



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:56 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 Full wwPDB EM Validation 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:

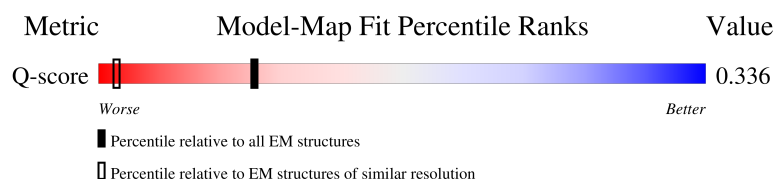
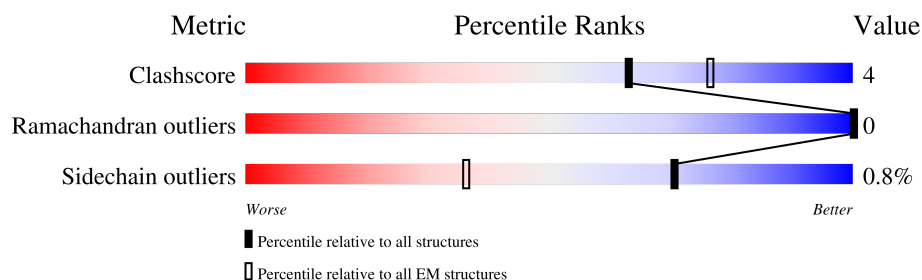
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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	
1	C	3056	
2	B	28	
2	D	28	

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.

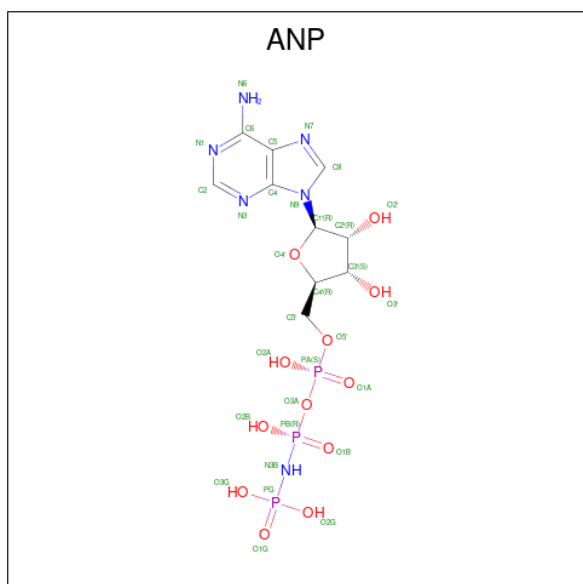
- Molecule 1 is a protein called Serine-protein kinase ATM.

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 (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
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	

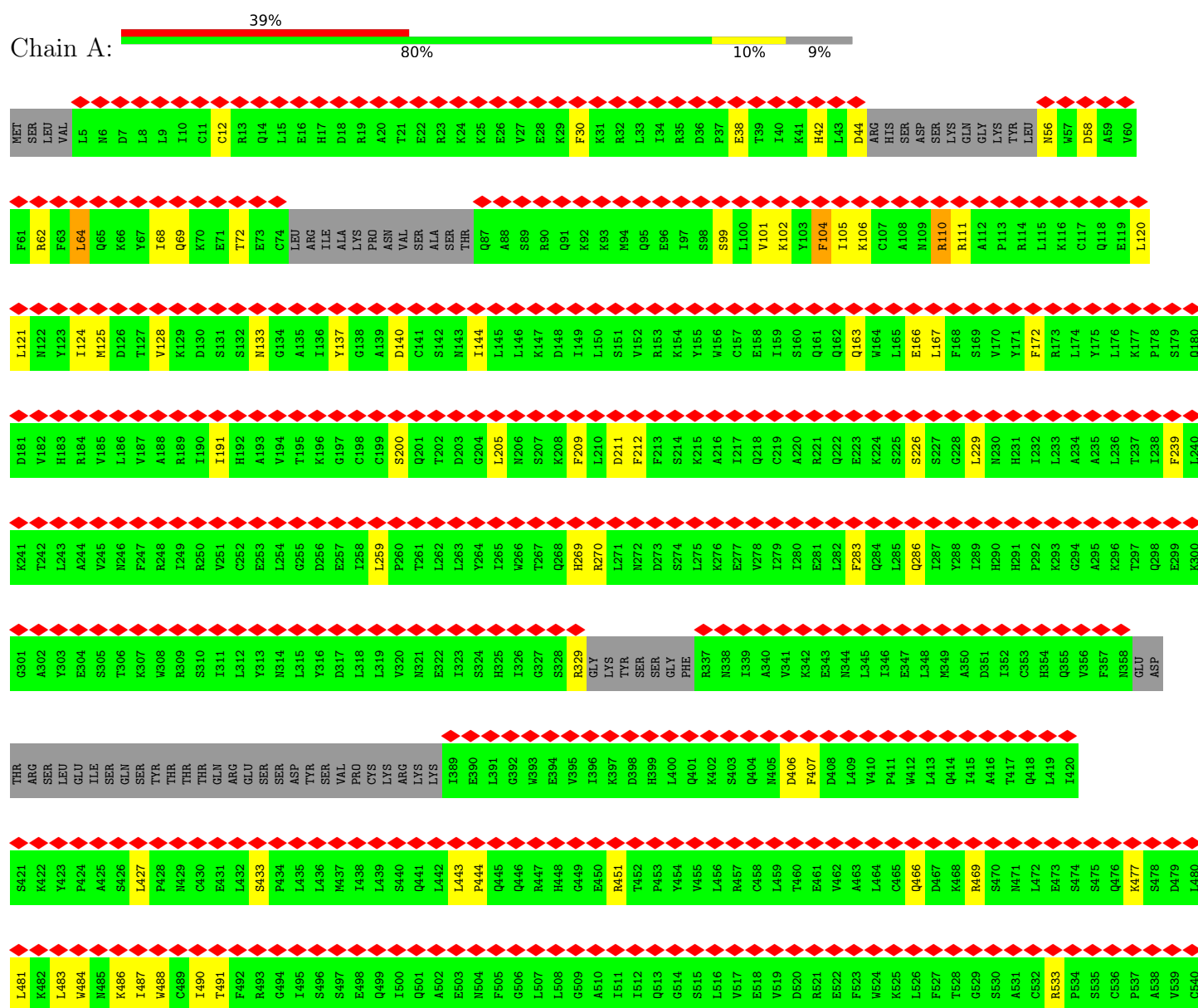
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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.

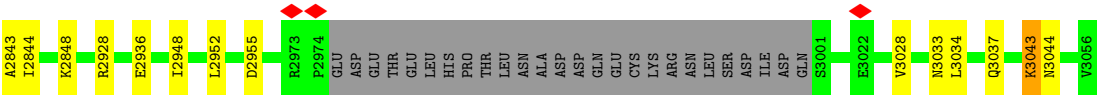
• Molecule 1: Serine-protein kinase ATM



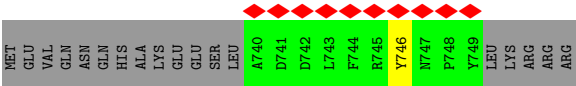
E1267	R1204	PRO	M1081	V1021	L961	L901	ASP	Q781	L721	D661	S601	C541
V1268	R1205	E1142	H1082	I1022	P962	K902	THR	L782	L722	F662	N602	L542
L1206	L1206	T1143	H1083	G1023	M963	F903	GLY	C783	V723	L663	F603	T543
S1270	L1208	L1144	Q1084	A1024	E964	L904	ASN	T784	G724	T664	P604	L544
I1271	D1208	D1145	V1085	F1025	D965	C905	LEU	R785	V725	ILE	H605	A545
A1272	M1210	E1146	R1086	W1026	V966	L906	MET	C786	L726	VAL	L606	L546
M1273	F1209	T1147	M1087	H1027	L967	V967	GLU	L787	G727	GLU	V607	L547
Q1274	A1211	Y1148	L1088	L1028	L967	V967	VAL	S788	G728	CYS	L608	T548
I1275	L1214	M1149	A1089	T1029	L969	T909	ASP	Y789	Y729	GLY	E609	S549
Q1276	D1215	R1150	A1090	K1030	L970	T910	GLN	N789	C730	ILE	K610	I550
E1277	Y1216	K1151	E1091	E1031	K971	A911	SER	C790	G730	GLU	I611	I551
L1217	L1217	S1152	S1092	R1032	P972	Q912	MET	K792	Y731	HIS	L612	P552
W1279	L1219	V1153	I1093	K1033	L973	T913	LEU	K793	G732	GLN	V613	G553
K1280	L1154	L1154	M1094	I1034	S974	N914	PHE	S794	G733	SER	S614	T554
S1281	L1155	L1155	L1095	I1035	N975	T915	ASN	F795	G734	SER	L615	
L1282	L1222	T1156	L1096	F1036	V976	V916	ASN	N796	I735	ILE	L616	VAL
L1283	N1223	L1157	F1097	S1037	C977	S917	TYR	K797	A736		T616	LYS
L1284	L1224	T1158	Q1098	R1038	S978	F918	PRO	I798	E737		M617	MET
D1285	Q1225	A1159	D1099	I1039	S978	R918	ASP	A799	E738		K618	ILE
	D1226	V1160	T1100	M1040	Y980	A920	SER	S800	E739		V682	GLU
I1290	T1227	V1161	K1101	A1041	R981	A921	VAL	G801	Y741		C620	GLN
N1293	E1228		GLY	L1042	R982	D922	ASP	F802	K742		K621	ASN
H1299	Y1229	S1165	SER	V1043	D983	I923	ALA	F803	S743		A622	CYS
F1298	N1230		ARG	M1044	Q984	R924	ASN	L804	E744		M624	VAL
A1299	L1231	C1168	SER	C1045	D985	R925	GLU	R805	L745		N625	ASN
Y1300	S1232	E1169	LEU	T1046	D985	K926	PRO	L806	F746		F626	ARG
E1301	S1233	I1170	L1108	K1047	V986	K926	GLY	L807	Q747		F627	SER
C1302	F1234	Q1171	K1109	T1048	C987	L928	GLU	T808	K748		L690	GLY
T1303	P1235	A1172	A1110	L1049	C988	N929	GLN	S809	A749		D691	ILE
R1304	F1236	L1173	L1111	L1050	T989	L930		K810	K750		R692	GLN
D1305	I1237	F1174	P1112	E1051	I990	D932		M812	S751		C693	GLN
S1306	L1238	A1175	L1113	A1052	N991	S933		N813	L752		L694	ASN
G1307	L1239	L1176	K1114	D1053	L992	S934		D814	M753		L695	ASN
M1308	N1240	C1177	L1115	P1054	V994	S934		Q754	C633		C633	ASN
Y1241	T1241	K1178	Q1116	P1056	H996	T935		I815	GLU		GLU	ASN
T1242	N1243	S1179	Q1117	S1056	L996	T935		A816	LEU		HIS	ASN
N1243	I1244	V1180	T1118	K1057	V997	E937		D817	GLY		HIS	ASN
E1245	T1246	K1181	A1119	W1058	H998	P938		L885	GLN		GLN	ASN
A1315	F1247	E1182	F1120	A1059	V998	T939		I818	LYS		LYS	ASN
T1314	T1248	M1183	E1121	I1060	K999	T939		C819	ASP		ASP	ASN
A1316	L1249	G1184	M1122	L1061	N1000	K940		K820	GLU		GLU	ASN
K1317	L1250	L1185	A1123	M1062	L1001	S941		S821	LEU		LEU	ASN
V1318	S1250	E1186	Y1124	V1063	G1002	L942		L822	S644		S644	ASN
Y1319	C1251	P1187	L1125	M1064	Q1003	H943		A823	F645		F645	ASN
D1320	Y1252	H1188	K1126	G1065	S1004	L944		S824	S646		S646	ASN
M1321	K1253	V1190	A1127	K1066	M1005	H945		F825	E647		E647	ASN
L1322	V1254	K1191	Q1128	D1067	M1006	M946		K766	V648		V648	ASN
L1255		K1192	E1129	F1068	D1007	Y947		T767	E649		E649	ASN
H1258	L1259	V1193	G1130	P1069	S1008	L948		N768	E650		E650	ASN
V1260	L1261	L1194	M1131	V1070	E1009	M949		S712	L651		L651	ASN
L1261	R1262	K1196	E1133	E1072	N1010	L950		T713	F652		F652	ASN
S1324		V1197	SER	V1073	T1011	L951		T714	Q654		Q654	ASN
E1325	L1269	L1198	H1328	F1074	D1012	K952		V716	T655		T655	ASN
M1326	V1260	E1195	S1198	T1075	R1013	E953		I773	G774		G774	ASN
L1327	L1261	K1196	S1199	Q1015	A1014	L954		T771	C718		C718	ASN
L1328	R1263	V1197	SER	G1016	A1014	P955		R772	L776		L776	ASN
E1329	S1263	T1200	ALA	F1077	Q1016	G956		L715	S719		S719	ASN
M1329	F1265	F1201	GLU	Q1017	F1077	E957		I773	R720		R720	ASN
L1332	D1266	G1202	ASN	F1018	F1018	E958		I773	M660		M660	ASN
D1333		Y1203		A1079	T1020	P960						

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	L243	Y303	LEU	Y423	L483	T543	F603	L663	L723	C783	ASN	F903	M963
R184	A244	E304	GLU	P424	W484	L544	P604	T664	G724	T784	ASN	L904	E964
V185	V245	E305	ILE	A425	M485	A545	H605	I1E	V725	R785	LEU	C905	D965
L186	N246	S306	SER	S426	K486	L546	L606	VAL	L726	C786	MET	N906	V966
V187	F247	T307	GLN	L427	L487	T547	V607	GLU	G727	L787	GLU	C907	L967
A188	R248	W308	TYR	P428	W488	T548	L608	CYS	C728	S788	GLU	V908	E968
R189	R249	R309	THR	M429	C489	S549	E609	ILE	Y729	M789	ASP	T909	L969
I190	R250	S310	THR	C430	L490	I550	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	P552	L612	HIS	M732	K792	MET	Q912	P972
A193	E253	Y313	GLU	S433	R493	G553	V613	GLN	G733	K793	ASN	T913	L973
V194	L254	N314	SER	P434	G494	T554	S614	SER	V734	S794	PHE	N914	S974
T195	G255	L315	ASP	L435	I495	L555	L615	ILE	I735	F795	ASN	T915	N975
K196	D256	Y316	TYR	L436	S496	T556	L616	VAL	A736	W796	ASP	V916	V976
G197	E257	D317	VAL	M437	S497	T557	T617	LYS	E737	K797	TYR	S917	C977
C198	I258	L318	PRO	I438	E498	L558	K618	F680	E738	L798	PRO	F918	S978
C199	L259	L319	CYS	L439	Q499	L559	N619	V682	E739	A799	SER	R919	L979
S200	P260	V320	LYS	S440	I500	L560	C620	H683	A740	S800	VAL	A920	Y980
Q201	T261	N321	ARG	Q441	Q501	M561	K621	Q684	Y741	G801	SER	A921	R981
T202	L262	I322	LYS	L442	A502	L562	A622	N685	K742	F802	ASP	D922	R982
D203	L263	I323	LYS	L443	E503	L563	A623	L686	S743	F803	ALA	I923	D983
G204	Y264	S324	ARG	P444	N504	L564	M624	E688	E744	L804	GLU	R924	Q984
L205	L265	H325	LYS	Q445	F505	L565	N625	Y688	L745	R805	PRO	R925	D985
N206	W266	I326	GLY	Q446	G506	L566	F626	S689	F746	L806	GLY	K926	V986
S207	T267	G327	GLY	R447	L507	S571	F627	L690	Q747	L807	GLU	L927	C987
K208	Q268	S328	GLY	H448	L508	S572	Q628	D691	K748	T808	GLN	L928	K988
F209	H269	R329	GLY	G449	G509	L572	S629	R692	A749	S809	THR	M929	T989
L210	R270	L396	LYS	E450	A510	K573	V630	C693	K750	K810	THR	N930	I990
D211	L271	T397	TYR	R451	I511	S574	P631	L694	S751	L811	THR	I931	L991
F212	N272	S398	SER	T452	I512	S575	E632	L695	L752	M812	THR	D932	N992
F213	D273	S399	SER	Y453	Q513	L576	C633	G696	W753	H813	THR	S933	H993
S214	S274	L400	GLY	P454	G514	M577	HIS	L697	Q754	D814	THR	S934	V994
K215	L275	PHE	GLY	V455	S515	K578	HIS	S698	C755	L815	THR	T935	L995
A216	K276	R337	GLY	L456	L516	W579	GLN	E699	A756	A816	THR	L936	H996
I217	E277	N338	GLY	R457	V517	L580	LYS	Q700	G757	D817	THR	E937	V997
Q218	V278	I339	GLY	C458	E518	L581	ASP	L701	E758	L818	THR	T939	K999
C219	I279	A340	GLY	L459	V519	F582	LYS	L702	S759	C819	THR	K940	N1000
A220	I280	V341	GLY	T460	D520	Y583	GLU	W703	L760	K820	THR	S941	L1001
R221	E281	K342	GLY	E461	R521	Q584	LEU	W704	T761	S821	THR	L942	G1002
Q222	L282	E343	GLY	V462	E522	L585	S644	Y705	L762	L822	THR	L943	L1003
E223	F283	N344	GLY	A463	F523	E586	F645	S706	F763	A823	THR	L944	Q1003
K224	Q284	L345	GLY	L464	N524	ASP	S646	S707	K764	S824	THR	K892	S1004
S225	L285	I346	GLY	C465	K525	LEU	E647	E708	W765	F825	THR	Q893	H945
Q226	Q286	E347	GLY	Q466	L526	ASN	V648	L709	K766	L826	THR	D894	N946
S227	I287	L348	GLY	D467	F527	SER	E649	T710	T767	L826	THR	L895	D1007
G228	Y288	M349	GLY	K468	T528	THR	E650	W711	W768	LYS	THR	L896	S1008
L229	I289	A350	GLY	R469	G529	THR	L651	S712	E769	PRO	THR	F897	E1009
N230	H290	D351	GLY	S470	S530	THR	F652	E713	E770	PHE	THR	L898	L1010
H231	H291	I352	GLY	M471	A531	THR	L653	T714	F771	ARG	THR	D899	L951
I232	P292	C353	GLY	L472	C532	THR	Q654	L715	I772	GLY	THR	K952	T1011
L233	K293	H354	GLY	E473	R533	THR	T655	W716	I773	VAL	THR	E953	R1012
A234	G294	Q355	GLY	S474	P534	THR	T656	R717	G774	GLU	THR	L954	D1013
A235	V295	L356	GLY	S475	S535	THR	F657	C718	S775	SER	THR	P955	Q1015
L236	K296	N358	GLY	Q476	C536	THR	L658	S719	L776	GLU	THR	Q956	G1016
I237	T297	I358	GLY	K477	P537	THR	K659	R720	R777	GLU	THR	E957	Q1017
I238	Q298	N358	GLY	S478	A538	THR	M660		R778	ASP	THR	F1018	L1019
F239	E299	ASP	ASP	D479	V539	THR			W780		THR	Y959	P960
L240	K300			L480	C540								

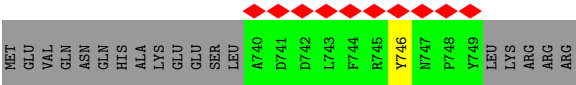
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GLU	HIS	LYS	ILE	GLN	THR	ASN	R2436	Y2437	T2438	T2439	K2440	T2441	Q2442	R2443	E2444	D2448	E2449	R2459	E2479	R2506	S2546	M2550	L2561	T2573	LYS	PRO	GLU	VAL	ALA	ARG	ARG	SER	ARG	ILE	THR	LYS	ASN	VAL	PRO	LYS	S2591	T2609	R2612	Q2615	R2618														
M2239	D2240	T2260	R2263	K2279	S2285	C2286	G2287	V2288	E2294	R2295	M2315	D2320	C2323	A2324	A2325	N2326	N2327	L2345	E2351	A2368	G2369	N2370	Y2371	D2372	G2373	E2374	S2375	K2383	M2384	Q2397	R2400	T2401	M2405	R2419	A2420	K2421	F2422	GLU	VAL	GLY	LEU	ARG																	
L1845	N1855	F1869	C1873	L1874	R1875	H1876	PHE	GLN	GLN	THR	THR	THR	THR	THR	PRO	PRO	ALA	ASN	LEU	ASP	SER	GLU	SER	SER	GLU	GLY	HIS	PHE	PHE	ARG	C1899	L1901	M1909	D1963	M1967	E1971	K1972	R1973	S1974	ALA	ALA	PHE	GLU	GLU	GLY	GLN	SER	T1984	T1985	S1990	E2238								
D1641	K1656	T1662	S1673	V1678	I1686	A1687	I1688	S1691	K1692	D1693	A1694	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	V1841																						
D1452	I1453	K1454	S1455	A1460	W1461	I1476	Q1478	R1479	P1480	S1481	C1482	I1483	M1484	D1485	R1489	L1493	V1501	C1502	Q1503	V1528	E1533	V1534	Q1535	Y1544	M1549	E1553	D1567	H1568	S1599	V1600	S1601	V1602	D1603	D1604	A1605	L1608	T1609	R1610	R1618	D1626	M1638																		
H1334	L1335	L1347	P1354	ALA	ASN	SER	ALA	SER	GLN	THR	ASP	LEU	CYS	ASP	PHE	SER	GLY	D1371	L1372	D1373	P1378	I1386	K1387	A1388	T1393	S1394	N1395	C1396	H1397	K1398	T1399	K1400	L1401	K1402	L1405	D1413	Q1425	E1428	K1434	T1438	I1439	H1443	L1449	L1450	K1451														
E1267	V1268	K1269	S1270	I1271	A1272	N1273	Q1274	I1275	Q1276	E1277	D1278	W1279	S1281	L1282	I1283	L1284	D1285	I1290	H1293	F1298	A1299	Y1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320	K1321	L1322	K1323	L1327	L1328	S1329	K1330	Q1331	I1332	D1333							
R1204	R1205	L1206	E1207	D1208	F1209	M1210	A1211	L1214	D1215	Y1216	L1217	E1220	W1221	L1222	M1223	L1224	Q1225	D1226	T1227	E1228	Y1229	M1230	L1231	S1232	E1233	F1234	P1235	F1236	I1237	L1238	L1239	M1240	Y1241	T1242	M1243	E1244	E1245	D1246	F1247	L1248	R1249	S1250	C1251	Y1252	K1253	V1254	L1255	H1258	L1259	V1260	K1261	R1262	S1263	H1264	F1265	D1266			
PRO	E1142	T1143	L1144	D1145	E1146	I1147	Y1148	N1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	W1161	S1165	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	G1177	K1178	S1179	W1180	K1181	E1182	N1183	G1184	N1185	E1186	P1187	H1188	L1189	V1190	K1191	A1192	V1193	L1194	E1195	K1196	V1197	S1198	E1199	T1200	F1201	G1202	Y1203		
N1081	H1082	H1083	Q1084	V1085	R1086	N1087	L1088	A1089	A1090	E1091	S1092	I1093	N1094	R1095	L1096	F1097	Q1098	D1099	T1100	K1101	GLY	ASP	SER	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	H1135	SER	ALA	GLU	ASN
V1021	I1022	G1023	A1024	F1025	W1026	L1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	S1037	V1038	R1039	T1040	M1041	A1042	L1043	N1044	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	D1053	P1054	V1055	S1056	K1057	A1058	A1059	I1060	L1061	N1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	N1070	L1071	E1072	V1073	F1074	T1075	Q1076	F1077	L1078	A1079	D1080



● 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: 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 ⓘ

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.

All (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
1:A:1271:ILE:O	1:A:1275:ILE:HB	1.76	0.85
1:C:2665:PRO:HD3	1:C:2683:ILE:HD11	1.73	0.71
1:A:2665:PRO:HD3	1:A:2683:ILE:HD11	1.73	0.71
1:A:1309:ALA:O	1:A:1312:ARG:N	2.27	0.68
1:C:1298:PHE:O	1:C:1312:ARG:NH1	2.27	0.68
1:A:1298:PHE:O	1:A:1312:ARG:NH1	2.27	0.68
1:C:1309:ALA:O	1:C:1312:ARG:N	2.27	0.66
1:C:1971:GLU:OE1	1:C:1971:GLU:HA	1.94	0.66
1:A:1971:GLU:HA	1:A:1971:GLU:OE1	1.94	0.66
1:C:1317:LYS:O	1:C:1321:MET:HG2	1.99	0.63
1:A:58:ASP:O	1:A:62:ARG:HG2	1.99	0.62
1:A:1317:LYS:O	1:A:1321:MET:HG2	1.99	0.62
1:A:2506:ARG:HG3	1:A:2506:ARG:NH1	2.04	0.62
1:C:58:ASP:O	1:C:62:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2401:ILE:HG22	1:C:2405:MET:HE2	1.82	0.62
1:A:427:LEU:O	1:A:469:ARG:NH2	2.28	0.61
1:A:2401:ILE:HG22	1:A:2405:MET:HE2	1.82	0.61
1:C:427:LEU:O	1:C:469:ARG:NH2	2.28	0.61
1:C:2550:MET:HE1	1:C:2609:ILE:HA	1.82	0.61
1:A:2550:MET:HE1	1:A:2609:ILE:HA	1.82	0.60
1:C:2745:THR:HG22	1:C:2750:LEU:HD12	1.83	0.60
1:A:466:GLN:OE1	1:A:484:TRP:NE1	2.33	0.60
1:A:2101:GLN:HA	1:A:2104:TRP:CD1	2.37	0.60
1:C:466:GLN:OE1	1:C:484:TRP:NE1	2.33	0.60
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.83	0.59
1:C:1771:ARG:NH1	1:C:1773:LYS:O	2.36	0.59
1:C:2506:ARG:HG3	1:C:2506:ARG:NH1	2.04	0.59
1:A:1771:ARG:NH1	1:A:1773:LYS:O	2.36	0.58
1:C:2101:GLN:HA	1:C:2104:TRP:CD1	2.37	0.58
1:A:1450:LEU:HD11	1:A:1501:VAL:HG22	1.86	0.58
1:C:1450:LEU:HD11	1:C:1501:VAL:HG22	1.86	0.58
1:C:329:ARG:NH2	1:C:407:PHE:O	2.36	0.57
1:C:804:LEU:HD21	1:C:911:ALA:HA	1.85	0.57
1:A:804:LEU:HD21	1:A:911:ALA:HA	1.85	0.57
1:C:2723:ARG:NH1	1:C:2955:ASP:OD2	2.38	0.57
1:A:1963:ASP:O	1:A:1967:MET:HG2	2.05	0.56
1:A:2723:ARG:NH1	1:A:2955:ASP:OD2	2.38	0.56
1:A:44:ASP:OD2	1:A:56:ASN:N	2.38	0.56
1:A:329:ARG:NH2	1:A:407:PHE:O	2.36	0.56
1:A:1827:LEU:HD22	1:A:1837:PHE:HZ	1.70	0.56
1:C:2727:VAL:O	1:C:2731:VAL:HG23	2.06	0.56
1:C:44:ASP:OD2	1:C:56:ASN:N	2.38	0.56
1:A:543:THR:HB	1:A:611:ILE:HD11	1.87	0.56
1:C:1963:ASP:O	1:C:1967:MET:HG2	2.05	0.56
1:A:486:LYS:O	1:A:490:ILE:HD12	2.06	0.56
1:C:1827:LEU:HD22	1:C:1837:PHE:HZ	1.70	0.56
1:C:1309:ALA:O	1:C:1313:GLU:OE1	2.24	0.55
1:C:486:LYS:O	1:C:490:ILE:HD12	2.06	0.55
1:A:1309:ALA:O	1:A:1313:GLU:OE1	2.24	0.55
1:A:2727:VAL:O	1:A:2731:VAL:HG23	2.06	0.55
1:C:1176:LEU:O	1:C:1180:VAL:HG23	2.06	0.55
1:A:1176:LEU:O	1:A:1180:VAL:HG23	2.06	0.54
1:C:1656:LYS:NZ	1:C:2161:ARG:O	2.38	0.54
1:A:1040:MET:HG3	1:A:1085:VAL:HG22	1.89	0.54
1:A:1806:ILE:HG21	1:A:1835:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:THR:HB	1:C:611:ILE:HD11	1.87	0.54
1:A:1656:LYS:NZ	1:A:2161:ARG:O	2.38	0.54
1:C:2615:GLN:OE1	1:C:2618:ARG:NH1	2.40	0.54
1:C:1040:MET:HG3	1:C:1085:VAL:HG22	1.89	0.54
1:C:2151:ARG:NH2	1:C:2183:GLU:OE1	2.38	0.54
1:C:2397:GLN:OE1	1:C:2400:ARG:NH1	2.41	0.54
1:A:2384:MET:HE1	1:A:2479:GLU:HB2	1.90	0.54
1:A:2615:GLN:OE1	1:A:2618:ARG:NH1	2.40	0.54
1:C:2731:VAL:HG22	1:C:2952:LEU:HD21	1.90	0.53
1:C:2421:LYS:HA	1:C:2441:VAL:HG11	1.89	0.53
1:A:406:ASP:OD1	1:A:451:ARG:NH1	2.42	0.53
1:A:1688:ILE:HD13	1:A:2163:LEU:HD13	1.91	0.53
1:C:2384:MET:HE1	1:C:2479:GLU:HB2	1.90	0.53
1:A:2421:LYS:HA	1:A:2441:VAL:HG11	1.89	0.53
1:C:1806:ILE:HG21	1:C:1835:THR:HG23	1.89	0.53
1:A:2731:VAL:HG22	1:A:2952:LEU:HD21	1.90	0.53
1:A:2105:ARG:NH2	1:A:2221:GLU:OE1	2.42	0.52
1:C:1688:ILE:HD13	1:C:2163:LEU:HD13	1.91	0.52
1:C:406:ASP:OD1	1:C:451:ARG:NH1	2.42	0.52
1:C:773:ILE:HG21	1:C:892:LYS:HB3	1.90	0.52
1:C:2105:ARG:NH2	1:C:2221:GLU:OE1	2.42	0.52
1:A:101:VAL:O	1:A:105:ILE:HG12	2.10	0.52
1:A:970:LEU:HD21	1:A:997:VAL:HG11	1.92	0.52
1:C:2405:MET:HE1	1:C:2459:ARG:HD2	1.91	0.52
1:C:101:VAL:O	1:C:105:ILE:HG12	2.10	0.52
1:A:773:ILE:HG21	1:A:892:LYS:HB3	1.90	0.52
1:A:2405:MET:HE1	1:A:2459:ARG:HD2	1.91	0.52
1:A:2397:GLN:OE1	1:A:2400:ARG:NH1	2.41	0.52
1:A:716:VAL:HG21	1:A:779:MET:HG3	1.92	0.51
1:C:1275:ILE:HG21	1:C:1282:LEU:HD11	1.92	0.51
1:C:2326:ASN:OD1	1:C:2327:ASN:N	2.42	0.51
1:C:970:LEU:HD21	1:C:997:VAL:HG11	1.92	0.51
1:C:991:LEU:HA	1:C:994:VAL:HG12	1.93	0.51
1:C:1476:ILE:O	1:C:1479:ARG:NH1	2.45	0.50
1:C:2699:PRO:HB2	1:C:2715:LEU:HD11	1.93	0.50
1:A:1753:TYR:OH	1:A:1758:ASP:OD1	2.30	0.50
1:C:1311:GLN:HA	1:C:1314:THR:HG22	1.94	0.50
1:A:38:GLU:O	1:A:42:HIS:ND1	2.45	0.50
1:A:1264:HIS:HB3	1:A:1267:GLU:OE1	2.12	0.50
1:A:1476:ILE:O	1:A:1479:ARG:NH1	2.45	0.50
1:C:716:VAL:HG21	1:C:779:MET:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.45	0.50
1:C:2279:LYS:NZ	1:C:2295:GLU:OE2	2.45	0.50
1:A:1275:ILE:HG21	1:A:1282:LEU:HD11	1.92	0.50
1:A:2705:VAL:HG22	1:A:2711:GLU:HG2	1.94	0.50
1:A:991:LEU:HA	1:A:994:VAL:HG12	1.93	0.49
1:C:609:GLU:HG3	1:C:721:LEU:HD12	1.94	0.49
1:C:1687:ALA:HB1	1:C:2843:ALA:HB1	1.94	0.49
1:C:1875:ARG:O	1:C:1876:HIS:ND1	2.45	0.49
1:C:1990:SER:OG	1:C:2002:GLN:HG3	2.13	0.49
1:A:259:LEU:HD11	1:A:286:GLN:HG3	1.94	0.49
1:C:2705:VAL:HG22	1:C:2711:GLU:HG2	1.94	0.49
1:C:271:LEU:HB3	1:C:276:LYS:HZ1	1.77	0.49
1:C:2722:LEU:HD12	1:C:2765:GLY:HA3	1.95	0.49
1:A:1311:GLN:HA	1:A:1314:THR:HG22	1.94	0.49
1:C:1264:HIS:HB3	1:C:1267:GLU:OE1	2.12	0.49
1:A:1020:THR:HG21	2:B:746:TYR:HB2	1.95	0.49
1:A:2699:PRO:HB2	1:A:2715:LEU:HD11	1.93	0.49
1:A:2722:LEU:HD12	1:A:2765:GLY:HA3	1.95	0.49
1:C:259:LEU:HD11	1:C:286:GLN:HG3	1.94	0.49
1:C:1753:TYR:OH	1:C:1758:ASP:OD1	2.30	0.49
1:C:1993:SER:O	1:C:1997:THR:OG1	2.28	0.49
1:C:38:GLU:O	1:C:42:HIS:ND1	2.45	0.49
1:C:1453:ILE:HD11	1:C:1461:TRP:CD2	2.48	0.49
1:A:1687:ALA:HB1	1:A:2843:ALA:HB1	1.94	0.48
1:A:1718:LEU:HA	1:A:1721:THR:HG22	1.95	0.48
1:A:2326:ASN:OD1	1:A:2327:ASN:N	2.42	0.48
1:C:1145:ASP:OD1	1:C:1145:ASP:N	2.46	0.48
1:A:925:ARG:O	1:A:929:MET:HG2	2.13	0.48
1:A:2260:ILE:HG12	1:A:2263:ARG:HH21	1.78	0.48
1:A:1453:ILE:HD11	1:A:1461:TRP:CD2	2.48	0.48
1:A:2151:ARG:NH2	1:A:2183:GLU:OE1	2.38	0.48
1:A:2546:SER:O	1:A:2550:MET:HG2	2.13	0.48
1:C:925:ARG:O	1:C:929:MET:HG2	2.13	0.48
1:A:2734:MET:HE3	1:A:2734:MET:HA	1.96	0.48
1:A:609:GLU:HG3	1:A:721:LEU:HD12	1.94	0.48
1:A:1601:SER:HB2	1:A:1610:ARG:HH21	1.78	0.48
1:C:104:PHE:CD1	1:C:104:PHE:C	2.92	0.48
1:C:1601:SER:HB2	1:C:1610:ARG:HH21	1.78	0.48
1:C:2734:MET:HE3	1:C:2734:MET:HA	1.96	0.48
1:C:2260:ILE:HG12	1:C:2263:ARG:HH21	1.78	0.48
1:A:1638:ASN:ND2	1:A:1641:ASP:OD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2345:LEU:HD13	1:A:2351:GLU:HG3	1.95	0.48
1:A:104:PHE:CD1	1:A:104:PHE:C	2.92	0.48
1:A:1990:SER:OG	1:A:2002:GLN:HG3	2.13	0.48
1:A:2279:LYS:NZ	1:A:2295:GLU:OE2	2.45	0.48
1:A:1216:TYR:HD2	1:A:1378:PRO:HG3	1.79	0.48
1:A:2368:ALA:HB1	1:A:2383:LYS:HG2	1.96	0.48
1:C:1020:THR:HG21	2:D:746:TYR:HB2	1.95	0.48
1:C:2156:GLU:O	1:C:2160:LYS:HG3	2.14	0.48
1:C:1216:TYR:HD2	1:C:1378:PRO:HG3	1.79	0.47
1:C:1604:ASP:OD1	1:C:1605:ALA:N	2.47	0.47
1:C:1270:SER:O	1:C:1273:ASN:N	2.47	0.47
1:C:1686:ILE:HG12	1:C:2167:TYR:HE2	1.79	0.47
1:A:1270:SER:O	1:A:1273:ASN:N	2.47	0.47
1:A:2156:GLU:O	1:A:2160:LYS:HG3	2.14	0.47
1:C:1638:ASN:ND2	1:C:1641:ASP:OD2	2.47	0.47
1:C:2368:ALA:HB1	1:C:2383:LYS:HG2	1.96	0.47
1:A:1114:LYS:HG3	1:A:1115:LEU:HD12	1.97	0.47
1:A:1272:ALA:O	1:A:1275:ILE:HG22	2.15	0.47
1:A:1993:SER:O	1:A:1997:THR:OG1	2.28	0.47
1:C:1114:LYS:HG3	1:C:1115:LEU:HD12	1.97	0.47
1:C:1123:ALA:HB1	1:C:1157:LEU:HD11	1.97	0.47
1:C:2546:SER:O	1:C:2550:MET:HG2	2.13	0.47
1:A:1145:ASP:OD1	1:A:1145:ASP:N	2.46	0.47
1:A:1604:ASP:OD1	1:A:1605:ALA:N	2.47	0.47
1:C:2288:VAL:HG11	1:C:2315:MET:HG2	1.97	0.47
1:C:397:LYS:NZ	1:C:431:GLU:OE1	2.40	0.47
1:C:736:ALA:HB3	1:C:739:GLU:HG3	1.96	0.47
1:C:1270:SER:HA	1:C:1273:ASN:ND2	2.30	0.47
1:C:2345:LEU:HD13	1:C:2351:GLU:HG3	1.95	0.47
1:A:1824:LEU:HD13	1:A:1845:LEU:HD23	1.96	0.47
1:C:1718:LEU:HA	1:C:1721:THR:HG22	1.95	0.47
1:C:2263:ARG:NE	1:C:2294:GLU:OE2	2.46	0.47
1:A:1123:ALA:HB1	1:A:1157:LEU:HD11	1.97	0.47
1:A:2936:GLU:HG3	1:A:3028:VAL:HG11	1.97	0.47
1:A:1686:ILE:HG12	1:A:2167:TYR:HE2	1.79	0.46
1:C:1528:VAL:O	1:C:1535:GLN:NE2	2.47	0.46
1:A:1270:SER:HA	1:A:1273:ASN:ND2	2.30	0.46
1:C:2928:ARG:NH1	1:C:3033:ASN:OD1	2.48	0.46
1:A:736:ALA:HB3	1:A:739:GLU:HG3	1.96	0.46
1:C:2936:GLU:HG3	1:C:3028:VAL:HG11	1.97	0.46
1:A:1460:ALA:HB2	1:A:1766:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.48	0.46
1:C:1272:ALA:O	1:C:1275:ILE:HG22	2.15	0.46
1:A:2288:VAL:HG11	1:A:2315:MET:HG2	1.97	0.46
1:C:64:LEU:O	1:C:68:ILE:HG12	2.16	0.46
1:C:1460:ALA:HB2	1:C:1766:PRO:HB3	1.96	0.46
1:C:1824:LEU:HD13	1:C:1845:LEU:HD23	1.96	0.46
1:C:2672:ASP:OD2	1:C:2674:THR:OG1	2.33	0.46
1:A:209:PHE:O	1:A:212:PHE:HB2	2.16	0.46
1:A:2506:ARG:HH11	1:A:2506:ARG:CG	2.14	0.46
1:C:3034:LEU:HD12	1:C:3037:GLN:HE21	1.81	0.46
1:C:2719:ARG:HG2	1:C:2763:ARG:NH2	2.31	0.46
1:A:99:SER:HA	1:A:102:LYS:HG2	1.98	0.46
1:C:140:ASP:O	1:C:144:ILE:HG12	2.16	0.46
1:A:64:LEU:O	1:A:68:ILE:HG12	2.16	0.45
1:A:140:ASP:O	1:A:144:ILE:HG12	2.16	0.45
1:A:2687:LYS:NZ	1:A:2711:GLU:OE2	2.39	0.45
1:A:684:GLN:NE2	1:A:688:GLU:OE2	2.50	0.45
1:A:2672:ASP:OD2	1:A:2674:THR:OG1	2.33	0.45
1:C:209:PHE:O	1:C:212:PHE:HB2	2.16	0.45
1:C:443:LEU:N	1:C:444:PRO:HD3	2.31	0.45
1:C:1027:HIS:HB2	1:C:1063:VAL:HG21	1.98	0.45
1:A:1281:SER:HA	1:A:1284:THR:HG22	1.99	0.45
1:A:1405:LEU:HD21	1:A:1449:LEU:HD23	1.99	0.45
1:C:99:SER:HA	1:C:102:LYS:HG2	1.98	0.45
1:A:613:VAL:O	1:A:617:MET:HG2	2.17	0.45
1:A:1047:LYS:HD3	1:A:1092:SER:HB3	1.99	0.45
1:A:1528:VAL:O	1:A:1535:GLN:NE2	2.47	0.45
1:A:2814:GLU:OE1	1:A:2814:GLU:N	2.50	0.45
1:C:1780:PHE:CE2	1:C:1782:LYS:HG3	2.52	0.45
1:A:269:HIS:CG	1:A:270:ARG:H	2.35	0.45
1:A:2656:LEU:HD23	1:A:2659:LEU:HD11	1.99	0.45
1:C:684:GLN:NE2	1:C:688:GLU:OE2	2.50	0.45
1:C:1405:LEU:HD21	1:C:1449:LEU:HD23	1.99	0.45
1:A:259:LEU:HG	1:A:283:PHE:HE1	1.82	0.45
1:A:2719:ARG:HG2	1:A:2763:ARG:NH2	2.31	0.45
1:C:259:LEU:HG	1:C:283:PHE:HE1	1.82	0.45
1:C:2448:ASP:OD1	1:C:2449:GLU:N	2.50	0.45
1:C:2814:GLU:N	1:C:2814:GLU:OE1	2.50	0.45
1:A:1780:PHE:CE2	1:A:1782:LYS:HG3	2.52	0.45
1:A:1434:LYS:O	1:A:1438:ILE:HG12	2.17	0.44
1:A:1873:CYS:SG	1:A:1901:LEU:HD22	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3034:LEU:HD12	1:A:3037:GLN:HE21	1.81	0.44
1:C:1626:ASP:N	1:C:1626:ASP:OD1	2.50	0.44
1:A:2041:MET:HE2	1:A:2044:LYS:HD2	1.99	0.44
1:A:2448:ASP:OD1	1:A:2449:GLU:N	2.50	0.44
1:C:613:VAL:O	1:C:617:MET:HG2	2.17	0.44
1:A:1027:HIS:HB2	1:A:1063:VAL:HG21	1.98	0.44
1:A:443:LEU:N	1:A:444:PRO:HD3	2.31	0.44
1:C:1265:PHE:HA	1:C:1268:VAL:HG12	1.98	0.44
1:A:2263:ARG:NE	1:A:2294:GLU:OE2	2.46	0.44
1:C:780:MET:HE3	1:C:900:MET:HG2	1.99	0.44
1:C:1425:GLN:O	1:C:1428:GLU:HG3	2.18	0.44
1:C:1434:LYS:O	1:C:1438:ILE:HG12	2.17	0.44
1:C:172:PHE:HA	1:C:191:ILE:HD11	2.00	0.44
1:C:269:HIS:CG	1:C:270:ARG:H	2.35	0.44
1:C:1112:PRO:HB2	1:C:1115:LEU:HD13	2.00	0.44
1:A:780:MET:HE3	1:A:900:MET:HG2	1.99	0.44
1:A:2635:ALA:HA	1:A:2638:TRP:CZ3	2.53	0.44
1:C:120:LEU:O	1:C:124:ILE:HG12	2.18	0.44
1:C:2844:ILE:O	1:C:2848:LYS:HG2	2.18	0.44
1:C:2948:ILE:O	1:C:2952:LEU:HD13	2.18	0.43
1:A:172:PHE:HA	1:A:191:ILE:HD11	2.00	0.43
1:A:1187:PRO:O	1:A:1191:LYS:HB2	2.18	0.43
1:A:1265:PHE:HA	1:A:1268:VAL:HG12	1.98	0.43
1:A:1626:ASP:OD1	1:A:1626:ASP:N	2.50	0.43
1:C:1131:MET:HG2	1:C:1150:ARG:HB3	2.00	0.43
1:C:1489:ARG:HG3	1:C:1489:ARG:HH11	1.83	0.43
1:A:1425:GLN:O	1:A:1428:GLU:HG3	2.18	0.43
1:A:2844:ILE:O	1:A:2848:LYS:HG2	2.18	0.43
1:C:1263:SER:HB2	1:C:1321:MET:HE1	2.01	0.43
1:C:2656:LEU:HD23	1:C:2659:LEU:HD11	1.99	0.43
1:A:226:SER:HB2	1:A:229:LEU:HD12	2.01	0.43
1:C:1047:LYS:HD3	1:C:1092:SER:HB3	1.99	0.43
1:C:2778:GLU:O	1:C:2782:ASN:HB2	2.18	0.43
1:A:1489:ARG:HG3	1:A:1489:ARG:HH11	1.83	0.43
1:C:1251:CYS:O	1:C:1255:LEU:HD23	2.18	0.43
1:A:121:LEU:HD12	1:A:167:LEU:HD11	2.01	0.43
1:C:1281:SER:HA	1:C:1284:THR:HG22	1.99	0.43
1:C:1503:GLN:HG2	1:C:1544:TYR:CE2	2.54	0.43
1:C:1869:PHE:CE1	1:C:1909:MET:HG3	2.53	0.43
1:C:1873:CYS:SG	1:C:1901:LEU:HD22	2.58	0.43
1:C:2506:ARG:HH11	1:C:2506:ARG:CG	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2635:ALA:HA	1:C:2638:TRP:CZ3	2.53	0.43
1:A:1251:CYS:O	1:A:1255:LEU:HD23	2.18	0.43
1:A:2948:ILE:O	1:A:2952:LEU:HD13	2.18	0.43
1:C:226:SER:HB2	1:C:229:LEU:HD12	2.01	0.43
1:C:1187:PRO:O	1:C:1191:LYS:HB2	2.18	0.43
1:C:2041:MET:HE2	1:C:2044:LYS:HD2	1.99	0.43
1:C:2092:CYS:SG	1:C:2095:LEU:HD13	2.59	0.43
1:A:120:LEU:O	1:A:124:ILE:HG12	2.18	0.43
1:A:125:MET:HA	1:A:128:VAL:HG12	2.01	0.43
1:A:2778:GLU:O	1:A:2782:ASN:HB2	2.18	0.43
1:C:904:LEU:HD23	1:C:904:LEU:HA	1.91	0.43
1:A:1131:MET:HG2	1:A:1150:ARG:HB3	2.00	0.43
1:A:1263:SER:HB2	1:A:1321:MET:HE1	2.01	0.43
1:A:1503:GLN:HG2	1:A:1544:TYR:CE2	2.54	0.43
1:A:2092:CYS:SG	1:A:2095:LEU:HD13	2.59	0.42
1:A:2936:GLU:HG2	1:A:3028:VAL:HG21	2.01	0.42
1:A:533:ARG:HH21	1:A:597:PRO:HB3	1.84	0.42
1:C:121:LEU:HD12	1:C:167:LEU:HD11	2.01	0.42
1:A:205:LEU:HB2	1:A:239:PHE:CE1	2.55	0.42
1:A:545:ALA:O	1:A:549:SER:HB2	2.19	0.42
1:A:1302:GLY:HA2	1:A:1308:MET:HE1	2.02	0.42
1:C:2024:GLY:O	1:C:2025:LYS:HG3	2.19	0.42
1:A:1443:HIS:HB2	1:A:1493:LEU:HD21	2.02	0.42
1:A:1838:CYS:HA	1:A:1841:VAL:HG12	2.01	0.42
1:A:1869:PHE:CE1	1:A:1909:MET:HG3	2.53	0.42
1:C:205:LEU:HB2	1:C:239:PHE:CE1	2.55	0.42
1:C:2550:MET:SD	1:C:2612:ARG:HD2	2.59	0.42
1:A:1112:PRO:HB2	1:A:1115:LEU:HD13	2.00	0.42
1:A:1186:GLU:HB3	1:A:1188:HIS:CE1	2.54	0.42
1:C:533:ARG:HH21	1:C:597:PRO:HB3	1.84	0.42
1:C:1186:GLU:HB3	1:C:1188:HIS:CE1	2.54	0.42
1:C:2561:LEU:HD23	1:C:2561:LEU:HA	1.93	0.42
1:C:1124:TYR:O	1:C:1128:GLN:HG2	2.20	0.42
1:C:1222:LEU:HB3	1:C:1262:ARG:HH21	1.84	0.42
1:C:1322:LEU:HA	1:C:1327:LEU:HD12	2.02	0.42
1:A:2550:MET:SD	1:A:2612:ARG:HD2	2.59	0.42
1:C:110:ARG:NH2	1:C:111:ARG:HE	2.18	0.42
1:C:545:ALA:O	1:C:549:SER:HB2	2.19	0.42
1:C:1131:MET:HB3	1:C:1131:MET:HE2	1.83	0.42
1:C:1302:GLY:HA2	1:C:1308:MET:HE1	2.02	0.42
1:A:2692:LEU:HA	1:A:2692:LEU:HD23	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:TRP:HA	1:C:491:THR:HG22	2.02	0.42
1:C:2936:GLU:HG2	1:C:3028:VAL:HG21	2.01	0.42
1:C:133:ASN:HB3	1:C:137:TYR:HD2	1.85	0.42
1:C:1702:LEU:HD23	1:C:1702:LEU:HA	1.94	0.42
1:C:3034:LEU:O	1:C:3037:GLN:HG3	2.20	0.42
1:A:621:LYS:O	1:A:625:ASN:ND2	2.49	0.42
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.89	0.42
1:C:125:MET:HA	1:C:128:VAL:HG12	2.01	0.42
1:A:477:LYS:O	1:A:481:LEU:HD23	2.20	0.41
1:A:1124:TYR:O	1:A:1128:GLN:HG2	2.20	0.41
1:A:2024:GLY:O	1:A:2025:LYS:HG3	2.19	0.41
1:C:1567:ASP:O	1:C:1568:HIS:ND1	2.53	0.41
1:A:106:LYS:O	1:A:110:ARG:HB2	2.20	0.41
1:A:163:GLN:HA	1:A:166:GLU:HG2	2.02	0.41
1:A:1567:ASP:O	1:A:1568:HIS:ND1	2.53	0.41
1:A:2440:LYS:O	1:A:2444:GLU:HG2	2.21	0.41
1:A:815:ILE:HG23	1:A:900:MET:HE2	2.02	0.41
1:A:2667:MET:HE1	1:A:2681:VAL:HB	2.01	0.41
1:A:1322:LEU:HA	1:A:1327:LEU:HD12	2.02	0.41
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	2.03	0.41
1:A:483:LEU:O	1:A:487:ILE:HG23	2.21	0.41
1:A:488:TRP:HA	1:A:491:THR:HG22	2.02	0.41
1:A:1618:ARG:HD2	1:A:1673:SER:HB3	2.01	0.41
1:C:1710:TRP:O	1:C:1714:MET:HG2	2.20	0.41
1:A:133:ASN:HB3	1:A:137:TYR:HD2	1.85	0.41
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.91	0.41
1:A:2561:LEU:HD23	1:A:2561:LEU:HA	1.93	0.41
1:C:163:GLN:HA	1:C:166:GLU:HG2	2.02	0.41
1:C:1443:HIS:HB2	1:C:1493:LEU:HD21	2.02	0.41
1:A:110:ARG:NH2	1:A:111:ARG:HE	2.18	0.41
1:A:1710:TRP:O	1:A:1714:MET:HG2	2.20	0.41
1:A:3034:LEU:O	1:A:3037:GLN:HG3	2.20	0.41
1:C:211:ASP:OD1	1:C:212:PHE:N	2.54	0.41
1:C:954:LEU:HD23	1:C:954:LEU:HA	1.90	0.41
1:C:2667:MET:HE1	1:C:2681:VAL:HB	2.01	0.41
1:A:1071:ASN:OD1	1:A:1072:GLU:N	2.54	0.41
1:C:12:CYS:HA	1:C:30:PHE:HZ	1.85	0.41
1:C:477:LYS:O	1:C:481:LEU:HD23	2.20	0.41
1:C:815:ILE:HG23	1:C:900:MET:HE2	2.02	0.41
1:A:102:LYS:HE3	1:A:144:ILE:HD11	2.03	0.41
1:A:1131:MET:HE2	1:A:1131:MET:HB3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:ALA:O	1:A:1310:GLN:C	2.64	0.41
1:C:125:MET:C	1:C:129:LYS:HZ2	2.29	0.41
1:C:1071:ASN:OD1	1:C:1072:GLU:N	2.54	0.41
1:C:1618:ARG:HD2	1:C:1673:SER:HB3	2.01	0.41
1:A:12:CYS:HA	1:A:30:PHE:HZ	1.85	0.41
1:A:1222:LEU:HB3	1:A:1262:ARG:HH21	1.84	0.41
1:A:3043:LYS:HG3	1:A:3044:ASN:N	2.36	0.41
1:C:963:MET:HE2	1:C:1011:THR:HA	2.03	0.41
1:C:1838:CYS:HA	1:C:1841:VAL:HG12	2.01	0.41
1:C:2440:LYS:O	1:C:2444:GLU:HG2	2.21	0.41
1:A:2865:ILE:HD13	1:A:2865:ILE:HA	1.94	0.40
1:C:1876:HIS:O	1:C:1899:CYS:N	2.54	0.40
1:C:2401:ILE:HG21	1:C:2459:ARG:HB2	2.03	0.40
1:A:211:ASP:OD1	1:A:212:PHE:N	2.54	0.40
1:A:1599:SER:O	1:A:1602:VAL:HG22	2.21	0.40
1:C:1599:SER:O	1:C:1602:VAL:HG22	2.21	0.40
1:C:94:MET:O	1:C:97:ILE:HG22	2.21	0.40
1:A:69:GLN:HA	1:A:72:THR:HG22	2.04	0.40
1:C:3043:LYS:HG3	1:C:3044:ASN:N	2.36	0.40
1:A:963:MET:HE2	1:A:1011:THR:HA	2.03	0.40
1:A:1876:HIS:O	1:A:1899:CYS:N	2.54	0.40
1:A:3048:LEU:HD13	1:A:3052:TRP:CZ3	2.56	0.40
1:C:102:LYS:HE3	1:C:144:ILE:HD11	2.03	0.40
1:C:106:LYS:O	1:C:110:ARG:HB2	2.20	0.40
1:C:808:THR:O	1:C:812:MET:HG2	2.22	0.40
1:C:1608:LEU:HD21	1:C:1662:THR:O	2.22	0.40
1:C:1678:VAL:O	1:C:1678:VAL:HG13	2.21	0.40

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%)	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

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	104	PHE
1	A	110	ARG
1	A	200	SER
1	A	433	SER
1	A	1040	MET
1	A	1145	ASP
1	A	1262	ARG
1	A	1275	ILE
1	A	1312	ARG
1	A	1313	GLU
1	A	1347	LEU
1	A	1386	ILE

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Mol	Chain	Res	Type
1	A	1478	GLN
1	A	1971	GLU
1	A	2506	ARG
1	A	2734	MET
1	A	2784	GLU
1	A	3043	LYS
1	C	64	LEU
1	C	104	PHE
1	C	110	ARG
1	C	200	SER
1	C	433	SER
1	C	1040	MET
1	C	1145	ASP
1	C	1262	ARG
1	C	1275	ILE
1	C	1312	ARG
1	C	1313	GLU
1	C	1347	LEU
1	C	1386	ILE
1	C	1478	GLN
1	C	1971	GLU
1	C	2506	ARG
1	C	2734	MET
1	C	2784	GLU
1	C	3043	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	218	GLN
1	A	290	HIS
1	A	399	HIS
1	A	628	GLN
1	A	1044	ASN
1	A	1535	GLN
1	A	1554	ASN
1	A	1640	GLN
1	A	1765	GLN
1	A	1825	GLN
1	A	1937	ASN
1	A	2061	GLN

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Mol	Chain	Res	Type
1	A	2070	ASN
1	A	2206	GLN
1	A	2243	GLN
1	A	2399	GLN
1	A	2542	ASN
1	A	2554	HIS
1	A	2673	HIS
1	A	2809	GLN
1	A	2826	ASN
1	A	3037	GLN
1	C	65	GLN
1	C	162	GLN
1	C	163	GLN
1	C	180	GLN
1	C	218	GLN
1	C	290	HIS
1	C	584	GLN
1	C	628	GLN
1	C	778	ASN
1	C	1044	ASN
1	C	1554	ASN
1	C	1620	GLN
1	C	1640	GLN
1	C	1765	GLN
1	C	1825	GLN
1	C	1937	ASN
1	C	2061	GLN
1	C	2070	ASN
1	C	2206	GLN
1	C	2243	GLN
1	C	2469	ASN
1	C	2542	ASN
1	C	2554	HIS
1	C	2673	HIS
1	C	2800	GLN
1	C	2809	GLN
1	C	2826	ASN
1	C	3037	GLN

5.3.3 RNA ⓘ

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
3	ANP	C	3101	-	-	4/18/38/38	0/3/3/3

All (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
3	C	3101	ANP	PB-O1B	2.44	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3101	ANP	PB-O3A	-2.41	1.56	1.59
3	C	3101	ANP	PB-O3A	-2.41	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

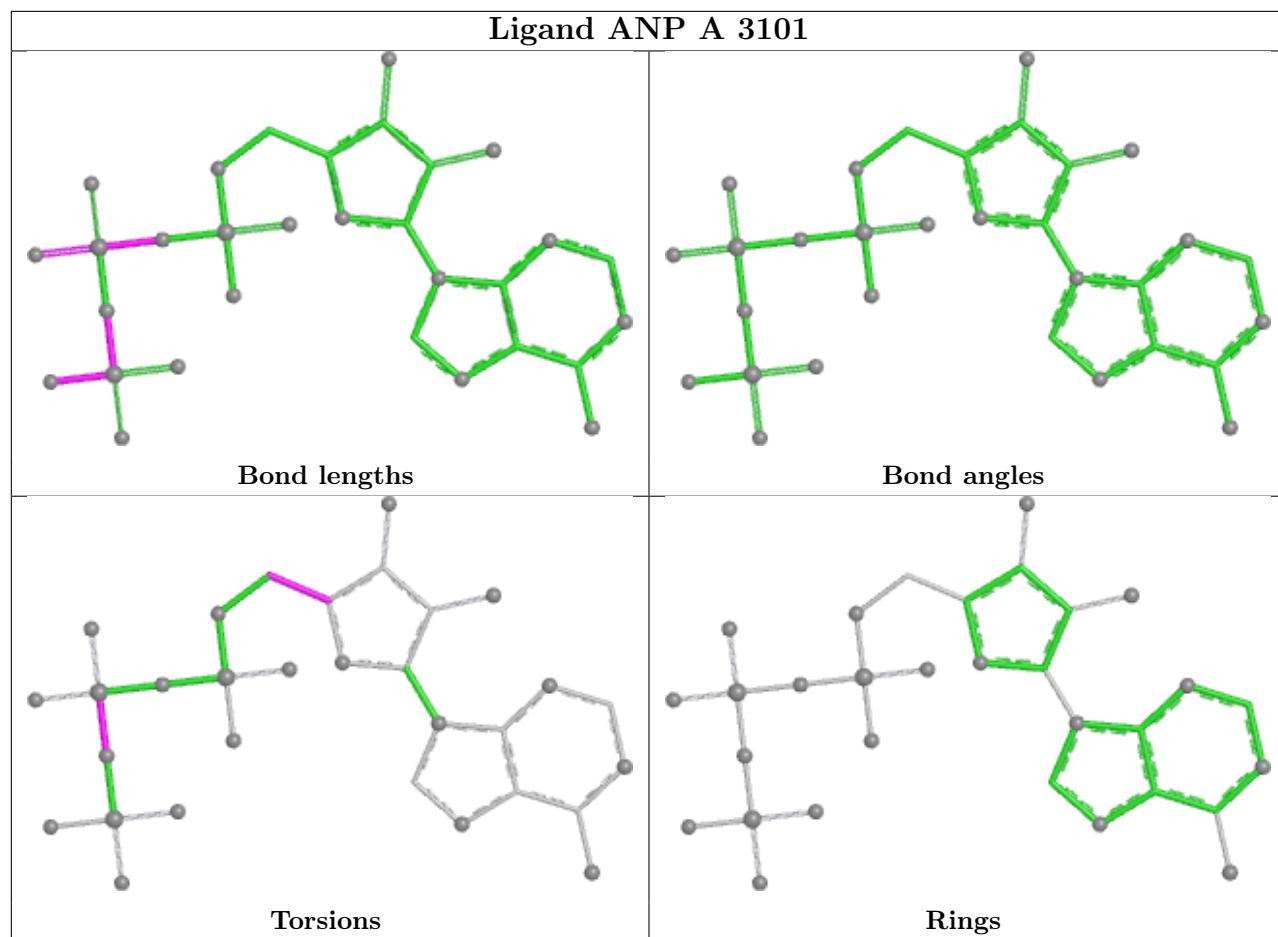
All (8) torsion outliers are listed below:

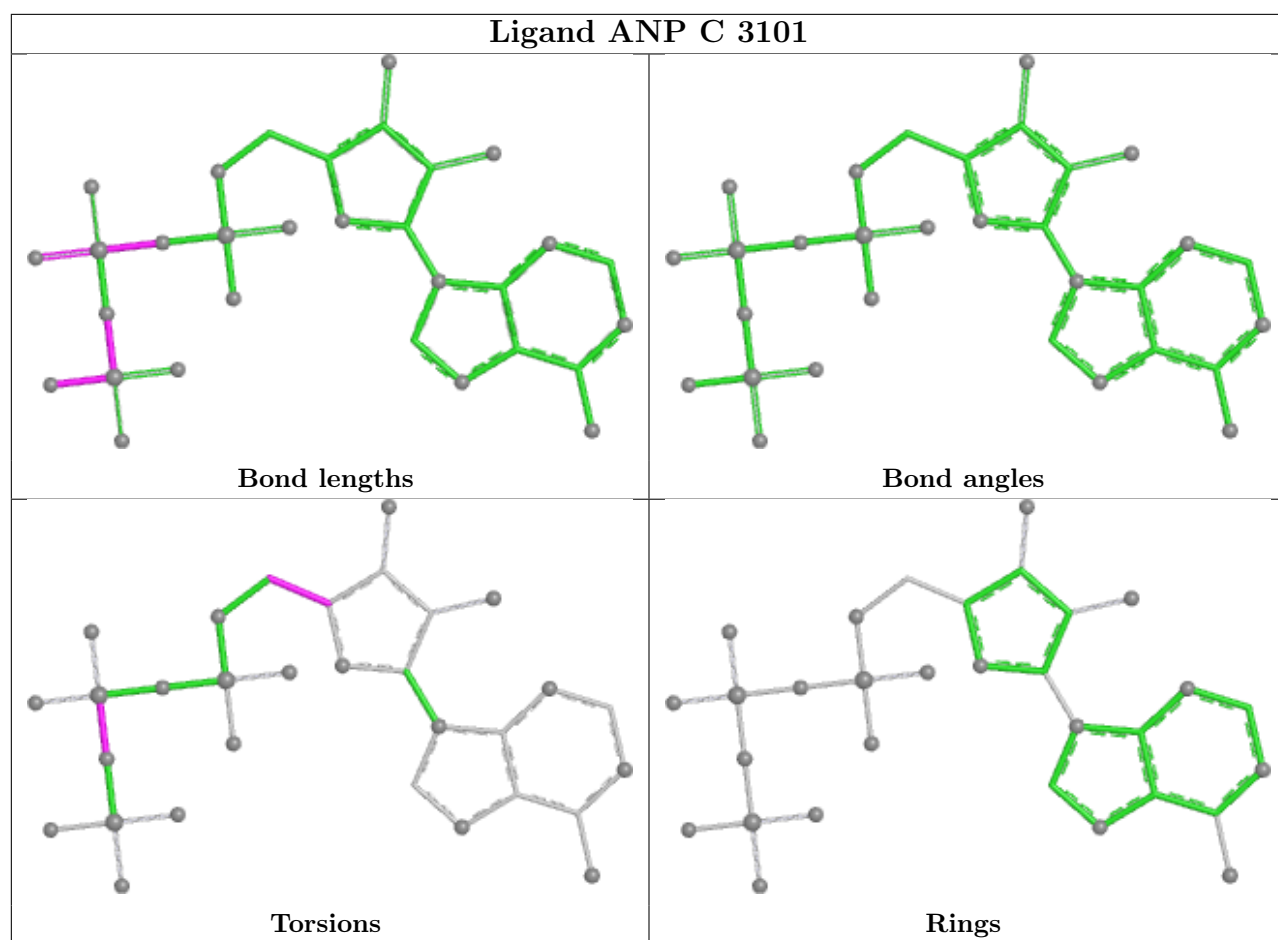
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PG-N3B-PB-O1B
3	C	3101	ANP	PG-N3B-PB-O1B
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	C	3101	ANP	O4'-C4'-C5'-O5'
3	C	3101	ANP	C3'-C4'-C5'-O5'
3	A	3101	ANP	PG-N3B-PB-O3A
3	C	3101	ANP	PG-N3B-PB-O3A

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.

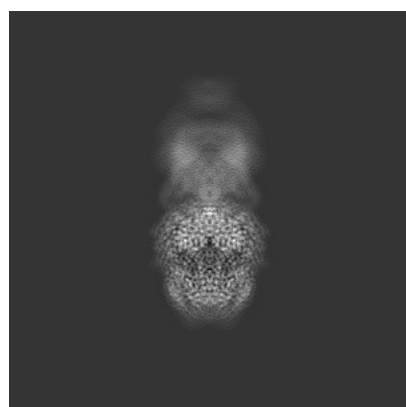
6 Map visualisation [i](#)

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.

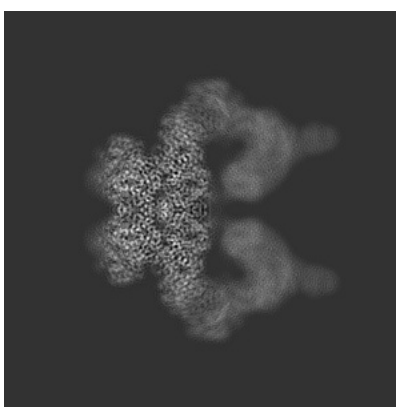
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

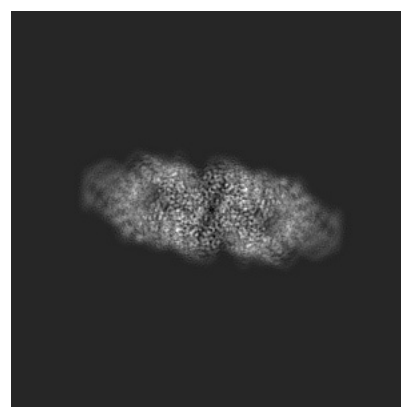
6.1.1 Primary map



X



Y

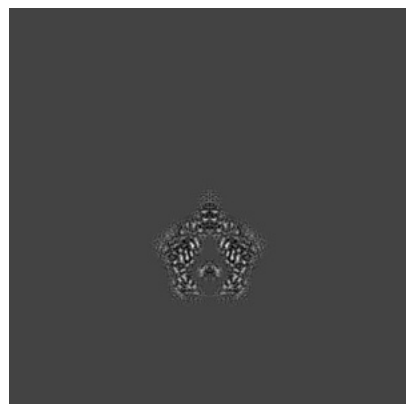


Z

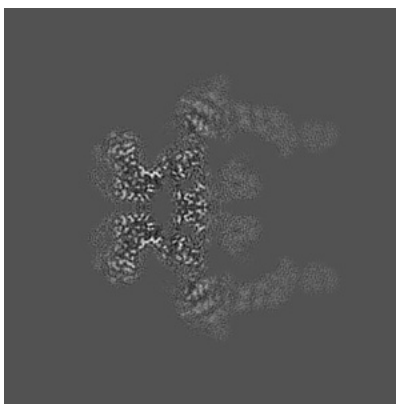
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

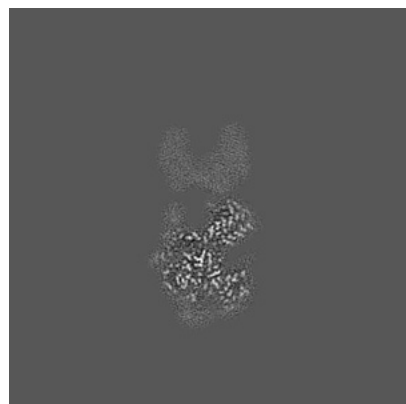


Z Index: 150

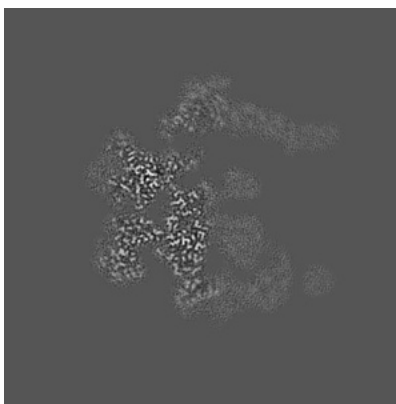
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

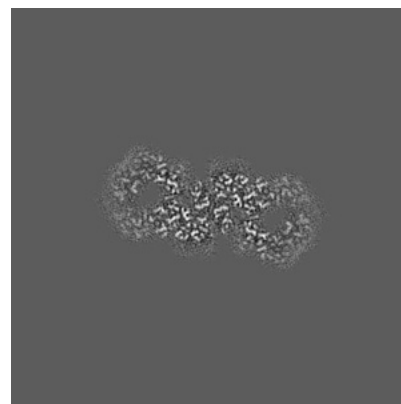
6.3.1 Primary map



X Index: 175



Y Index: 144

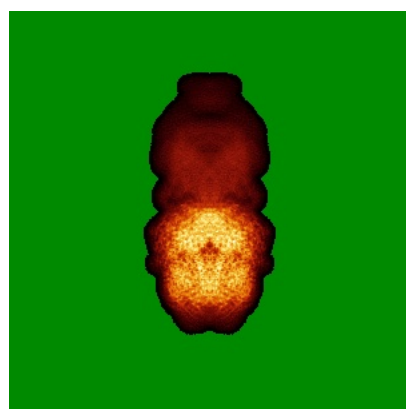


Z Index: 131

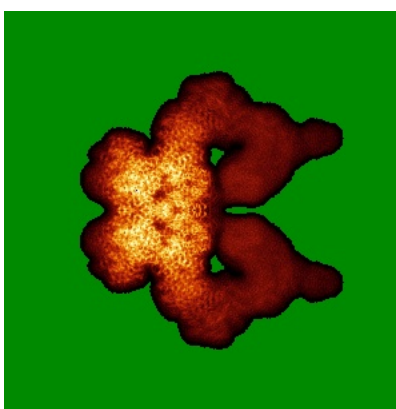
The images above show the largest variance slices of the map in three orthogonal directions.

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

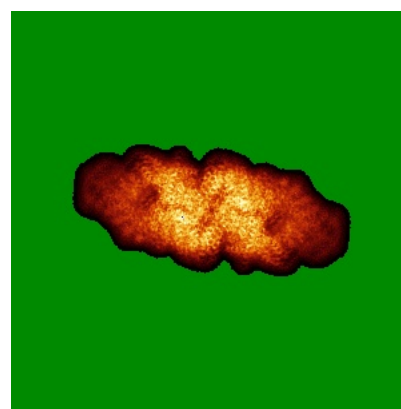
6.4.1 Primary map



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

This section was not generated.

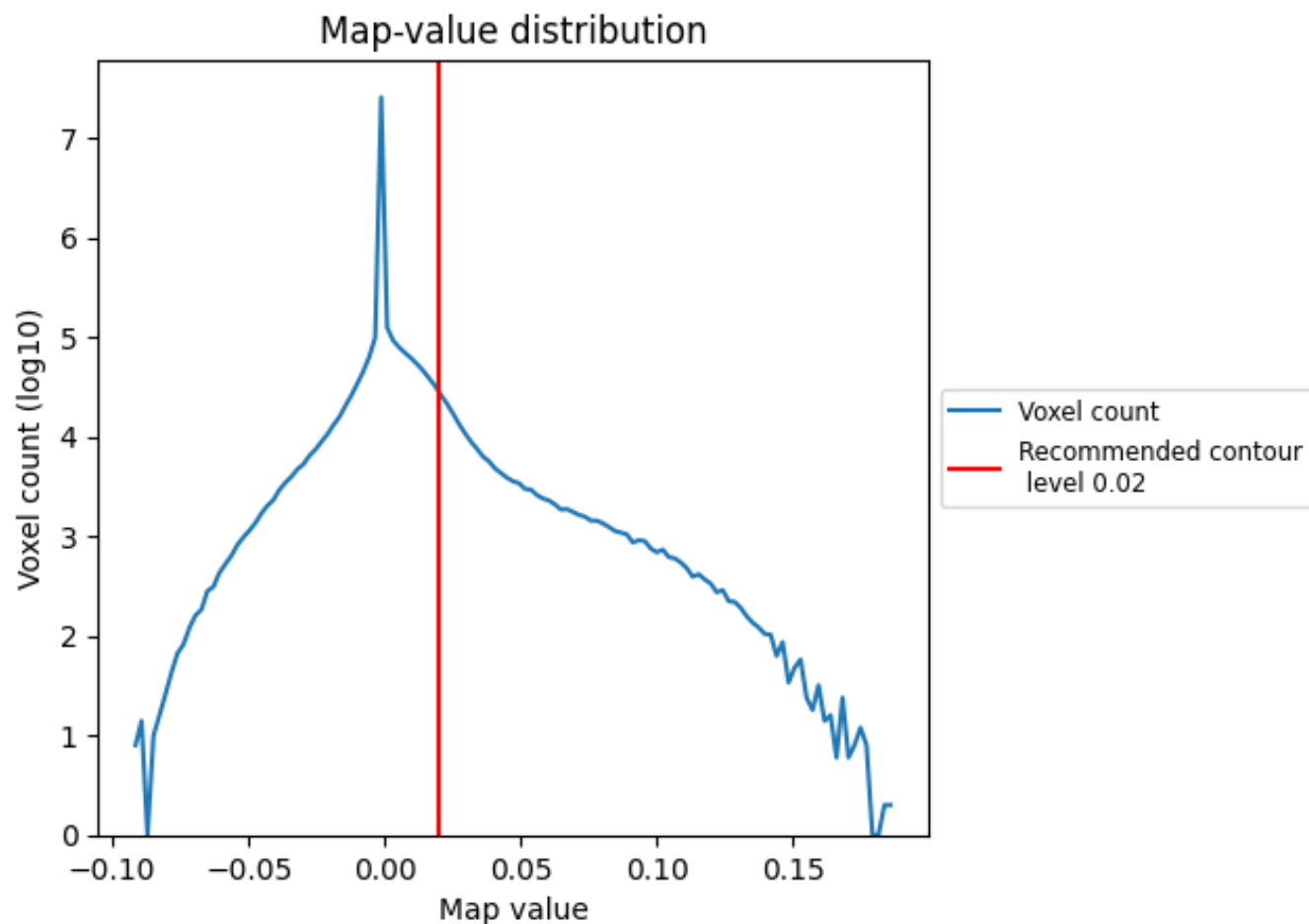
6.6 Mask visualisation

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

7 Map analysis [i](#)

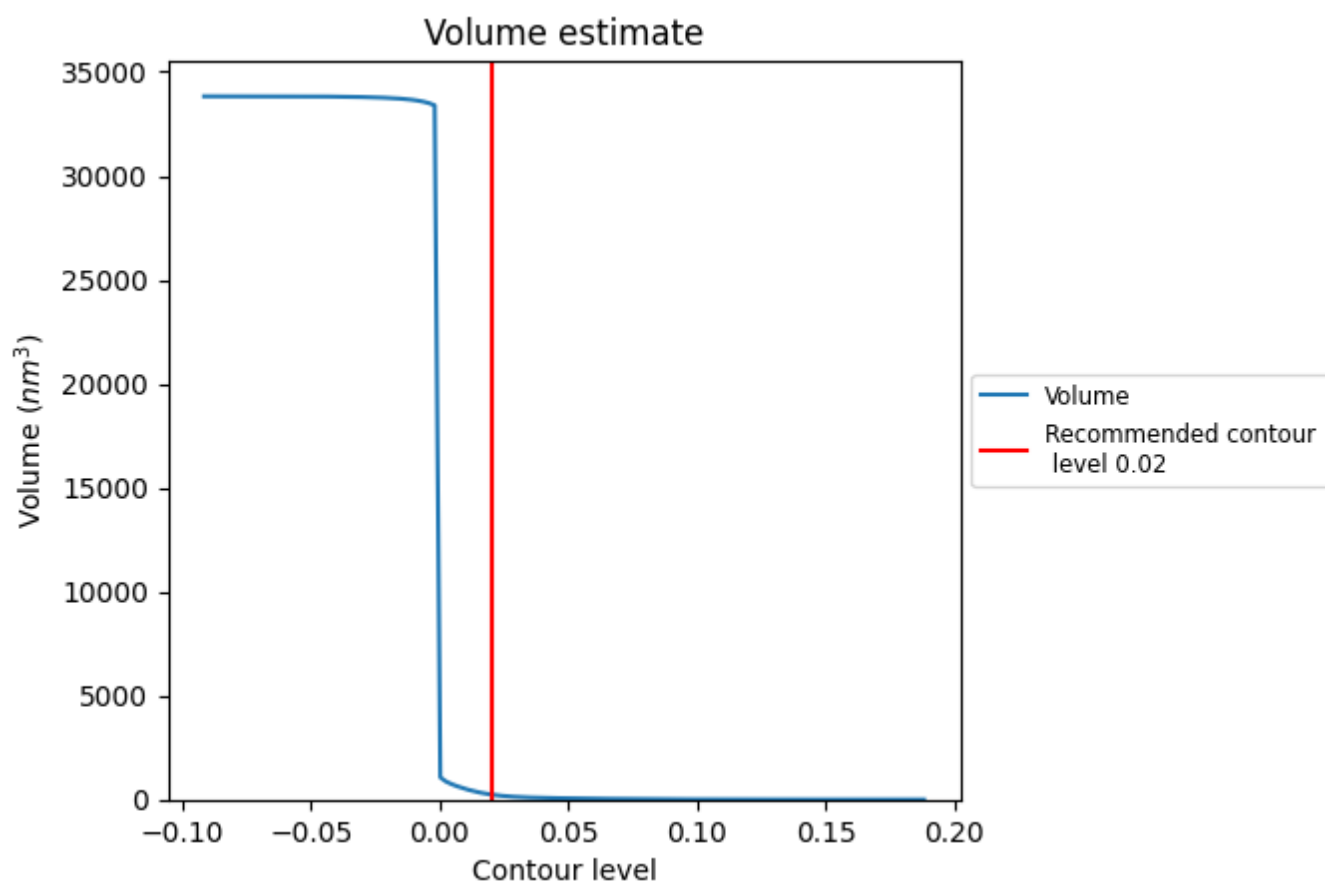
This section contains the results of statistical analysis of the map.

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.

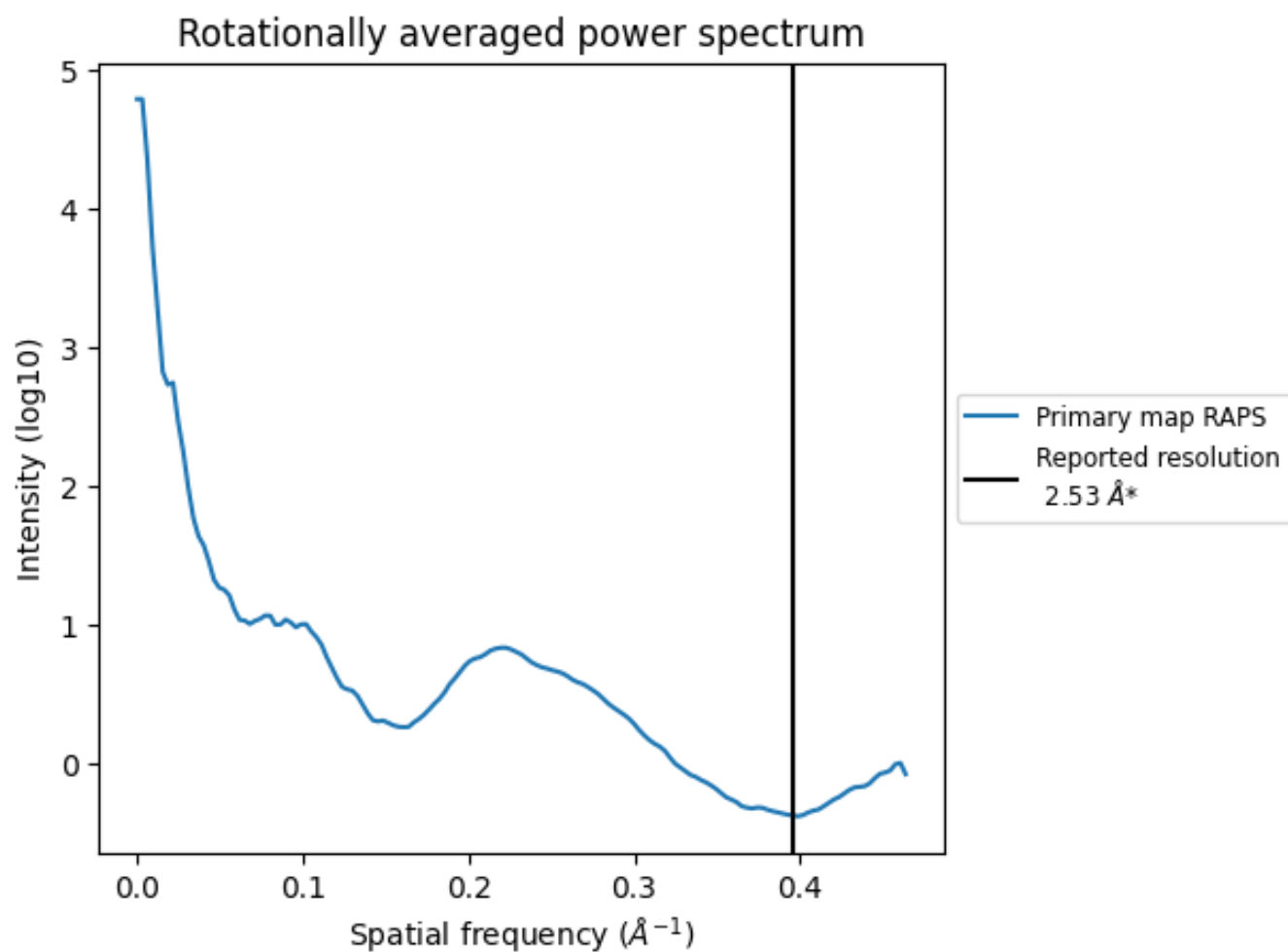
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 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 ⓘ

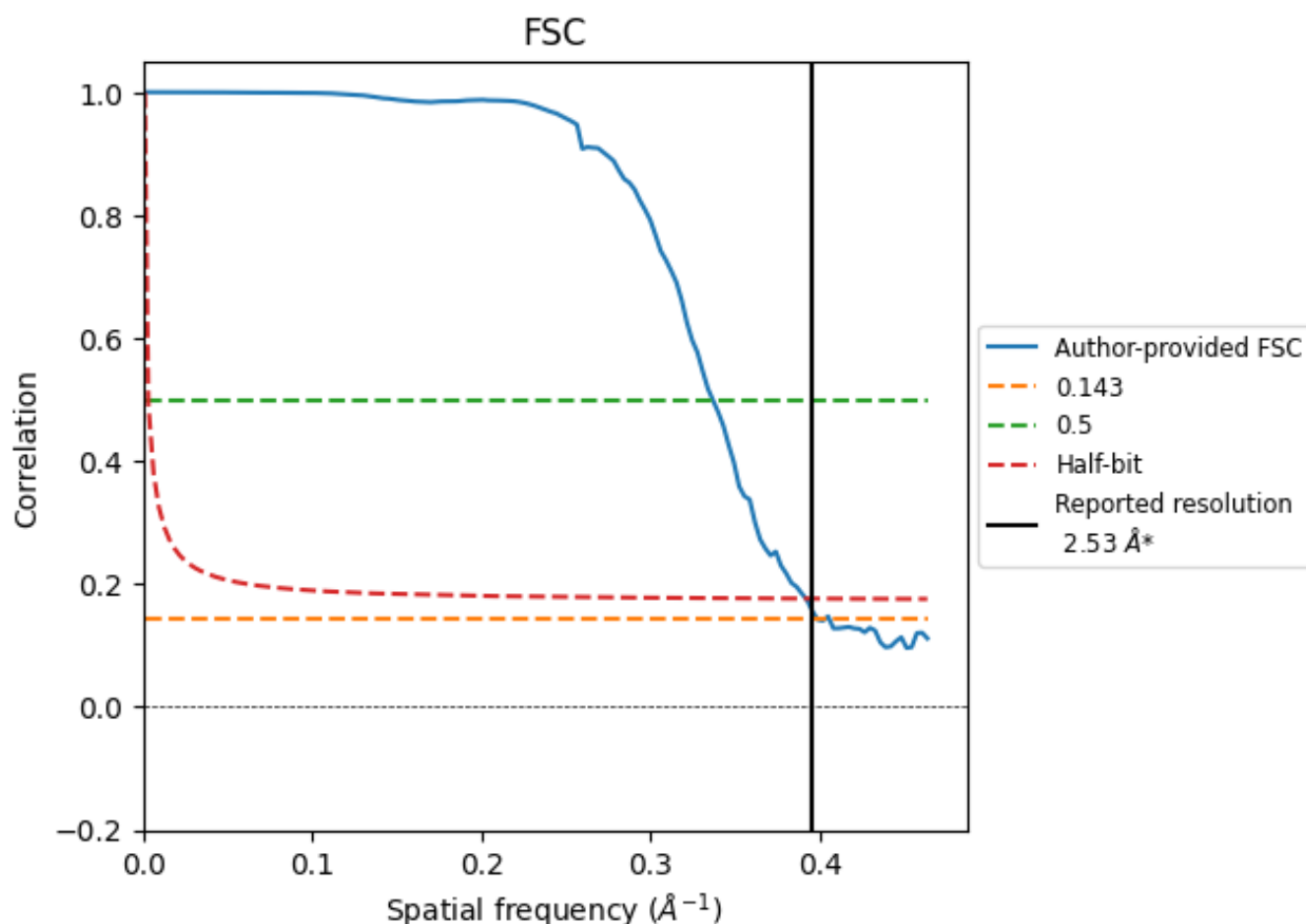


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 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.

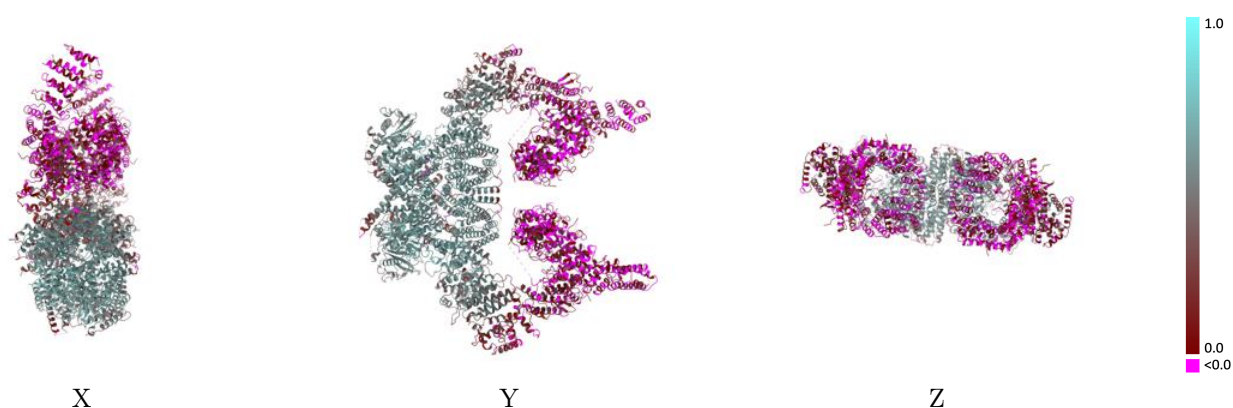
9 Map-model fit [i](#)

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](#)

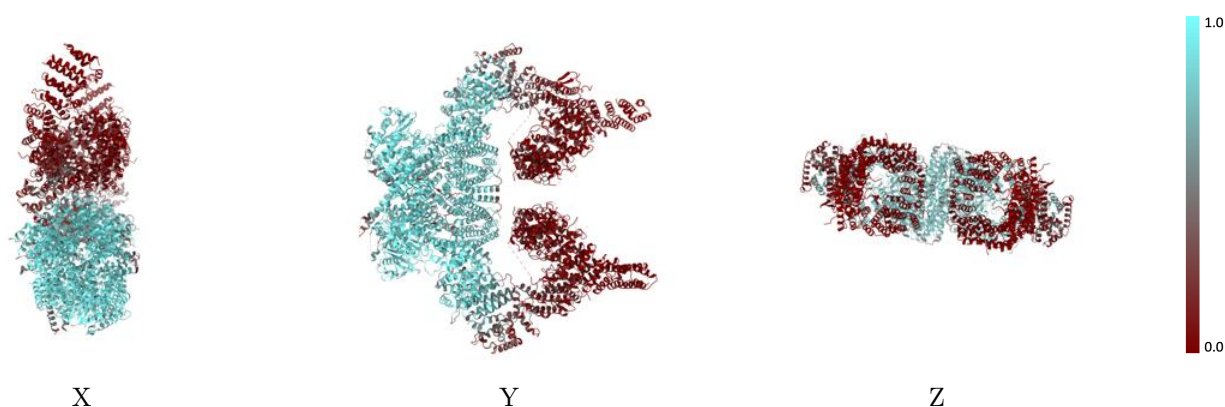
This section was not generated.

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



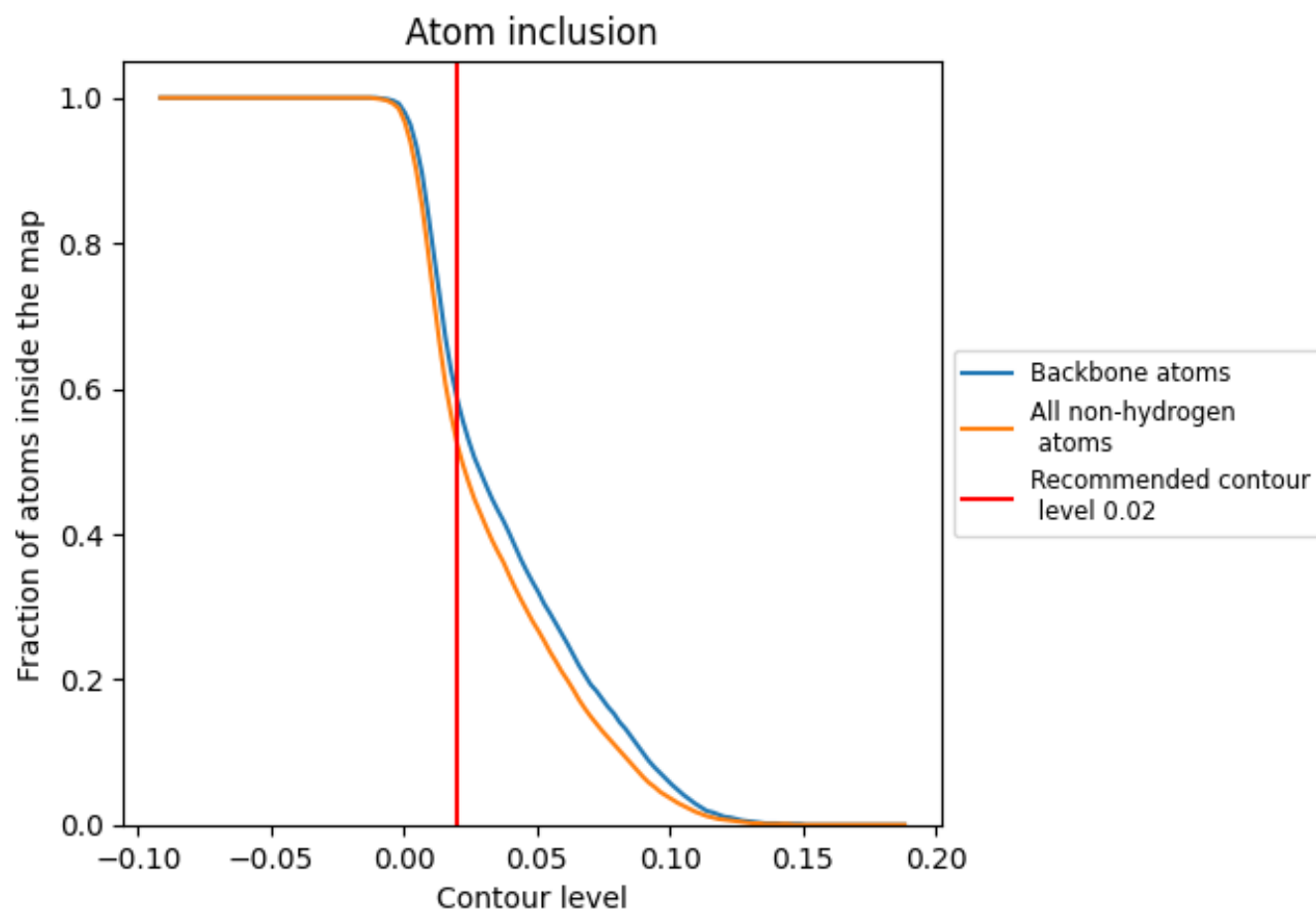
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.5240	0.3360
A	0.5260	0.3370
B	0.0250	0.0430
C	0.5260	0.3380
D	0.0250	0.0470

