



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:55 AM UTC

PDB ID : 7SID / pdb_00007sid
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

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:

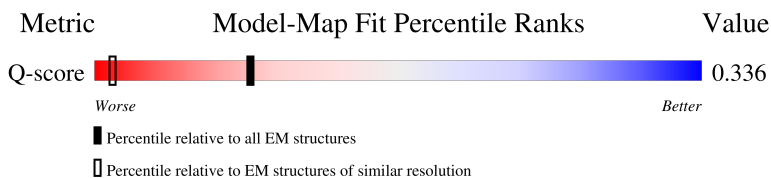
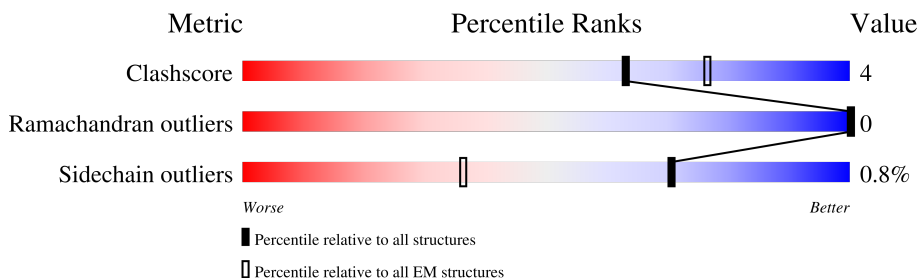
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7309 (2.03 - 3.03)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3056	<p>39% (Poor fit), 80% (0 outliers), 10% (1 outlier), 9% (2 outliers), 9% (3+ outliers), 9% (Not modelled)</p>
1	C	3056	<p>39% (Poor fit), 80% (0 outliers), 10% (1 outlier), 9% (2 outliers), 9% (3+ outliers), 9% (Not modelled)</p>
2	B	28	<p>36% (Poor fit), 32% (0 outliers), 64% (Not modelled)</p>
2	D	28	<p>36% (Poor fit), 32% (0 outliers), 64% (Not modelled)</p>

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.

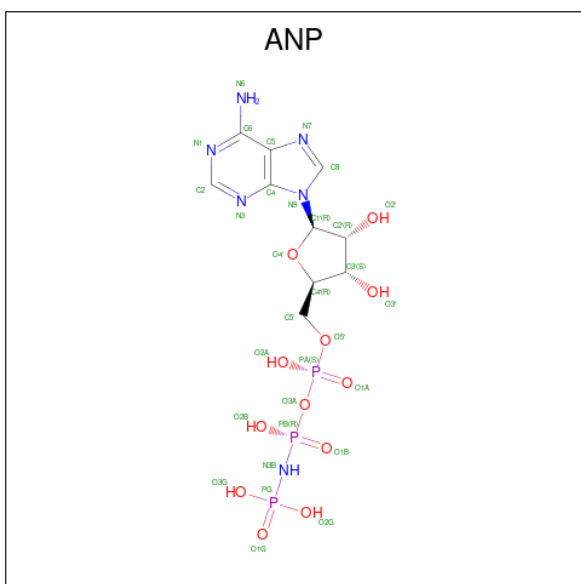
- Molecule 1 is a protein called Serine-protein kinase ATM.

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

- Molecule 2 is a protein called Nibrin.

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

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

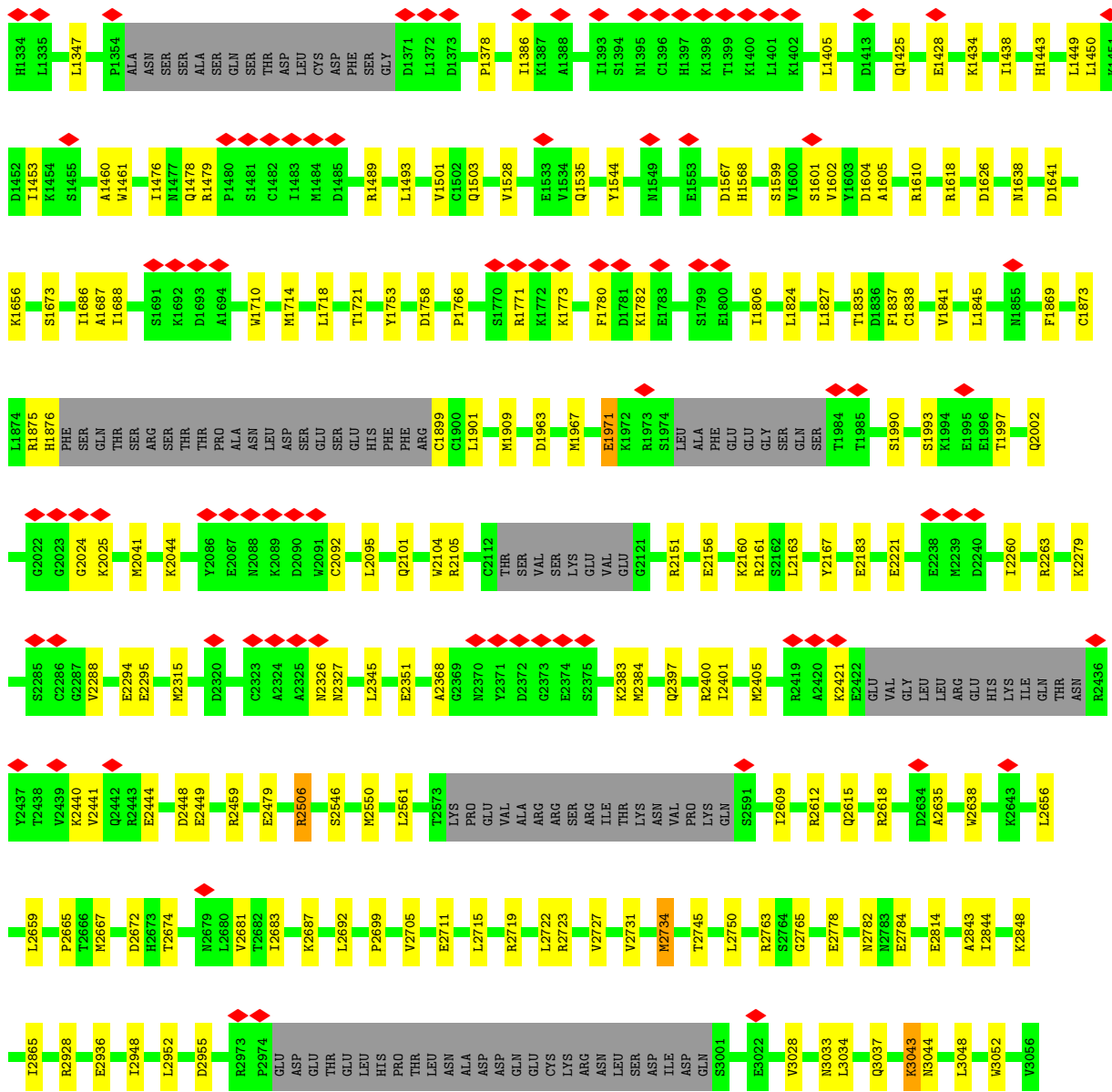


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	6	12	3	0
3	C	1	31	10	6	12	3	0

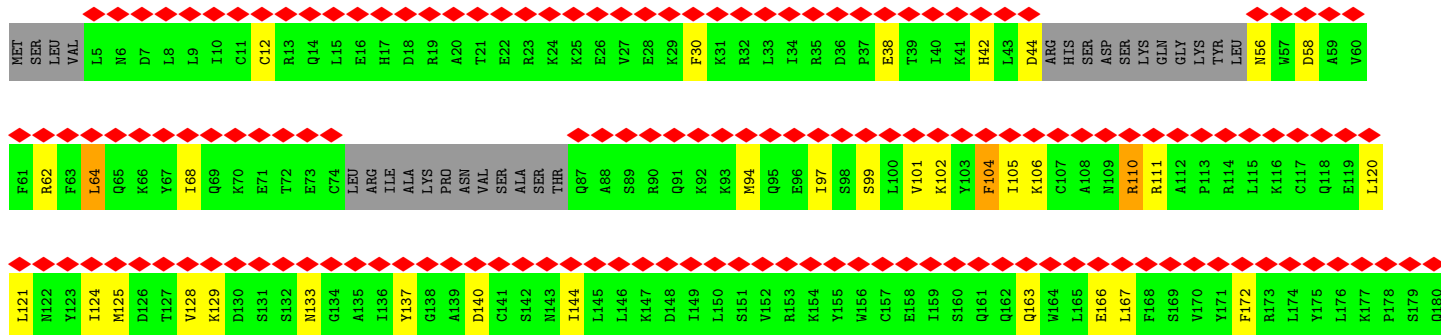
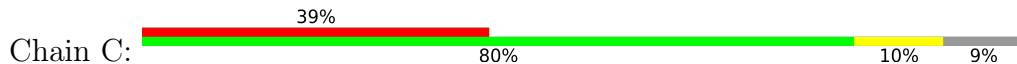
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

E1267	V1268	K1269	S1270	I1271	A1272	M1273	Q1274	I1275	Q1276	D1277	L1278	M1279	D1278	I1281	L1282	I1283	T1284	D1285	I1290	M1293	F1298	A1299	Y1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	Y1318	Y1319	D1320	M1321	L1322	K1323	S1324	E1325	M1326	L1327	L1328	G1329	K1330	Q1331	I1332	D1333			
R1204	R1205	L1206	E1207	D1208	F1209	M1210	A1211	L1214	D1215	Y1216	L1217	E1220	W1221	L1222	N1223	L1224	Q1225	D1226	T1227	E1228	Y1229	M1230	L1231	S1232	S1233	F1234	P1235	F1236	I1237	L1238	L1239	N1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	Y1248	R1249	S1250	C1251	Y1252	K1253	V1254	L1255	H1258	L1259	V1260	I1261	R1262	S1263	H1264	Q1265	D1266			
M1081	H1082	H1083	Q1084	V1085	R1086	M1087	L1088	A1089	A1090	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	T1100	K1101	GLY	ASP	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1111	P1112	L1113	L1114	L1115	Q1116	Q1117	T1118	A1119	F1120	E1121	M1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1132	E1133	M1134	SER	HIS	SER	ALA	ASN	
PRO	E1142	T1143	L1144	D1145	E1146	I1147	Y1148	M1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	T1158	A1159	V1160	V1161	S1165	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	L1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	M1183	G1184	L1185	E1186	P1187	H1188	L1189	V1190	K1191	K1192	V1193	L1194	E1195	K1196	L1197	S1198	E1199	T1200	F1201	G1202	Y1203		
V1021	I1022	G1023	F1024	F1025	W1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	D1044	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	D1053	P1054	Y1055	S1056	K1057	W1058	A1059	I1060	L1061	N1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	V1070	M1071	E1072	V1073	F1074	T1075	Q1076	F1077	L1078	A1079	D1080
L901	K902	F903	L904	C905	L906	C907	V908	T909	T910	A911	Q912	T913	N914	T915	V916	S917	F918	R919	A920	A921	D922	I923	R924	R925	K926	L927	L928	M929	L930	I931	D932	S933	S934	T935	L936	E937	P938	T939	K940	S941	L942	H943	L944	H945	N946	Y947	L948	M949	L950	L951	K952	E953	L954	P955	G956	E957	E958	Y959	P960
L961	P962	M963	E964	D965	V966	L967	E968	L969	L970	K971	P972	L973	S974	N975	V976	C977	S978	L979	Y980	R981	R982	D983	Q984	D985	V986	C987	K988	T989	L990	N991	N992	H993	V994	L995	H996	V997	K998	M1000	L1001	G1002	Q1003	S1004	M1005	M1006	D1007	S1008	E1009	M1010	T1011	R1012	D1013	A1014	Q1015	G1016	Q1017	L1018	L1019	T1020	
Q781	L782	C783	T784	R785	L786	L787	S788	M789	C790	Y791	K792	G793	S794	P795	N796	K797	I798	A799	S900	G901	F902	F903	L904	R905	L906	L907	T908	S909	K910	L911	M912	L913	D914	I915	A916	D917	I918	C919	K920	S921	A923	S924	F925	I926	L927	P928	PHE	ASP	ARG	GLY	GLU	VAL	GLU	SER	MET	GLU	ASP		
L721	L722	V723	G724	V725	L726	G727	C728	Y729	C730	Y731	G732	G733	V734	I735	A736	E737	E738	E739	A740	Y741	K742	S743	E744	L745	F746	Q747	K748	A749	K750	S751	L752	L753	Q754	C755	A756	E758	S759	I760	T761	L762	F763	K764	N765	K766	I767	T768	E769	E770	F771	L772	I773	G774	S775	L776	R777	M778	M779	M780	
D661	F662	L663	T664	ILE	VAL	ARG	GLU	CYS	GLY	ILE	GLU	LYS	HIS	GLN	SER	ILE	G679	F680	S681	V682	H683	Q684	A740	E685	S688	L689	D691	R692	C693	L694	L695	G696	L697	S698	E699	Q700	L701	L702	I703	N704	Y705	S706	S707	E708	I709	T710	N711	S712	F713	T714	L715	V716	R717	C718	S719	R720			
S601	N602	F603	P604	H605	L606	V607	L608	E609	K610	I611	L612	V613	S614	L615	T616	M617	K618	N619	C620	K621	A622	A623	M624	N625	F626	F627	Q628	S629	V630	P631	R632	C633	GLU	HIS	HIS	GLN	LYS	ASP	LYS	GLU	GLU	LEU	SER	T993	E994	V995	P996	P997	I998	L999	H600								

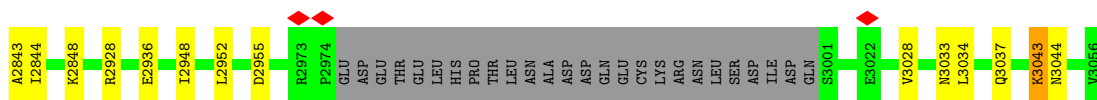


● Molecule 1: Serine-protein kinase ATM

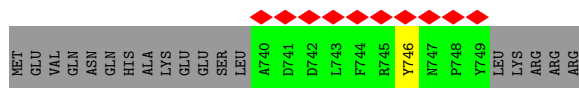


L961	P962	M963	E964	D965	V966	L967	E968	L969	L970	K971	P972	L973	S974	N975	V976	C977	S978	L979	Y980	R981	D982	D983	Q984	D985	V986	C987	K988	T989	I990	L991	N992	H993	V994	L995	H996	V997	K998	N999	L1000	L1001	G1002	Q1003	S1004	L1005	M1006	D1007	S1008	E1009	N1010	T1011	R1012	D1013	Q1014	Q1015	G1016	Q1017	F1018	L1019	P960		
L901	K902	F903	L904	C905	L906	C907	V908	T909	T910	A911	Q912	T913	N914	T915	V916	S917	F918	R919	A920	A921	D922	I923	Q924	R925	K926	L927	L928	M929	L930	I931	D932	S933	S934	T935	L936	E937	P938	T939	K940	S941	L942	L943	H944	H945	M946	Y947	L948	M949	L950	L951	K952	L953	L954	P955	Q956	E957	E958	Y959			
D181	V182	H183	R184	V185	L186	V187	A188	R189	I190	I191	H192	A193	V194	T195	K196	G197	C198	C199	S200	Q201	T202	D203	G204	L205	N206	N207	K208	F209	L210	D211	F212	F213	S214	K215	A216	I217	Q218	C219	A220	R221	E222	E223	K224	S225	S226	S227	G228	L229	N230	H231	I232	L233	A234	A235	L236	T237	I238	F239	L240		
K241	T242	L243	A244	V245	N246	F247	R248	I249	R250	V251	C252	E253	L254	G255	D256	E257	I258	L259	P260	T261	L262	L263	Y264	I265	V266	T267	Q268	H269	R270	L271	N272	D273	S274	L275	K276	E277	V278	I279	I280	E281	L282	F283	Q284	L285	Q286	I287	Y288	I289	H290	H291	P292	K293	G294	A295	K296	T297	Q298	E299	K300		
G301	A302	Y303	E304	S305	T306	K307	W308	R309	S310	I311	L312	Y313	N314	L315	Y316	D317	L318	L319	V320	N321	E322	I323	S324	H325	I326	G327	S328	R329	GLY	LYS	TYR	SER	SER	GLY	PHE	R337	N338	I339	A340	V341	K342	E343	N344	L345	I346	E347	L348	M349	A350	D351	H291	C353	H354	Q355	V356	F357	N358	ASP			
THR	ARG	LEU	GLU	ILE	SER	GLN	TYR	THR	THR	THR	GLN	ARG	GLU	SER	SER	ASP	TYR	VAL	PRO	CYS	LYS	ARG	LYS	I389	E390	L391	G392	W393	E394	V395	I396	K397	D398	H399	L400	PHE	Q401	N338	S403	Q404	A340	M405	F407	D408	L409	V410	P411	W412	L413	Q414	A350	I415	A416	T417	H354	Q355	V356	F357	N358	ASP	
S421	K422	Y423	P424	A425	S426	L427	P428	M429	C430	E431	L432	S433	P434	L435	L436	M437	I438	L439	S440	Q441	L442	L443	P444	Q445	Q446	R447	H448	G449	E450	R451	T452	P453	Y454	V455	L456	R457	C458	L459	T460	E461	A462	A463	L464	C465	Q466	D467	K468	A469	S470	M471	L472	E473	S474	S475	Q476	K477	D478	L480			
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C541	L542	T543	L544	A545	L546	T547	T548	S549	L550	V551	P552	G553	T554	VAL	LYS	MET	GLY	ILE	GLU	GLN	ASN	MET	A502	E503	N504	F505	G506	L507	L508	G509	A510	I511	I512	Q513	G514	S515	L516	V517	E518	V519	D520	R521	E522	F523	N524	K525	L526	F527	T528	G529	S530	A531	C532	R533	E534	S535	C536	P537	A538	V539	C540
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D661	F662	L663	T664	ILE	VAL	ARG	GLU	CYS	GLY	ILE	GLU	LYS	HIS	SER	ILE	G679	F680	S681	V682	H683	Q684	N685	L686	K687	E688	S689	L690	D691	R692	L694	L695	G696	L697	S698	E699	Q700	L701	L702	M703	W704	Y705	S706	S707	E708	I709	T710	M711	S712	E713	T714	L715	V716	R717	C718	S719	D658	K659	M660			
L721	L722	W723	G724	W725	L726	G727	C728	Y729	C730	Y731	M732	G733	W734	I735	A736	E737	E738	E739	A740	Y741	K742	S743	E744	L745	F746	Q747	K748	A749	K750	S751	L752	W753	Q754	C755	A756	G757	E758	S759	L760	T761	L762	F763	K764	W765	K766	T767	M768	E769	L770	F771	R772	I773	G774	S775	L776	R777	M778	W779	M780		
Q781	L782	C783	T784	R785	C786	L787	S788	M789	C790	T791	K792	K793	S794	F795	M796	K797	I798	A799	S800	G801	F802	F803	L804	R805	L806	L807	T808	S809	K810	L811	M812	H813	D814	I815	A816	D817	C819	K820	S821	A823	S824	F825	LYS	LYS	PRO	PHE	ASP	ARG	GLY	GLU	VAL	L776	L777	M778	W779	M780					
ASP	THR	ASN	ASN	LEU	MET	GLU	VAL	GLU	ASP	GLN	SER	MET	ASN	PHE	ASN	ASP	TYR	PRO	ASP	SER	SER	VAL	SER	PRO	GLY	GLU	SER	GLN	S877	T878	I879	O880	A881	T882	M883	P884	A886	E887	E888	N1000	H889	S891	K892	Q893	D894	L895	L896	F897	L898	L899	D899	M900									

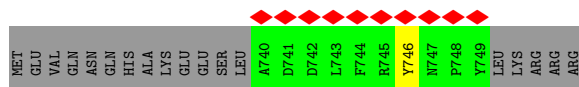
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H1021	I1022	G1023	A1024	F1025	M1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	D1053	P1054	Y1055	K1056	T1057	M1058	A1059	I1060	L1061	N1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	V1070	M1071	E1072	V1073	F1074	T1075	Q1076	F1077	L1078	A1079	
N1081	H1082	H1083	Q1084	V1085	R1086	M1087	L1088	A1089	A1090	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	K1100	K1101	GLY	ASP	SER	ARG	LEU	L1108	K1109	A1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	F1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	R1132	E1133	M1134	SER	HIS	SER	ALA	GLU	ASN
PRO	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	V1161	S1165	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	M1183	G1184	L1185	E1186	P1187	H1188	L1189	V1190	K1191	K1192	V1193	L1194	E1195	K1196	V1197	S1198	E1199	T1200	F1201	G1202	Y1203		
R1204	R1205	L1206	E1207	D1208	F1209	M1210	A1211	L1214	D1215	Y1216	L1217	E1220	M1221	L1222	M1223	L1224	Q1225	D1226	T1227	E1228	Y1229	M1230	L1231	S1232	S1233	F1234	F1235	F1236	I1237	L1238	L1239	M1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	Y1248	R1249	S1250	C1251	Y1252	M1253	V1254	L1255	H1258	L1259	I1261	R1262	S1263	H1264	Q1331	F1265	D1266		
E1267	V1268	K1269	S1270	I1271	A1272	Q1274	I1275	Q1276	E1277	D1278	M1279	K1280	S1281	L1282	L1283	T1284	D1285	I1290	M1293	F1298	A1299	V1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320	M1321	L1322	K1323	S1324	E1325	M1326	L1327	L1328	G1329	K1330	Q1331	I1332	D1333			
H1334	L1335	L1347	P1354	ALA	ASN	SER	SER	ALA	SER	GLN	THR	ASP	LEU	CYS	ASP	PHE	SER	GLY	D1371	L1372	D1373	P1378	I1386	K1387	A1388	I1393	S1394	M1395	C1396	H1397	K1398	T1399	K1400	L1401	K1402	L1405	D1413	Q1425	E1428	K1434	I1438	H1443	L1449	L1450	K1461													
D1462	I1463	K1464	S1465	A1466	M1461	I1476	M1477	Q1478	R1479	P1480	S1481	C1482	I1483	M1484	D1485	R1489	L1493	V1501	Q1502	V1528	E1533	V1534	Q1535	Y1544	M1549	E1553	D1567	H1568	S1599	S1601	V1602	D1604	A1605	L1608	T1609	R1610	R1618	D1626	M1638																			
D1641	K1656	T1662	S1673	V1678	I1686	A1687	I1688	S1691	K1692	D1693	A1694	L1702	M1710	M1714	L1718	T1721	Y1753	D1758	P1766	S1770	R1771	K1772	K1773	F1780	D1781	K1782	E1783	S1799	E1800	I1806	L1824	L1827	T1835	D1836	C1838	V1841																						
L1845	M1855	F1869	C1873	L1874	R1875	H1876	PHE	SER	GLN	THR	ARG	ALA	ASN	LEU	ASP	SER	GLU	SER	GLU	GLU	HIS	PHE	PHE	ARG	C1899	L1901	M1909	D1963	M1967	E1971	K1972	R1973	S1974	ALA	PHE	GLU	GLU	GLY	SER	GLN	T1984	T1985	S1990															
S1993	K1994	E1995	E1996	T1997	Q2002	G2022	G2023	G2024	K2025	M2041	K2044	Y2086	E2087	M2088	K2089	D2090	W2091	C2092	L2095	Q2101	W2104	R2105	C2112	THR	SER	VAL	SER	LYS	GLU	VAL	GLU	G2121	R2151	E2156	K2160	R2161	S2162	L2163	Y2167	E2183	E2221	E2238																
M2239	D2240	I2260	R2263	K2279	S2285	C2286	G2287	V2288	E2294	E2295	M2315	D2320	C2323	A2324	A2325	N2326	N2327	L2345	E2351	A2368	G2369	N2370	Y2371	D2372	G2373	E2374	S2375	K2383	M2384	R2400	I2401	M2405	R2419	A2420	K2421	E2422	GLU	VAL	GLY	LEU	ARG																	
GLU	HIS	LYS	ILE	GLN	THR	ASN	R2436	Y2437	T2438	K2440	V2441	Q2442	R2443	E2444	D2448	E2449	R2459	E2479	R2506	S2546	M2550	L2561	T2573	PRO	GLU	VAL	ALA	ARG	SER	ARG	ILE	THR	LYS	ASN	VAL	PRO	LYS	G2591	I2609	R2612	Q2615	R2618																



• 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 (\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 (\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: ANP, MG

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	0.11	0/22624	0.28	1/30565 (0.0%)
1	C	0.11	0/22624	0.28	1/30565 (0.0%)
2	B	0.11	0/85	0.30	0/115
2	D	0.11	0/85	0.30	0/115
All	All	0.11	0/45418	0.28	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	8.04	130.17	114.10
1	C	1313	GLU	CA-CB-CG	8.04	130.17	114.10

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	187	0
1	C	22210	0	22392	187	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	374	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 374 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 [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	A	2469/2780 (89%)	2450 (99%)	19 (1%)	73	88
1	C	2469/2780 (89%)	2450 (99%)	19 (1%)	73	88
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%)	4916 (99%)	38 (1%)	70	88

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1312	ARG
1	C	2734	MET
1	C	1313	GLU
1	C	1478	GLN
1	C	3043	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	HIS
1	C	1640	GLN
1	C	2826	ASN

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Mol	Chain	Res	Type
1	C	584	GLN
1	C	1044	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	3101	-	33,33,33	0.94	4 (12%)	45,52,52	0.58	0
3	ANP	C	3101	-	33,33,33	0.94	4 (12%)	45,52,52	0.58	0

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	A	3101	-	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	3101	-	-	4/18/38/38	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

There are no bond angle outliers.

There are no chirality outliers.

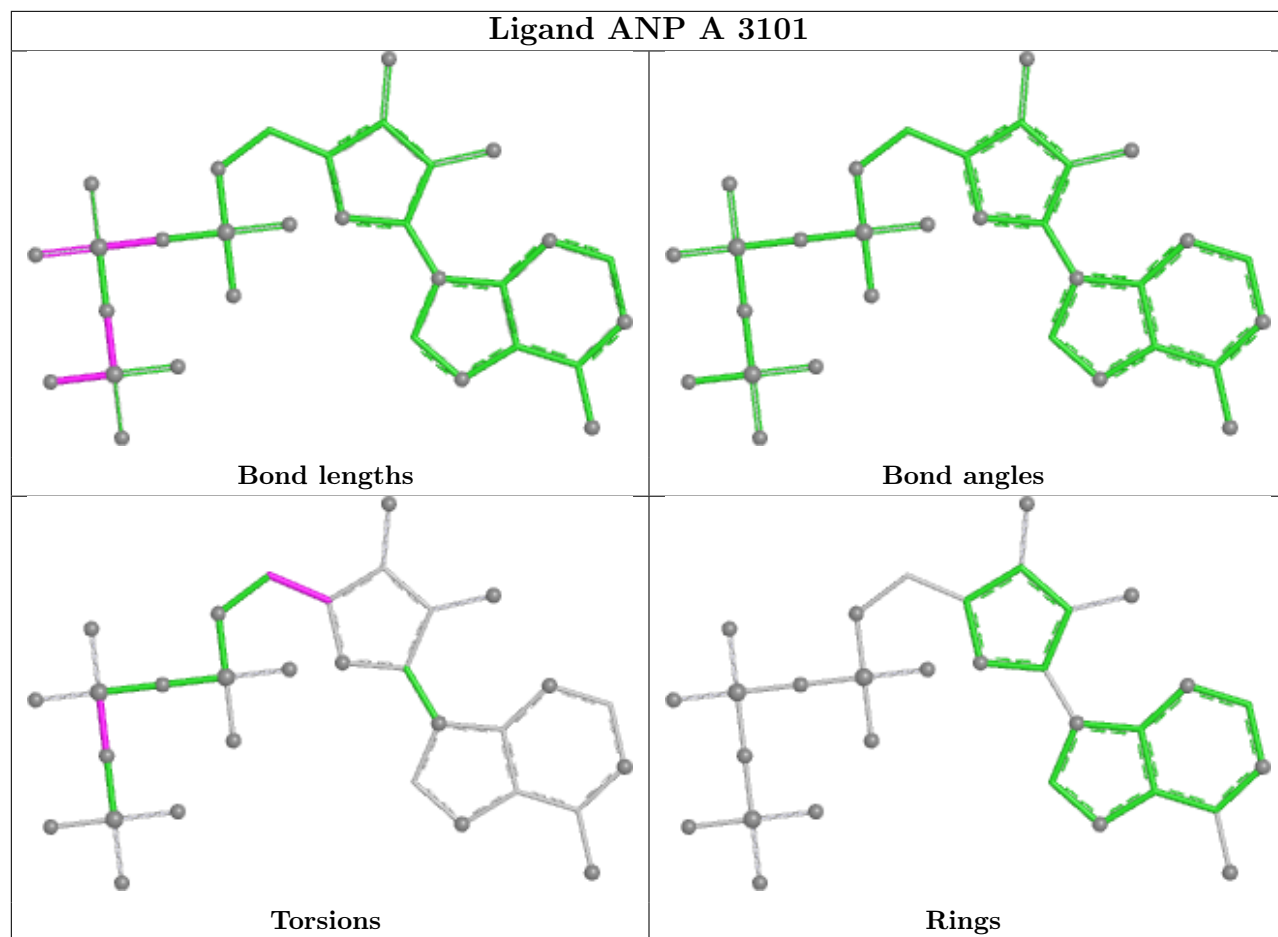
5 of 8 torsion outliers are listed below:

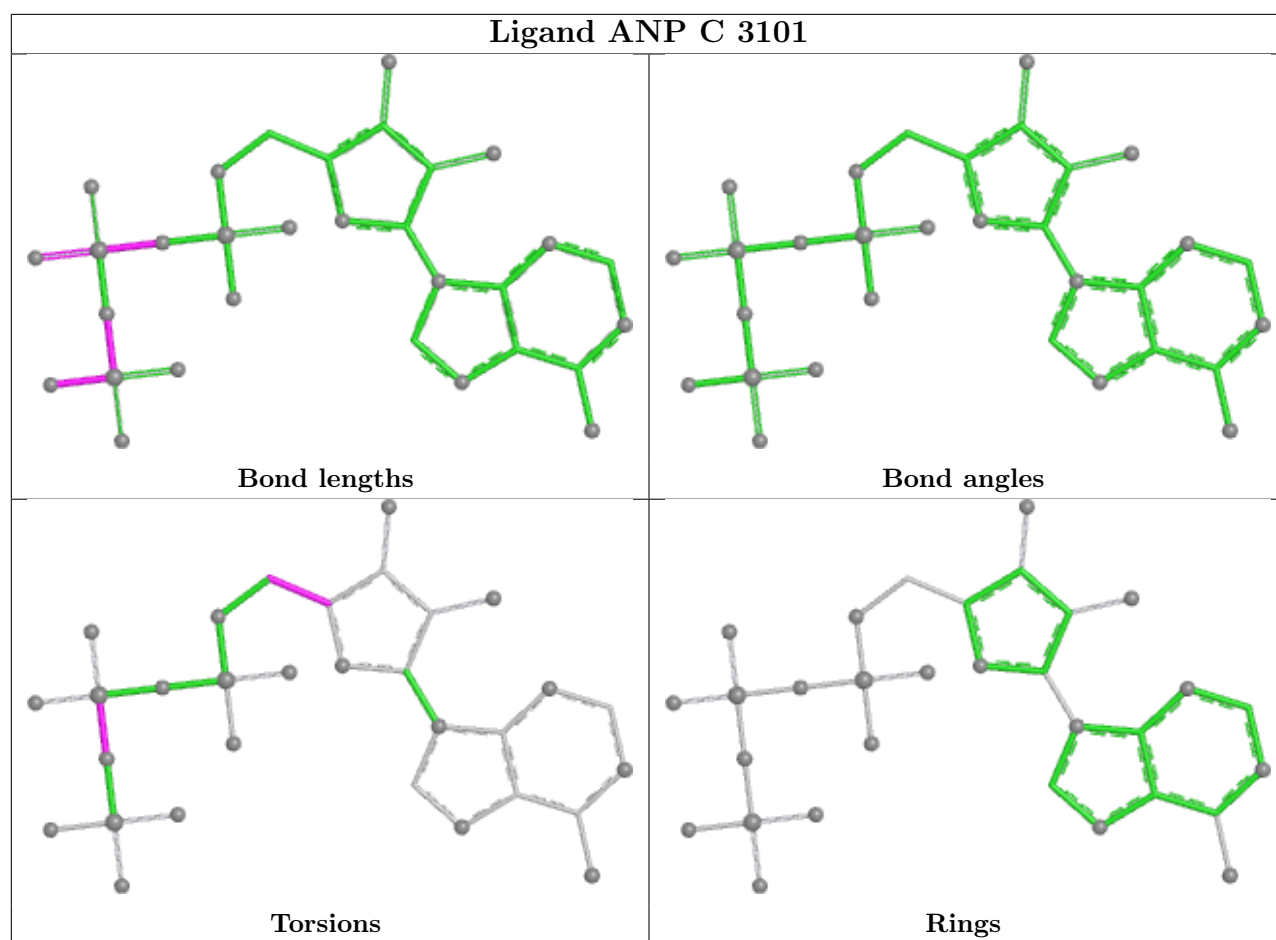
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PG-N3B-PB-O1B
3	C	3101	ANP	PG-N3B-PB-O1B
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	C	3101	ANP	O4'-C4'-C5'-O5'

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.

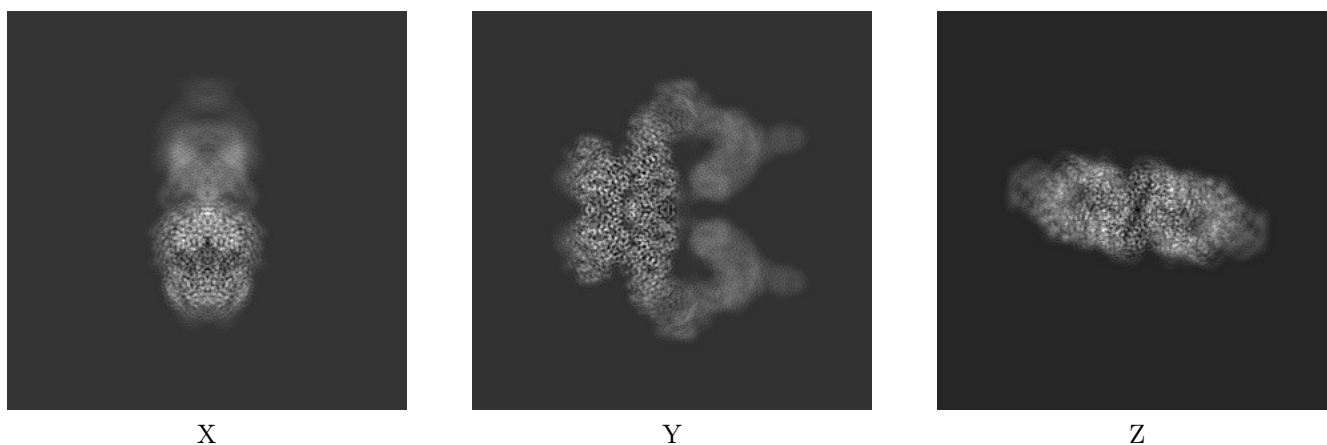
6 Map visualisation [i](#)

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](#)

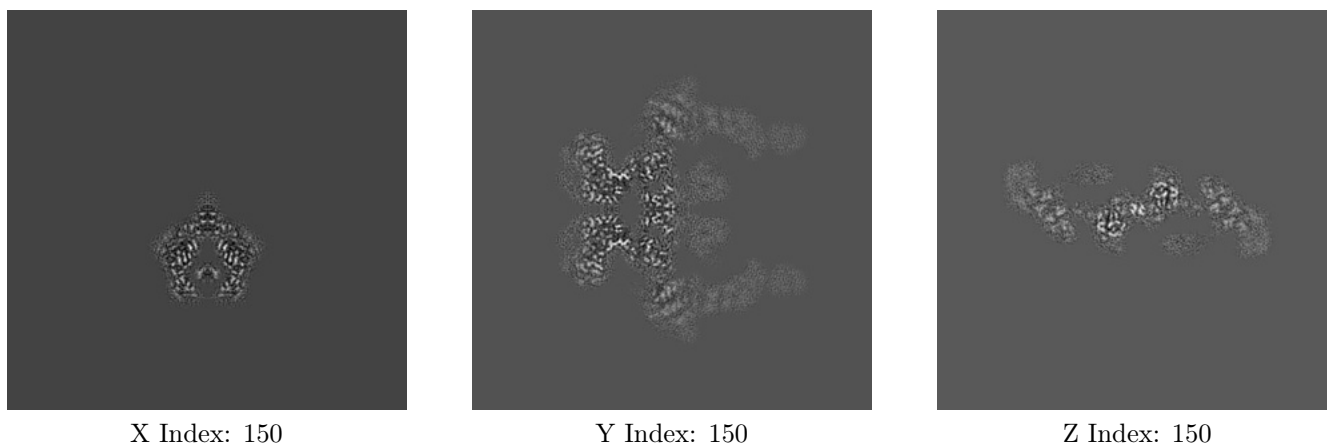
6.1.1 Primary map



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

6.2 Central slices [i](#)

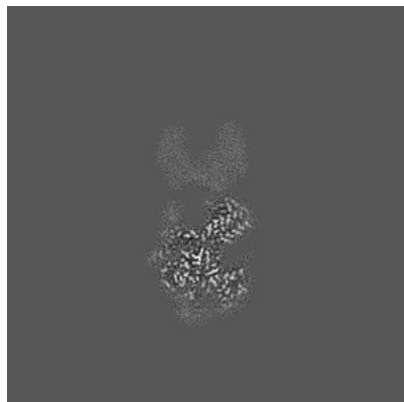
6.2.1 Primary map



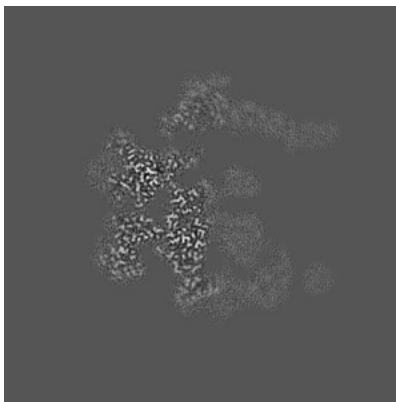
The images above show central slices of the map in three orthogonal directions.

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

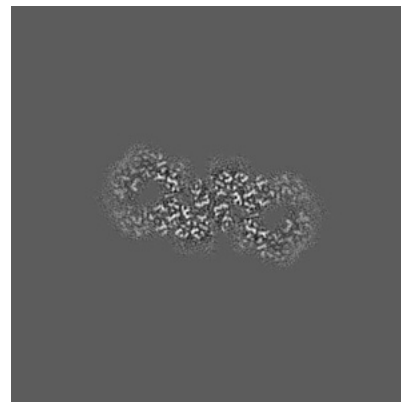
6.3.1 Primary map



X Index: 175



Y Index: 144

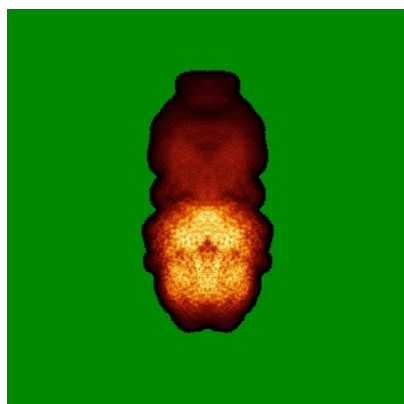


Z Index: 131

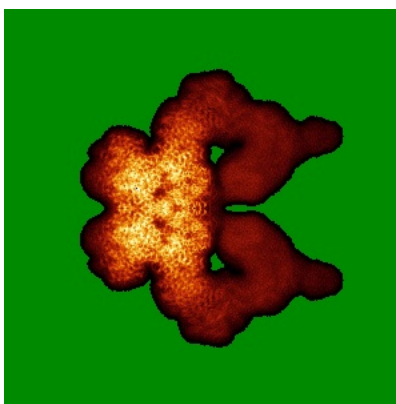
The images above show the largest variance slices of the map in three orthogonal directions.

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

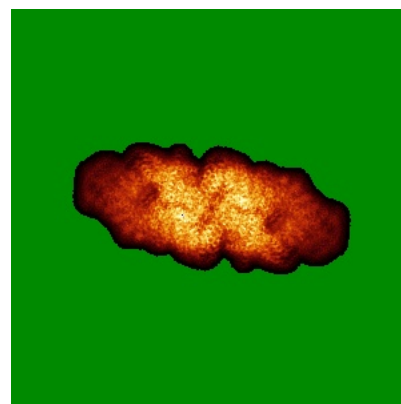
6.4.1 Primary map



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

This section was not generated.

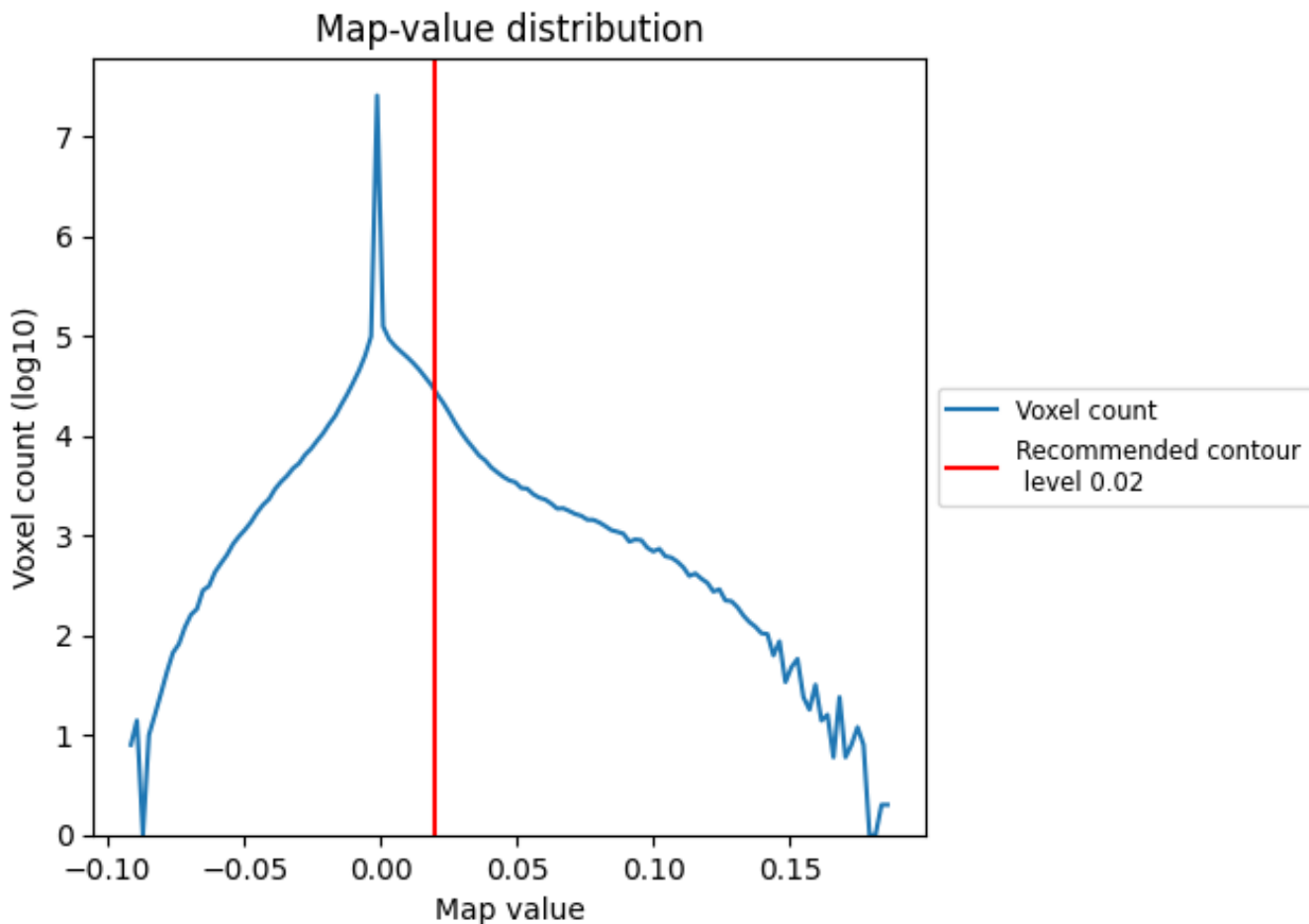
6.6 Mask visualisation

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

7 Map analysis [i](#)

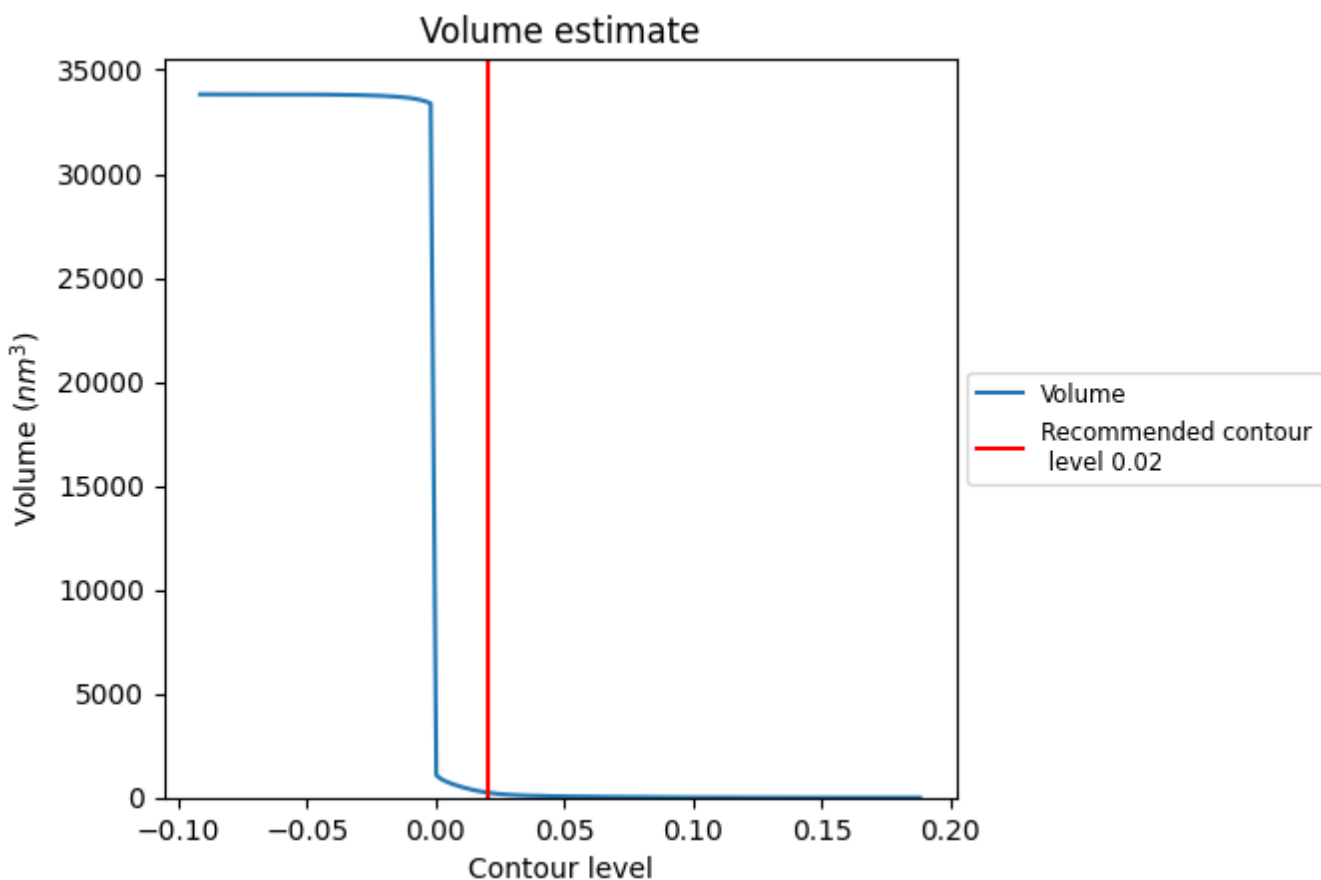
This section contains the results of statistical analysis of the map.

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.

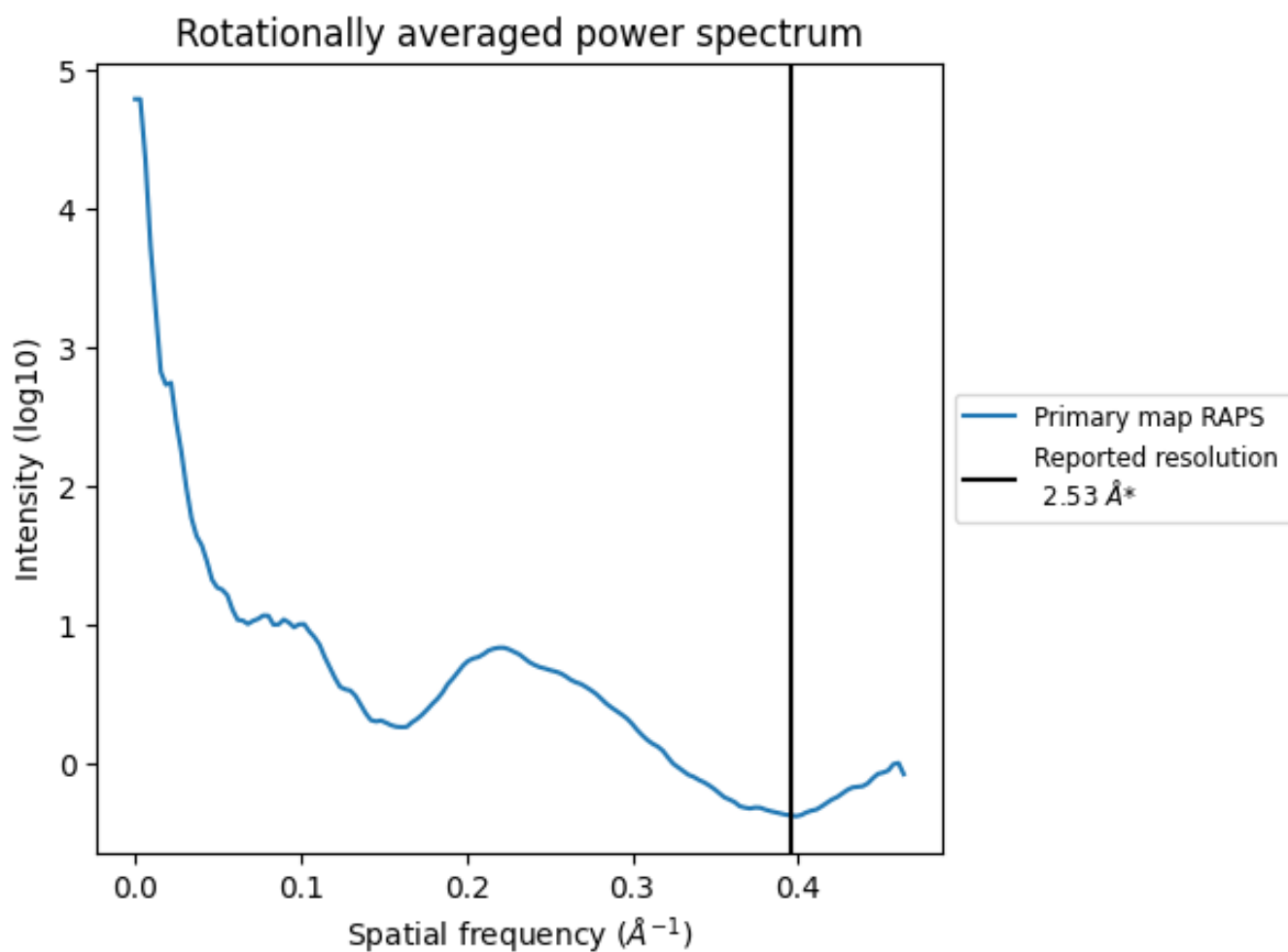
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 242 nm^3 ; 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 i

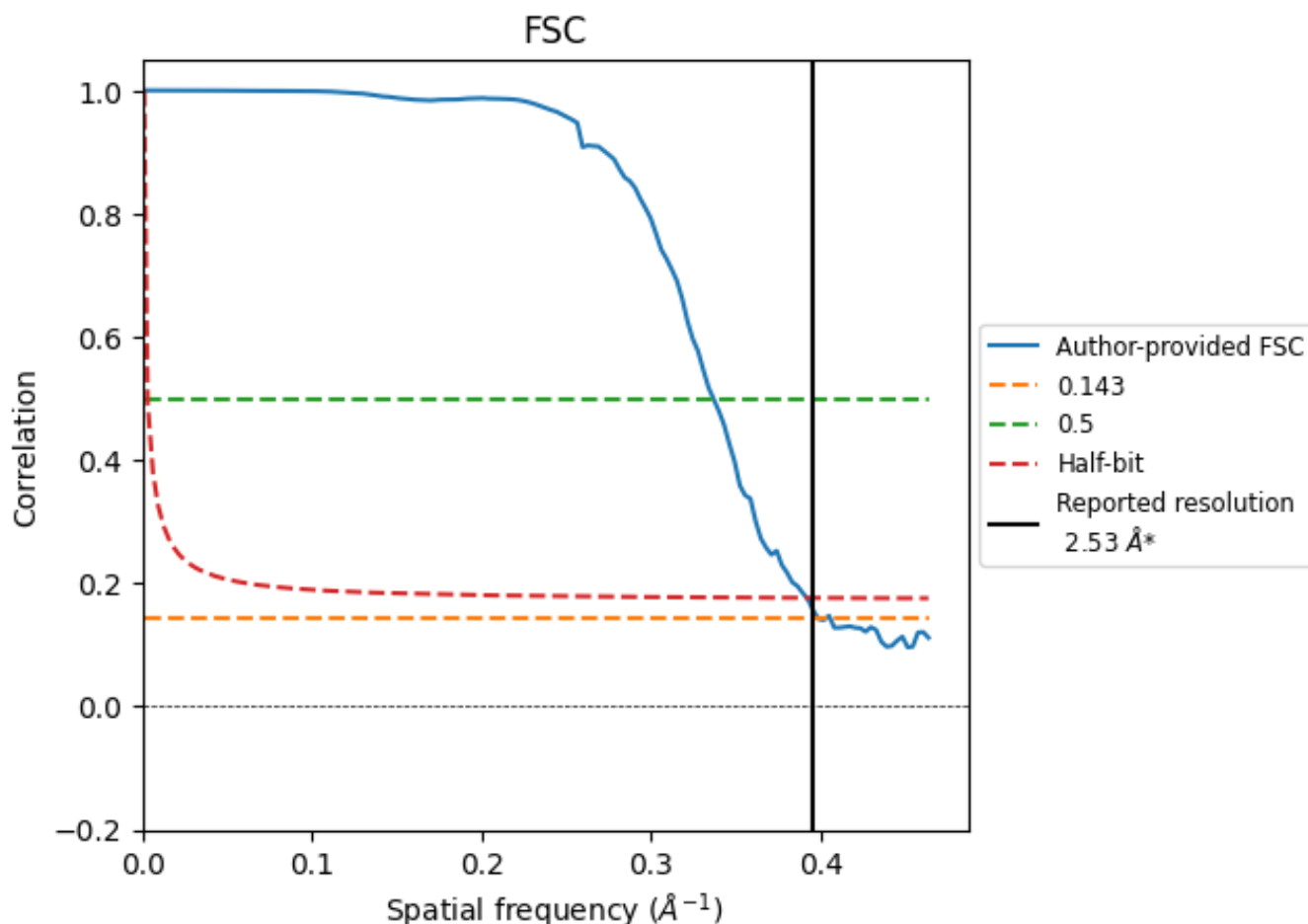


*Reported resolution corresponds to spatial frequency of 0.395 \AA^{-1}

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 0.395 Å⁻¹

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.

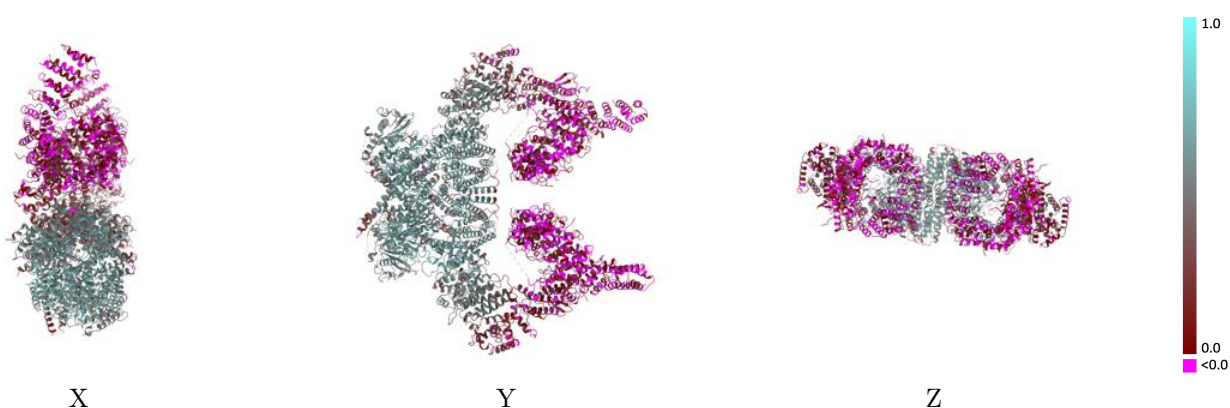
9 Map-model fit [i](#)

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](#)

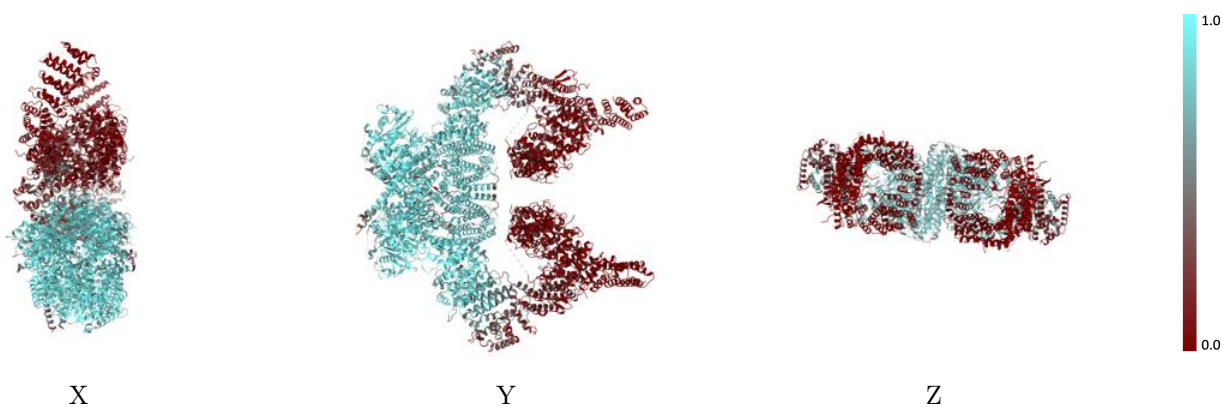
This section was not generated.

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



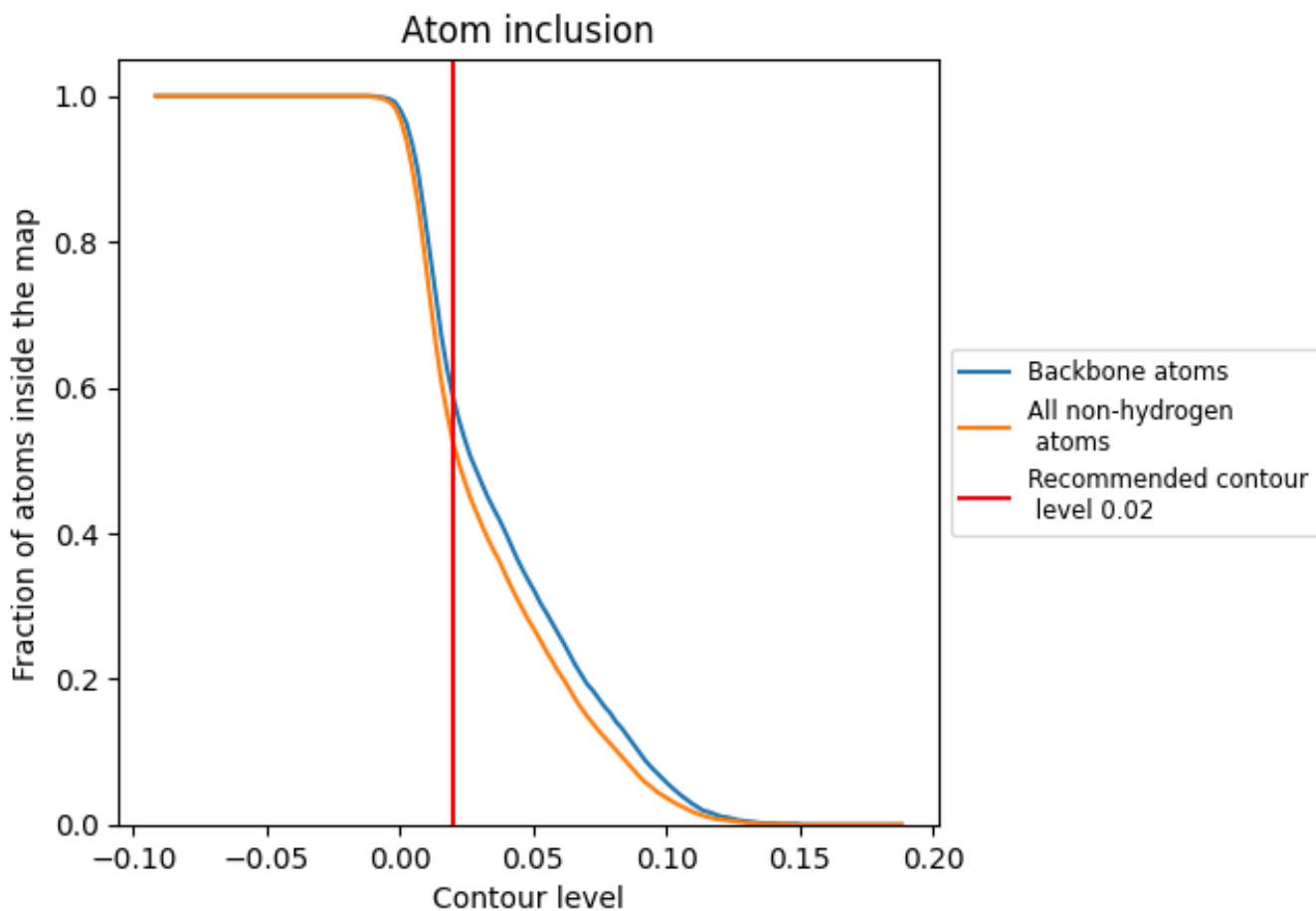
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.5240	 0.3360
A	 0.5260	 0.3370
B	 0.0250	 0.0430
C	 0.5260	 0.3380
D	 0.0250	 0.0470

