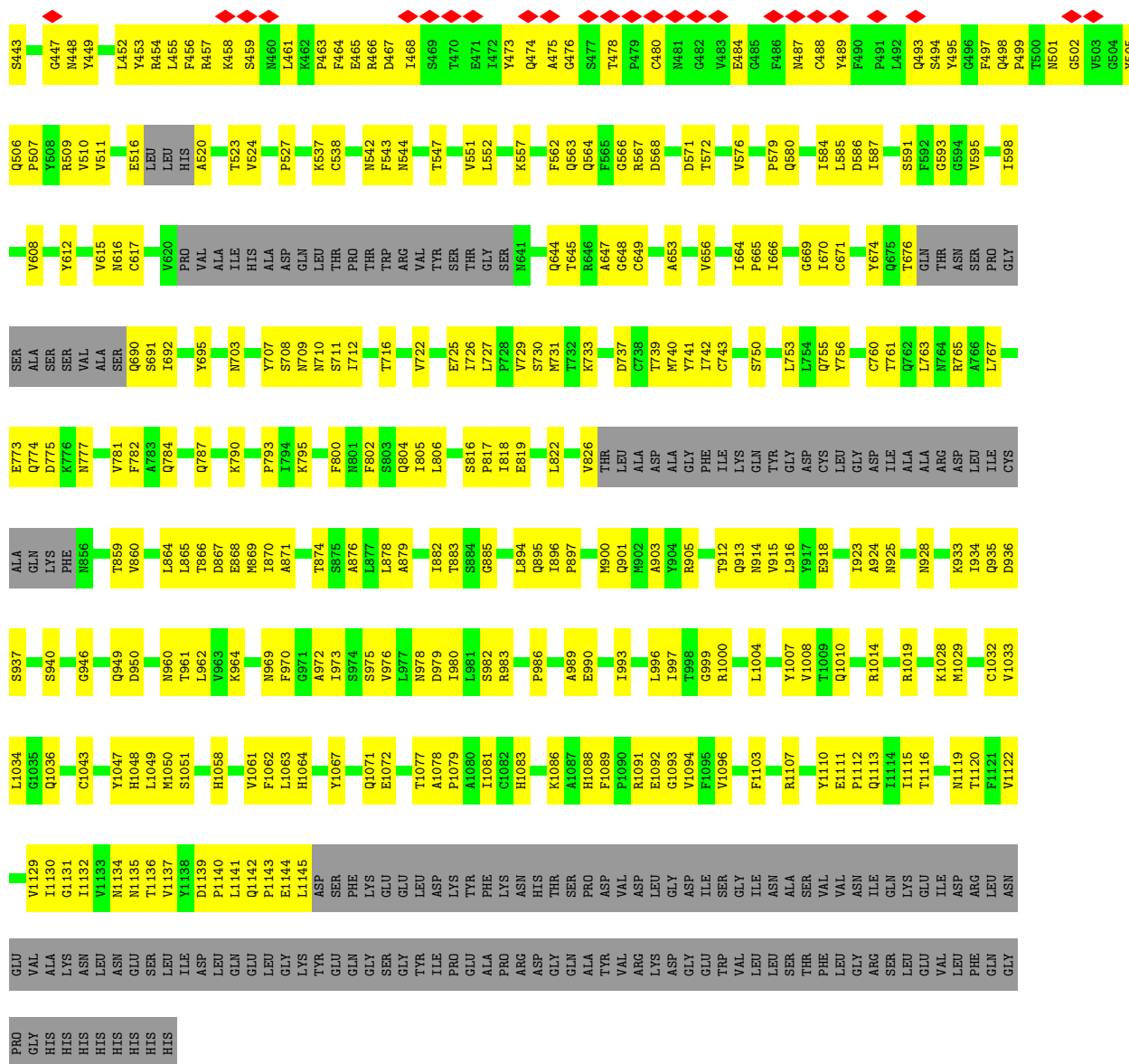
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

V781	E868	Q949	L1034	T1120	ASP
F782	M869	Q949	G1035	ASP	LEU
A783	A871	N953	Q1036	V1137	GLN
Q784		N953	R1039	L1141	GLY
V785	T874	N955	C1043	L1145	LEU
K786		L959	G1046	ASP	LYS
Q787	L877	Y963	Y1047	PHE	TYR
	A879	L966	H1048	GLY	GLN
	G880	S867	L1049	GLY	GLY
	T881	S868	M1050	GLY	GLY
F800	T883	N969	S1061	LEU	TYR
M801	S884	F970	F1052	ASP	ILE
F802	G885	G971	S1055	PRO	GLY
S803	Q804	A972	H1058	GLY	GLY
Q805	T887	L977	G1059	ASN	PRO
I805	F888	N978	F1062	HIS	ARG
L806	Q895	I896	L1063	THR	ASP
E819	P897	Y980	H1064	GLN	GLY
V826	M900	Q901	V1065	ALA	ALA
THR	Q901	Y904	T1066	VAL	TYR
LEU	Y904	R905	Q1071	ASP	VAL
ALA	R905	PHE	E1072	GLY	ARG
ASP	F906	ILE	F1075	ASP	LYS
GLY	N907	GLN	T1076	ILE	GLY
PHE	G908	TYR	T1077	GLY	TRP
ILE	V911	GLY	A1078	ILE	VAL
LYS	N914	GLY	A1080	ALA	LEU
GLN	V915	CYS	I1081	SER	THR
TYR	L916	ASP	C1082	VAL	THR
GLY	Y917	LEU	H1083	VAL	PHE
ASP	E918	ASP	Q1005	VAL	LEU
ILE	N919	ILE	K1086	ASN	GLY
ALA	Q920	ALA	A1087	GLN	SER
ALA	K921	ALA	H1088	LYS	SER
ARG	L922	ARG	Q1010	GLY	LEU
ASP	I923	ASP	Q1011	ILE	VAL
LEU	A924	LEU	V1094	ASP	LEU
ILE	N925	ILE	F1095	PHE	PHE
CYS	Q926	CYS	V1096	GLY	GLN
ALA	F927	ALA	R1019	ASN	PRO
GLN	N928	GLN	L1024	VAL	GLY
LYS	S929	LYS	A1025	HIS	HIS
PHE	A930	PHE	T1026	HIS	HIS
N856	K933	N856	Y1110	ASN	HIS
G857	I934	G857	I1114	ASN	HIS
L858	Q935	L858	I1115	GLY	HIS
	S939		D1118	LEU	HIS
L864	L945		N1119	ILE	HIS
L865					
T866					
D867					

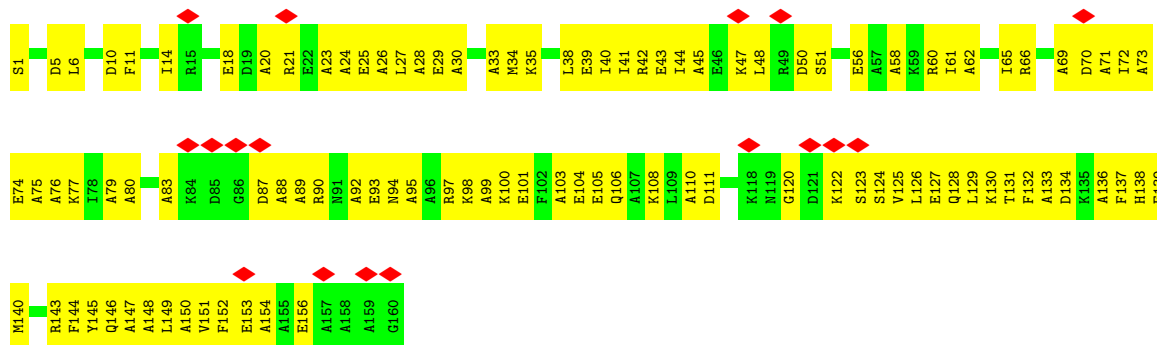
• Molecule 1: Spike glycoprotein

Chain B:  43% 36% 21%

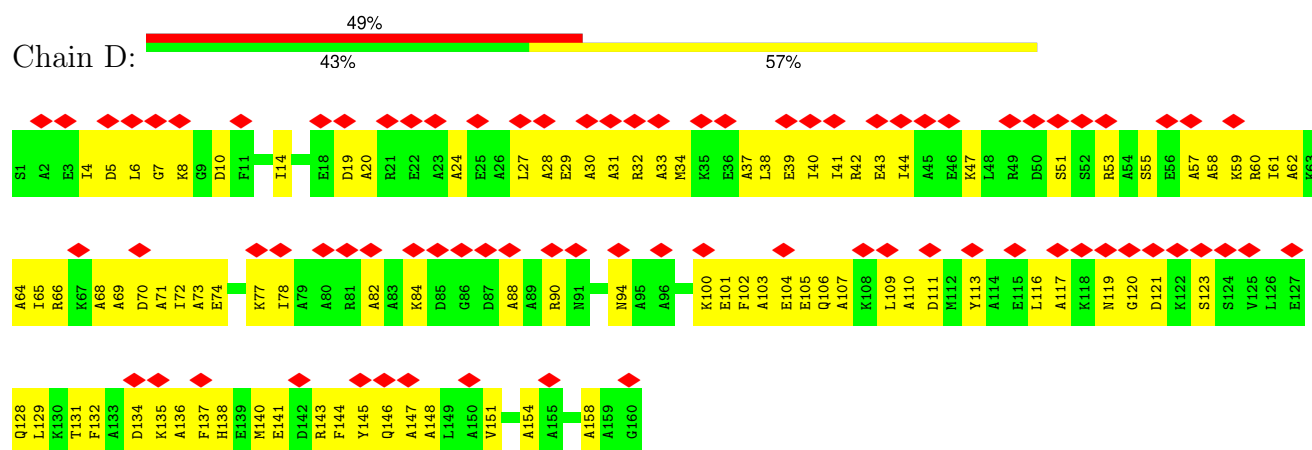
MET	SER	Y160	SER	Y160	SER	V341	L425	S494	Q580
PHE	GLY	M165	THR	M165	THR	F342	P426	Y495	T581
VAL	ASN	C166	ASN	C166	GLY	F429	F429	G496	L582
LEU	THR	GLN	THR	GLN	TRP	T430	T430	F497	E583
VAL	LYS	S172	LYS	S172	THR	G431	G431	Q498	I584
LEU	ARG	GLN	ARG	GLN	ALA	V350	V350	N501	L585
LEU	PHE	PHE	PHE	PHE	GLY	V350	V350	G502	D586
PRO	N81	N81	N81	N81	ALA	A435	A435	V510	L587
LEU	N81	N81	N81	N81	A263	W353	W353	Y505	T588
SER	N82	N82	N82	N82	A264	N354	N354	Q506	G594
GLN	N83	N83	N83	N83	Y269	R355	R355	P507	V595
VAL	L84	L84	L84	L84	L270	K356	K356	Y508	
CYS	P85	P85	P85	P85	L271	N360	N360	R509	
ASN	F86	F86	F86	F86	Q271	C361	C361	V511	T598
THR	G89	G89	G89	G89	P272	S362	S362	S443	T599
LYS	F92	F92	F92	F92	T274	D364	D364	S443	G601
ASN	E96	E96	E96	E96	F275	A363	A363	K444	T602
THR	I101	I101	I101	I101	L276	Y365	Y365	G447	N603
THR	R102	R102	R102	R102		S366	S366	N448	
LEU	G103	G103	G103	G103	Y279	V367	V367	N450	V608
PRO	W104	W104	W104	W104	N280	L368	L368	L451	A609
VAL	F106	F106	F106	F106	E281	Y369	Y369	L452	V610
ASP	G107	G107	G107	G107	N282	N370	N370	L453	L611
GLY	T108	T108	T108	T108	C283	F374	F374	L455	V615
TRP	F109	F109	F109	F109	T284	S375	S375	L457	N616
VAL	F32	F32	F32	F32		T376	T376	K458	C617
LEU	Y37	Y37	Y37	Y37	D290	P384	P384	S459	T618
LEU	D111	D111	D111	D111	C291	L293	L293	N460	F619
SER	S112	S112	S112	S112	A292	D294	D294	L461	P620
THR	T124	T124	T124	T124	L295	L296	L296	K462	VAL
THR	C131	C131	C131	C131	P295	L296	L296	F463	ALA
THR	E132	E132	E132	E132	S205	L390	L390	K464	ILE
LEU	F133	F133	F133	F133	S206	C391	C391	F466	GLY
THR	Q134	Q134	Q134	Q134	S297	F392	F392	R466	ASP
THR	F135	F135	F135	F135	V308	T393	T393	D467	GLN
LEU	C136	C136	C136	C136	E309	D398	D398	L472	THR
VAL	G142	G142	G142	G142	G311	S399	S399	Y473	LEU
VAL	V143	V143	V143	V143	Q312	F400	F400	Q474	THR
LEU	T143	T143	T143	T143	Y313	V401	V401	A475	PRO
LEU	F55	F55	F55	F55	Q314	I402	I402		THR
LEU	F58	F58	F58	F58	T315	R403	R403	T478	TRP
GLY	S60	S60	S60	S60	S316	Q409	Q409	F479	ARG
GLY	N61	N61	N61	N61	N317	I410	I410	C480	VAL
PRO	M64	M64	M64	M64	E324	A411	A411	V483	THR
GLY	F65	F65	F65	F65	S325	Q414	Q414	E484	SER
GLY	H66	H66	H66	H66	T326	K417	K417	C485	GLY
ALA	ALA	ALA	ALA	ALA	V327	I418	I418	F486	
ILE	ILE	ILE	ILE	ILE	F329	C488	C488	N487	N641
LEU	LEU	LEU	LEU	LEU	T332	Y489	Y489	F490	Q644
GLY	GLY	GLY	GLY	GLY	C336	P491	P491	L492	T645
HIS	HIS	HIS	HIS	HIS	F337	L493	L493	V575	G646
HIS	HIS	HIS	HIS	HIS	F338	Q493	Q493	V576	A647
HIS	HIS	HIS	HIS	HIS				R577	V656



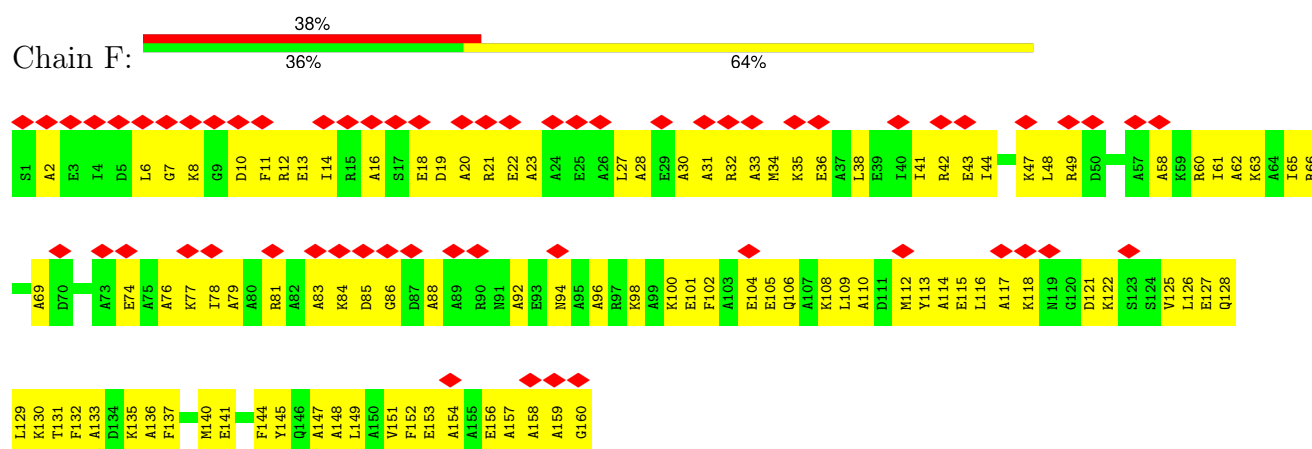
• Molecule 2: CTC-445.2 inhibitor



• Molecule 2: CTC-445.2 inhibitor



- Molecule 2: CTC-445.2 inhibitor



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26038	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.469	Depositor
Minimum map value	-0.216	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	375.40802, 375.40802, 375.40802	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/7605	0.50	1/10385 (0.0%)
1	B	0.44	0/7607	0.55	1/10391 (0.0%)
1	C	0.43	0/7607	0.55	6/10389 (0.1%)
2	D	0.18	0/1215	0.45	0/1620
2	E	0.21	0/1215	0.40	0/1620
2	F	0.21	0/1215	0.50	0/1620
All	All	0.40	0/26464	0.52	8/36025 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	PRO	CA-N-CD	-8.96	99.45	112.00
1	A	384	PRO	CA-N-CD	-8.79	99.69	112.00
1	C	328	ARG	N-CA-C	8.53	119.52	108.34
1	C	330	PRO	N-CA-C	7.40	127.71	112.47
1	C	329	PHE	CA-C-N	6.94	128.52	119.84

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	7433	0	6943	446	0
1	B	7435	0	6926	439	0
1	C	7435	0	6933	492	0
2	D	1207	0	1203	78	0
2	E	1207	0	1203	89	0
2	F	1207	0	1203	91	0
3	G	28	0	25	1	0
3	H	28	0	25	2	0
4	A	112	0	104	3	0
4	B	154	0	143	12	0
4	C	112	0	104	2	0
All	All	26358	0	24812	1556	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 30.

The worst 5 of 1556 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HD2	1:C:495:TYR:CE1	1.35	1.60
1:C:374:PHE:CD1	1:C:434:ILE:CG2	1.87	1.57
1:A:357:ARG:HG2	1:A:396:TYR:CE1	1.36	1.55
1:C:329:PHE:CG	1:C:330:PRO:HD3	1.46	1.51
1:C:374:PHE:CD1	1:C:434:ILE:HG22	1.49	1.45

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	977/1257 (78%)	868 (89%)	109 (11%)	0	100	100
1	B	982/1257 (78%)	835 (85%)	142 (14%)	5 (0%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	977/1257 (78%)	864 (88%)	111 (11%)	2 (0%)	44	77
2	D	158/160 (99%)	146 (92%)	12 (8%)	0	100	100
2	E	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
2	F	158/160 (99%)	145 (92%)	13 (8%)	0	100	100
All	All	3410/4251 (80%)	2999 (88%)	404 (12%)	7 (0%)	45	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ILE
1	B	531	THR
1	C	329	PHE
1	C	330	PRO
1	B	528	LYS

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	747/1096 (68%)	745 (100%)	2 (0%)	91	92
1	B	741/1096 (68%)	739 (100%)	2 (0%)	91	92
1	C	747/1096 (68%)	744 (100%)	3 (0%)	89	91
2	D	107/107 (100%)	107 (100%)	0	100	100
2	E	107/107 (100%)	107 (100%)	0	100	100
2	F	107/107 (100%)	107 (100%)	0	100	100
All	All	2556/3609 (71%)	2549 (100%)	7 (0%)	90	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	329	PHE
1	C	329	PHE

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Mol	Chain	Res	Type
1	C	895	GLN
1	C	331	ASN
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	644	GLN
1	C	1142	GLN
1	C	394	ASN
2	F	106	GLN
1	C	913	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.44	0	17,19,21	0.58	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	H	1	1,3	14,14,15	0.47	0	17,19,21	1.07	1 (5%)
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O4-C4-C3	3.38	118.35	110.38

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

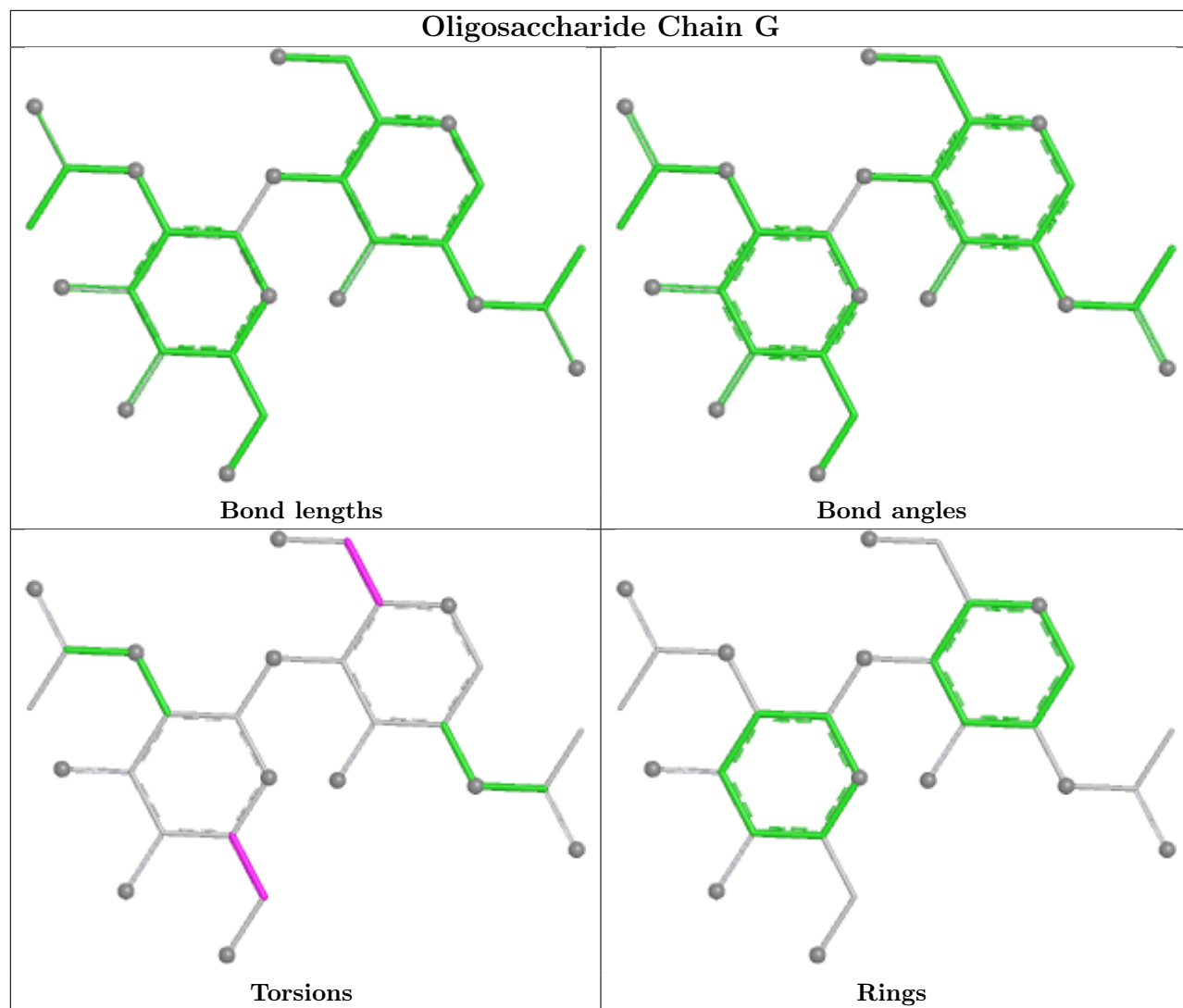
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C3-C2-N2-C7
3	H	2	NAG	O7-C7-N2-C2

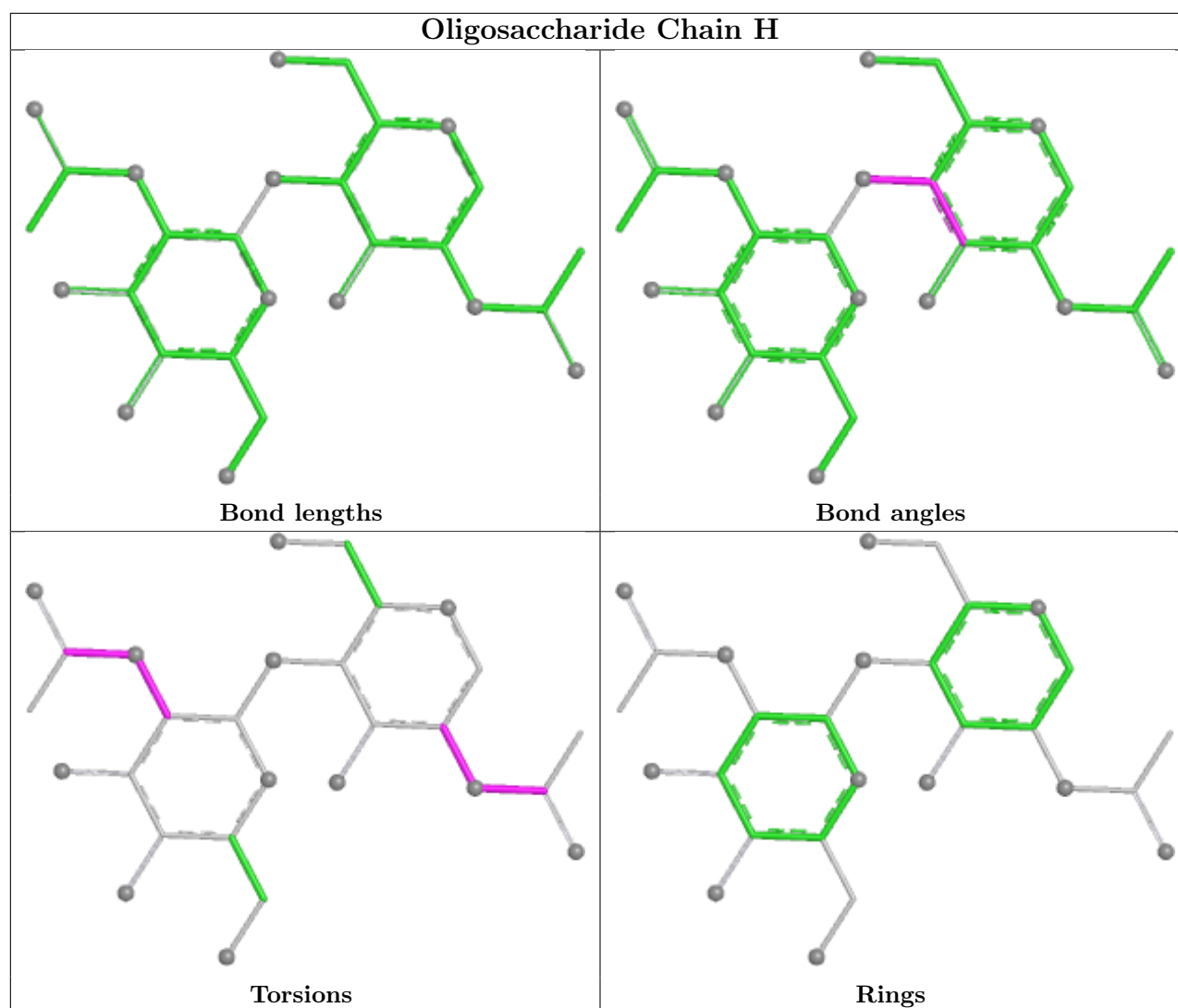
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	NAG	2	0
3	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1307	1	14,14,15	0.40	0	17,19,21	0.52	0
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	B	1309	1	14,14,15	0.47	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1301	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1306	1	14,14,15	0.61	0	17,19,21	0.42	0
4	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	0.46	0
4	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.37	0
4	NAG	B	1308	1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	A	1305	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	C	1302	1	14,14,15	0.47	0	17,19,21	0.42	0
4	NAG	A	1302	1	14,14,15	0.31	0	17,19,21	0.42	0
4	NAG	A	1308	1	14,14,15	0.27	0	17,19,21	0.37	0
4	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.55	0
4	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	B	1311	1	14,14,15	0.26	0	17,19,21	0.72	0
4	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	C	1306	1	14,14,15	0.59	0	17,19,21	0.38	0
4	NAG	A	1303	1	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	B	1302	1	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	C	1304	1	14,14,15	0.36	0	17,19,21	0.50	0
4	NAG	B	1305	1	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.56	0
4	NAG	C	1308	1	14,14,15	0.44	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	NAG	2	0
4	B	1304	NAG	1	0
4	B	1309	NAG	1	0
4	B	1306	NAG	1	0
4	A	1301	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	NAG	7	0
4	B	1310	NAG	1	0
4	C	1306	NAG	2	0
4	B	1307	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

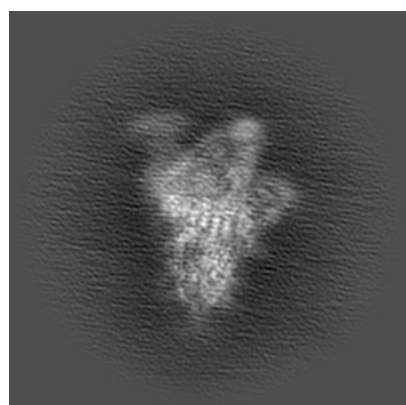
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22916. These allow visual inspection of the internal detail of the map and identification of artifacts.

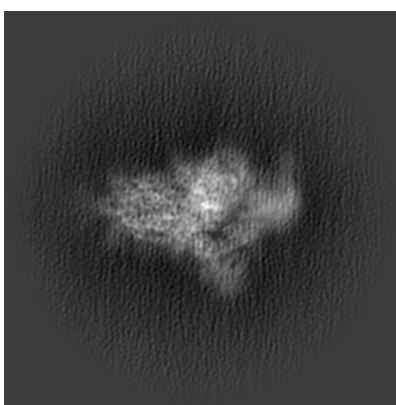
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

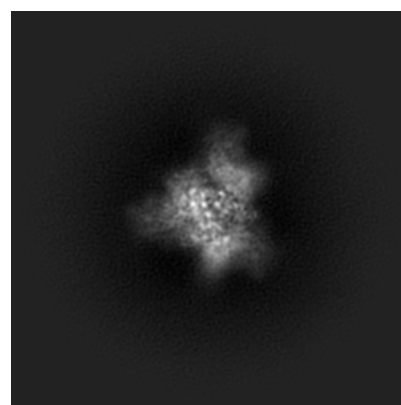
6.1.1 Primary map



X



Y

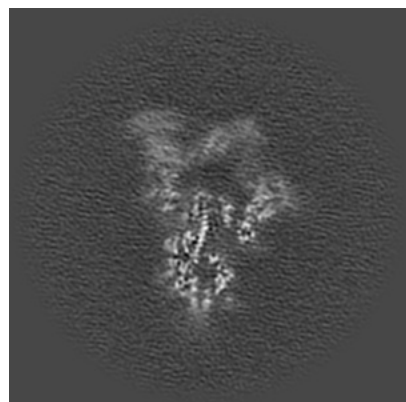


Z

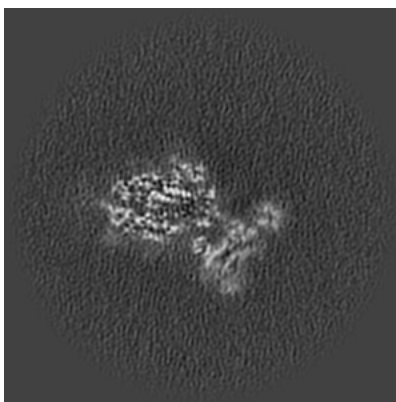
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

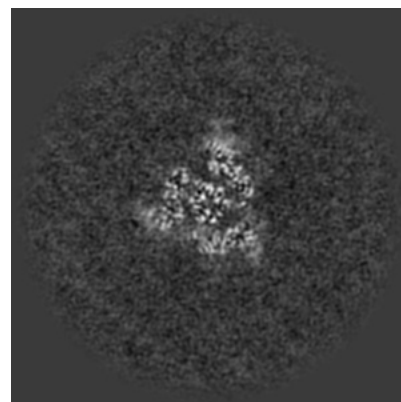
6.2.1 Primary map



X Index: 216



Y Index: 216

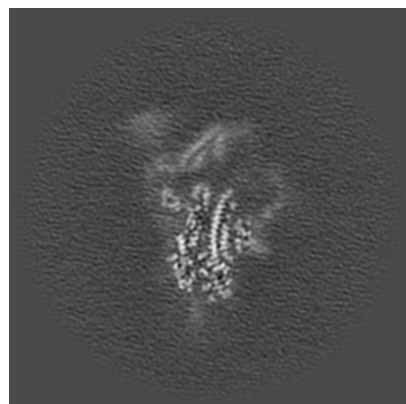


Z Index: 216

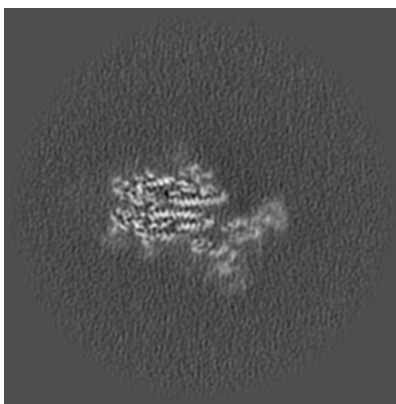
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

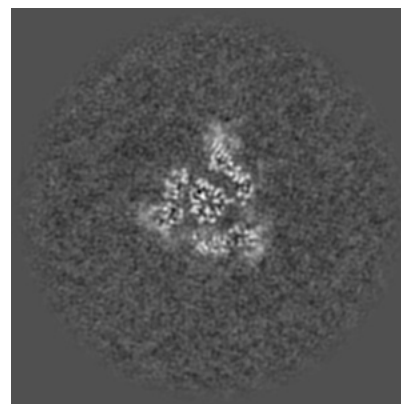
6.3.1 Primary map



X Index: 208



Y Index: 222

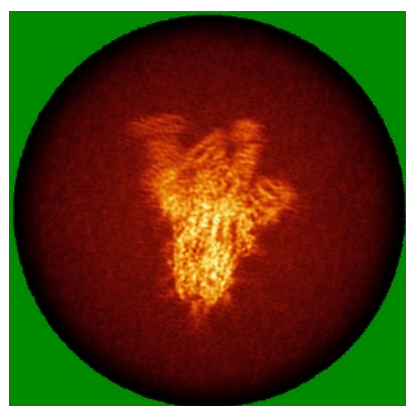


Z Index: 218

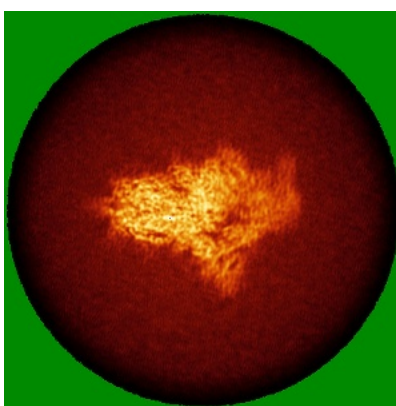
The images above show the largest variance slices of the map in three orthogonal directions.

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

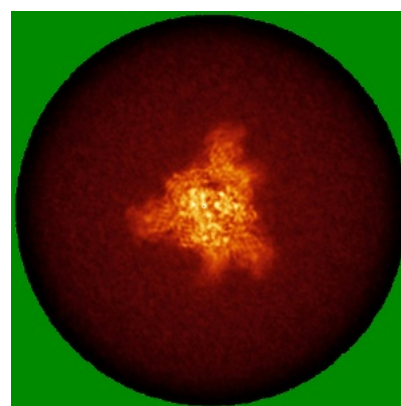
6.4.1 Primary map



X



Y



Z

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

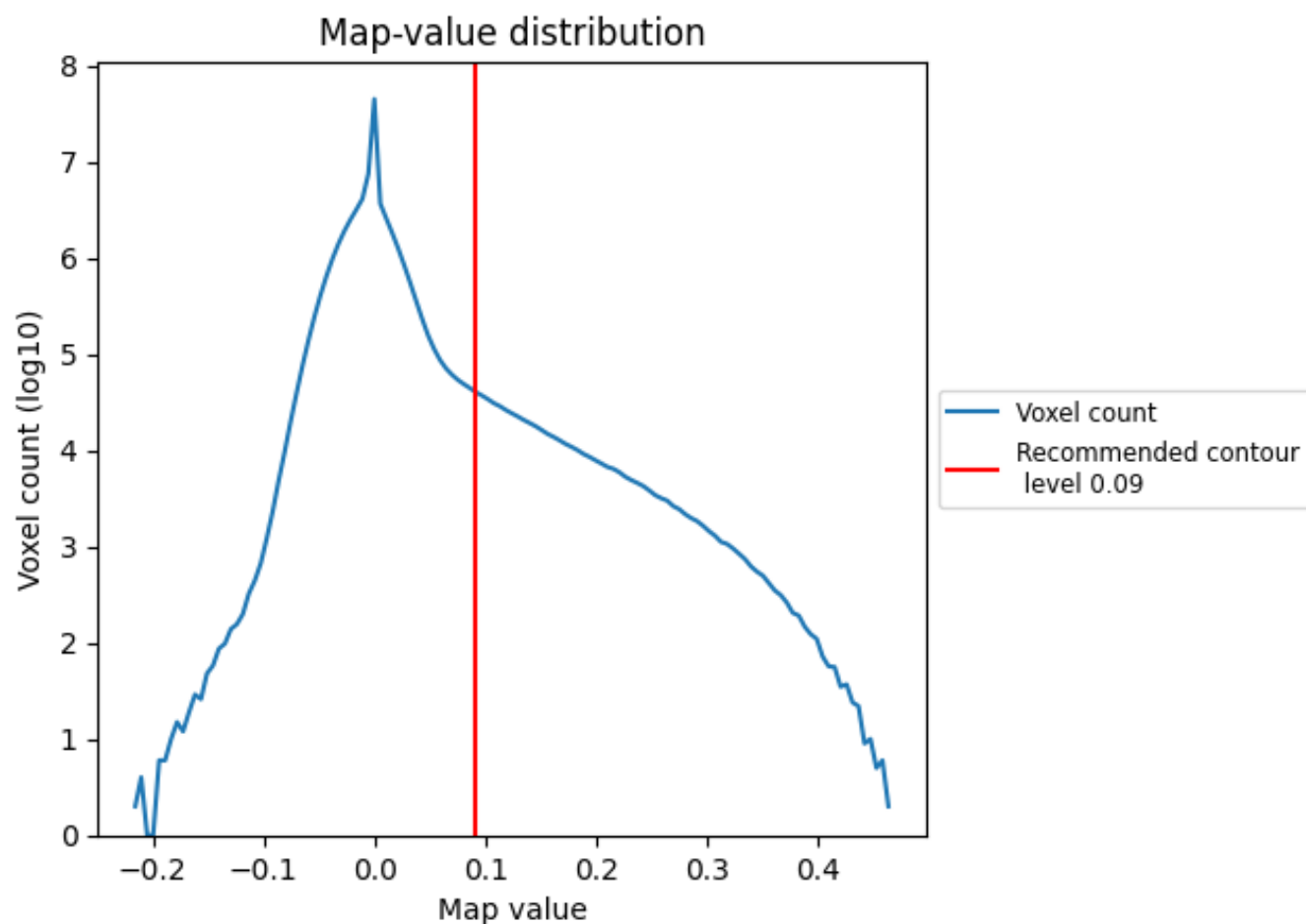
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

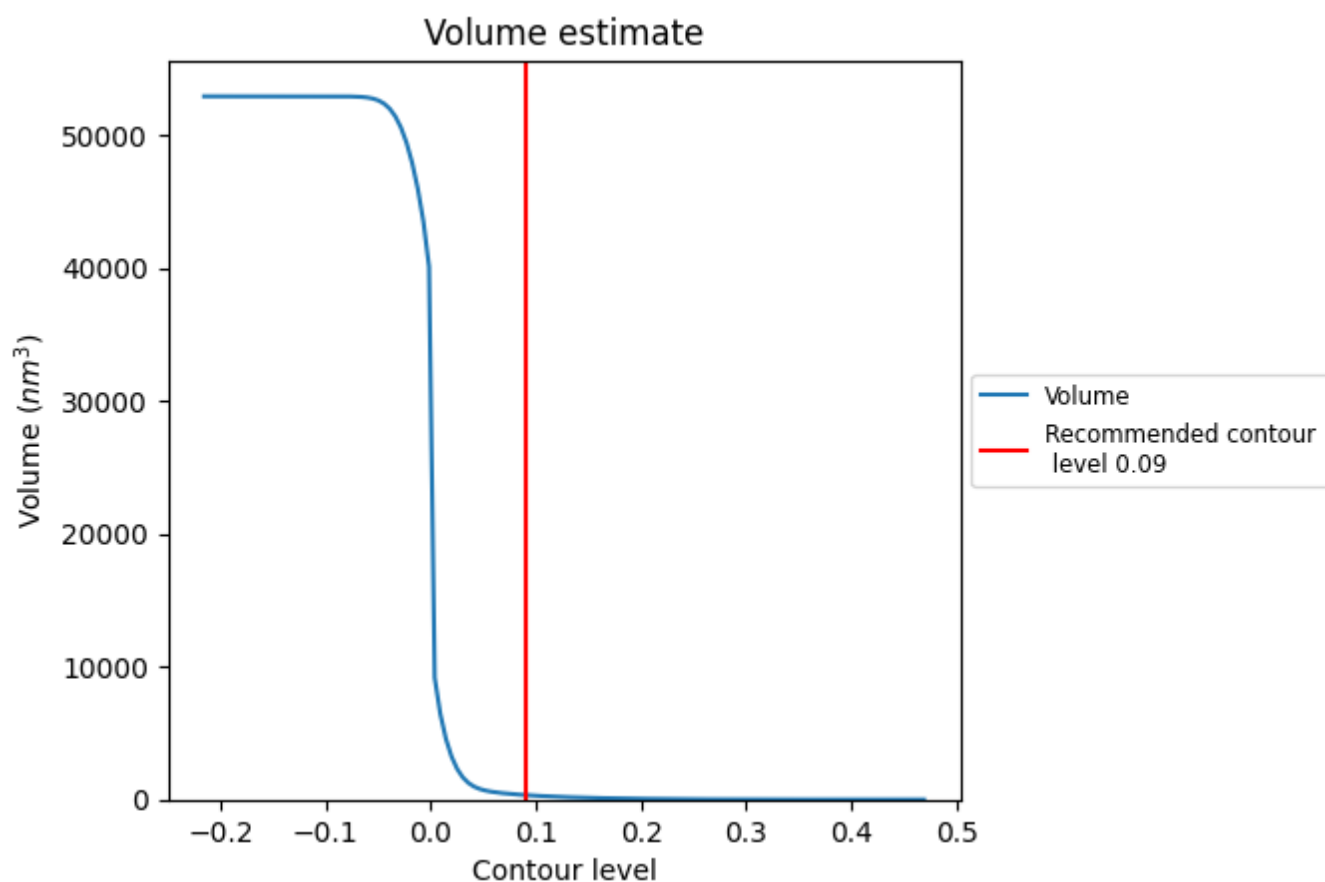
This section contains the results of statistical analysis of the map.

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.

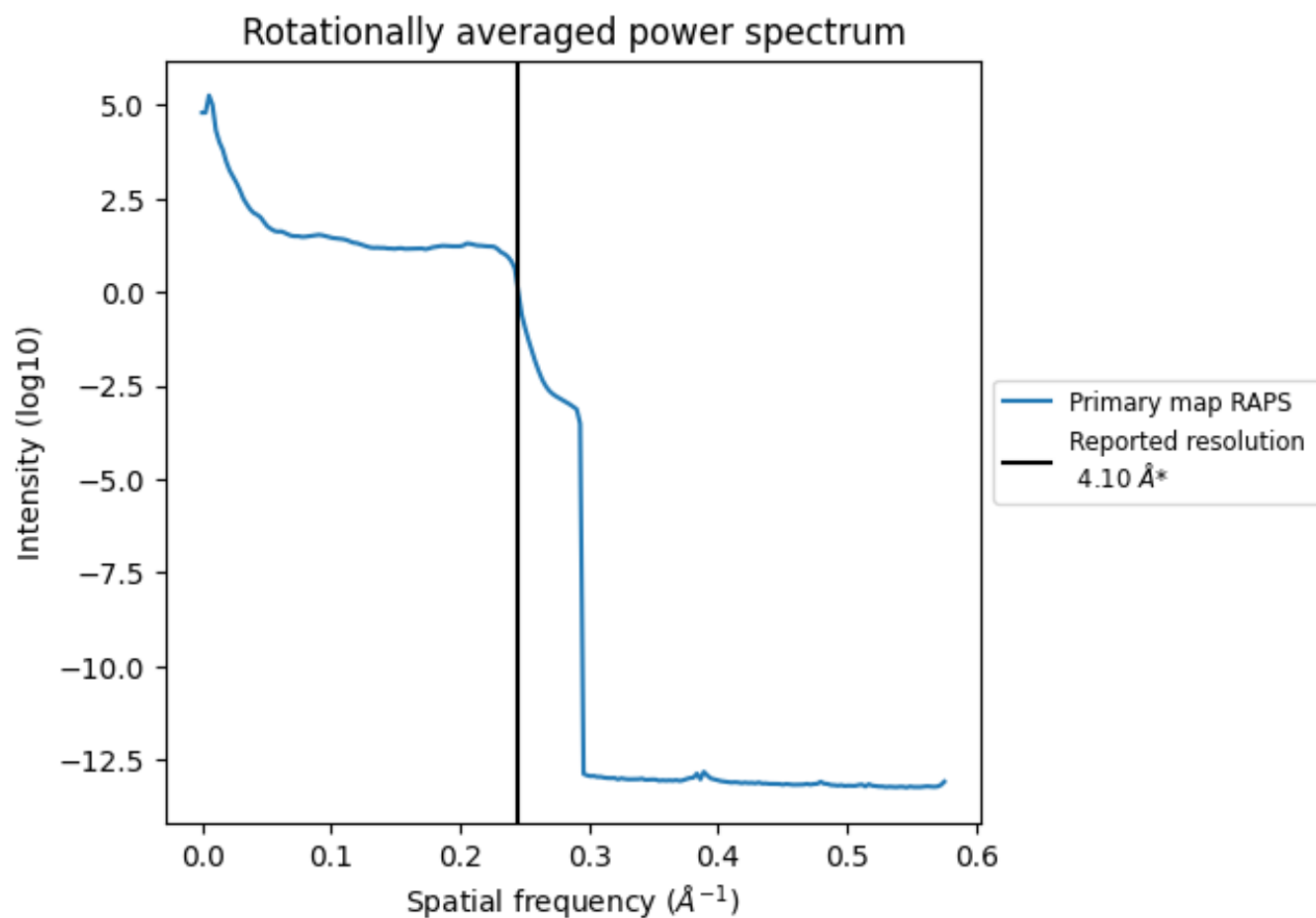
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 ⓘ

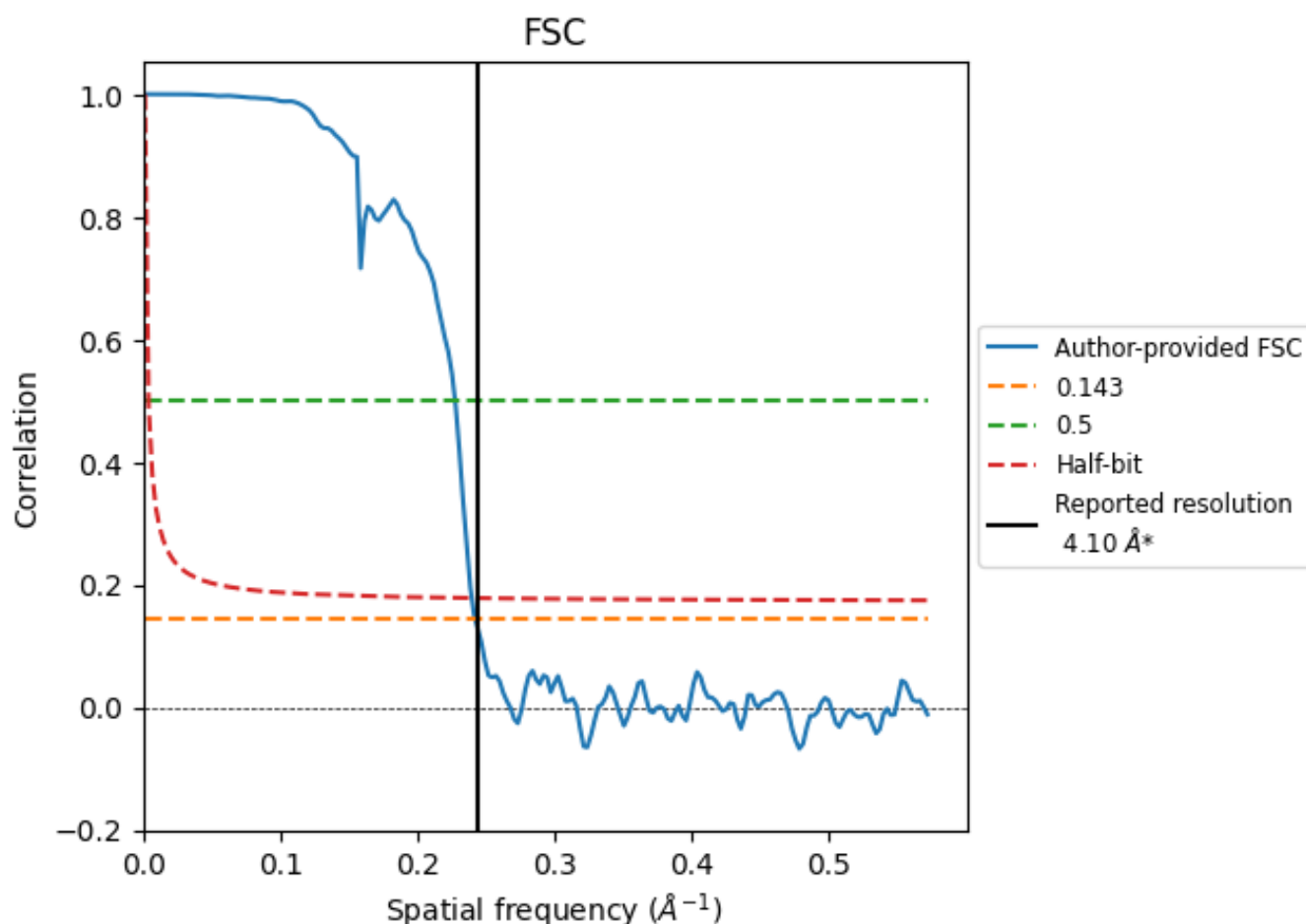


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

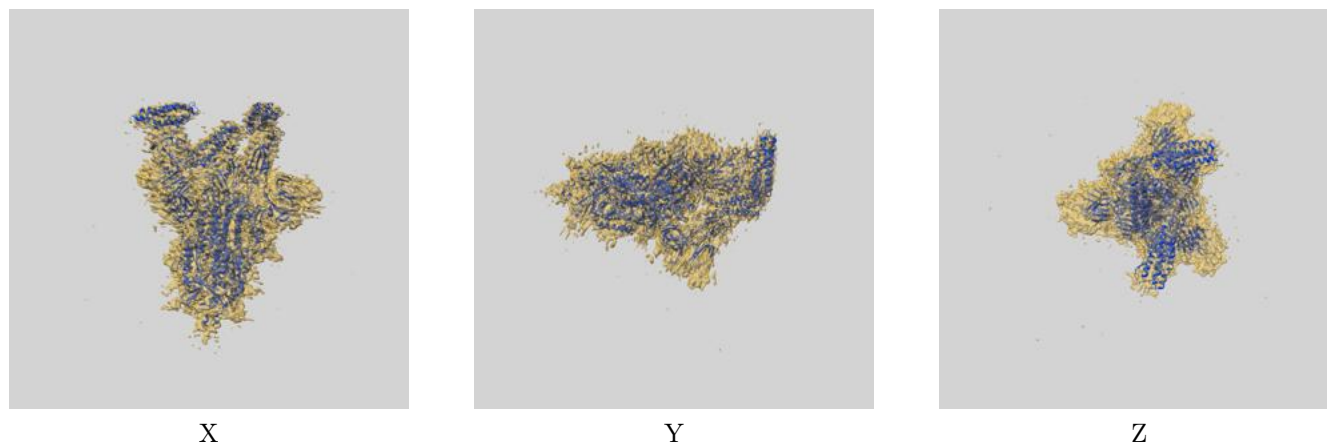
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.13	4.40	4.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22916 and PDB model 7KL9. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



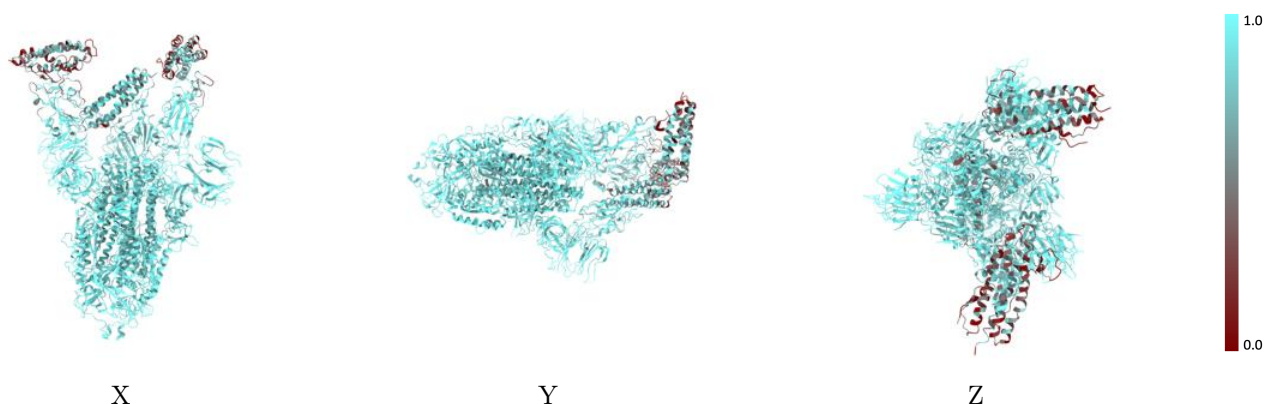
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



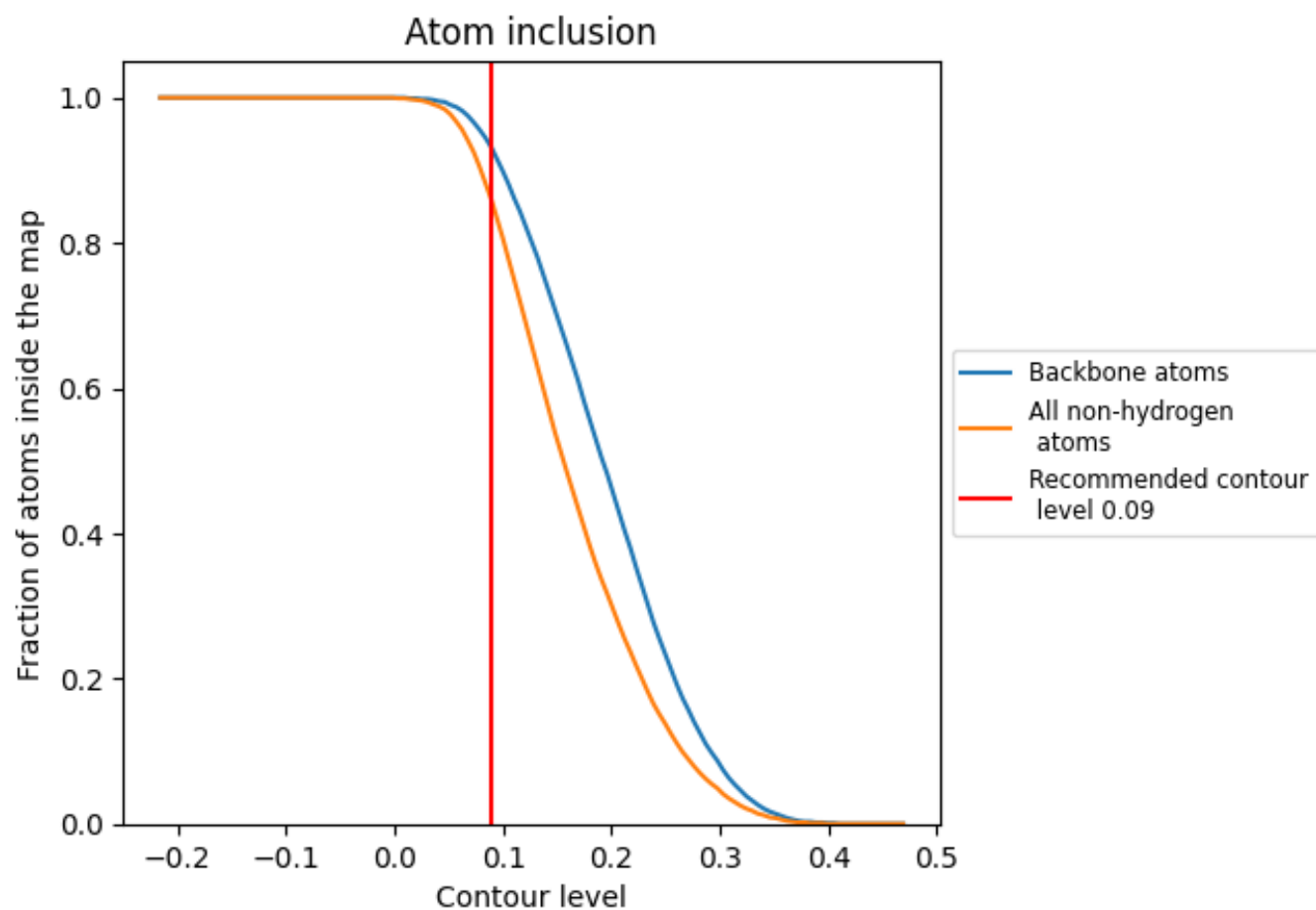
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8570	<div></div> 0.3520
A	<div></div> 0.9020	<div></div> 0.3670
B	<div></div> 0.9160	<div></div> 0.3870
C	<div></div> 0.8890	<div></div> 0.3640
D	<div></div> 0.4280	<div></div> 0.2250
E	<div></div> 0.7490	<div></div> 0.2460
F	<div></div> 0.5300	<div></div> 0.2030
G	<div></div> 0.6790	<div></div> 0.3280
H	<div></div> 1.0000	<div></div> 0.4070

1.0

0.0

<0.0