



## wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 02:20 PM EST

PDB ID : 7SID  
EMDB ID : EMD-25141  
Title : Human ATM Dimer Bound to Nbs1  
Authors : Warren, C.; Pavletich, N.P.  
Deposited on : 2021-10-13  
Resolution : 2.53 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.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

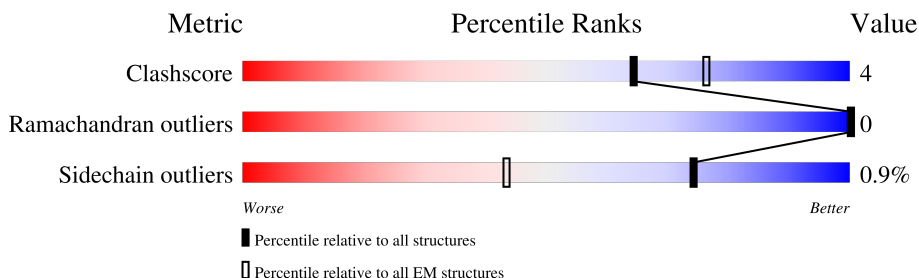
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	3056	<div> <div>39%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	3056	<div> <div>39%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
2	B	28	<div> <div>36%</div> <div> <div>32%</div> <div>64%</div> </div> </div>
2	D	28	<div> <div>36%</div> <div> <div>32%</div> <div>64%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 44650 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.

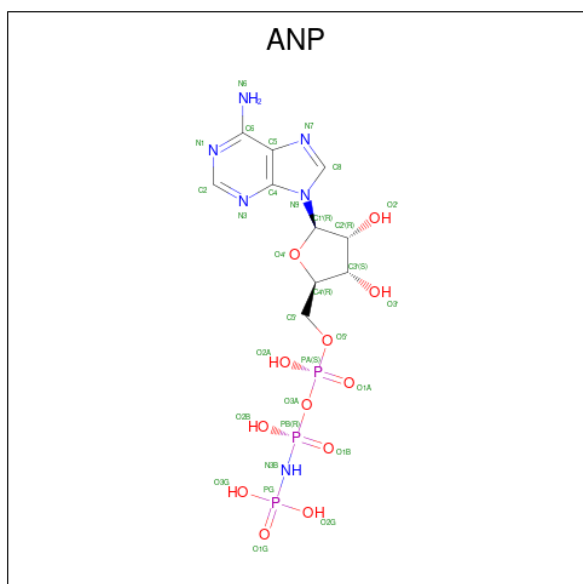
- Molecule 1 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		
1	C	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		

- Molecule 2 is a protein called Nibrin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	10	Total	C	N	O	0	0
			83	53	14	16		
2	D	10	Total	C	N	O	0	0
			83	53	14	16		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

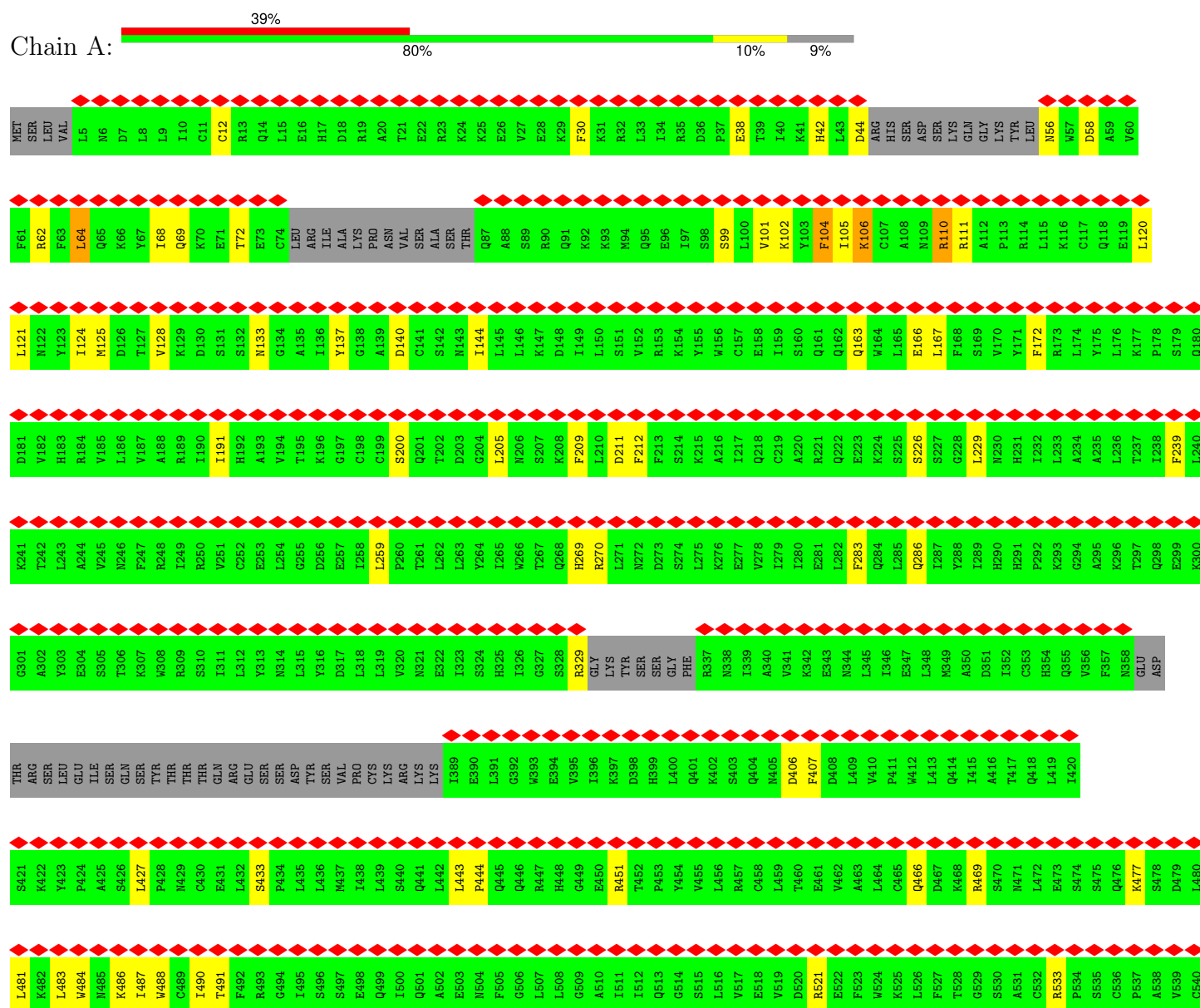
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

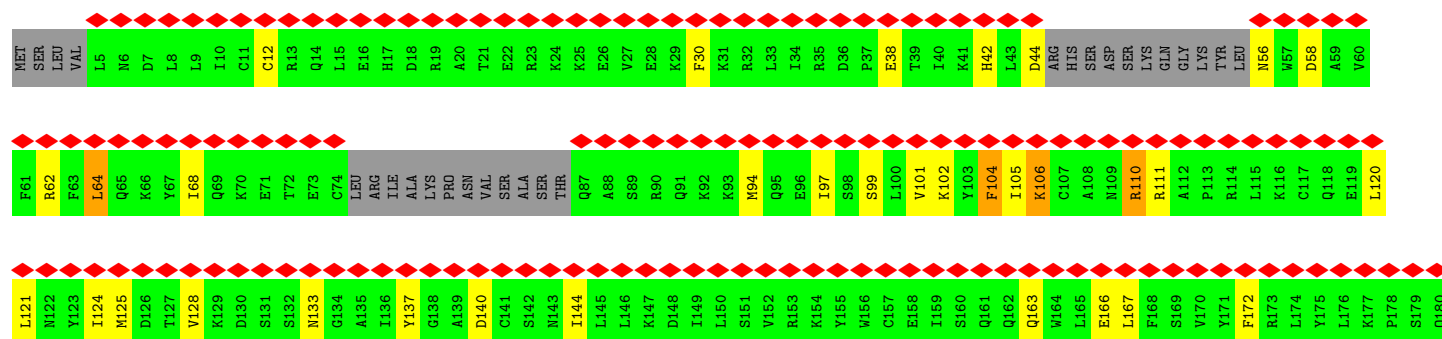
### 3 Residue-property plots

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: Serine-protein kinase ATM



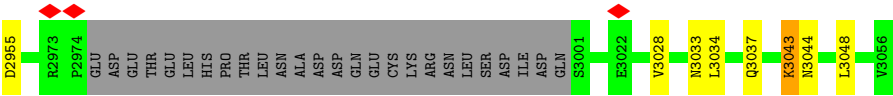
E1267	R1204	PRO	M1081	V1021	L961	L901	Q781	L721	D661	S601	C541
V1268	R1205	E1142	H1082	I1022	P962	K902	L782	L722	F662	N602	L542
K1269	L1206	T1143	H1083	G1023	M963	F903	GLY	L723	L663	F803	T543
S1270	D1208	L1144	Q1084	A1024	E964	L904	ASN	G724	T664	P604	L544
I1271	F1209	D1145	V1085	F1025	D965	C905	MET	V725	ILE	H605	A545
A1272	M1210	E1146	R1086	W1026	V966	L906	GLU	L726	VAL	L606	L546
Q1273	A1211	I1147	M1087	H1027	L967	C907	VAL	G727	ARG	V607	T547
M1274		Y1148	L1088	L1028	E968	V908	GLU	C728	GLU	L608	
I1275	L1214	M1149	A1089	T1029	L969	V909	ASP	Y729	CYS	T548	
Q1276	D1215	R1150	A1090	K1030	E970	T910	GLN	C730	GLY	E609	Y549
Y1216	Y1216	K1151	E1091	E1031	L970	A911	SER	T731	ILE	K610	I550
L1217		S1092	S1092	R1032	P972	Q912	MET	M732	LYS	I611	V551
		V1153	I1093	K1033	L973	T913	ASN	G733	HIS	L612	P552
E1220	W1219	L1154	M1094	Y1034	S974	N914	LEU	V734	GLN	V613	G553
W1221	K1220	L1095	L1095	I1035	N975	T915	PHE	V735	SER	S614	T554
L1222	L1222	L1096	L1096	F1036	V976	V916	ASN	I735	SER	L615	VAL
N1223	N1223	F1097	F1097	S1037	C977	S917	ASP	A736	ILE	T616	LYS
L1224	L1224	Q1098	Q1098	V1038	S978	F918	TYR	E737	G679	M617	MET
Q1225	Q1225	A1099	D1099	R1039	S978	R918	PRO	E738	F680	K619	GLY
D1226	D1226	T1100	T1100	M1040	L979	R919	ASP	E739	S681	V682	ILE
T1227	T1227	K1101	K1101	A1041	V980	A920	SER	A740	V683	C620	GLU
E1228	E1228	GLY	GLY	L1042	R981	A921	VAL	Y741	Q684	K621	GLN
Y1229	Y1229	ASP	ASP	V1043	R982	D922	ALA	K742	N685	A622	MET
N1230	N1230	SER	SER	M1044	Q984	I923	ASN	E743	L686	A623	CYS
L1231	L1231	ARG	ARG	C1045	D985	R924	GLU	E744	K687	M624	VAL
S1232	S1232	L1046	L1046	K1047	D985	R925	PRO	L745	E688	N625	ASN
S1233	S1233				V986	K926	GLY	F746	S689	F626	ARG
E1301	E1301	K1170	L1108	T1048	V986	L926	GLU	Q747	L690	F627	SER
F1234	F1234	Q1171	K1109	L1049	K988	L928	SER	K748	D691	Q628	
P1235	P1235	A1172	A1110	L1050	T989	M929	GLN	A749	R692	S629	
R1304	R1304	L1173	L1111	L1050	T989	L928		K750	C693	V630	
I1237	I1237	F1174	P1112	E1051	P1112	M929		S751	L694	P631	
L1238	L1238	A1175	L1113	A1052	L991	L930		M753	L695	E632	
L1239	L1239	L1176	K1114	D1053	N992	D932		Q754	G696	C633	
N1240	N1240	C1177	L1115	P1054	H993	S933		C755	L697		
Y1241	Y1241	K1178	Q1116	Y1055	V994	S934		E756	GLU		
T1242	T1242	S1179	Q1117	S1056	L995	T935		A756	HIS		
N1243	N1243	V1180	T1118	K1057	H996	L936		G757	GLN		
E1244	E1244	K1181	A1119	W1058	V997	E937		E758	LYS		
E1245	E1245	E1182	F1120	A1059	V998	P938		S759	ASP		
D1246	D1246	M1183	E1121	I1060	K1000	T939		L701	LYS		
F1247	F1247	G1184	E1122	L1061	N1000	K940		L702	ASP		
Y1248	Y1248	L1185	M1122	L1061	L1000	S941		N703	GLU		
L1316	L1316	L1185	A1123	M1062	L1001	S941		T761	LEU		
K1317	K1317	E1186	Y1124	V1063	G1002	L942		L762	S644		
V1318	V1318	P1187	L1125	M1064	Q1003	H943		F763	F645		
Y1319	C1251	H1188	K1126	S1004	S1004	L944		K764	S646		
D1320	Y1252	L1189	A1127	K1066	H945	L944		N765	E647		
M1321	K1253	V1190	Q1128	M1006	M1006	M946		K766	V648		
L1322	V1254	K1191	Q1129	D1067	D1007	Y947		T767	I709		
	L1255	K1192	G1130	F1068	S1008	L948		L767	ASN		
K1323		V1193	M1131	P1069	E1009	M949		T768	E650		
H1258	H1258	L1194	R1132	K1259	S1008	L948		E769	L651		
S1324	L1259	E1195	L1132	M1010	N1010	L950		F769	F652		
M1326	V1260	K1196	E1133	T1071	T1011	K951		F771	E713		
L1327	L1261	V1197	M1134	V1073	E1072	K952		R772	L715		
R1262	R1262	SER	SER	F1074	D1013	E953		I773	V716		
S1263	S1263	H1328	H1328	T1075	A1014	L954		G774	R717		
K1330	K1330	E1199	SER	Q1076	A1014	L954		S775	T656		
Q1331	Q1331	T1200	ALA	F1077	Q1015	P955		L776	C718		
F1265	F1265	F1201	GLU	Q1017	Q1016	G956		R777	S719		
D1266	D1266	G1202	ASN	L1078	F1018	E958		M778	K659		
D1333	D1333	Y1203		A1079	L1019	P960		M779	M660		



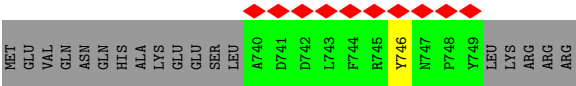
D181	K241	G301	L481	C541	S601	D661	L721	Q781	L901	L961
V182	T242	A302	K482	L542	N602	F662	L722	L782	K902	P962
H183	L243	Y303	L483	T543	F603	L663	L723	C783	K903	M963
R184	A244	E304	W484	L544	P604	T664	L724	T784	L904	E964
V185	V245	S305	W485	A545	H605	I1E	L725	R785	C905	D965
L186	N246	T306	K486	L546	L606	VAL	L726	C786	L906	V966
V187	F247	K307	L487	T547	V607	GLU	L727	L787	C907	L967
A188	R248	W308	W488	T548	L608	CYS	L728	S788	V908	E968
R189	R249	R309	C489	S549	E609	GLY	L729	W789	T909	L969
I190	R250	T310	L490	I550	K610	I1E	C730	GLU	T910	L970
I191	V251	I311	T491	V551	L611	LYS	L731	L791	A911	K971
H192	C252	L312	F492	P552	L612	HIS	L732	K792	Q912	P972
A193	E253	Y313	R493	G553	V613	GLN	L733	L793	T913	L973
V194	L254	N314	G494	T554	S614	SER	L734	S794	N914	S974
T195	G255	L315	L495	T555	L615	I1E	L735	F795	T915	N975
K196	D256	Y316	S496	VAL	L616	G679	A736	W796	V916	V976
G197	E257	D317	S497	GLY	T616	F680	E737	K797	S917	C977
C198	I258	L318	E498	ILE	K618	S681	E738	T798	F918	S978
C199	L259	L319	Q499	GLN	N619	V682	E739	A799	R919	L979
S200	P260	V320	I500	ASN	C620	H683	A740	S800	A920	Y980
Q201	T261	N321	Q501	MET	K621	Q684	Y741	G801	A921	R981
T202	L262	I322	A502	CYS	A622	N685	K742	F802	D922	R982
D203	L263	I323	E503	GLU	A623	L686	S743	F803	I923	D983
G204	Y264	S324	N504	VAL	M624	K687	E744	L804	R924	Q984
L205	L265	H325	F505	ARG	N625	E688	L745	R805	R925	D985
N206	W266	I326	G506	SER	F626	S689	F746	L806	K926	V986
S207	T267	G327	L507	P570	F627	L690	Q747	L807	L927	C987
K208	Q268	S328	L508	GLU	Q628	D691	K748	T808	L928	K988
F209	H269	R329	G509	L572	S629	R692	A749	S809	N929	T989
L210	R270	L396	A510	K573	V630	C693	K750	K810	L930	I990
D211	L271	T397	I511	E574	P631	L694	S751	L811	I931	L991
F212	N272	S398	I512	S575	E632	L695	L752	N812	D932	N992
F213	D273	SER	Q513	T576	C633	G696	L753	H813	S933	H993
S214	S274	GLY	L454	M577	HIS	HIS	Q754	D814	S934	L994
K215	L275	PHE	V455	K578	GLU	HIS	C755	L815	T935	L995
A216	K276	R337	L456	W579	GLN	HIS	A756	A816	L936	H996
I217	E277	N338	L457	L580	LYS	LYS	G757	D817	E937	V997
Q218	V278	I339	R457	L581	ASP	Q700	E758	L818	T939	K999
C219	I279	A340	C458	P582	LYS	L702	S759	C819	K940	N1000
A220	I280	V341	L459	V519	GLU	L703	L760	K820	S941	L1001
R221	E281	K342	T460	D520	LEU	W704	T761	S821	L942	G1002
Q222	L282	E343	E461	R521	S644	L705	L762	L822	H943	Q1003
E223	F283	N344	V462	F523	F645	S706	F763	L823	L944	S1004
K224	Q284	V410	L464	N524	S646	S707	K764	S824	K892	S1005
S225	L285	I346	C465	K525	E547	E708	N765	F825	Q893	H945
Q226	Q286	E347	Q466	L526	V648	I709	K766	I826	D894	M1006
S227	I287	L348	D467	F527	E549	T710	T767	L826	L895	D1007
G228	Y288	M349	K468	T528	E650	N711	W768	L826	L896	S1008
L229	I289	A350	R469	G529	L651	S712	E769	L895	F897	E1009
N230	H290	D351	S470	S530	F652	E713	E770	ASP	L898	N1010
H231	H291	C353	M471	A531	L653	T714	F771	ARG	D899	T1011
I232	P292	H354	L472	G532	Q654	L715	R772	GLY	R900	R1012
L233	K293	Q355	E473	R533	T655	V716	I773	VAL		D1013
A234	G294	V356	S474	P534	T656	R717	G774	GLU		A1014
A235	A295	F357	S475	T528	L656	C718	S775	SER		P955
L236	K296	N358	Q476	G535	F657	S719	L776	GLU		Q1015
I237	T297	GLU	K477	S536	K659	S719	R777	MET		G1016
I238	Q298	ASP	S478	A538	M660	R720	R778	GLU		Q1017
F239	E299		D479	V539			W779	ASP		F1018
L240	K300		L480	C540			M780			L1019



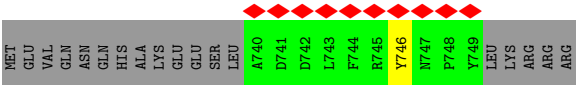




● Molecule 2: Nibrin



● Molecule 2: Nibrin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224367	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 ( $e^-/\text{\AA}^2$ )	51.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	323.4, 323.4, 323.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.078, 1.078, 1.078	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: MG, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/22624	0.45	1/30565 (0.0%)
1	C	0.24	0/22624	0.45	1/30565 (0.0%)
2	B	0.28	0/85	0.45	0/115
2	D	0.28	0/85	0.45	0/115
All	All	0.24	0/45418	0.45	2/61360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1313	GLU	CA-CB-CG	7.62	130.17	113.40
1	C	1313	GLU	CA-CB-CG	7.62	130.17	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1262	ARG	Sidechain
1	C	1262	ARG	Sidechain

## 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	A	22210	0	22392	177	0
1	C	22210	0	22392	174	0
2	B	83	0	69	1	0
2	D	83	0	69	1	0
3	A	31	0	13	0	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	44650	0	44948	350	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 350 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2506:ARG:HG3	1:C:2506:ARG:HH11	1.27	0.98
1:A:2506:ARG:HG3	1:A:2506:ARG:HH11	1.28	0.97
1:C:1313:GLU:OE1	1:C:1313:GLU:N	2.07	0.87
1:A:1313:GLU:OE1	1:A:1313:GLU:N	2.07	0.87
1:C:1271:ILE:O	1:C:1275:ILE:HB	1.76	0.86

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	2735/3056 (90%)	2688 (98%)	47 (2%)	0	100	100
1	C	2735/3056 (90%)	2688 (98%)	47 (2%)	0	100	100
2	B	8/28 (29%)	8 (100%)	0	0	100	100
2	D	8/28 (29%)	8 (100%)	0	0	100	100
All	All	5486/6168 (89%)	5392 (98%)	94 (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	
1	A	2469/2780 (89%)	2446 (99%)	23 (1%)	75	89
1	C	2469/2780 (89%)	2446 (99%)	23 (1%)	75	89
2	B	8/26 (31%)	8 (100%)	0	100	100
2	D	8/26 (31%)	8 (100%)	0	100	100
All	All	4954/5612 (88%)	4908 (99%)	46 (1%)	74	89

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	433	SER
1	C	1347	LEU
1	C	521	ARG
1	C	1275	ILE
1	C	1478	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1640	GLN
1	C	65	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1128	GLN
1	C	1640	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	ANP	C	3101	-	29,33,33	1.15	4 (13%)	31,52,52	0.82	1 (3%)
3	ANP	A	3101	-	29,33,33	1.15	4 (13%)	31,52,52	0.82	1 (3%)

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
3	ANP	C	3101	-	-	4/14/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	3101	-	-	4/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3101	ANP	PG-O1G	2.53	1.50	1.46
3	C	3101	ANP	PG-O1G	2.53	1.50	1.46
3	A	3101	ANP	PG-N3B	2.44	1.69	1.63
3	C	3101	ANP	PG-N3B	2.44	1.69	1.63
3	A	3101	ANP	PB-O1B	2.44	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3101	ANP	C5-C6-N6	2.16	123.61	120.31
3	C	3101	ANP	C5-C6-N6	2.16	123.61	120.31

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

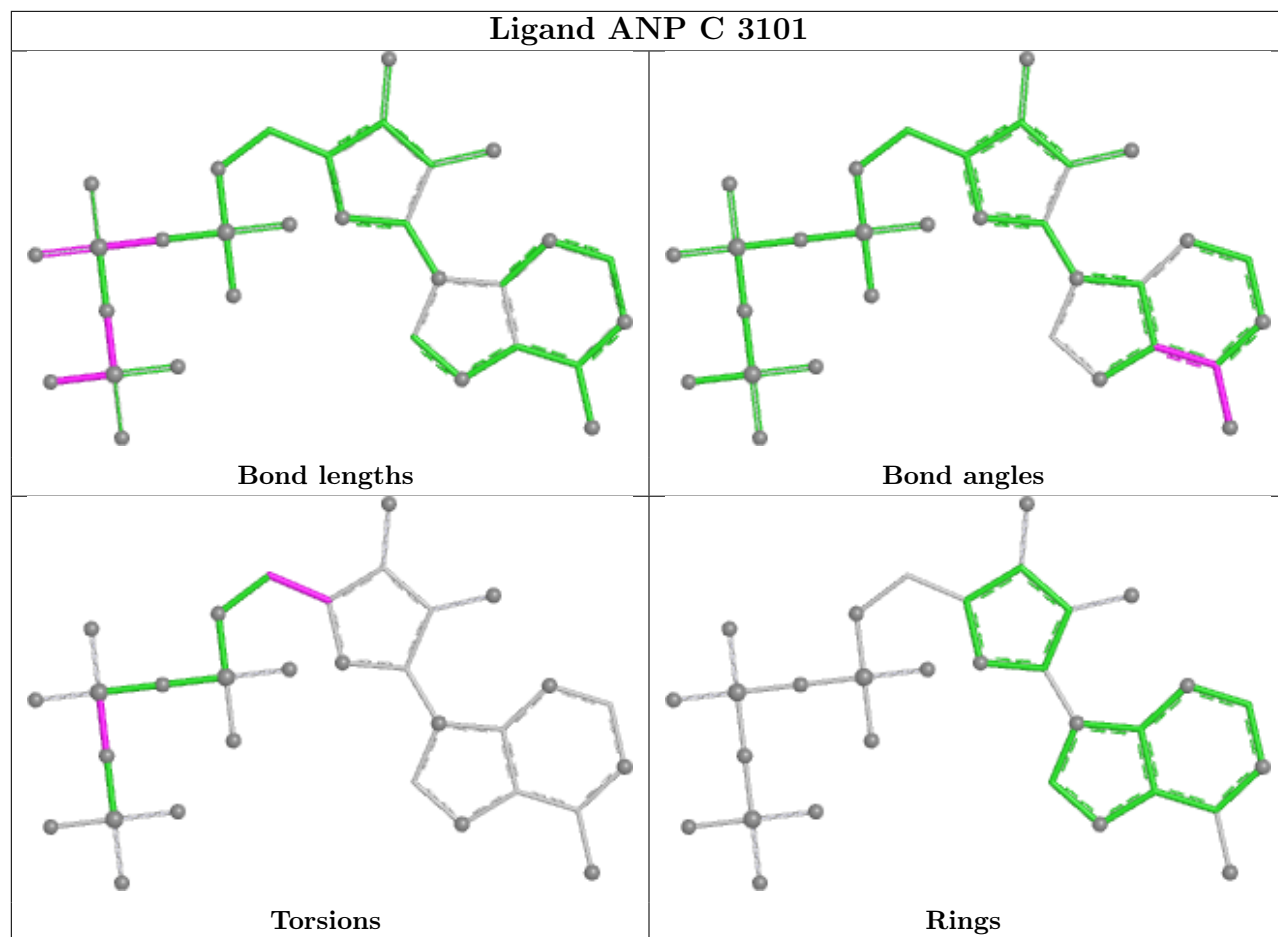
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PG-N3B-PB-O1B
3	C	3101	ANP	PG-N3B-PB-O1B
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	C	3101	ANP	O4'-C4'-C5'-O5'

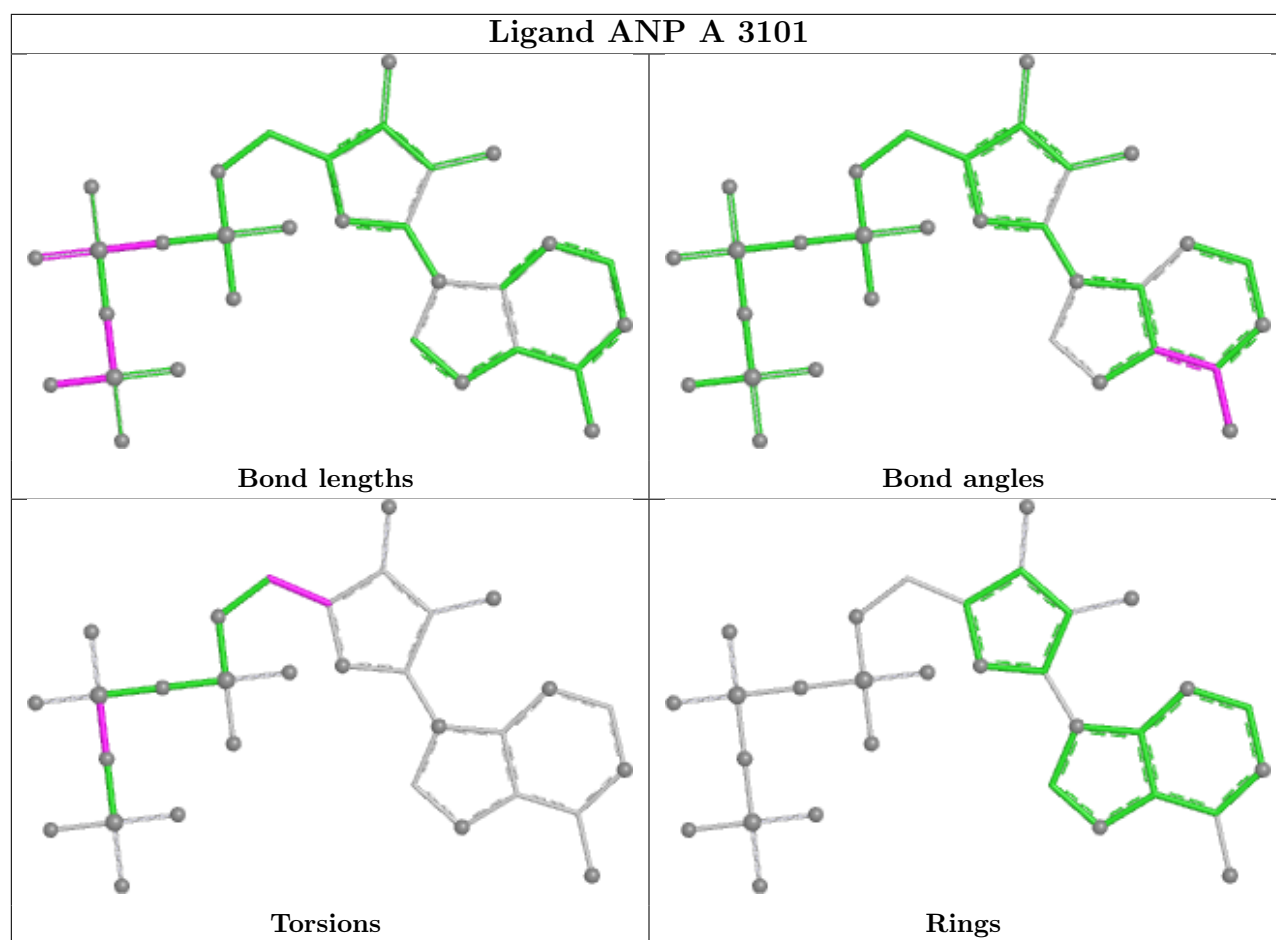
There are no ring outliers.

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.

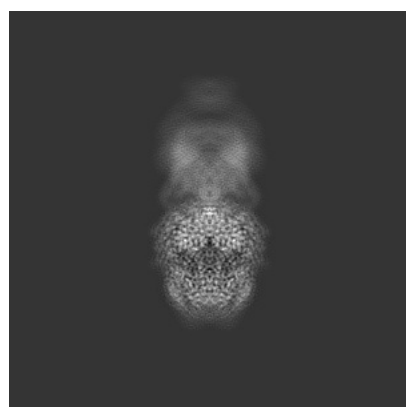
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25141. These allow visual inspection of the internal detail of the map and identification of artifacts.

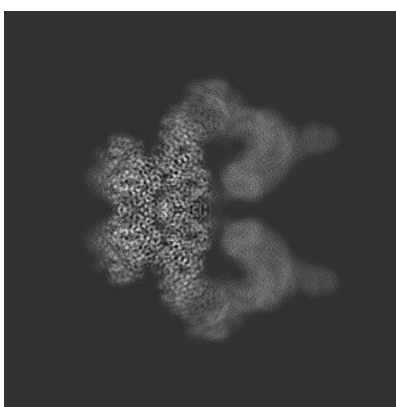
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

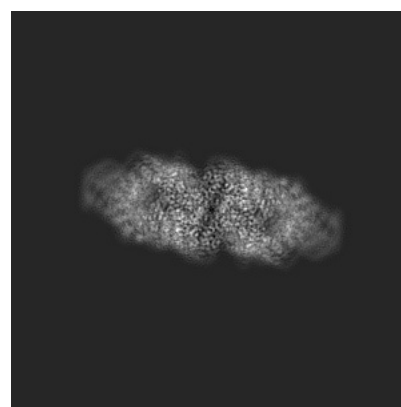
#### 6.1.1 Primary map



X



Y

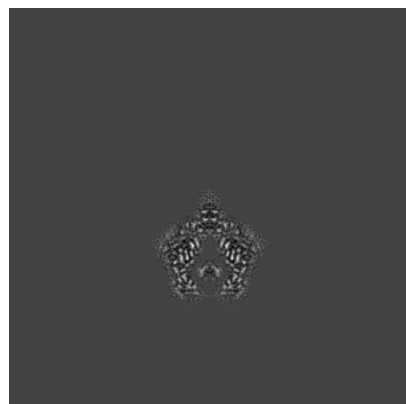


Z

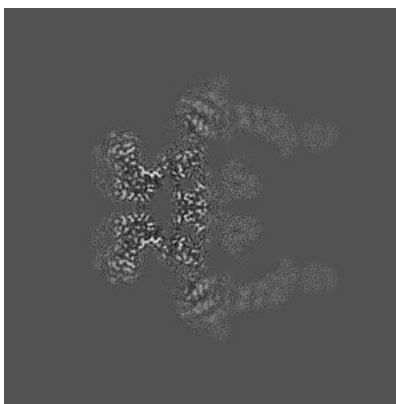
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 150



Y Index: 150

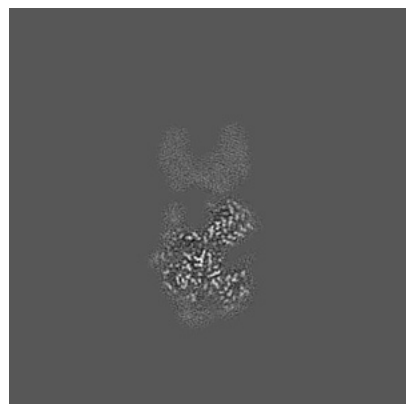


Z Index: 150

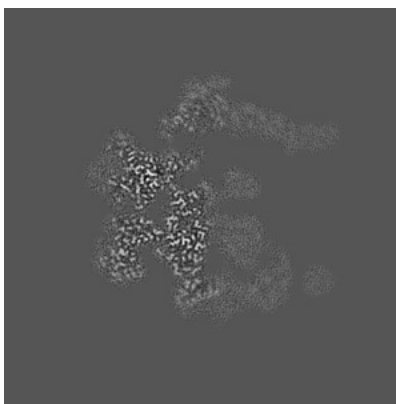
The images above show central slices of the map in three orthogonal directions.

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

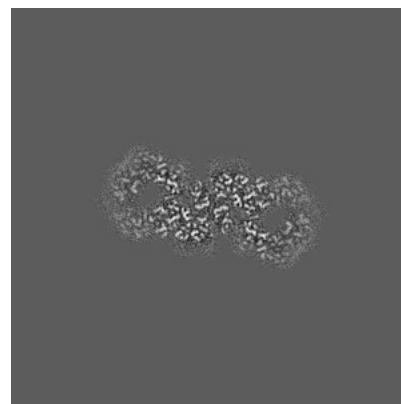
### 6.3.1 Primary map



X Index: 175



Y Index: 144

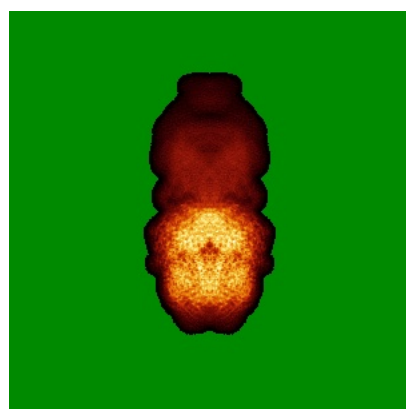


Z Index: 131

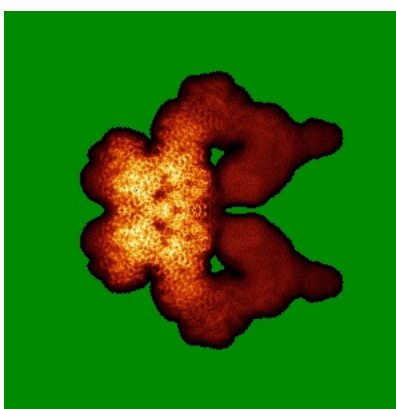
The images above show the largest variance slices of the map in three orthogonal directions.

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

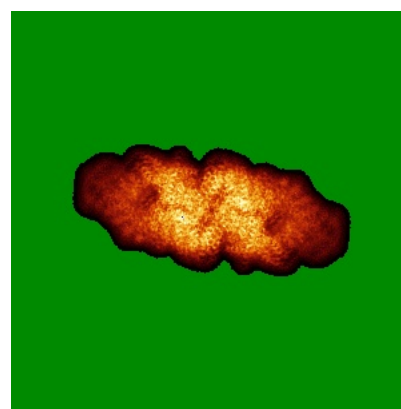
### 6.4.1 Primary map



X



Y

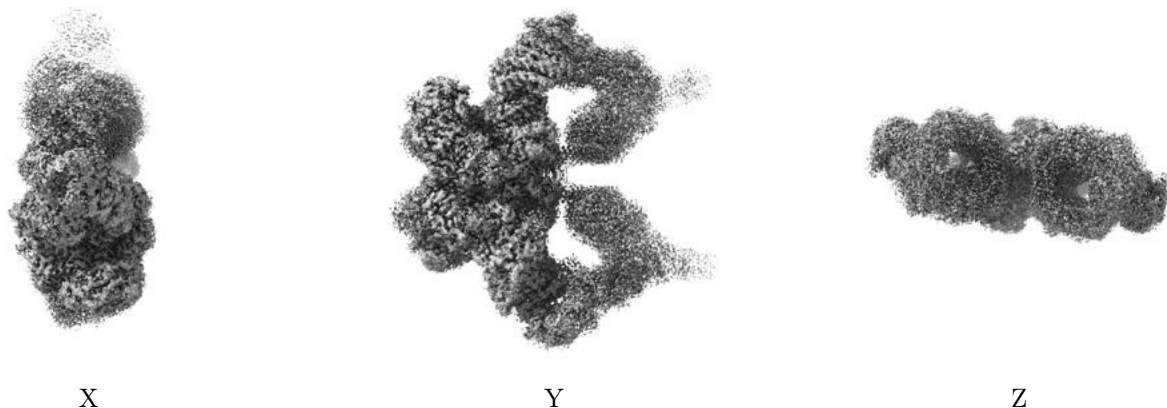


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

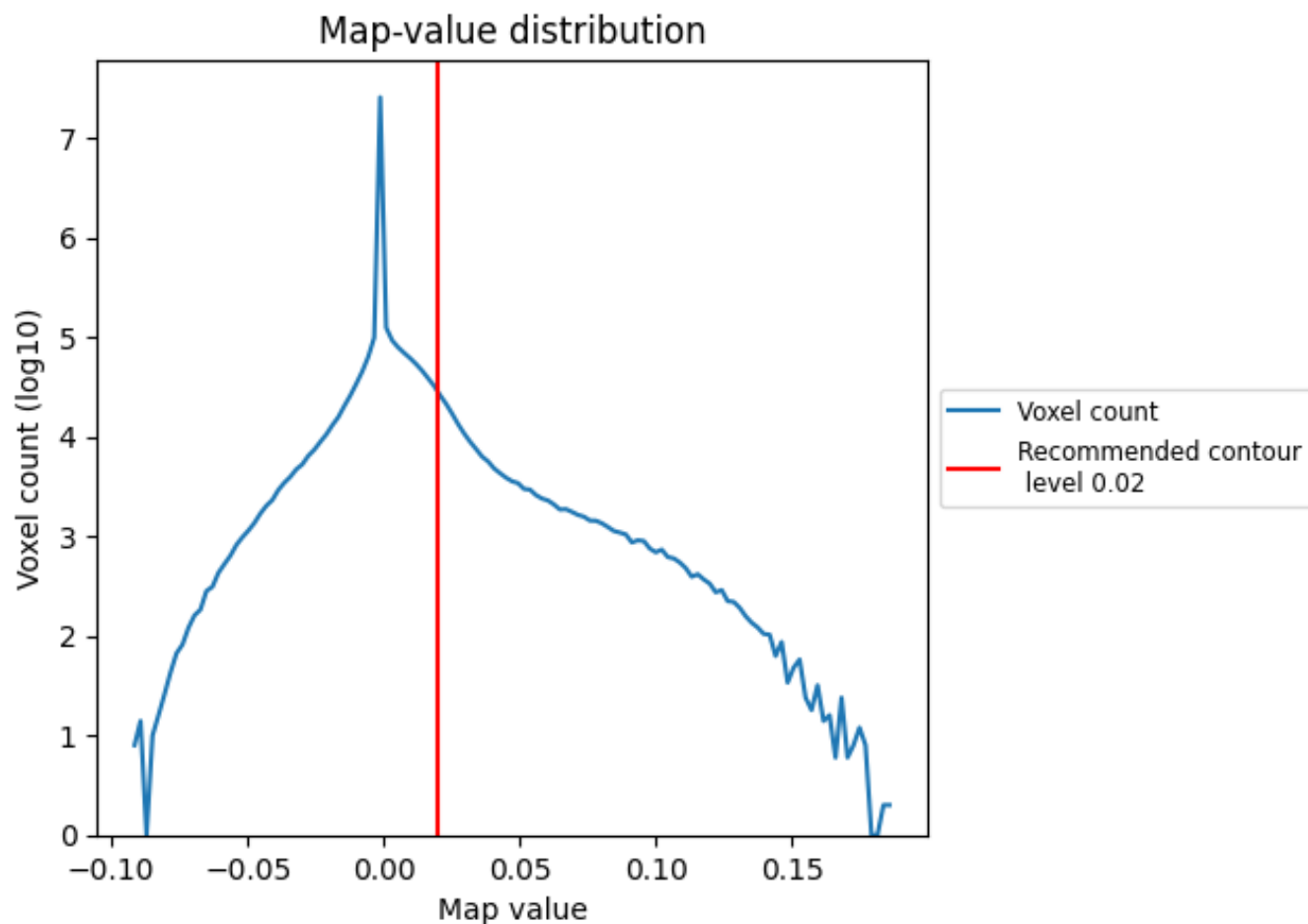
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

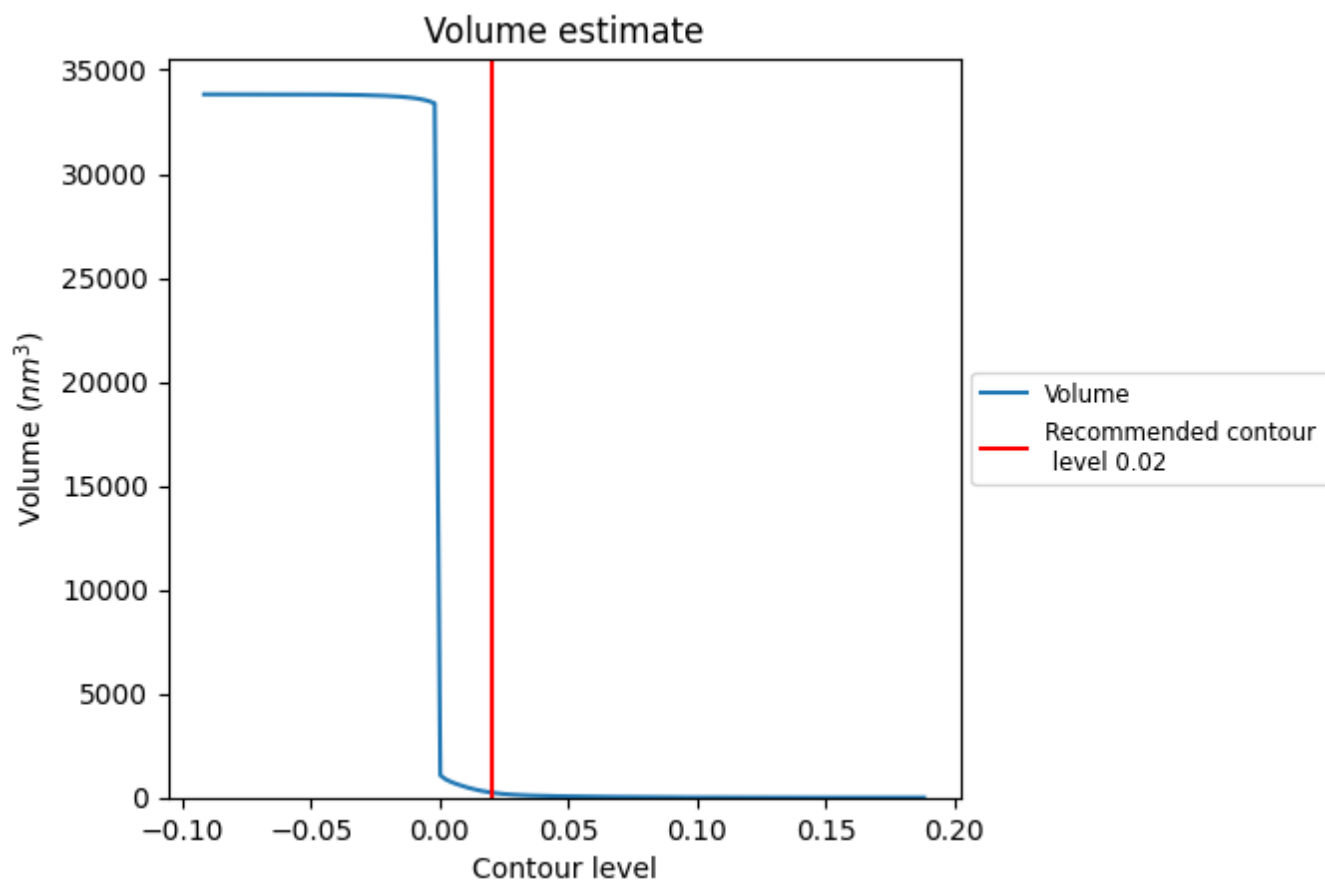
This section contains the results of statistical analysis of the map.

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



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

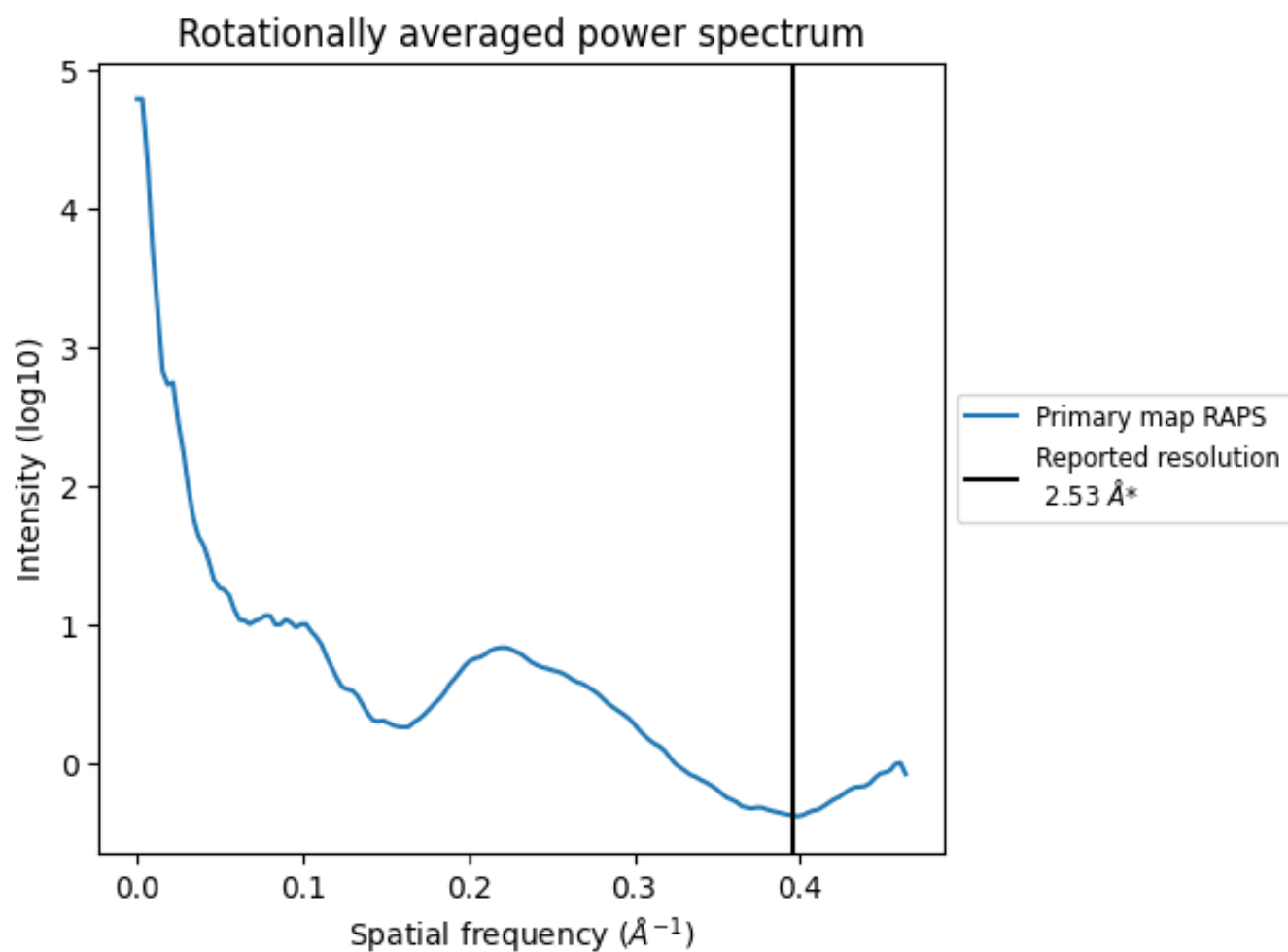
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm<sup>3</sup>; this corresponds to an approximate mass of 218 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 ⓘ



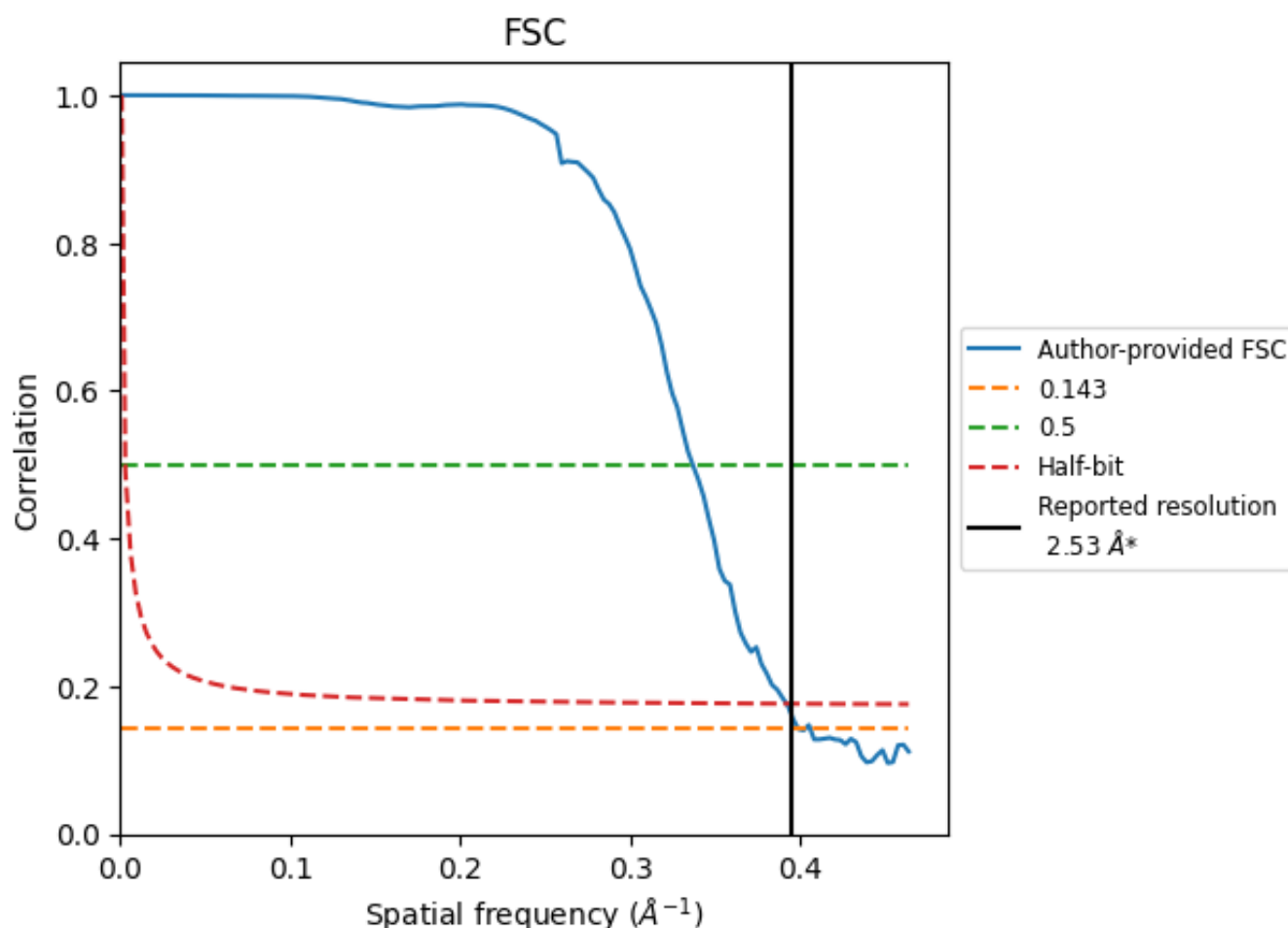
\*Reported resolution corresponds to spatial frequency of 0.395 Å<sup>-1</sup>



## 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 0.395 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

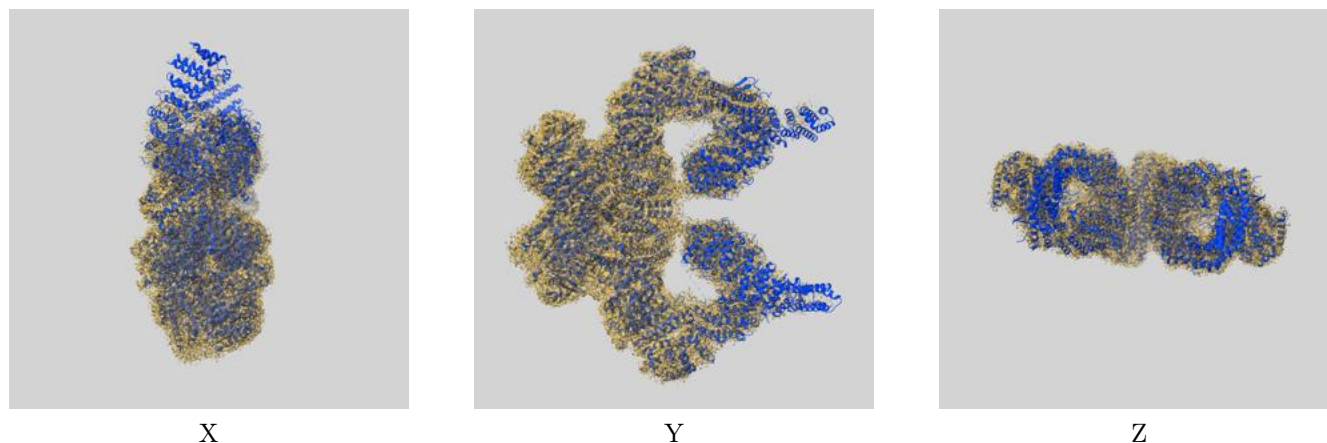
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.51	2.97	2.55
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

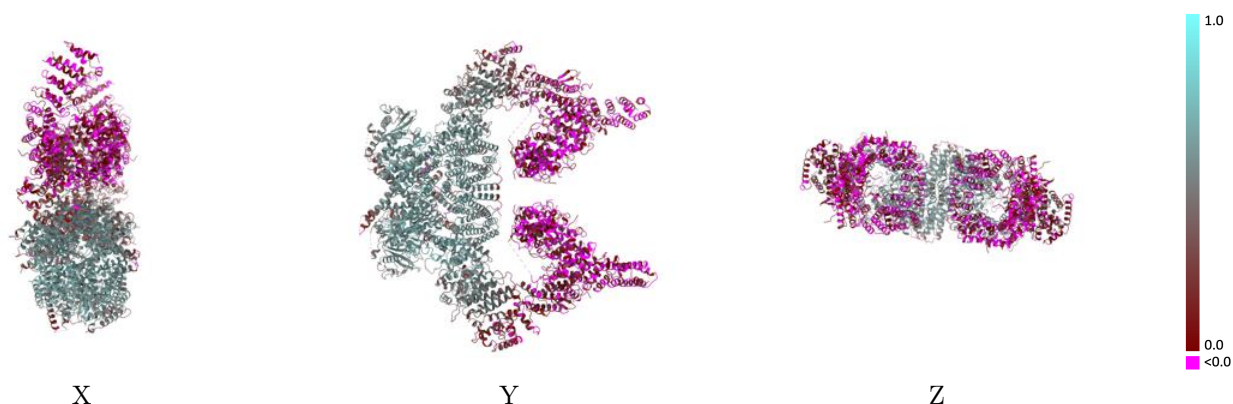
This section contains information regarding the fit between EMDB map EMD-25141 and PDB model 7SID. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



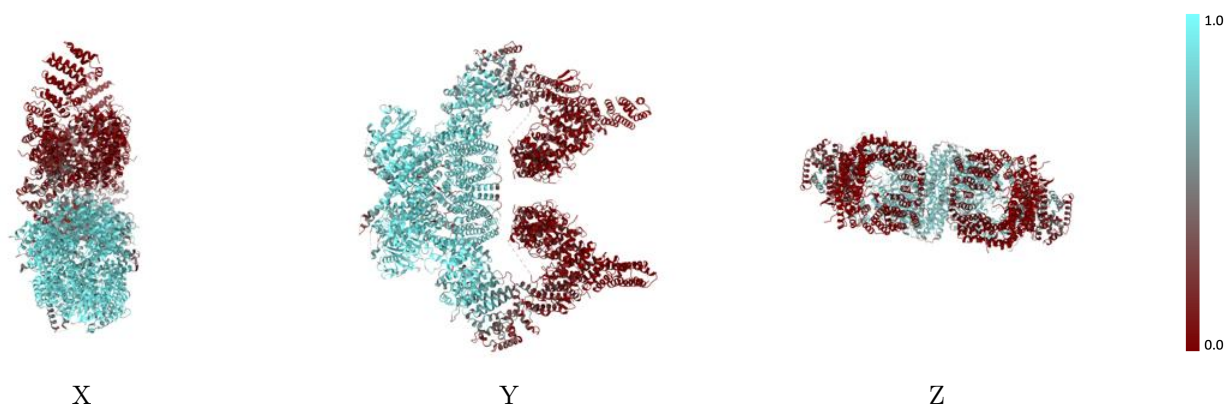
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



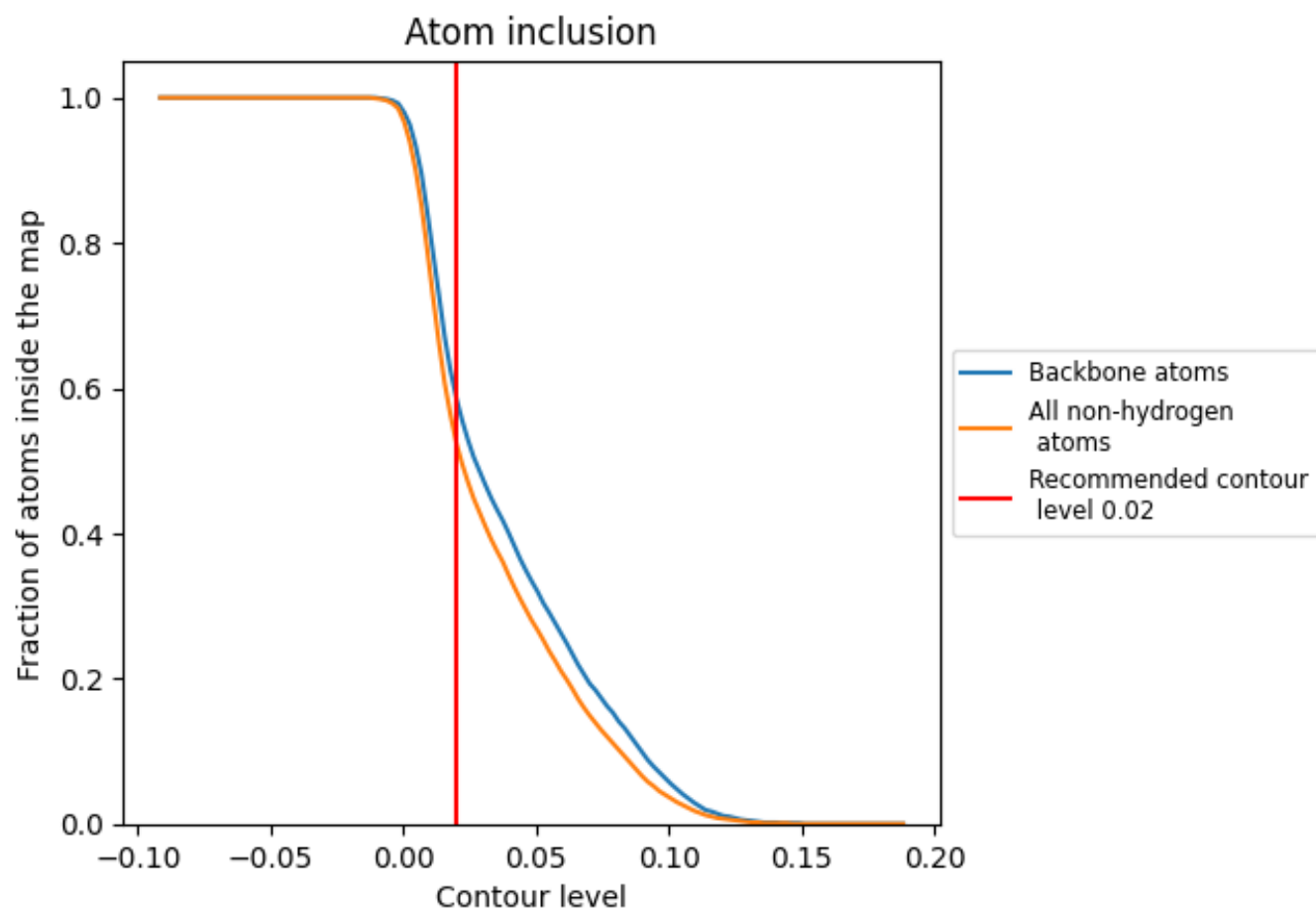
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 52% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5240	<div></div> 0.3360
A	<div></div> 0.5260	<div></div> 0.3370
B	<div></div> 0.0250	<div></div> 0.0430
C	<div></div> 0.5260	<div></div> 0.3380
D	<div></div> 0.0250	<div></div> 0.0470

