



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:37 PM UTC

PDB ID : 7DZY / pdb_00007dzy
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:

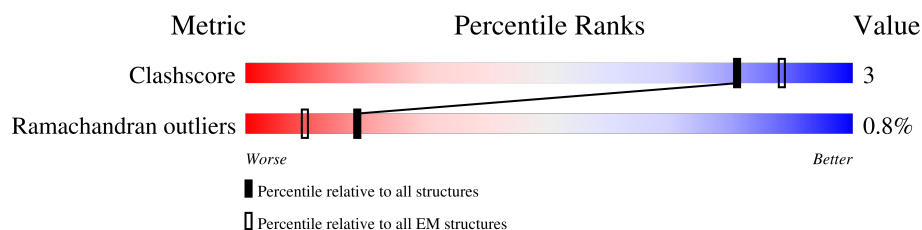
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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	229148	23984
Ramachandran outliers	224038	23583

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% 85% 10%
1	B	1249	73% 85% 10%
1	C	1249	71% 84% 5% 10%
2	H	225	100% 95% 5%
2	M	225	100% 95% 5%
2	O	225	100% 95% 5%
3	L	266	80% 78% 20%
3	N	266	80% 78% 20%
3	P	266	80% 78% 20%

2 Entry composition

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
1	A	1121	Total	C	N	O	0	0
			4484	2242	1121	1121		
1	B	1121	Total	C	N	O	0	0
			4484	2242	1121	1121		
1	C	1121	Total	C	N	O	0	0
			4484	2242	1121	1121		

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		

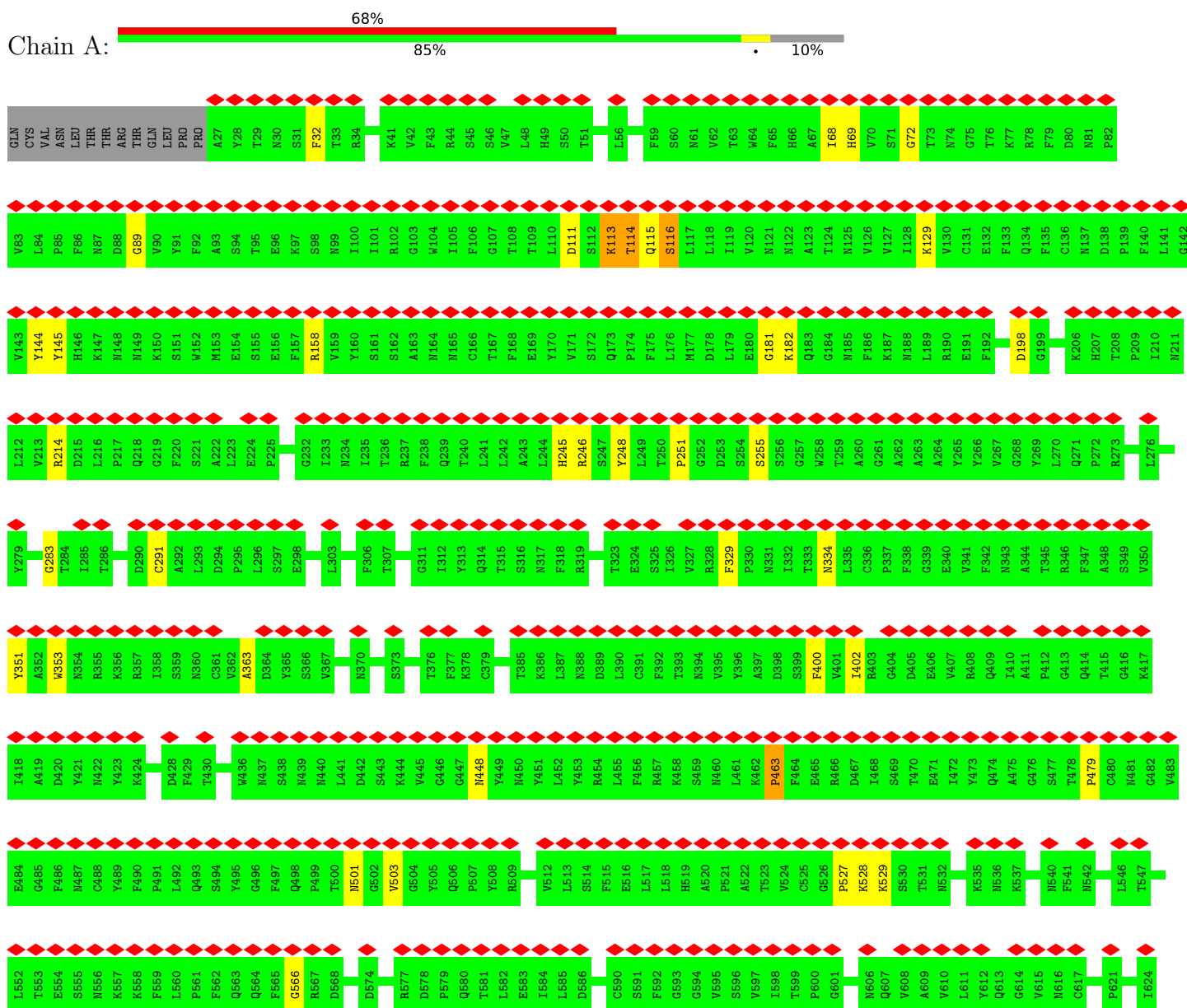
- Molecule 3 is a protein called Fab light chain of enhancing antibody 2490.

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		

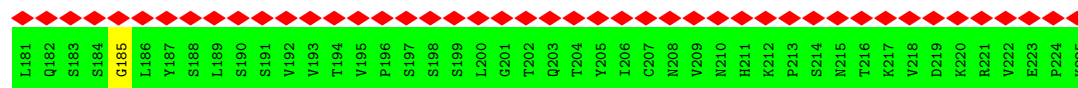
3 Residue-property plots

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.

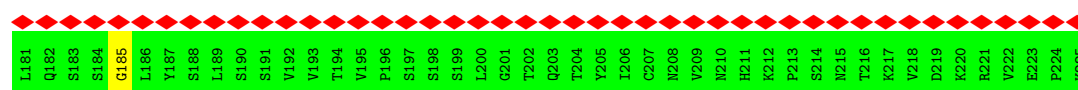
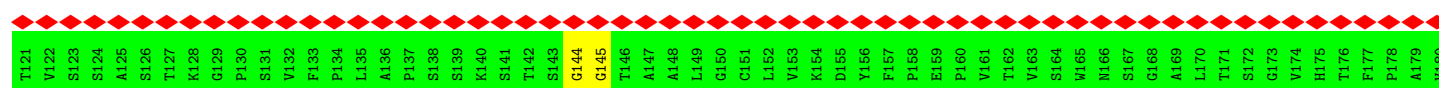
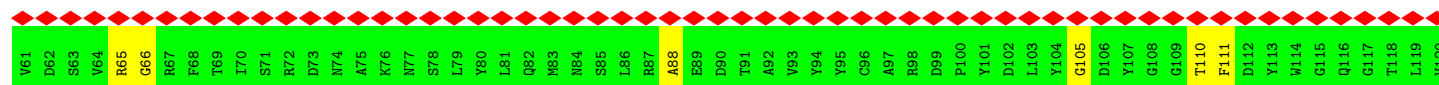
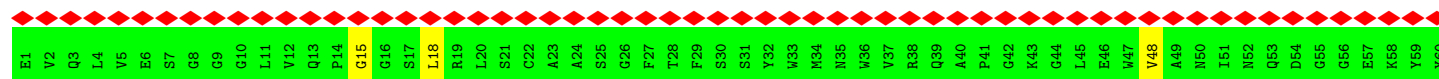
• Molecule 1: Spike glycoprotein



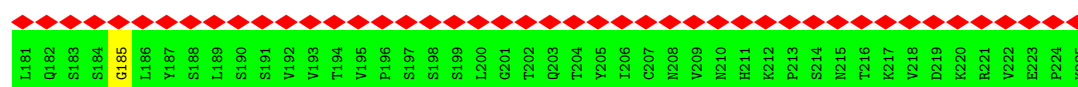
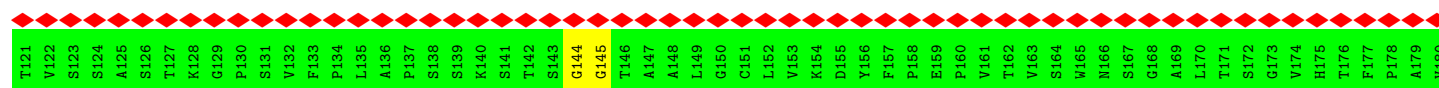
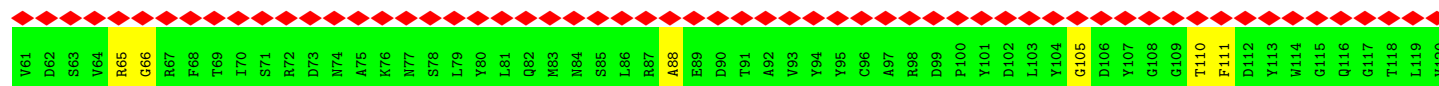
F194	K195	N196	I197	D198	G199	Y200	F201	K202	I203	Y204	S205	K206	H207	T208	P209	N211	L212	V213	R214	D215	L216	P217	Q218	G219	F220	S221	A222	L223	E224	P225	L226	V227	D228	L229	P230	I231	G232	I233	N234	I235	T236	R237	F238	Q239	T240	L241	L242	A243	L244	H245	R246	S247	Y248	L249	T250	P251	G252	D253	
S254	S255	S256	G257	W258	T259	A260	G261	A262	A263	A264	Y265	Y266	V267	G268	Y269	L270	Q271	P272	R273	T274	F275	L276	L277	K278	Y279	N280	E281	N282	G283	T284	I285	T286	D287	A288	Y289	D290	C291	A292	L293	D294	P295	L296	S297	E298	T299	S305	I312	Y313	Q314	T315	S316	N317	F318	R319	V320	Q321	P322		
T323	E324	S325	I326	S327	R328	F329	P330	N331	I332	T333	N334	L335	C336	P337	F338	G339	E340	V341	F342	R343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	W353	N354	R355	L356	R357	I358	S359	N360	C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	A371	A372	S373	F374	S375	T376	F377	K378	C379	G381	V382	
S383	P384	K386	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	A397	D398	S399	F400	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	N422	Y423	K424	L425	P426	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	P463	F464	E465	R466	D467	I468	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	N508	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	Y569	A570	D571	T572	D574	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	Y612	Q613	G614	V615	N616	C617	S618	E619	V620	P621	V622	A623	L624		
H625	A626	D627	Q628	L629	T630	P631	T632	A633	V635	V636	S637	T638	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	G677	T678	N679	S680	P681	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	T712	A713	L714	P715	T716	N717	F718	T719	L720	S721	V722	T723	T724	E725	L726	L727	P728	Y729	S730	H731	V736	D737	C738	R739	H740	Y741	L742	C743	G744	D745	S746	T747	N751	Q755	T756	G757	S758	F759				
C760	T761	Q762	R765	A771	D775	F782	A783	Q784	Y785	K786	Q787	L788	Y789	K790	T791	P792	F793	L794	K795	T796	F797	G798	G799	F800	N801	R802	V803	Q804	L805	L806	P807	D808	P809	S810	K811	P812	S813	K814	R815	S816	F817	D820	L821	L822	F823	N824	K825	V826	T827	L828	A829	D830	A831						
G838	D839	C840	L841	D842	D843	L844	A845	A846	B847	Q853	R854	H855	N856	L861	P862	T866	L870	A871	T874	S875	A879	C890	T881	L882	T883	S884	F888	C889	A890	C891	L896	P897	F898	A899	N902	A903	Y904	R905	F906	N907	Q908	L909	Q910	V911	T912	Q913	N914	V915	L916	Y917									
E918	N919	Q920	K921	L922	I923	A924	N925	Q926	F927	N928	S929	A930	I931	C932	K933	D936	S937	L938	S939	S940	T941	Q946	K947	L948	Q949	D950	V951	V952	N953	Q954	N955	A956	Q957	L958	L959	V963	L966	S967	S968	S975	H976	L981	P987	E990	Y991	Q992	I993	D994	R995	L996									
I997	T998	G999	R1000	L1001	Q1002	S1003	L1004	Q1005	T1006	Y1007	V1008	T1009	Q1010	Q1011	Q1012	L1013	R1014	A1015	A1016	E1017	I1018	R1019	A1020	S1021	A1022	N1023	A1026	T1027	E1031	C1032	V1033	L1034	G1035	Q1036	S1037	K1038	R1039	D1041	F1042	C1043	G1044	K1045	G1046	Y1047	H1048	S1051	Q1054	G1059	L1063	H1064	V1065	T1066							



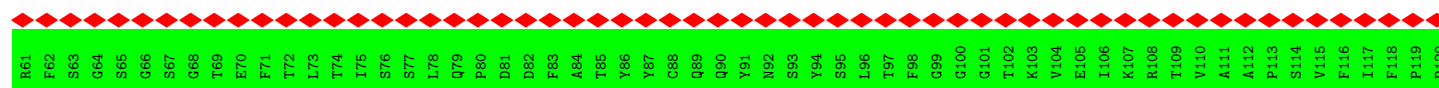
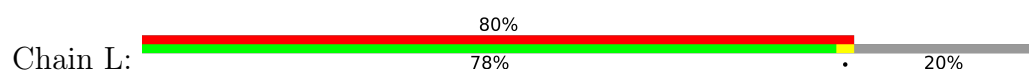
• Molecule 2: Fab Heavy chain of enhancing antibody 2490



• Molecule 2: Fab Heavy chain of enhancing antibody 2490

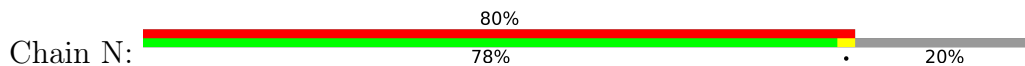


• Molecule 3: Fab light chain of enhancing antibody 2490



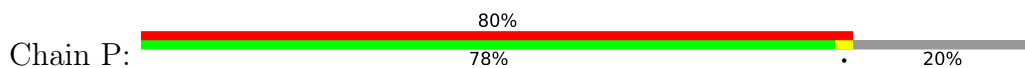
L181	S182	K183	A184	D185	Y186	E187	K188	H189	K190	V191	Y192	A193	C194	E195	V196	T197	H198	Q199	G200	L201	S202	S203	P204	V205	T206	K207	S208	F209	N210	R211	G212	E213	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	SER	LEU	SER	THR	THR	LEU	SER	LYS	ALA	ASP	TYR	GLU			
S121	D122	E123	Q124	L125	K126	S127	G128	T129	A130	S131	V132	V133	C134	L135	L136	N137	N138	F139	Y140	P141	R142	E143	A144	K145	V146	Q147	W148	K149	V150	D151	N152	A153	L154	Q155	S156	G157	N158	S159	Q160	E161	S162	V163	T164	E165	Q166	D167	S168	K169	D170	S171	T172	Y173	S174	L175	S176	S177	T178	L179	T180

• Molecule 3: Fab light chain of enhancing antibody 2490



D1	I2	Q3	M4	T5	Q6	S7	P8	S9	T10	L11	S12	L13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	S28	I29	S30	S31	W32	L33	A34	W35	Y36	Q37	Q38	R39	P40	R41	K42	A43	P44	V45	E105	I106	K107	R108	T109	V110	A111	S112	P113	S114	V115	F116	I117	F118	P119	S60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
R61	F62	S63	G64	S65	G66	S67	G68	T69	E70	F71	T72	L73	T74	I75	S76	S77	L78	Q79	P80	D81	D82	F83	A84	T85	Y86	Y87	C88	Q89	Q90	Y91	N92	S93	Y94	S95	L96	T97	F98	G99	G100	G101	T102	K103	V104	E105	I106	K107	R108	T109	V110	A111	S112	P113	S114	V115	F116	I117	F118	P119	E120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
S121	D122	E123	Q124	L125	K126	S127	G128	T129	A130	S131	V132	V133	C134	L135	L136	N137	N138	F139	Y140	P141	R142	E143	A144	K145	V146	Q147	W148	K149	V150	D151	N152	A153	L154	Q155	S156	G157	N158	S159	Q160	E161	S162	V163	T164	E165	Q166	D167	S168	K169	D170	S171	T172	Y173	S174	L175	S176	S177	T178	L179	T180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L181	S182	K183	A184	D185	Y186	E187	K188	H189	K190	V191	Y192	A193	C194	E195	V196	T197	H198	Q199	G200	L201	S202	S203	P204	V205	T206	K207	S208	F209	N210	R211	G212	E213	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	SER	LEU	SER	THR	THR	LEU	SER	LYS	ALA	ASP	TYR	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					

• Molecule 3: Fab light chain of enhancing antibody 2490



D1	I2	Q3	M4	T5	Q6	S7	P8	S9	T10	L11	S12	L13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	S28	I29	S30	S31	W32	L33	A34	W35	Y36	Q37	Q38	K39	P40	R41	K42	A43	P44	K45	L46	L47	I48	Y49	K50	A51	S52	T53	L54	E55	S56	G57	V58	P59	S60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
R61	F62	S63	G64	S65	G66	S67	G68	T69	E70	F71	T72	L73	T74	I75	S76	S77	L78	Q79	P80	D81	D82	F83	A84	T85	Y86	Y87	C88	Q89	Q90	Y91	N92	S93	Y94	S95	L96	T97	F98	G99	G100	G101	T102	K103	V104	E105	I106	K107	R108	T109	V110	A111	A112	P113	S114	V115	F116	I117	F118	P119	P120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
S121	D122	E123	Q124	L125	K126	S127	G128	T129	A130	S131	V132	V133	C134	L135	L136	N137	N138	F139	Y140	P141	R142	E143	A144	K145	V146	Q147	W148	K149	V150	D151	N152	A153	L154	Q155	S156	G157	N158	S159	Q160	E161	S162	V163	T164	E165	Q166	D167	S168	K169	D170	S171	T172	Y173	S174	L175	S176	S177	T178	L179	T180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
L181	S182	K183	A184	D185	Y186	E187	K188	H189	K190	V191	Y192	A193	C194	E195	V196	T197	H198	Q199	G200	L201	S202	S203	P204	V205	T206	K207	S208	F209	N210	R211	G212	E213	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	SER	LEU	SER	THR	THR	LEU	SER	LYS	ALA	ASP	TYR	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

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 (Å)	334.4, 334.4, 334.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	1.56	2/4483 (0.0%)	1.66	62/5602 (1.1%)
1	B	1.60	8/4483 (0.2%)	1.75	63/5602 (1.1%)
1	C	1.64	13/4483 (0.3%)	1.77	81/5602 (1.4%)
2	H	1.55	1/899 (0.1%)	1.58	14/1122 (1.2%)
2	M	1.54	1/899 (0.1%)	1.58	15/1122 (1.3%)
2	O	1.54	1/899 (0.1%)	1.58	14/1122 (1.2%)
3	L	1.47	0/851	1.46	7/1062 (0.7%)
3	N	1.47	0/851	1.46	7/1062 (0.7%)
3	P	1.47	0/851	1.46	7/1062 (0.7%)
All	All	1.58	26/18699 (0.1%)	1.67	270/23358 (1.2%)

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	B	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	843	ASP	CA-C	14.59	1.73	1.52
1	C	841	LEU	N-CA	14.55	1.65	1.46
1	B	586	ASP	C-N	13.07	1.46	1.33
1	B	587	ILE	N-CA	12.12	1.59	1.46
1	C	840	CYS	C-N	12.06	1.50	1.33
1	C	841	LEU	CA-C	11.18	1.67	1.52
1	C	843	ASP	C-N	10.47	1.47	1.33
1	B	854	LYS	CA-C	-9.93	1.39	1.52
1	C	842	GLY	CA-C	9.79	1.64	1.52
1	C	840	CYS	N-CA	-8.31	1.36	1.46
1	C	841	LEU	C-N	8.00	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	843	ASP	N-CA	7.90	1.56	1.46
1	C	844	ILE	N-CA	7.77	1.55	1.46
1	B	574	ASP	CA-C	7.74	1.61	1.52
1	B	588	THR	CA-C	-6.84	1.44	1.52
2	H	105	GLY	CA-C	-6.61	1.42	1.52
2	O	105	GLY	CA-C	-6.57	1.42	1.52
2	M	105	GLY	CA-C	-6.57	1.42	1.52
1	B	290	ASP	C-N	-6.48	1.25	1.33
1	C	290	ASP	C-N	-6.14	1.25	1.33
1	A	145	TYR	CA-C	-5.79	1.45	1.52
1	C	844	ILE	CA-C	5.76	1.60	1.52
1	B	574	ASP	C-N	5.67	1.40	1.33
1	C	842	GLY	C-N	5.40	1.41	1.33
1	B	588	THR	C-N	-5.39	1.26	1.33
1	A	246	ARG	CA-C	-5.23	1.46	1.52

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	840	CYS	CA-C-O	-29.09	90.74	120.70
1	B	574	ASP	CA-C-N	25.32	162.60	121.58
1	B	574	ASP	C-N-CA	25.32	162.60	121.58
1	C	843	ASP	CA-C-N	18.10	146.12	120.42
1	C	843	ASP	C-N-CA	18.10	146.12	120.42
1	B	586	ASP	CA-C-N	17.07	146.26	122.01
1	B	586	ASP	C-N-CA	17.07	146.26	122.01
1	C	844	ILE	N-CA-C	16.73	127.62	110.72
1	B	854	LYS	CA-C-N	-16.23	94.45	122.36
1	B	854	LYS	C-N-CA	-16.23	94.45	122.36
1	C	843	ASP	N-CA-C	15.66	131.65	112.54
1	B	587	ILE	N-CA-C	13.96	129.06	107.98
1	C	842	GLY	CA-C-N	12.55	141.68	120.72
1	C	842	GLY	C-N-CA	12.55	141.68	120.72
1	B	574	ASP	N-CA-C	11.96	128.59	112.68
1	A	251	PRO	N-CA-C	-11.70	92.14	111.68
1	B	586	ASP	CA-C-O	-11.24	108.23	121.05
1	A	1098	ASN	N-CA-C	-10.94	95.08	110.50
1	C	840	CYS	CA-C-N	10.91	142.39	121.54
1	C	840	CYS	C-N-CA	10.91	142.39	121.54
1	C	841	LEU	N-CA-C	10.72	133.63	110.80
1	A	198	ASP	CA-C-N	-10.09	109.47	123.08
1	A	198	ASP	C-N-CA	-10.09	109.47	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	847	ARG	N-CA-C	-10.08	100.29	111.28
1	C	840	CYS	N-CA-C	10.04	121.99	111.14
1	A	1085	GLY	N-CA-C	-9.31	101.76	115.63
1	B	1129	VAL	N-CA-C	9.09	122.42	111.05
1	C	840	CYS	O-C-N	8.44	131.21	122.09
1	C	841	LEU	CA-C-N	8.42	141.43	122.07
1	C	841	LEU	C-N-CA	8.42	141.43	122.07
2	M	144	GLY	N-CA-C	-8.28	105.23	115.08
2	O	144	GLY	N-CA-C	-8.27	105.24	115.08
2	H	144	GLY	N-CA-C	-8.25	105.27	115.08
1	C	519	HIS	N-CA-C	-8.17	102.61	112.58
1	A	503	VAL	CA-C-N	8.15	130.61	120.34
1	A	503	VAL	C-N-CA	8.15	130.61	120.34
1	C	842	GLY	N-CA-C	8.05	120.60	110.29
1	B	1085	GLY	N-CA-C	-7.83	103.92	114.95
1	C	409	GLN	CA-C-N	-7.74	113.33	122.22
1	C	409	GLN	C-N-CA	-7.74	113.33	122.22
1	A	245	HIS	CA-C-N	-7.66	110.54	122.87
1	A	245	HIS	C-N-CA	-7.66	110.54	122.87
1	A	214	ARG	N-CA-C	-7.65	102.94	111.28
1	C	144	TYR	CA-C-N	-7.65	112.21	122.99
1	C	144	TYR	C-N-CA	-7.65	112.21	122.99
1	C	1085	GLY	N-CA-C	-7.62	104.56	114.85
1	B	575	ALA	N-CA-C	7.57	120.41	107.93
1	A	363	ALA	CA-C-N	7.51	134.90	122.66
1	A	363	ALA	C-N-CA	7.51	134.90	122.66
1	C	844	ILE	O-C-N	-7.28	114.33	121.83
1	A	69	HIS	CA-C-N	-7.03	113.54	123.11
1	A	69	HIS	C-N-CA	-7.03	113.54	123.11
1	B	855	PHE	N-CA-C	-7.02	105.24	113.88
1	C	970	PHE	O-C-N	-6.99	113.29	122.59
1	A	501	ASN	N-CA-C	6.96	118.95	111.36
1	C	89	GLY	CA-C-N	-6.96	113.27	122.94
1	C	89	GLY	C-N-CA	-6.96	113.27	122.94
1	A	527	PRO	CA-C-N	6.84	134.60	121.54
1	A	527	PRO	C-N-CA	6.84	134.60	121.54
1	C	844	ILE	CA-C-N	6.82	130.11	120.28
1	C	844	ILE	C-N-CA	6.82	130.11	120.28
1	B	97	LYS	N-CA-C	-6.81	103.79	111.07
1	C	89	GLY	N-CA-C	-6.80	102.87	110.96
1	B	283	GLY	N-CA-C	-6.78	105.74	115.64
2	O	66	GLY	CA-C-N	6.73	129.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	66	GLY	C-N-CA	6.73	129.84	120.29
2	H	66	GLY	CA-C-N	6.70	129.80	120.29
2	H	66	GLY	C-N-CA	6.70	129.80	120.29
2	M	66	GLY	CA-C-N	6.69	129.79	120.29
2	M	66	GLY	C-N-CA	6.69	129.79	120.29
1	C	383	SER	N-CA-C	-6.66	101.67	109.93
1	A	129	LYS	CA-C-N	6.65	131.54	120.64
1	A	129	LYS	C-N-CA	6.65	131.54	120.64
1	B	129	LYS	CA-C-N	6.65	132.06	121.09
1	B	129	LYS	C-N-CA	6.65	132.06	121.09
1	C	1044	GLY	N-CA-C	-6.62	105.66	111.95
1	B	742	ILE	CA-C-N	6.61	134.34	122.38
1	B	742	ILE	C-N-CA	6.61	134.34	122.38
1	C	1128	VAL	N-CA-C	6.59	116.73	110.53
1	B	448	ASN	CA-C-N	6.58	131.72	120.72
1	B	448	ASN	C-N-CA	6.58	131.72	120.72
1	A	68	ILE	CA-C-N	-6.56	114.23	123.03
1	A	68	ILE	C-N-CA	-6.56	114.23	123.03
1	C	1107	ARG	N-CA-C	6.52	118.18	111.14
1	B	1128	VAL	CA-C-N	6.47	130.69	120.47
1	B	1128	VAL	C-N-CA	6.47	130.69	120.47
1	C	261	GLY	CA-C-N	6.46	130.13	120.31
1	C	261	GLY	C-N-CA	6.46	130.13	120.31
1	C	843	ASP	O-C-N	-6.43	113.81	122.43
1	A	1044	GLY	N-CA-C	-6.39	105.52	112.04
1	A	448	ASN	CA-C-N	6.39	132.32	121.14
1	A	448	ASN	C-N-CA	6.39	132.32	121.14
1	C	245	HIS	CA-C-N	-6.38	113.38	122.94
1	C	245	HIS	C-N-CA	-6.38	113.38	122.94
1	A	248	TYR	N-CA-C	-6.36	104.27	111.07
1	B	331	ASN	CA-C-N	6.32	130.66	120.30
1	B	331	ASN	C-N-CA	6.32	130.66	120.30
2	H	48	VAL	N-CA-C	6.32	116.95	110.82
1	B	586	ASP	O-C-N	6.31	130.46	123.01
2	M	48	VAL	N-CA-C	6.31	116.94	110.82
2	O	48	VAL	N-CA-C	6.28	116.91	110.82
1	A	1091	ARG	N-CA-C	-6.23	104.57	111.36
1	B	798	GLY	N-CA-C	-6.22	106.12	115.32
1	A	351	TYR	CA-C-N	6.19	133.65	121.58
1	A	351	TYR	C-N-CA	6.19	133.65	121.58
1	C	251	PRO	N-CA-C	-6.18	101.35	111.68
1	C	842	GLY	O-C-N	-6.17	114.61	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	GLY	N-CA-C	-6.15	107.21	115.21
1	C	363	ALA	CA-C-N	6.15	134.54	122.61
1	C	363	ALA	C-N-CA	6.15	134.54	122.61
1	B	251	PRO	N-CA-C	-6.13	101.46	111.21
2	O	111	PHE	CA-C-N	6.06	128.69	120.44
2	O	111	PHE	C-N-CA	6.06	128.69	120.44
2	H	111	PHE	CA-C-N	6.06	128.68	120.44
2	H	111	PHE	C-N-CA	6.06	128.68	120.44
2	M	111	PHE	CA-C-N	6.05	128.66	120.44
2	M	111	PHE	C-N-CA	6.05	128.66	120.44
1	B	743	CYS	N-CA-C	6.03	120.64	113.16
1	B	371	SER	CA-C-N	6.02	129.46	120.31
1	B	371	SER	C-N-CA	6.02	129.46	120.31
3	N	28	SER	CA-C-N	6.02	130.10	121.02
3	N	28	SER	C-N-CA	6.02	130.10	121.02
1	B	244	LEU	CA-C-N	6.01	133.31	121.58
1	B	244	LEU	C-N-CA	6.01	133.31	121.58
1	A	182	LYS	N-CA-C	-6.00	101.32	109.54
3	L	28	SER	CA-C-N	6.00	130.08	121.02
3	L	28	SER	C-N-CA	6.00	130.08	121.02
3	P	28	SER	CA-C-N	5.99	130.07	121.02
3	P	28	SER	C-N-CA	5.99	130.07	121.02
1	B	496	GLY	CA-C-N	-5.99	113.72	122.65
1	B	496	GLY	C-N-CA	-5.99	113.72	122.65
1	B	684	ALA	N-CA-C	-5.98	102.82	110.53
1	C	970	PHE	N-CA-C	-5.97	98.07	110.80
1	B	1044	GLY	N-CA-C	-5.97	106.28	111.95
1	A	115	GLN	N-CA-C	-5.97	106.09	113.19
1	B	122	ASN	N-CA-C	-5.92	102.18	110.35
1	C	214	ARG	N-CA-C	-5.91	104.84	111.28
1	C	912	THR	CA-C-N	5.91	128.79	120.28
1	C	912	THR	C-N-CA	5.91	128.79	120.28
1	B	490	PHE	N-CA-C	-5.89	102.35	109.83
2	H	185	GLY	N-CA-C	-5.89	106.97	115.27
2	M	185	GLY	N-CA-C	-5.87	106.99	115.27
2	O	185	GLY	N-CA-C	-5.86	107.01	115.27
1	A	463	PRO	CA-C-N	-5.84	112.22	122.62
1	A	463	PRO	C-N-CA	-5.84	112.22	122.62
1	A	89	GLY	CA-C-N	-5.83	115.01	123.06
1	A	89	GLY	C-N-CA	-5.83	115.01	123.06
1	C	351	TYR	CA-C-N	5.81	132.91	121.58
1	C	351	TYR	C-N-CA	5.81	132.91	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	LEU	N-CA-C	-5.76	105.09	111.71
1	A	329	PHE	CA-C-N	5.75	125.73	120.03
1	A	329	PHE	C-N-CA	5.75	125.73	120.03
2	M	105	GLY	CA-C-O	-5.75	113.92	121.51
1	C	469	SER	CA-C-N	5.75	131.20	121.14
1	C	469	SER	C-N-CA	5.75	131.20	121.14
2	O	105	GLY	CA-C-O	-5.75	113.92	121.51
2	H	105	GLY	CA-C-O	-5.73	113.94	121.51
1	B	469	SER	CA-C-N	5.70	131.12	121.14
1	B	469	SER	C-N-CA	5.70	131.12	121.14
1	A	1033	VAL	CA-C-N	5.70	130.24	120.72
1	A	1033	VAL	C-N-CA	5.70	130.24	120.72
1	B	246	ARG	N-CA-C	-5.66	105.20	111.71
1	A	113	LYS	CA-C-N	-5.65	113.32	122.36
1	A	113	LYS	C-N-CA	-5.65	113.32	122.36
1	C	400	PHE	CA-C-N	5.64	130.49	122.09
1	C	400	PHE	C-N-CA	5.64	130.49	122.09
1	A	400	PHE	CA-C-N	5.62	130.47	122.09
1	A	400	PHE	C-N-CA	5.62	130.47	122.09
1	C	801	ASN	CA-C-N	5.59	130.92	121.14
1	C	801	ASN	C-N-CA	5.59	130.92	121.14
1	A	796	ASP	CA-C-N	5.58	132.45	122.06
1	A	796	ASP	C-N-CA	5.58	132.45	122.06
1	A	283	GLY	N-CA-C	-5.53	107.14	115.32
3	N	151	ASP	CA-C-N	5.50	129.94	122.07
3	N	151	ASP	C-N-CA	5.50	129.94	122.07
3	L	151	ASP	CA-C-N	5.50	129.93	122.07
3	L	151	ASP	C-N-CA	5.50	129.93	122.07
1	A	144	TYR	CA-C-N	-5.50	115.25	123.00
1	A	144	TYR	C-N-CA	-5.50	115.25	123.00
3	P	151	ASP	CA-C-N	5.50	129.93	122.07
3	P	151	ASP	C-N-CA	5.50	129.93	122.07
1	A	857	GLY	N-CA-C	-5.43	107.04	114.64
1	B	700	GLY	N-CA-C	-5.41	106.11	111.85
1	C	448	ASN	CA-C-N	5.41	130.60	121.14
1	C	448	ASN	C-N-CA	5.41	130.60	121.14
1	C	336	CYS	N-CA-C	-5.39	102.69	110.40
1	C	613	GLN	CA-C-N	5.37	128.21	120.11
1	C	613	GLN	C-N-CA	5.37	128.21	120.11
1	A	985	ASP	N-CA-C	-5.36	103.97	110.13
1	A	743	CYS	N-CA-C	5.35	119.81	113.28
1	C	839	ASP	N-CA-C	-5.34	104.87	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LYS	CA-C-N	5.34	131.19	122.81
1	A	182	LYS	C-N-CA	5.34	131.19	122.81
1	C	504	GLY	CA-C-N	5.33	132.59	121.94
1	C	504	GLY	C-N-CA	5.33	132.59	121.94
1	B	1070	ALA	N-CA-C	5.32	119.69	111.56
1	B	709	ASN	CA-C-N	-5.30	115.92	123.03
1	B	709	ASN	C-N-CA	-5.30	115.92	123.03
2	M	18	LEU	CA-C-N	-5.29	115.32	122.77
2	M	18	LEU	C-N-CA	-5.29	115.32	122.77
1	C	129	LYS	CA-C-N	5.28	129.31	120.64
1	C	129	LYS	C-N-CA	5.28	129.31	120.64
2	H	18	LEU	CA-C-N	-5.28	115.32	122.77
2	H	18	LEU	C-N-CA	-5.28	115.32	122.77
2	O	18	LEU	CA-C-N	-5.28	115.32	122.77
2	O	18	LEU	C-N-CA	-5.28	115.32	122.77
1	A	114	THR	CA-C-N	5.28	133.88	121.52
1	A	114	THR	C-N-CA	5.28	133.88	121.52
1	B	526	GLY	CA-C-N	5.28	125.28	120.21
1	B	526	GLY	C-N-CA	5.28	125.28	120.21
1	A	181	GLY	N-CA-C	-5.27	100.68	113.18
1	A	1070	ALA	N-CA-C	5.25	119.59	111.56
1	C	247	SER	CA-C-N	5.24	127.31	120.28
1	C	247	SER	C-N-CA	5.24	127.31	120.28
2	H	88	ALA	CA-C-N	5.24	127.83	120.28
2	H	88	ALA	C-N-CA	5.24	127.83	120.28
1	C	211	ASN	N-CA-C	-5.23	101.68	109.11
1	A	246	ARG	CA-C-O	-5.23	115.25	121.16
1	B	1107	ARG	N-CA-C	5.23	117.89	111.82
1	B	941	THR	CA-C-N	5.21	128.22	120.31
1	B	941	THR	C-N-CA	5.21	128.22	120.31
1	C	120	VAL	CA-C-N	-5.20	115.77	123.05
1	C	120	VAL	C-N-CA	-5.20	115.77	123.05
2	O	88	ALA	CA-C-N	5.18	127.74	120.28
2	O	88	ALA	C-N-CA	5.18	127.74	120.28
2	M	88	ALA	CA-C-N	5.17	127.73	120.28
2	M	88	ALA	C-N-CA	5.17	127.73	120.28
1	C	95	THR	CA-C-N	5.17	131.01	121.70
1	C	95	THR	C-N-CA	5.17	131.01	121.70
1	B	261	GLY	CA-C-N	5.17	128.05	120.71
1	B	261	GLY	C-N-CA	5.17	128.05	120.71
3	P	189	HIS	CA-C-N	5.16	129.32	120.71
3	P	189	HIS	C-N-CA	5.16	129.32	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	TYR	CA-C-N	-5.16	115.88	123.00
1	B	453	TYR	C-N-CA	-5.16	115.88	123.00
3	N	189	HIS	CA-C-N	5.13	129.28	120.71
3	N	189	HIS	C-N-CA	5.13	129.28	120.71
3	N	190	LYS	N-CA-C	5.13	117.66	111.40
3	L	189	HIS	CA-C-N	5.13	129.27	120.71
3	L	189	HIS	C-N-CA	5.13	129.27	120.71
1	C	384	PRO	N-CA-C	-5.12	106.74	113.65
2	H	145	GLY	N-CA-C	-5.12	104.37	112.66
2	H	65	ARG	N-CA-C	5.11	117.25	111.11
2	M	145	GLY	N-CA-C	-5.11	104.38	112.66
2	O	145	GLY	N-CA-C	-5.11	104.39	112.66
1	C	172	SER	CA-C-N	5.10	128.41	120.60
1	C	172	SER	C-N-CA	5.10	128.41	120.60
3	P	190	LYS	N-CA-C	5.09	117.62	111.40
1	A	291	CYS	CA-C-N	5.09	129.22	120.72
1	A	291	CYS	C-N-CA	5.09	129.22	120.72
2	O	65	ARG	N-CA-C	5.09	117.22	111.11
2	M	65	ARG	N-CA-C	5.08	117.21	111.11
1	C	381	GLY	CA-C-N	-5.08	115.14	122.45
1	C	381	GLY	C-N-CA	-5.08	115.14	122.45
1	B	291	CYS	CA-C-N	5.07	129.19	120.72
1	B	291	CYS	C-N-CA	5.07	129.19	120.72
3	L	190	LYS	N-CA-C	5.07	117.59	111.40
1	B	1125	ASN	CA-C-N	5.06	128.01	120.31
1	B	1125	ASN	C-N-CA	5.06	128.01	120.31
1	B	157	PHE	CA-C-N	-5.06	116.25	123.03
1	B	157	PHE	C-N-CA	-5.06	116.25	123.03
1	B	569	ILE	N-CA-C	-5.06	105.46	110.62
1	C	423	TYR	CA-C-N	-5.04	115.66	122.77
1	C	423	TYR	C-N-CA	-5.04	115.66	122.77
1	B	747	THR	N-CA-C	-5.04	105.86	111.36
1	A	246	ARG	N-CA-C	-5.03	101.96	109.95
1	C	293	LEU	N-CA-C	5.03	116.45	111.07
1	A	479	PRO	CA-C-N	5.02	127.42	120.29
1	A	479	PRO	C-N-CA	5.02	127.42	120.29
2	M	15	GLY	N-CA-C	-5.02	108.72	114.69

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	1220	46	0
1	C	4484	0	1220	44	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	5136	61	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 3.

All (61) 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:575:ALA:H	1:C:843:ASP:C	1.83	0.86
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:575:ALA:H	1:C:843:ASP:CA	1.93	0.80
1:B:182:LYS:O	1:B:261:GLY:HA3	1.82	0.79
1:B:575:ALA:H	1:C:844:ILE:N	1.84	0.75
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:143:VAL:C	1:B:245:HIS:H	2.04	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:574:ASP:C	1:C:845:ALA:H	2.06	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:C	1:C:840:CYS:C	2.67	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:142:GLY:HA3	1:B:244:LEU:C	2.28	0.59
1:B:575:ALA:C	1:C:843:ASP:N	2.62	0.58
1:B:575:ALA:C	1:C:843:ASP:H	2.14	0.56
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:C:729:VAL:N	1:C:1059:GLY:HA2	2.25	0.52
1:A:114:THR:C	1:A:116:SER:H	2.18	0.51
1:B:574:ASP:CA	1:C:843:ASP:C	2.83	0.51
1:B:575:ALA:N	1:C:843:ASP:CA	2.71	0.50
1:C:199:GLY:CA	1:C:232:GLY:HA2	2.42	0.50
1:B:586:ASP:C	1:C:841:LEU:C	2.80	0.50
1:B:575:ALA:N	1:C:843:ASP:C	2.62	0.49
1:B:143:VAL:N	1:B:245:HIS:N	2.61	0.48
1:B:575:ALA:N	1:C:842:GLY:C	2.72	0.47
1:B:142:GLY:CA	1:B:244:LEU:N	2.78	0.47
1:B:588:THR:N	1:C:841:LEU:CA	2.78	0.47
1:A:111:ASP:C	1:A:113:LYS:H	2.21	0.46
1:B:586:ASP:O	1:C:841:LEU:N	2.47	0.46
1:C:122:ASN:C	1:C:124:THR:H	2.23	0.46
1:B:587:ILE:N	1:C:841:LEU:C	2.74	0.46
1:B:574:ASP:H	1:C:843:ASP:CA	2.29	0.45
1:B:574:ASP:H	1:C:843:ASP:C	2.24	0.44
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:587:ILE:N	1:C:842:GLY:N	2.66	0.43
1:B:587:ILE:CA	1:C:841:LEU:C	2.91	0.43
1:C:121:ASN:C	1:C:123:ALA:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ILE:CA	1:C:841:LEU:N	2.83	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:B:587:ILE:N	1:C:840:CYS:C	2.79	0.41
1:C:371:SER:C	1:C:373:SER:H	2.27	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 [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	1119/1249 (90%)	1064 (95%)	43 (4%)	12 (1%)	11	43
1	B	1119/1249 (90%)	1071 (96%)	39 (4%)	9 (1%)	16	49
1	C	1119/1249 (90%)	1050 (94%)	58 (5%)	11 (1%)	12	45
2	H	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	30	61
2	M	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	30	61
2	O	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	30	61
3	L	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	24	57
3	N	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	24	57
3	P	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	24	57
All	All	4659/5220 (89%)	4448 (96%)	173 (4%)	38 (1%)	18	49

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	463	PRO

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Mol	Chain	Res	Type
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
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 ⓘ

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 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.

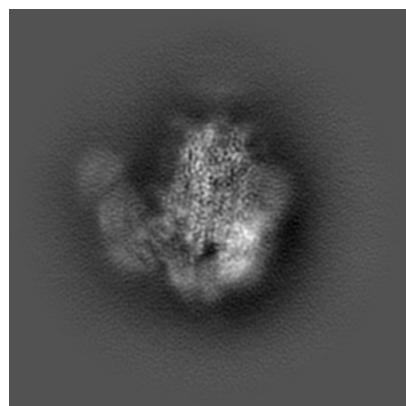
6 Map visualisation [i](#)

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

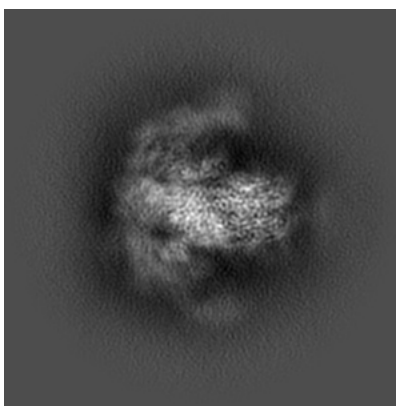
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

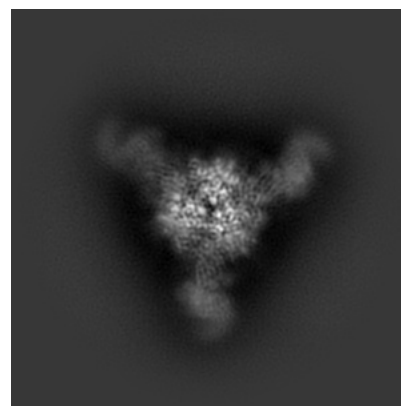
6.1.1 Primary map



X

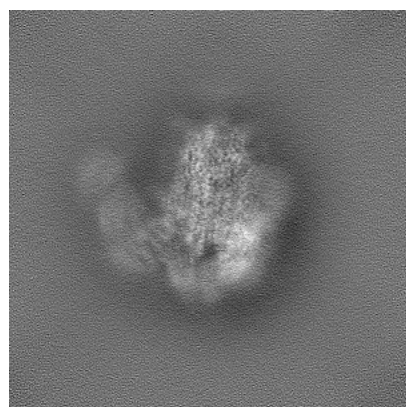


Y

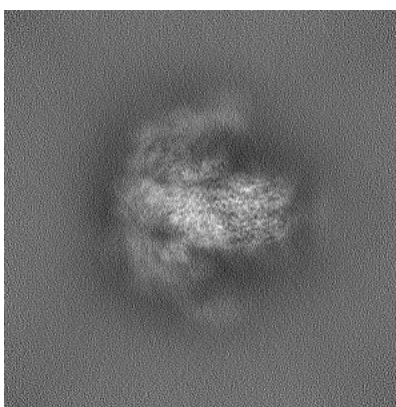


Z

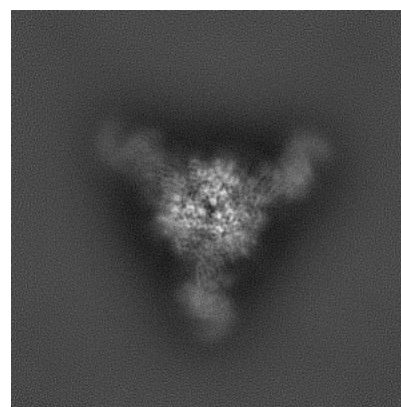
6.1.2 Raw map



X



Y

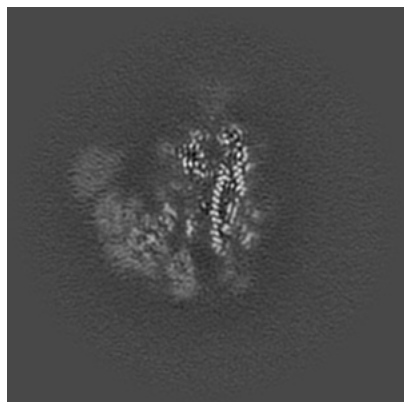


Z

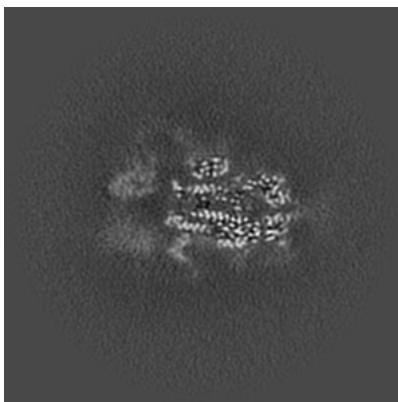
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

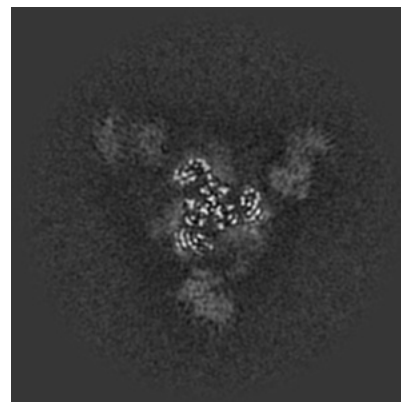
6.2.1 Primary map



X Index: 190

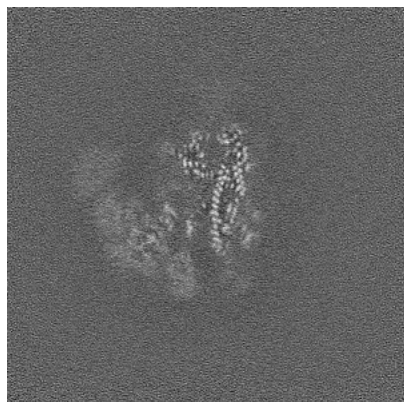


Y Index: 190

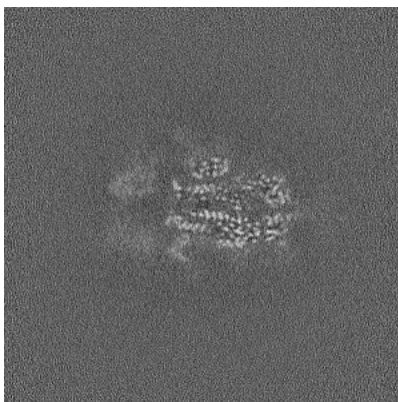


Z Index: 190

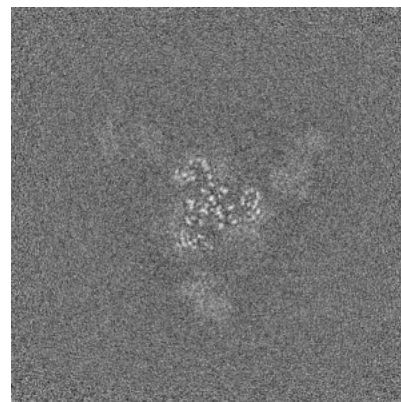
6.2.2 Raw map



X Index: 190



Y Index: 190

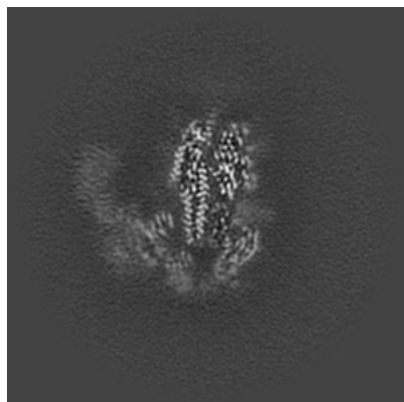


Z Index: 190

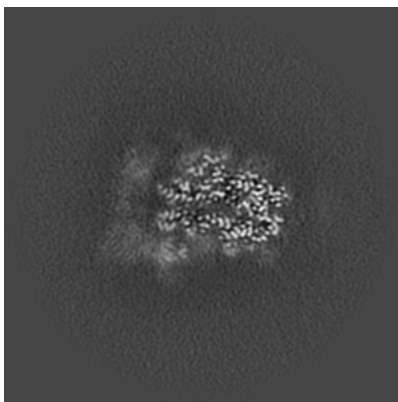
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

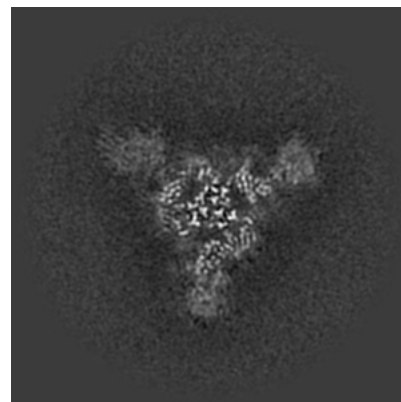
6.3.1 Primary map



X Index: 197

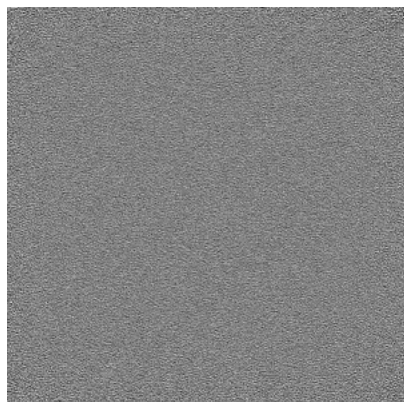


Y Index: 180

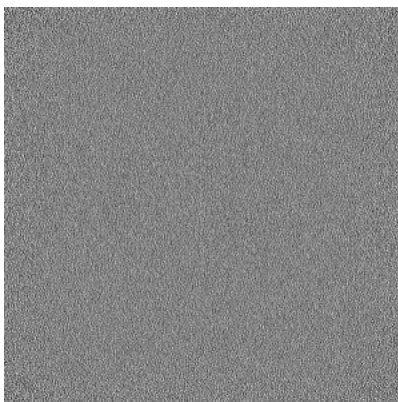


Z Index: 173

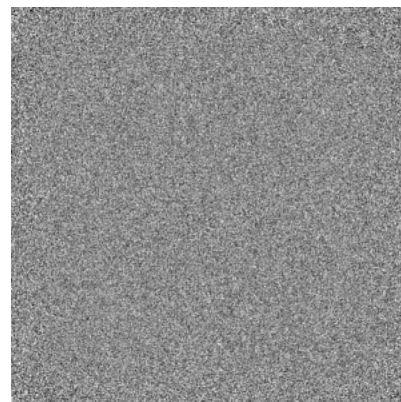
6.3.2 Raw map



X Index: 0



Y Index: 0

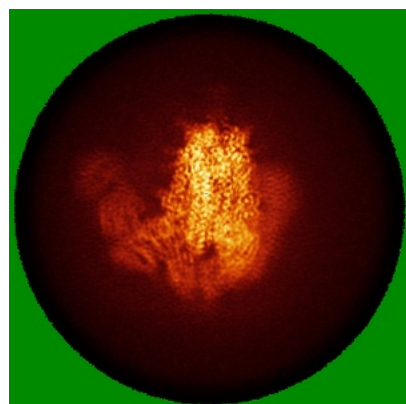


Z Index: 379

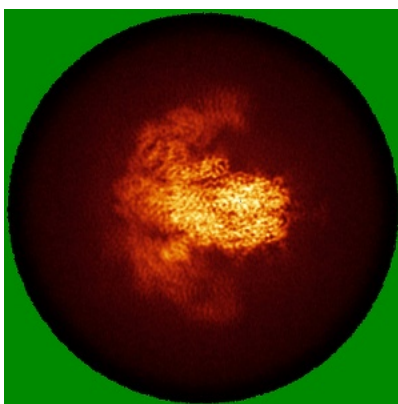
The images above show the largest variance slices of the map in three orthogonal directions.

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

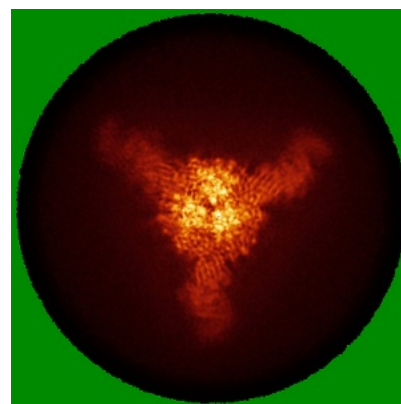
6.4.1 Primary map



X

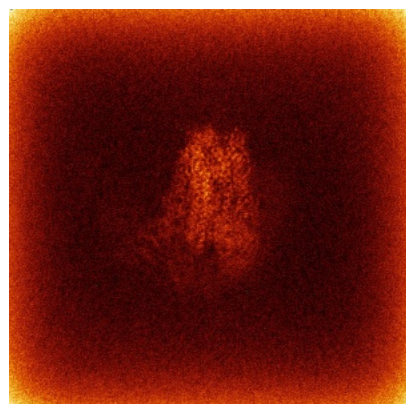


Y

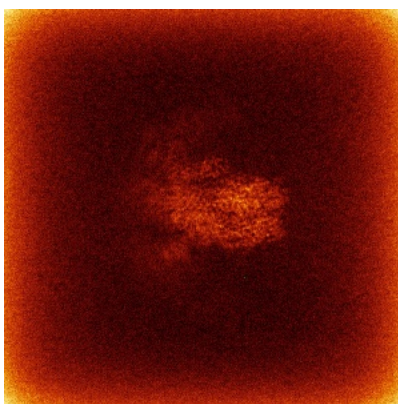


Z

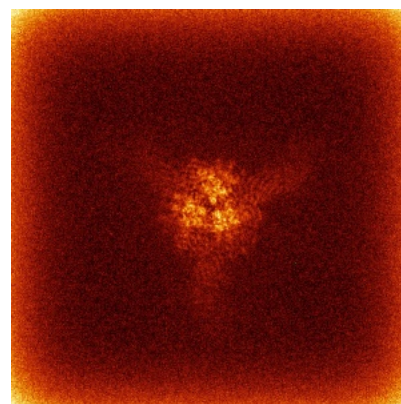
6.4.2 Raw map



X



Y

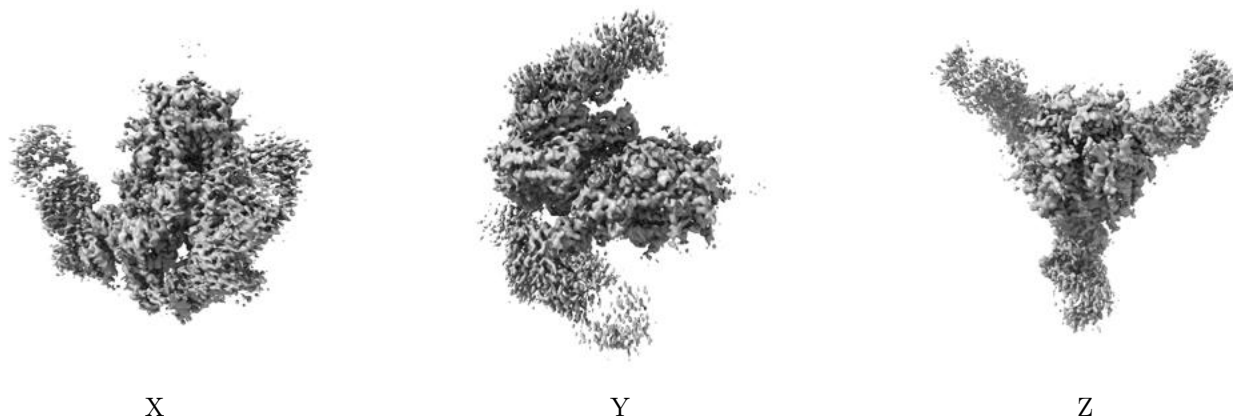


Z

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

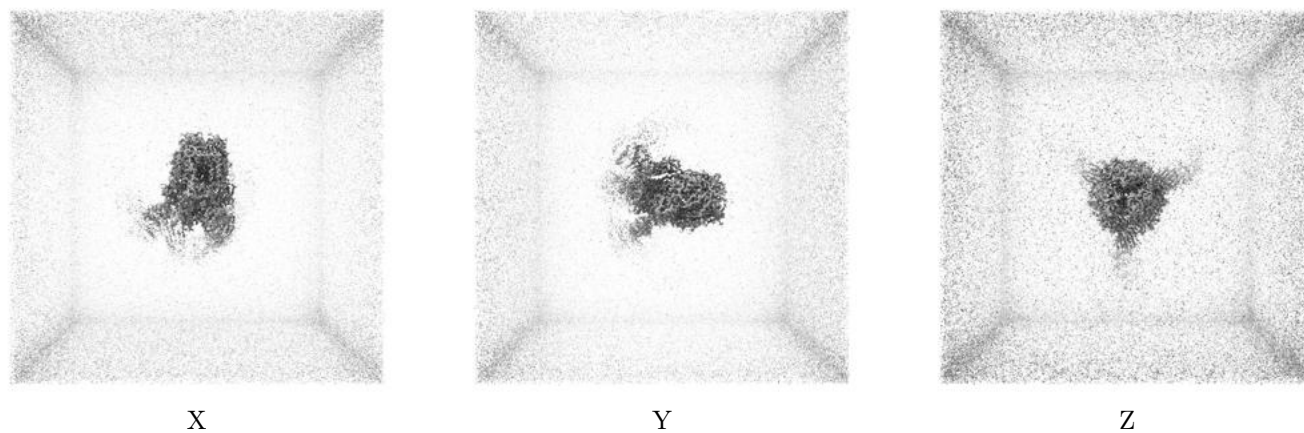
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

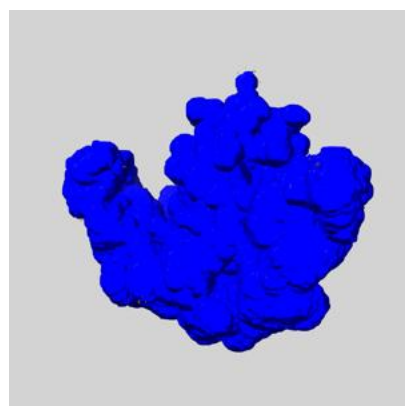
6.6 Mask visualisation [i](#)

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

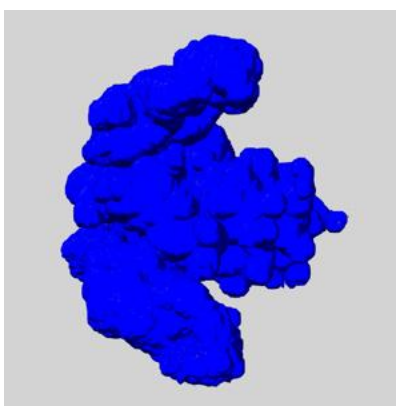
A mask typically either:

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

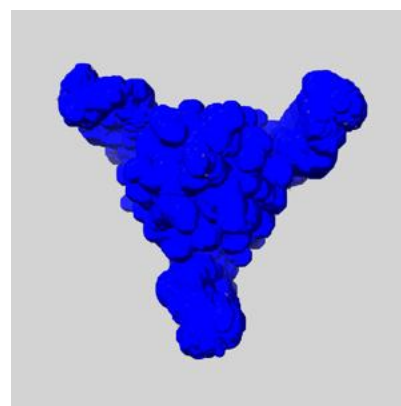
6.6.1 emd_30921_msk_1.map [i](#)



X



Y

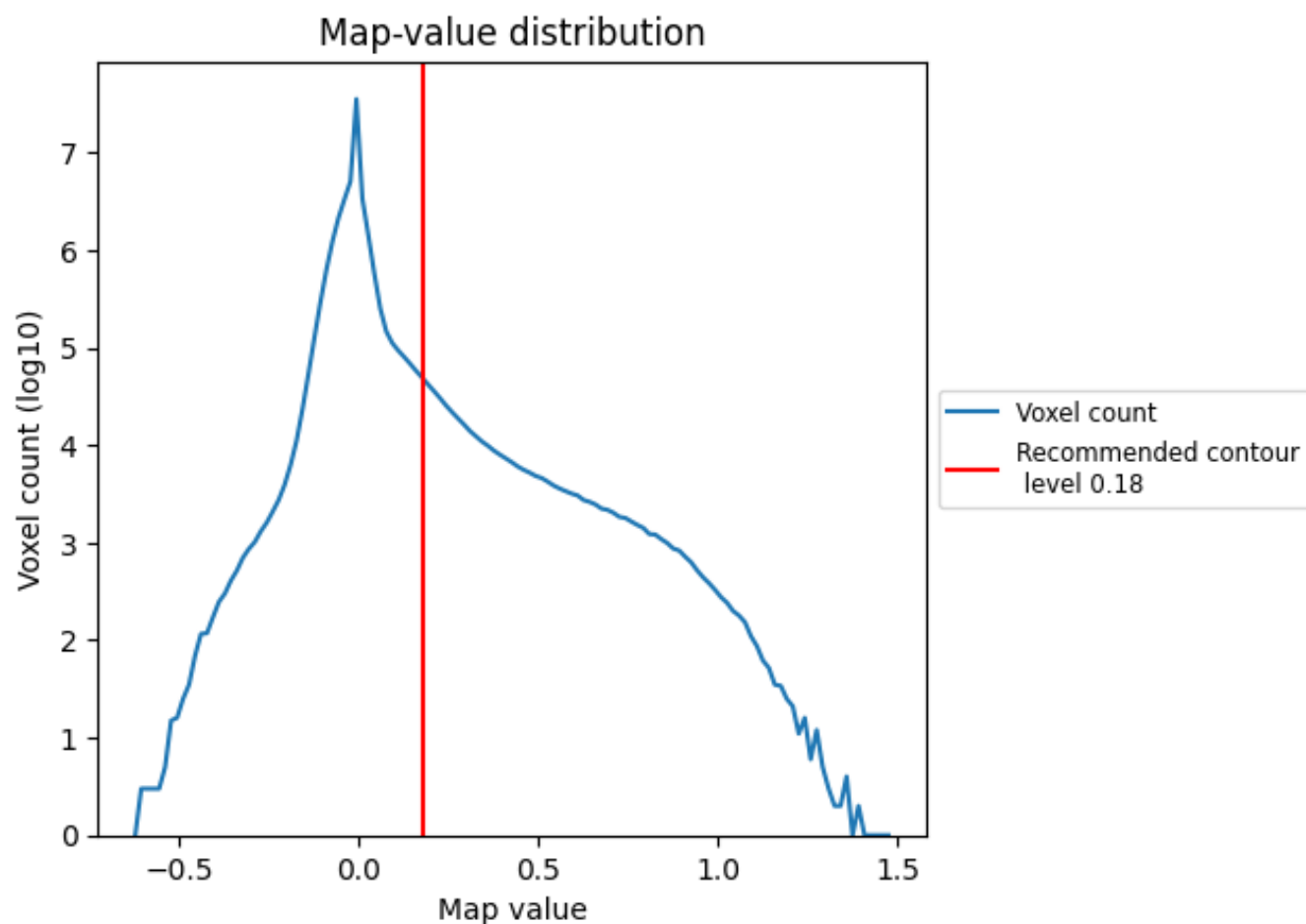


Z

7 Map analysis [i](#)

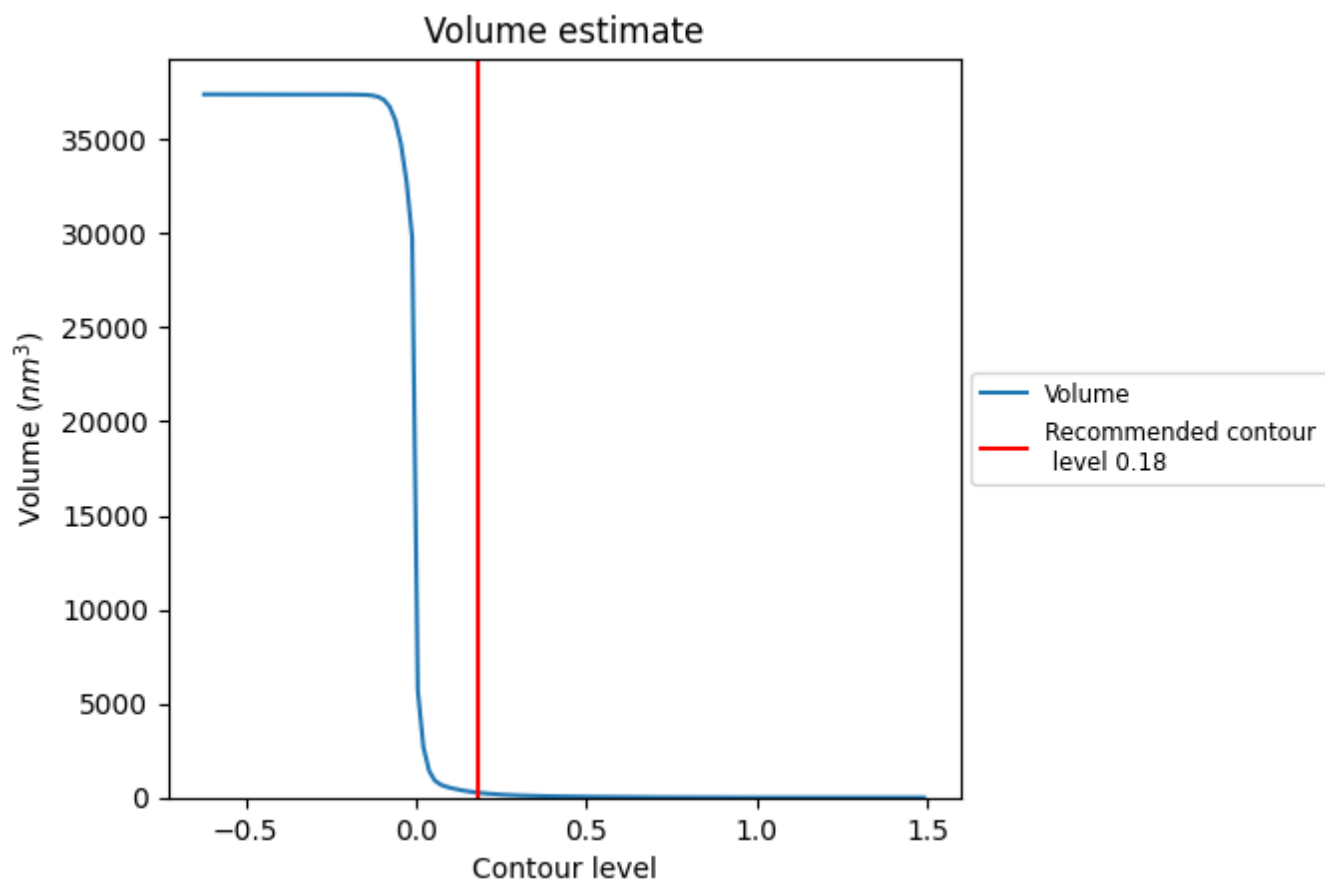
This section contains the results of statistical analysis of the map.

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.

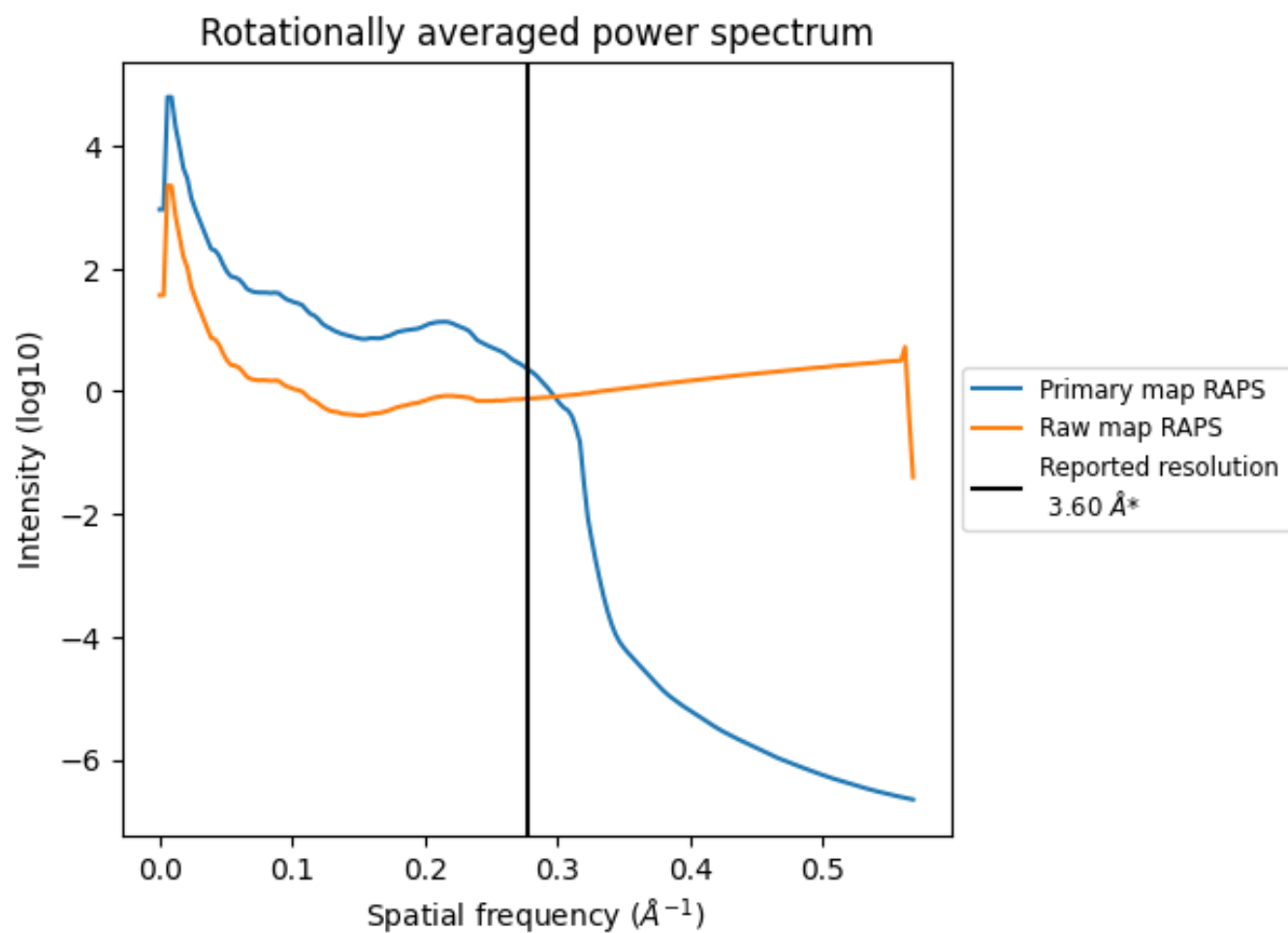
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm^3 ; 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 ⓘ

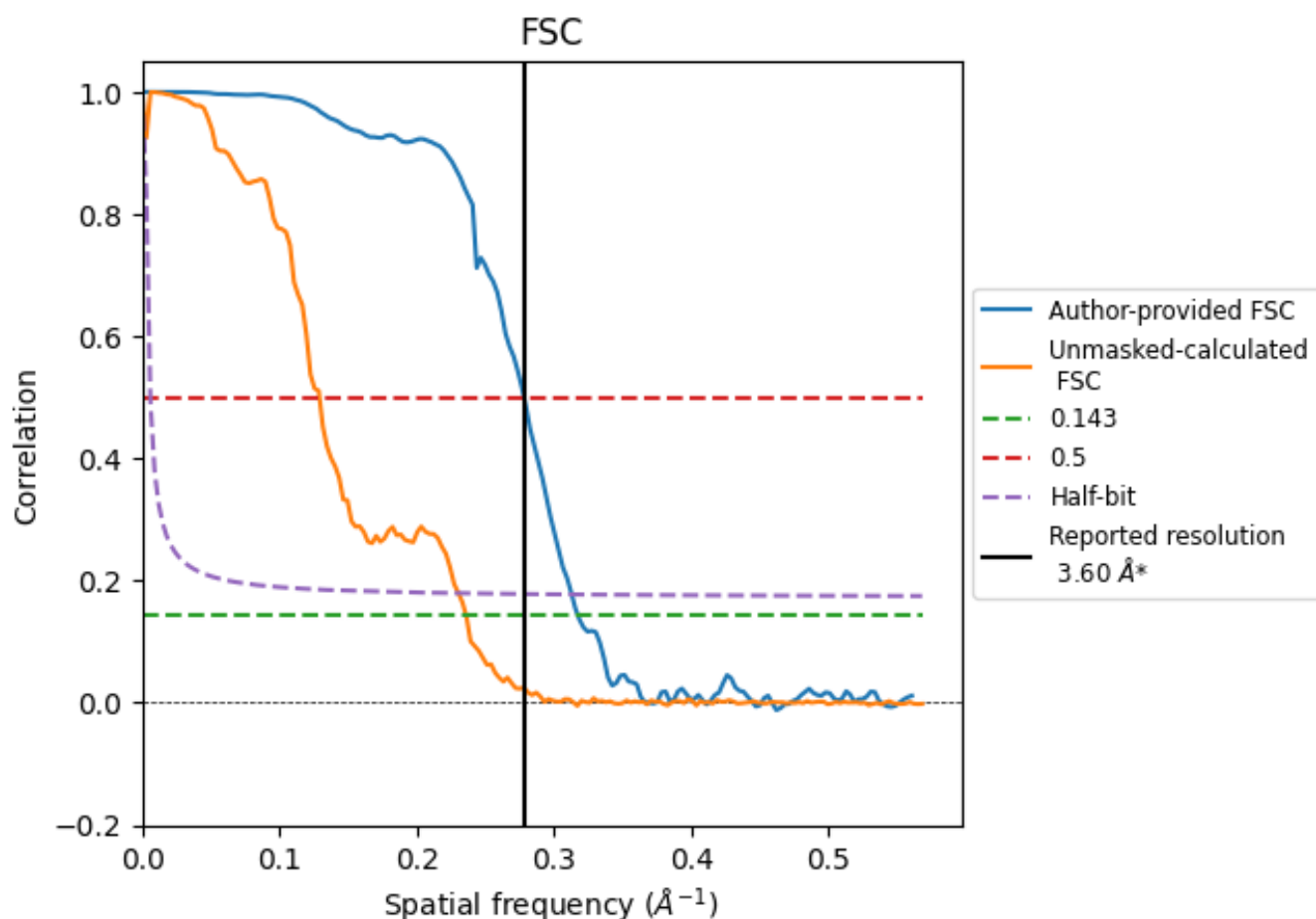


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $\text{\AA}^{-1}$

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

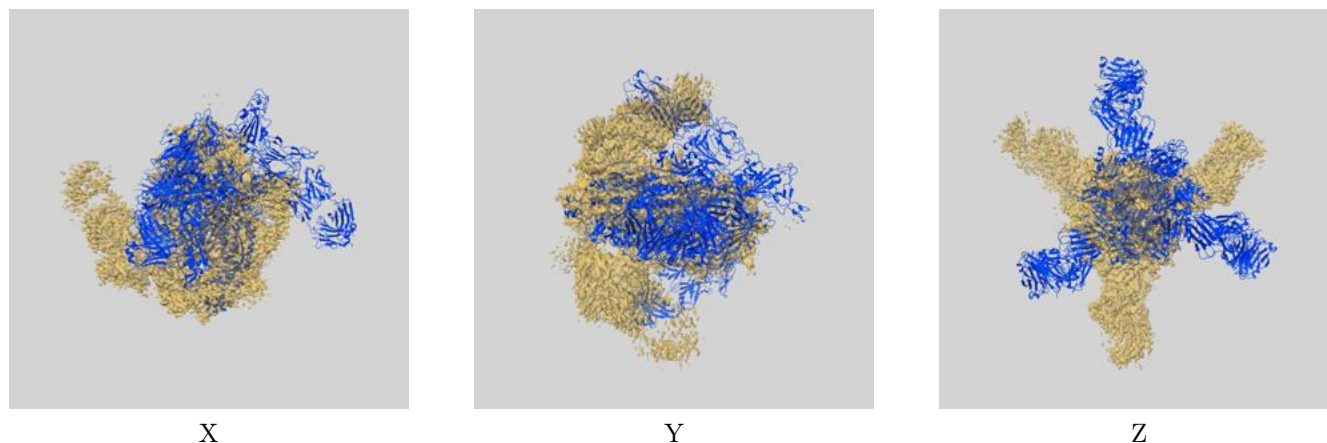
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 3.6 by more than 10 %

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](#)

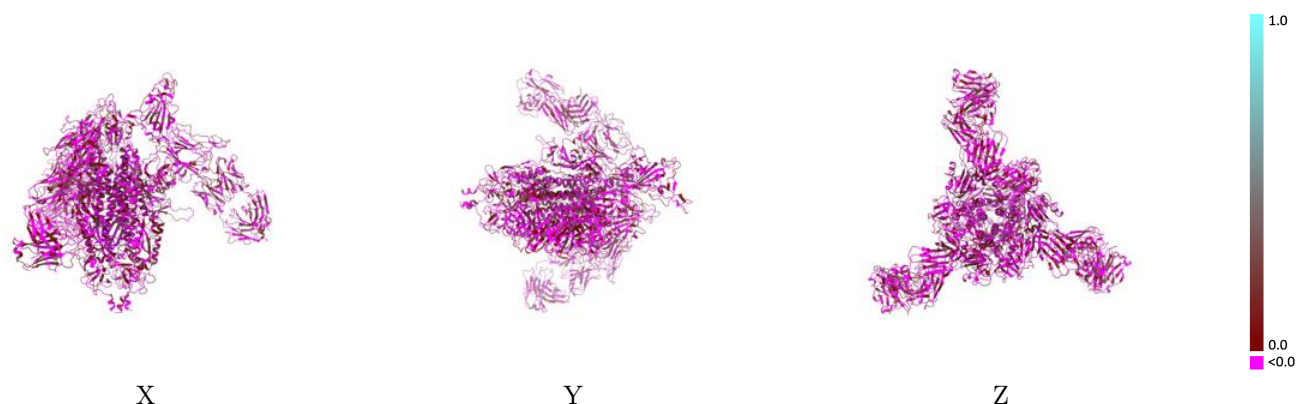
This section contains information regarding the fit between EMDB map EMD-30921 and PDB model 7DZY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



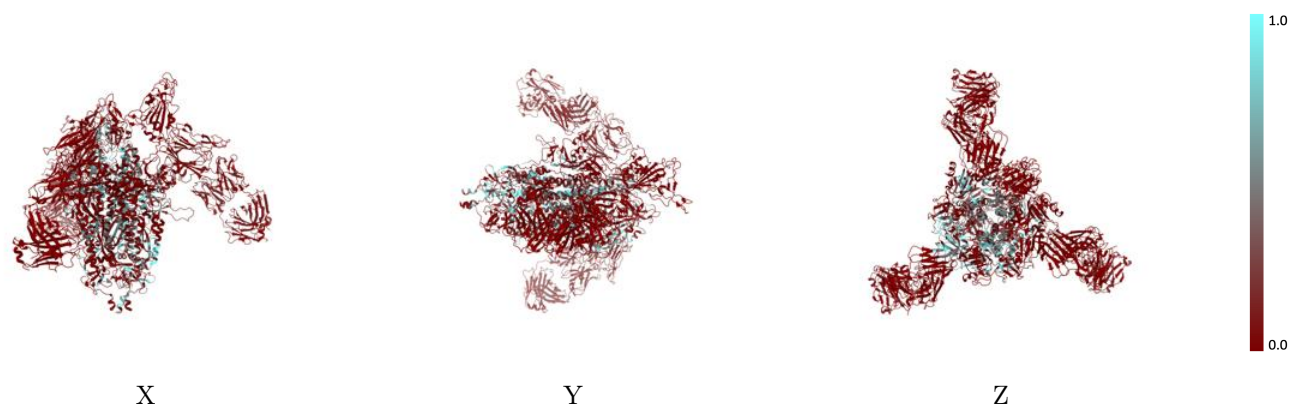
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



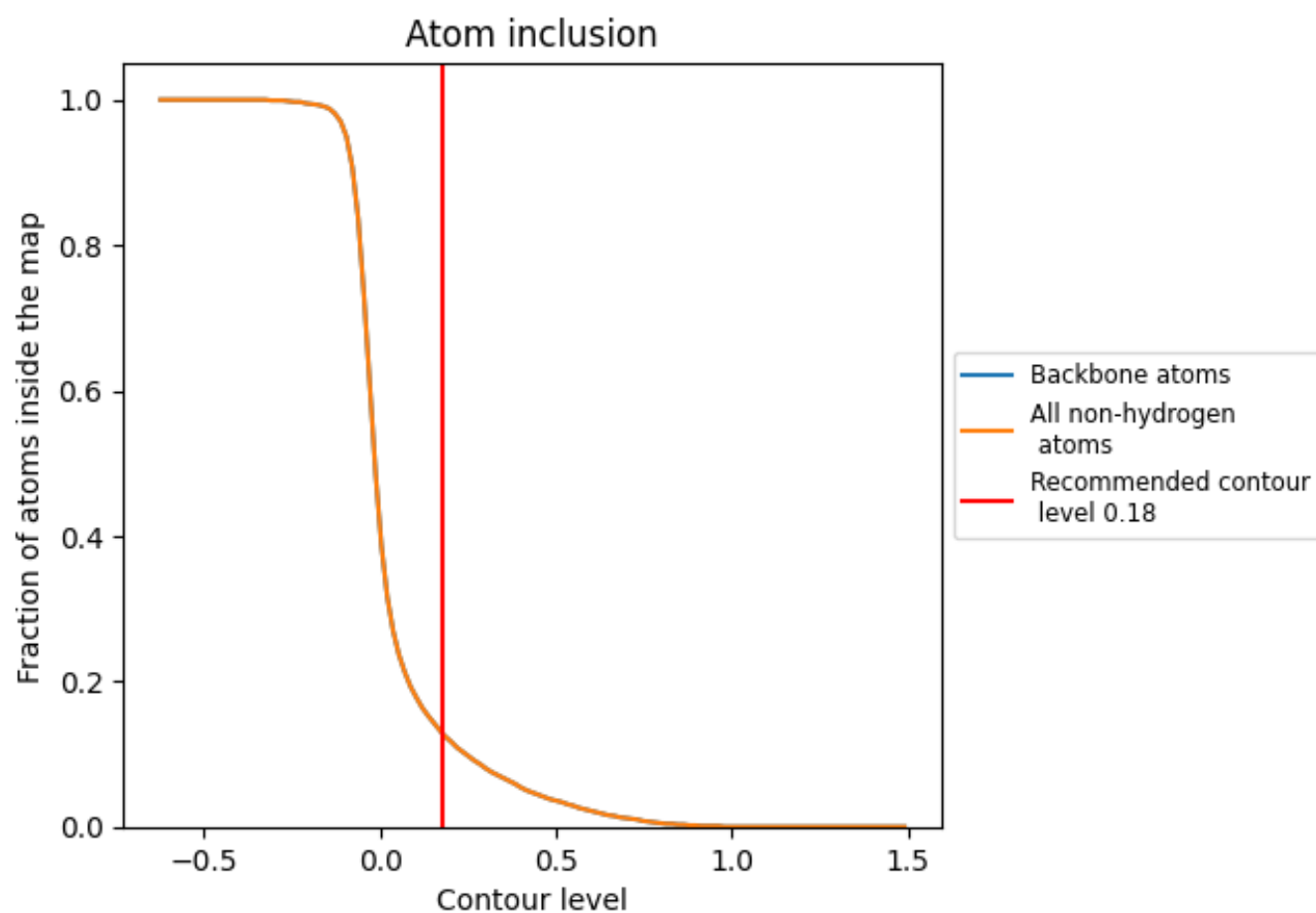
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

1.0
0.0
-0.0