



wwPDB EM Validation Summary Report ⓘ

May 5, 2026 – 04:35 pm BST

PDB ID : 9R3D / pdb_00009r3d
EMDB ID : EMD-53554
Title : Cryo-EM structure of the human pre-Bact-OTS complex (whole map)
Authors : Zhang, Z.; Kumar, V.; Zhong, J.; Dybkov, O.; Kastner, B.; Urlaub, H.;
Luhmann, R.
Deposited on : 2025-05-04
Resolution : 3.12 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

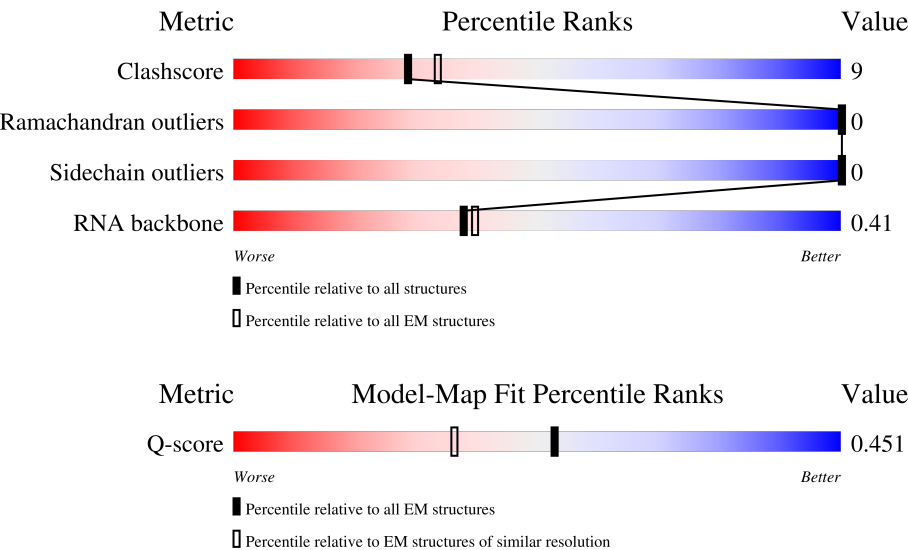
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.12 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14478 (2.62 - 3.62)

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 <=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	5	77	<div><div>19%</div><div>47%</div><div>39%</div><div>14%</div></div>
2	6	85	<div><div>26%</div><div>45%</div><div>49%</div><div>6%</div></div>
3	B	2136	<div><div>36%</div><div>39%</div><div>59%</div></div>

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Mol	Chain	Length	Quality of chain
4	C	972	
5	I	312	
6	K	439	
7	Q	144	
8	T	1098	
9	X	641	
10	Z	29	
11	q	73	
12	r	199	
13	P7	579	
14	A	2335	
15	P	420	
16	t	520	
17	S1	526	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 41862 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 RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	77	Total	C	N	O	P	0	0
			1620	726	271	546	77		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	85	Total	C	N	O	P	0	0
			1821	815	340	581	85		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	868	Total	C	N	O	0	0
			4369	2633	868	868		

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	843	Total	C	N	O	S	0	0
			6649	4250	1117	1249	33		

- Molecule 5 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	184	Total	C	N	O	S	0	0
			1521	978	256	277	10		

- Molecule 6 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	137	Total	C	N	O	S	0	0
			940	590	169	179	2		

- Molecule 7 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	142	Total	C	N	O	S	0	0
			1173	738	216	208	11		

- Molecule 8 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	224	Total	C	N	O	S	0	0
			1691	1035	326	328	2		

- Molecule 9 is a protein called WW domain-binding protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	35	Total	C	N	O	S	0	0
			291	177	62	48	4		

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	29	Total	C	N	O	P	0	0
			619	277	113	200	29		

- Molecule 11 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	73	Total	C	N	O	S	0	0
			599	383	103	109	4		

- Molecule 12 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	89	Total	C	N	O	S	0	0
			728	452	137	132	7		

- Molecule 13 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P7	18	Total	C	N	O	0	0
			92	56	18	18		

- Molecule 14 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	2208	Total	C	N	O	S	1	0
			17219	11011	3064	3074	70		

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	161	Total	C	N	O	S	0	0
			1309	825	232	236	16		

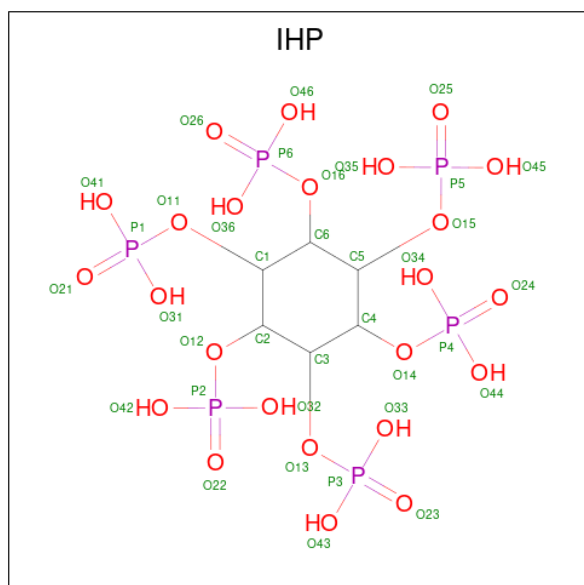
- Molecule 16 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	t	83	Total	C	N	O	S	0	0
			661	428	107	125	1		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S1	80	Total	C	N	O	S	0	0
			524	322	100	100	2		

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

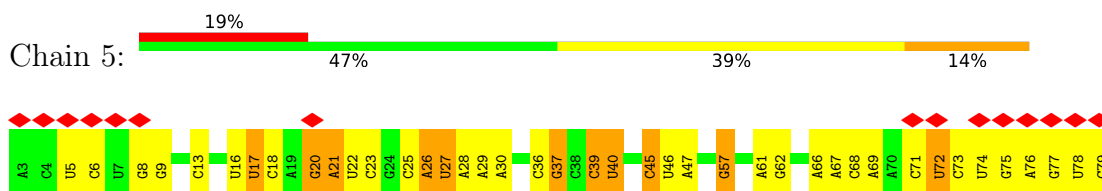


Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			36	6	24	6	

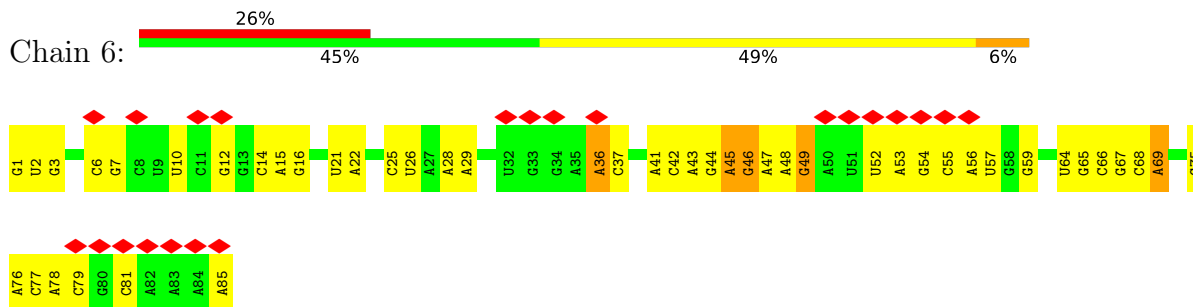
3 Residue-property plots

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.

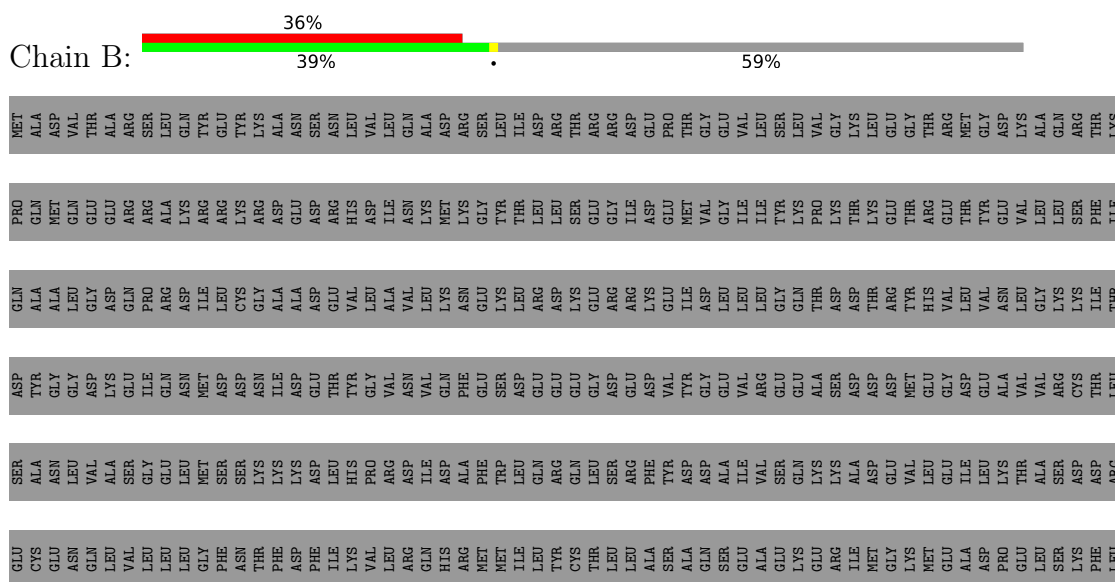
• Molecule 1: U5 snRNA



• Molecule 2: U6 snRNA



• Molecule 3: U5 small nuclear ribonucleoprotein 200 kDa helicase

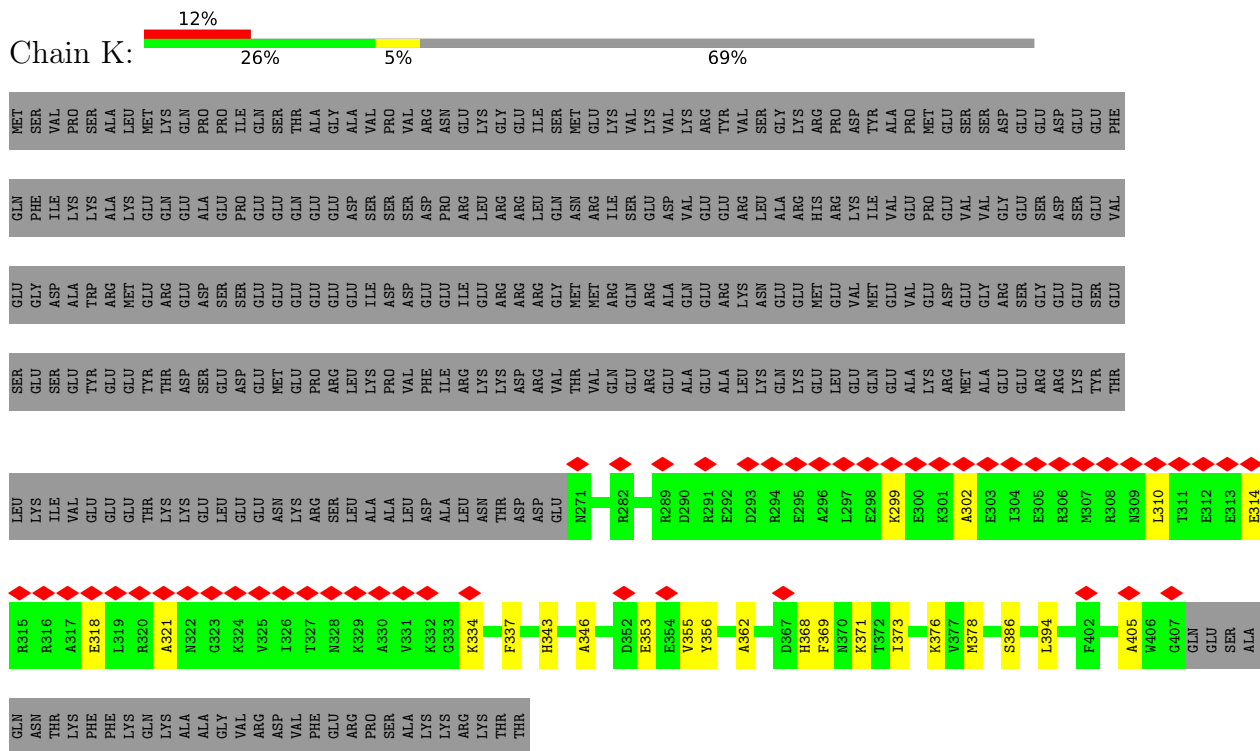


TTR	GLN	LEU	HIS	GLU	THR	GLU	LYS	GLU	ASP	LEU	ILE	ARG	GLU	ARG	SER	ARG	ARG	GLU	VAL	ARG	GLN	SER	GLN	MET	ASP	THR	ASP	LEU	GLU	THR	MET	ASP	LEU	GLN	GLY	GLU	ALA	LEU	ALA	PRO	ARG	GLN	VAL	LEU	ASP	LEU	GLU	LEU	VAL	PHE	THR	GLN	G419	S420						
H421	F422	M423	A424	K425	K426	R427	C428	Q429	L430	P431	D432	G433	S434	F435	R436	R437	Q438	R439	K440	G441	Y442	E443	E444	V445	V446	V447	P448	A449	L450	K451	P452	P453	K453	P454	F455	G456	S457	E458	E459	Q460	L461	L462	P463	V464	E465	K466	L467	P468	K469	Y470	A471	Q472	A473	G474	F475	E476	G477	F478	K479	T480
L481	M482	R483	I484	Q485	S486	K487	L488	Y489	R490	A491	D492	L493	E494	T495	D496	E497	N498	L499	L500	L501	C502	A503	P504	T505	G506	A507	G508	K509	T510	N511	V512	A513	L514	M515	C516	M517	L518	R519	E520	L521	G522	K523	H524	I525	N526	M527	D528	G529	T530	I531	N532	V533	D534	D535	F536	K537	I538	I539	Y540	
I541	A542	P543	M544	R545	S546	L547	Q548	Q549	E550	M551	V552	G553	S554	F555	G556	K557	R558	L559	A560	T561	Y562	G563	I564	T565	V566	A567	E568	L569	T570	G571	D572	H573	Q574	L575	C576	K577	E578	E579	I580	S581	A582	T583	Q584	I585	I586	V587	C588	T589	P590	E591	K592	V593	D594	I595	I596	T597	R598	K599	G600	
G601	E602	R603	T604	Y605	T606	Q607	L608	V609	R610	L611	I612	G613	L614	D615	E616	I617	H618	L619	L620	H621	D622	D623	R624	G625	P626	V627	L628	E629	A630	L631	V632	A633	R634	A635	I636	R637	N638	I639	E640	M641	T642	Q643	E644	D645	V646	R647	L648	I649	G650	L651	S652	A653	T654	L655	P656	N657	Y658	E659	D660	
V661	A662	T663	F664	L665	R666	V667	D668	P669	A670	K671	G672	L673	F674	Y675	F676	D677	N678	S679	F680	R681	P682	V683	P684	L685	E686	Q687	T688	Y689	V690	G691	L692	T693	E694	K695	K696	A697	S698	K699	R700	F701	Q702	I703	M704	N705	E706	I707	V708	Y709	E710	K711	I712	M713	E714	H715	A716	G717	K718	N719	Q720	
V721	L722	V723	F724	V725	H726	S727	R728	K729	E730	T731	G732	K733	T734	A735	R736	A737	L738	R739	D740	H741	C742	L743	E744	K745	D746	T747	L748	G749	L750	F751	L752	R753	E754	G755	S756	A757	S758	T759	E760	V761	L762	R763	T764	E765	A766	E767	Q768	C769	K770	N771	L772	K775	D776	L777	L778	P779	Y780	G781		
F782	A783	I784	H785	H786	A787	G788	M789	T790	R791	V792	D793	R794	T795	L796	V797	E798	D799	L800	F801	A802	D803	K804	H805	L806	Q807	V808	L809	V810	S811	T812	A813	T814	L815	A816	M817	C818	V819	N820	L821	P822	A823	H824	T825	V826	I827	T828	K829	G830	T831	Q832	V833	H834	S835	K836	E837	K838	G839	R840	H841	
T842	E843	L844	G845	A846	L847	D848	T849	L850	Q851	H852	L853	G854	R855	A856	G857	R858	P859	Q860	Y861	D862	T863	K864	G865	E866	G867	T868	L869	T870	S871	H872	G873	C874	L875	E876	L877	Q877	Y878	Y879	L880	S881	L882	L883	N884	Q885	Q886	L887	P888	T889	E890	S891	Q892	H893	H894	S895	K896	L897	P898	D899	M900	L901
N902	A903	E904	I905	V906	L907	Q908	N909	V910	Q911	N912	A913	K914	D915	A916	W919	L920	G921	A923	Y924	L925	Y926	I927	R928	N929	L930	R931	S932	P933	T934	L935	Y936	G937	I938	S939	H940	D941	D942	L943	K944	G945	D946	P947	L948	L949	D950	Q951	R952	R953	L954	D955	L956	V957	H958	T959	A960	A961	L962			
M963	L964	D965	K966	N967	N968	L969	V970	K971	Y972	D973	K974	K975	T976	G977	N978	F979	Q980	V981	T982	E983	L984	G985	I987	A988	H989	H990	Y991	Y992	L993	T994	N995	D996	T997	V998	Y1001	N1002	Q1003	L1004	L1005	K1006	P1007	T1008	L1009	S1010	E1011	I1012	R1016	V1017	F1018	S1019	L1020	S1021	S1022	F1024	K1025					
N1026	I1027	T1028	V1029	R1030	E1031	E1032	E1033	K1034	L1035	A1036	L1037	P1045	I1046	K1049	E1050	S1051	I1052	E1053	E1054	P1055	S1056	A1057	K1058	I1059	L1063	Q1064	A1065	F1066	Q1069	L1070	K1071	L1072	E1073	G1074	F1075	A1076	L1077	M1078	A1079	D1080	M1081	V1082	Y1083	Y1084	T1085	Q1086	S1087	A1088	G1089	R1090	L1091	M1092	R1093	A1094	I1095					
F1096	E1097	I1098	V1099	L1100	M1101	R1102	G1103	V1104	A1105	Q1106	T1107	T1108	D1109	K1110	N1113	L1114	C1115	K1116	M1117	I1118	D1119	K1120	R1121	Q1124	S1125	M1126	C1127	P1128	R1129	Q1130	Q1131	F1132	R1133	K1134	L1135	P1136	E1137	E1138	V1139	V1140	I1143	E1144	K1145	K1146	N1147	F1148	P1149	F1150	E1151	R1152	L1153	Y1154	D1155	L1156	N1157	H1158				

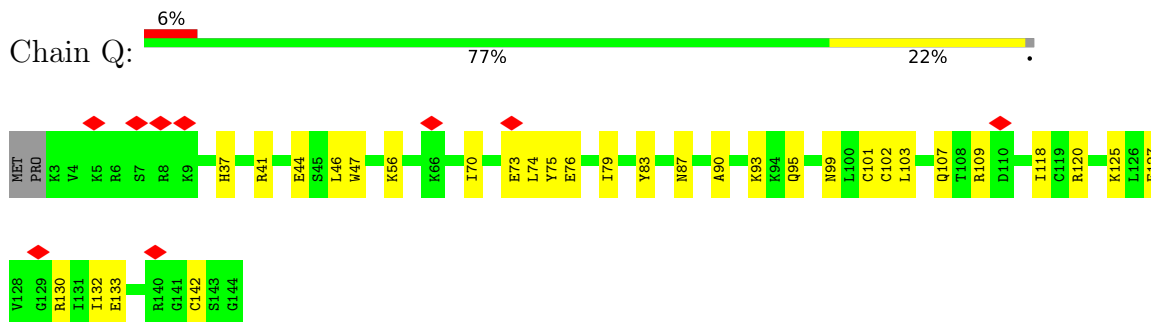




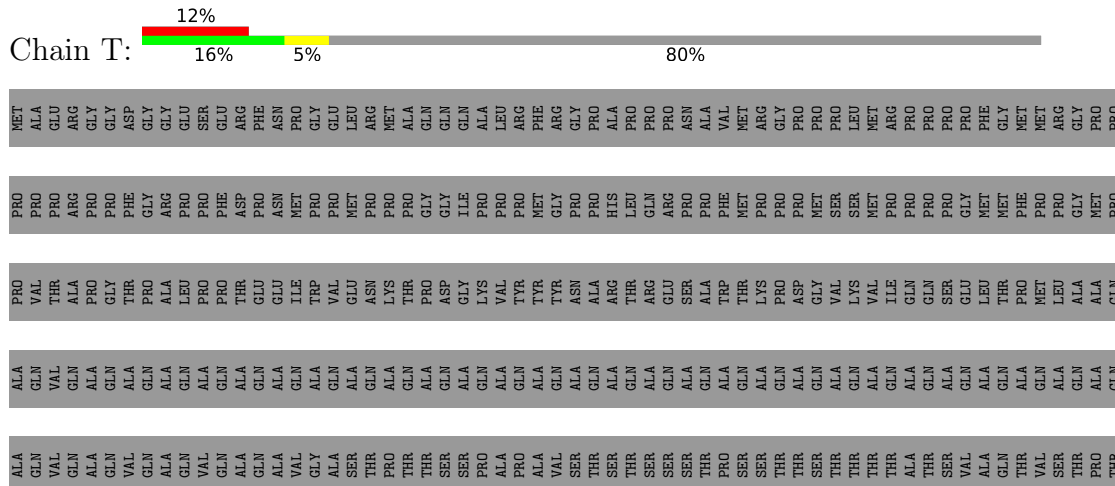
Chain K:

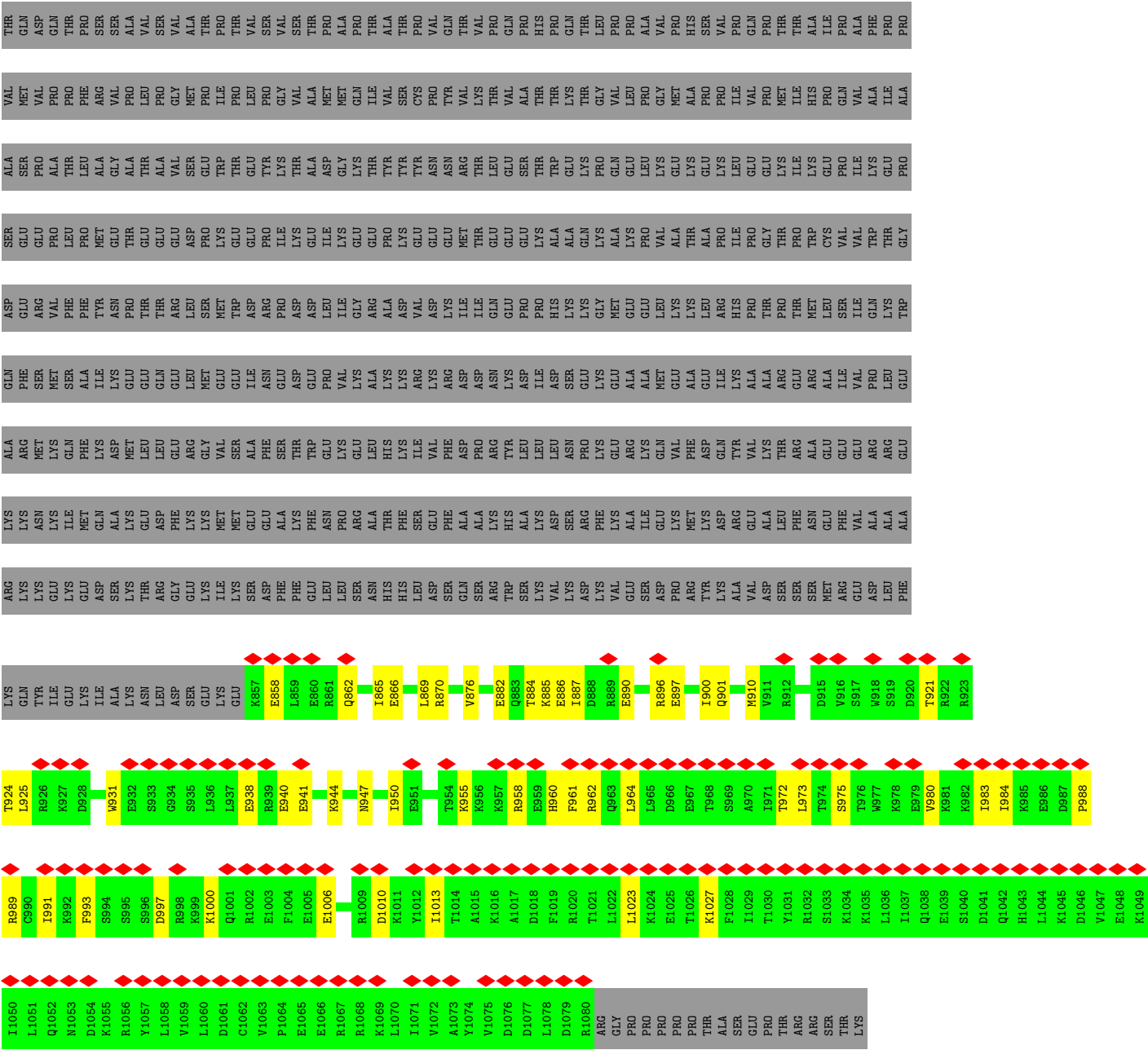


Chain Q:

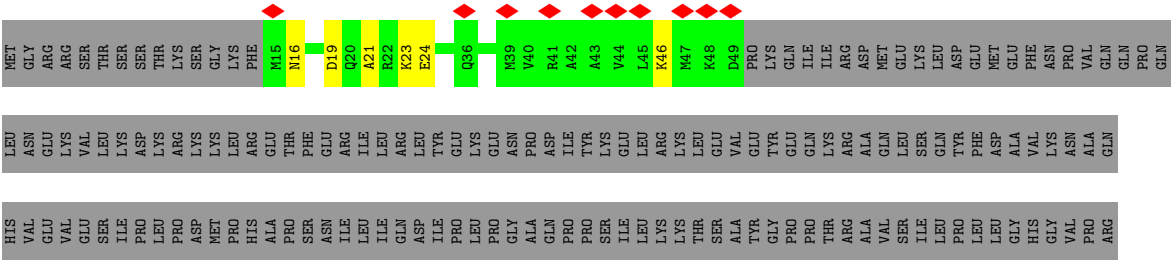


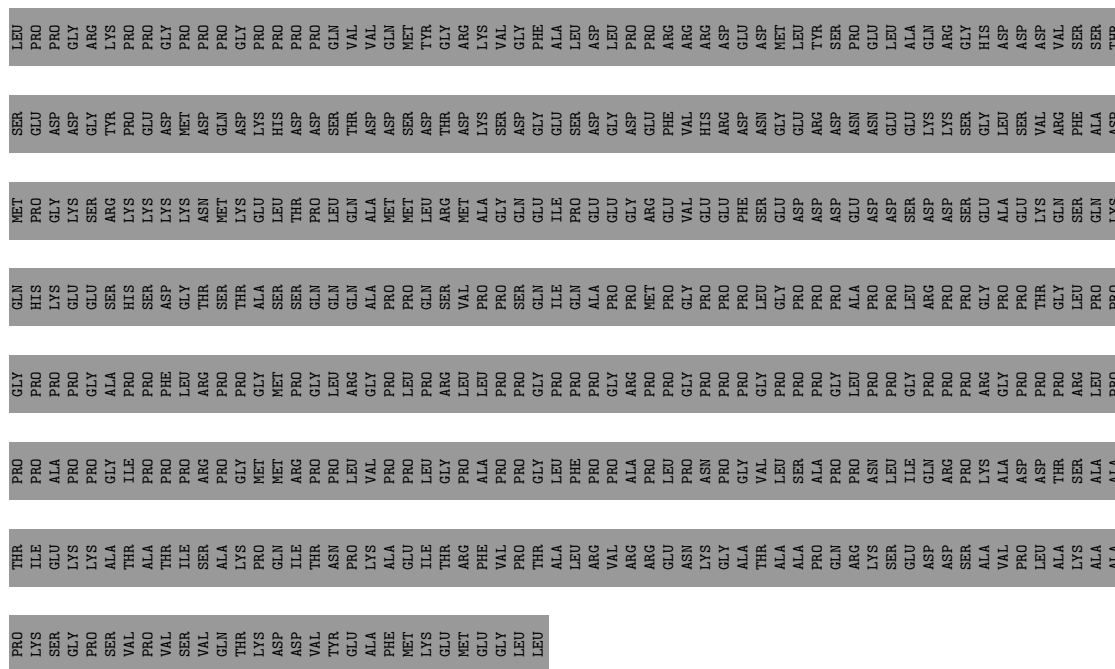
Chain T:



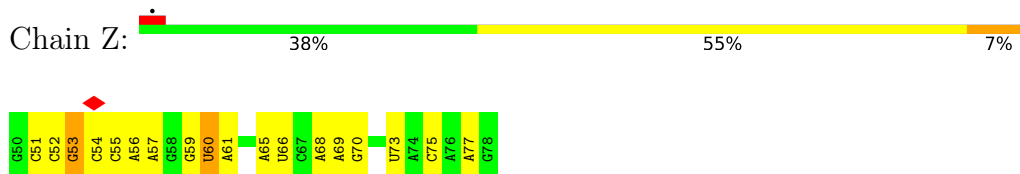


• Molecule 9: WW domain-binding protein 11

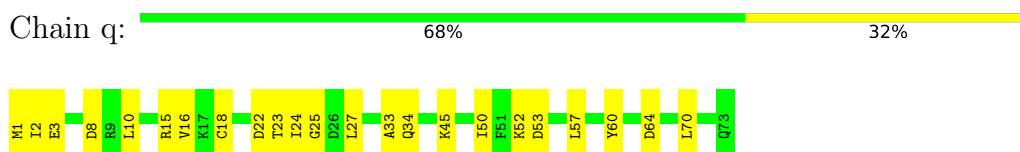




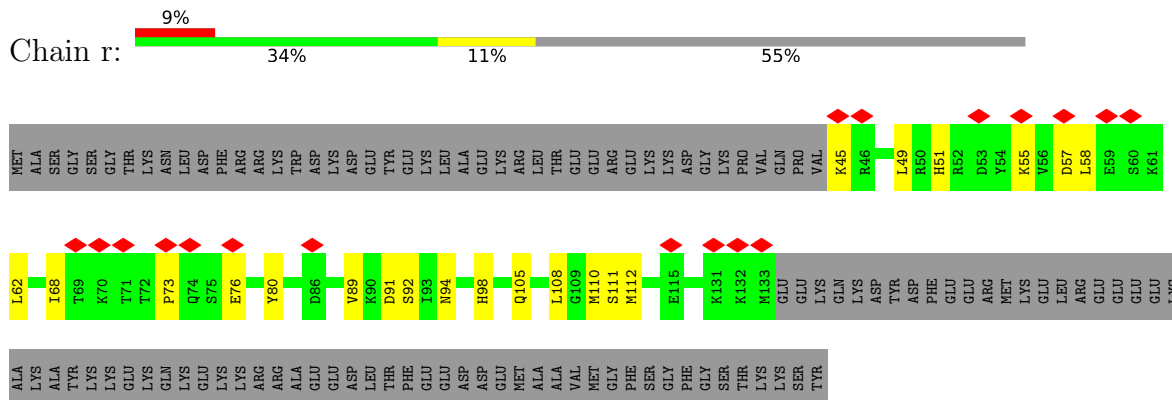
- Molecule 10: pre-mRNA



- Molecule 11: Ubiquitin-like protein 5



- Molecule 12: Zinc finger matrin-type protein 2



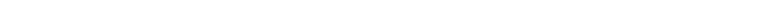
- Molecule 13: Pre-mRNA-processing factor 17

97%

97%

[illegible]

- Molecule 14: Pre-mRNA-processing-splicing factor 8

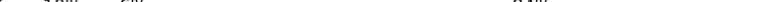
Chain A:  26% 73% 21% 5%

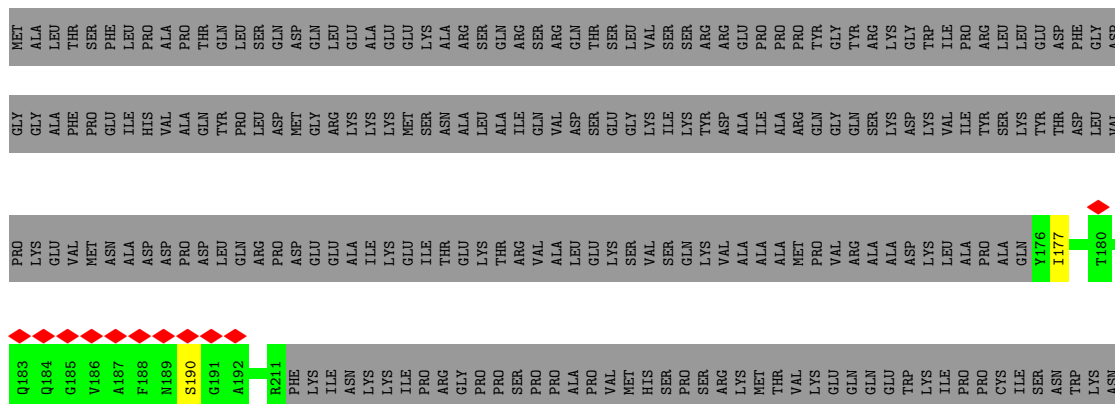
[illegible]

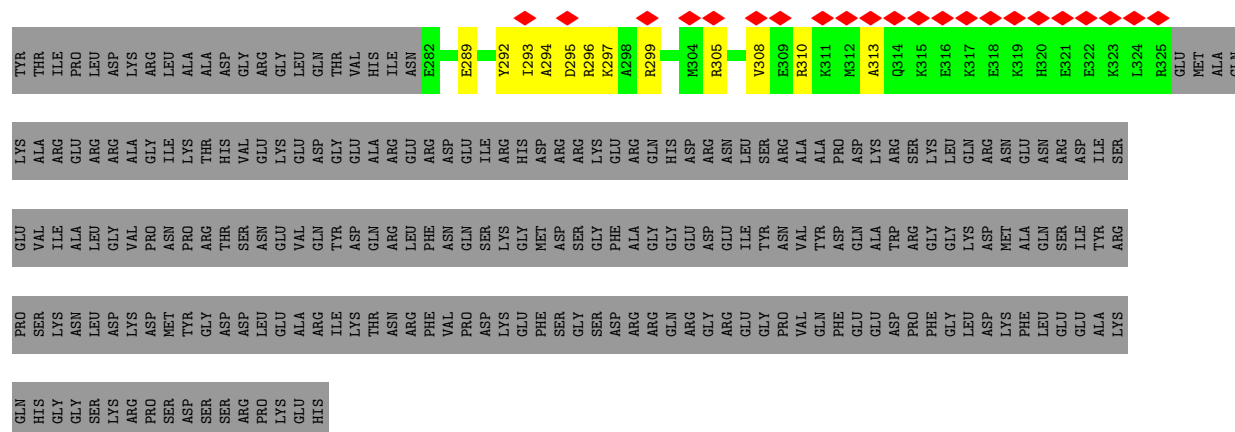




LEU	PRO	VAL	TLE	THR	Y156	P93	ALA	MET
PRO	PRO	VAL	VAL	THR		194	THR	
SER	SER	GLY	ASN	TYR	R159	Q95	SER	
PRO	ARG	ARG	VAL	VAL	N160	V96	LEU	
PRO	GLY	GLY	GLY	P162	R161	R97	GLY	
ALA	LEU	LEU	LEU	H163	H163	G100	SER	
VAL	ASN	VAL	GLY	I164	I164		ASN	
ASN	LYS	ASP	THR	E172	E172	LEU	THR	
ILE	GLY	TLE	THR	R175	R175	SER	THR	
ALA	ARG	THR	THR	E178	E178	PHE	ARG	
PRO	SER	GLU	THR	G179	G179	ASP	GLN	
LEU	THR	THR	THR			MET	TRP	
PRO	ALA	ASP	ALA	R182	R182	LYS	TRP	
PRO	ALA	ASN	LEU	H183	H183	SER	E16	
GLY	GLY	ASN	ARG	E184	E184	ASP	D17	
ILE	LYS	HIS	HIS	P185	P185	VAL	A18	
PRO	GLU	PHE	GLU	P186	P186	ASN	L23	
PRO	LYS	TYR	TYR	T187	T187	LYS	C24	
PRO	LYS	GLN	GLN	P188	P188	GLU	Q25	
PRO	ASP	PHE	PHE	D189	D189	TYR	T26	
PRO	GLY	GLY	GLY	P189	P189	THR	C27	
PRO	THR	ILE	ILE	D190	D190	GLN		
GLY	THR	ARG	THR	D191	D191	ASN	E39	
GLY	ASP	THR	THR	P192	P192	MET		
PRO	SER	THR	TLE	L193	L193	GLU	E44	
HIS	GLY	THR	THR	A194	A194	ARG	C45	
PRO	ILE	VAL	VAL	D195	D195	GLU	K46	
PHE	LYS	GLN	GLN	Q196	Q196	ILE	I47	
HIS	LEU	VAL	VAL	N197	N197	SER	C48	
PRO	GLU	ARG	ARG	I198	I198	ASN	A49	
MET	MET	GLN	GLN	K199	K199	R50	R50	
GLY	VAL	GLN	GLN	D200	D200	ASP	P51	
PRO	PRO	CYS	CYS	E201	E201	GLY	F52	
PRO	GLY	ALA	ALA			THR	T53	
PRO	LEU	PHE	PHE	T205	T205	ARG	R56	
PRO	PRO	TLE	TLE	N206	N206	PRO		
PHE	GLY	GLN	GLN			VAL	V61	
MET	LEU	PHE	PHE	V209	V209	GLY	R62	
ARG	LEU	ALA	ALA	A210	A210	MET	M63	
ALA	PRO	THR	THR	D211	D211	LEU	R64	
PRO	PRO	ARG	ARG			GLY	F65	
GLY	PRO	GLN	GLN	R216	R216	LYS		
PRO	PRO	ALA	ALA	A217	A217	ALA	V70	
ILE	ALA	ALA	ALA	T218	T218	THR	C71	
HIS	GLU	VAL	VAL	T219	T219	SER		
TYR	GLU	ALA	ALA	M220	M220	THR	L77	
PRO	GLU	ALA	ALA			SER	K78	
SER	GLU	ALA	ALA			D145		
GLN	GLU	GLY	GLY			M146		
ASP	SER	LYS	LYS	ARG	ARG	L150	T83	
PRO	PRO	ALA	ALA	PRO	PRO	A151	C84	
GLN	ASN	PHE	PHE	LEU	LEU	ASP	R85	
ARG	TYR	ASN	ASN	ASP	ASP	T152	L86	
MET	PHE	LYS	LYS	PRO	PRO	T153		
GLY	ASN	LEU	LEU	GLU	GLU	T154	E89	
							L92	

Chain t: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.359	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.055	Depositor
Map size (\AA)	540.0, 540.0, 540.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	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: IHP

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	5	0.08	0/1806	0.16	0/2807
2	6	0.07	0/2040	0.16	0/3178
3	B	0.08	0/4406	0.23	0/6169
4	C	0.12	0/6798	0.29	0/9234
5	I	0.10	0/1551	0.27	0/2090
6	K	0.12	0/958	0.31	0/1303
7	Q	0.11	0/1198	0.26	0/1605
8	T	0.12	0/1709	0.31	0/2297
9	X	0.10	0/291	0.26	0/379
10	Z	0.07	0/692	0.16	0/1076
11	q	0.12	0/609	0.29	0/819
12	r	0.08	0/736	0.22	0/978
13	P7	0.07	0/92	0.18	0/128
14	A	0.12	0/17678	0.29	0/24071
15	P	0.09	0/1338	0.25	0/1802
16	t	0.11	0/675	0.31	0/921
17	S1	0.07	0/528	0.23	0/715
All	All	0.11	0/43105	0.27	0/59572

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5	1620	0	822	23	0
2	6	1821	0	921	26	0
3	B	4369	0	2122	20	0
4	C	6649	0	6673	155	0
5	I	1521	0	1544	33	0
6	K	940	0	740	21	0
7	Q	1173	0	1182	25	0
8	T	1691	0	1516	32	0
9	X	291	0	326	4	0
10	Z	619	0	314	10	0
11	q	599	0	613	17	0
12	r	728	0	759	17	0
13	P7	92	0	46	1	0
14	A	17219	0	16116	355	0
15	P	1309	0	1311	31	0
16	t	661	0	661	21	0
17	S1	524	0	424	11	0
18	A	36	0	6	0	0
All	All	41862	0	36096	725	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 9.

The worst 5 of 725 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)
14:A:1005:ILE:HG22	14:A:1009:MET:HE3	1.62	0.81
14:A:2303:GLU:HG3	14:A:2305:TYR:H	1.45	0.80
4:C:731:SER:HB3	4:C:747:ASP:H	1.49	0.77
7:Q:133:GLU:HG3	15:P:178:GLU:HG3	1.67	0.77
14:A:909:TYR:HB2	14:A:1033:GLY:HA3	1.67	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	866/2136 (40%)	839 (97%)	27 (3%)	0	100	100
4	C	841/972 (86%)	813 (97%)	28 (3%)	0	100	100
5	I	182/312 (58%)	179 (98%)	3 (2%)	0	100	100
6	K	135/439 (31%)	130 (96%)	5 (4%)	0	100	100
7	Q	140/144 (97%)	140 (100%)	0	0	100	100
8	T	222/1098 (20%)	219 (99%)	3 (1%)	0	100	100
9	X	33/641 (5%)	33 (100%)	0	0	100	100
11	q	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
12	r	87/199 (44%)	86 (99%)	1 (1%)	0	100	100
13	P7	16/579 (3%)	16 (100%)	0	0	100	100
14	A	2199/2335 (94%)	2144 (98%)	55 (2%)	0	100	100
15	P	157/420 (37%)	155 (99%)	2 (1%)	0	100	100
16	t	79/520 (15%)	75 (95%)	4 (5%)	0	100	100
17	S1	76/526 (14%)	76 (100%)	0	0	100	100
All	All	5104/10394 (49%)	4974 (98%)	130 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	38/1908 (2%)	38 (100%)	0	100	100
4	C	745/866 (86%)	745 (100%)	0	100	100
5	I	167/293 (57%)	167 (100%)	0	100	100
6	K	67/395 (17%)	67 (100%)	0	100	100
7	Q	128/130 (98%)	128 (100%)	0	100	100
8	T	151/956 (16%)	151 (100%)	0	100	100
9	X	31/554 (6%)	31 (100%)	0	100	100
11	q	66/66 (100%)	66 (100%)	0	100	100
12	r	84/181 (46%)	84 (100%)	0	100	100
13	P7	1/502 (0%)	1 (100%)	0	100	100
14	A	1692/2108 (80%)	1692 (100%)	0	100	100
15	P	146/361 (40%)	146 (100%)	0	100	100
16	t	75/456 (16%)	75 (100%)	0	100	100
17	S1	33/450 (7%)	33 (100%)	0	100	100
All	All	3424/9226 (37%)	3424 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
14	A	1096	HIS
14	A	1373	GLN
15	P	196	GLN
14	A	1159	ASN
14	A	1399	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	76/77 (98%)	22 (28%)	0
10	Z	28/29 (96%)	9 (32%)	1 (3%)
2	6	84/85 (98%)	24 (28%)	0
All	All	188/191 (98%)	55 (29%)	1 (0%)

5 of 55 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	16	U
1	5	17	U
1	5	20	G
1	5	21	A
1	5	22	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	Z	54	C

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	IHP	A	2401	-	36,36,36	0.77	0	54,60,60	1.17	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	IHP	A	2401	-	-	5/30/54/54	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	2401	IHP	C3-C2-C1	3.55	118.19	110.41
18	A	2401	IHP	C5-C4-C3	2.28	115.40	110.41
18	A	2401	IHP	C4-C3-C2	2.17	115.16	110.41

There are no chirality outliers.

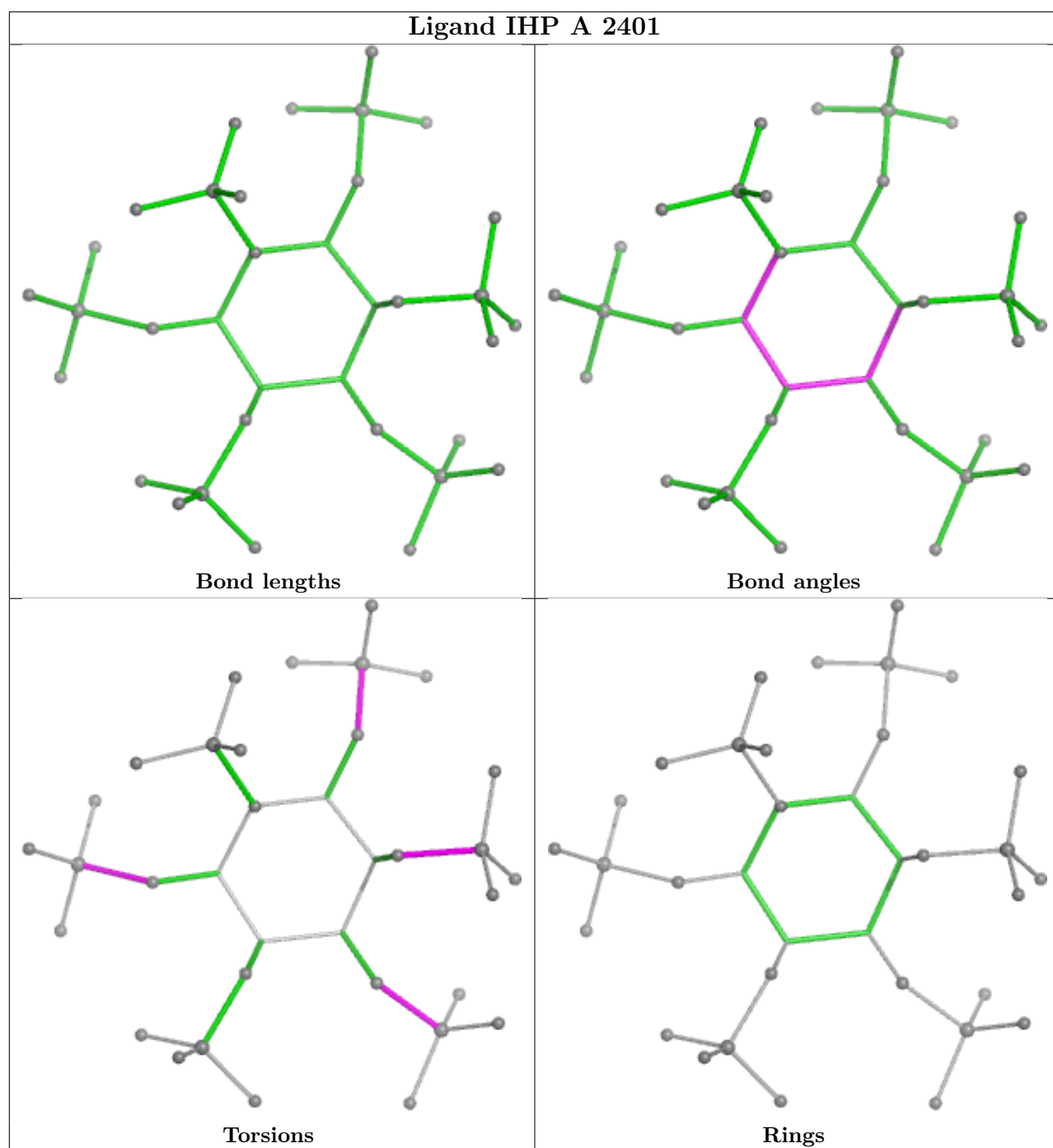
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C1-O11-P1-O21
18	A	2401	IHP	C6-O16-P6-O46
18	A	2401	IHP	C4-O14-P4-O34
18	A	2401	IHP	C2-O12-P2-O22
18	A	2401	IHP	C2-O12-P2-O42

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

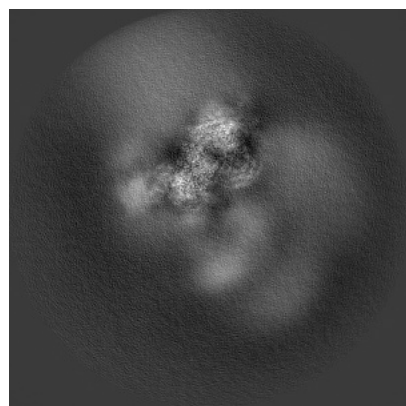
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53554. These allow visual inspection of the internal detail of the map and identification of artifacts.

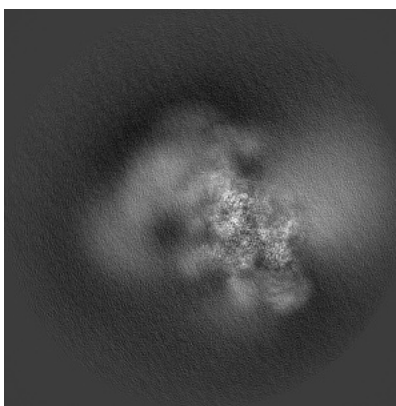
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

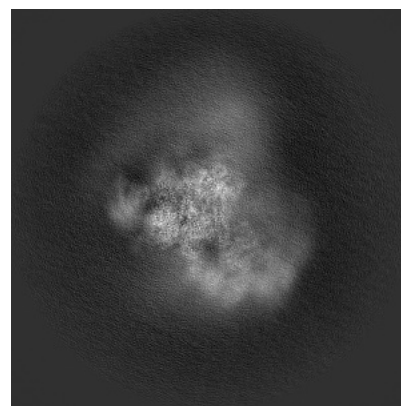
6.1.1 Primary map



X

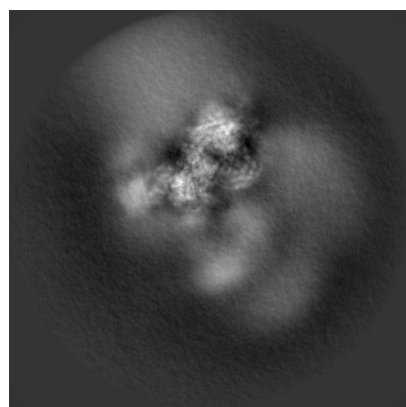


Y

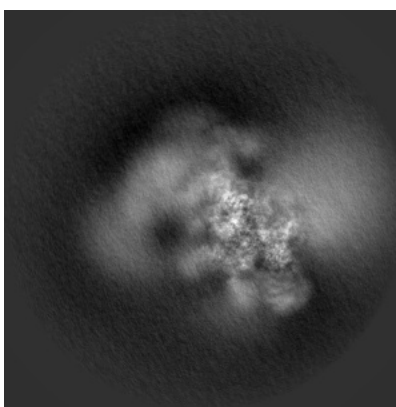


Z

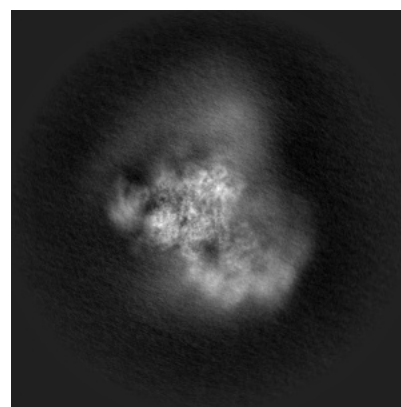
6.1.2 Raw map



X



Y

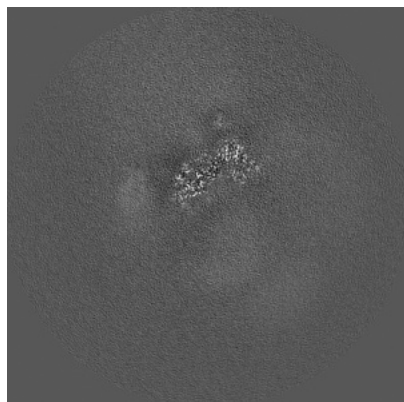


Z

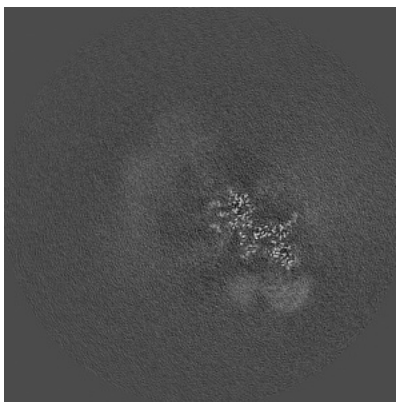
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

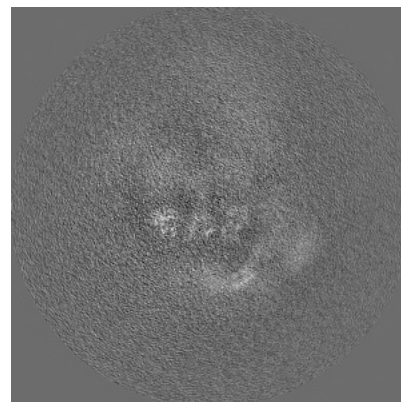
6.2.1 Primary map



X Index: 200

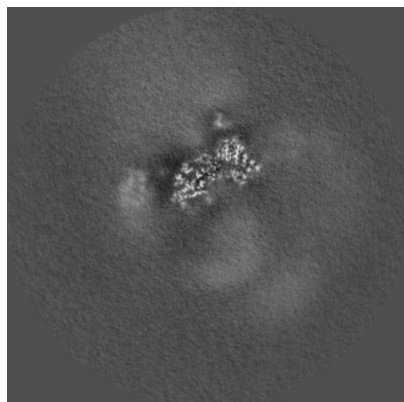


Y Index: 200

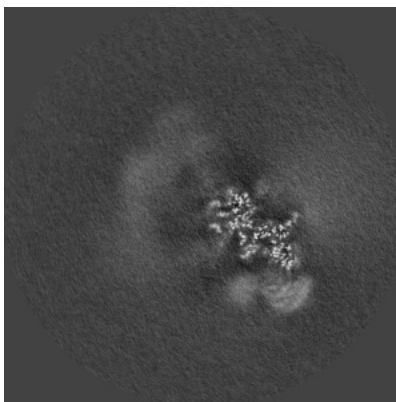


Z Index: 200

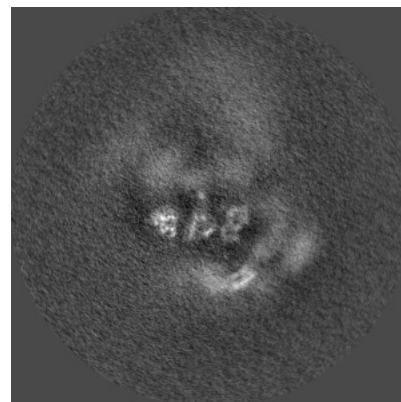
6.2.2 Raw map



X Index: 200



Y Index: 200

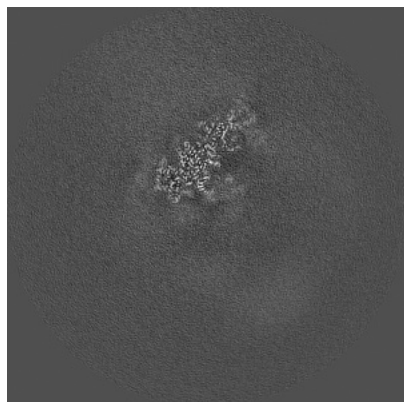


Z Index: 200

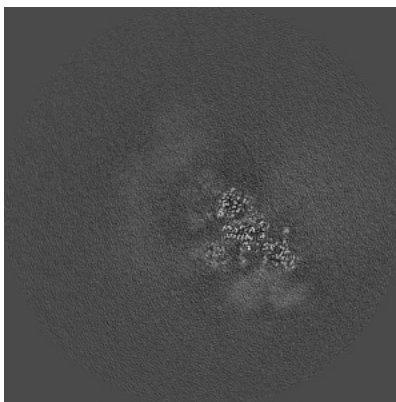
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

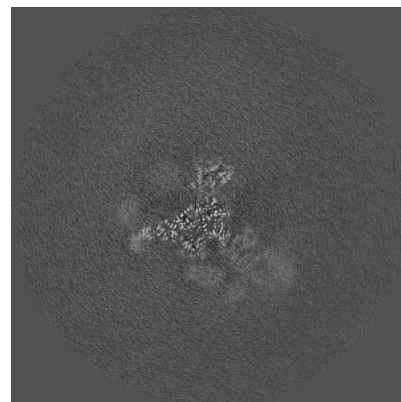
6.3.1 Primary map



X Index: 179

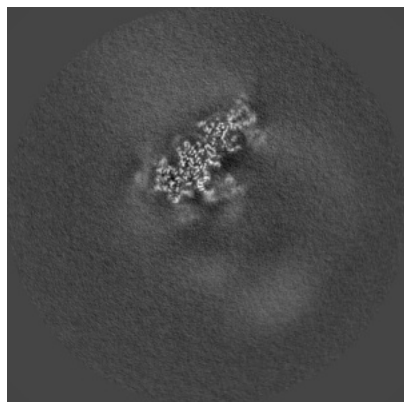


Y Index: 191

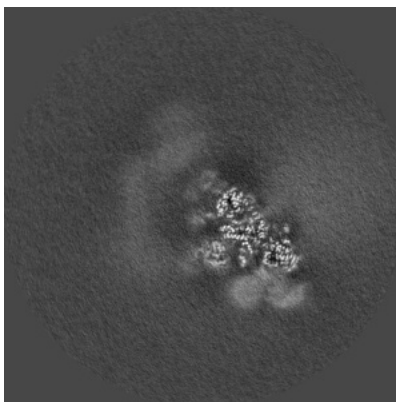


Z Index: 230

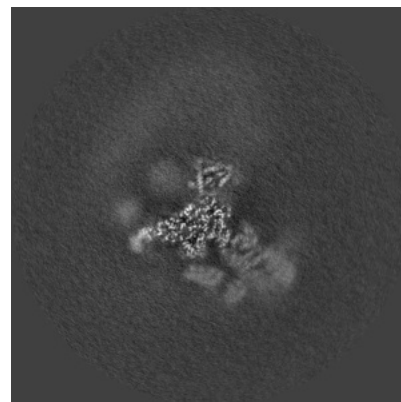
6.3.2 Raw map



X Index: 179



Y Index: 192

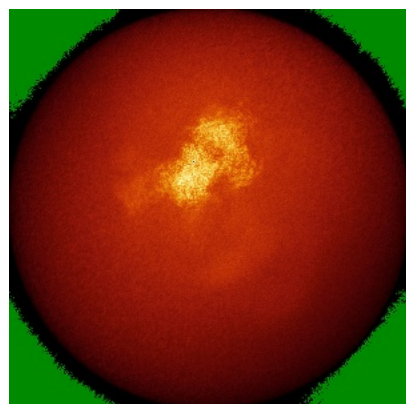


Z Index: 229

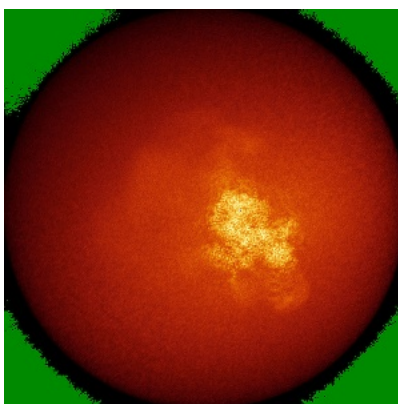
The images above show the largest variance slices of the map in three orthogonal directions.

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

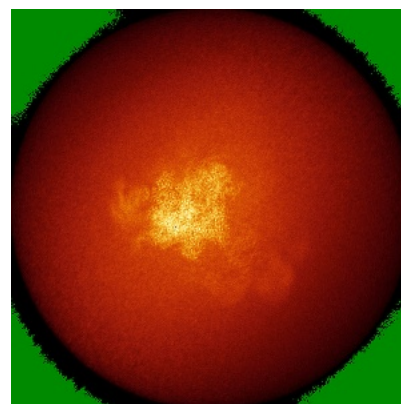
6.4.1 Primary map



X

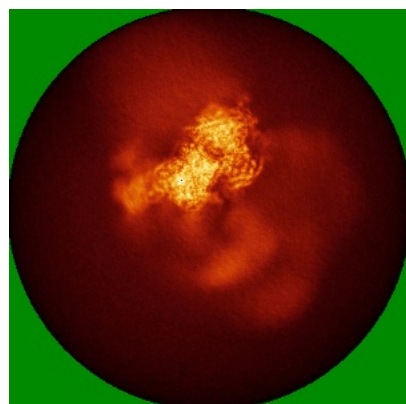


Y

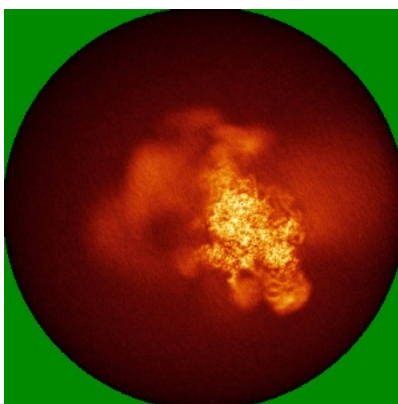


Z

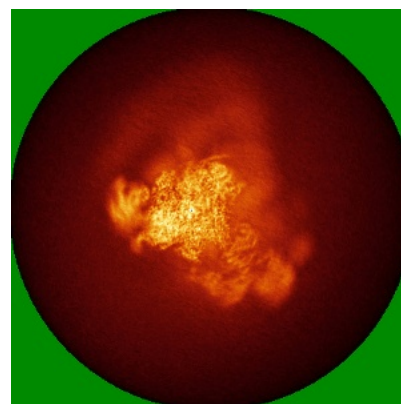
6.4.2 Raw map



X



Y

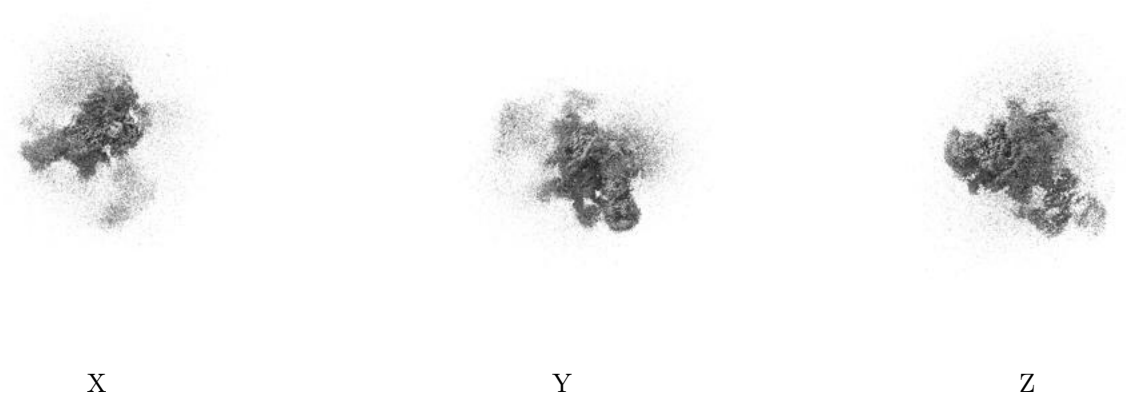


Z

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.

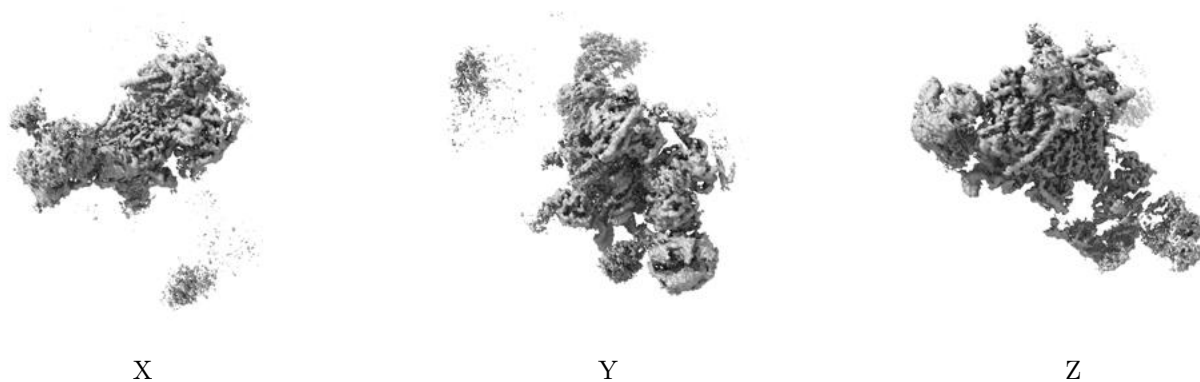
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

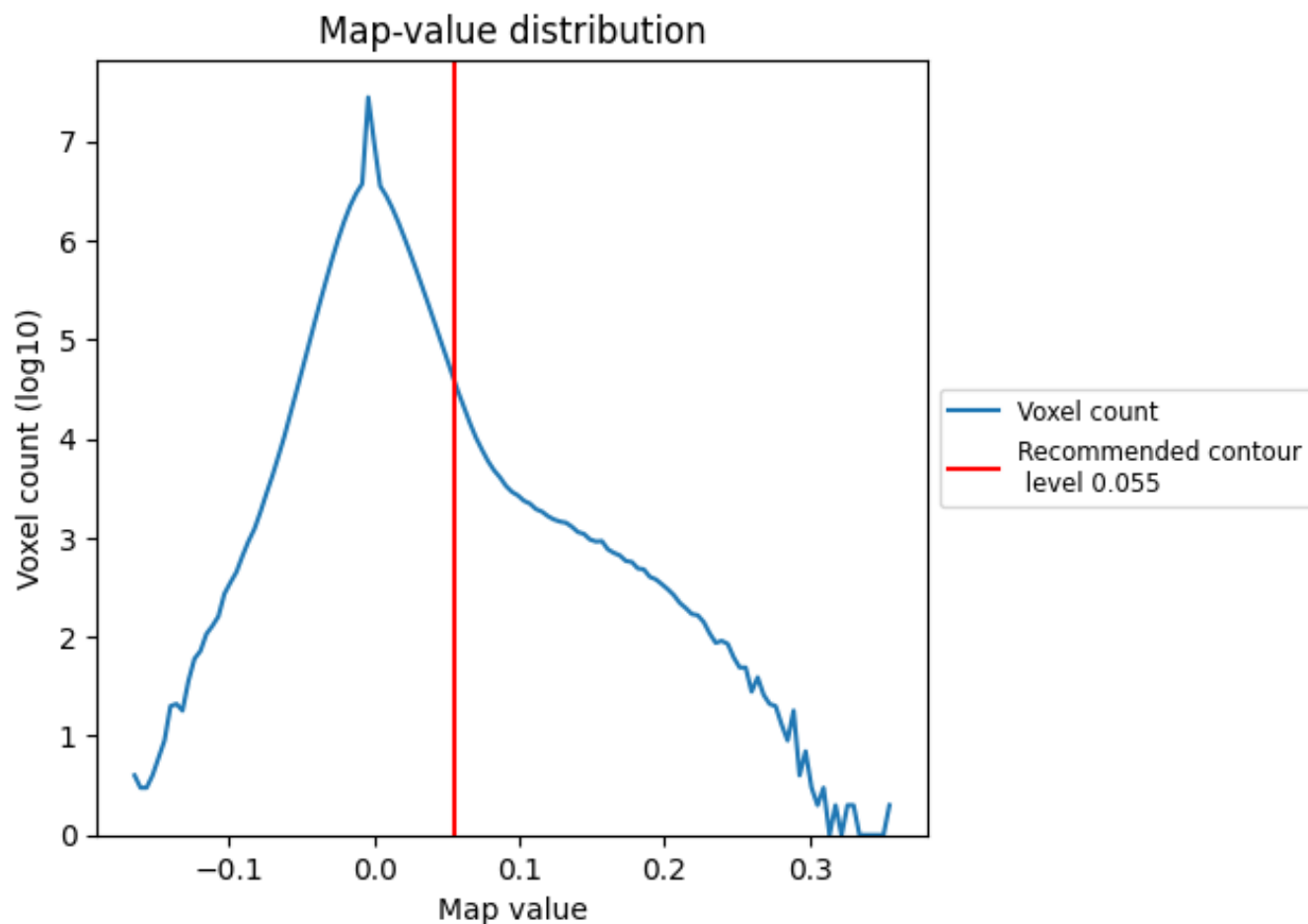
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

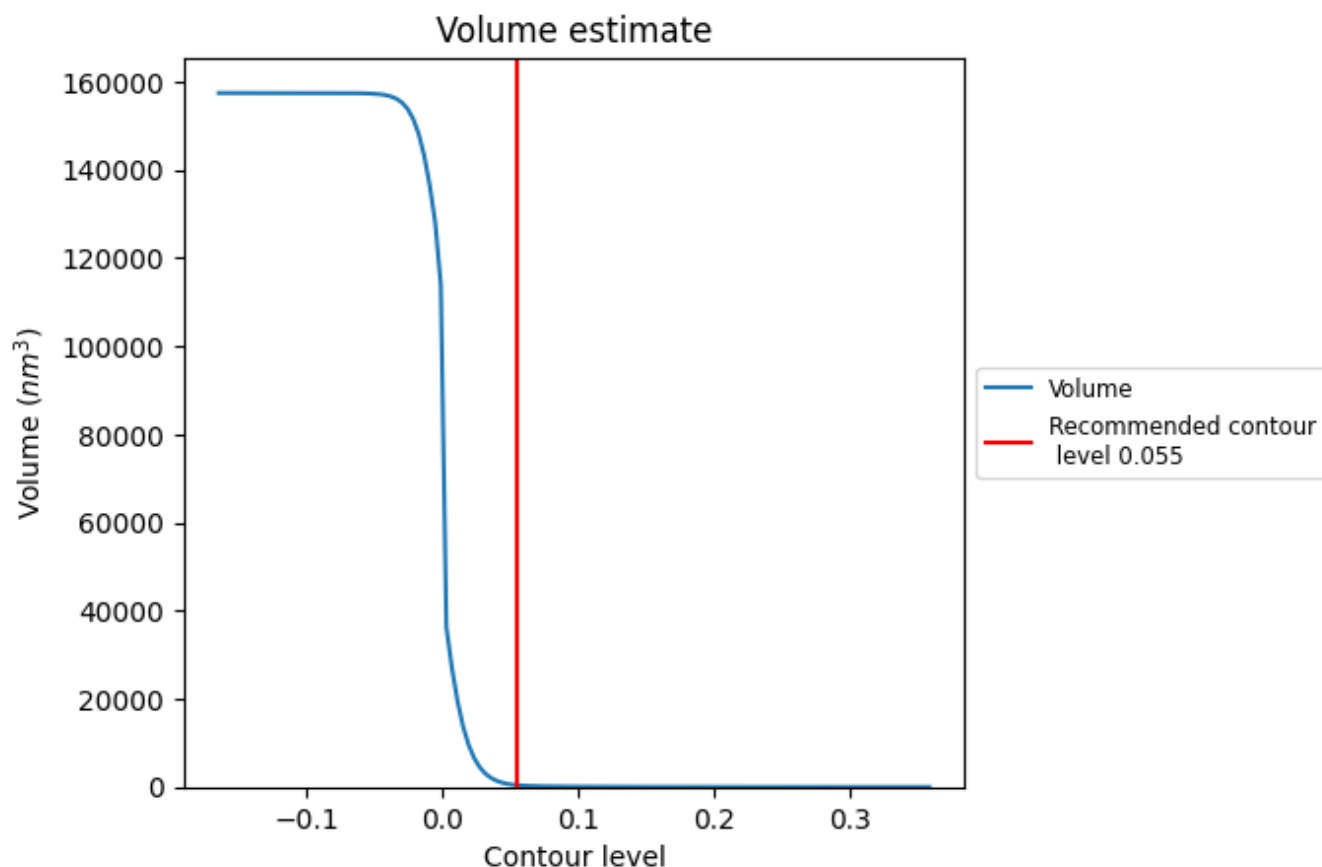
This section contains the results of statistical analysis of the map.

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.

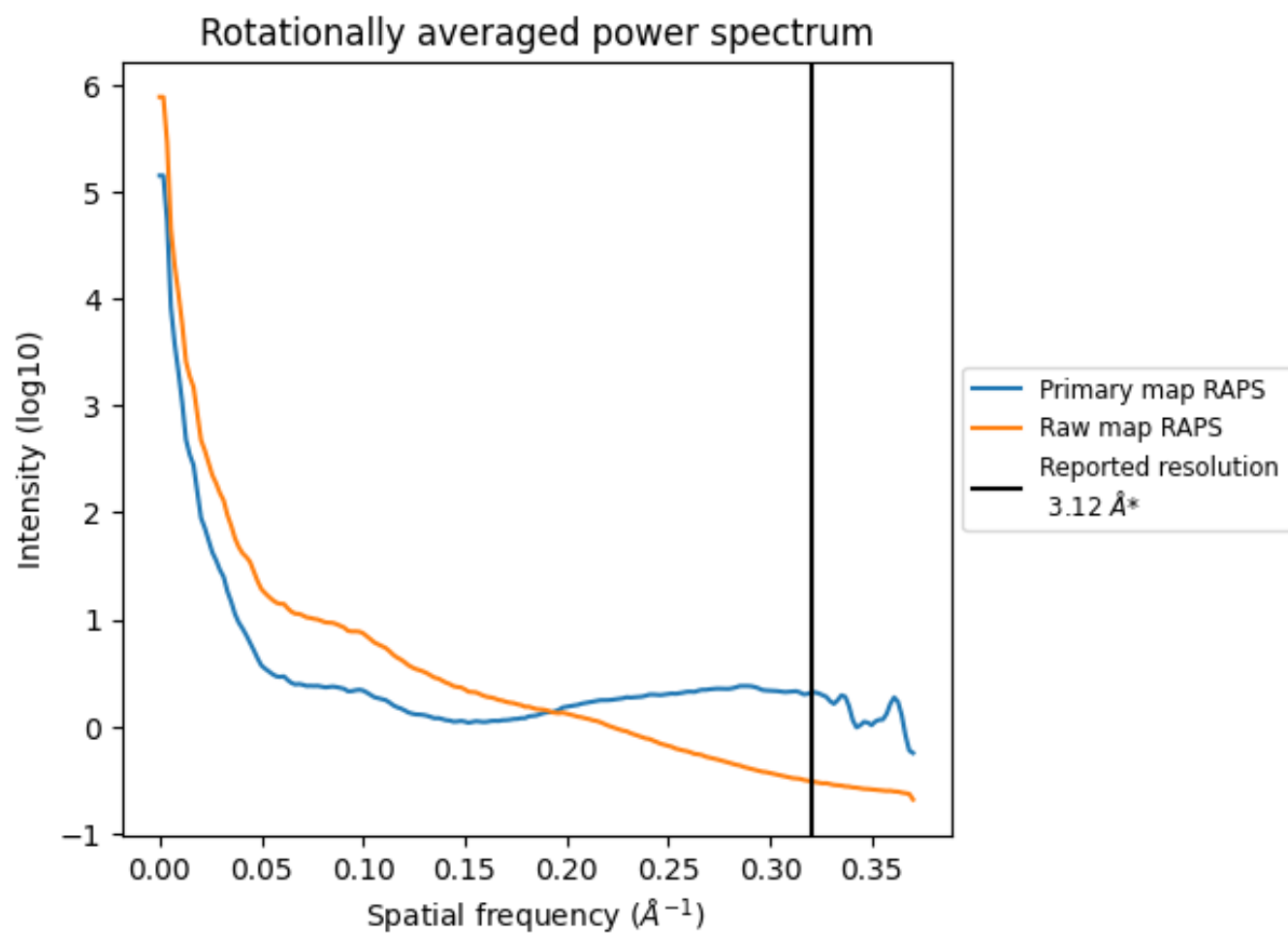
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 407 nm³; this corresponds to an approximate mass of 367 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 ⓘ

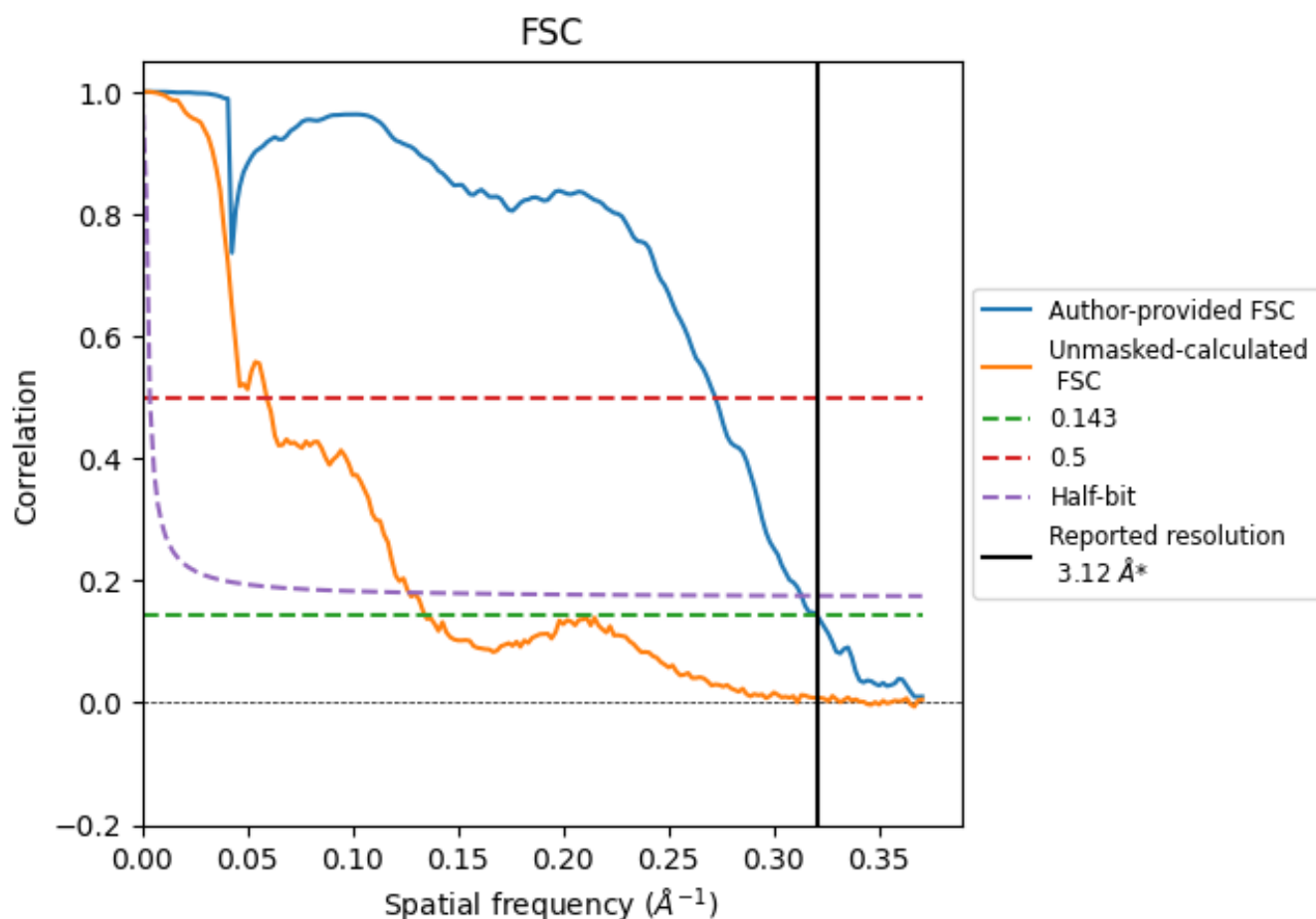


*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

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 0.321 Å⁻¹

8.2 Resolution estimates [i](#)

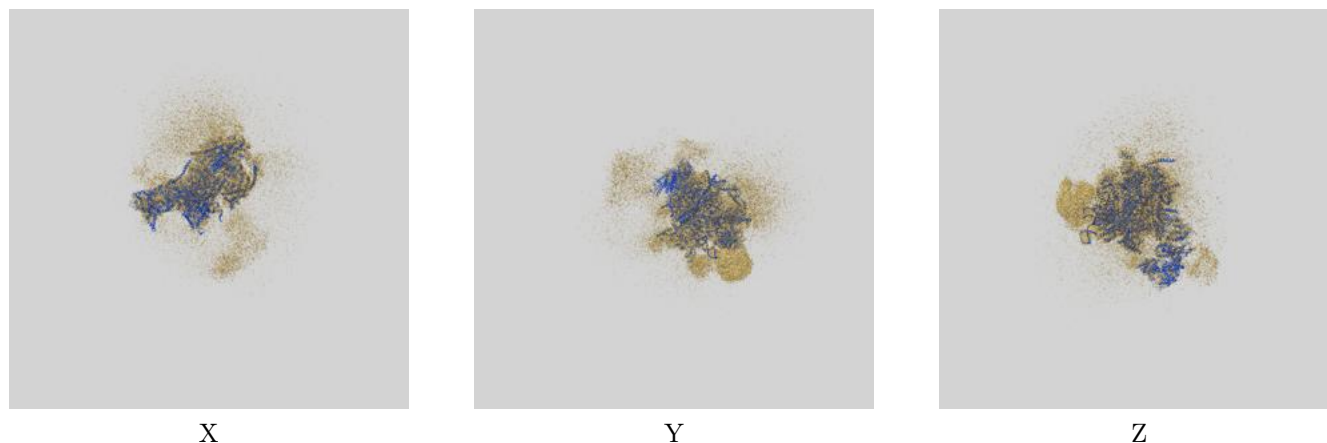
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.12	3.67	3.19
Unmasked-calculated*	7.44	16.92	7.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.44 differs from the reported value 3.12 by more than 10 %

9 Map-model fit [i](#)

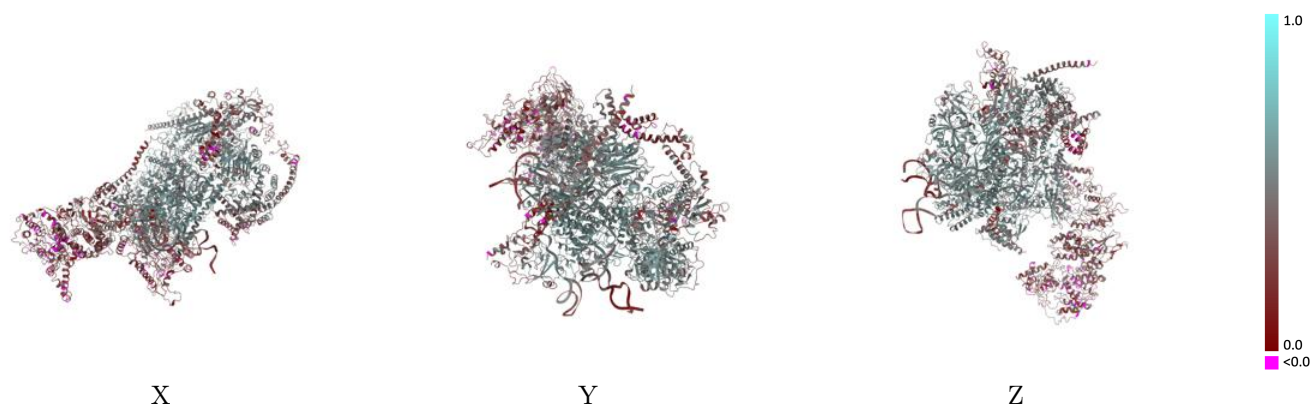
This section contains information regarding the fit between EMDB map EMD-53554 and PDB model 9R3D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



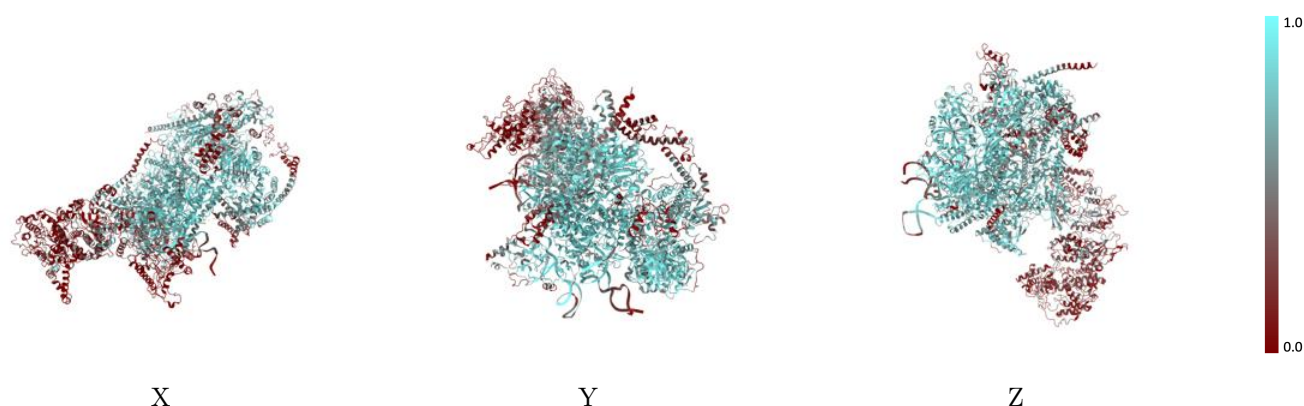
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



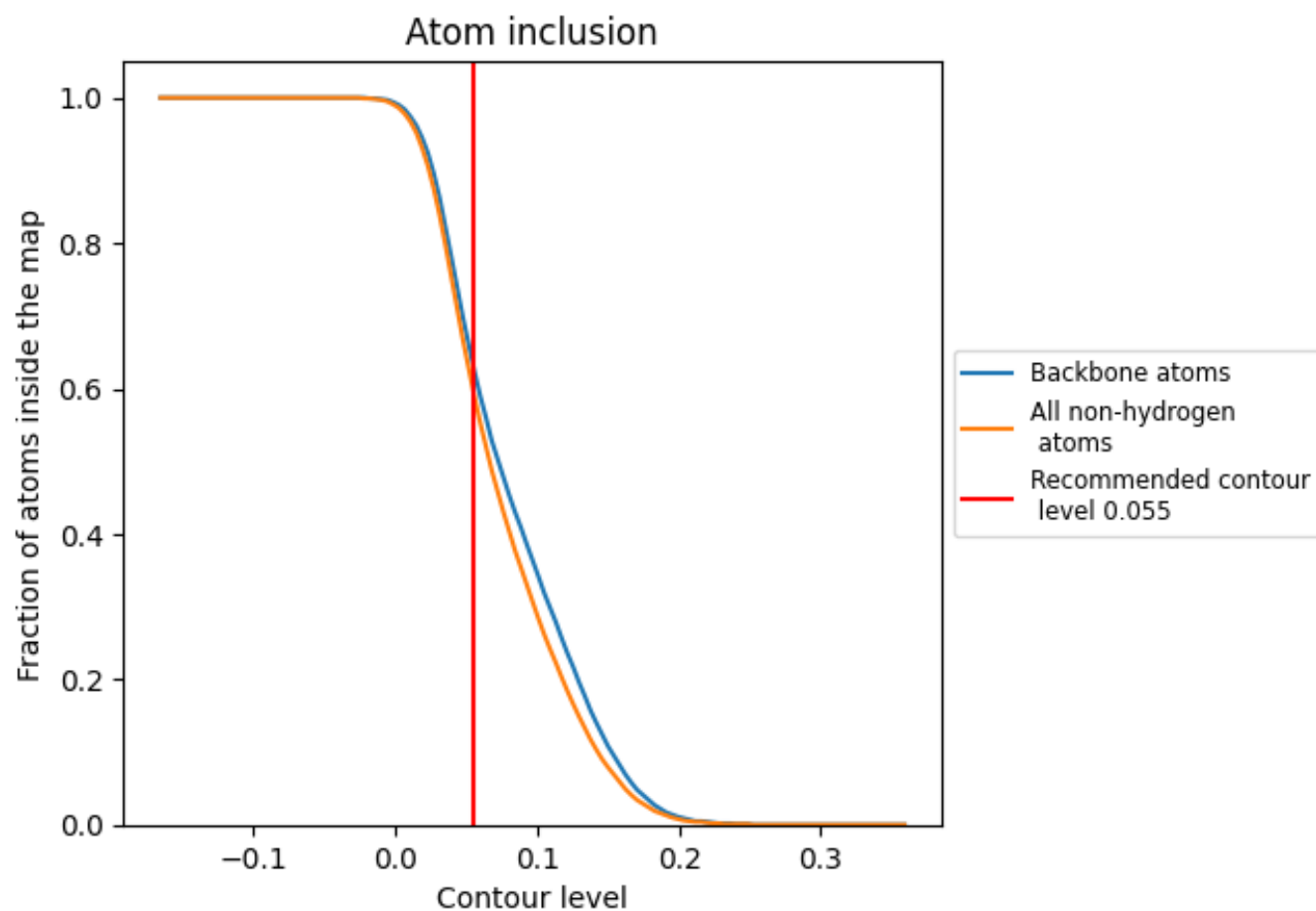
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 60% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5990	 0.4510
5	 0.7320	 0.4370
6	 0.6540	 0.4070
A	 0.6400	 0.4800
B	 0.1600	 0.2660
C	 0.7450	 0.5150
I	 0.7550	 0.5370
K	 0.5820	 0.4780
P	 0.6530	 0.4380
P7	 0.3480	 0.3380
Q	 0.7550	 0.5140
S1	 0.5110	 0.3960
T	 0.3560	 0.3460
X	 0.5230	 0.4570
Z	 0.8080	 0.4740
q	 0.8140	 0.5770
r	 0.6300	 0.4840
t	 0.1210	 0.2560

