



Full wwPDB EM Validation Report ⓘ

Jul 24, 2023 – 12:28 PM JST

PDB ID : 7DZY
EMDB ID : EMD-30921
Title : Spike protein from SARS-CoV2 with Fab fragment of enhancing antibody 2490
Authors : Liu, Y.; Soh, W.T.; Li, S.; Kishikawa, J.; Hirose, M.; Kato, T.; Standley, D.;
Okada, M.; Arase, H.
Deposited on : 2021-01-26
Resolution : 3.60 Å (reported)
Based on initial models : 7KEW, 5K8M

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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

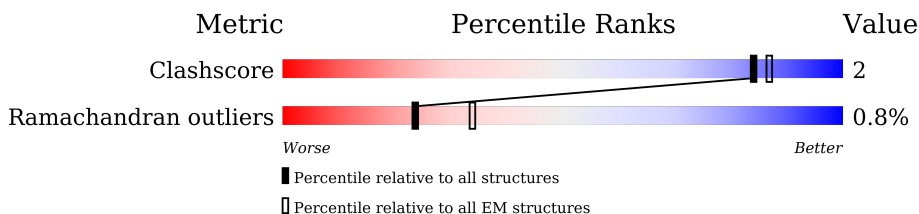
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	1249	68% 88% 10%
1	B	1249	73% 88% 10%
1	C	1249	71% 88% 10%
2	H	225	100% 99%
2	M	225	100% 99%
2	O	225	100% 99%
3	L	266	80% 80% 20%
3	N	266	80% 80% 20%
3	P	266	80% 80% 20%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 18708 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
			Total	C	N	O		
1	A	1121	4484	2242	1121	1121	0	0
1	B	1121	4484	2242	1121	1121	0	0
1	C	1121	4484	2242	1121	1121	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLN	-	expression tag	UNP P0DTC2
A	15	CYS	-	expression tag	UNP P0DTC2
A	16	VAL	-	expression tag	UNP P0DTC2
A	17	ASN	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	THR	-	expression tag	UNP P0DTC2
A	20	THR	-	expression tag	UNP P0DTC2
A	21	ARG	-	expression tag	UNP P0DTC2
A	22	THR	-	expression tag	UNP P0DTC2
A	23	GLN	-	expression tag	UNP P0DTC2
A	24	LEU	-	expression tag	UNP P0DTC2
A	25	PRO	-	expression tag	UNP P0DTC2
A	26	PRO	-	expression tag	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	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
A	1258	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
B	14	GLN	-	expression tag	UNP P0DTC2
B	15	CYS	-	expression tag	UNP P0DTC2
B	16	VAL	-	expression tag	UNP P0DTC2
B	17	ASN	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	THR	-	expression tag	UNP P0DTC2
B	20	THR	-	expression tag	UNP P0DTC2
B	21	ARG	-	expression tag	UNP P0DTC2
B	22	THR	-	expression tag	UNP P0DTC2
B	23	GLN	-	expression tag	UNP P0DTC2
B	24	LEU	-	expression tag	UNP P0DTC2
B	25	PRO	-	expression tag	UNP P0DTC2
B	26	PRO	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	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
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
C	14	GLN	-	expression tag	UNP P0DTC2
C	15	CYS	-	expression tag	UNP P0DTC2
C	16	VAL	-	expression tag	UNP P0DTC2
C	17	ASN	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	THR	-	expression tag	UNP P0DTC2
C	20	THR	-	expression tag	UNP P0DTC2
C	21	ARG	-	expression tag	UNP P0DTC2
C	22	THR	-	expression tag	UNP P0DTC2
C	23	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	LEU	-	expression tag	UNP P0DTC2
C	25	PRO	-	expression tag	UNP P0DTC2
C	26	PRO	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab Heavy chain of enhancing antibody 2490.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	225	Total	C	N	O	0	0
			900	450	225	225		
2	M	225	Total	C	N	O	0	0
			900	450	225	225		
2	O	225	Total	C	N	O	0	0
			900	450	225	225		

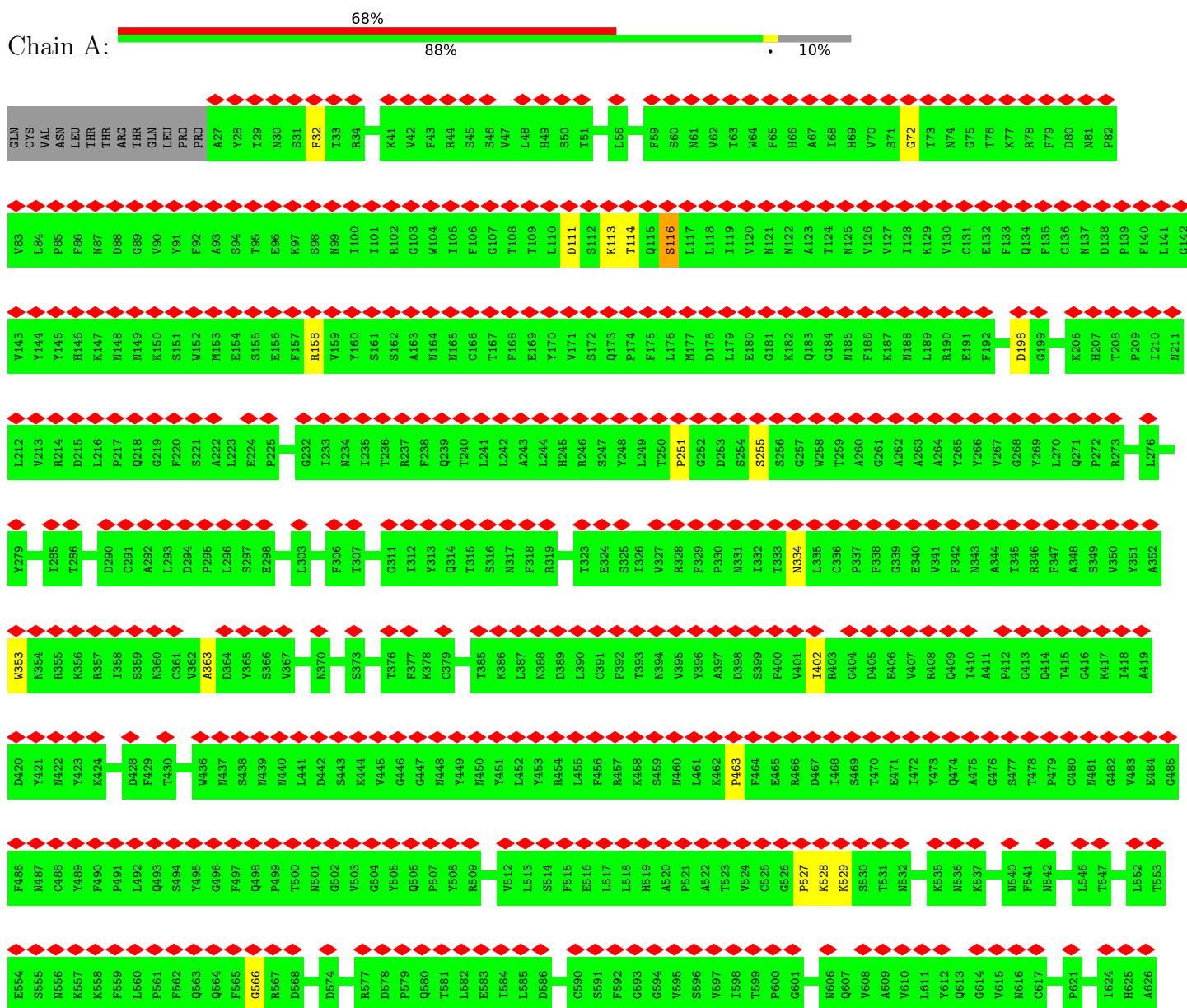
- Molecule 3 is a protein called Fab light chain of enhancing antibody 2490.

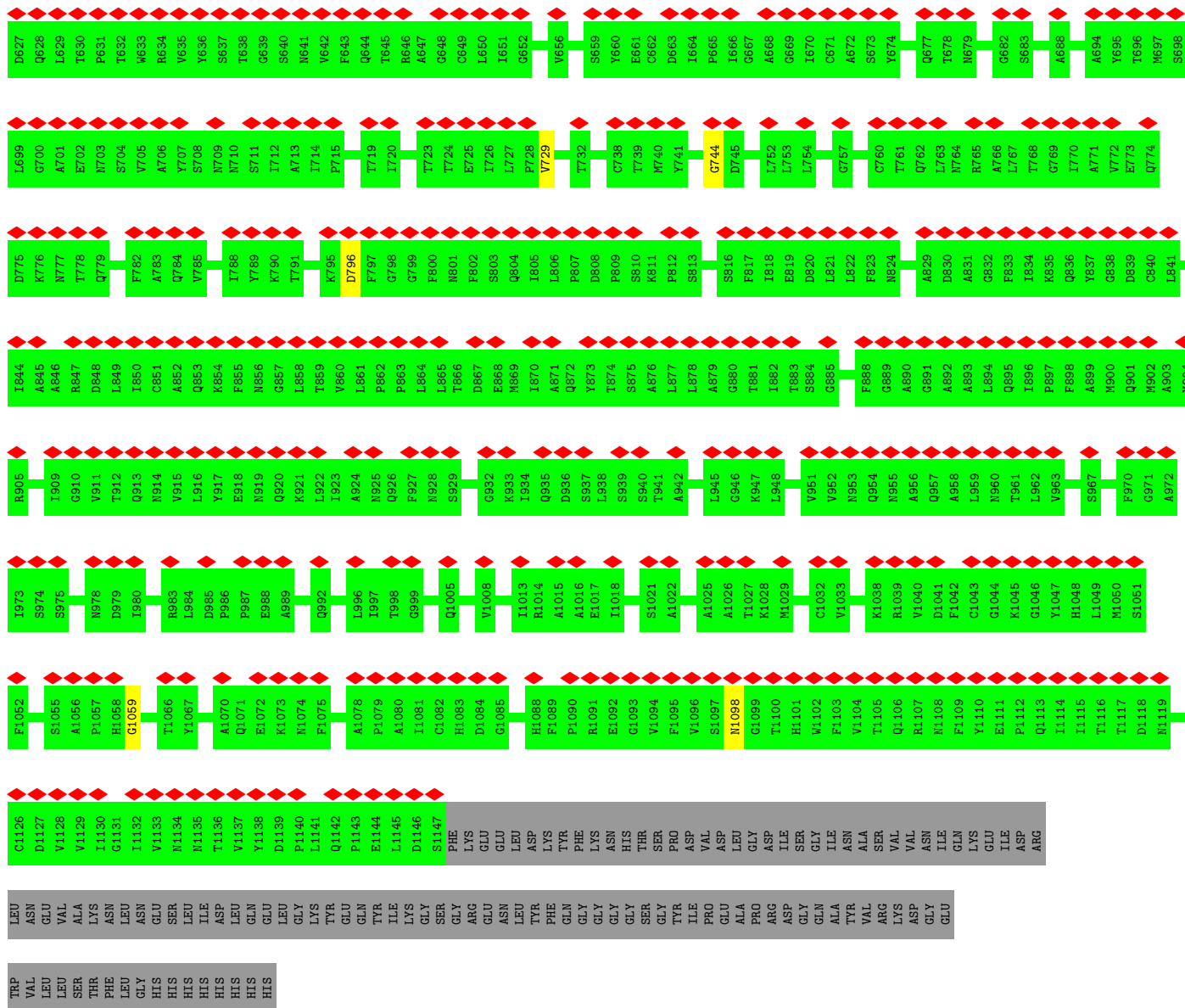
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	213	Total	C	N	O	0	0
			852	426	213	213		
3	N	213	Total	C	N	O	0	0
			852	426	213	213		
3	P	213	Total	C	N	O	0	0
			852	426	213	213		

3 Residue-property plots

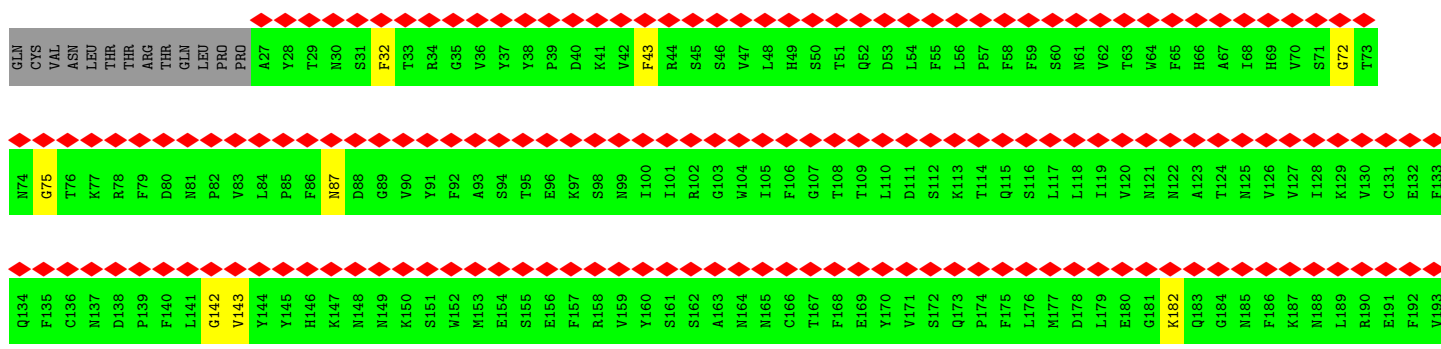
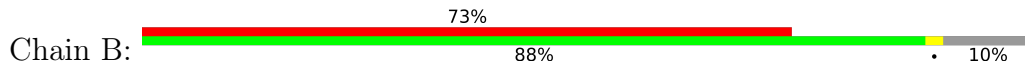
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

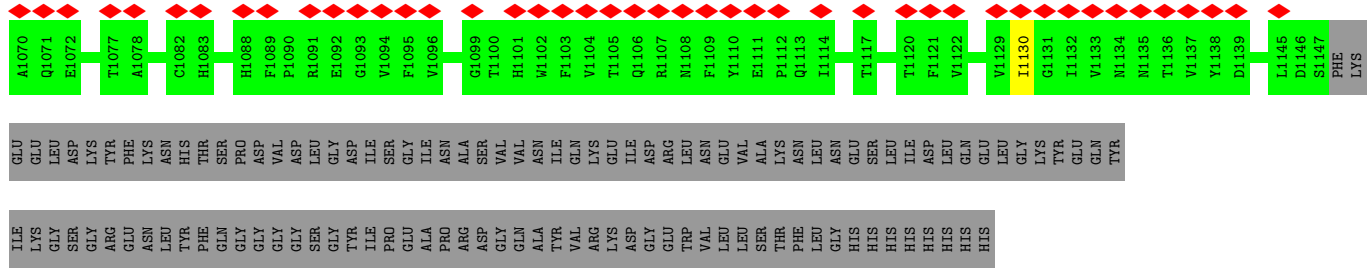




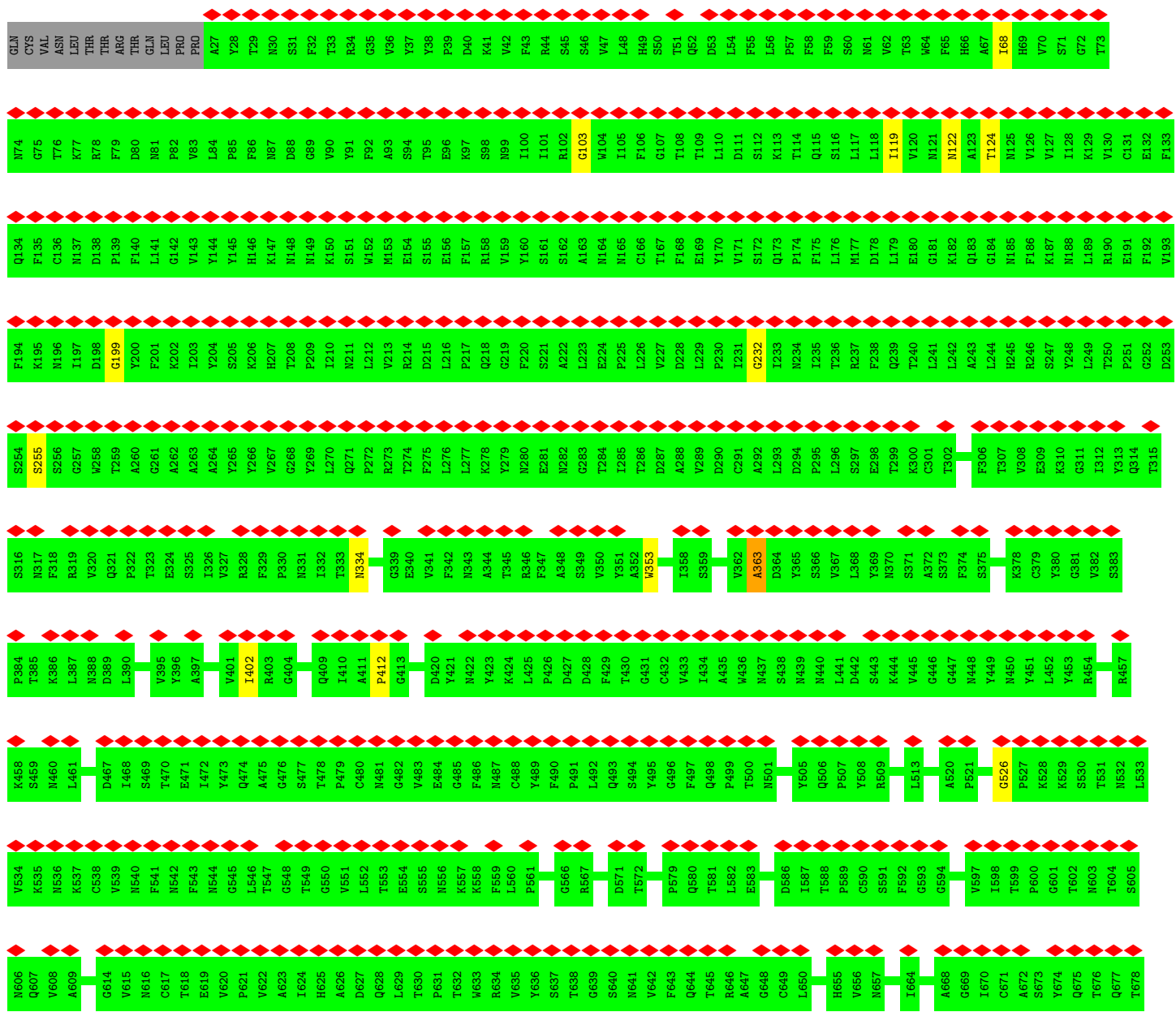
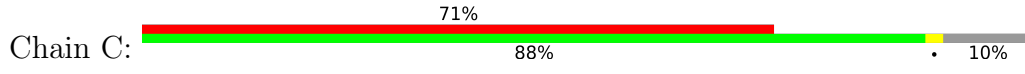
● Molecule 1: Spike glycoprotein

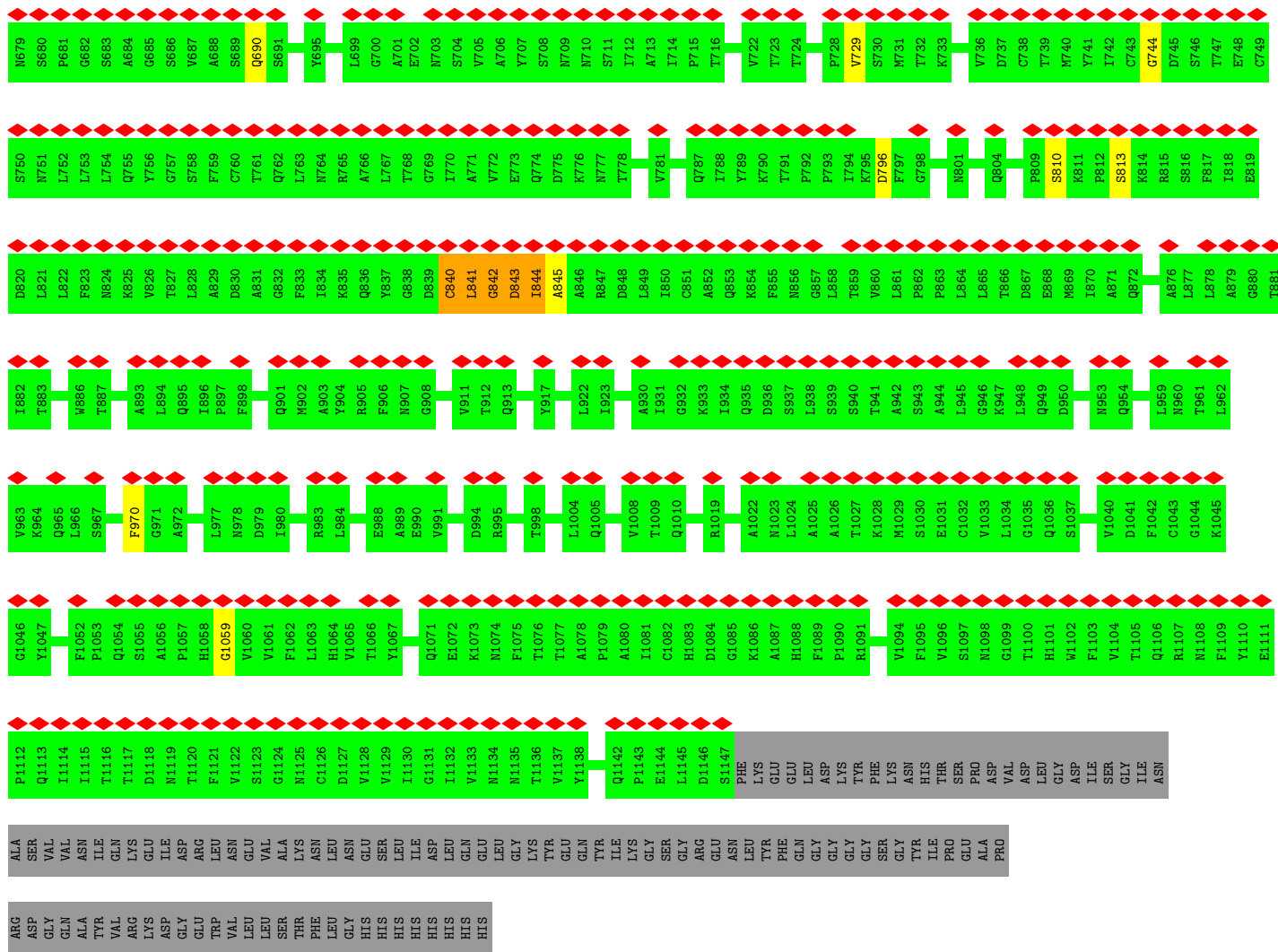


F194	K195	N196	I197	D198	G199	Y200	F201	A262	K202	I203	Y204	S205	K206	H207	T208	P209	I210	N211	V212	V213	R214	D215	L216	P217	Q218	G219	F220	S221	A222	L223	E224	P225	L226	V227	D228	L229	P230	I231	G232	I233	N234	I235	T236	R237	F238	Q239	T240	L241	L242	A243	L244	H245	R246	S247	Y248	L249	T250	P251	G252	D253
S254	S255	S256	G257	W258	T259	A260	G261	A262	N331	A263	A264	Y265	Y266	Y267	G268	Y269	L270	Q271	P272	R273	T274	N343	A344	L276	L277	K278	Y279	N280	E281	N282	G283	T284	I285	T286	D287	A288	V289	D290	C291	A292	L293	D294	P295	T296	S297	F298	T299	S305	I312	Y313	Q314	T315	S316	N317	F318	R319	V320	P321	P322	
T323	E324	S325	I326	R327	R328	F329	P330	N331	I332	T333	N334	L335	C336	P337	F338	G339	E340	V341	F342	R343	R403	A344	T345	R346	F347	A348	S349	V350	Y351	A352	W353	N354	R355	T356	R357	I358	S359	N360	C361	V362	A363	A364	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F374	S375	S376	F377	K378	C379	N380	G381	V382
S383	P384	T385	K386	L387	N388	D389	L390	C391	F392	T393	N394	Y395	Y396	A397	D398	S399	F400	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	A412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	N422	Y423	K424	L425	A426	D427	D428	F429	T430	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	
S443	K444	V445	G446	G447	N448	Y449	N450	Y451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	K462	F463	F464	E465	R466	D467	A468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485	F486	N487	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	
V503	G504	Y505	Q506	P507	Y508	R509	V510	V511	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540	F541	N542	F543	N544	G545	L546	T547	G548	T549	G550	V551	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	
Q563	Q564	F565	G566	R567	D568	L569	A570	D571	L572	T573	A574	A575	V576	R577	D578	P579	Q580	T581	L582	E583	L584	L585	D586	L587	T588	P589	C590	S591	F592	G593	G594	V595	S596	V597	G601	T602	N603	T604	S605	N606	Q607	V608	A609	V610	L611	V612	Q613	G614	V615	N616	C617	T618	S619	V620	P621	V622	L624			
H625	A626	D627	Q628	L629	T630	P631	T632	A633	R634	V635	V636	S637	T638	G639	S640	N641	V642	F643	Q644	T645	R646	A647	G648	C649	L650	L651	G652	A653	E654	H655	V656	N657	N658	S659	V660	E661	C662	A668	G669	L670	C671	A672	S673	V674	Q675	T676	Q677	N678	N679	S680	F681	G682	S683	A684	G685	S686	V687	A688		
S689	Q690	S691	T692	L693	A694	Y695	T696	H697	S698	L699	G700	A701	E702	S706	N709	N710	S711	L712	A713	L714	F715	G716	N717	F718	T719	L720	S721	V722	T723	L724	E725	L726	P727	Y729	S730	W731	V736	D737	C738	T739	W740	Y741	L742	D745	S746	N751	Q755	Y756	G757	S758	F759	C760	T761							
Q762	R765	A771	D775	F782	A783	Q784	V785	K786	Q787	L788	Y789	K790	T791	F792	F793	L794	K795	F796	G798	G799	F800	N801	F802	S803	Q804	L806	P807	D808	P809	S810	K811	F812	S813	K814	R815	S816	F817	D820	L821	L822	F823	N824	K825	V826	T827	L828	D830	A831	G838	D839										
C840	L841	G842	D843	I844	A845	A846	R847	Q853	R854	F855	N856	L861	P862	T866	I870	A871	T874	S875	A879	C880	T881	L882	T883	S884	F888	G889	Q890	A891	I896	P897	F898	A899	N902	A903	Y904	R905	F906	N907	G908	I909	G910	V911	T912	Q913	N914	Y915	L916	Y917	E918	N919										
Q920	K921	L922	I923	A924	N925	Q926	F927	N928	S929	A930	I931	G932	K933	D936	S937	L938	S939	S940	G946	K947	L948	Q949	D950	V951	V952	N953	Q954	A956	Q957	Q958	L959	V963	V964	L966	F967	S968	S975	N978	L981	P987	E990	V991	Q992	I993	D994	R995	L996	I997	T998	G999										
R1000	L1001	Q1002	S1003	L1004	Q1005	T1006	Y1007	V1008	T1009	Q1010	Q1011	L1012	I1013	R1014	A1015	A1016	E1017	I1018	R1019	A1020	S1021	A1022	N1023	A1026	T1027	E1031	C1032	V1033	L1034	G1035	Q1036	A958	S1037	K1038	R1039	V1040	D1041	F1042	C1043	G1044	K1045	G1046	Y1047	H1048	S1051	Q1054	G1059	L1063	H1064	V1065	T1066	Y1067	V1068	P1069						

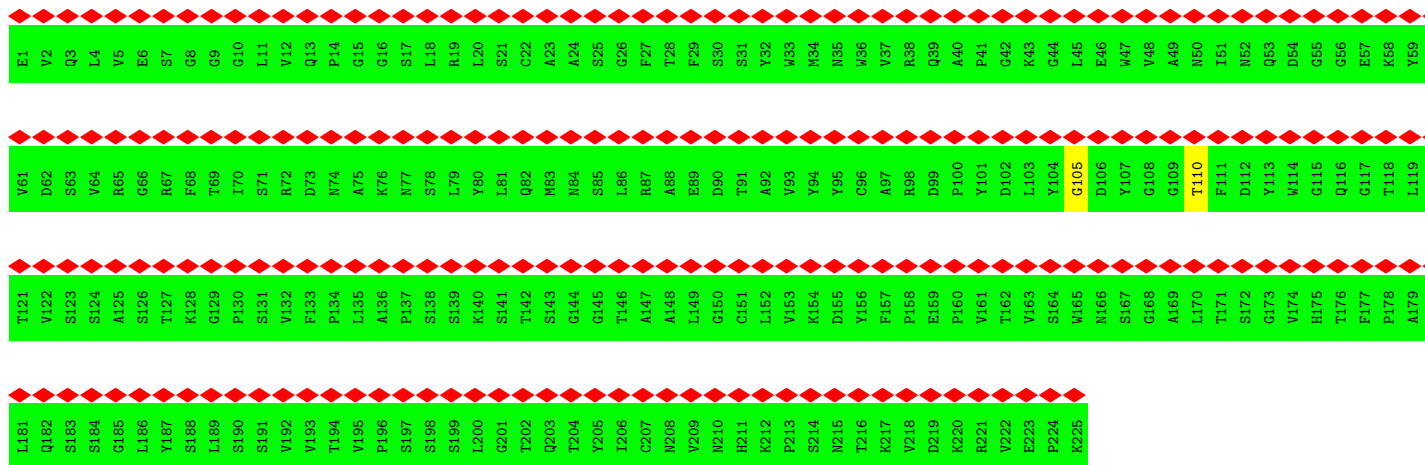


• Molecule 1: Spike glycoprotein

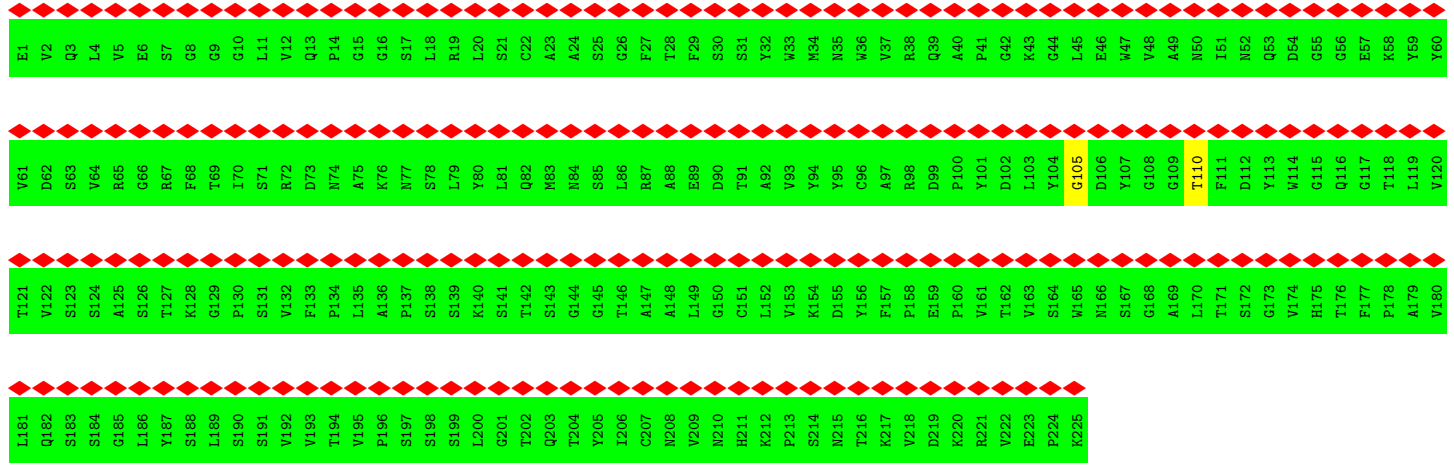




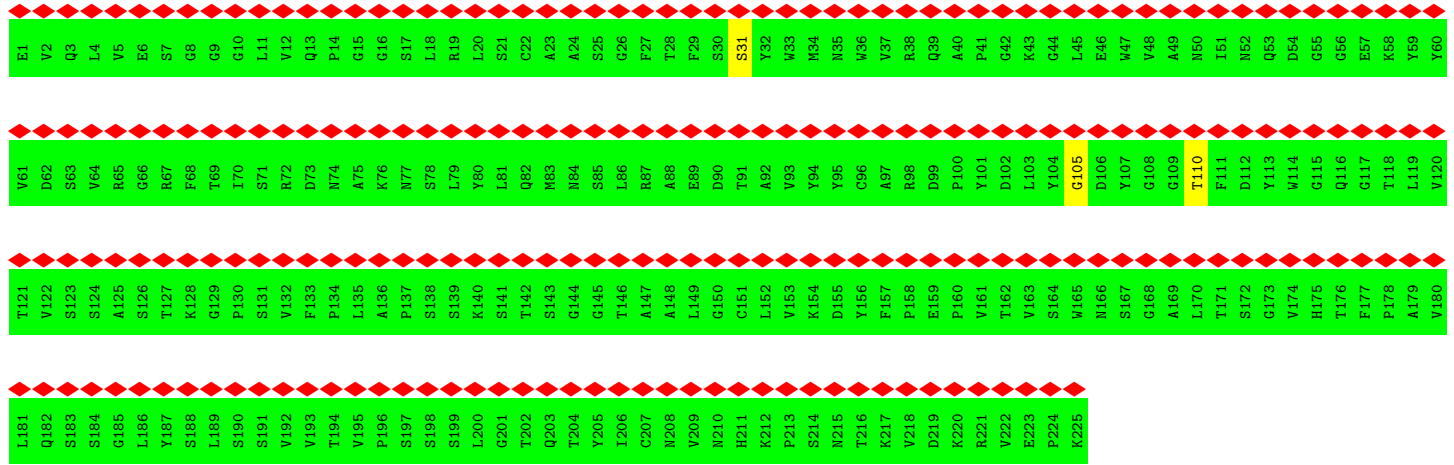
● Molecule 2: Fab Heavy chain of enhancing antibody 2490



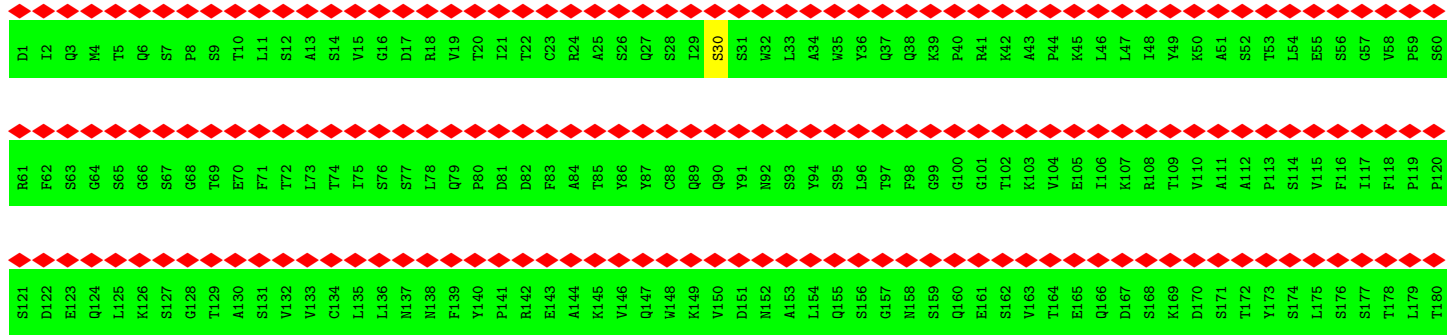
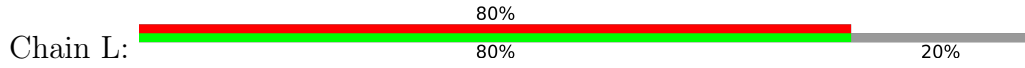
● Molecule 2: Fab Heavy chain of enhancing antibody 2490

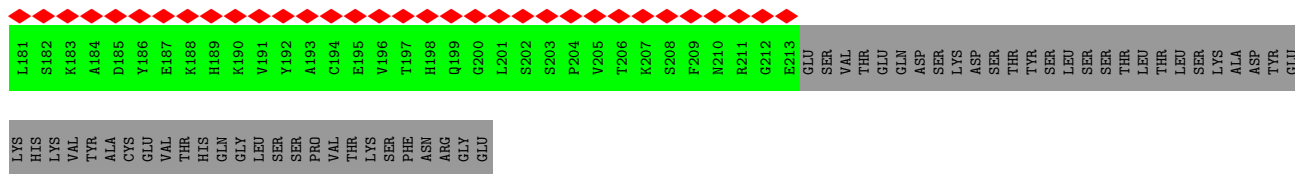


• Molecule 2: Fab Heavy chain of enhancing antibody 2490

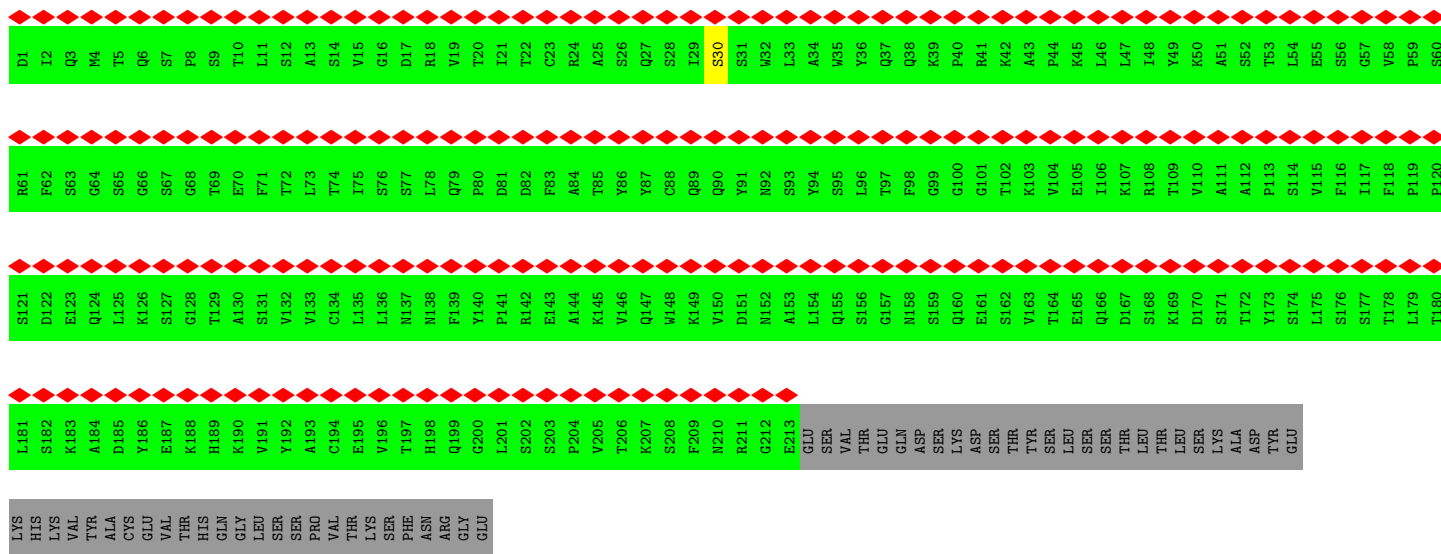


• Molecule 3: Fab light chain of enhancing antibody 2490

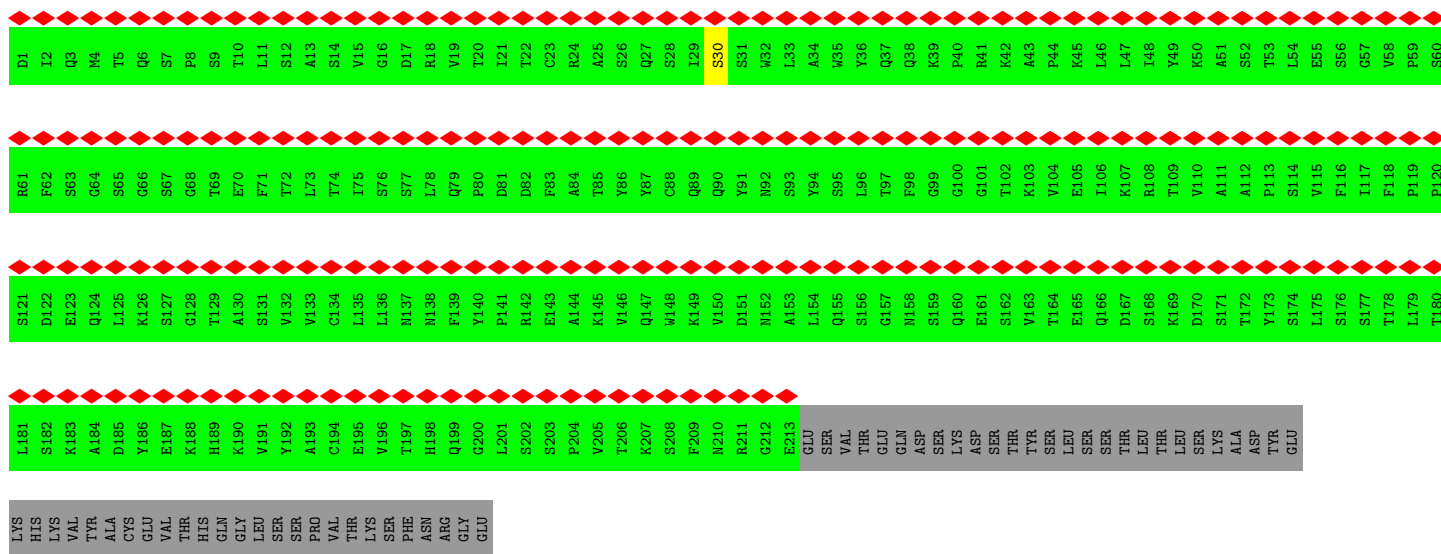




• Molecule 3: Fab light chain of enhancing antibody 2490



• Molecule 3: Fab light chain of enhancing antibody 2490



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131312	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.491	Depositor
Minimum map value	-0.623	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.18	Depositor
Map size (\AA)	334.4, 334.4, 334.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.92	0/4483	0.90	5/5602 (0.1%)
1	B	0.94	3/4483 (0.1%)	0.92	7/5602 (0.1%)
1	C	0.97	8/4483 (0.2%)	0.95	16/5602 (0.3%)
2	H	0.95	1/899 (0.1%)	0.88	0/1122
2	M	0.95	1/899 (0.1%)	0.88	0/1122
2	O	0.95	1/899 (0.1%)	0.88	0/1122
3	L	0.88	0/851	0.77	0/1062
3	N	0.88	0/851	0.77	0/1062
3	P	0.88	0/851	0.77	0/1062
All	All	0.94	14/18699 (0.1%)	0.90	28/23358 (0.1%)

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	B	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	841	LEU	N-CA	9.30	1.65	1.46
1	C	842	GLY	CA-C	8.08	1.64	1.51
1	C	843	ASP	CA-C	7.75	1.73	1.52
1	C	840	CYS	C-N	7.18	1.50	1.34
1	C	841	LEU	C-N	6.91	1.45	1.33
1	B	587	ILE	N-CA	6.72	1.59	1.46
2	H	105	GLY	CA-C	-6.21	1.42	1.51
2	O	105	GLY	CA-C	-6.17	1.42	1.51
2	M	105	GLY	CA-C	-6.17	1.42	1.51
1	C	841	LEU	CA-C	5.69	1.67	1.52
1	C	843	ASP	C-N	5.67	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	ASP	C-N	5.42	1.46	1.34
1	B	854	LYS	CA-C	-5.19	1.39	1.52
1	C	843	ASP	N-CA	5.18	1.56	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	ASP	C-N-CA	16.36	162.60	121.70
1	C	840	CYS	CA-C-O	-13.98	90.74	120.10
1	B	854	LYS	C-N-CA	-10.90	94.45	121.70
1	B	586	ASP	C-N-CA	9.82	146.26	121.70
1	C	843	ASP	C-N-CA	9.77	146.12	121.70
1	C	840	CYS	CA-C-N	9.48	138.05	117.20
1	C	841	LEU	C-N-CA	9.11	141.43	122.30
1	C	841	LEU	N-CA-C	8.38	133.63	111.00
1	C	840	CYS	C-N-CA	8.27	142.39	121.70
1	C	842	GLY	C-N-CA	7.99	141.68	121.70
1	A	251	PRO	N-CA-C	-7.67	92.14	112.10
1	C	843	ASP	N-CA-C	7.65	131.65	111.00
1	B	587	ILE	N-CA-C	6.69	129.06	111.00
1	B	574	ASP	N-CA-C	6.52	128.59	111.00
1	C	844	ILE	N-CA-C	6.16	127.62	111.00
1	A	198	ASP	C-N-CA	-6.11	109.47	122.30
1	A	1098	ASN	N-CA-C	-5.90	95.08	111.00
1	C	843	ASP	CA-C-N	5.85	130.07	117.20
1	C	970	PHE	O-C-N	-5.83	113.29	123.20
1	B	586	ASP	CA-C-O	-5.65	108.23	120.10
1	C	843	ASP	O-C-N	-5.55	113.81	122.70
1	C	840	CYS	O-C-N	5.32	131.21	122.70
1	A	363	ALA	C-N-CA	5.28	134.90	121.70
1	C	844	ILE	O-C-N	-5.23	114.33	122.70
1	A	527	PRO	C-N-CA	5.16	134.60	121.70
1	C	363	ALA	C-N-CA	5.13	134.54	121.70
1	B	742	ILE	C-N-CA	5.05	134.34	121.70
1	C	842	GLY	O-C-N	-5.05	114.61	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	853	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	4484	0	1220	7	0
1	B	4484	0	1219	41	0
1	C	4484	0	1220	37	0
2	H	900	0	263	0	0
2	M	900	0	263	0	0
2	O	900	0	263	2	0
3	L	852	0	229	0	0
3	N	852	0	229	0	0
3	P	852	0	229	0	0
All	All	18708	0	5135	54	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 2.

All (54) 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:B:587:ILE:CA	1:C:841:LEU:CA	2.55	0.84
1:B:575:ALA:N	1:C:844:ILE:N	2.28	0.81
1:B:182:LYS:O	1:B:261:GLY:HA3	1.82	0.79
1:B:199:GLY:O	1:B:232:GLY:HA2	1.85	0.75
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.57	0.69
1:A:72:GLY:H	2:O:31:SER:CA	2.06	0.69
1:B:575:ALA:N	1:C:844:ILE:H	1.92	0.68
1:B:142:GLY:HA2	1:B:244:LEU:N	2.11	0.65
1:B:729:VAL:H	1:B:1059:GLY:HA2	1.62	0.65
1:B:575:ALA:CA	1:C:844:ILE:H	2.10	0.64
1:B:575:ALA:N	1:C:843:ASP:N	2.44	0.64
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.79	0.63
1:B:587:ILE:N	1:C:840:CYS:O	2.32	0.63
1:B:587:ILE:CA	1:C:842:GLY:H	2.12	0.62
1:B:143:VAL:N	1:B:245:HIS:H	1.98	0.62
1:B:587:ILE:CA	1:C:842:GLY:N	2.62	0.61
1:C:363:ALA:O	1:C:526:GLY:HA2	2.00	0.61
1:B:143:VAL:C	1:B:245:HIS:H	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASP:C	1:C:845:ALA:H	2.06	0.58
1:B:575:ALA:N	1:C:843:ASP:CA	2.71	0.54
1:B:142:GLY:HA3	1:B:244:LEU:C	2.28	0.54
1:A:72:GLY:N	2:O:31:SER:CA	2.71	0.54
1:A:729:VAL:H	1:A:1059:GLY:HA2	1.71	0.54
1:B:574:ASP:O	1:B:587:ILE:N	2.36	0.54
1:B:574:ASP:N	1:C:843:ASP:CA	2.71	0.54
1:B:575:ALA:N	1:C:843:ASP:C	2.62	0.53
1:B:587:ILE:C	1:C:840:CYS:C	2.67	0.53
1:B:575:ALA:C	1:C:843:ASP:N	2.62	0.53
1:C:729:VAL:N	1:C:1059:GLY:HA2	2.25	0.52
1:B:575:ALA:C	1:C:843:ASP:H	2.14	0.51
1:C:199:GLY:CA	1:C:232:GLY:HA2	2.42	0.50
1:B:143:VAL:N	1:B:245:HIS:N	2.61	0.48
1:B:142:GLY:CA	1:B:244:LEU:N	2.78	0.47
1:A:114:THR:C	1:A:116:SER:H	2.18	0.47
1:B:588:THR:N	1:C:841:LEU:CA	2.78	0.47
1:B:586:ASP:O	1:C:841:LEU:N	2.47	0.46
1:B:574:ASP:CA	1:C:843:ASP:C	2.83	0.46
1:B:574:ASP:H	1:C:843:ASP:CA	2.29	0.45
1:A:566:GLY:HA2	1:B:43:PHE:O	2.18	0.44
1:B:575:ALA:CA	1:C:843:ASP:N	2.81	0.44
1:B:587:ILE:N	1:C:841:LEU:CA	2.81	0.43
1:B:588:THR:N	1:C:841:LEU:N	2.66	0.43
1:B:575:ALA:O	1:C:843:ASP:CA	2.66	0.43
1:B:575:ALA:N	1:C:842:GLY:C	2.72	0.43
1:B:587:ILE:N	1:C:842:GLY:N	2.66	0.43
1:B:587:ILE:CA	1:C:841:LEU:N	2.83	0.42
1:A:111:ASP:C	1:A:113:LYS:H	2.21	0.42
1:B:586:ASP:O	1:C:841:LEU:CA	2.68	0.42
1:A:729:VAL:N	1:A:1059:GLY:HA2	2.33	0.41
1:C:122:ASN:C	1:C:124:THR:H	2.23	0.41
1:B:587:ILE:N	1:C:841:LEU:C	2.74	0.41
1:B:574:ASP:H	1:C:843:ASP:C	2.24	0.41
1:B:586:ASP:C	1:C:841:LEU:C	2.80	0.41
1:C:103:GLY:HA3	1:C:119:ILE:O	2.21	0.41

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	1119/1249 (90%)	1064 (95%)	43 (4%)	12 (1%)	14	53
1	B	1119/1249 (90%)	1071 (96%)	39 (4%)	9 (1%)	19	59
1	C	1119/1249 (90%)	1050 (94%)	58 (5%)	11 (1%)	15	55
2	H	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
2	M	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
2	O	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
3	L	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
3	N	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
3	P	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
All	All	4659/5220 (89%)	4448 (96%)	173 (4%)	38 (1%)	24	59

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	463	PRO
1	A	528	LYS
1	A	529	LYS
1	A	796	ASP
1	B	571	ASP
1	B	854	LYS
1	C	353	TRP
1	C	796	ASP
1	C	810	SER
1	A	116	SER
1	A	334	ASN
1	A	744	GLY
1	B	796	ASP
1	B	1130	ILE
1	C	744	GLY

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Mol	Chain	Res	Type
1	B	87	ASN
1	C	334	ASN
1	C	402	ILE
1	C	412	PRO
1	C	690	GLN
2	H	110	THR
3	L	30	SER
2	M	110	THR
3	N	30	SER
2	O	110	THR
3	P	30	SER
1	A	158	ARG
1	A	353	TRP
1	B	32	PHE
1	B	333	THR
1	C	68	ILE
1	C	813	SER
1	B	72	GLY
1	A	32	PHE
1	C	255	SER
1	A	402	ILE
1	B	75	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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.

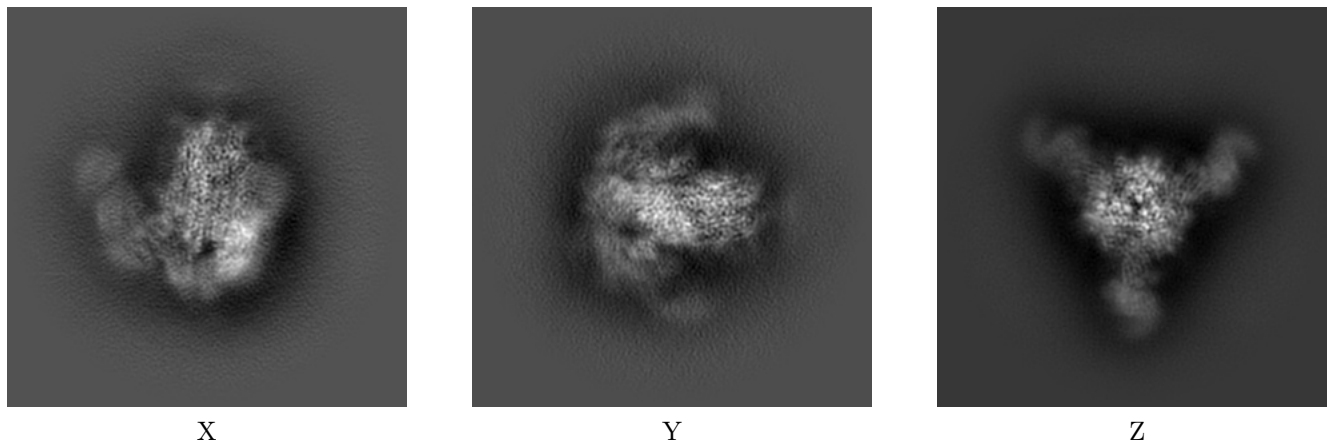
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30921. These allow visual inspection of the internal detail of the map and identification of artifacts.

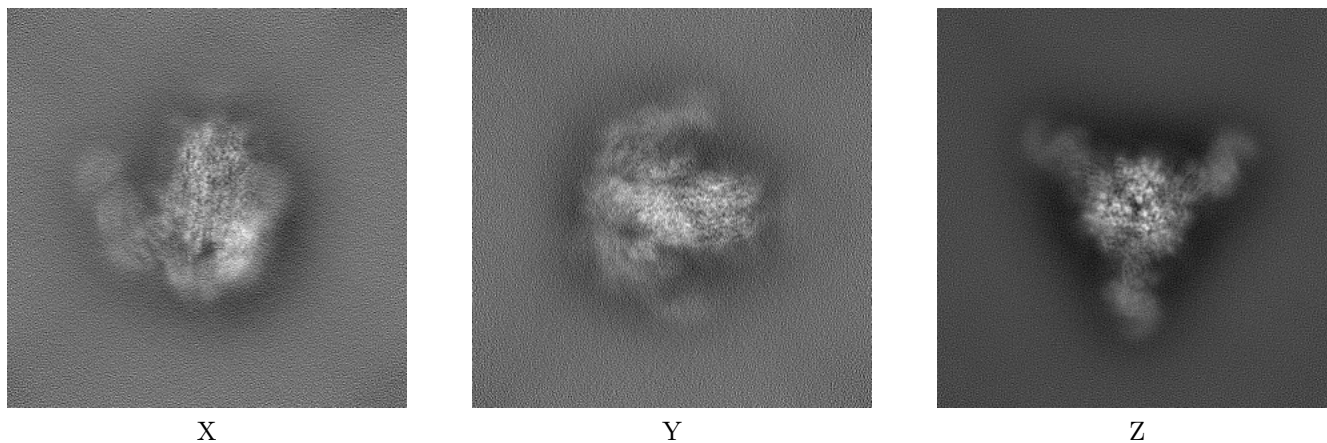
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



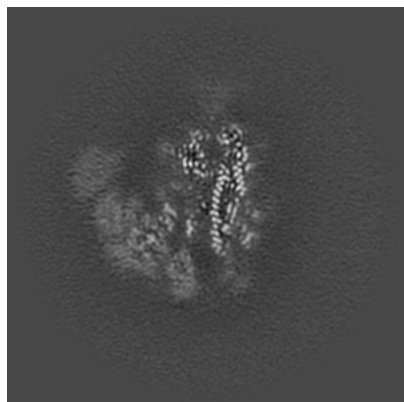
6.1.2 Raw map



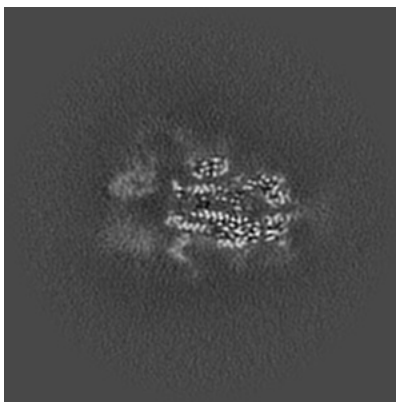
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

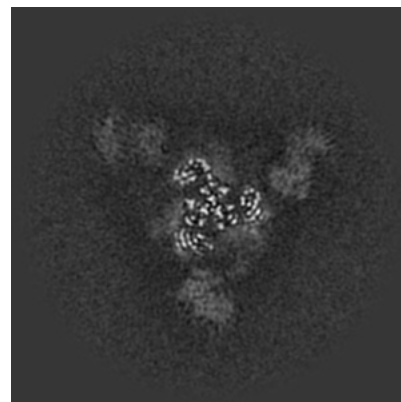
6.2.1 Primary map



X Index: 190

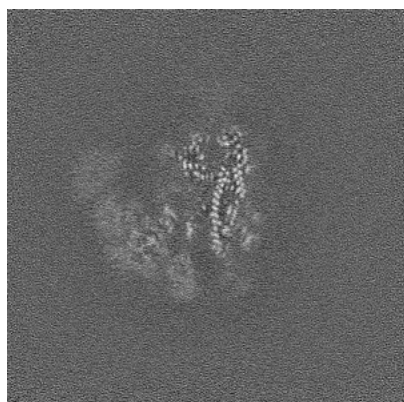


Y Index: 190

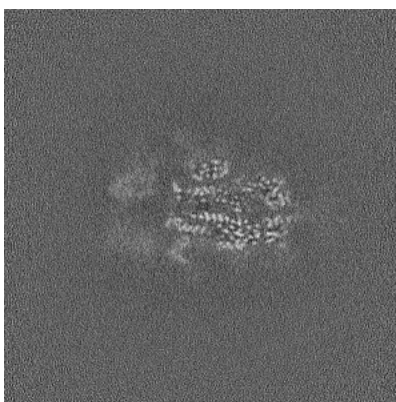


Z Index: 190

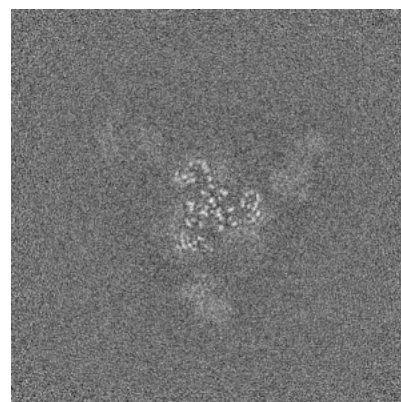
6.2.2 Raw map



X Index: 190



Y Index: 190

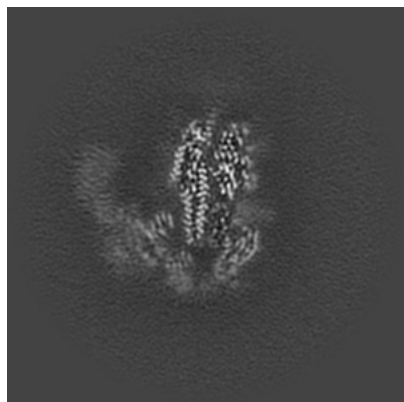


Z Index: 190

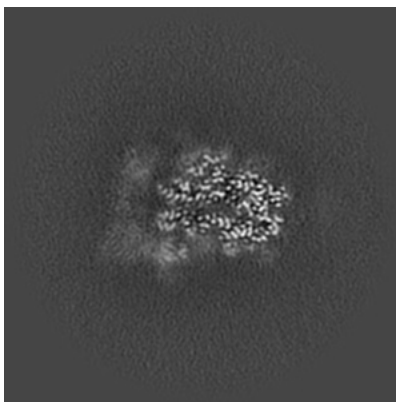
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

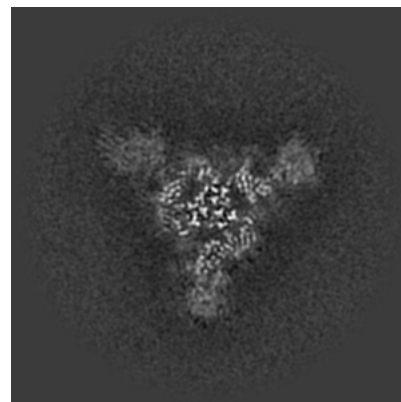
6.3.1 Primary map



X Index: 197

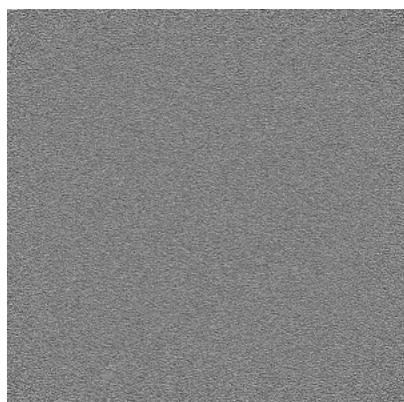


Y Index: 180

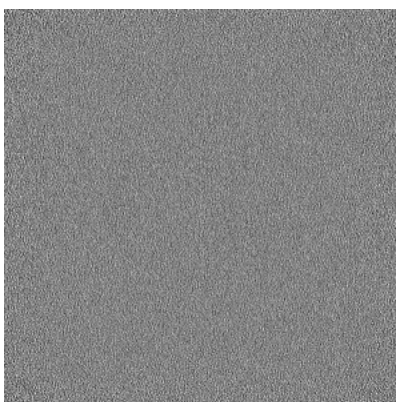


Z Index: 173

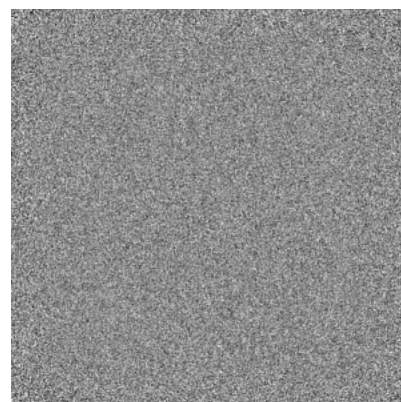
6.3.2 Raw map



X Index: 0



Y Index: 0

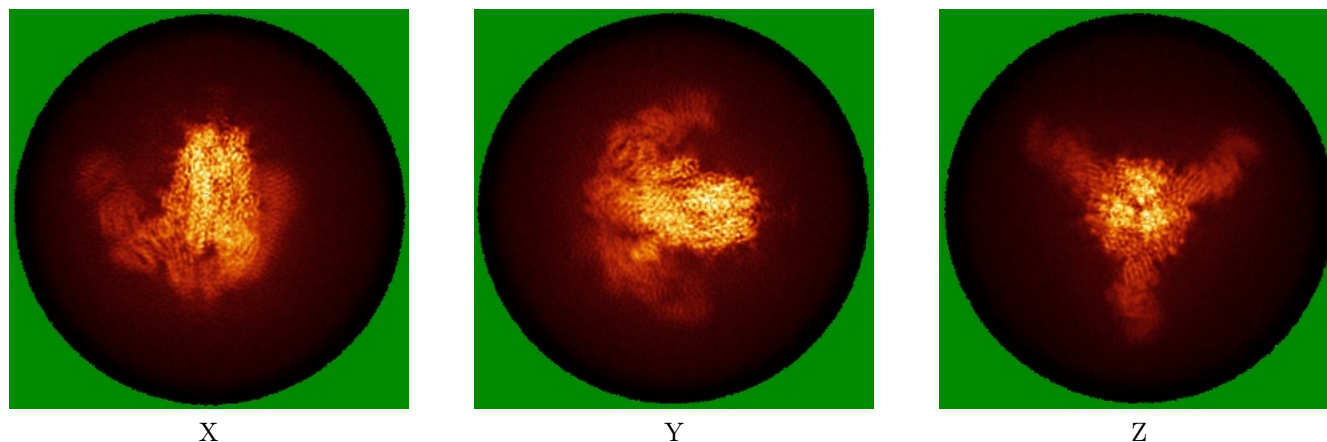


Z Index: 379

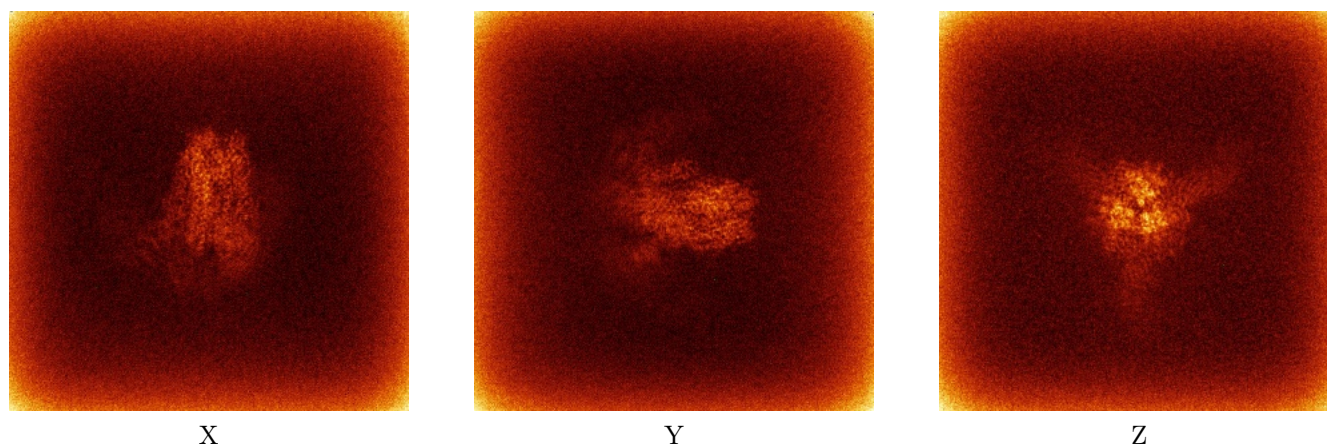
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



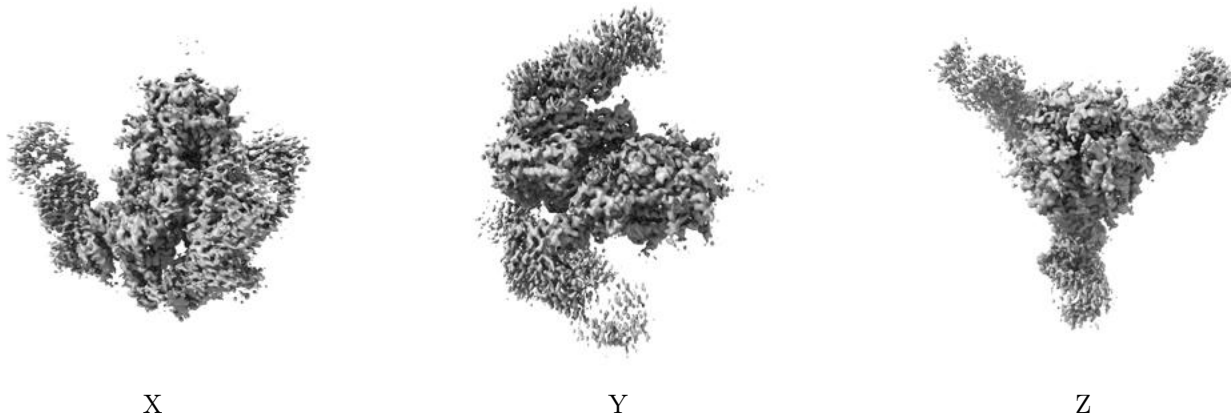
6.4.2 Raw map



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.

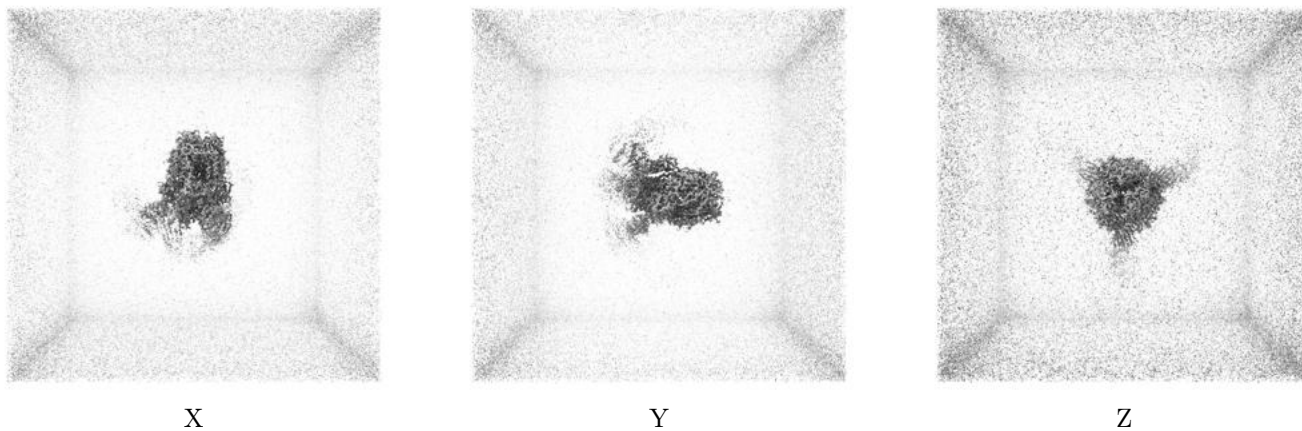
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

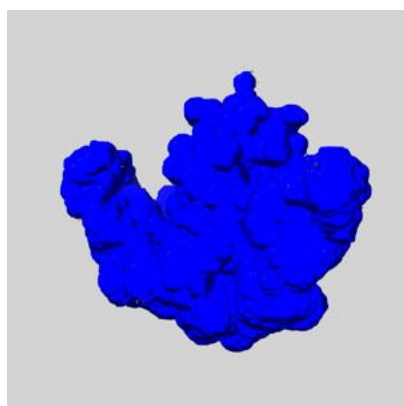
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

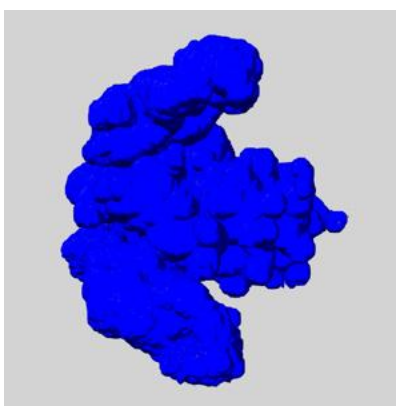
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

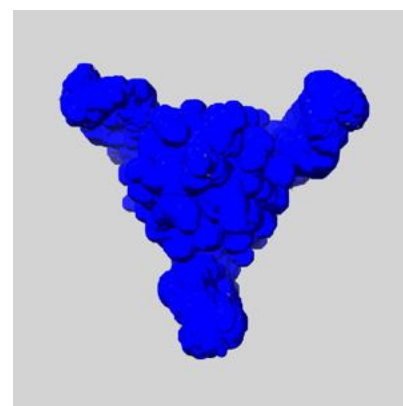
6.6.1 emd_30921_msk_1.map [i](#)



X



Y

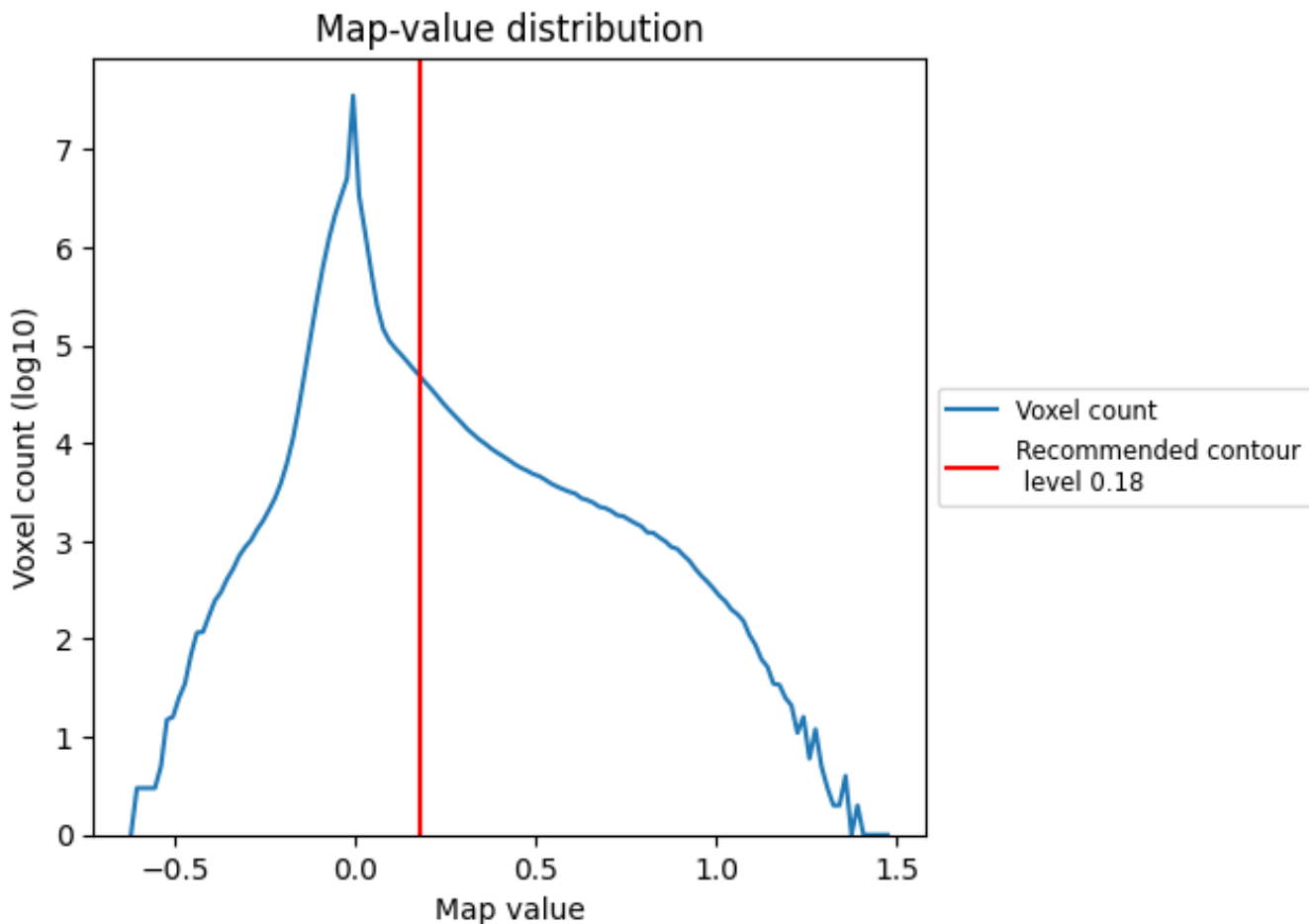


Z

7 Map analysis [i](#)

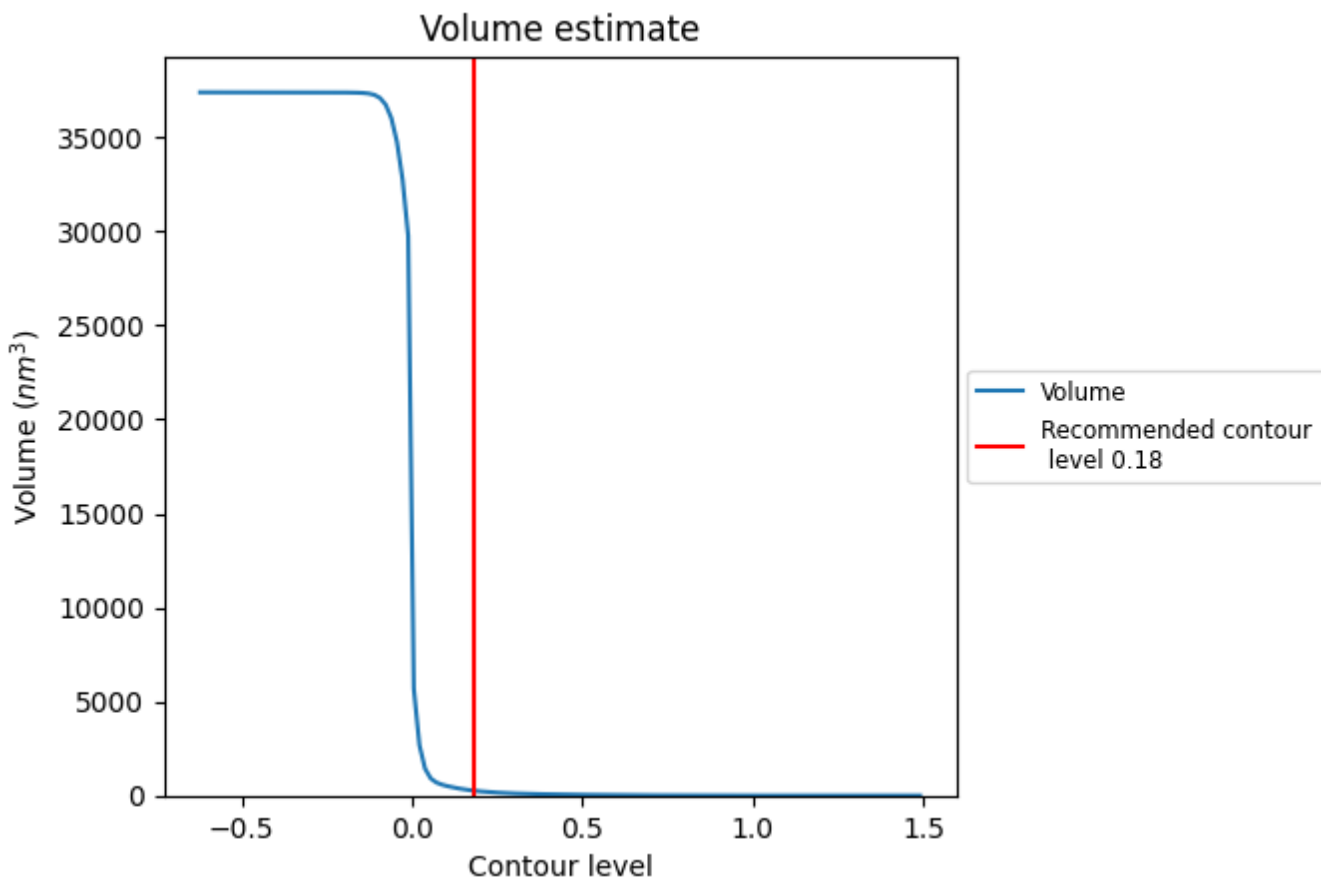
This section contains the results of statistical analysis of the map.

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.

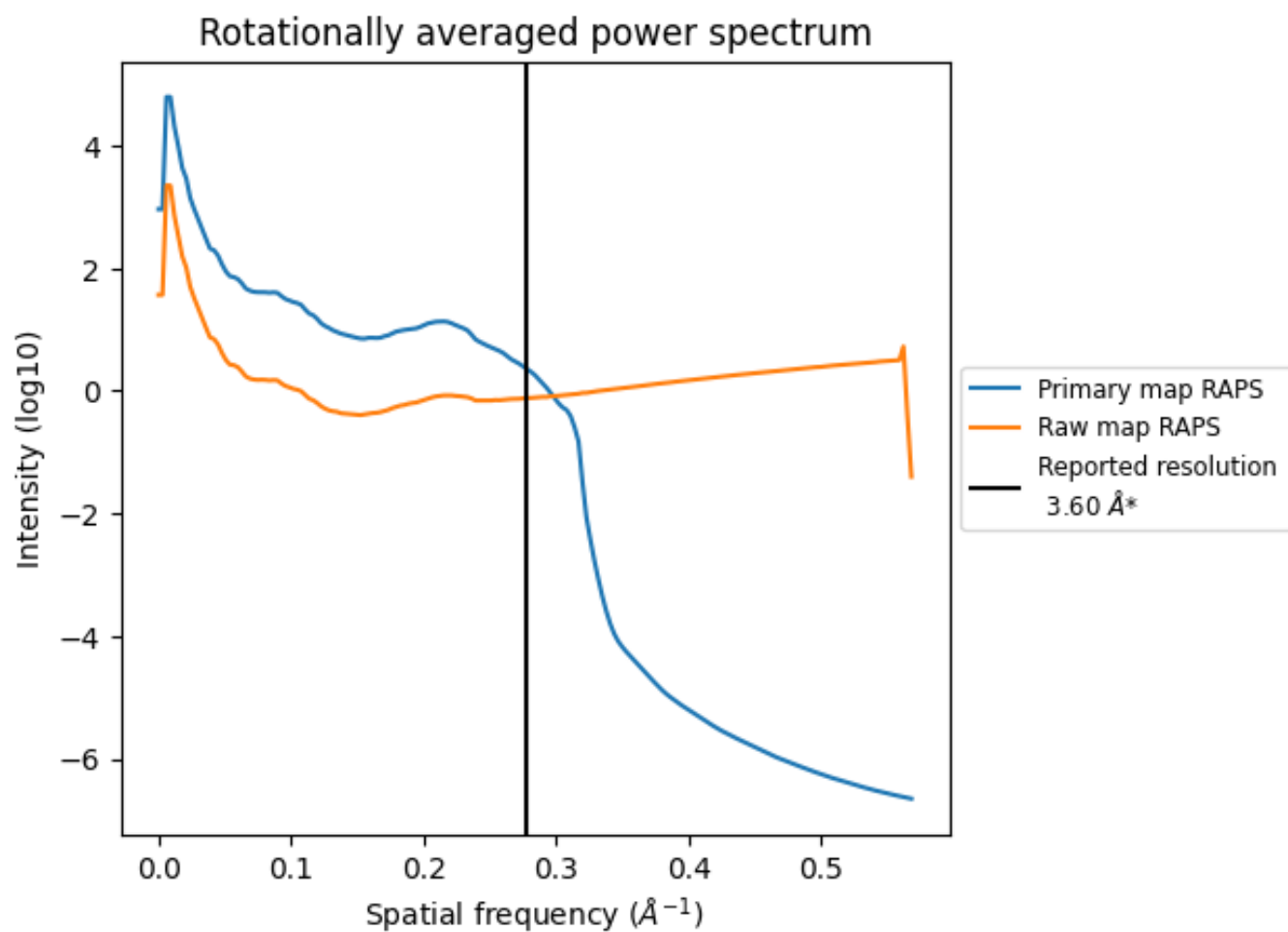
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm³; this corresponds to an approximate mass of 238 kDa.

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

7.3 Rotationally averaged power spectrum i

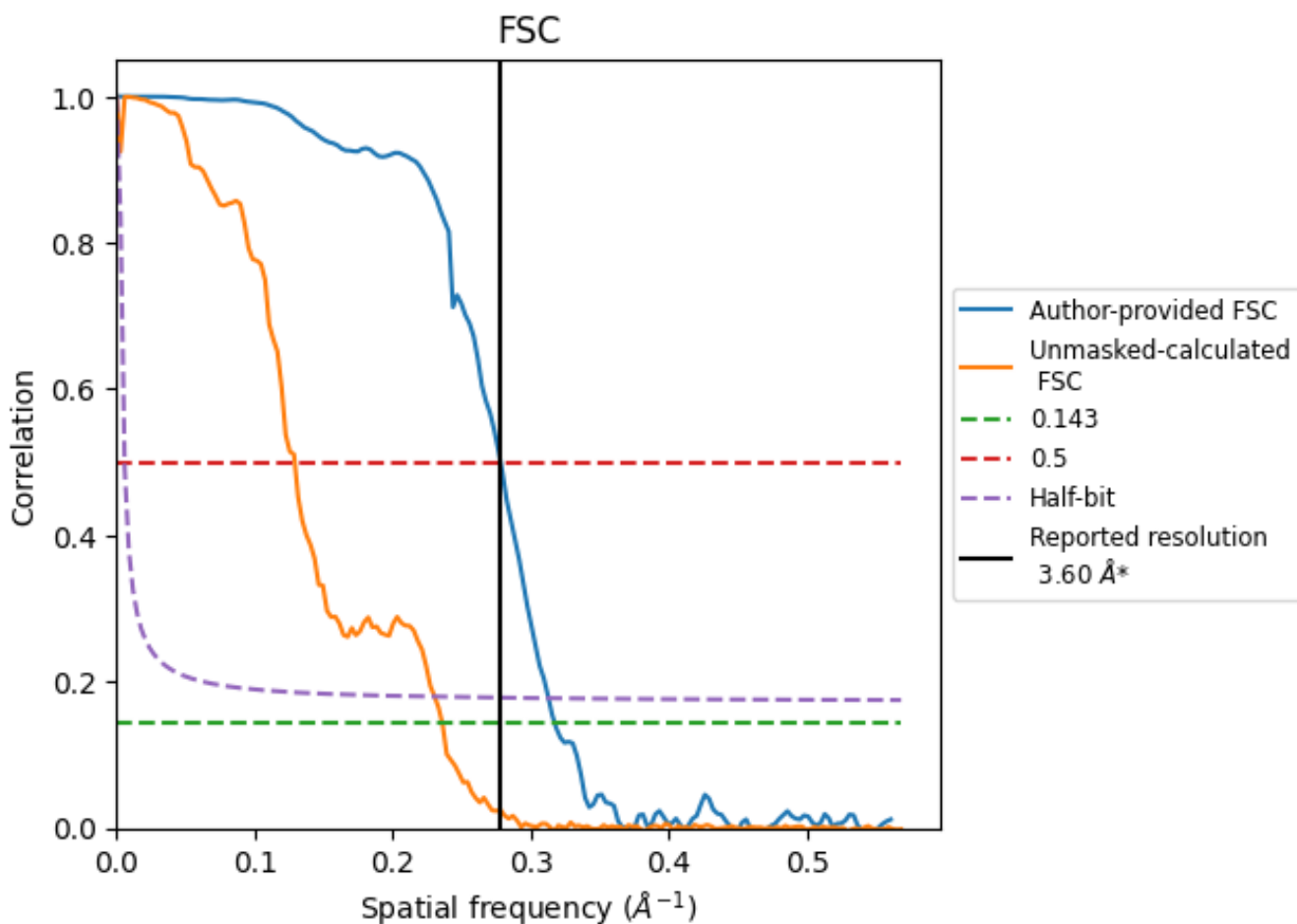


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278\AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.15	3.59	3.20
Unmasked-calculated*	4.24	7.75	4.34

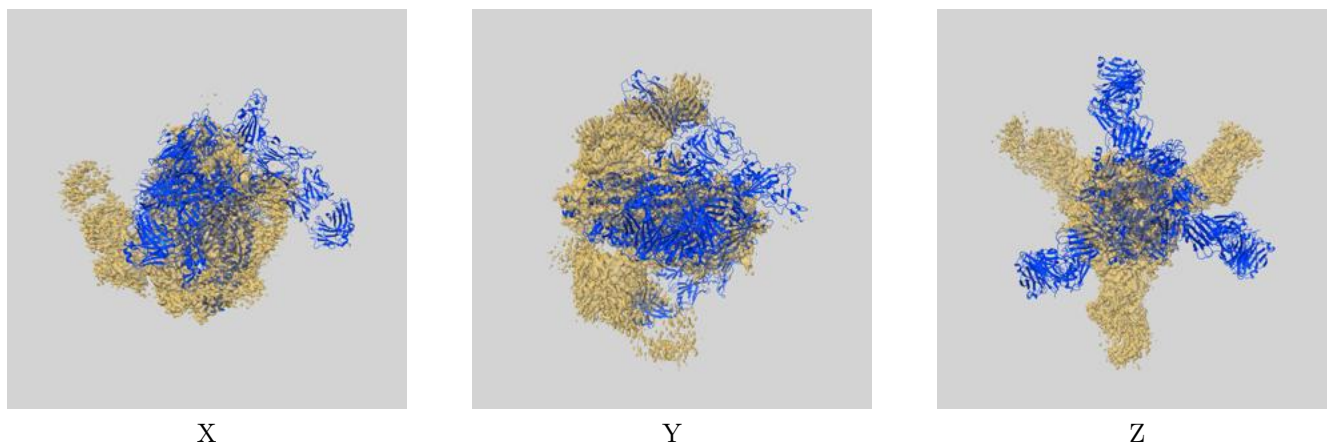
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

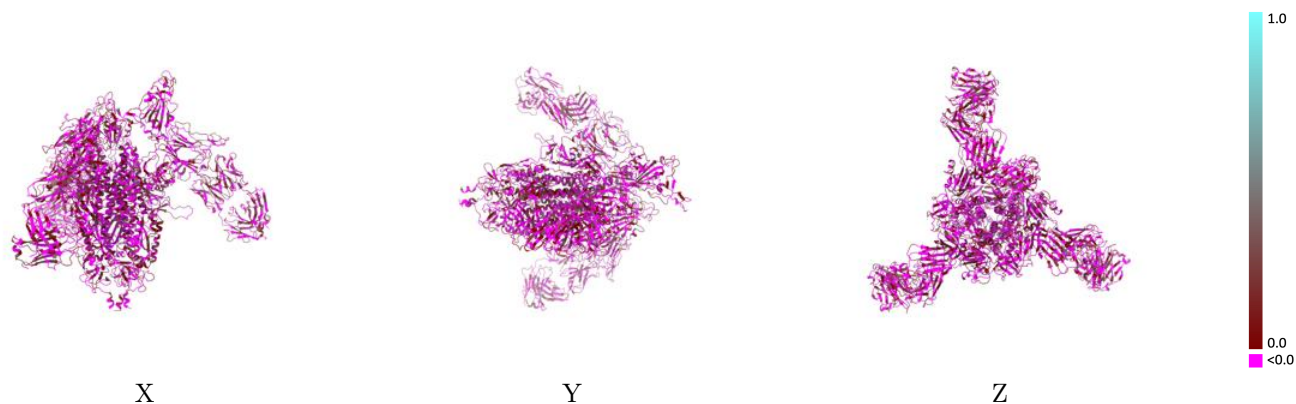
This section contains information regarding the fit between EMDB map EMD-30921 and PDB model 7DZY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



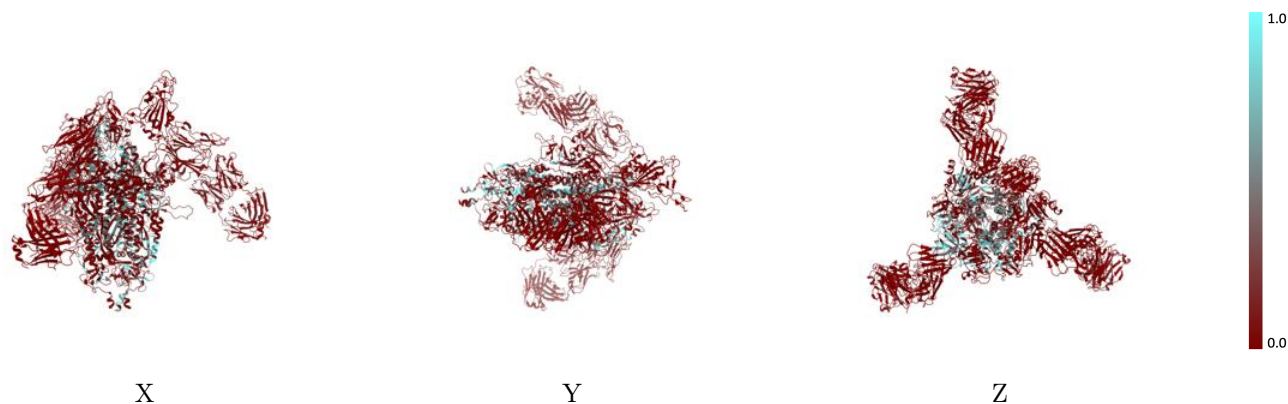
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



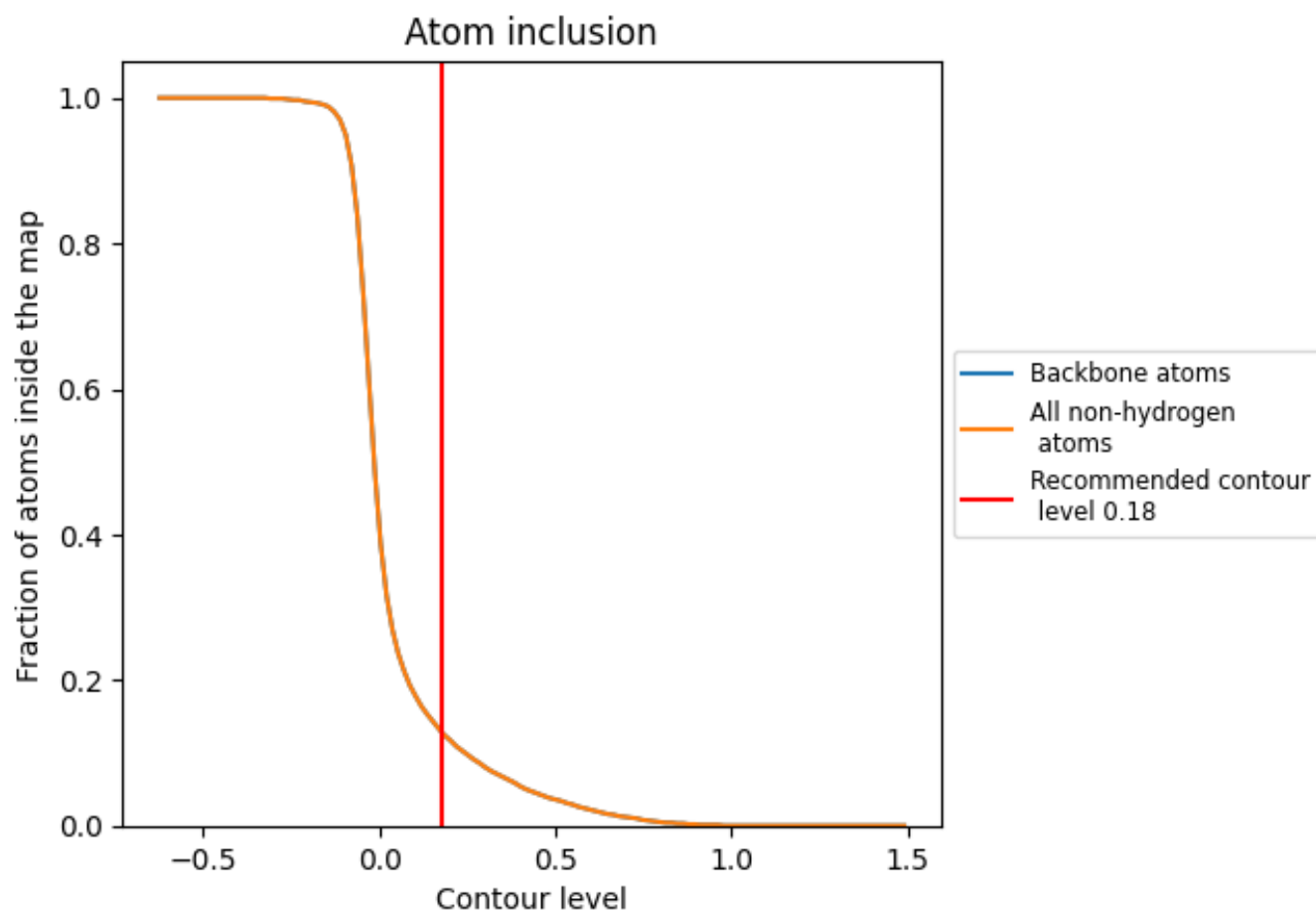
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 13% of all backbone atoms, 13% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1270	 -0.0100
A	 0.2020	 -0.0270
B	 0.1500	 -0.0140
C	 0.1780	 0.0000
H	 0.0000	 0.0010
L	 0.0000	 0.0260
M	 0.0000	 -0.0080
N	 0.0000	 0.0050
O	 0.0000	 -0.0250
P	 0.0000	 -0.0040

