



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 12:20 PM JST

PDB ID : 5X5F
EMDB ID : EMD-6707
Title : Prefusion structure of MERS-CoV spike glycoprotein, conformation 2
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 4.20 Å(reported)

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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

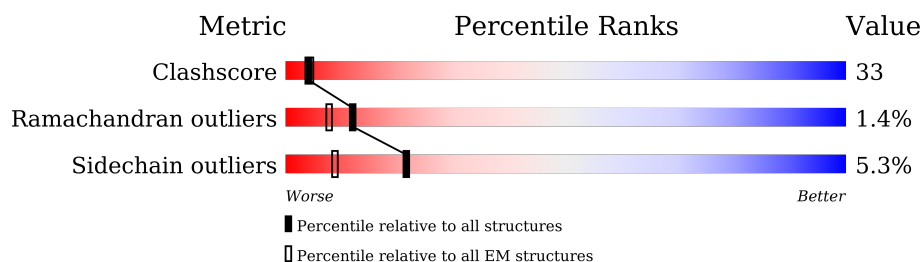
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	1323	<div> <div>55%</div> <div>57%</div> <div>24%</div> <div>• •</div> <div>14%</div> </div>
1	B	1323	<div> <div>52%</div> <div>57%</div> <div>24%</div> <div>• •</div> <div>14%</div> </div>
1	C	1323	<div> <div>54%</div> <div>59%</div> <div>23%</div> <div>• •</div> <div>14%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26422 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 S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8810	5601	1458	1700	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
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B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

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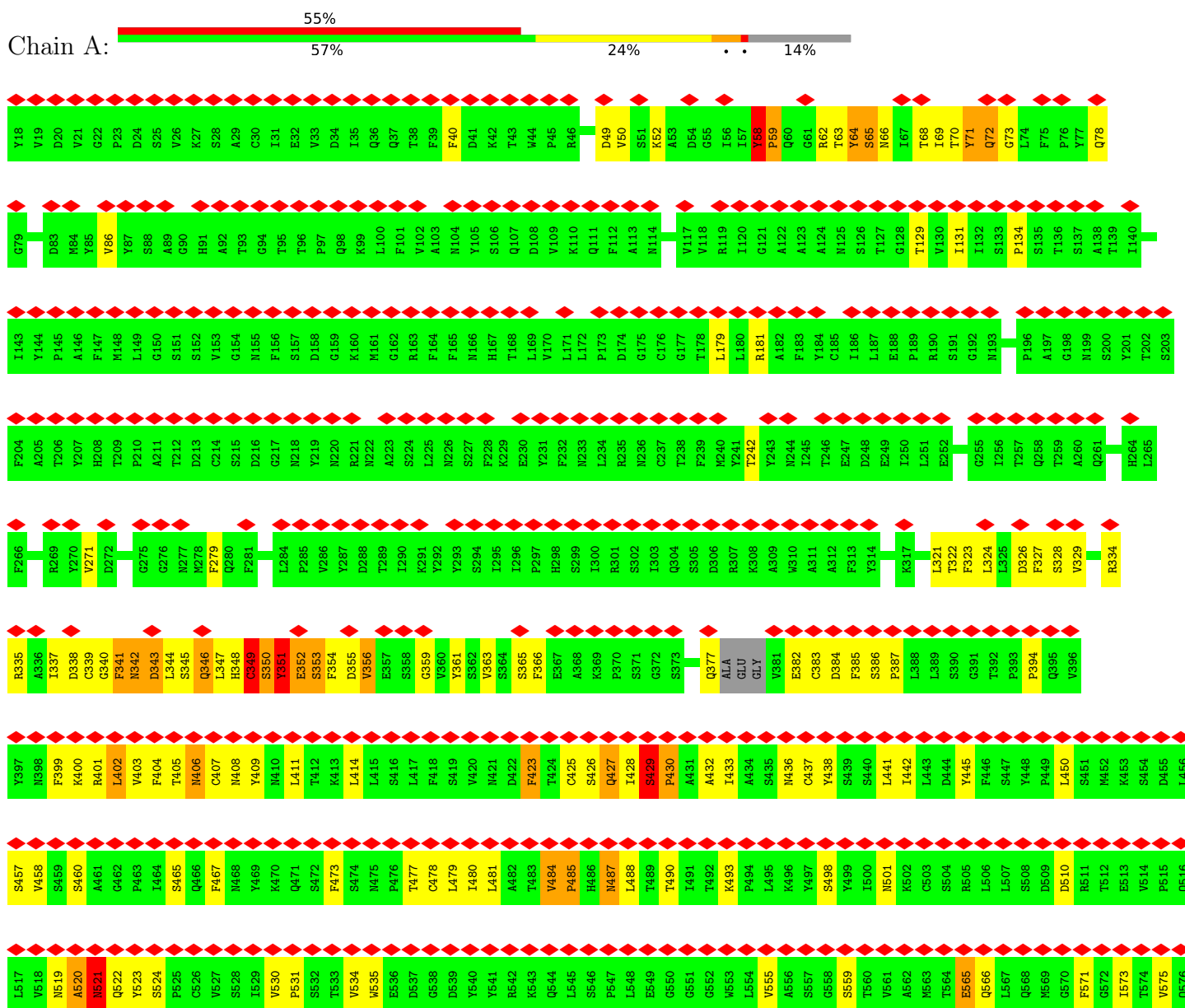
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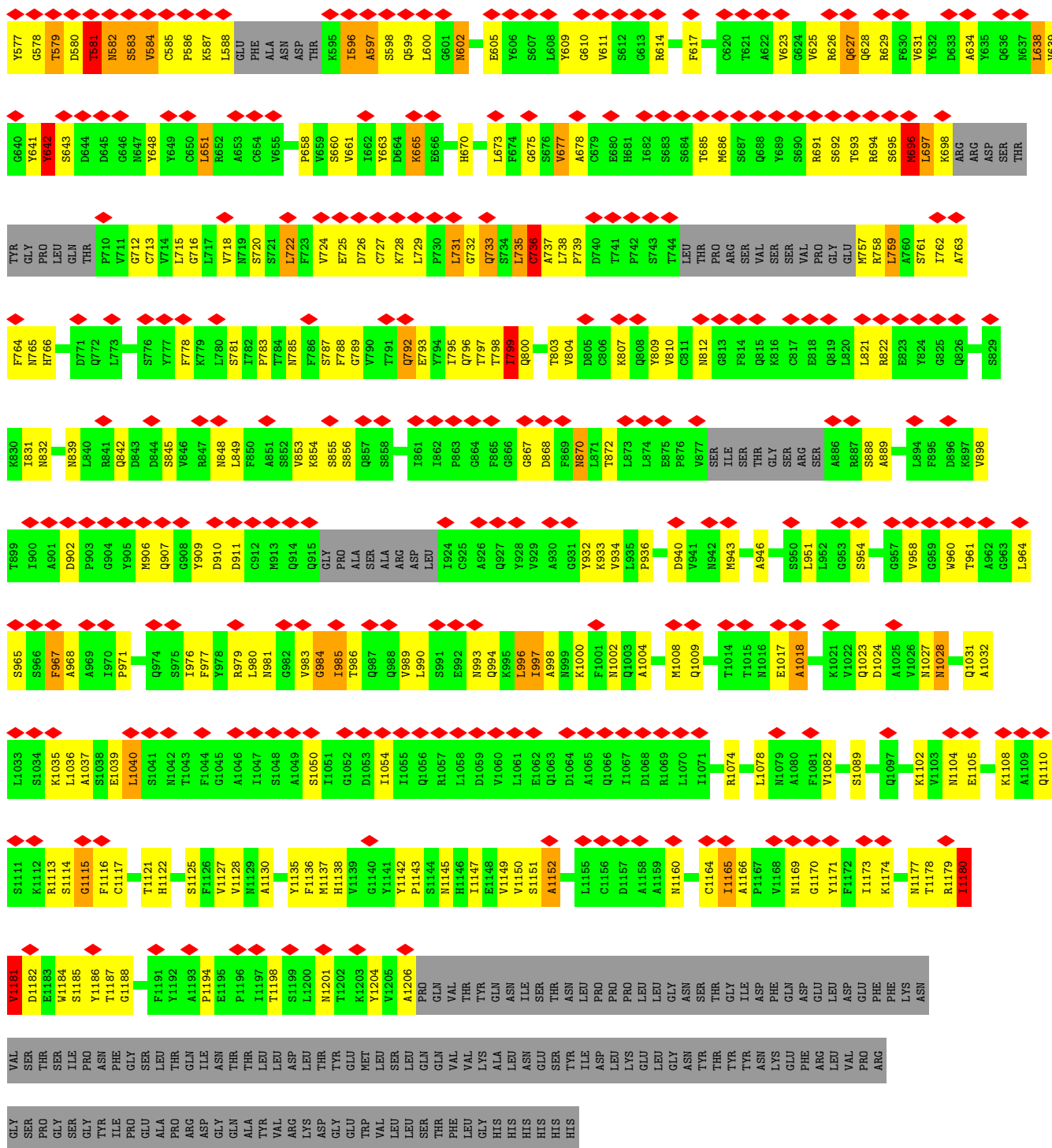
Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

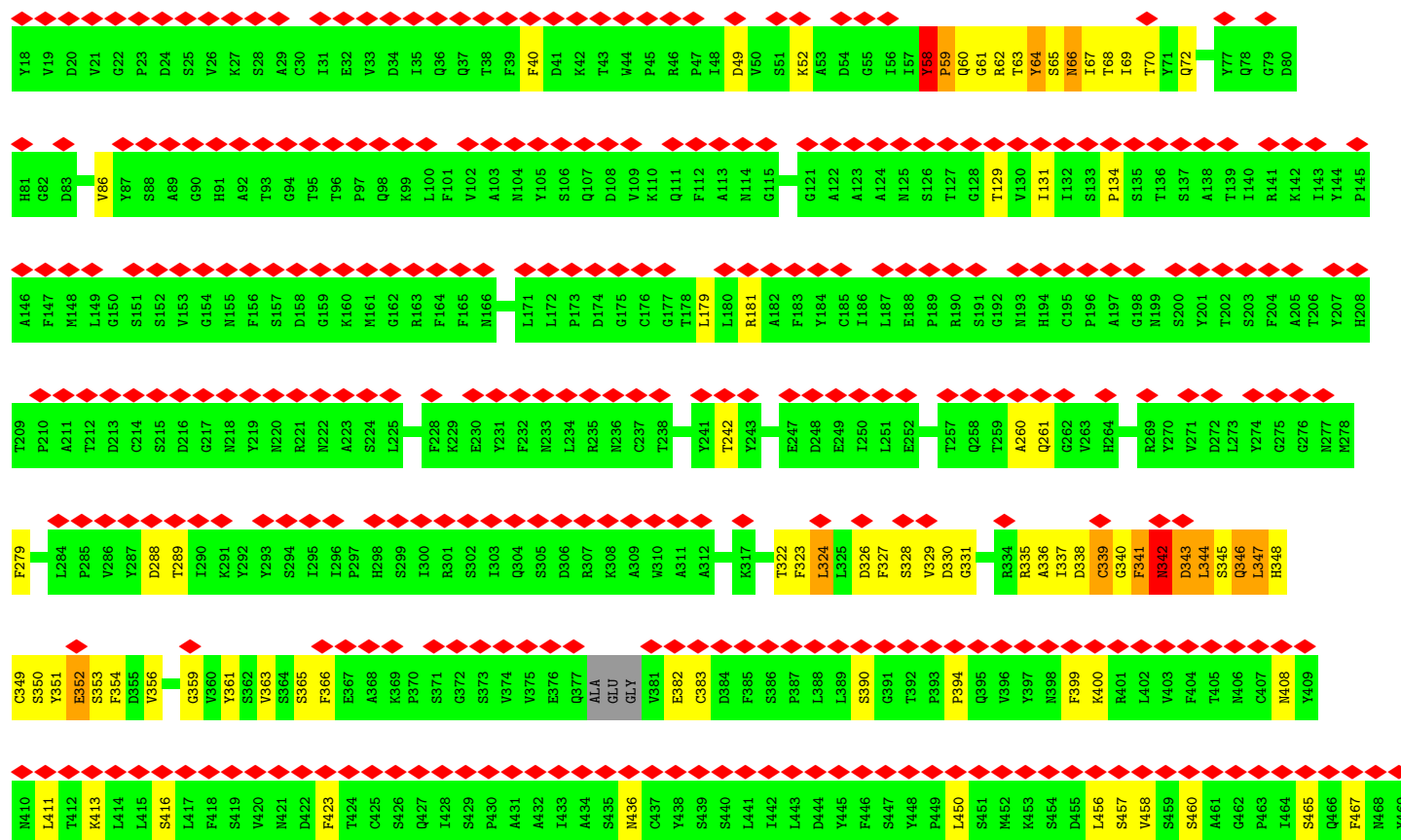
• Molecule 1: S protein





ALA	SER	V853	S781	C713	G647	V584	SS24	I464	F404	N342	V271	Y207	A146	Y85
ARG	ALA	K854	I782	V714	Y648	C585	P625	S465	T405	D343	D272	H208	F147	V86
ASP	ARG	S855	T783	L715	Y649	P586	C526	Q466	N406	L344	L273	T209	M148	Y87
LEU	ASP	S856	N785	G716	C650	K587	V527	F467	C407	S445	Y274	P210	L149	S88
I924	I924	S857	F786	L717	L651	L588	SS28	N468	N408	L347	G275	A211	G150	A89
C925	C925	S858	H718	W719	R652	GLU	I529	Y469	Y409	H348	G276	T212	S151	G90
A926	A926	S859	F788	S720	A653	PHE	V530	K470	N410	C949	F279	D213	S152	H91
Q927	Q927	T791	C654	S721	C654	ALA	P631	Q471	L411	S350	Q280	C214	V153	A92
Y928	Y928	L722	V655	F723	V655	ASP	SS32	S472	T412	E352	F281	S215	G154	T93
V929	V929	W724	P658	W724	P658	THR	T533	F473	K413	S353	A282	D216	M155	G94
A930	A930	E725	S660	E725	S660	K595	V534	S474	L414	F354	T283	G217	F156	T95
G931	G931	Y794	V661	D726	V661	I596	V535	N475	L415	D355	L284	N218	S157	T96
X332	X332	T795	I662	C727	I662	O599	E536	P476	S416	P285	L284	Y219	D158	P97
K933	K933	T797	V663	K728	V663	L600	D537	T477	F418	P285	L284	N220	G159	Q98
V934	V934	T798	D664	L729	D664	N602	D539	C478	S419	Y286	T286	R221	K160	K99
D868	D868	K665	G665	L730	G665	E605	Y540	N487	V420	Y286	T286	R222	M161	L100
L935	L935	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	F101
P336	P336	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	R163	V102
D940	D940	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
M943	M943	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A946	A946	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
L951	L951	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S954	S954	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G957	G957	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
V958	V958	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
W960	W960	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T961	T961	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A962	A962	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G963	G963	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
L964	L964	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S965	S965	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
F967	F967	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A968	A968	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
P971	P971	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I976	I976	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
F977	F977	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Y978	Y978	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
R979	R979	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
L980	L980	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
N981	N981	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
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G984	G984	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I985	I985	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T986	T986	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Q987	Q987	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G988	G988	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
V989	V989	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
L990	L990	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I105	I105	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S106	S106	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Q107	Q107	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
D108	D108	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
V109	V109	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
K110	K110	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Q111	Q111	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
F112	F112	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A113	A113	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
M114	M114	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G115	G115	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
F116	F116	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
V117	V117	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
W118	W118	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
R119	R119	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I120	I120	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G121	G121	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
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I123	I123	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A124	A124	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
M125	M125	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S126	S126	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T127	T127	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G128	G128	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T129	T129	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
V130	V130	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I131	I131	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I132	I132	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S133	S133	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
P134	P134	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S135	S135	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T136	T136	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S137	S137	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A138	A138	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T139	T139	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I140	I140	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
R141	R141	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
K142	K142	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Y201	Y201	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T202	T202	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S203	S203	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
F204	F204	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
A205	A205	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T206	T206	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
I256	I256	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
T257	T257	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
Q258	Q258	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
N193	N193	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
P196	P196	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S197	S197	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
G198	G198	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
N199	N199	K665	G665	L730	G665	E605	Y541	N487	V420	Y286	T286	R222	G162	
S200</														

- Molecule 1: S protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0595	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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	0.58	6/9006 (0.1%)	0.81	29/12245 (0.2%)
1	B	0.51	1/9006 (0.0%)	0.80	24/12245 (0.2%)
1	C	0.51	1/9010 (0.0%)	0.78	22/12250 (0.2%)
All	All	0.53	8/27022 (0.0%)	0.80	75/36740 (0.2%)

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
1	A	0	20
1	B	0	20
1	C	0	19
All	All	0	59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	CYS	N-CA	-15.13	1.16	1.46
1	A	349	CYS	C-O	9.59	1.41	1.23
1	A	349	CYS	CB-SG	-8.35	1.68	1.82
1	A	696	MET	N-CA	6.67	1.59	1.46
1	A	59	PRO	N-CD	5.22	1.55	1.47

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	735	LEU	CA-CB-CG	11.61	142.00	115.30
1	B	735	LEU	CA-CB-CG	11.58	141.93	115.30
1	A	735	LEU	CA-CB-CG	11.51	141.78	115.30
1	A	349	CYS	O-C-N	-11.07	104.98	122.70
1	A	1040	LEU	CA-CB-CG	7.84	133.32	115.30

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	520	ALA	Mainchain
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	65	SER	Peptide
1	A	733	GLN	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	8806	0	8507	678	0
1	B	8806	0	8504	766	0
1	C	8810	0	8512	581	0
All	All	26422	0	25523	1686	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 33.

The worst 5 of 1686 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:339:CYS:SG	1:C:349:CYS:HB2	1.35	1.62
1:B:344:LEU:CD2	1:B:670:HIS:HB3	1.16	1.61
1:A:583:SER:HB2	1:A:609:TYR:CE1	1.37	1.60
1:C:335:ARG:HB3	1:C:354:PHE:CE2	1.34	1.60
1:B:344:LEU:HD22	1:B:670:HIS:CB	1.16	1.58

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	1128/1323 (85%)	964 (86%)	147 (13%)	17 (2%)	8	40
1	B	1128/1323 (85%)	965 (86%)	147 (13%)	16 (1%)	9	40
1	C	1128/1323 (85%)	966 (86%)	147 (13%)	15 (1%)	10	42
All	All	3384/3969 (85%)	2895 (86%)	441 (13%)	48 (1%)	12	40

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	SER
1	A	584	VAL
1	A	596	ILE
1	A	597	ALA
1	A	797	THR

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	973/1143 (85%)	919 (94%)	54 (6%)	18	42
1	B	973/1143 (85%)	923 (95%)	50 (5%)	20	44
1	C	974/1143 (85%)	924 (95%)	50 (5%)	20	44
All	All	2920/3429 (85%)	2766 (95%)	154 (5%)	21	43

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	352	GLU
1	C	870	ASN
1	C	458	VAL
1	C	555	VAL
1	C	1059	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	599	GLN
1	C	848	ASN
1	B	839	ASN
1	C	842	GLN
1	C	1028	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

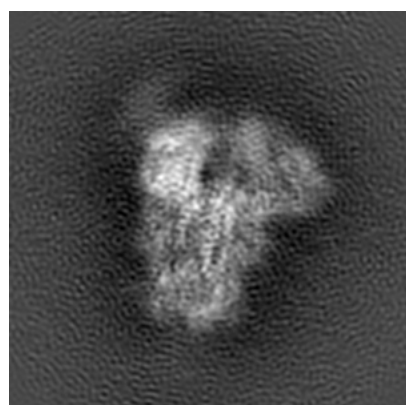
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6707. These allow visual inspection of the internal detail of the map and identification of artifacts.

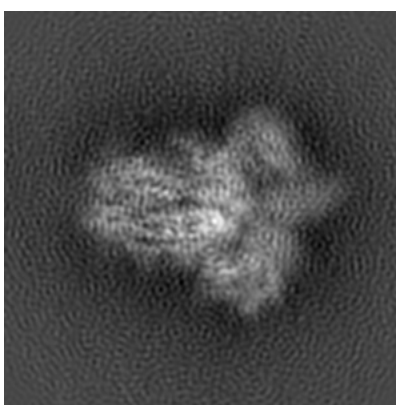
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

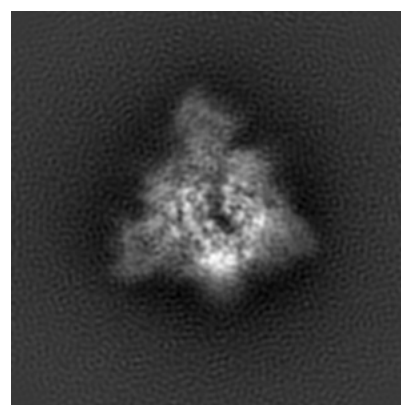
6.1.1 Primary map



X



Y

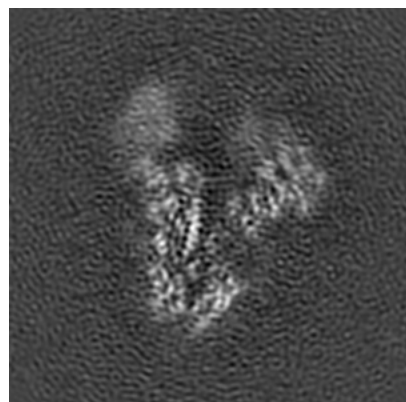


Z

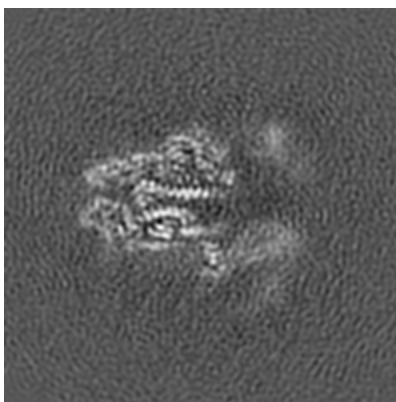
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

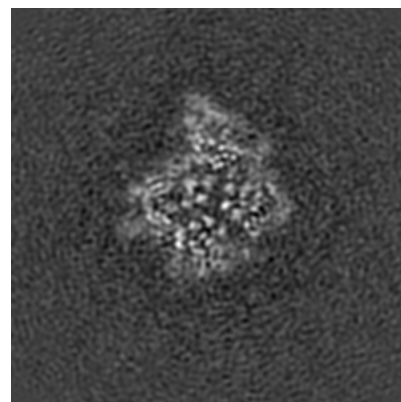
6.2.1 Primary map



X Index: 100



Y Index: 100

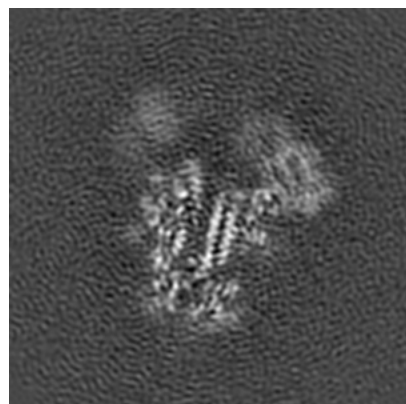


Z Index: 100

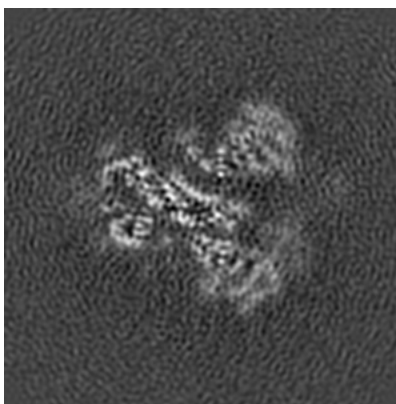
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

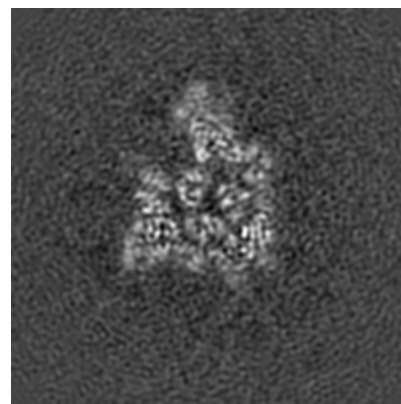
6.3.1 Primary map



X Index: 96



Y Index: 87

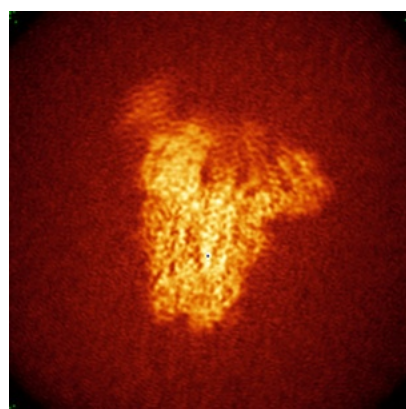


Z Index: 108

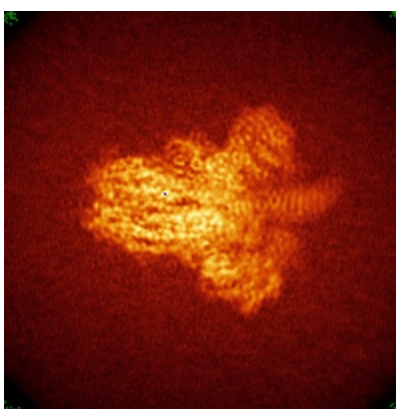
The images above show the largest variance slices of the map in three orthogonal directions.

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

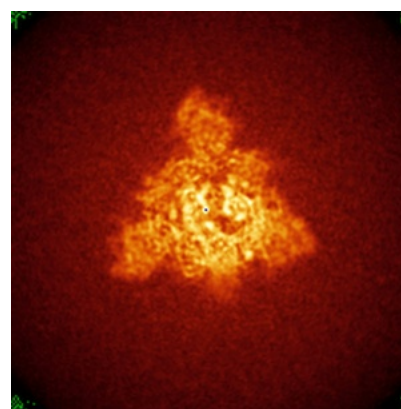
6.4.1 Primary map



X



Y

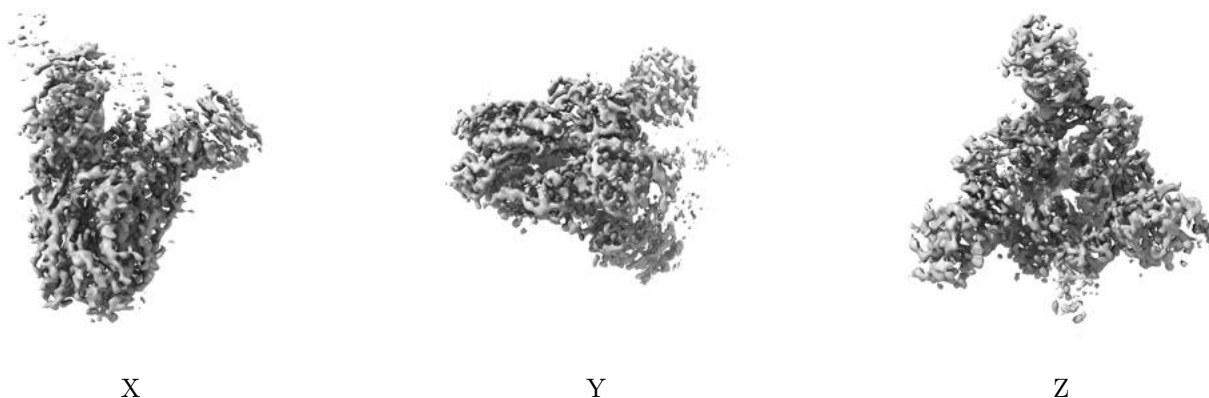


Z

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 0.0595. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

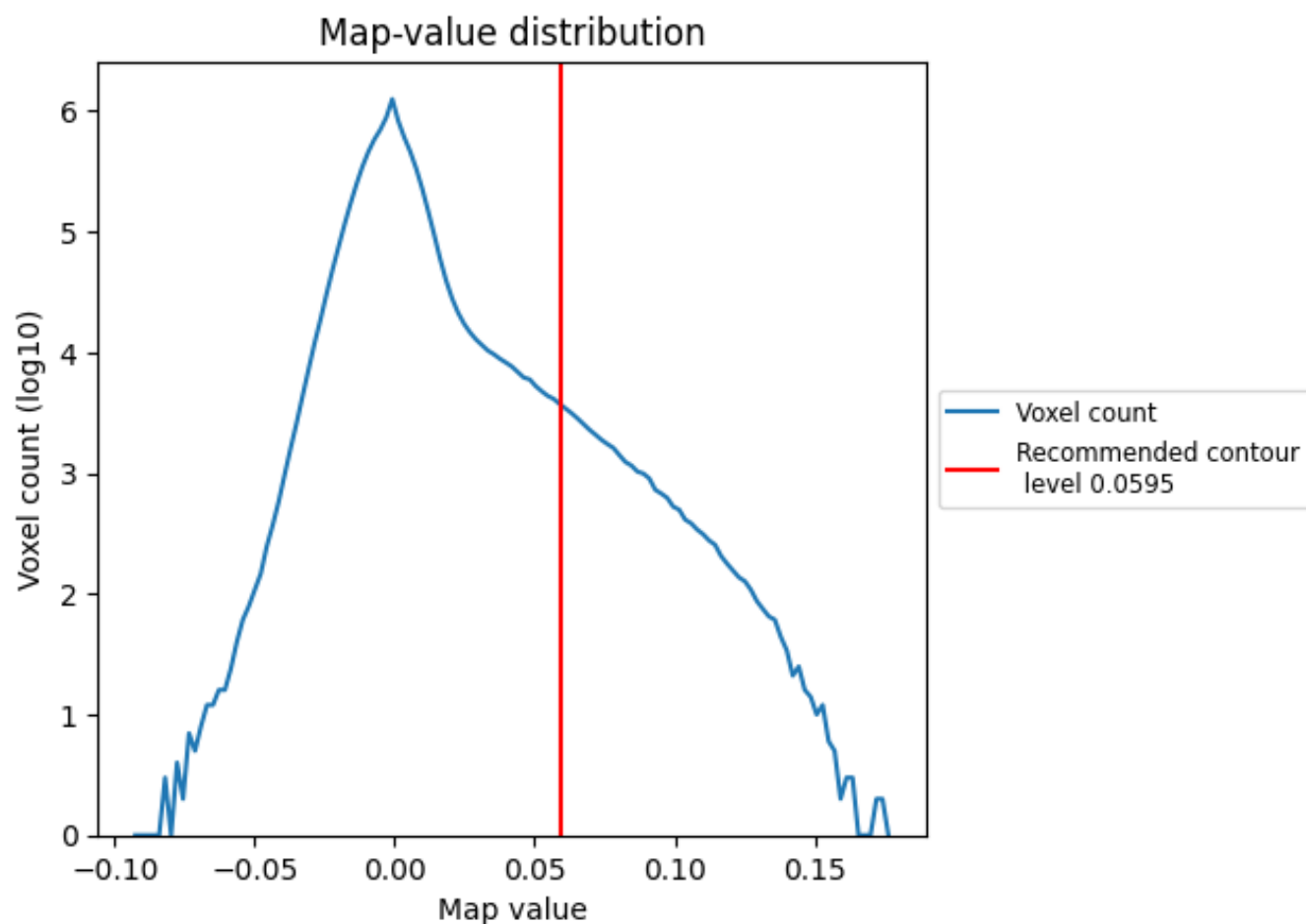
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

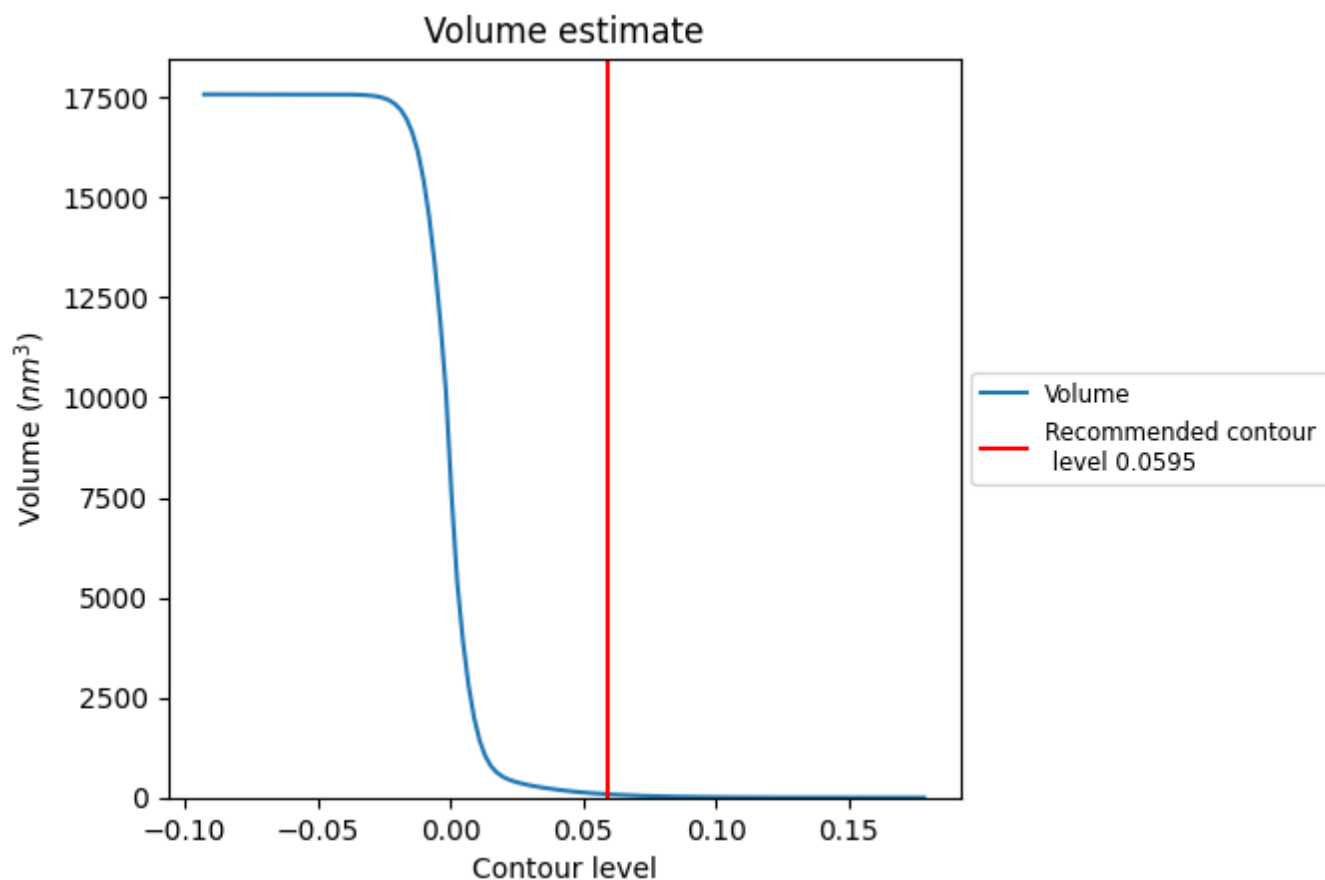
This section contains the results of statistical analysis of the map.

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.

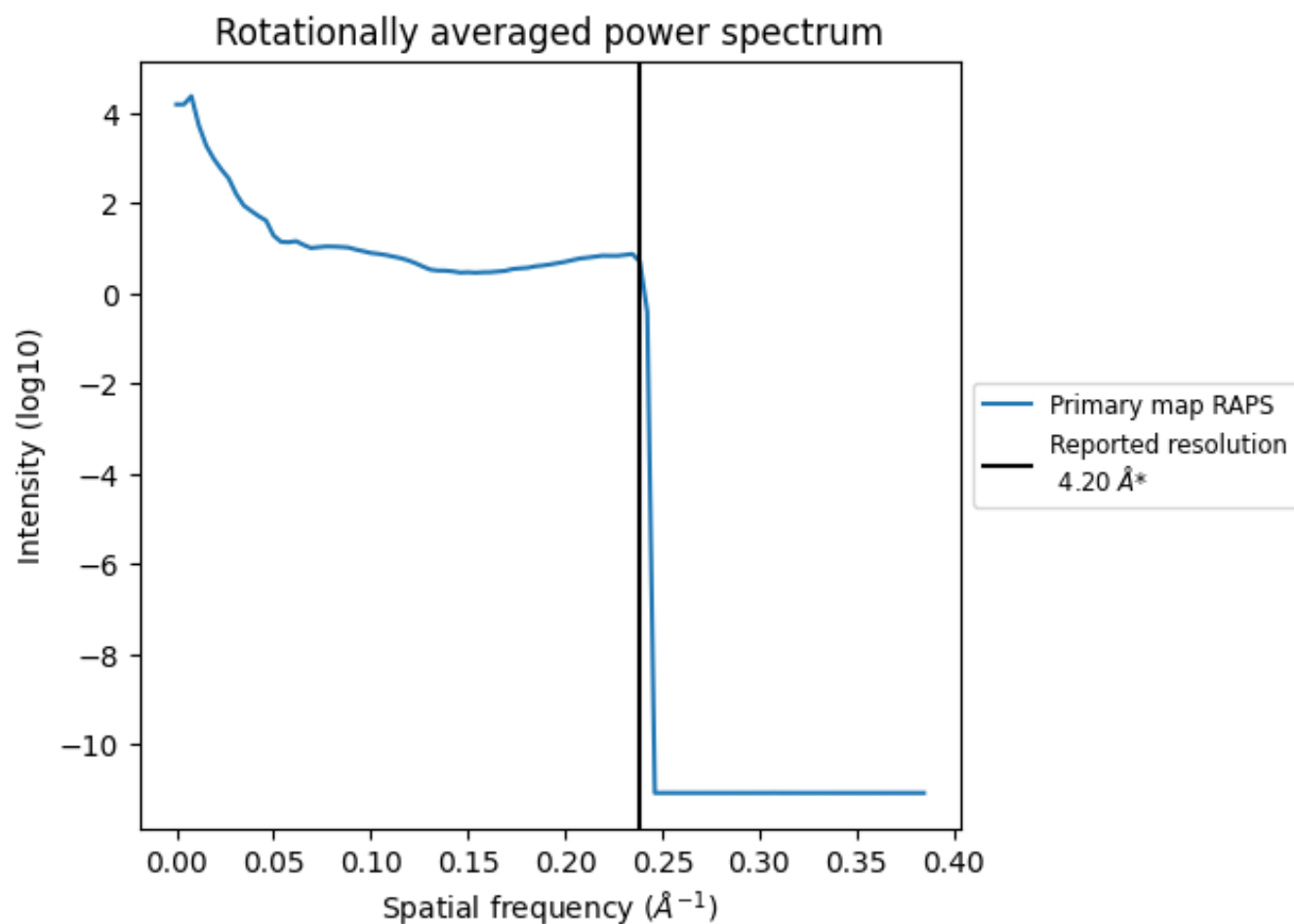
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 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 0.238 Å⁻¹

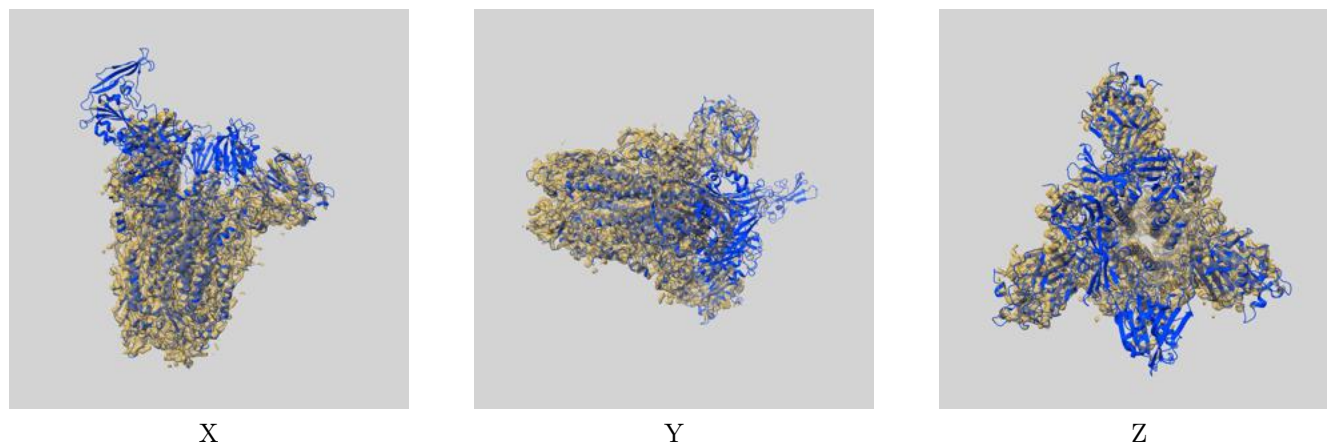
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

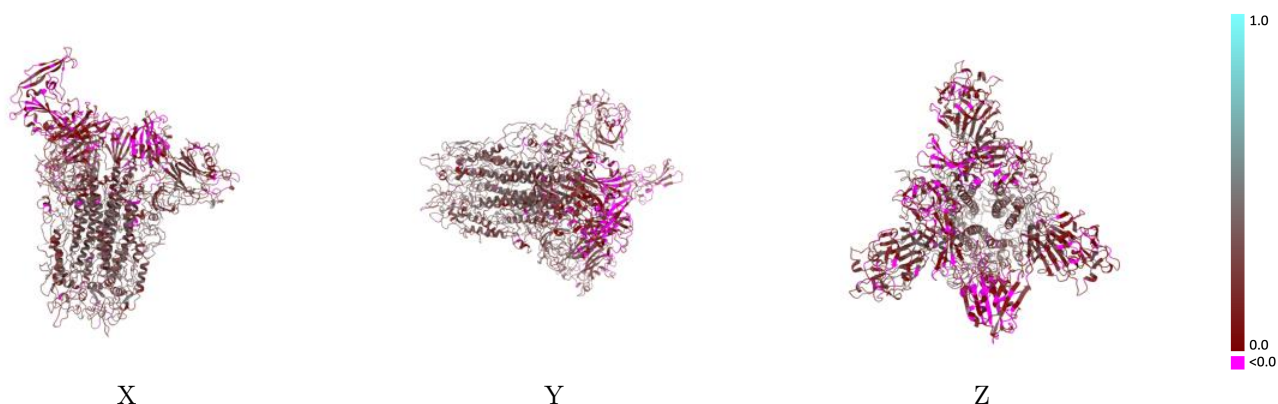
This section contains information regarding the fit between EMDB map EMD-6707 and PDB model 5X5F. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



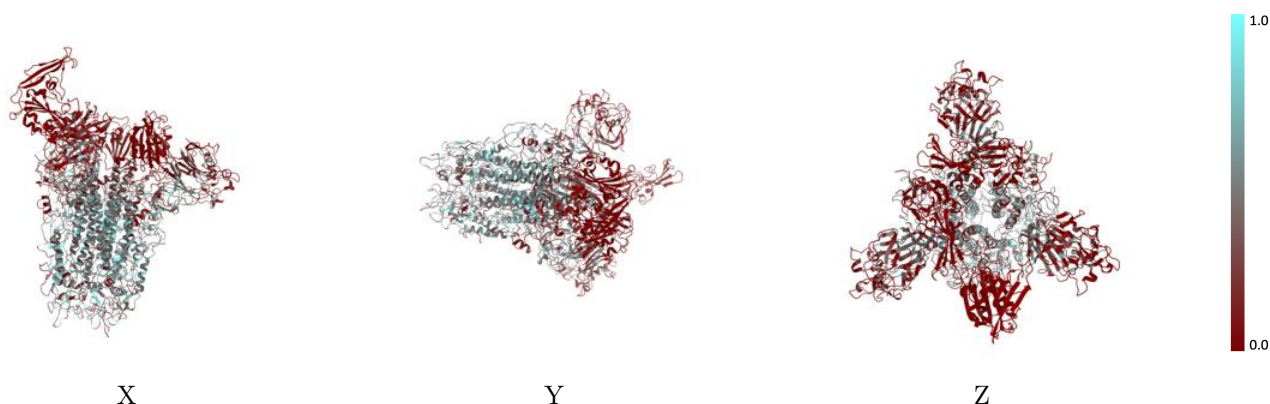
The images above show the 3D surface view of the map at the recommended contour level 0.0595 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



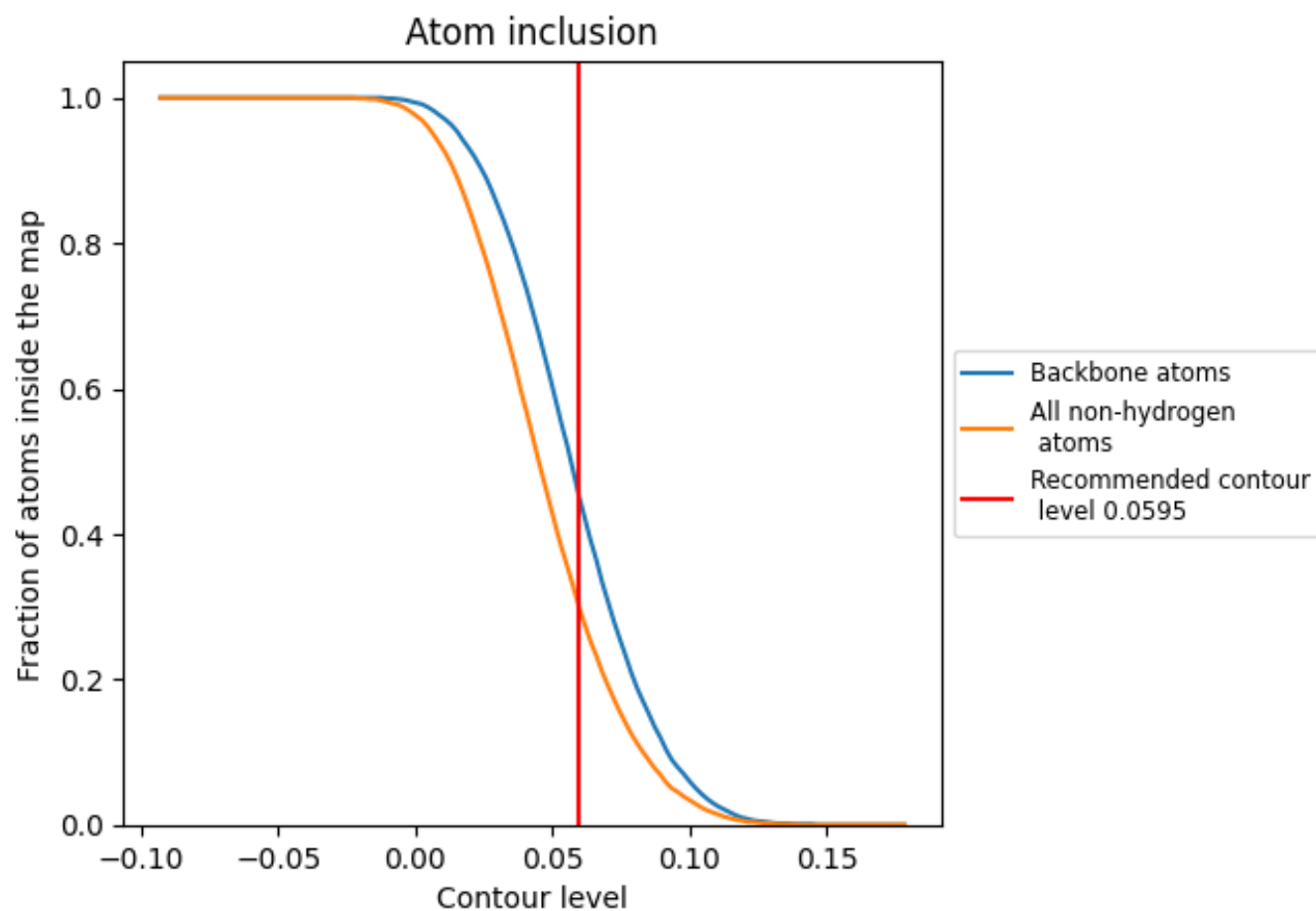
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0595).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 30% 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 (0.0595) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3050	<div></div> 0.2240
A	<div></div> 0.2890	<div></div> 0.2110
B	<div></div> 0.3180	<div></div> 0.2350
C	<div></div> 0.3090	<div></div> 0.2270

