



## wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 07:35 pm GMT

PDB ID : 6ZLW  
EMDB ID : EMD-11276  
Title : SARS-CoV-2 Nsp1 bound to the human 40S ribosomal subunit  
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2020-07-01  
Resolution : 2.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

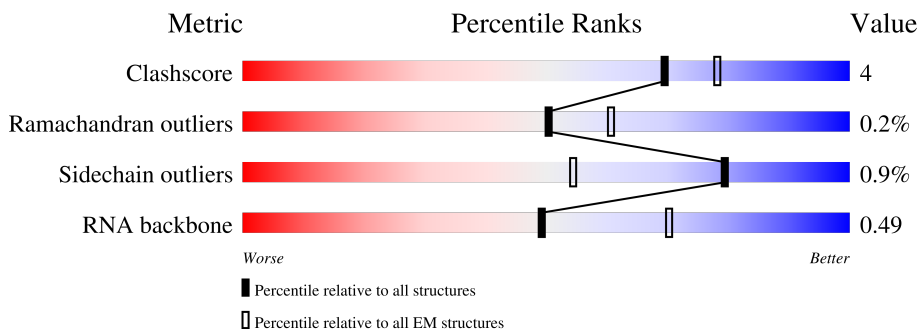
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 2.60 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
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	B	295	
2	C	264	
3	D	293	
4	E	263	
5	F	243	
6	G	249	
7	H	194	


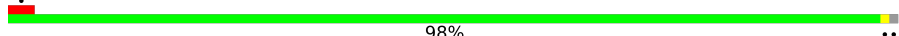


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Mol	Chain	Length	Quality of chain
8	I	208	86% 12% ..
9	J	194	82% 10% • 7%
10	K	204	79% 12% • 7%
11	L	158	83% 13% •
12	M	165	53% 5% 41%
13	N	151	87% 12% •
14	O	132	5% 83% 10% 7%
15	P	151	81% 7% • 11%
16	Q	145	72% 10% 17%
17	R	146	80% 14% • 5%
18	S	135	87% 11% •
19	T	152	78% 16% 6%
20	U	145	92% 7% •
21	V	119	71% 13% • 15%
22	W	130	90% 9% •
23	X	143	85% 13% ..
24	Y	133	86% 8% 7%
25	Z	83	92% 7% •
26	a	125	57% 42%
27	b	84	96% ..
28	c	115	88% 12%
29	d	69	83% 6% 12%
30	e	59	85% • 12%
31	f	56	93% • •
32	g	156	43% 54%

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Mol	Chain	Length	Quality of chain
33	h	25	 88% 12%
34	j	317	 98% ..
35	2	1868	 54% 26% 8% • 11%
36	i	180	 18% 82%

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 74568 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 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	218	Total	C	N	O	S	0	0
			1682	1090	289	293	10		

- Molecule 4 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	225	Total	C	N	O	S	0	0
			1748	1115	315	311	7		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	186	1501	957	276	267	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	205	1682	1056	331	290	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	180	1499	955	300	242	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	189	1495	934	284	270	7	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	151	1229	782	230	211	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	97	816	533	144	133	6	0	0

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	149	1202	770	228	203	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	135	Total	C	N	O	S	0	0
			1006	616	198	186	6		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 17 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 19 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 20 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	101	803	504	153	142	4	0	0

- Molecule 22 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	129	1034	659	193	176	6	0	0

- Molecule 23 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	141	1098	693	219	183	3	0	0

- Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	124	1014	641	198	170	5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	82	625	384	116	120	5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	72	574	368	104	101	1	0	0

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	82	640	402	118	113	7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S26.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 30 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	52	Total	C	N	O	S	0	0
			403	246	89	67	1		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	72	Total	C	N	O	S	0	0
			591	372	114	98	7		

- Molecule 33 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	22	Total	C	N	O	S	0	0
			213	130	57	23	3		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	2	1665	35552	15869	6385	11633	1665	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

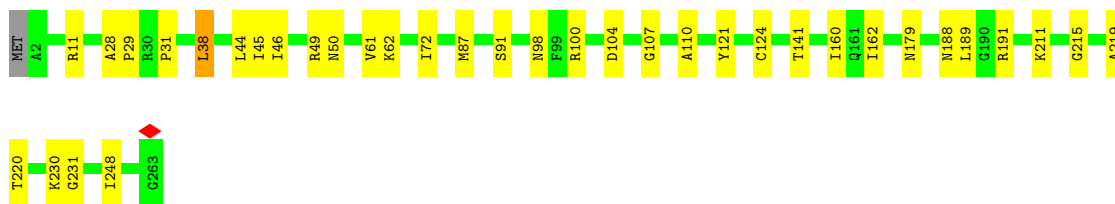
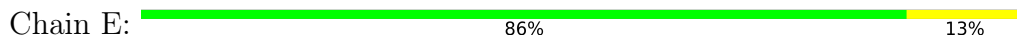
- Molecule 36 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	i	33	261	159	47	54	1	0	0

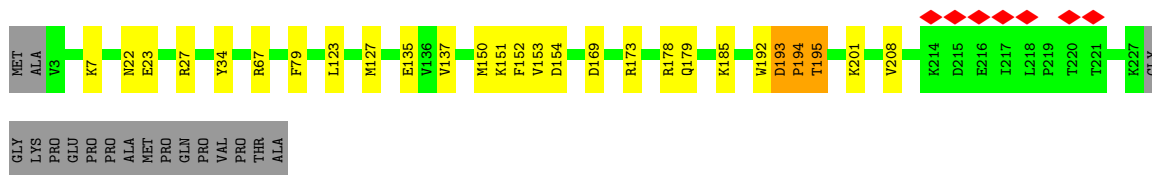
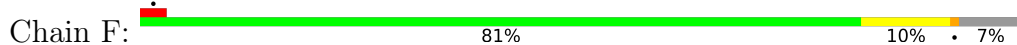
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	c	1	Total	Zn	0
			1	1	
37	f	1	Total	Zn	0
			1	1	
37	g	1	Total	Zn	0
			1	1	

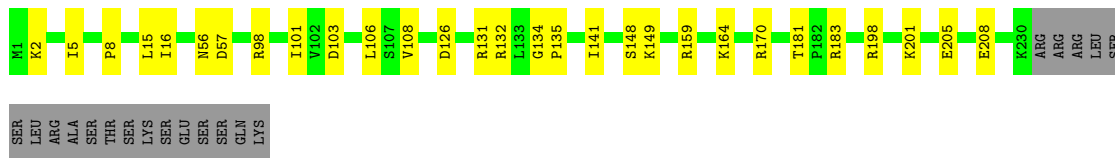
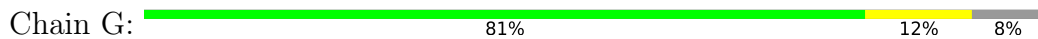




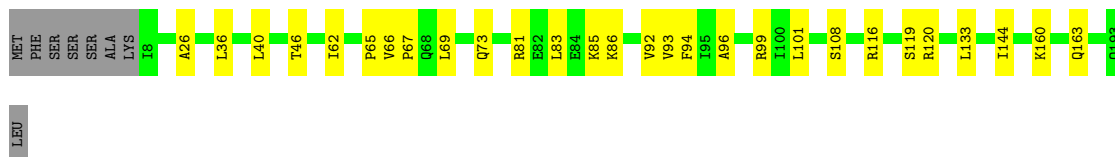
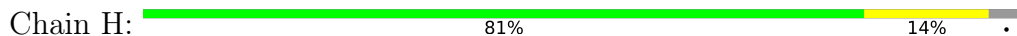
- Molecule 5: 40S ribosomal protein S3



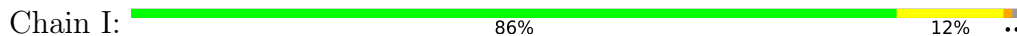
- Molecule 6: 40S ribosomal protein S6



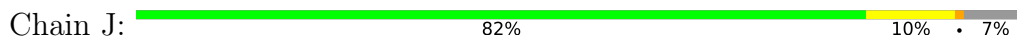
- Molecule 7: 40S ribosomal protein S7



- Molecule 8: 40S ribosomal protein S8

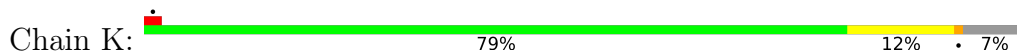


- Molecule 9: 40S ribosomal protein S9

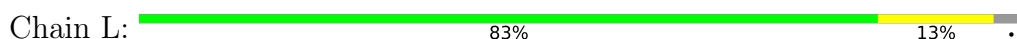




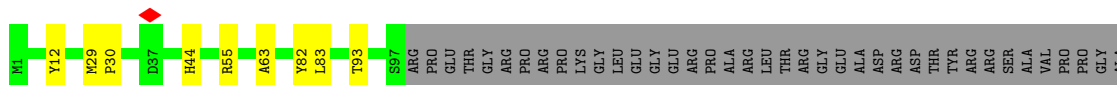
• Molecule 10: 40S ribosomal protein S5



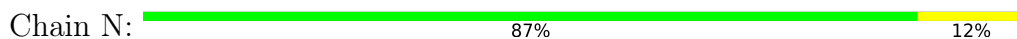
• Molecule 11: 40S ribosomal protein S11



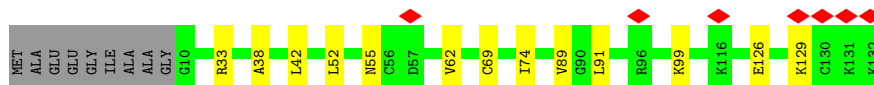
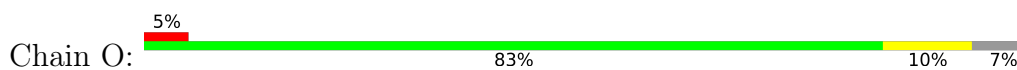
• Molecule 12: 40S ribosomal protein S10



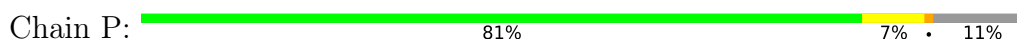
• Molecule 13: 40S ribosomal protein S13



• Molecule 14: 40S ribosomal protein S12



• Molecule 15: 40S ribosomal protein S14

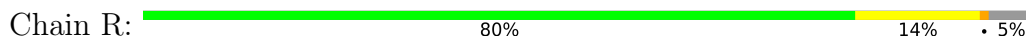




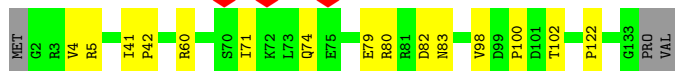
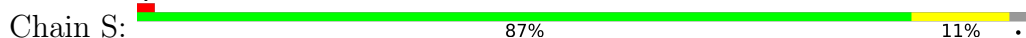
• Molecule 16: 40S ribosomal protein S15



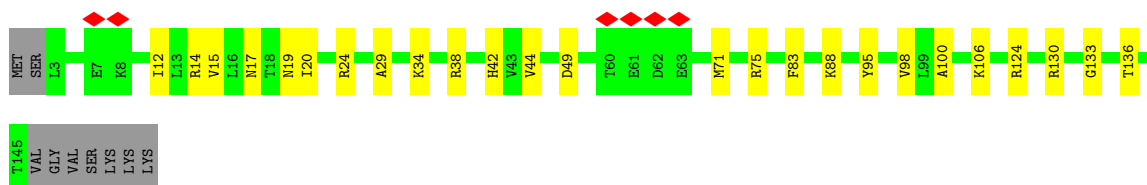
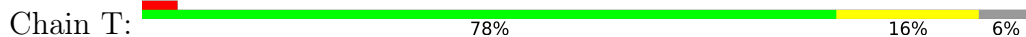
• Molecule 17: 40S ribosomal protein S16



• Molecule 18: 40S ribosomal protein S17



• Molecule 19: 40S ribosomal protein S18



• Molecule 20: 40S ribosomal protein S19



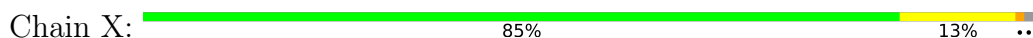
• Molecule 21: 40S ribosomal protein S20



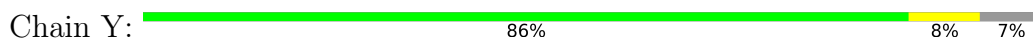
• Molecule 22: 40S ribosomal protein S15a



• Molecule 23: 40S ribosomal protein S23



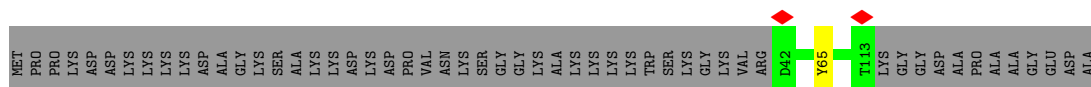
• Molecule 24: 40S ribosomal protein S24



• Molecule 25: 40S ribosomal protein S21



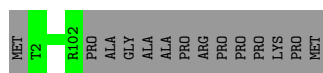
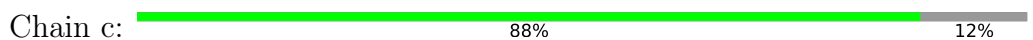
• Molecule 26: 40S ribosomal protein S25



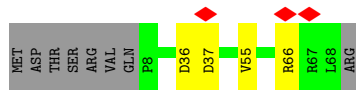
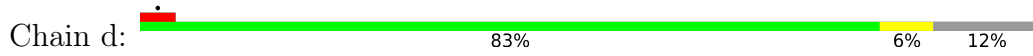
• Molecule 27: 40S ribosomal protein S27



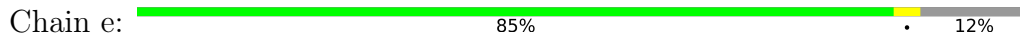
• Molecule 28: 40S ribosomal protein S26



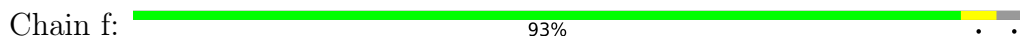
- Molecule 29: 40S ribosomal protein S28



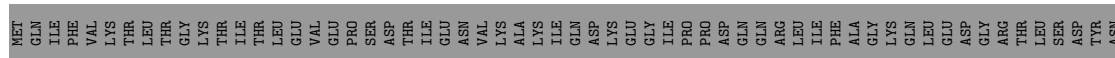
- Molecule 30: 40S ribosomal protein S30



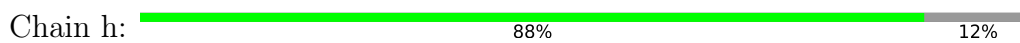
- Molecule 31: 40S ribosomal protein S29



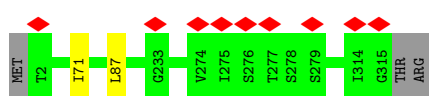
- Molecule 32: Ubiquitin-40S ribosomal protein S27a



- Molecule 33: 60S ribosomal protein L41



- Molecule 34: Receptor of activated protein C kinase 1



- Molecule 35: 18S ribosomal RNA





U1	U115	U214	G	C369	C472	U566	A684	U	C792	G878	G991	U1111	C1213	U1314
A2	U116	G225	C	G370	A473	C567	G685	C	G793	C879	A992	U1112	A1214	U1315
C3	C117	A	U	G373	G474	C568	U666	C	A794	C880	A996	U1113	C1215	G1318
C4	C118	U	U	G374	C475	A569	U667	C	C797	U887	A997	U1114	C1216	G1319
U5	U119	C	U	G377	A476	C570	A668	C	U799	U890	A998	U1115	A1217	G1320
G6	U120	A	U	C382	G482	U572	A669	C	U800	G891	G999	C1117	C1218	G1324
U12	C127	A	U	C383	U487	U573	A670	C	U801	G892	U1002	U1118	G1224	G1325
G16	U128	A	A	G384	U488	U574	A671	C	C803	U896	G1010	U1119	U1225	G1326
C17	C129	A	A	U384	A489	U575	A672	C	U803	U899	G1011	U1120	A1228	U1327
G16	G130	C	A	G385	U489	U576	G673	U	C804	C900	A1011	U1121	G1229	G1327
U	C	C	A	C386	C492	U577	G683	C	U808	G901	A1012	A1122	C1230	G1330
U21	C	A	A	C387	U495	U578	A685	C	A809	G902	U1013	C1123	C1231	U1333
C	U	A	A	U388	A494	U579	U686	C	A810	A903	U1016	G1126	U1232	U1334
C30	C	A	A	A389	U495	U580	C687	C	A811	A904	U1017	G1127	G1233	G1334
G33	C	C	C	A390	C496	U581	U688	U	A812	U914	U1018	G1128	C1234	G1335
G41	C	G	G	C391	C496	U582	U	C	A813	U914	U1019	G1129	G1235	C1336
U44	U140	C	C	A398	A500	U583	U	C	U814	A919	U1022	G1130	G1236	C1337
A45	C	C	C	C399	C501	U584	U	C	G821	A920	A1023	G1131	C1237	U1342
A46	U143	C	C	C400	C502	U585	U	C	U822	A921	A1030	G1132	U1238	U1343
C49	U144	C	C	A401	A508	U586	U	C	U823	G925	U1038	U1137	U1239	G1348
G56	G145	C	C	C402	G509	U587	U	C	C824	G926	U1039	C1138	U1240	U1359
U57	G146	C	C	G407	A516	U588	U	C	A830	G928	G1040	C1139	U1241	U1368
C58	U149	C	C	A408	A516	U589	U	C	C833	G929	G1041	G1140	A1251	U1369
A64	A150	C	C	C409	A516	U590	U	C	C834	C930	U1044	A1143	C1252	C1363
G66	U160	C	C	A409	A516	U591	U	C	C	C931	C1047	A1144	A1253	G1366
C67	C162	C	C	U416	A516	U592	U	C	C	C932	G1048	A1145	G1257	U1371
A68	U163	C	C	U417	A516	U593	U	C	C	C933	A1049	A1148	G1258	U1372
C69	G164	C	C	A418	A516	U594	U	C	C	C934	A1050	A1149	A1259	C1373
G70	U165	C	C	U419	A516	U595	U	C	C	C935	A1060	C1153	C1261	C1374
C71	A164	C	C	C419	A516	U596	U	C	C	C936	U1061	U1154	A1265	A1378
C72	G165	C	C	U420	A516	U597	U	C	C	C937	A1062	G1157	A1266	A1382
G73	C168	C	C	G421	A516	U598	U	C	C	C938	C1075	U1161	C1269	C1389
G74	U178	C	C	U422	A516	U599	U	C	C	C939	C1078	G1165	G1270	G1396
U76	C179	C	C	U423	A516	U600	U	C	C	C940	U1081	G1171	C1271	U1397
C78	G180	C	C	U427	A516	U601	U	C	C	C941	A1082	G1171	G1274	G1398
A79	A181	C	C	U428	A516	U602	U	C	C	C942	A1083	A1189	G1275	G1399
C83	C182	C	C	A433	A516	U603	U	C	C	C943	A1084	A1190	A1276	A1401
G86	G184	C	C	C434	A516	U604	U	C	C	C944	C1085	U1191	C1277	A1402
A99	C188	C	C	U438	A516	U605	U	C	C	C945	G1089	U1192	A1278	C1403
G190	U189	C	C	G438	A516	U606	U	C	C	C946	G1090	A1195	C1279	U1404
C191	G190	C	C	C337	A516	U607	U	C	C	C947	C1091	A1195	C1292	A1405
A191	A191	C	C	G338	A516	U608	U	C	C	C948	G1096	U1201	A1301	G1406
G206	G206	C	C	C339	A516	U609	U	C	C	C949	G1097	U1202	G1302	U1407
U105	U105	C	C	C334	A516	U610	U	C	C	C950	C1098	G1203	C1303	G1411
G113	A209	C	C	C334	A516	U611	U	C	C	C951	G1099	G1207	C1309	G1412
G114	G213	C	C	U	A364	U612	U	C	C	C952	A1100	G1211	C1309	G1413
		C	C	U368	G471	U613	U	C	C	C953	U1101	G1212	A1313	C1415
						U614	U	C	C	C954	G1102			
						U538	U	C	C	C955				
						U541	U	C	C	C956				
						U542	U	C	C	C957				
						C543	U	C	C	C958				
						U544	U	C	C	C959				
						G547	U	C	C	C960				
						C548	U	C	C	C961				
						C549	U	C	C	C962				
						C550	U	C	C	C963				
						U651	U	C	C	C964				
						U652	U	C	C	C965				
						U553	U	C	C	C966				
						A554	U	C	C	C967				
						A555	U	C	C	C968				
						U556	U	C	C	C969				
						G559	U	C	C	C970				
						A560	U	C	C	C971				
						A561	U	C	C	C972				
						U562	U	C	C	C973				
						G563	U	C	C	C974				



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173060	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 ( $e^-/\text{\AA}^2$ )	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	43.872	Depositor
Minimum map value	-25.766	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.716	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	B	0.36	0/1661	0.57	0/2259
2	C	0.32	0/1756	0.55	0/2350
3	D	0.39	0/1718	0.56	0/2322
4	E	0.38	0/2118	0.62	1/2849 (0.0%)
5	F	0.44	0/1776	0.57	0/2392
6	G	0.33	0/1885	0.54	0/2510
7	H	0.30	0/1524	0.58	0/2042
8	I	0.39	0/1711	0.60	1/2282 (0.0%)
9	J	0.39	0/1524	0.62	1/2035 (0.0%)
10	K	0.44	0/1516	0.63	0/2037
11	L	0.46	1/1250 (0.1%)	0.60	0/1673
12	M	0.48	0/840	0.58	0/1133
13	N	0.35	0/1226	0.54	0/1649
14	O	0.31	0/963	0.61	0/1291
15	P	0.37	0/1019	0.57	0/1367
16	Q	0.47	0/1003	0.63	0/1341
17	R	0.52	0/1126	0.68	1/1506 (0.1%)
18	S	0.38	0/1080	0.58	0/1449
19	T	0.47	0/1202	0.68	1/1610 (0.1%)
20	U	0.54	0/1142	0.66	0/1530
21	V	0.39	0/813	0.58	0/1092
22	W	0.39	0/1051	0.59	0/1406
23	X	0.42	0/1116	0.62	0/1490
24	Y	0.37	0/1031	0.58	0/1370
25	Z	0.37	0/631	0.55	0/844
26	a	0.45	0/580	0.66	0/780
27	b	0.39	0/653	0.63	0/876
28	c	0.39	0/828	0.54	0/1109
29	d	0.47	0/481	0.77	2/643 (0.3%)
30	e	0.37	0/406	0.61	0/534
31	f	0.53	0/466	0.68	0/618
32	g	0.37	0/602	0.62	0/795

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	h	0.28	0/214	0.52	0/272
34	j	0.42	0/2497	0.61	1/3399 (0.0%)
35	2	0.90	2/39754 (0.0%)	1.27	398/61950 (0.6%)
36	i	0.33	0/266	0.54	0/358
All	All	0.70	3/79429 (0.0%)	1.01	406/115163 (0.4%)

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
5	F	0	2
10	K	0	2
12	M	0	1
17	R	0	1
18	S	0	1
20	U	0	1
22	W	0	1
23	X	0	1
24	Y	0	1
27	b	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	131	CYS	CB-SG	-5.66	1.72	1.81
35	2	1229	G	C8-N7	-5.24	1.27	1.30
35	2	1229	G	N7-C5	-5.01	1.36	1.39

The worst 5 of 406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	501	C	N1-C2-O2	14.95	127.87	118.90
35	2	501	C	C2-N1-C1'	14.19	134.41	118.80
35	2	501	C	N3-C2-O2	-12.69	113.02	121.90
35	2	1618	C	N3-C2-O2	-12.13	113.41	121.90
35	2	356	C	N1-C2-O2	11.77	125.96	118.90

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	194	PRO	Peptide
5	F	195	THR	Peptide
10	K	165	ASN	Peptide
10	K	40	ALA	Peptide
12	M	63	ALA	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	B	1624	0	1634	16	0
2	C	1729	0	1803	15	0
3	D	1682	0	1769	19	0
4	E	2076	0	2177	22	0
5	F	1748	0	1844	20	0
6	G	1862	0	2018	21	0
7	H	1501	0	1593	18	0
8	I	1682	0	1769	17	0
9	J	1499	0	1618	17	0
10	K	1495	0	1549	15	0
11	L	1229	0	1302	13	0
12	M	816	0	841	5	0
13	N	1202	0	1289	12	0
14	O	953	0	990	7	0
15	P	1006	0	1030	6	0
16	Q	984	0	1028	10	0
17	R	1109	0	1174	13	0
18	S	1066	0	1116	9	0
19	T	1184	0	1244	14	0
20	U	1122	0	1153	6	0
21	V	803	0	873	11	0
22	W	1034	0	1080	7	0
23	X	1098	0	1167	12	0
24	Y	1014	0	1082	5	0
25	Z	625	0	628	6	0
26	a	574	0	627	0	0
27	b	640	0	665	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	814	0	864	0	0
29	d	479	0	507	0	0
30	e	403	0	432	0	0
31	f	455	0	446	0	0
32	g	591	0	622	0	0
33	h	213	0	258	0	0
34	j	2440	0	2396	0	0
35	2	35552	0	17949	160	0
36	i	261	0	229	0	0
37	c	1	0	0	0	0
37	f	1	0	0	0	0
37	g	1	0	0	0	0
All	All	74568	0	58766	387	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 4.

The worst 5 of 387 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)
35:2:925:G:H1	35:2:1017:U:H3	1.02	0.90
35:2:1729:U:H3	35:2:1805:G:H1	1.26	0.81
17:R:11:GLN:HE21	17:R:71:ARG:HH12	1.36	0.74
20:U:76:THR:HG22	20:U:94:ARG:HB3	1.73	0.70
19:T:133:GLY:HA3	35:2:1623:A:H5''	1.75	0.69

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	B	204/295 (69%)	195 (96%)	9 (4%)	0	100	100
2	C	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
3	D	216/293 (74%)	211 (98%)	5 (2%)	0	100	100
4	E	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
5	F	223/243 (92%)	211 (95%)	10 (4%)	2 (1%)	17	35
6	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
7	H	184/194 (95%)	179 (97%)	5 (3%)	0	100	100
8	I	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
9	J	178/194 (92%)	170 (96%)	7 (4%)	1 (1%)	25	47
10	K	187/204 (92%)	176 (94%)	8 (4%)	3 (2%)	9	19
11	L	149/158 (94%)	140 (94%)	9 (6%)	0	100	100
12	M	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
13	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
14	O	121/132 (92%)	118 (98%)	3 (2%)	0	100	100
15	P	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
16	Q	118/145 (81%)	116 (98%)	2 (2%)	0	100	100
17	R	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
18	S	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
19	T	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
20	U	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
21	V	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
22	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
23	X	139/143 (97%)	135 (97%)	3 (2%)	1 (1%)	22	43
24	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
25	Z	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
26	a	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
27	b	80/84 (95%)	72 (90%)	8 (10%)	0	100	100
28	c	99/115 (86%)	99 (100%)	0	0	100	100
29	d	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
30	e	48/59 (81%)	45 (94%)	2 (4%)	1 (2%)	7	13
31	f	52/56 (93%)	50 (96%)	0	2 (4%)	3	4
32	g	70/156 (45%)	62 (89%)	6 (9%)	2 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	20/25 (80%)	20 (100%)	0	0	100	100
34	j	312/317 (98%)	293 (94%)	19 (6%)	0	100	100
36	i	31/180 (17%)	29 (94%)	2 (6%)	0	100	100
All	All	4815/5681 (85%)	4625 (96%)	178 (4%)	12 (0%)	50	71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	K	166	ILE
32	g	89	LYS
9	J	161	LEU
10	K	41	VAL
32	g	83	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	172/243 (71%)	171 (99%)	1 (1%)	86	95
2	C	194/231 (84%)	194 (100%)	0	100	100
3	D	182/225 (81%)	180 (99%)	2 (1%)	73	88
4	E	224/225 (100%)	223 (100%)	1 (0%)	91	97
5	F	188/202 (93%)	187 (100%)	1 (0%)	88	96
6	G	200/218 (92%)	200 (100%)	0	100	100
7	H	167/174 (96%)	167 (100%)	0	100	100
8	I	178/180 (99%)	176 (99%)	2 (1%)	73	88
9	J	160/168 (95%)	158 (99%)	2 (1%)	69	86
10	K	159/170 (94%)	157 (99%)	2 (1%)	69	86
11	L	135/142 (95%)	133 (98%)	2 (2%)	65	83
12	M	88/136 (65%)	87 (99%)	1 (1%)	73	88
13	N	130/131 (99%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	104/108 (96%)	103 (99%)	1 (1%)	76	90
15	P	104/119 (87%)	100 (96%)	4 (4%)	33	59
16	Q	107/130 (82%)	106 (99%)	1 (1%)	78	91
17	R	115/121 (95%)	115 (100%)	0	100	100
18	S	118/122 (97%)	117 (99%)	1 (1%)	81	92
19	T	124/132 (94%)	123 (99%)	1 (1%)	81	92
20	U	114/115 (99%)	113 (99%)	1 (1%)	78	91
21	V	93/107 (87%)	91 (98%)	2 (2%)	52	76
22	W	112/113 (99%)	111 (99%)	1 (1%)	78	91
23	X	113/115 (98%)	111 (98%)	2 (2%)	59	80
24	Y	108/115 (94%)	108 (100%)	0	100	100
25	Z	66/67 (98%)	66 (100%)	0	100	100
26	a	64/103 (62%)	63 (98%)	1 (2%)	62	82
27	b	74/76 (97%)	74 (100%)	0	100	100
28	c	88/98 (90%)	88 (100%)	0	100	100
29	d	54/62 (87%)	52 (96%)	2 (4%)	34	60
30	e	40/48 (83%)	39 (98%)	1 (2%)	47	73
31	f	48/49 (98%)	48 (100%)	0	100	100
32	g	65/140 (46%)	62 (95%)	3 (5%)	27	51
33	h	21/24 (88%)	21 (100%)	0	100	100
34	j	272/275 (99%)	271 (100%)	1 (0%)	91	97
36	i	27/151 (18%)	27 (100%)	0	100	100
All	All	4208/4835 (87%)	4172 (99%)	36 (1%)	79	91

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	a	65	TYR
34	j	71	ILE
29	d	55	VAL
32	g	85	TYR
11	L	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
17	R	142	GLN
25	Z	47	ASN
18	S	83	ASN
23	X	46	HIS
28	c	25	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	2	1655/1868 (88%)	407 (24%)	41 (2%)

5 of 407 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	2	2	A
35	2	3	C
35	2	17	C
35	2	33	G
35	2	41	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	2	1438	A
35	2	1623	A
35	2	1440	C
35	2	1558	C
35	2	1734	G

## 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1550:G	O3'	1551:U	P	4.52

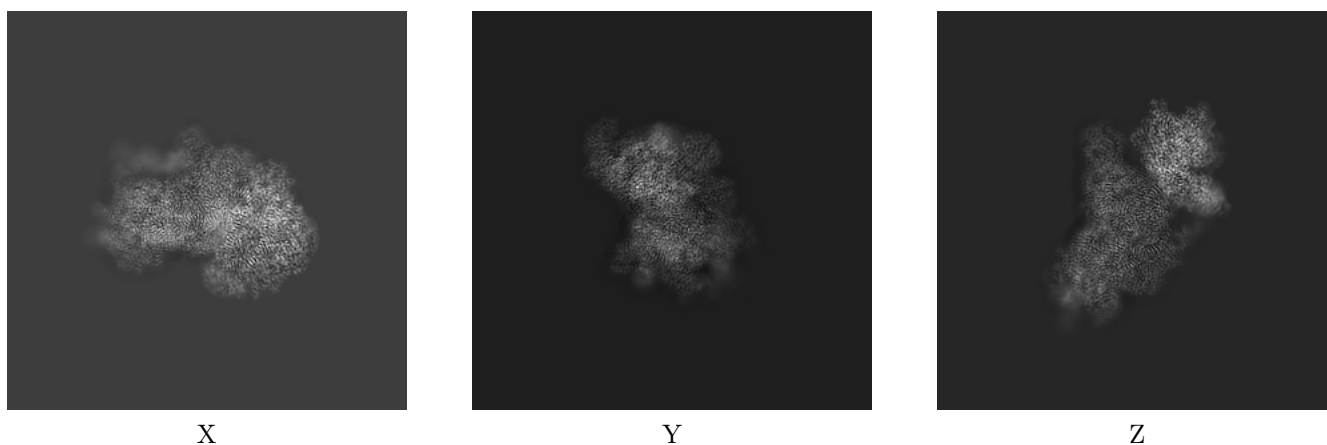
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11276. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

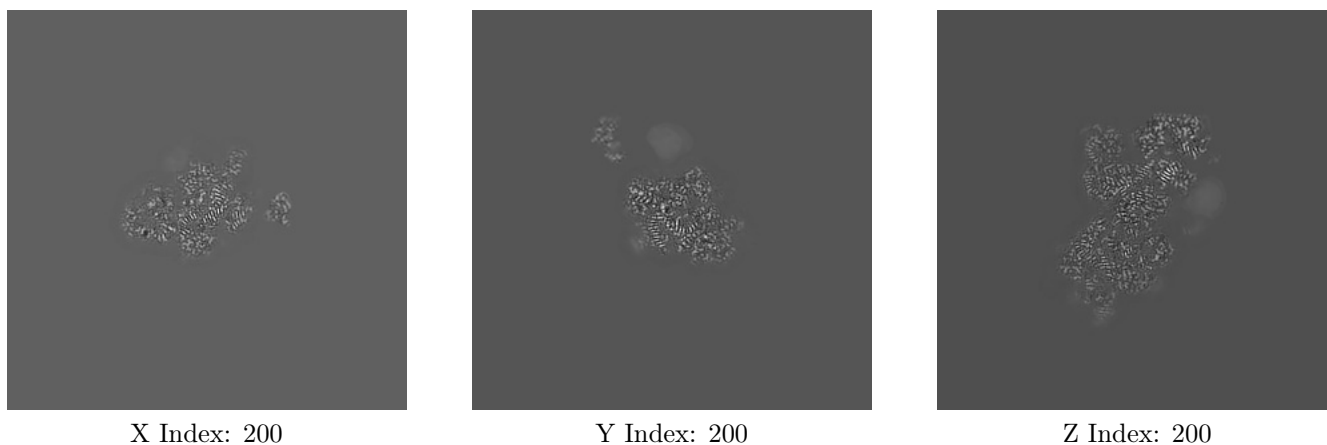
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

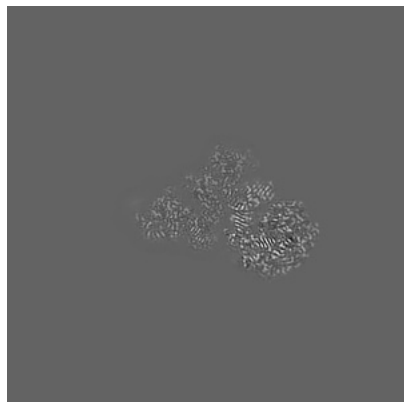
#### 6.2.1 Primary map



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

## 6.3 Largest variance slices [i](#)

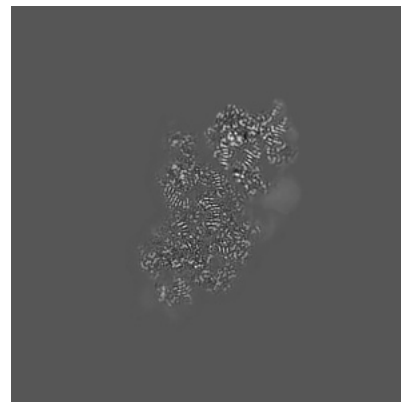
### 6.3.1 Primary map



X Index: 224



Y Index: 269



Z Index: 191

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

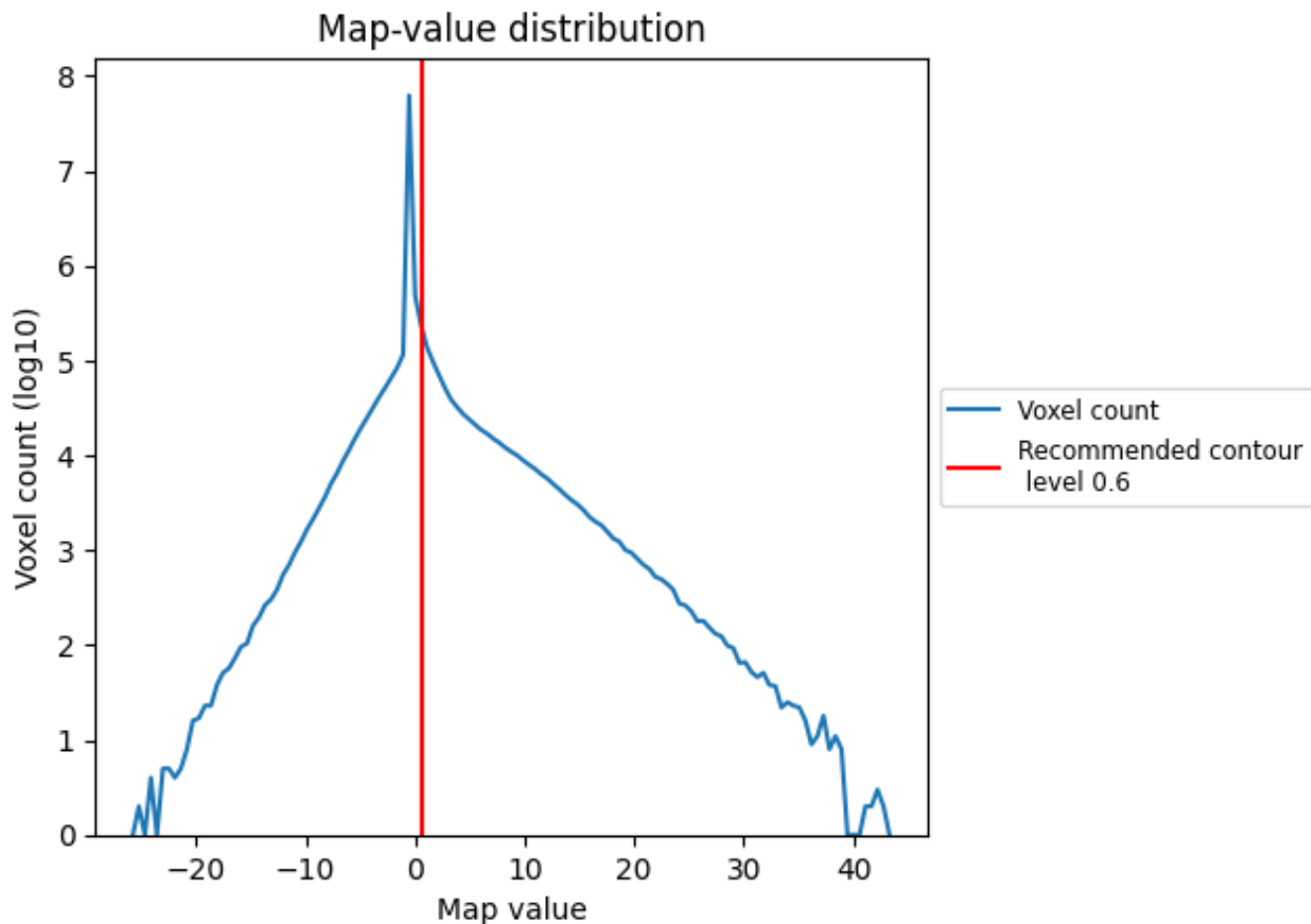
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

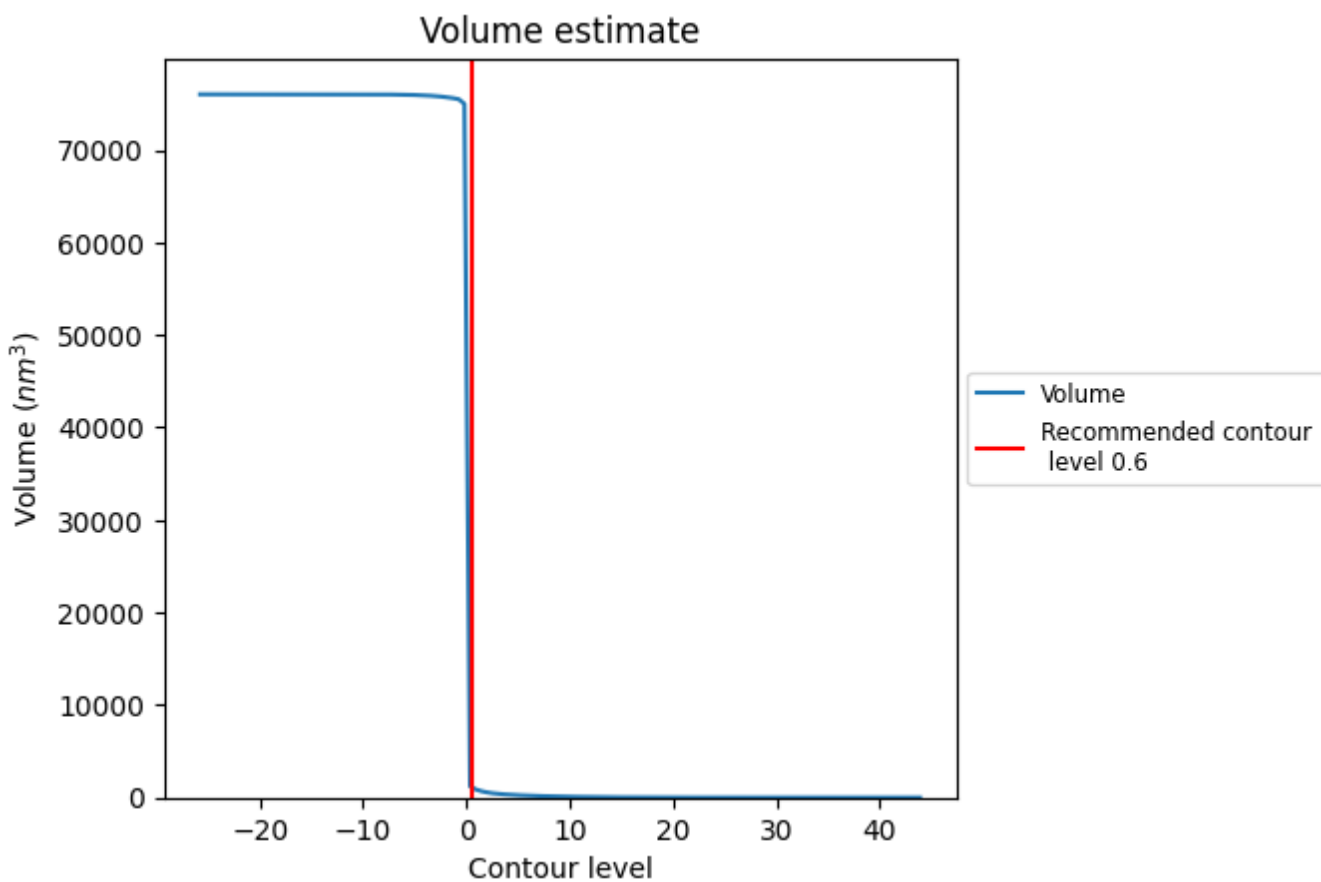
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



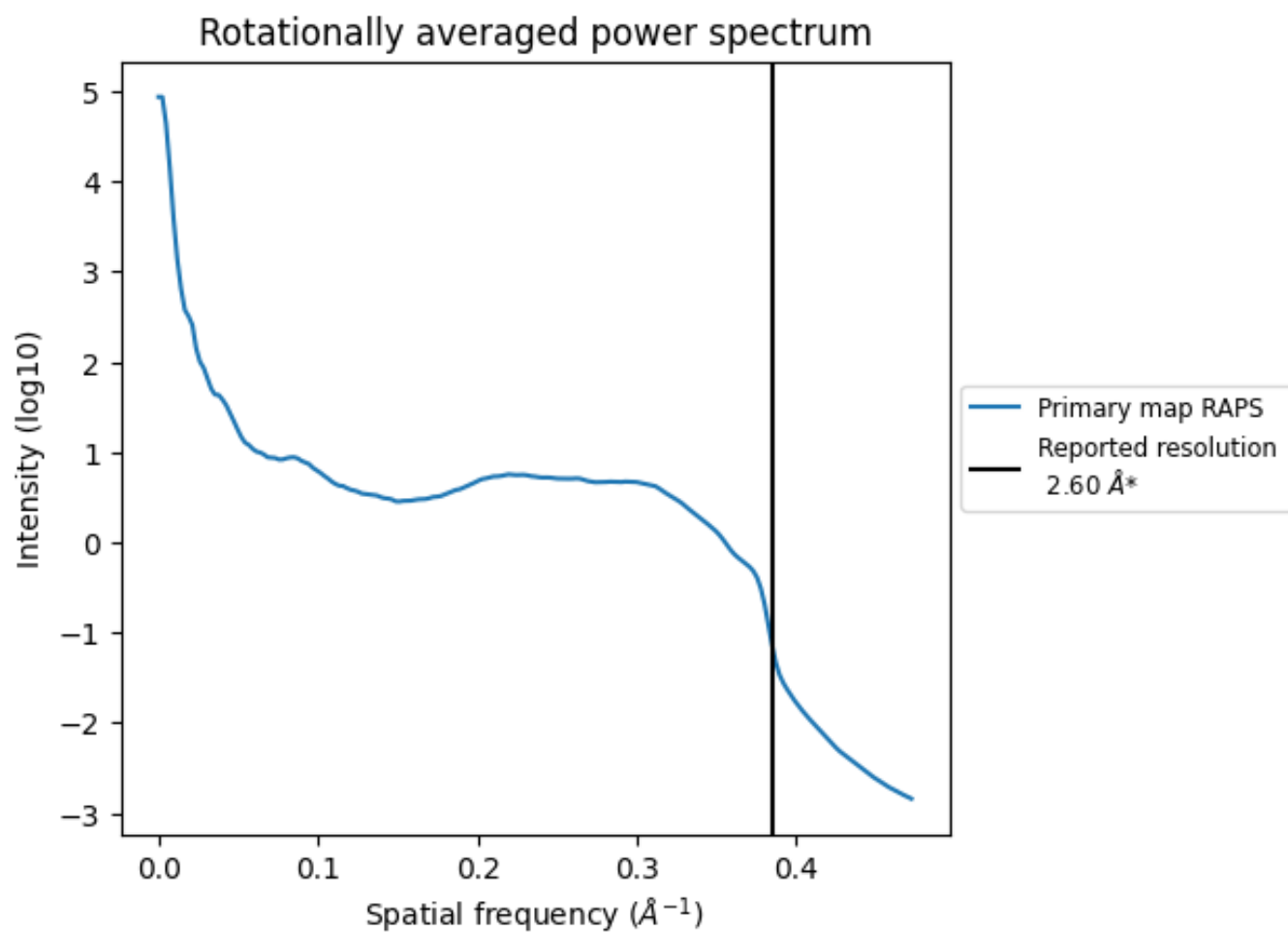
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1067 nm<sup>3</sup>; this corresponds to an approximate mass of 964 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 0.385 Å<sup>-1</sup>

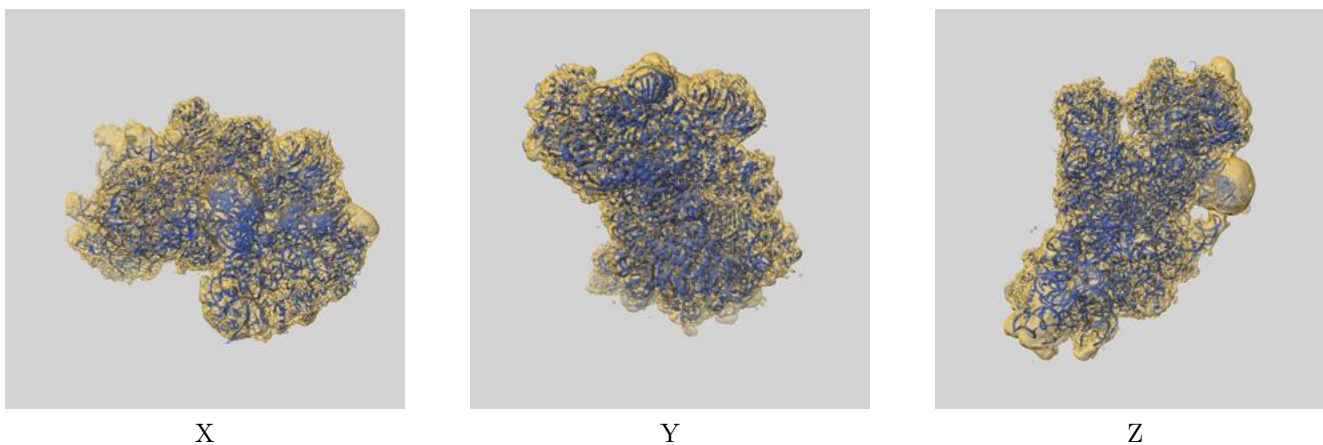
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

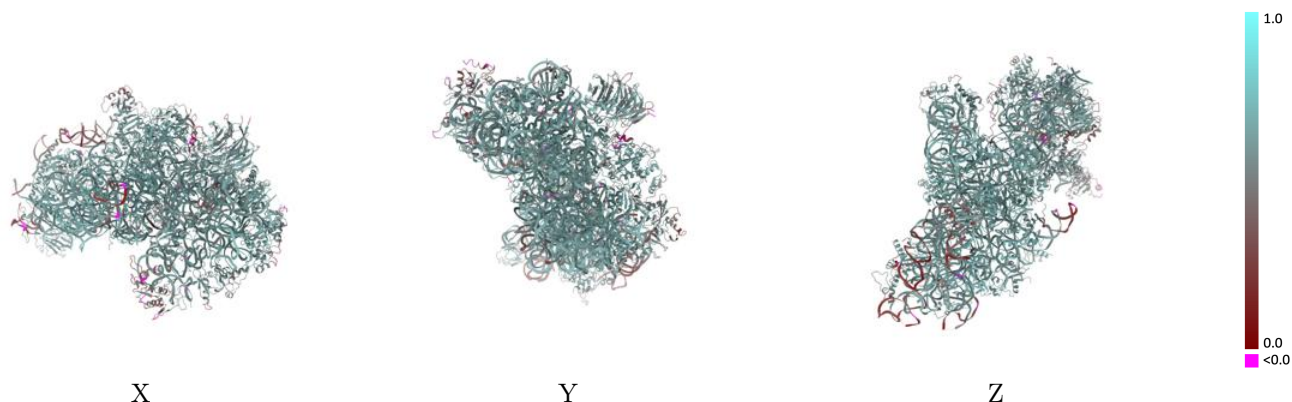
This section contains information regarding the fit between EMDB map EMD-11276 and PDB model 6ZLW. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



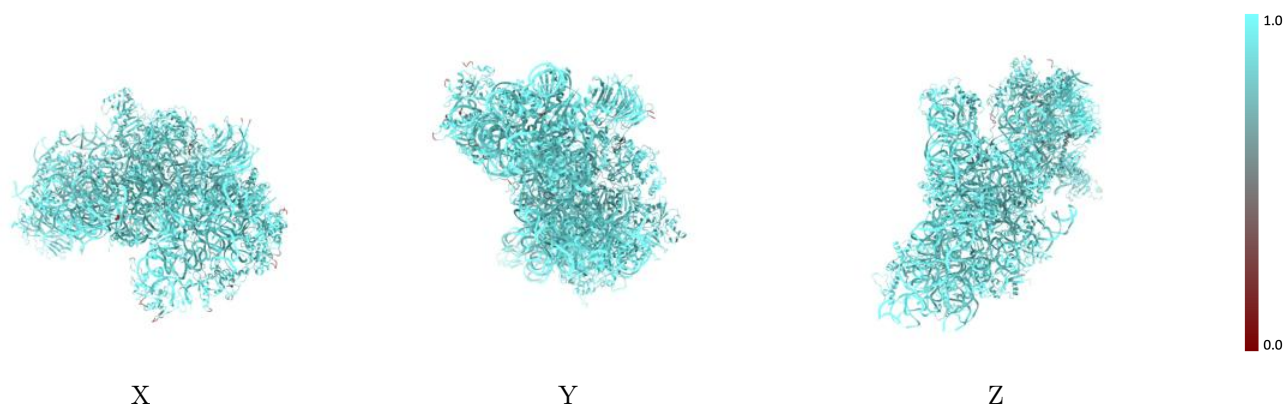
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



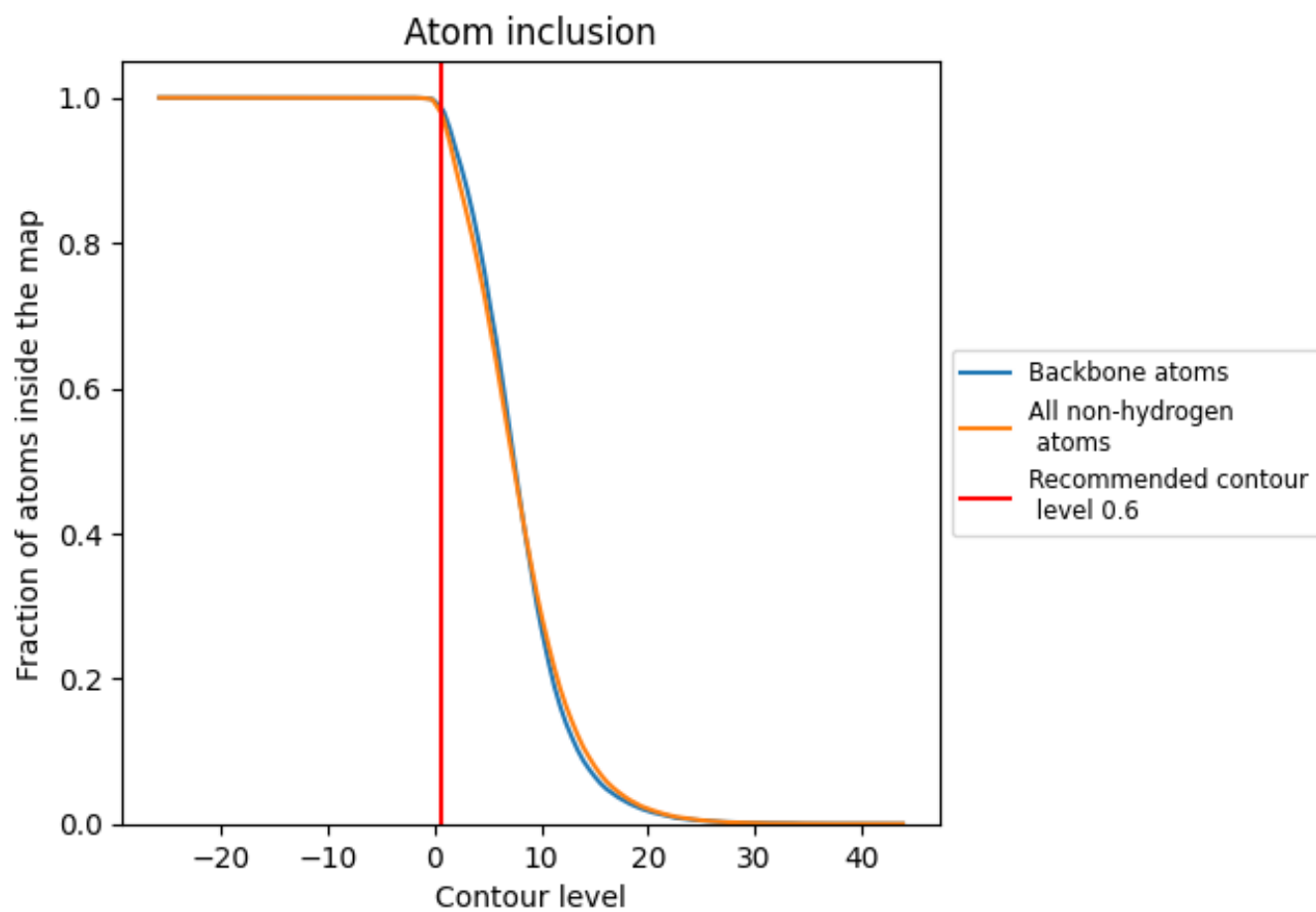
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9796	 0.5950
2	 0.9936	 0.6080
B	 0.9817	 0.6240
C	 0.9747	 0.6020
D	 0.9903	 0.6510
E	 0.9877	 0.6470
F	 0.9548	 0.5420
G	 0.9856	 0.5770
H	 0.9443	 0.5000
I	 0.9827	 0.6010
J	 0.9882	 0.6470
K	 0.9484	 0.5670
L	 0.9774	 0.6130
M	 0.9749	 0.5750
N	 0.9906	 0.6230
O	 0.8850	 0.3610
P	 0.9744	 0.5920
Q	 0.9382	 0.5510
R	 0.9925	 0.6260
S	 0.9411	 0.5180
T	 0.9201	 0.5390
U	 0.9542	 0.5930
V	 0.9731	 0.5370
W	 0.9901	 0.6580
X	 0.9832	 0.6420
Y	 0.9868	 0.6210
Z	 0.9771	 0.6230
a	 0.9234	 0.5440
b	 0.9729	 0.5820
c	 0.9706	 0.6120
d	 0.9046	 0.5020
e	 0.9768	 0.6010
f	 0.9817	 0.6170
g	 0.8957	 0.4450
h	 0.9897	 0.6010



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Chain	Atom inclusion	Q-score
i	 0.9804	 0.6280
j	 0.9553	 0.5480