



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 07:46 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

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:

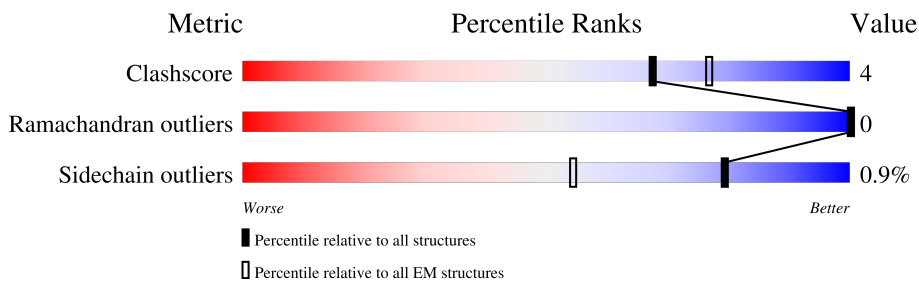
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.53 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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)</p>
1	C	3056	<p>39% (Poor fit), 80% (0 outliers), 10% (1 outlier), 9% (2 outliers), 9% (3+ outliers)</p>
2	B	28	<p>36% (Poor fit), 32% (0 outliers), 64% (1 outlier)</p>
2	D	28	<p>36% (Poor fit), 32% (0 outliers), 64% (1 outlier)</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.

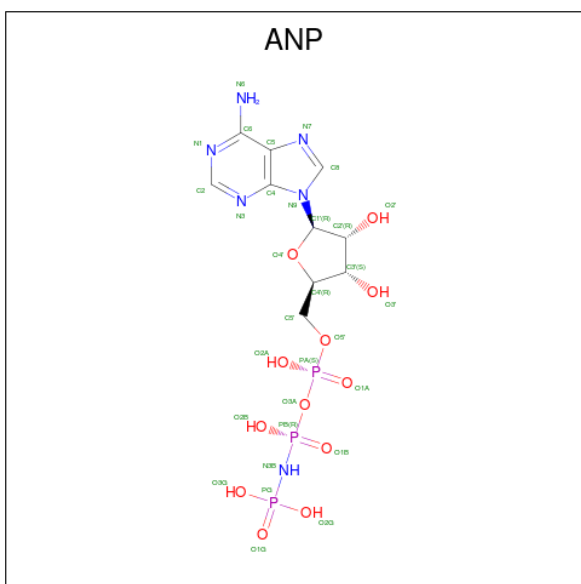
- Molecule 1 is a protein called Serine-protein kinase ATM.

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 (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	

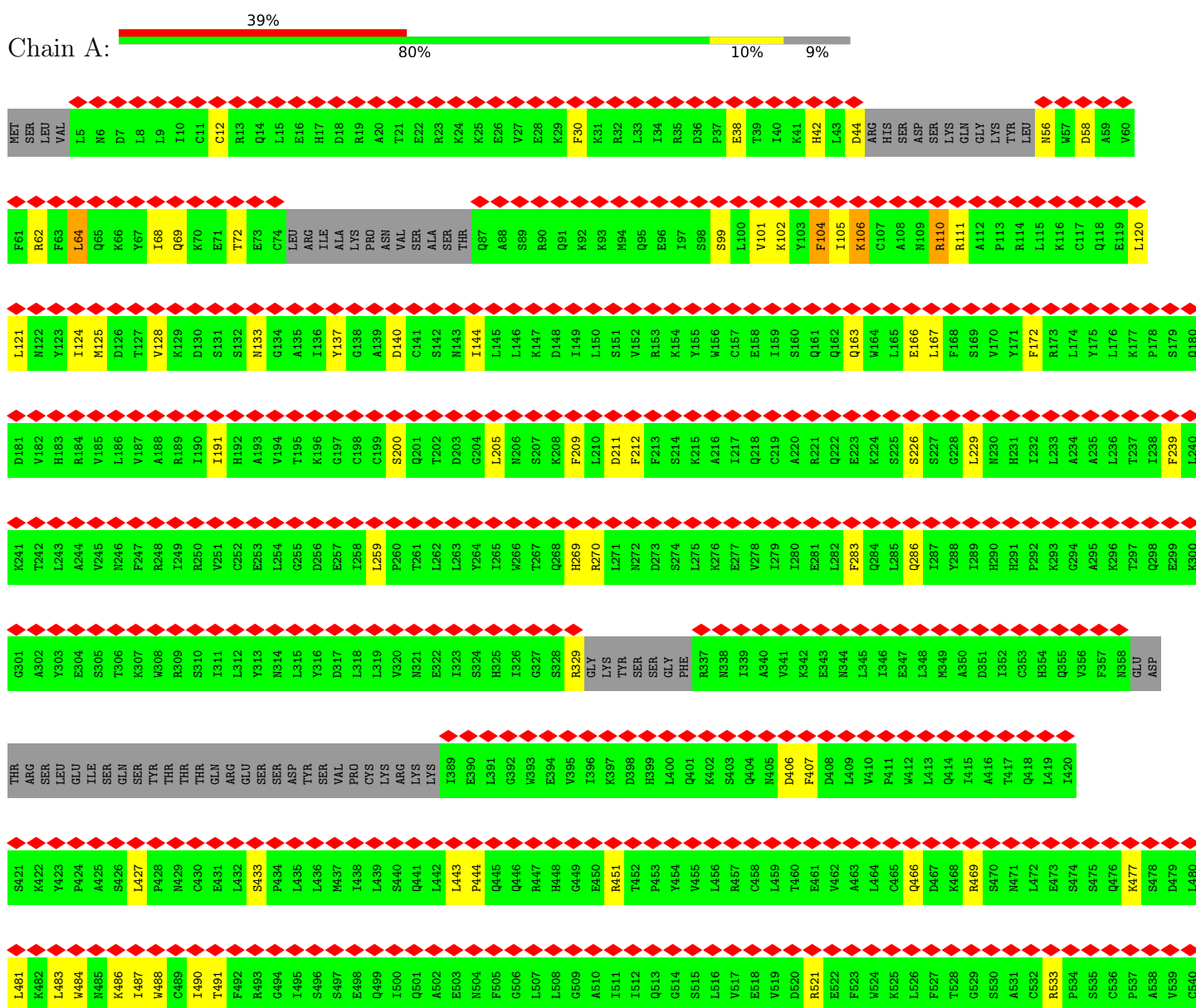
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

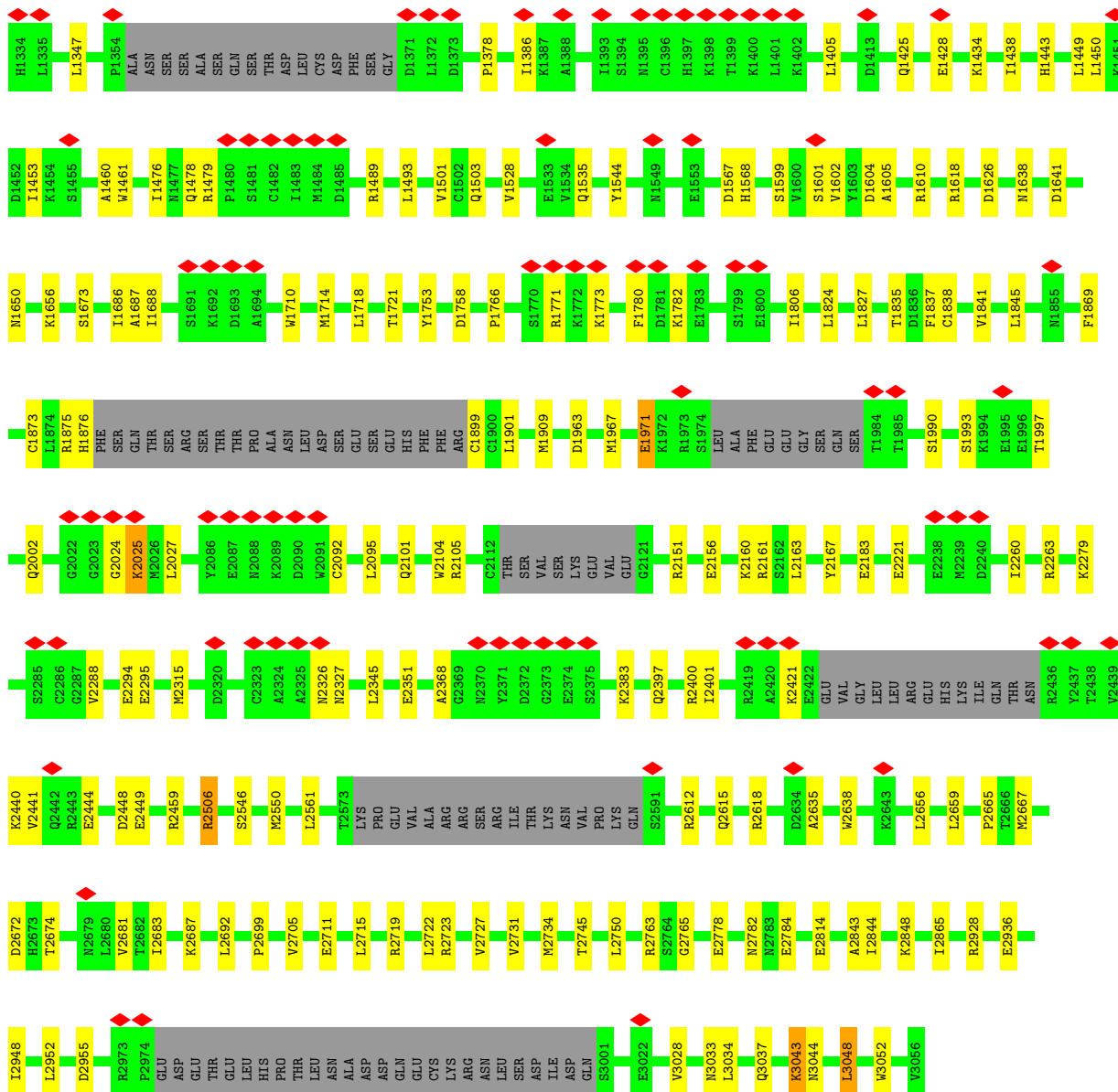
3 Residue-property plots

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.

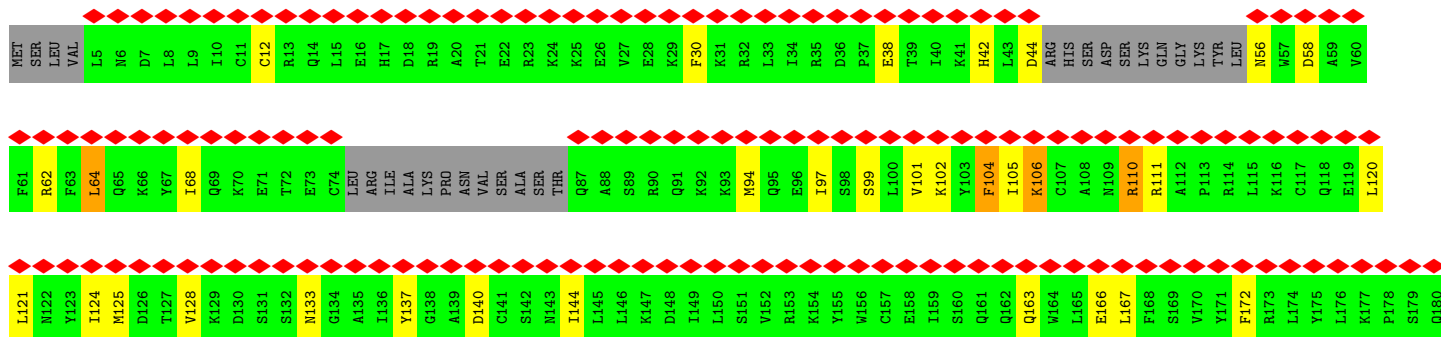
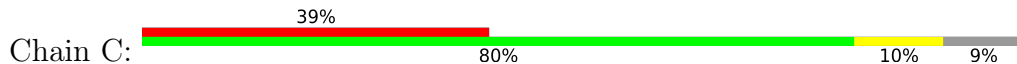
- Molecule 1: Serine-protein kinase ATM



E1267	V1268	K1269	S1270	I1271	A1272	M1273	Q1274	I1275	Q1276	D1277	D1278	M1279	K1280	S1281	L1282	L1283	T1284	D1285	I1290	M1293	F1298	A1299	Y1300	E1301	G1302	F1303	R1304	D1305	S1306	G1307	A1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	Y1318	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	F1235	L1236	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	F1265	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	ARC	LEU	L1108	K1109	A1110	L1111	P1112	L1113	K1114	L1115	Q1116	T1117	T1118	A1119	F1120	E1121	M1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1132	L1133	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	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	A1024	F1025	W1026	H1027	L1028	T1029	K1030	E1031	R1032	L1033	Y1034	I1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	N1044	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	E1071	N1072	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	N929	L930	I931	D932	S933	R934	T935	L936	E937	P938	T939	K940	S941	L942	H943	L944	H945	N946	Y947	L948	N949	L950	L951	K952	E953	L954	P955	G956	E957	E958	Y959	P960	
L961	P962	M963	E964	D965	V966	L967	E968	L969	K971	P972	L973	S974	N975	V976	C977	S978	L979	Y980	R981	R982	D983	Q984	D985	V986	C987	K988	T989	L990	L991	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	F1018	L1019	T1020			
L721	L722	V723	T724	W725	L726	G727	C728	Y729	C730	Y731	G732	V733	V734	I735	A736	E737	E738	E739	A740	Y741	K742	S743	E744	L745	F746	Q747	K748	A749	K750	S751	L752	G753	Q754	C755	A756	E758	S759	I760	T761	L762	F763	K764	N765	K766	I767	T770	N771	E770	E771	L772	I773	G774	S775	L776	R777	M778	M779	M780		
Q781	L782	C783	T784	R785	L786	L787	S788	M789	C790	T791	K792	S793	W794	P795	N796	K797	I798	A799	S900	G901	F902	F903	L904	R905	L906	L907	T908	S909	K910	L911	M912	N913	D914	I915	A916	D917	I918	C919	K920	S921	L922	A923	S924	F925	I926	L927	P928	PHE	ASP	ARG	GLY	GLU	VAL	GLU	SER	MET	GLU	ASP		
ASP	THR	ASN	GLY	LEU	MET	GLU	GLU	ASP	GLN	SER	MET	ASN	LEU	PHE	ASN	ASP	PRO	SER	SER	VAL	SER	ASP	ALA	ASN	GLU	PRO	GLY	GLU	SER	GLN	S977	T978	I979	G980	I982	A981	N983	P984	L985	S986	L988	E987	E988	Y989	L990	S991	K992	Q993	D994	L995	L996	F997	D998	N990						
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	R629	V630	P631	G632	C633	GLU	HIS	HIS	GLN	GLM	LYS	ASP	LYS	GLU	GLU	LEU	S644	F645	S646	E647	V648	E649	E650	L651	F652	L653	Q654	T655	R656	F657	D658	K659	M660
C541	L542	T543	L544	A545	L546	T547	T548	S549	I550	V551	P552	G553	VAL	L554	LYS	MET	GLY	ILE	GLU	GLN	ASN	MET	CYS	GLU	VAL	ASN	ARG	SER	F570	S571	L572	K573	E574	S575	I576	M577	K578	W579	L580	L581	F582	Y583	Q584	L585	E586	GLY	ASP	LEU	GLU	ASN	SER	T593	E594	V595	P596	P597	I598	L599	H600	

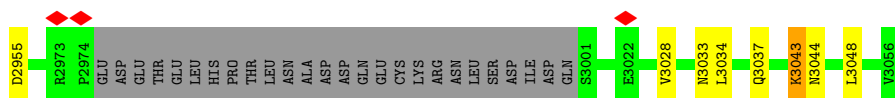


● Molecule 1: Serine-protein kinase ATM

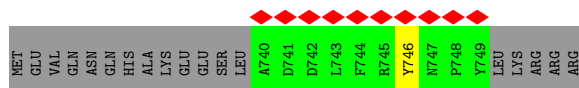


D181	K241	G301	THR	S421	L481	C541	S601	D661	L721	Q781	ASP	L901	L961
V182	T242	A302	ARG	K422	K482	L542	N602	F662	L722	L782	THR	K902	P962
H183	T243	Y303	SER	Y423	L483	T543	F603	L663	W723	C783	ASN	F903	M963
R184	A244	E304	GLU	P424	W484	L544	P604	T664	G724	T784	ASN	L904	E964
V185	V245	S305	ILE	A425	M485	A545	H605	IIE	W725	R785	LEU	C905	D965
L186	V246	T306	SER	S426	K486	L546	L606	VAL	L726	C786	MET	N906	V966
V187	F247	R307	GLN	L427	L487	T547	V607	ARG	G727	L787	GLU	C907	L967
A188	R248	W308	THR	P428	W488	T548	L608	CYS	C728	S788	GLY	V908	E968
R189	I249	R309	THR	M429	C489	S549	E609	IIE	Y729	M789	ASP	T909	L969
I190	R250	S310	THR	C430	L489	L550	K610	GLU	C730	C790	GLN	T910	L970
I191	V251	I311	GLN	E431	T491	V551	L611	LYS	Y731	T791	SER	A911	K971
H192	C252	L312	ARG	L432	F492	P652	L612	HIS	M732	K792	MET	Q912	P972
A193	E253	Y313	GLU	S433	R493	G653	W613	GLN	G733	K793	ASN	T913	L973
V194	L254	N314	SER	P434	G494	T554	S614	SER	W734	S794	PHE	N914	S974
T195	G255	L315	ASP	L435	I495	VAL	L615	SER	I735	F795	ASN	T915	N975
K196	D256	Y316	TRP	L436	S496	LYS	T616	IIE	A736	W796	ASP	V916	V976
G197	E257	D317	VAL	M437	S497	MET	M617	F680	E737	K797	TYR	S917	C977
C198	I258	L318	PRO	I438	E498	ILE	K618	G681	E738	I798	PRO	F918	S978
C199	L259	L319	CYS	I439	Q499	GLU	N619	V682	E739	A799	SER	R919	L979
S200	P260	V320	LYS	S440	I500	ASN	C620	H683	A740	S800	VAL	A920	Y980
Q201	T261	N321	LYS	Q441	Q501	MET	K621	Q684	Y741	G801	SER	A921	R981
T202	L262	I323	LYS	L442	A502	VAL	A622	N685	K742	F802	ASP	D922	R982
D203	L263	I323	LYS	L443	E503	GLU	A623	L686	S743	F803	ALA	I923	D983
G204	Y264	S324	ARG	P444	N504	VAL	M624	L687	E744	L804	GLY	R924	Q984
L205	I265	H325	ARG	Q445	F505	ARG	N625	E688	L745	R805	PRO	R925	D985
N206	V266	I326	LYS	Q446	G506	SER	F626	S689	F746	L806	GLY	K926	V986
N207	T267	G327	LYS	R447	L507	F570	F627	L690	Q747	L807	GLU	L927	C987
K208	Q268	S328	LYS	H448	L508	L572	Q628	D691	K748	T808	GLN	L928	K988
F209	H269	R329	GLY	G449	G509	L577	S629	R692	A749	S809	THR	M929	T989
L210	R270	N330	LYS	E450	A510	K573	V630	C693	K750	K810	THR	L930	I990
D211	L271	N338	TYR	R451	I511	E574	P631	L694	S751	L811	THR	I931	L991
F212	N272	D398	SER	T452	I512	S675	E632	L695	L752	M812	THR	D932	N992
F213	D273	SER	SER	P453	Q513	L576	C633	G696	W753	M813	THR	S933	H993
S214	S274	GLY	GLY	Y454	G514	M677	GLU	L697	Q754	D814	THR	S934	L994
K215	L275	PHE	PHE	V455	S515	K578	HIS	S698	C755	I815	THR	T935	L995
A216	K276	R337	K402	L456	L516	W579	GLN	E699	A756	A816	THR	L936	H996
I217	E277	N338	K402	R457	L517	W579	LYS	Q700	G757	D817	THR	E937	V997
Q218	I339	I339	S403	C458	E518	L580	ASP	L701	E758	L818	THR	P938	K998
C219	A340	A340	Q404	L459	V519	F582	LYS	L702	S759	C819	THR	K940	N999
A220	I280	V341	M405	L460	D520	Y683	GLU	M703	L760	K820	THR	L941	L1000
R221	E281	I280	D406	T460	R521	Q584	LEU	W704	T761	S821	THR	S941	L1001
E222	E281	E281	D408	E461	E522	L585	S644	Y705	L762	L822	THR	L942	G1002
E223	F283	N344	L409	A463	F523	E586	F645	S706	F763	A823	THR	H943	Q1003
K224	Q284	L345	V410	L464	N524	ASP	S646	S707	K764	S824	THR	L944	S1004
S225	L285	I346	P411	C465	K525	LEU	E547	E708	W765	F825	THR	H945	M1005
S226	Q286	E347	W412	Q466	L526	GLU	V648	I709	K766	K826	THR	M946	M1006
S227	I287	L348	L413	D467	F527	ASN	E549	T710	T767	L827	THR	Y947	D1007
G228	Y288	M349	Q414	K468	T528	SER	E650	M711	W768	L828	THR	L948	S1008
L229	I289	A350	I415	R469	G529	T593	L651	S712	E769	F829	THR	M949	E1009
N230	H290	D351	A416	S470	S530	E594	F652	E713	E770	A830	THR	L950	E1009
H231	H291	I352	T417	M471	A531	V595	L653	T714	F771	ARG	THR	L951	T1011
I232	P292	C353	Q418	L472	C532	P597	Q654	L715	R772	GLY	THR	K952	R1012
L233	K293	H354	H354	E473	R533	L598	T655	W716	I773	GLU	THR	L953	D1013
A234	G294	Q355	Q355	S474	E534	L599	T656	R717	G774	VAL	THR	L954	A1014
A235	A295	V356	V356	S475	S535	L599	F657	C718	S775	SER	THR	P955	Q1015
L236	K296	F357	F357	Q476	C536	H600	D658	S719	L776	GLU	THR	Q956	G1016
I237	T297	N358	N358	K477	P537		K659	R720	R777	ASP	THR	E957	Q1017
I238	Q298	GLU	GLU	S478	A538		M660		W778		THR	F1018	F1018
F239	E299	ASP	ASP	D479	V539				W780		THR	L1019	L1019
L240	K300			L480	C540						THR	P960	T1020

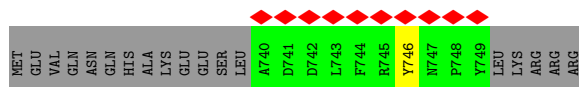
L2659	L2665	D2672	H2673	T2674	N2679	L2683	P2699	V2705	E2711	L2715	R2719	L2722	R2723	V2727	V2731	R2734	T2745	L2750	R2763	G2764	G2765	E2778	N2782	N2783	E2784	E2814	A2843	L2844	K2848	R2928	E2936	L2948	L2952	THR	ASN	R2436	Y2437	T2438	V2439	K2440	Q2442	R2443	E2444	D2448	E2449	R2459	R2506	S2546	M2550	L2561	T2573	PRO	GLU	VAL	ALA	ARG	ARG	ARG	ILE	THR	LYS	ASN	VAL	PRO	LYS	GLN	S2591	R2612	Q2615	R2618	D2634	A2635	V2638	K2643	L2656	D1841	M1850	K1856	T1862	S1873	V1878	I1886	A1887	I1888	S1891	K1892	D1893	A1894	L1702	W1710	M1714	L1718	T1721	Y1753	D1758	P1766	S1770	R1771	K1772	K1773	F1780	D1781	K1782	E1783	S1799	E1800	I1806	L1824	L1827	T1835	D1836	F1837	C1838	D1452	I1453	K1454	S1455	A1460	W1461	I1476	M1477	Q1478	R1479	P1480	S1481	I1483	M1484	D1485	R1489	L1493	V1501	G1502	Q1503	V1528	E1533	V1534	Q1535	Y1544	N1549	E1553	D1567	H1568	S1599	V1600	S1601	V1602	I1603	D1604	A1605	L1608	T1609	R1610	R1618	D1626	M1638	H1334	L1335	L1347	P1354	ALA	ASN	SER	SER	ALA	ALA	GLN	SER	THR	ASP	LEU	CYS	ASP	PHE	SER	GLY	D1371	L1372	D1373	P1378	I1386	K1387	A1388	I1393	S1394	N1395	C1396	H1397	L1398	T1399	K1400	L1401	K1402	L1405	D1413	Q1425	E1428	K1434	I1438	H1443	L1449	L1450	K1461	E1267	V1268	K1269	S1270	I1271	A1272	N1273	Q1274	I1275	Q1276	E1277	D1278	W1279	K1280	S1281	L1282	L1283	T1284	D1285	I1290	N1293	F1298	A1299	V1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	V1319	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	M1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	L1248	E1249	S1250	C1251	Y1252	K1253	V1254	L1255	H1258	L1259	I1261	R1262	S1263	H1264	Q1265	D1266	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	V1021	I1022	G1023	A1024	F1025	W1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	N1044	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	L1053	P1054	V1055	S1056	K1057	M1058	A1059	L1060	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	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	PRO	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	M1100	K1101	GLY	ASP	SER	SER	ARG	ARG	LEU	L1108	K1109	A1110	L1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	M1120	E1121	N1122	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	G1130	M1131	E1133	M1134	SER	HIS	SER	ALA	ALA	GLU	ASN	E1142	T1143	L1144	D1145	E1146	I1147	M1149	R1150	K1151	S1152	E1091	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• 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	0.24	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 [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%)	2446 (99%)	23 (1%)	78	91
1	C	2469/2780 (89%)	2446 (99%)	23 (1%)	78	91
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%)	79	91

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

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

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 monosaccharides 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	C	3101	-	29,33,33	1.10	4 (13%)	31,52,52	1.07	2 (6%)
3	ANP	A	3101	-	29,33,33	1.10	4 (13%)	31,52,52	1.07	2 (6%)

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-N3B	2.44	1.69	1.63
3	C	3101	ANP	PG-N3B	2.44	1.69	1.63
3	A	3101	ANP	PG-O1G	2.44	1.50	1.46
3	C	3101	ANP	PG-O1G	2.44	1.50	1.46
3	A	3101	ANP	PB-O3A	-2.37	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3101	ANP	PB-O3A-PA	-3.74	119.44	132.62
3	C	3101	ANP	PB-O3A-PA	-3.74	119.44	132.62
3	A	3101	ANP	C5-C6-N6	2.14	123.61	120.35
3	C	3101	ANP	C5-C6-N6	2.14	123.61	120.35

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

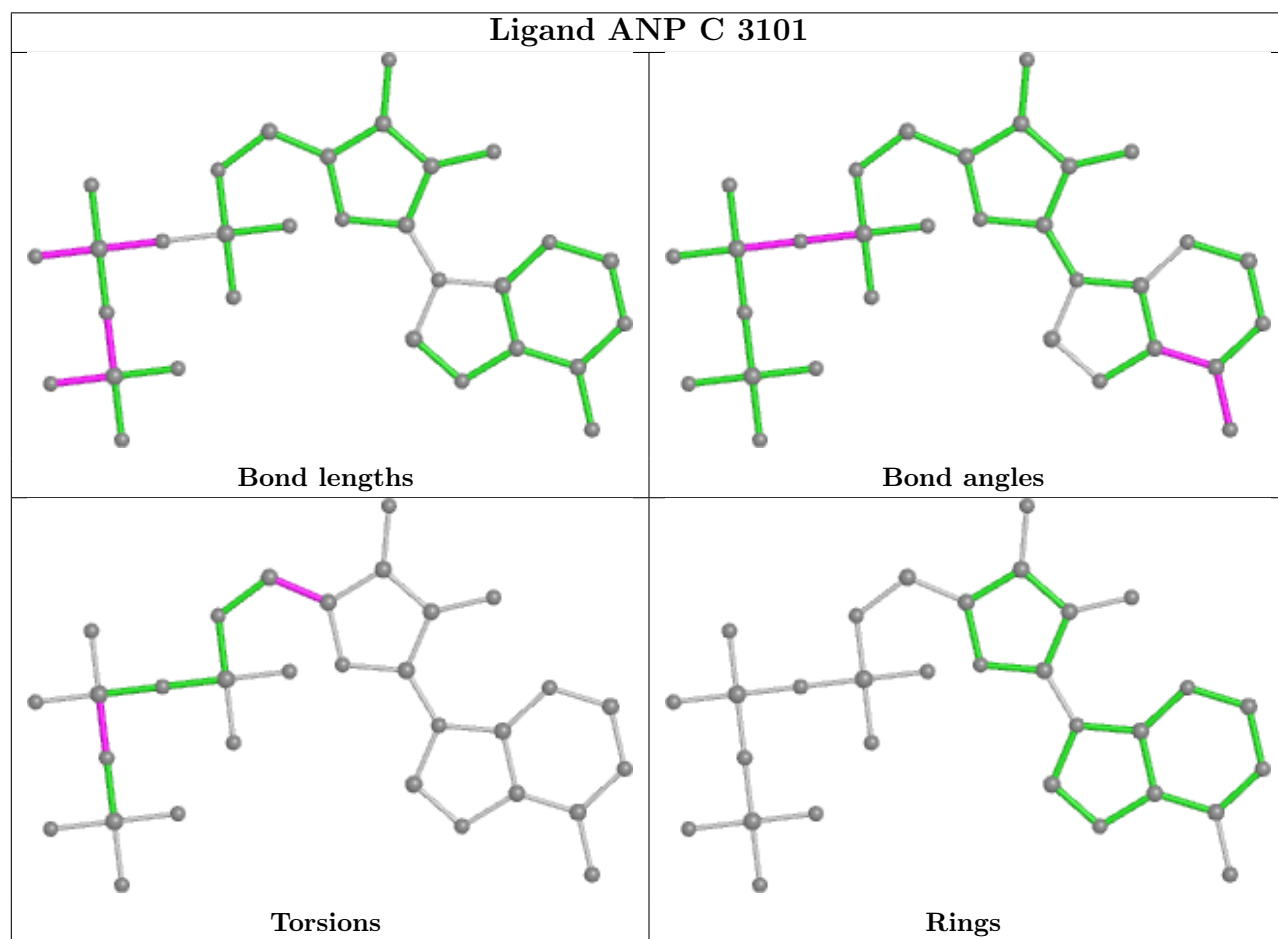
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PG-N3B-PB-O1B
3	C	3101	ANP	PG-N3B-PB-O1B
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	C	3101	ANP	O4'-C4'-C5'-O5'

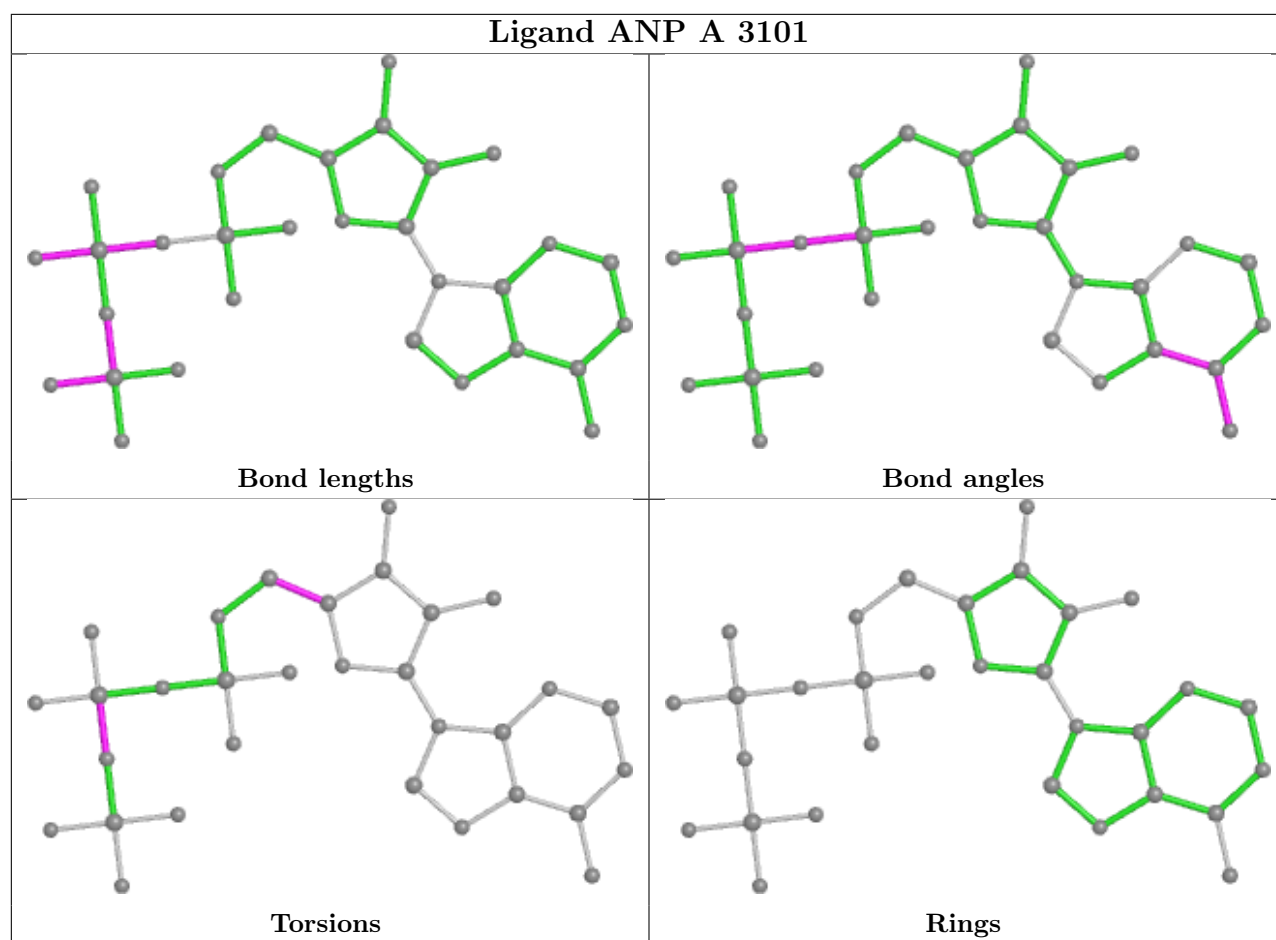
There are no ring outliers.

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.

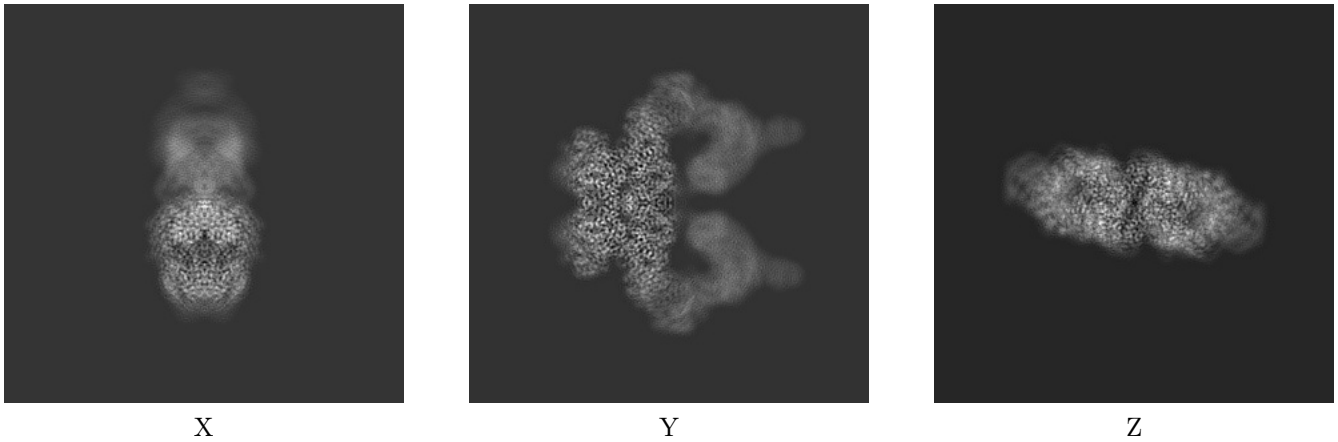
6 Map visualisation [i](#)

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](#)

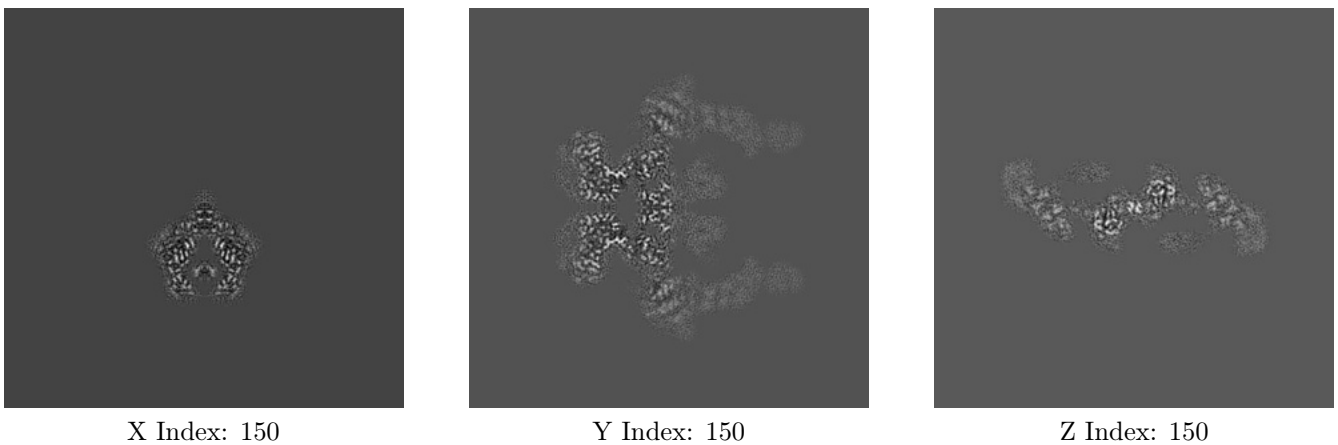
6.1.1 Primary map



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

6.2 Central slices [i](#)

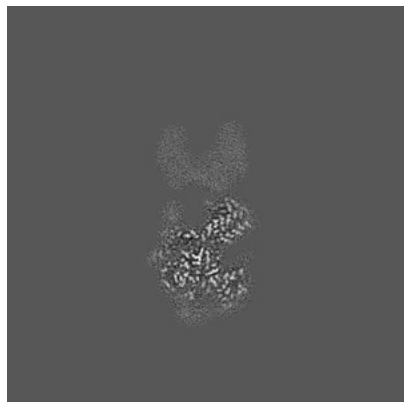
6.2.1 Primary map



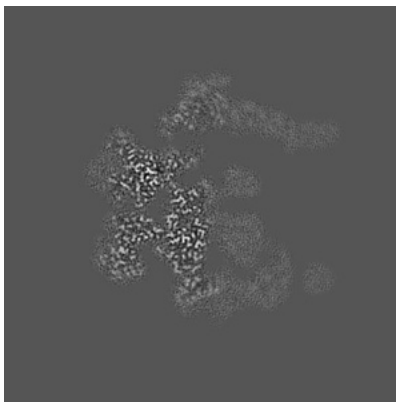
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

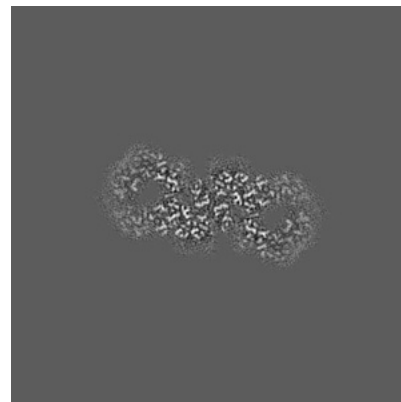
6.3.1 Primary map



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 surface views [i](#)

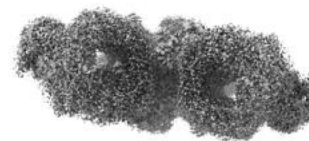
6.4.1 Primary map



X



Y



Z

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

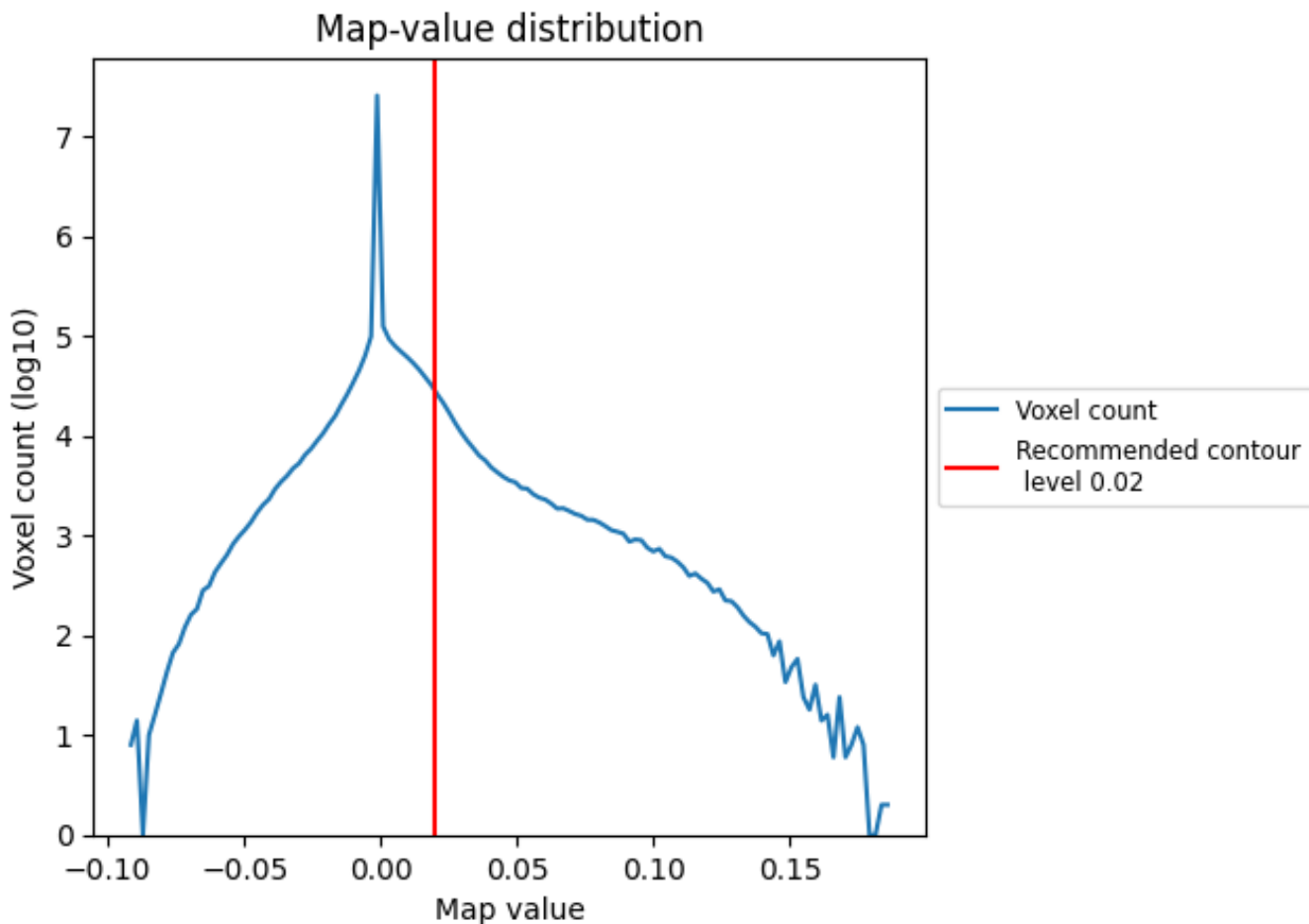
6.5 Mask visualisation

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

7 Map analysis [i](#)

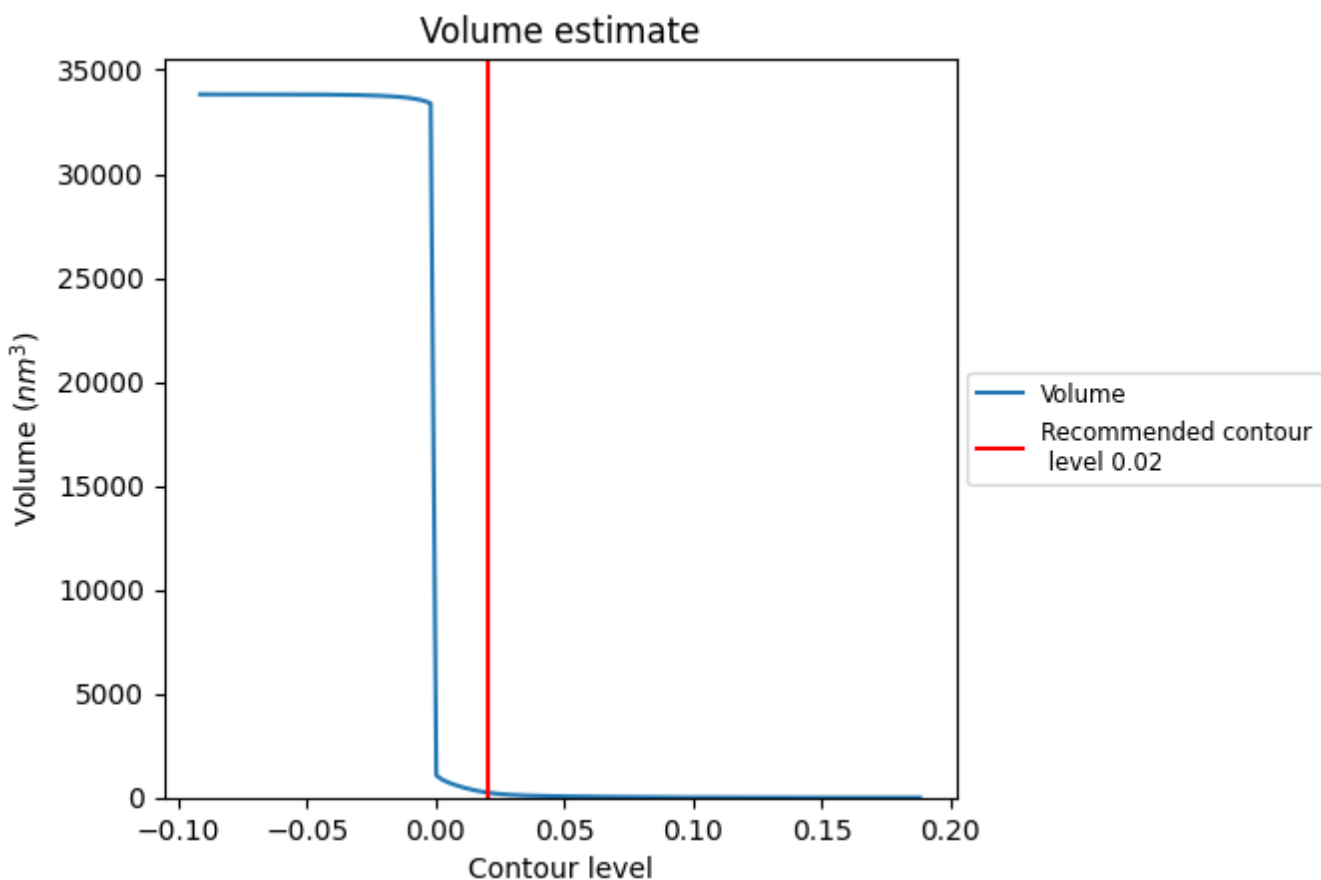
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

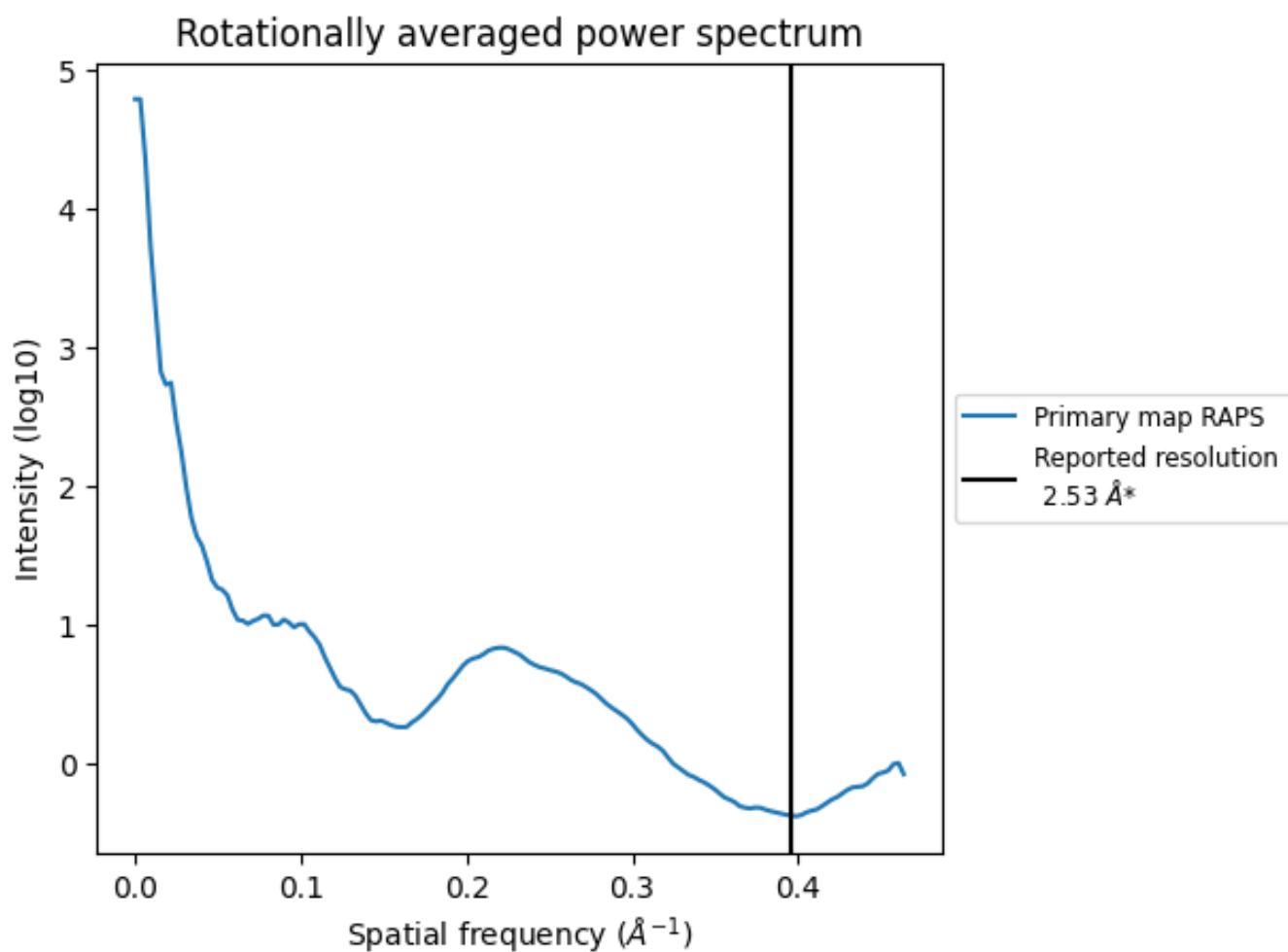
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 242 nm³; 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

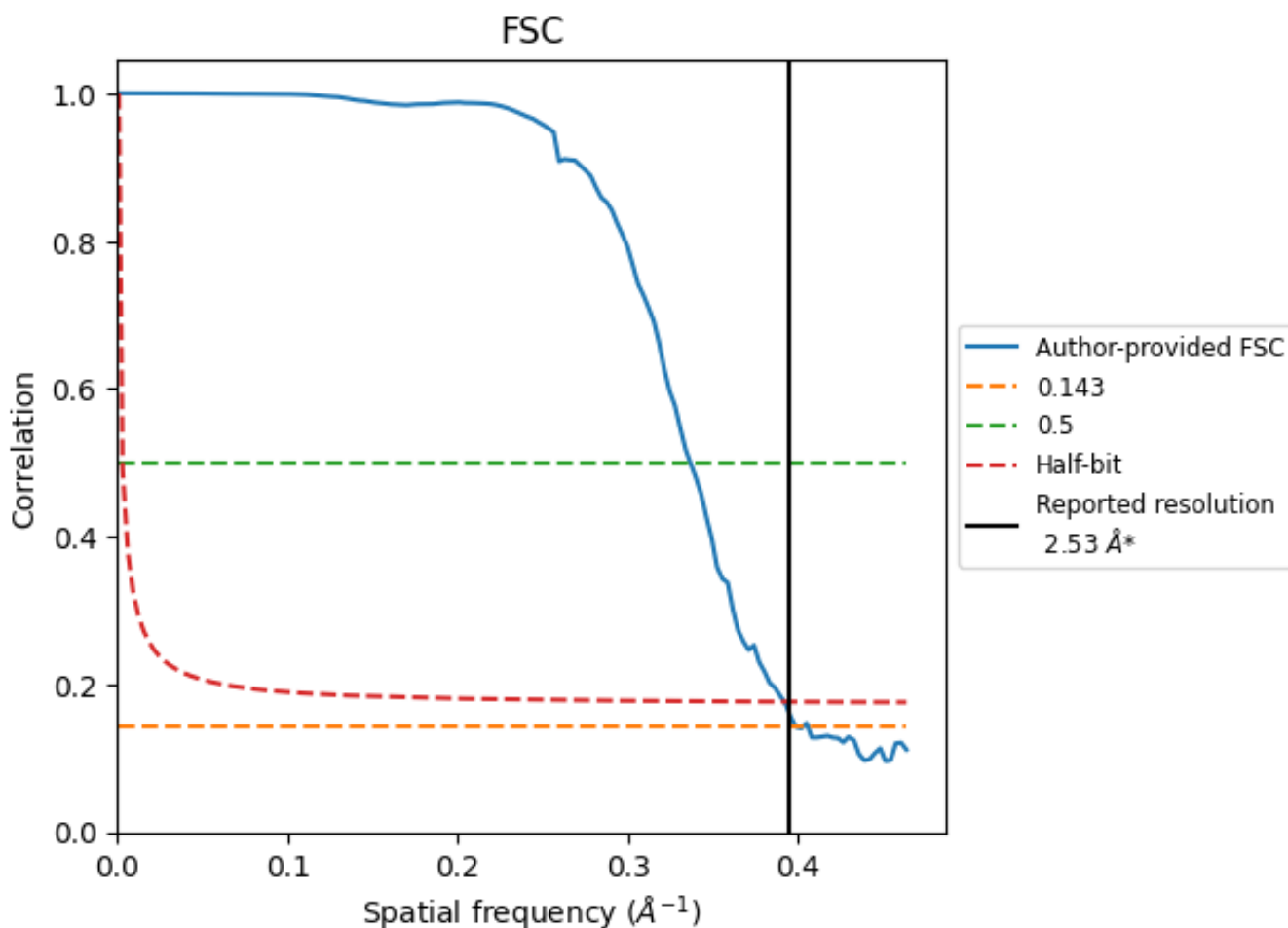


*Reported resolution corresponds to spatial frequency of 0.395 \AA^{-1}

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](#)

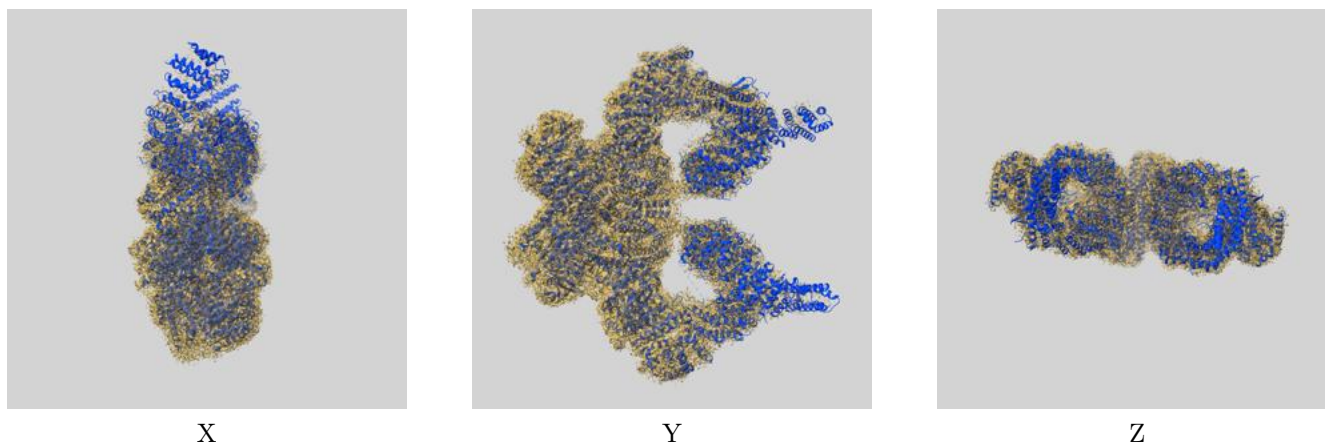
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.51	2.97	2.55
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

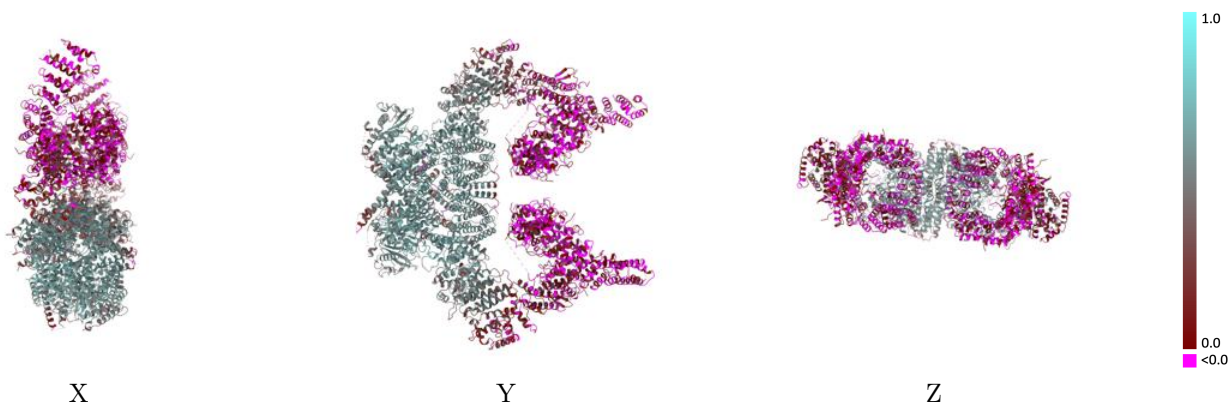
This section contains information regarding the fit between EMDB map EMD-25141 and PDB model 7SID. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



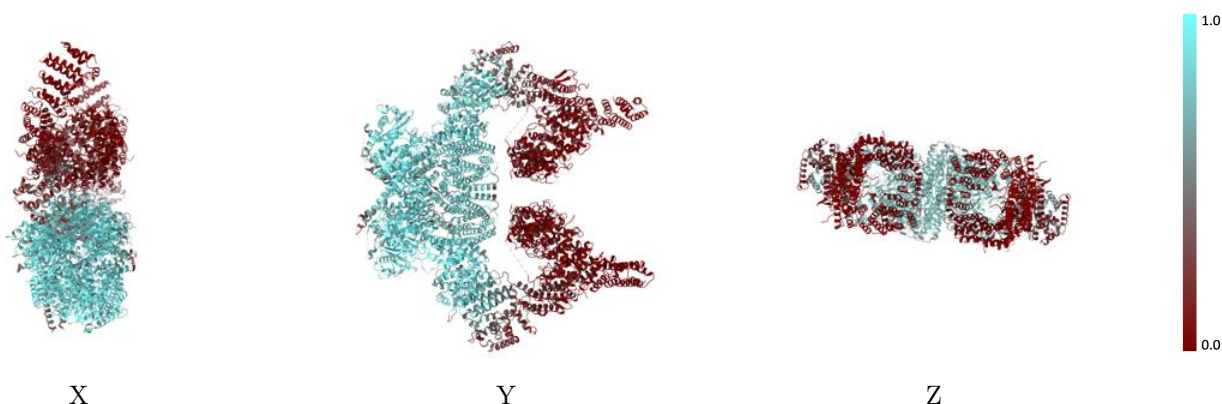
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



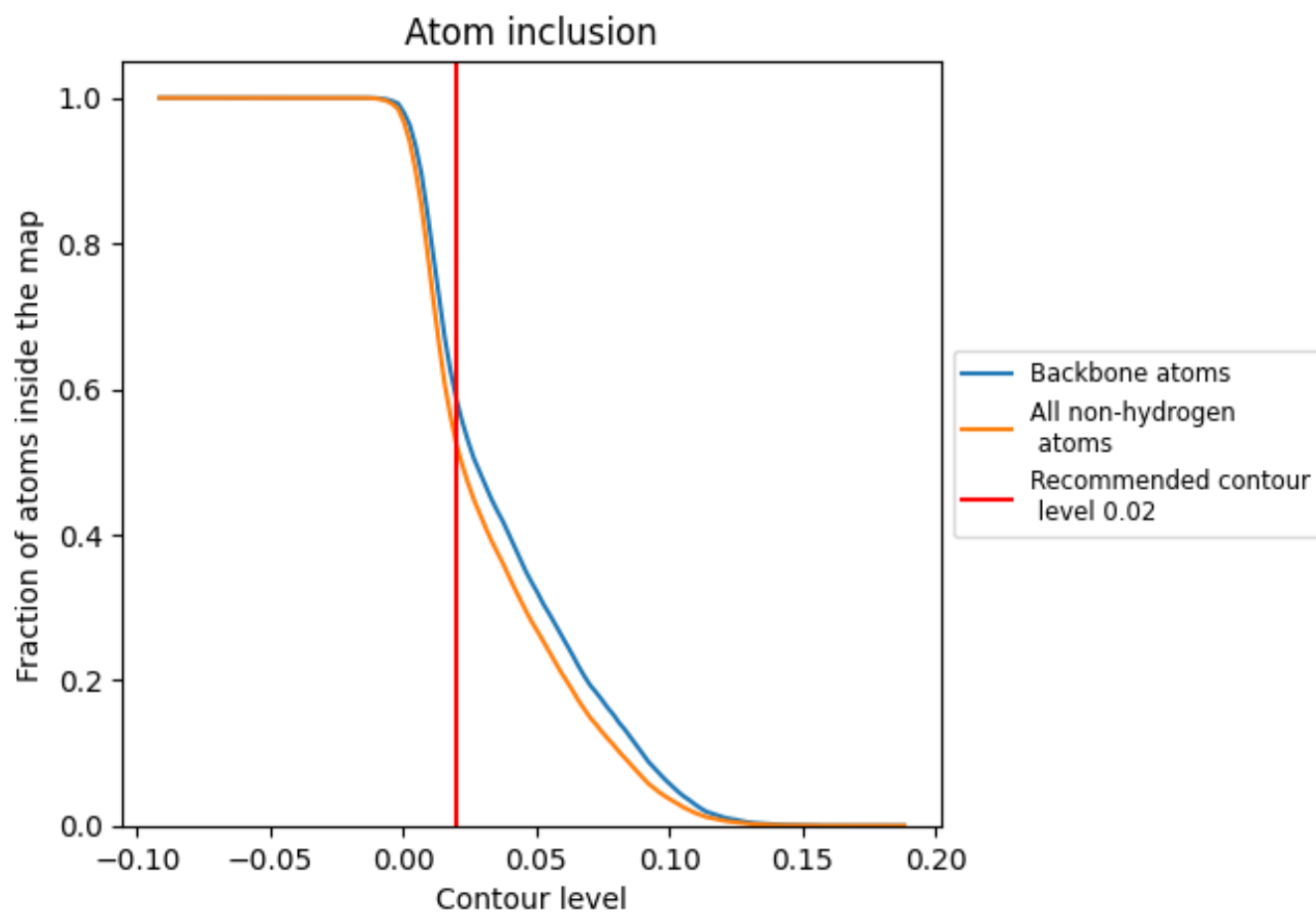
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [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	 0.5243	 0.3360
A	 0.5261	 0.3370
B	 0.0250	 0.0430
C	 0.5261	 0.3380
D	 0.0250	 0.0470

