



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:10 PM UTC

PDB ID : 7SIC / pdb_00007sic
EMDB ID : EMD-25140
Title : Human ATM Dimer
Authors : Warren, C.; Pavletich, N.P.
Deposited on : 2021-10-13
Resolution : 2.51 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

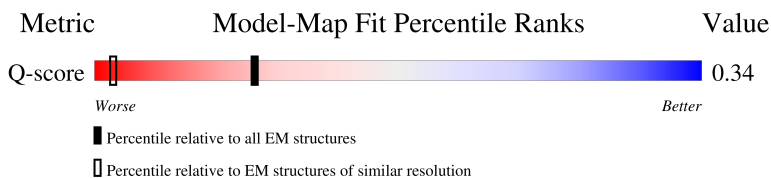
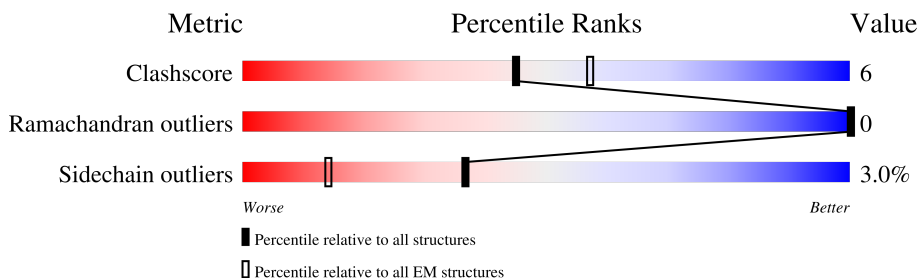
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.51 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	7159 (2.01 - 3.01)

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	44% 75% 16% 9%
1	B	3056	44% 75% 15% 9%

2 Entry composition [i](#)

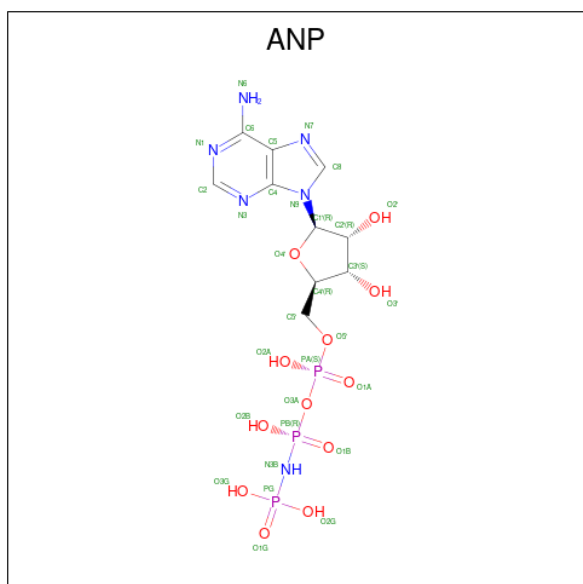
There are 3 unique types of molecules in this entry. The entry contains 44484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	B	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		

- Molecule 2 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
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

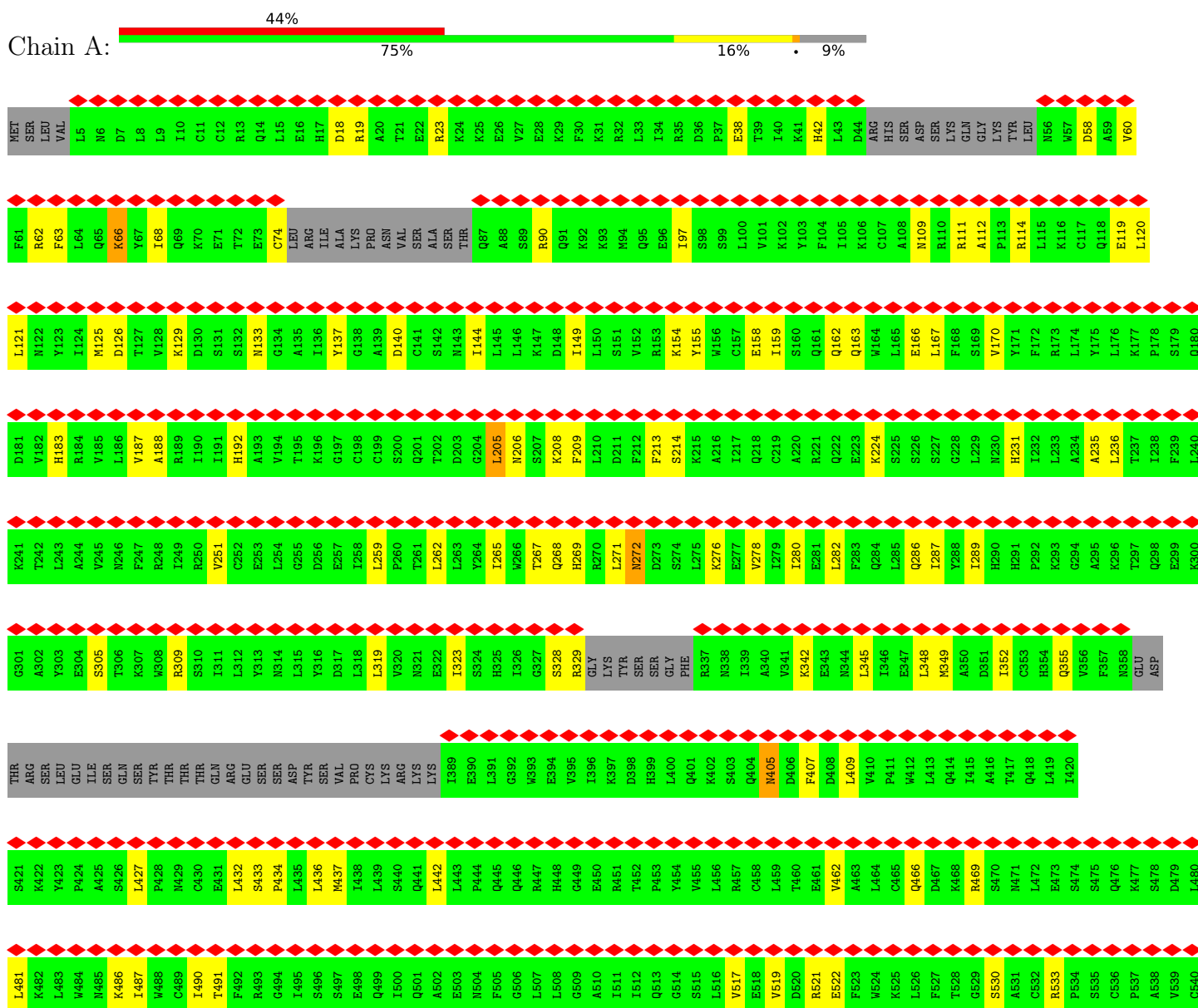
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Mg 1	0
3	B	1	Total 1	Mg 1	0

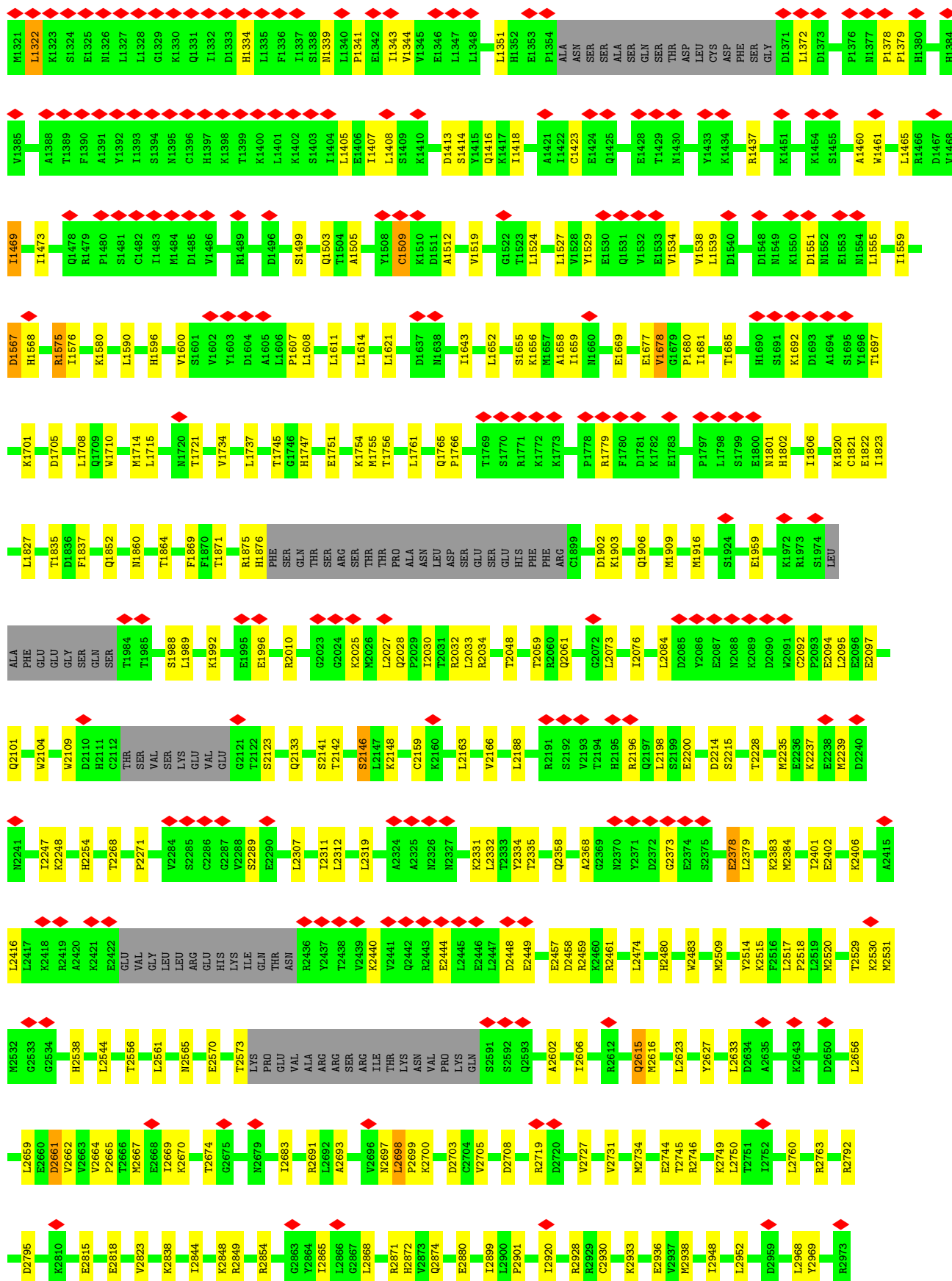
3 Residue-property plots

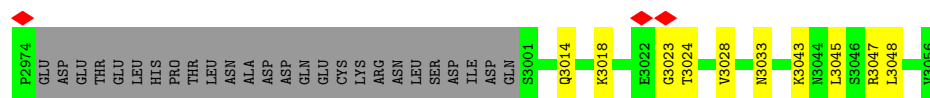
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

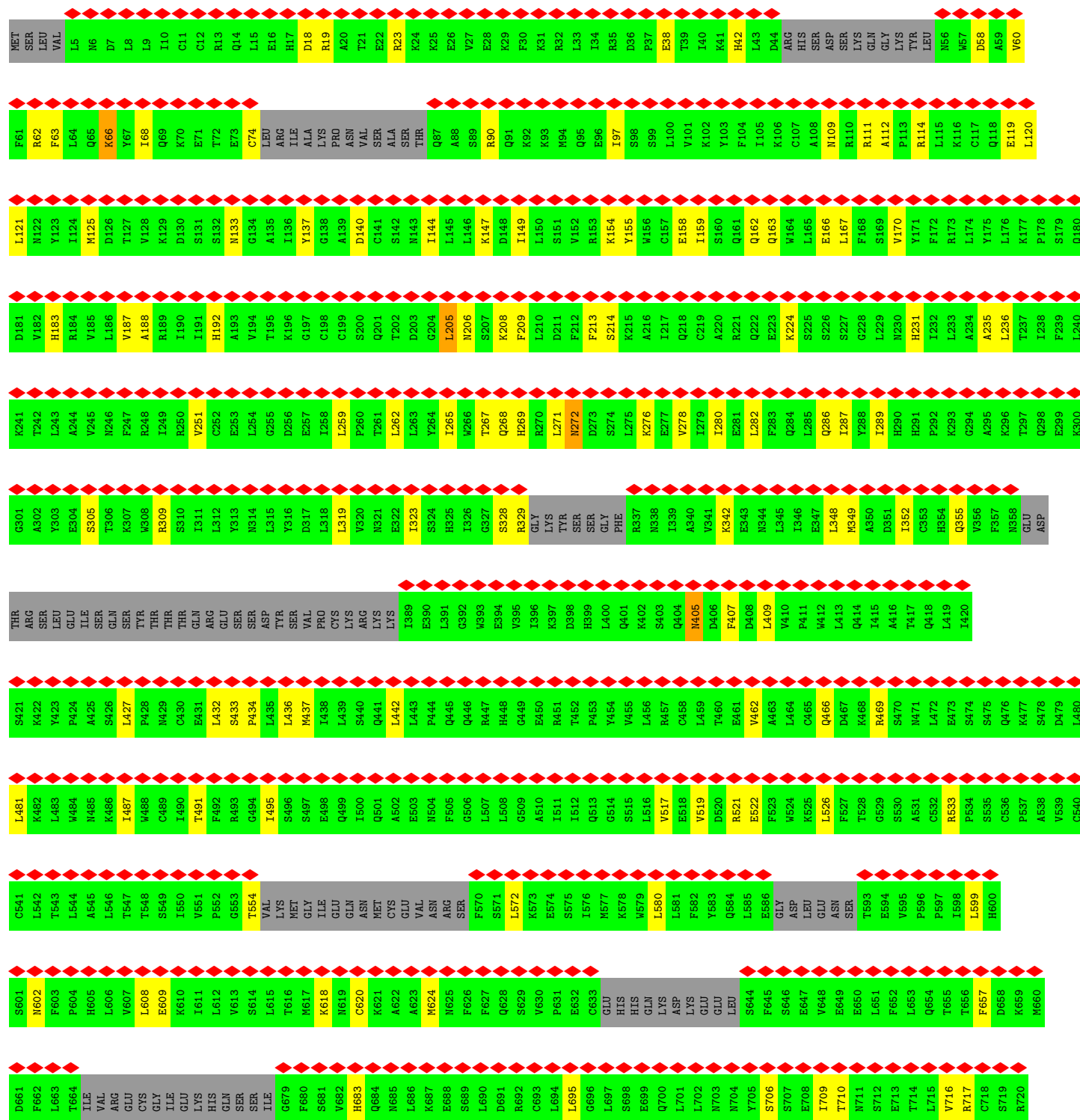
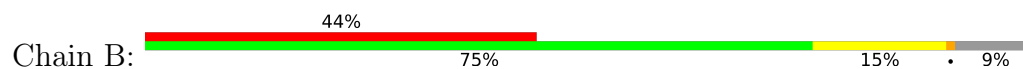


I1261	R1262	S1263	H1264	F1265	D1266	E1267	V1268	K1269	S1270	I1271	A1272	M1273	K1274	I1275	Q1276	E1277	D1278	W1279	K1280	S1281	L1282	L1283	T1284	D1285	C1286	D1287	F1288	P1289	K1290	I1291	V1292	I1293	L1294	L1295	P1296	Y1297	F1298	A1299	Y1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	R1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320
F1201	G1202	Y1203	R1204	R1205	L1206	E1207	D1208	F1209	M1210	A1211	S1212	H1213	L1214	D1215	Y1216	L1217	V1218	E1219	E1220	W1221	L1222	N1223	L1224	Q1225	D1226	T1227	E1228	Y1229	K1230	L1231	S1232	S1233	F1234	P1235	F1236	I1237	L1238	L1239	N1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	Y1248	R1249	S1250	C1251	K1252	K1253	V1254	L1255	P1256	P1257	H1258	L1259	V1260
N1081	H1082	Q1084	V1085	R1086	M1087	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	M1122	A1123	Y1124	G1125	L1126	A1127	Q1128	E1129	G1130	M1131	R1132	E1133	M1134	SER	HIS	SER	ALA	GLU	ASN	
PRO	E1142	T1143	D1145	E1146	T1147	Y1148	M1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	V1161	L1162	S1163	C1164	S1165	P1166	I1167	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	N1183	G1184	L1185	E1186	P1187	H1188	L1189	V1190	K1191	K1192	V1193	L1194	E1195	K1196	V1197	S1198	E1199	T1200	
N1081	H1082	Q1084	V1085	R1086	M1087	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	M1122	A1123	Y1124	G1125	L1126	A1127	Q1128	E1129	G1130	M1131	R1132	E1133	M1134	SER	HIS	SER	ALA	GLU	ASN	
PRO	E1142	T1143	D1145	E1146	T1147	Y1148	M1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	V1161	L1162	S1163	C1164	S1165	P1166	I1167	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	N1183	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	S1212	H1213	L1214	D1215	Y1216	L1217	V1218	E1219	E1220	W1221	L1222	N1223	L1224	Q1225	D1226	T1227	E1228	Y1229	K1230	L1231	S1232	S1233	F1234	P1235	F1236	I1237	L1238	L1239	N1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	Y1248	R1249	S1250	C1251	K1252	K1253	V1254	L1255	P1256	P1257	H1258	L1259	V1260
C541	L542	T543	L544	A545	L546	T547	T548	S549	I550	V551	P552	G553	T554	VAL	LYS	MET	GLY	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	
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	E632	C633	GLU	HIS	HIS	GLN	LYS	ASP	LYS	GLU	GLU	LEU	S644	F645	S646	E647	V648	E649	E650	L651	F652	L653	Q654	T655	T656	F657	D658	K659	M660
D661	F662	L663	T664	ILE	VAL	ARG	GLU	CYS	GLY	ILE	GLU	LYS	HIS	GLN	SER	ILE	G679	F680	S681	V682	H683	Q684	A685	L686	K687	E688	S689	L690	D691	R692	C693	L694	L695	G696	L697	S698	E699	Q700	L701	L702	N703	N704	Y705	S706	S707	E708	I709	T710	N711	S712	E713	T714	L715	V716	R717	C718	S719	R720	
L721	L722	V723	G724	V725	L726	G727	G728	Y729	G730	Y731	M732	G733	V734	I735	A736	E737	E738	E739	A740	Y741	K742	S743	E744	L745	L746	Q747	K748	A749	K750	S751	L752	M753	Q754	C755	A756	G757	E758	S759	I760	T761	L762	F763	K764	N765	K766	T767	N768	E769	E770	F771	R772	I773	G774	S775	L776	R777	M779	M780	
Q781	L782	C783	T784	R785	C786	L787	S788	M789	C790	T791	K792	K793	S794	F795	N796	K797	I798	A799	S800	G801	F802	F803	L804	R805	L806	L807	T808	S809	K810	L811	M812	N813	D814	I815	A816	D817	I818	C819	K820	S821	A823	S824	F825	I826	LYS	LYS	PRO	PHE	ASP	ARG	GLY	GLU	VAL	SER	MET	GLU	ASP		
ASP	THR	ASN	GLY	ASN	LEU	MET	GLU	GLU	GLN	SER	MET	ASN	PHE	ASN	ASP	TYR	PRO	ASP	SER	VAL	SER	ALA	ASN	GLU	PRO	GLY	GLU	SER	GLN	S877	T878	I879	G880	A881	I882	N883	P884	L885	A886	E887	E888	Y889	L890	S891	K892	Q893	D894	L895	L896	F897	L898	D899	M900						
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	I990	L991	N992	H993	V994	L995	H996	V997	V998	K999	M1000	L1001	G1002	Q1003	S1004	M1005	M1006	D1007	S1008	E1009	M1010	T1011	R1012	D1013	A1014	Q1015	G1016	Q1017	F1018	L1019	T1020
V1021	T1022	G1023	A1024	F1025	W1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	T1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	N1044	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	D1053	P1054	Y1055	S1056	K1057	W1058	A1059	L1060	L1061	N1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	V1070	M1071	E1072	V1073	F1074	T1075	Q1076	F1077	L1078	A1079	D1080
N1081	H1082	Q1084	V1085	R1086	M1087	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	M1122	A1123	Y1124	G1125	L1126	A1127	Q1128	E1129	G1130	M1131	R1132	E1133	M1134	SER	HIS	SER	ALA	GLU	ASN	
PRO	E1142	T1143	L1144	D1145	E1146	T1147	Y1148	M1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	V1161	L1162	S1163	C1164	S1165	P1166	I1167	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	N1183	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	S1212	H1213	L1214	D1215	Y1216	L1217	V1218	E1219	E1220	W1221	L1222	N1223	L1224	Q1225	D1226	T1227	E1228	Y1229	K1230	L1231	S1232	S1233	F1234	P1235	F1236	I1237	L1238	L1239	N1240	Y1241	T1242	N1243	I1244	E1245	D1246	F1247	Y1248	R1249	S1250	C1251	K1252	K1253	V1254	L1255	P1256	P1257	H1258	L1259	V1260
I1261	R1262	S1263	H1264	F1265	D1266	E1267	V1268	K1269	S1270	I1271	A1272	M1273	K1274	I1275	Q1276	E1277	D1278	W1279	K1280	S1281	L1282	L1283	T1284	D1285	C1286	D1287	F1288	P1289	K1290	I1291	V1292	I1293	L1294	L1295	P1296	Y1297	F1298	A1299	Y1300	E1301	G1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	R1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320

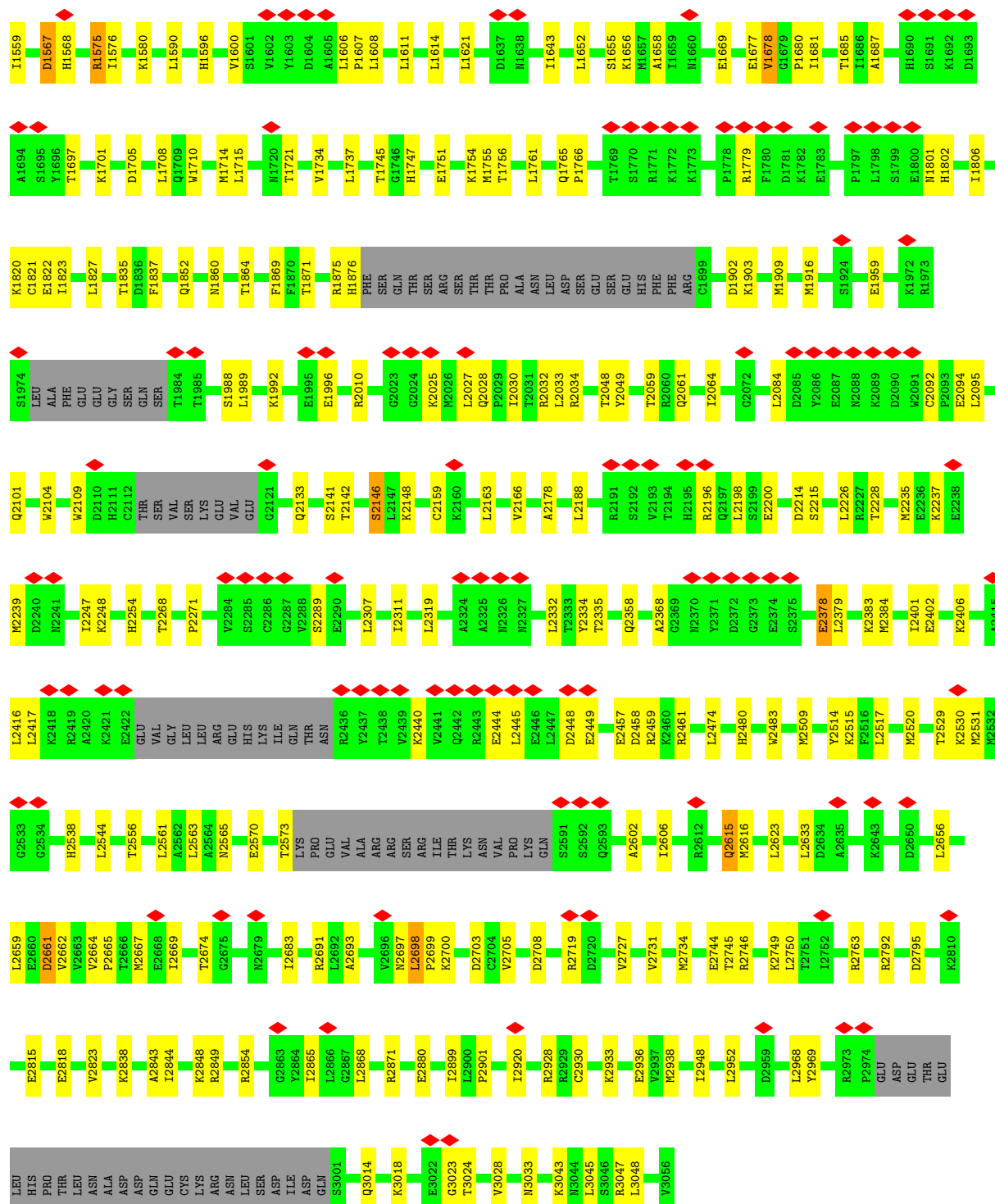




● Molecule 1: Serine-protein kinase ATM



I1469	I1473	Q1478	R1479	P1480	A1391	Y1392	I1393	S1394	F1329	K1330	Q1331	I1332	D1333	H1334	L1335	F1336	I1337	S1338	M1339	L1340	P1341	E1342	I1343	V1344	V1345	E1346	L1347	L1348	L1351	H1352	E1353	P1354	ALA	ASN	SER	SER	ALA	SER	GLN	THR	ASP	LEU	CYS	PHE	SER	GLY	D1371	L1372	D1373	P1376	N1377	P1378	P1379	H1380	H1384									
V1385	A1388	T1389	F1390	A1391	Y1392	L1393	S1394	N1395	C1396	H1397	K1398	T1399	K1400	L1401	K1402	S1403	I1404	L1405	E1406	I1407	L1408	S1409	K1410	D1413	Y1415	Q1416	I1417	I1418	A1421	I1422	C1423	E1424	Q1425	E1428	T1429	N1430	Y1433	K1434	R1437	K1451	K1454	S1455	A1460	W1461	L1465	R1466	V1468																	
I1469	I1473	Q1478	R1479	P1480	A1391	Y1392	I1393	S1394	F1329	K1330	Q1331	I1332	D1333	H1334	L1335	F1336	I1337	S1338	M1339	L1340	P1341	E1342	I1343	V1344	V1345	E1346	L1347	L1348	L1351	H1352	E1353	P1354	ALA	ASN	SER	SER	ALA	SER	GLN	THR	ASP	LEU	CYS	PHE	SER	GLY	D1371	L1372	D1373	P1376	N1377	P1378	P1379	H1380	H1384									
V1385	A1388	T1389	F1390	A1391	Y1392	L1393	S1394	N1395	C1396	H1397	K1398	T1399	K1400	L1401	K1402	S1403	I1404	L1405	E1406	I1407	L1408	S1409	K1410	D1413	Y1415	Q1416	I1417	I1418	A1421	I1422	C1423	E1424	Q1425	E1428	T1429	N1430	Y1433	K1434	R1437	K1451	K1454	S1455	A1460	W1461	L1465	R1466	V1468																	
Q781	L782	C783	T784	R785	C786	L787	S788	N789	C790	Y791	K792	K793	S794	P795	N796	K797	I798	A799	S800	G801	ASP	F802	F803	L804	R805	L806	L807	T808	S809	K810	L811	M812	N813	D814	I815	P884	A816	L885	D817	I818	C819	K820	S821	L822	A823	S824	F825	I826	LVS	LVS	PRO	PHE	ASP	ARG	GLY	GLU	VAL	GLU	SER	MET	GLU	ASP		
ASP	THR	ASN	GLY	ASN	LEU	MET	GLU	VAL	GLU	ASP	GLN	SER	SER	ASN	PHE	ASN	ASP	TYR	PRO	ASP	SER	SER	VAL	SER	ASP	ALA	ASN	GLU	PRO	GLY	SER	GLN	S877	T878	I879	G880	A881	I882	S934	T935	L936	E937	P938	T939	K940	S941	L942	L943	L944	H945	M946	Y947	L948	M949	L950	L951	K952	E953	P955	G956	E957	E958	Y959	P960
L961	P962	M963	E964	C965	V966	L967	E968	L969	L970	K971	P972	L973	S974	M975	V976	S977	L979	Y980	A981	D982	D983	Q984	D985	V986	C987	K988	T989	L990	L991	N992	H993	L994	H996	V997	V998	K999	M1000	L1001	G1002	Q1003	S1004	N1005	M1006	D1007	S1008	E1009	M1010	T1011	R1012	D1013	A1014	Q1015	G1016	Q1017	F1018	L1019	T1020							
V1021	I1022	G1023	A1024	F1025	V1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	S1037	V1038	R1039	M1040	A1041	L1042	V1043	N1044	C1045	L1046	K1047	T1048	L1049	E1051	A1052	D1053	P1054	Y1055	S1056	K1057	W1058	A1059	T1060	L1061	N1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	V1070	N1071	E1072	F1073	T1074	T1075	Q1076	F1077	L1078	A1079	D1080						
M1081	H1082	Q1083	Q1084	V1085	M1086	M1087	L1088	A1089	A1090	E1091	S1092	I1093	M1094	R1095	L1096	F1097	Q1098	D1099	T1100	K1101	GLY	ASP	SER	ARG	LEU	L1108	K1109	A1110	L1111	P1112	L1113	K1114	L1115	Q1116	Q1117	T1118	A1119	F1120	E1121	M1122	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	Y1148	N1149	R1150	K1151	S1152	V1153	L1154	L1155	T1156	L1157	I1158	A1159	V1160	V1161	L1162	S1163	C1164	S1165	P1166	I1167	C1168	E1169	K1170	Q1171	A1172	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	M1183	G1184	L1185	E1186	P1187	H1188	L1189	V1190	K1191	L1192	V1193	L1194	E1195	K1196	V1197	S1198	T1200						
F1201	G1202	Y1203	R1204	L1205	L1206	E1207	D1208	F1209	M1210	A1211	H1212	H1213	L1214	D1215	Y1216	L1217	V1218	E1219	W1220	S1221	L1222	N1223	L1224	Q1225	D1226	T1227	E1228	N1229	L1230	L1231	S1232	S1233	F1234	P1235	F1236	I1237	L1238	F1239	Y1240	E1241	G1242	T1243	I1244	E1245	D1246	F1247	N1248	S1249	C1250	Q1251	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320			
I1261	R1262	S1263	H1264	F1265	D1266	E1267	V1268	K1269	S1270	I1271	A1272	N1273	N1274	Q1275	I1276	E1277	I1278	W1279	K1280	S1281	L1282	L1283	T1284	D1285	C1286	F1287	P1288	K1289	I1290	L1291	N1292	N1293	I1294	L1295	P1296	Y1297	F1298	A1299	Y1300	E1301	S1302	T1303	R1304	D1305	S1306	G1307	M1308	A1309	Q1310	Q1311	R1312	E1313	T1314	A1315	T1316	K1317	V1318	Y1319	D1320					
M1321	L1322	K1323	S1324	N1325	L1326	L1327	L1328	G1329	K1330	Q1331	M1332	D1333	H1334	L1335	F1336	I1337	S1338	M1339	L1340	P1341	E1342	I1343	V1344	V1345	E1346	L1347	L1348	L1351	H1352	E1353	P1354	ALA	ASN	SER	SER	ALA	SER	GLN	THR	ASP	LEU	CYS	PHE	SER	GLY	D1371	L1372	D1373	P1376	N1377	P1378	P1379	H1380	H1384										
V1385	A1388	T1389	F1390	A1391	Y1392	L1393	S1394	N1395	C1396	H1397	K1398	T1399	K1400	L1401	K1402	S1403	I1404	L1405	E1406	I1407	L1408	S1409	K1410	D1413	Y1415	Q1416	I1417	I1418	A1421	I1422	C1423	E1424	Q1425	E1428	T1429	N1430	Y1433	K1434	R1437	K1451	K1454	S1455	A1460	W1461	L1465	R1466	V1468																	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	303604	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 ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/22624	0.30	0/30565
1	B	0.11	0/22624	0.30	0/30565
All	All	0.11	0/45248	0.30	0/61130

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22210	0	22392	292	0
1	B	22210	0	22392	286	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	44484	0	44810	566	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 6.

All (566) 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:B:1312:ARG:HG3	1:B:1312:ARG:HH11	1.31	0.95
1:A:1312:ARG:HG3	1:A:1312:ARG:HH11	1.31	0.93
1:B:2458:ASP:OD1	1:B:2461:ARG:NH2	2.23	0.71
1:B:1509:CYS:HB2	1:B:1512:ALA:HB2	1.73	0.71
1:A:1509:CYS:HB2	1:A:1512:ALA:HB2	1.73	0.71
1:A:272:ASN:OD1	1:A:272:ASN:N	2.19	0.70
1:A:2458:ASP:OD1	1:A:2461:ARG:NH2	2.23	0.70
1:A:1988:SER:OG	1:A:1992:LYS:NZ	2.26	0.69
1:B:1988:SER:OG	1:B:1992:LYS:NZ	2.26	0.69
1:B:63:PHE:HD1	1:B:66:LYS:HZ1	1.41	0.68
1:B:272:ASN:OD1	1:B:272:ASN:N	2.19	0.68
1:A:2480:HIS:HB3	1:A:2483:TRP:HD1	1.58	0.68
1:A:2061:GLN:HG2	1:A:2084:LEU:HD21	1.76	0.67
1:A:3043:LYS:HE3	1:A:3047:ARG:NH2	2.10	0.67
1:B:2480:HIS:HB3	1:B:2483:TRP:HD1	1.58	0.67
1:B:1685:THR:HG23	1:B:2166:VAL:HG21	1.76	0.67
1:B:3043:LYS:HE3	1:B:3047:ARG:NH2	2.10	0.67
1:A:1685:THR:HG23	1:A:2166:VAL:HG21	1.76	0.67
1:A:2030:ILE:HD12	1:A:2030:ILE:H	1.60	0.67
1:B:2061:GLN:HG2	1:B:2084:LEU:HD21	1.76	0.67
1:B:2030:ILE:HD12	1:B:2030:ILE:H	1.60	0.66
1:A:319:LEU:HD23	1:A:349:MET:HG2	1.78	0.66
1:A:427:LEU:O	1:A:469:ARG:NH2	2.25	0.66
1:A:1131:MET:HG2	1:A:1150:ARG:HB3	1.76	0.66
1:B:319:LEU:HD23	1:B:349:MET:HG2	1.78	0.66
1:B:1131:MET:HG2	1:B:1150:ARG:HB3	1.76	0.66
1:A:329:ARG:NH2	1:A:407:PHE:O	2.29	0.65
1:B:329:ARG:NH2	1:B:407:PHE:O	2.29	0.65
1:A:1290:ILE:O	1:A:1294:ILE:HD12	1.97	0.65
1:A:1294:ILE:HG23	1:A:1315:ALA:HB1	1.79	0.65
1:A:2969:TYR:OH	2:A:3101:ANP:O2G	2.15	0.64
1:B:1310:GLN:HE21	1:B:1311:GLN:HE21	1.45	0.64
1:A:1310:GLN:HE21	1:A:1311:GLN:HE21	1.45	0.64
1:B:1290:ILE:O	1:B:1294:ILE:HD12	1.97	0.64
1:B:1223:ASN:OD1	1:B:1262:ARG:NH2	2.32	0.63
1:B:1294:ILE:HG23	1:B:1315:ALA:HB1	1.79	0.63
1:A:1215:ASP:OD2	1:A:1258:HIS:NE2	2.28	0.63
1:B:602:ASN:OD1	1:B:717:ARG:NH1	2.32	0.63
1:B:2368:ALA:HB1	1:B:2383:LYS:HG2	1.80	0.62
1:B:1747:HIS:O	1:B:1751:GLU:HG2	1.99	0.62
1:B:68:ILE:HD12	1:B:97:ILE:HD12	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2744:GLU:HG2	1:B:2933:LYS:HD2	1.81	0.62
1:A:2368:ALA:HB1	1:A:2383:LYS:HG2	1.80	0.62
1:A:2744:GLU:HG2	1:A:2933:LYS:HD2	1.81	0.62
1:A:1223:ASN:OD1	1:A:1262:ARG:NH2	2.32	0.62
1:A:1294:ILE:HG21	1:A:1319:TYR:HB2	1.82	0.62
1:A:1351:LEU:O	1:A:1437:ARG:NH1	2.32	0.62
1:B:1351:LEU:O	1:B:1437:ARG:NH1	2.32	0.62
1:A:1747:HIS:O	1:A:1751:GLU:HG2	1.99	0.61
1:B:2969:TYR:OH	2:B:3101:ANP:O2G	2.15	0.61
1:A:68:ILE:HD12	1:A:97:ILE:HD12	1.82	0.61
1:A:602:ASN:OD1	1:A:717:ARG:NH1	2.32	0.61
1:A:2142:THR:O	1:A:2146:SER:OG	2.19	0.61
1:B:1294:ILE:HG21	1:B:1319:TYR:HB2	1.82	0.60
1:B:2214:ASP:OD1	1:B:2746:ARG:NH1	2.34	0.60
1:A:2664:VAL:HB	1:A:2667:MET:HG3	1.84	0.60
1:A:2697:ASN:HD22	1:A:2719:ARG:HG3	1.66	0.60
1:A:2214:ASP:OD1	1:A:2746:ARG:NH1	2.34	0.60
1:B:2656:LEU:HD13	1:B:2659:LEU:HD11	1.84	0.60
1:B:2142:THR:O	1:B:2146:SER:OG	2.19	0.60
1:B:2378:GLU:OE1	1:B:2378:GLU:N	2.20	0.60
1:B:2697:ASN:HD22	1:B:2719:ARG:HG3	1.66	0.60
1:B:2401:ILE:HG21	1:B:2459:ARG:HB2	1.84	0.60
1:A:125:MET:HE2	1:A:125:MET:HA	1.84	0.59
1:A:1652:LEU:HD13	1:A:2163:LEU:HD21	1.84	0.59
1:B:1652:LEU:HD13	1:B:2163:LEU:HD21	1.84	0.59
1:B:2188:LEU:HD11	1:B:2198:LEU:HD22	1.85	0.59
1:A:3045:LEU:HA	1:A:3048:LEU:HD12	1.85	0.59
1:B:125:MET:HA	1:B:125:MET:HE2	1.84	0.59
1:B:1215:ASP:OD2	1:B:1258:HIS:NE2	2.28	0.59
1:A:2188:LEU:HD11	1:A:2198:LEU:HD22	1.85	0.59
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	1.84	0.59
1:B:2520:MET:HG2	1:B:2556:THR:HG22	1.85	0.59
1:A:2448:ASP:OD2	1:A:2449:GLU:N	2.36	0.59
1:B:2448:ASP:OD2	1:B:2449:GLU:N	2.36	0.59
1:B:2928:ARG:NH1	1:B:3033:ASN:OD1	2.35	0.59
1:A:1251:CYS:O	1:A:1255:LEU:HG	2.02	0.59
1:A:2520:MET:HG2	1:A:2556:THR:HG22	1.85	0.59
1:A:205:LEU:HD23	1:A:205:LEU:H	1.67	0.59
1:B:3045:LEU:HA	1:B:3048:LEU:HD12	1.85	0.59
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.35	0.58
1:A:1575:ARG:HB3	1:A:1575:ARG:HH11	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1916:MET:HE3	1:B:1916:MET:HA	1.86	0.58
1:B:2664:VAL:HB	1:B:2667:MET:HG3	1.84	0.58
1:A:2633:LEU:HB3	1:A:2700:LYS:HE2	1.85	0.58
1:A:2656:LEU:HD13	1:A:2659:LEU:HD11	1.84	0.58
1:A:618:LYS:HG2	1:A:683:HIS:CD2	2.39	0.58
1:B:1312:ARG:HG3	1:B:1312:ARG:NH1	2.07	0.58
1:B:1575:ARG:HH11	1:B:1575:ARG:HB3	1.68	0.58
1:B:618:LYS:HG2	1:B:683:HIS:CD2	2.39	0.58
1:B:1251:CYS:O	1:B:1255:LEU:HG	2.02	0.58
1:B:205:LEU:HD23	1:B:205:LEU:H	1.67	0.58
1:A:1916:MET:HE3	1:A:1916:MET:HA	1.86	0.57
1:B:427:LEU:O	1:B:469:ARG:NH2	2.25	0.57
1:A:62:ARG:HB2	1:A:62:ARG:HH11	1.69	0.57
1:B:62:ARG:NH1	1:B:62:ARG:HB2	2.20	0.57
1:A:2719:ARG:HA	1:A:2763:ARG:HG2	1.87	0.56
1:A:2239:MET:HE2	1:A:2247:ILE:HD12	1.87	0.56
1:B:2633:LEU:HB3	1:B:2700:LYS:HE2	1.85	0.56
1:A:62:ARG:HB2	1:A:62:ARG:NH1	2.20	0.56
1:A:2101:GLN:HA	1:A:2104:TRP:CD1	2.40	0.56
1:A:2509:MET:HE1	1:A:2544:LEU:HB2	1.87	0.56
1:A:111:ARG:HE	1:A:114:ARG:HH22	1.52	0.56
1:B:62:ARG:HB2	1:B:62:ARG:HH11	1.69	0.56
1:B:2101:GLN:HA	1:B:2104:TRP:CD1	2.40	0.56
1:A:19:ARG:O	1:A:23:ARG:N	2.36	0.56
1:B:1208:ASP:N	1:B:1208:ASP:OD1	2.38	0.56
1:B:2509:MET:HE1	1:B:2544:LEU:HB2	1.87	0.56
1:B:162:GLN:HE21	1:B:162:GLN:C	2.13	0.56
1:A:1745:THR:OG1	1:A:1822:GLU:OE2	2.24	0.56
1:A:1208:ASP:OD1	1:A:1208:ASP:N	2.38	0.55
1:B:2239:MET:HE2	1:B:2247:ILE:HD12	1.87	0.55
1:B:2719:ARG:HA	1:B:2763:ARG:HG2	1.87	0.55
1:A:140:ASP:O	1:A:144:ILE:HD12	2.07	0.55
1:A:162:GLN:HE21	1:A:162:GLN:C	2.12	0.55
1:B:205:LEU:HD12	1:B:209:PHE:HD1	1.71	0.55
1:A:192:HIS:HA	1:A:235:ALA:HB2	1.88	0.55
1:A:487:ILE:O	1:A:491:THR:HG22	2.06	0.55
1:B:111:ARG:HE	1:B:114:ARG:HH22	1.52	0.55
1:B:192:HIS:HA	1:B:235:ALA:HB2	1.88	0.55
1:A:405:ASN:OD1	1:A:405:ASN:N	2.29	0.54
1:B:487:ILE:O	1:B:491:THR:HG22	2.06	0.54
1:B:1745:THR:OG1	1:B:1822:GLU:OE2	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:NH2	1:A:355:GLN:O	2.40	0.54
1:B:162:GLN:O	1:B:162:GLN:NE2	2.34	0.54
1:A:205:LEU:HD12	1:A:209:PHE:HD1	1.71	0.54
1:A:2196:ARG:O	1:A:2200:GLU:HG3	2.08	0.54
1:B:19:ARG:O	1:B:23:ARG:N	2.36	0.54
1:B:140:ASP:O	1:B:144:ILE:HD12	2.07	0.54
1:B:2402:GLU:OE2	1:B:2459:ARG:NE	2.32	0.54
1:A:2901:PRO:HB3	1:B:2444:GLU:OE1	2.08	0.54
1:B:1710:TRP:O	1:B:1714:MET:HG2	2.08	0.54
1:A:2968:LEU:HD11	1:B:2440:LYS:HD3	1.90	0.54
1:B:309:ARG:NH2	1:B:355:GLN:O	2.40	0.54
1:B:1959:GLU:OE2	1:B:2849:ARG:NH1	2.36	0.53
1:B:2196:ARG:O	1:B:2200:GLU:HG3	2.08	0.53
1:A:1182:GLU:OE2	1:A:1229:TYR:OH	2.26	0.53
1:A:2444:GLU:OE1	1:B:2901:PRO:HB3	2.08	0.53
1:B:1182:GLU:OE2	1:B:1229:TYR:OH	2.26	0.53
1:A:2936:GLU:HG3	1:A:3028:VAL:HG21	1.90	0.53
1:B:1318:VAL:O	1:B:1322:LEU:HD12	2.09	0.53
1:A:1567:ASP:O	1:A:1568:HIS:ND1	2.36	0.53
1:B:2936:GLU:HG3	1:B:3028:VAL:HG21	1.90	0.53
1:A:580:LEU:HD22	1:A:608:LEU:HD21	1.91	0.53
1:A:1318:VAL:O	1:A:1322:LEU:HD12	2.09	0.53
1:B:1343:ILE:H	1:B:1343:ILE:HD12	1.74	0.53
1:A:1710:TRP:O	1:A:1714:MET:HG2	2.08	0.52
1:A:2378:GLU:OE1	1:A:2378:GLU:N	2.20	0.52
1:A:1755:MET:SD	1:A:1755:MET:N	2.82	0.52
1:B:580:LEU:HD22	1:B:608:LEU:HD21	1.91	0.52
1:A:2440:LYS:HD3	1:B:2968:LEU:HD11	1.90	0.52
1:A:618:LYS:HG2	1:A:683:HIS:HD2	1.73	0.52
1:A:1312:ARG:HG3	1:A:1312:ARG:NH1	2.07	0.52
1:A:2697:ASN:HB3	1:A:2719:ARG:HD3	1.92	0.52
1:B:618:LYS:HG2	1:B:683:HIS:HD2	1.73	0.52
1:A:1551:ASP:OD1	1:A:1551:ASP:N	2.41	0.52
1:B:1755:MET:SD	1:B:1755:MET:N	2.82	0.52
1:B:2838:LYS:HE2	1:B:2880:GLU:HG2	1.92	0.52
1:A:74:CYS:O	1:A:90:ARG:NH1	2.37	0.52
1:A:162:GLN:O	1:A:162:GLN:NE2	2.34	0.52
1:A:1697:THR:O	1:A:1701:LYS:HG2	2.10	0.52
1:B:2697:ASN:HB3	1:B:2719:ARG:HD3	1.92	0.52
1:B:2094:GLU:H	1:B:2094:GLU:CD	2.18	0.51
1:A:1343:ILE:HD12	1:A:1343:ILE:H	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:ALA:HA	1:B:1214:LEU:HB2	1.91	0.51
1:B:405:ASN:OD1	1:B:405:ASN:N	2.29	0.51
1:B:2319:LEU:HD13	1:B:2334:TYR:HA	1.93	0.51
1:A:112:ALA:HB3	1:A:114:ARG:HH11	1.76	0.51
1:B:2745:THR:HG22	1:B:2750:LEU:HD12	1.93	0.51
1:A:2319:LEU:HD13	1:A:2334:TYR:HA	1.93	0.51
1:B:957:GLU:HB2	1:B:999:LYS:HB2	1.93	0.51
1:A:1211:ALA:HA	1:A:1214:LEU:HB2	1.91	0.50
1:A:1265:PHE:HA	1:A:1268:VAL:HG12	1.93	0.50
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.45	0.50
1:A:2094:GLU:CD	1:A:2094:GLU:H	2.18	0.50
1:A:2838:LYS:HE2	1:A:2880:GLU:HG2	1.92	0.50
1:B:1265:PHE:HA	1:B:1268:VAL:HG12	1.93	0.50
1:B:1697:THR:O	1:B:1701:LYS:HG2	2.10	0.50
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.93	0.50
1:B:112:ALA:HB3	1:B:114:ARG:HH11	1.76	0.50
1:B:1551:ASP:OD1	1:B:1551:ASP:N	2.41	0.50
1:A:599:LEU:O	1:A:717:ARG:NE	2.44	0.50
1:A:957:GLU:HB2	1:A:999:LYS:HB2	1.93	0.50
1:A:1334:HIS:HD1	1:A:1334:HIS:C	2.19	0.50
1:B:18:ASP:O	1:B:23:ARG:NH1	2.45	0.50
1:B:1992:LYS:O	1:B:1996:GLU:HG3	2.12	0.50
1:A:154:LYS:O	1:A:158:GLU:HG3	2.12	0.50
1:B:706:SER:N	1:B:710:THR:OG1	2.40	0.50
1:B:1655:SER:HB3	1:B:2159:CYS:SG	2.52	0.50
1:A:1655:SER:HB3	1:A:2159:CYS:SG	2.52	0.50
1:A:63:PHE:HD1	1:A:66:LYS:HZ1	1.60	0.50
1:B:1334:HIS:HD1	1:B:1334:HIS:C	2.19	0.50
1:B:521:ARG:HE	1:B:554:THR:HB	1.77	0.49
1:B:2570:GLU:CD	1:B:2570:GLU:H	2.20	0.49
1:A:18:ASP:O	1:A:23:ARG:NH1	2.45	0.49
1:A:1754:LYS:HG3	1:A:1755:MET:SD	2.52	0.49
1:B:1754:LYS:HG3	1:B:1755:MET:SD	2.52	0.49
1:A:521:ARG:HE	1:A:554:THR:HB	1.77	0.49
1:B:599:LEU:O	1:B:717:ARG:NE	2.44	0.49
1:B:1288:PRO:O	1:B:1292:VAL:HG13	2.13	0.49
1:B:154:LYS:O	1:B:158:GLU:HG3	2.12	0.49
1:A:409:LEU:HD11	1:A:442:LEU:HD11	1.94	0.49
1:B:1875:ARG:O	1:B:1876:HIS:ND1	2.46	0.49
1:A:1473:ILE:HD13	1:A:1519:VAL:HG22	1.95	0.49
1:B:1473:ILE:HD13	1:B:1519:VAL:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:PRO:HB3	1:A:976:VAL:HG22	1.94	0.49
1:B:938:PRO:HB3	1:B:976:VAL:HG22	1.94	0.49
1:B:2235:MET:HE2	1:B:2248:LYS:HA	1.94	0.49
1:A:2033:LEU:HD21	1:A:2048:THR:HB	1.95	0.49
1:B:409:LEU:HD11	1:B:442:LEU:HD11	1.94	0.49
1:A:1656:LYS:HD2	1:A:2163:LEU:HD12	1.95	0.48
1:A:2307:LEU:HD21	1:B:2032:ARG:HD3	1.95	0.48
1:B:1779:ARG:HH22	1:B:1820:LYS:HD2	1.78	0.48
1:A:1779:ARG:HH22	1:A:1820:LYS:HD2	1.78	0.48
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.46	0.48
1:A:2570:GLU:H	1:A:2570:GLU:CD	2.20	0.48
1:B:2033:LEU:HD21	1:B:2048:THR:HB	1.95	0.48
1:A:1288:PRO:O	1:A:1292:VAL:HG13	2.13	0.48
1:A:1344:VAL:HG11	1:A:1418:ILE:HD13	1.94	0.48
1:A:2235:MET:HE2	1:A:2248:LYS:HA	1.94	0.48
1:B:2727:VAL:O	1:B:2731:VAL:HG23	2.14	0.48
1:B:1413:ASP:N	1:B:1413:ASP:OD1	2.45	0.48
1:A:1652:LEU:HB3	1:A:2163:LEU:HD11	1.95	0.48
1:A:1992:LYS:O	1:A:1996:GLU:HG3	2.12	0.48
1:A:2727:VAL:O	1:A:2731:VAL:HG23	2.14	0.48
1:B:251:VAL:HG11	1:B:289:ILE:HD13	1.95	0.48
1:B:657:PHE:CZ	1:B:1155:LEU:HB3	2.49	0.48
1:B:1656:LYS:HD2	1:B:2163:LEU:HD12	1.95	0.48
1:B:74:CYS:O	1:B:90:ARG:NH1	2.37	0.47
1:A:2573:THR:O	1:A:2573:THR:OG1	2.28	0.47
1:A:2865:ILE:HG13	1:A:2938:MET:HG3	1.97	0.47
1:B:1344:VAL:HG11	1:B:1418:ILE:HD13	1.94	0.47
1:B:2228:THR:OG1	1:B:2254:HIS:NE2	2.39	0.47
1:A:624:MET:HE3	1:A:624:MET:HA	1.96	0.47
1:A:2228:THR:OG1	1:A:2254:HIS:NE2	2.39	0.47
1:B:432:LEU:HD21	1:B:466:GLN:HG3	1.97	0.47
1:B:1652:LEU:HB3	1:B:2163:LEU:HD11	1.95	0.47
1:B:1680:PRO:O	1:B:2215:SER:OG	2.26	0.47
1:A:1959:GLU:OE2	1:A:2849:ARG:NH1	2.36	0.47
1:A:1307:GLY:O	1:A:1311:GLN:NE2	2.48	0.47
1:A:2027:LEU:HD13	1:B:2311:ILE:HD11	1.97	0.47
1:A:2311:ILE:HD11	1:B:2027:LEU:HD13	1.97	0.47
1:A:2384:MET:HE3	1:A:2480:HIS:CE1	2.49	0.47
1:B:2384:MET:HE3	1:B:2480:HIS:CE1	2.49	0.47
1:B:2697:ASN:OD1	1:B:2697:ASN:N	2.42	0.47
1:A:119:GLU:OE1	1:A:119:GLU:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:O	1:A:269:HIS:HB2	2.15	0.47
1:B:624:MET:HE3	1:B:624:MET:HA	1.96	0.47
1:A:251:VAL:HG11	1:A:289:ILE:HD13	1.95	0.47
1:A:2032:ARG:HD3	1:B:2307:LEU:HD21	1.95	0.47
1:B:1307:GLY:O	1:B:1311:GLN:NE2	2.48	0.47
1:A:1341:PRO:HG3	1:A:1414:SER:HB2	1.97	0.47
1:A:2406:LYS:HB2	1:A:2406:LYS:HE3	1.73	0.47
1:A:2665:PRO:HD3	1:A:2683:ILE:HD11	1.96	0.47
1:B:2865:ILE:HG13	1:B:2938:MET:HG3	1.97	0.47
1:A:657:PHE:CZ	1:A:1155:LEU:HB3	2.49	0.46
1:A:1231:LEU:HD21	1:A:1255:LEU:HB3	1.97	0.46
1:A:2402:GLU:OE2	1:A:2459:ARG:NE	2.32	0.46
1:B:265:ILE:O	1:B:269:HIS:HB2	2.15	0.46
1:B:924:ARG:HD2	1:B:961:LEU:HD21	1.98	0.46
1:A:3014:GLN:HG2	1:A:3018:LYS:NZ	2.30	0.46
1:B:1827:LEU:HD22	1:B:1837:PHE:HZ	1.80	0.46
1:A:342:LYS:HB2	1:A:342:LYS:HE3	1.56	0.46
1:A:2731:VAL:HG21	1:A:2952:LEU:HD21	1.98	0.46
1:B:1231:LEU:HD21	1:B:1255:LEU:HB3	1.97	0.46
1:A:924:ARG:HD2	1:A:961:LEU:HD21	1.98	0.46
1:B:342:LYS:HB2	1:B:342:LYS:HE3	1.56	0.46
1:B:938:PRO:HB2	1:B:979:LEU:HD12	1.97	0.46
1:B:2665:PRO:HD3	1:B:2683:ILE:HD11	1.96	0.46
1:A:1669:GLU:HG3	1:A:2148:LYS:HG3	1.98	0.46
1:B:2025:LYS:HB2	1:B:2025:LYS:HE3	1.79	0.46
1:A:271:LEU:HB3	1:A:276:LYS:HD3	1.98	0.46
1:A:432:LEU:HD21	1:A:466:GLN:HG3	1.97	0.46
1:A:1596:HIS:O	1:A:1600:VAL:HG23	2.16	0.46
1:A:938:PRO:HB2	1:A:979:LEU:HD12	1.97	0.46
1:B:716:VAL:HG21	1:B:779:MET:HG3	1.98	0.46
1:B:1341:PRO:HG3	1:B:1414:SER:HB2	1.97	0.46
1:B:1596:HIS:O	1:B:1600:VAL:HG23	2.16	0.46
1:B:533:ARG:HG2	1:B:533:ARG:HH11	1.81	0.46
1:A:1678:VAL:HG23	1:A:1681:ILE:HD12	1.98	0.45
1:A:2667:MET:HE3	1:A:2667:MET:HB3	1.78	0.45
1:B:58:ASP:OD1	1:B:62:ARG:NH2	2.43	0.45
1:B:271:LEU:HB3	1:B:276:LYS:HD3	1.98	0.45
1:A:741:TYR:CE1	1:A:805:ARG:HD3	2.51	0.45
1:A:1680:PRO:O	1:A:2215:SER:OG	2.26	0.45
1:B:753:MET:HG2	1:B:806:LEU:HD13	1.98	0.45
1:B:1527:LEU:HB3	1:B:1538:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1669:GLU:HG3	1:B:2148:LYS:HG3	1.98	0.45
1:A:533:ARG:HG2	1:A:533:ARG:HH11	1.81	0.45
1:B:206:ASN:HD22	1:B:208:LYS:HG2	1.82	0.45
1:B:2474:LEU:O	1:B:2515:LYS:NZ	2.50	0.45
1:A:120:LEU:HG	1:A:149:ILE:HD11	1.99	0.45
1:A:967:LEU:HD11	1:A:1013:ASP:HB3	1.98	0.45
1:B:1715:LEU:HD22	1:B:1737:LEU:HD23	1.97	0.45
1:B:2237:LYS:HA	1:B:2237:LYS:HD3	1.70	0.45
1:B:3014:GLN:HG2	1:B:3018:LYS:NZ	2.30	0.45
1:A:109:ASN:ND2	1:A:155:TYR:OH	2.48	0.45
1:A:1527:LEU:HB3	1:A:1538:VAL:HG21	1.99	0.45
1:A:2474:LEU:O	1:A:2515:LYS:NZ	2.50	0.45
1:B:1567:ASP:O	1:B:1568:HIS:ND1	2.36	0.45
1:B:2358:GLN:HA	1:B:2358:GLN:OE1	2.17	0.45
1:A:1465:LEU:HD13	1:A:1469:ILE:HD12	1.99	0.45
1:A:2616:MET:HE2	1:A:2616:MET:HB3	1.83	0.45
1:B:2731:VAL:HG21	1:B:2952:LEU:HD21	1.98	0.45
1:A:60:VAL:HA	1:A:63:PHE:CD2	2.51	0.45
1:A:1034:TYR:HB3	1:A:1038:VAL:HB	1.98	0.45
1:A:2670:LYS:HB2	1:A:2670:LYS:HE2	1.68	0.45
1:A:1869:PHE:CE1	1:A:1909:MET:HG3	2.51	0.45
1:A:2763:ARG:NH1	1:A:2763:ARG:HB3	2.32	0.45
1:A:716:VAL:HG21	1:A:779:MET:HG3	1.98	0.45
1:A:1290:ILE:HG22	1:A:1294:ILE:CD1	2.47	0.45
1:A:2693:ALA:HB3	1:A:2699:PRO:HG2	1.99	0.45
1:B:741:TYR:CE1	1:B:805:ARG:HD3	2.51	0.45
1:B:1678:VAL:HG23	1:B:1681:ILE:HD12	1.98	0.45
1:B:2406:LYS:HE3	1:B:2406:LYS:HB2	1.73	0.45
1:A:183:HIS:O	1:A:187:VAL:HG23	2.16	0.45
1:A:753:MET:HG2	1:A:806:LEU:HD13	1.98	0.45
1:A:1257:PRO:O	1:A:1261:ILE:HG22	2.17	0.45
1:B:892:LYS:HD2	1:B:892:LYS:HA	1.74	0.45
1:B:967:LEU:HD11	1:B:1013:ASP:HB3	1.98	0.45
1:B:1257:PRO:O	1:B:1261:ILE:HG22	2.17	0.45
1:B:2025:LYS:HB3	1:B:2028:GLN:HG3	1.99	0.45
1:A:206:ASN:HD22	1:A:208:LYS:HG2	1.82	0.44
1:A:262:LEU:HD11	1:A:282:LEU:HD23	1.99	0.44
1:A:706:SER:N	1:A:710:THR:OG1	2.40	0.44
1:A:1460:ALA:HB2	1:A:1766:PRO:HB3	1.99	0.44
1:B:120:LEU:HG	1:B:149:ILE:HD11	1.99	0.44
1:B:159:ILE:HG23	1:B:163:GLN:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD11	1:B:282:LEU:HD23	1.99	0.44
1:B:609:GLU:HG2	1:B:724:GLY:HA3	1.99	0.44
1:B:1643:ILE:HD12	1:B:1643:ILE:HA	1.89	0.44
1:B:2514:TYR:HA	1:B:2517:LEU:HG	2.00	0.44
1:B:2531:MET:H	1:B:2538:HIS:HD2	1.65	0.44
1:A:159:ILE:HG23	1:A:163:GLN:HB2	2.00	0.44
1:A:1715:LEU:HD22	1:A:1737:LEU:HD23	1.97	0.44
1:A:1827:LEU:HD22	1:A:1837:PHE:HZ	1.80	0.44
1:B:109:ASN:ND2	1:B:155:TYR:OH	2.48	0.44
1:B:183:HIS:O	1:B:187:VAL:HG23	2.16	0.44
1:B:1802:HIS:HB2	1:B:1902:ASP:OD2	2.17	0.44
1:B:2763:ARG:HB3	1:B:2763:ARG:NH1	2.32	0.44
1:A:121:LEU:HD23	1:A:163:GLN:NE2	2.33	0.44
1:A:948:LEU:HB3	1:A:993:HIS:ND1	2.32	0.44
1:A:1607:PRO:HG2	1:A:1658:ALA:HA	1.99	0.44
1:A:2109:TRP:O	1:A:2133:GLN:NE2	2.51	0.44
1:B:60:VAL:HA	1:B:63:PHE:CD2	2.51	0.44
1:B:1761:LEU:O	1:B:1765:GLN:HG2	2.17	0.44
1:B:1869:PHE:CE1	1:B:1909:MET:HG3	2.51	0.44
1:B:2109:TRP:O	1:B:2133:GLN:NE2	2.51	0.44
1:B:2561:LEU:O	1:B:2565:ASN:N	2.48	0.44
1:A:780:MET:HG3	1:A:900:MET:HG2	1.99	0.44
1:B:224:LYS:HE3	1:B:269:HIS:HA	1.99	0.44
1:B:1378:PRO:HG2	1:B:1379:PRO:HD3	1.98	0.44
1:B:1460:ALA:HB2	1:B:1766:PRO:HB3	1.99	0.44
1:B:2616:MET:HB2	1:B:2661:ASP:HB3	2.00	0.44
1:A:1378:PRO:HG2	1:A:1379:PRO:HD3	1.98	0.44
1:A:1860:ASN:O	1:A:1864:THR:HG22	2.17	0.44
1:A:2025:LYS:HB3	1:A:2028:GLN:HG3	1.99	0.44
1:A:2358:GLN:OE1	1:A:2358:GLN:HA	2.17	0.44
1:A:2616:MET:HB2	1:A:2661:ASP:HB3	1.99	0.44
1:B:121:LEU:HD23	1:B:163:GLN:NE2	2.33	0.44
1:B:948:LEU:HB3	1:B:993:HIS:ND1	2.32	0.44
1:B:1465:LEU:HD13	1:B:1469:ILE:HD12	1.99	0.44
1:B:433:SER:O	1:B:437:MET:HG3	2.18	0.44
1:B:780:MET:HG3	1:B:900:MET:HG2	1.99	0.44
1:B:1860:ASN:O	1:B:1864:THR:HG22	2.17	0.44
1:A:433:SER:O	1:A:437:MET:HG3	2.18	0.44
1:A:790:CYS:SG	1:A:792:LYS:HG3	2.58	0.44
1:B:1034:TYR:HB3	1:B:1038:VAL:HB	1.98	0.44
1:B:1280:LYS:HD2	1:B:1280:LYS:HA	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3043:LYS:O	1:B:3047:ARG:HG3	2.18	0.44
1:A:706:SER:HB3	1:A:709:ILE:HG13	1.99	0.44
1:A:1117:GLN:NE2	1:A:1171:GLN:OE1	2.48	0.44
1:A:1802:HIS:HB2	1:A:1902:ASP:OD2	2.17	0.44
1:A:2514:TYR:HA	1:A:2517:LEU:HG	2.00	0.44
1:B:1465:LEU:HD21	1:B:1505:ALA:HB2	1.99	0.44
1:B:166:GLU:O	1:B:170:VAL:HG13	2.18	0.44
1:B:706:SER:HB3	1:B:709:ILE:HG13	1.99	0.44
1:A:1465:LEU:HD21	1:A:1505:ALA:HB2	1.99	0.43
1:A:2734:MET:HG2	1:A:2948:ILE:HD13	2.00	0.43
1:B:1607:PRO:HG2	1:B:1658:ALA:HA	1.99	0.43
1:B:2693:ALA:HB3	1:B:2699:PRO:HG2	1.99	0.43
1:A:267:THR:HG22	1:A:268:GLN:OE1	2.18	0.43
1:A:768:ASN:OD1	1:A:768:ASN:N	2.50	0.43
1:A:3043:LYS:O	1:A:3047:ARG:HG3	2.18	0.43
1:A:205:LEU:HD12	1:A:209:PHE:CD1	2.53	0.43
1:A:1066:LYS:HB3	1:A:1066:LYS:HE2	1.55	0.43
1:A:1761:LEU:O	1:A:1765:GLN:HG2	2.17	0.43
1:B:814:ASP:O	1:B:818:ILE:HG13	2.19	0.43
1:B:2749:LYS:HB2	1:B:2749:LYS:HE3	1.62	0.43
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.43
1:A:554:THR:HG22	1:A:572:LEU:HD22	2.00	0.43
1:A:609:GLU:HG2	1:A:724:GLY:HA3	1.99	0.43
1:B:554:THR:HG22	1:B:572:LEU:HD22	2.00	0.43
1:B:2417:LEU:HD23	1:B:2417:LEU:HA	1.70	0.43
1:A:166:GLU:O	1:A:170:VAL:HG13	2.18	0.43
1:A:2416:LEU:HD22	1:B:2899:ILE:HG22	2.00	0.43
1:A:2899:ILE:HG22	1:B:2416:LEU:HD22	2.00	0.43
1:B:119:GLU:OE1	1:B:119:GLU:N	2.46	0.43
1:A:319:LEU:HD22	1:A:352:ILE:HD12	2.00	0.43
1:A:2332:LEU:HD21	1:A:2379:LEU:HA	2.01	0.43
1:A:2531:MET:H	1:A:2538:HIS:HD2	1.65	0.43
1:A:2570:GLU:OE1	1:A:2570:GLU:N	2.51	0.43
1:A:2691:ARG:HG3	1:A:2691:ARG:HH11	1.84	0.43
1:B:433:SER:HB3	1:B:434:PRO:HD3	2.00	0.43
1:B:1608:LEU:HD23	1:B:1608:LEU:HA	1.83	0.43
1:A:2237:LYS:HA	1:A:2237:LYS:HD3	1.70	0.43
1:A:2335:THR:HG21	1:A:2368:ALA:HB2	2.01	0.43
1:A:2440:LYS:O	1:A:2444:GLU:HG2	2.19	0.43
1:A:2530:LYS:H	1:A:2530:LYS:HD3	1.84	0.43
1:B:133:ASN:HB3	1:B:137:TYR:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:HD1	1:A:66:LYS:NZ	2.16	0.43
1:A:2623:LEU:HD22	1:A:2662:VAL:HG11	2.01	0.43
1:B:259:LEU:HD11	1:B:286:GLN:HG3	2.01	0.43
1:B:2440:LYS:O	1:B:2444:GLU:HG2	2.19	0.43
1:B:2734:MET:HG2	1:B:2948:ILE:HD13	2.00	0.43
1:B:3043:LYS:HA	1:B:3043:LYS:HD2	1.85	0.43
1:B:319:LEU:HD22	1:B:352:ILE:HD12	2.00	0.43
1:B:790:CYS:SG	1:B:792:LYS:HG3	2.58	0.43
1:B:2570:GLU:OE1	1:B:2570:GLU:N	2.51	0.43
1:A:1294:ILE:HG22	1:A:1298:PHE:CE1	2.54	0.43
1:B:1290:ILE:HG22	1:B:1294:ILE:CD1	2.47	0.43
1:B:2332:LEU:HD21	1:B:2379:LEU:HA	2.01	0.43
1:A:38:GLU:O	1:A:42:HIS:HB2	2.19	0.42
1:A:224:LYS:HE3	1:A:269:HIS:HA	1.99	0.42
1:B:38:GLU:O	1:B:42:HIS:HB2	2.19	0.42
1:B:768:ASN:OD1	1:B:768:ASN:N	2.50	0.42
1:B:1093:ILE:HG21	1:B:1157:LEU:HD12	2.01	0.42
1:B:1294:ILE:HG22	1:B:1298:PHE:CE1	2.54	0.42
1:B:2602:ALA:O	1:B:2606:ILE:HG12	2.19	0.42
1:A:192:HIS:CE1	1:A:879:ILE:HG13	2.54	0.42
1:A:433:SER:HB3	1:A:434:PRO:HD3	2.00	0.42
1:A:1256:ILE:HG12	1:A:1268:VAL:HG23	2.01	0.42
1:A:2010:ARG:CZ	1:A:2034:ARG:HD2	2.49	0.42
1:A:2268:THR:C	1:A:2271:PRO:HD2	2.44	0.42
1:B:192:HIS:CE1	1:B:879:ILE:HG13	2.55	0.42
1:A:2561:LEU:O	1:A:2565:ASN:N	2.48	0.42
1:B:205:LEU:HD12	1:B:209:PHE:CD1	2.53	0.42
1:B:267:THR:HG22	1:B:268:GLN:OE1	2.18	0.42
1:B:1117:GLN:NE2	1:B:1171:GLN:OE1	2.48	0.42
1:B:1820:LYS:HB2	1:B:1852:GLN:HG3	2.02	0.42
1:B:2691:ARG:NH1	1:B:2691:ARG:HG3	2.34	0.42
1:A:760:ILE:HD11	1:A:780:MET:HE3	2.02	0.42
1:A:892:LYS:HA	1:A:892:LYS:HD2	1.74	0.42
1:A:1643:ILE:HD12	1:A:1643:ILE:HA	1.89	0.42
1:A:1820:LYS:HB2	1:A:1852:GLN:HG3	2.02	0.42
1:A:2312:LEU:HD12	1:A:2312:LEU:HA	1.88	0.42
1:B:1256:ILE:HG12	1:B:1268:VAL:HG23	2.01	0.42
1:B:2010:ARG:CZ	1:B:2034:ARG:HD2	2.49	0.42
1:B:2563:LEU:HD23	1:B:2563:LEU:HA	1.80	0.42
1:A:1093:ILE:HG21	1:A:1157:LEU:HD12	2.01	0.42
1:B:760:ILE:HD11	1:B:780:MET:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1536:LYS:HA	1:B:1536:LYS:HD2	1.85	0.42
1:B:1606:LEU:HD12	1:B:1606:LEU:HA	1.80	0.42
1:A:436:LEU:HD13	1:A:462:VAL:HG11	2.02	0.42
1:A:814:ASP:O	1:A:818:ILE:HG13	2.19	0.42
1:A:1705:ASP:HB3	1:A:1708:LEU:HG	2.00	0.42
1:A:2691:ARG:HG3	1:A:2691:ARG:NH1	2.34	0.42
1:B:188:ALA:HB1	1:B:231:HIS:HB2	2.02	0.42
1:A:530:SER:O	1:A:530:SER:OG	2.32	0.42
1:A:1405:LEU:HA	1:A:1408:LEU:HB2	2.02	0.42
1:A:3043:LYS:HD2	1:A:3043:LYS:HA	1.85	0.42
1:B:436:LEU:HD13	1:B:462:VAL:HG11	2.02	0.42
1:B:1499:SER:O	1:B:1503:GLN:HG3	2.20	0.42
1:B:2691:ARG:HG3	1:B:2691:ARG:HH11	1.84	0.42
1:B:2708:ASP:OD1	1:B:2708:ASP:N	2.53	0.42
1:A:259:LEU:HD11	1:A:286:GLN:HG3	2.01	0.42
1:A:822:LEU:HD23	1:A:897:PHE:HB2	2.02	0.42
1:A:2708:ASP:OD1	1:A:2708:ASP:N	2.53	0.42
1:B:822:LEU:HD23	1:B:897:PHE:HB2	2.02	0.42
1:B:1705:ASP:HB3	1:B:1708:LEU:HG	2.00	0.42
1:B:2268:THR:C	1:B:2271:PRO:HD2	2.44	0.42
1:A:2025:LYS:HB2	1:A:2025:LYS:HE3	1.79	0.42
1:A:2092:CYS:SG	1:A:2095:LEU:HB2	2.60	0.42
1:A:2602:ALA:O	1:A:2606:ILE:HG12	2.19	0.42
1:B:206:ASN:ND2	1:B:208:LYS:HG2	2.35	0.42
1:B:1461:TRP:CH2	1:B:1465:LEU:HD23	2.55	0.42
1:B:1590:LEU:HD11	1:B:1621:LEU:HD23	2.02	0.42
1:B:2792:ARG:NE	1:B:2795:ASP:OD2	2.52	0.42
1:A:133:ASN:HB3	1:A:137:TYR:HD2	1.84	0.42
1:A:1461:TRP:CH2	1:A:1465:LEU:HD23	2.55	0.42
1:A:2698:LEU:HD12	1:A:2698:LEU:H	1.85	0.42
1:A:2792:ARG:NE	1:A:2795:ASP:OD2	2.52	0.42
1:B:2335:THR:HG21	1:B:2368:ALA:HB2	2.01	0.42
1:A:621:LYS:O	1:A:625:ASN:ND2	2.49	0.41
1:A:1499:SER:O	1:A:1503:GLN:HG3	2.20	0.41
1:A:1555:LEU:O	1:A:1559:ILE:HG13	2.20	0.41
1:A:1608:LEU:HA	1:A:1608:LEU:HD23	1.83	0.41
1:B:805:ARG:HE	1:B:805:ARG:HB3	1.79	0.41
1:B:2573:THR:O	1:B:2573:THR:OG1	2.28	0.41
1:B:2623:LEU:HD22	1:B:2662:VAL:HG11	2.01	0.41
1:A:2854:ARG:HG2	1:A:2930:CYS:SG	2.60	0.41
1:B:2530:LYS:H	1:B:2530:LYS:HD3	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:ND2	1:A:208:LYS:HG2	2.35	0.41
1:B:2844:ILE:O	1:B:2848:LYS:HG2	2.21	0.41
1:A:1590:LEU:HD11	1:A:1621:LEU:HD23	2.02	0.41
1:A:2749:LYS:HE3	1:A:2749:LYS:HB2	1.62	0.41
1:A:3018:LYS:HE2	1:B:3023:GLY:O	2.20	0.41
1:B:1909:MET:HE3	1:B:1909:MET:HB3	1.84	0.41
1:A:1290:ILE:HG22	1:A:1294:ILE:HD11	2.03	0.41
1:A:1659:ILE:HD13	1:A:1659:ILE:HA	1.92	0.41
1:B:2092:CYS:SG	1:B:2095:LEU:HB2	2.60	0.41
1:A:213:PHE:CG	1:A:236:LEU:HD13	2.56	0.41
1:A:3023:GLY:O	1:B:3018:LYS:HE2	2.20	0.41
1:B:1398:LYS:H	1:B:1398:LYS:HG2	1.67	0.41
1:B:1416:GLN:NE2	1:B:1734:VAL:HG21	2.35	0.41
1:A:1539:LEU:HD13	1:A:1539:LEU:HA	1.91	0.41
1:A:1677:GLU:OE1	1:A:1677:GLU:HA	2.21	0.41
1:A:1903:LYS:HA	1:A:1903:LYS:HD3	1.90	0.41
1:A:2844:ILE:O	1:A:2848:LYS:HG2	2.21	0.41
1:B:2854:ARG:HG2	1:B:2930:CYS:SG	2.60	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.87	0.41
1:A:486:LYS:O	1:A:490:ILE:HG13	2.21	0.41
1:A:1821:CYS:SG	1:A:1823:ILE:HG13	2.60	0.41
1:A:2815:GLU:O	1:A:2818:GLU:HG3	2.21	0.41
1:A:2868:LEU:HG	1:A:2871:ARG:HD3	2.02	0.41
1:B:213:PHE:CG	1:B:236:LEU:HD13	2.56	0.41
1:B:1066:LYS:HB3	1:B:1066:LYS:HE2	1.55	0.41
1:B:1290:ILE:HG22	1:B:1294:ILE:HD11	2.03	0.41
1:B:1555:LEU:O	1:B:1559:ILE:HG13	2.20	0.41
1:B:1821:CYS:SG	1:B:1823:ILE:HG13	2.60	0.41
1:B:2815:GLU:O	1:B:2818:GLU:HG3	2.21	0.41
1:A:126:ASP:HA	1:A:129:LYS:HB2	2.03	0.41
1:A:657:PHE:HZ	1:A:1155:LEU:HB3	1.85	0.41
1:A:958:GLU:H	1:A:958:GLU:CD	2.20	0.41
1:A:1110:ALA:HB3	1:A:1372:LEU:HD21	2.03	0.41
1:A:1524:LEU:O	1:A:1527:LEU:HB2	2.21	0.41
1:B:147:LYS:HA	1:B:147:LYS:HD3	1.94	0.41
1:B:495:ILE:HG21	1:B:526:LEU:HD21	2.03	0.41
1:B:657:PHE:HZ	1:B:1155:LEU:HB3	1.85	0.41
1:B:1339:ASN:OD1	1:B:1339:ASN:N	2.54	0.41
1:B:1405:LEU:HA	1:B:1408:LEU:HB2	2.02	0.41
1:B:2163:LEU:HD23	1:B:2163:LEU:HA	1.89	0.41
1:B:2417:LEU:HD13	1:B:2445:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2868:LEU:HG	1:B:2871:ARG:HD3	2.02	0.41
1:B:2178:ALA:HB1	1:B:2226:LEU:HD23	2.03	0.41
1:B:2669:ILE:HD12	1:B:2669:ILE:N	2.36	0.41
1:A:188:ALA:HB1	1:A:231:HIS:HB2	2.02	0.40
1:A:280:ILE:HG23	1:A:348:LEU:HD22	2.03	0.40
1:A:2517:LEU:N	1:A:2518:PRO:HD2	2.36	0.40
1:A:2627:TYR:HB3	1:A:2760:LEU:HD13	2.03	0.40
1:B:1334:HIS:C	1:B:1334:HIS:ND1	2.79	0.40
1:B:1611:LEU:O	1:B:1614:LEU:HB2	2.21	0.40
1:B:2049:TYR:HB3	1:B:2064:ILE:HG13	2.03	0.40
1:A:1416:GLN:NE2	1:A:1734:VAL:HG21	2.35	0.40
1:A:2097:GLU:OE1	1:A:2123:SER:OG	2.37	0.40
1:B:1677:GLU:HA	1:B:1677:GLU:OE1	2.21	0.40
1:B:1903:LYS:HD3	1:B:1903:LYS:HA	1.90	0.40
1:A:58:ASP:OD1	1:A:62:ARG:NH2	2.43	0.40
1:A:1040:MET:HG3	1:A:1085:VAL:HG22	2.04	0.40
1:A:1611:LEU:O	1:A:1614:LEU:HB2	2.21	0.40
1:A:1692:LYS:HE3	1:A:1692:LYS:HB3	1.87	0.40
1:A:2331:LYS:HZ2	1:A:2373:GLY:H	1.70	0.40
1:A:2615:GLN:NE2	1:A:2615:GLN:O	2.53	0.40
1:B:280:ILE:HG23	1:B:348:LEU:HD22	2.03	0.40
1:B:1289:LYS:O	1:B:1293:ASN:ND2	2.53	0.40
1:B:1524:LEU:O	1:B:1527:LEU:HB2	2.21	0.40
1:B:2615:GLN:NE2	1:B:2615:GLN:O	2.53	0.40
1:A:2669:ILE:HD12	1:A:2669:ILE:N	2.36	0.40
1:A:2872:HIS:CE1	1:A:2874:GLN:HB2	2.57	0.40
1:B:2698:LEU:HD12	1:B:2698:LEU:H	1.85	0.40
1:A:1310:GLN:NE2	1:A:1311:GLN:HE21	2.15	0.40
1:A:1339:ASN:OD1	1:A:1339:ASN:N	2.54	0.40
1:A:1902:ASP:O	1:A:1906:GLN:HG3	2.21	0.40
1:A:2073:LEU:HD22	1:A:2076:ILE:HD12	2.03	0.40
1:B:1110:ALA:HB3	1:B:1372:LEU:HD21	2.03	0.40
1:B:1687:ALA:HB1	1:B:2843:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100
1	B	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100
All	All	5470/6112 (90%)	5374 (98%)	96 (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%)	2394 (97%)	75 (3%)	36	64
1	B	2469/2780 (89%)	2394 (97%)	75 (3%)	36	64
All	All	4938/5560 (89%)	4788 (97%)	150 (3%)	37	64

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	167	LEU
1	A	205	LEU
1	A	214	SER
1	A	272	ASN
1	A	278	VAL
1	A	287	ILE
1	A	305	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	ILE
1	A	328	SER
1	A	405	ASN
1	A	481	LEU
1	A	517	VAL
1	A	519	VAL
1	A	522	GLU
1	A	620	CYS
1	A	695	LEU
1	A	725	VAL
1	A	759	SER
1	A	791	THR
1	A	800	SER
1	A	898	LEU
1	A	909	THR
1	A	917	SER
1	A	929	MET
1	A	966	VAL
1	A	967	LEU
1	A	995	LEU
1	A	1021	VAL
1	A	1045	CYS
1	A	1063	VAL
1	A	1075	THR
1	A	1108	LEU
1	A	1143	THR
1	A	1167	ILE
1	A	1190	VAL
1	A	1208	ASP
1	A	1279	TRP
1	A	1285	ASP
1	A	1312	ARG
1	A	1322	LEU
1	A	1407	ILE
1	A	1423	CYS
1	A	1469	ILE
1	A	1509	CYS
1	A	1529	TYR
1	A	1534	VAL
1	A	1567	ASP
1	A	1575	ARG
1	A	1576	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1580	LYS
1	A	1678	VAL
1	A	1721	THR
1	A	1756	THR
1	A	1801	ASN
1	A	1806	ILE
1	A	1835	THR
1	A	1871	THR
1	A	1989	LEU
1	A	2059	THR
1	A	2141	SER
1	A	2146	SER
1	A	2289	SER
1	A	2378	GLU
1	A	2457	GLU
1	A	2529	THR
1	A	2615	GLN
1	A	2661	ASP
1	A	2674	THR
1	A	2698	LEU
1	A	2703	ASP
1	A	2705	VAL
1	A	2823	VAL
1	A	2920	ILE
1	A	3024	THR
1	B	66	LYS
1	B	167	LEU
1	B	205	LEU
1	B	214	SER
1	B	272	ASN
1	B	278	VAL
1	B	287	ILE
1	B	305	SER
1	B	323	ILE
1	B	328	SER
1	B	405	ASN
1	B	481	LEU
1	B	517	VAL
1	B	519	VAL
1	B	522	GLU
1	B	620	CYS
1	B	695	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	725	VAL
1	B	759	SER
1	B	791	THR
1	B	800	SER
1	B	898	LEU
1	B	909	THR
1	B	917	SER
1	B	929	MET
1	B	966	VAL
1	B	967	LEU
1	B	995	LEU
1	B	1021	VAL
1	B	1045	CYS
1	B	1063	VAL
1	B	1075	THR
1	B	1108	LEU
1	B	1143	THR
1	B	1167	ILE
1	B	1190	VAL
1	B	1208	ASP
1	B	1279	TRP
1	B	1285	ASP
1	B	1312	ARG
1	B	1322	LEU
1	B	1407	ILE
1	B	1423	CYS
1	B	1469	ILE
1	B	1509	CYS
1	B	1529	TYR
1	B	1534	VAL
1	B	1567	ASP
1	B	1575	ARG
1	B	1576	ILE
1	B	1580	LYS
1	B	1678	VAL
1	B	1721	THR
1	B	1756	THR
1	B	1801	ASN
1	B	1806	ILE
1	B	1835	THR
1	B	1871	THR
1	B	1989	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2059	THR
1	B	2141	SER
1	B	2146	SER
1	B	2289	SER
1	B	2378	GLU
1	B	2457	GLU
1	B	2529	THR
1	B	2615	GLN
1	B	2661	ASP
1	B	2674	THR
1	B	2698	LEU
1	B	2703	ASP
1	B	2705	VAL
1	B	2823	VAL
1	B	2920	ILE
1	B	3024	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	163	GLN
1	A	286	GLN
1	A	325	HIS
1	A	445	GLN
1	A	1027	HIS
1	A	1311	GLN
1	A	1549	ASN
1	A	1554	ASN
1	A	1906	GLN
1	A	2061	GLN
1	A	2292	GLN
1	A	2399	GLN
1	A	2469	ASN
1	A	2480	HIS
1	A	2538	HIS
1	A	2641	GLN
1	A	2658	ASN
1	A	2730	GLN
1	A	2742	ASN
1	B	118	GLN
1	B	163	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	286	GLN
1	B	445	GLN
1	B	1264	HIS
1	B	1311	GLN
1	B	1554	ASN
1	B	1825	GLN
1	B	1951	HIS
1	B	2061	GLN
1	B	2399	GLN
1	B	2469	ASN
1	B	2480	HIS
1	B	2538	HIS
1	B	2641	GLN
1	B	2658	ASN
1	B	2730	GLN
1	B	2742	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
2	ANP	A	3101	3	33,33,33	0.93	4 (12%)	45,52,52	0.54	0
2	ANP	B	3101	3	33,33,33	0.93	4 (12%)	45,52,52	0.54	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
2	ANP	A	3101	3	-	4/18/38/38	0/3/3/3
2	ANP	B	3101	3	-	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)
2	A	3101	ANP	PG-O1G	2.53	1.50	1.46
2	B	3101	ANP	PG-O1G	2.53	1.50	1.46
2	A	3101	ANP	PB-O3A	-2.43	1.56	1.59
2	B	3101	ANP	PB-O3A	-2.43	1.56	1.59
2	A	3101	ANP	PG-N3B	2.39	1.69	1.63
2	B	3101	ANP	PG-N3B	2.39	1.69	1.63
2	A	3101	ANP	PB-O1B	2.36	1.49	1.46
2	B	3101	ANP	PB-O1B	2.36	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

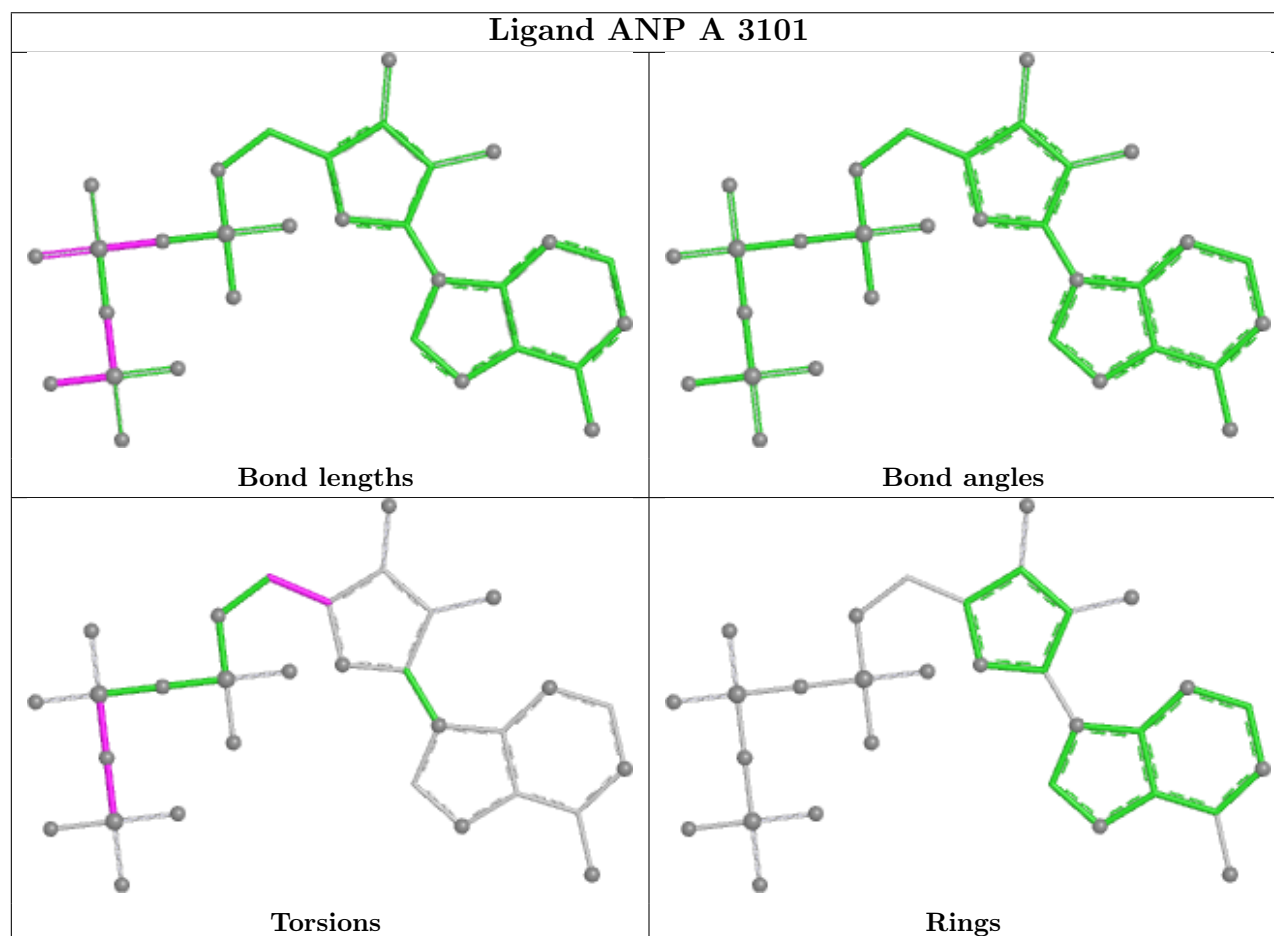
Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	PB-N3B-PG-O1G
2	A	3101	ANP	PG-N3B-PB-O1B
2	B	3101	ANP	PB-N3B-PG-O1G
2	B	3101	ANP	PG-N3B-PB-O1B
2	A	3101	ANP	O4'-C4'-C5'-O5'
2	B	3101	ANP	O4'-C4'-C5'-O5'
2	A	3101	ANP	C3'-C4'-C5'-O5'
2	B	3101	ANP	C3'-C4'-C5'-O5'

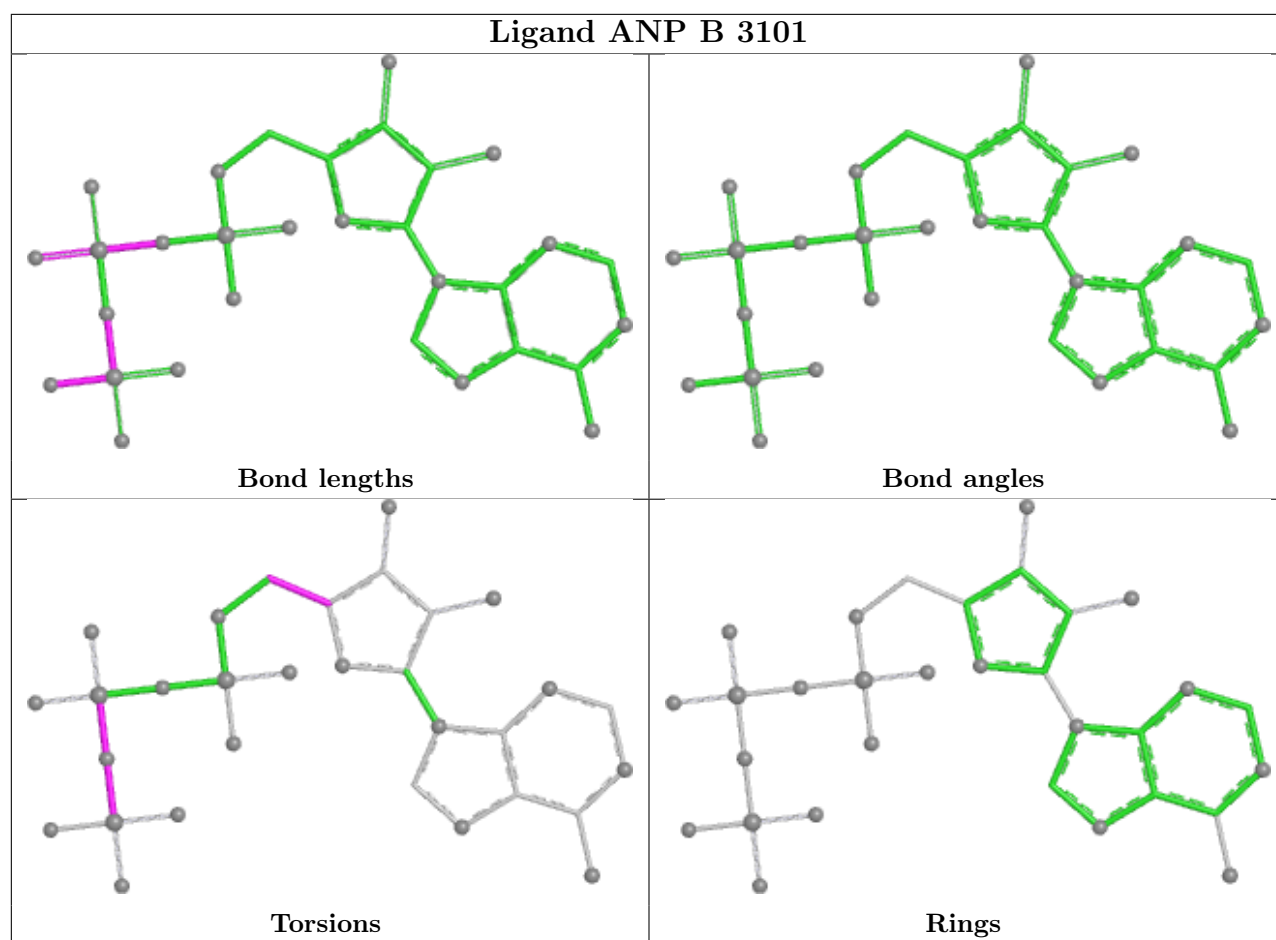
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3101	ANP	1	0
2	B	3101	ANP	1	0

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.

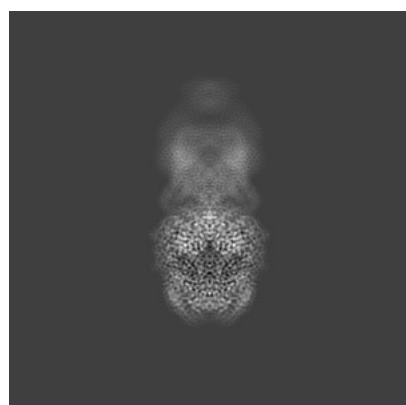
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25140. These allow visual inspection of the internal detail of the map and identification of artifacts.

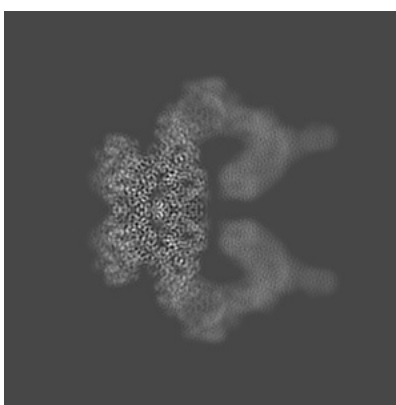
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

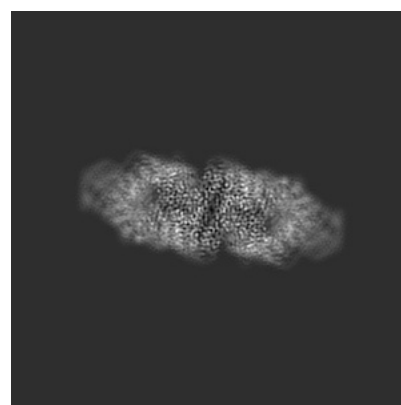
6.1.1 Primary map



X



Y

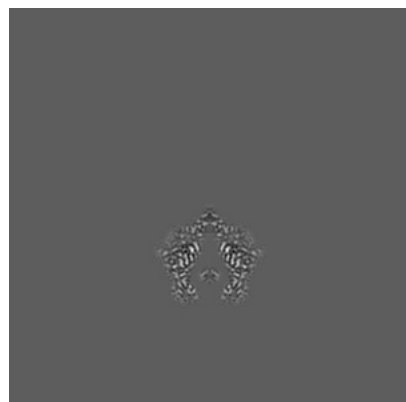


Z

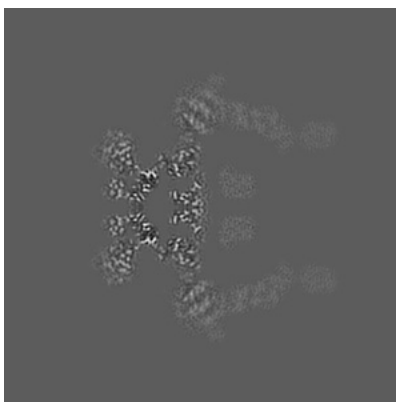
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

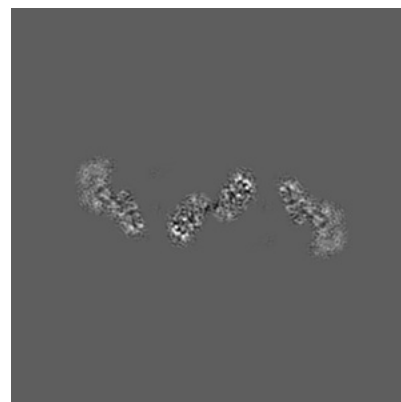
6.2.1 Primary map



X Index: 150



Y Index: 150

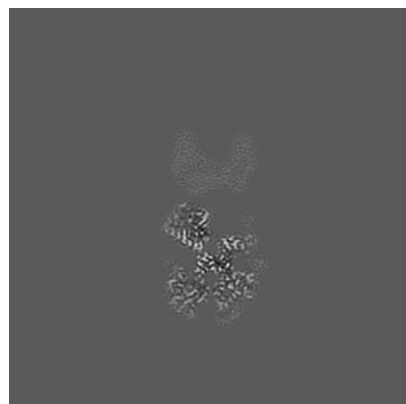


Z Index: 150

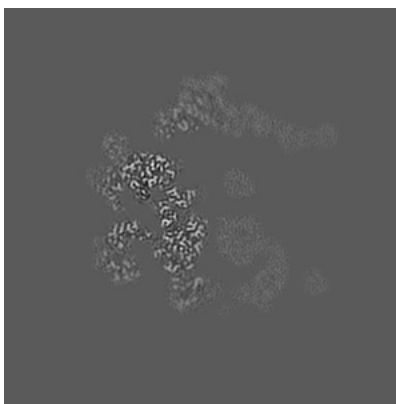
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

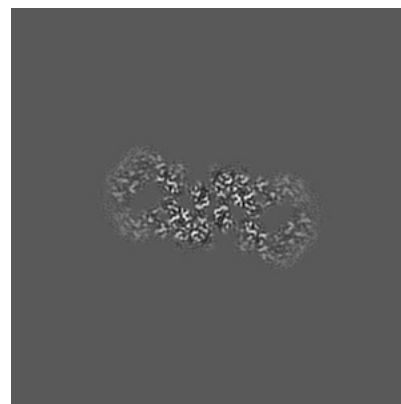
6.3.1 Primary map



X Index: 127



Y Index: 140

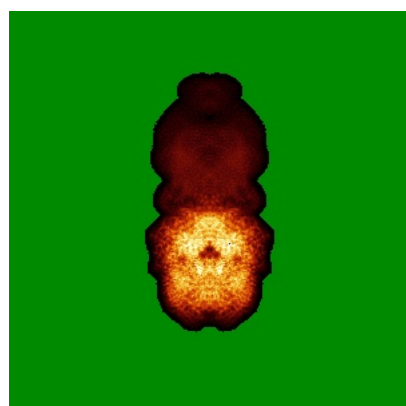


Z Index: 128

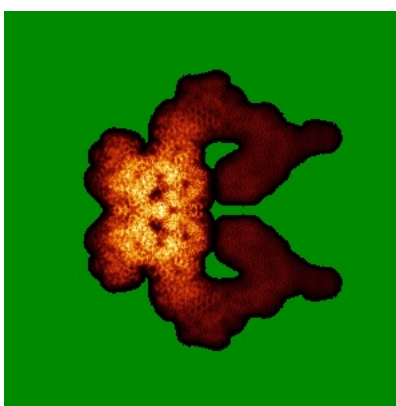
The images above show the largest variance slices of the map in three orthogonal directions.

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

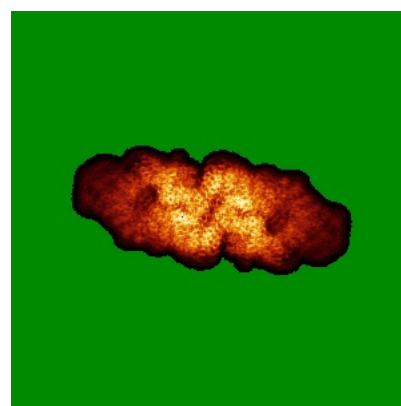
6.4.1 Primary map



X



Y

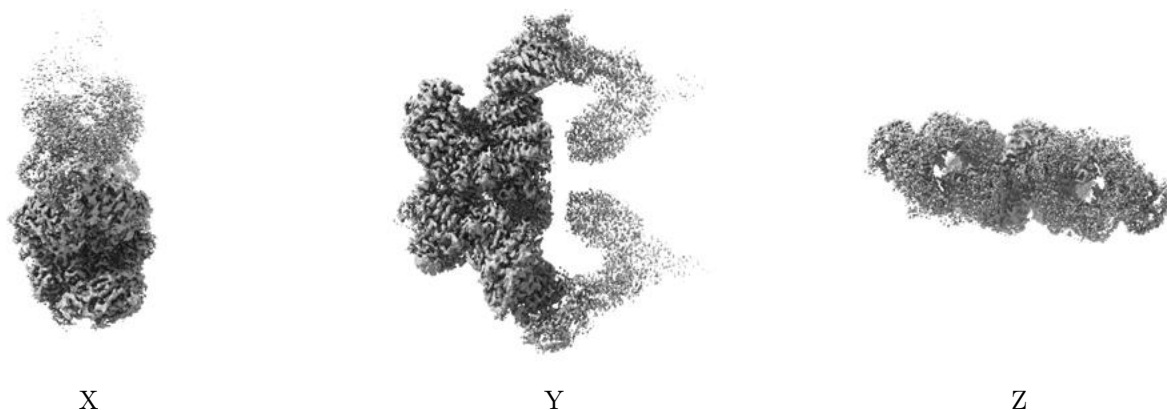


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

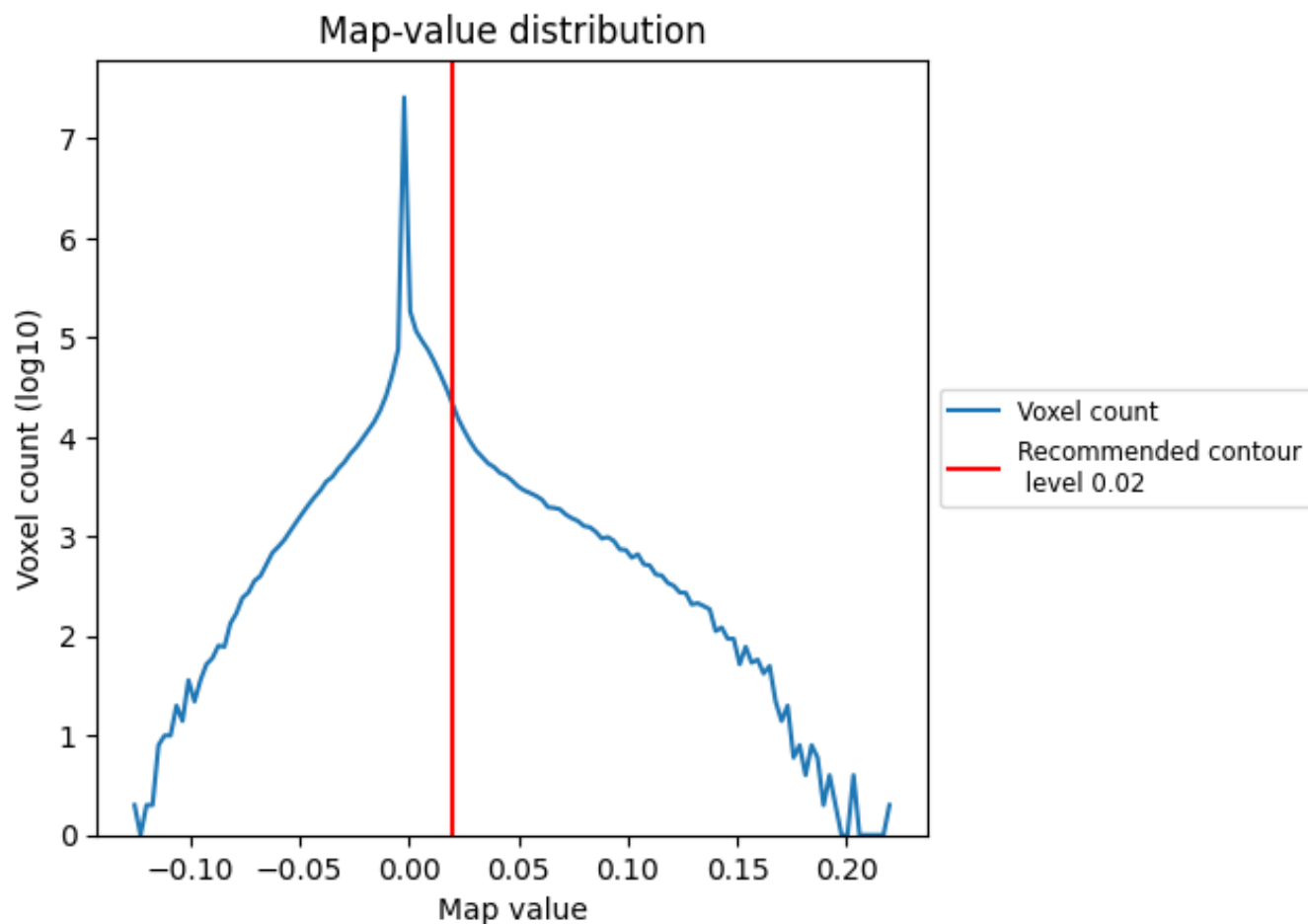
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

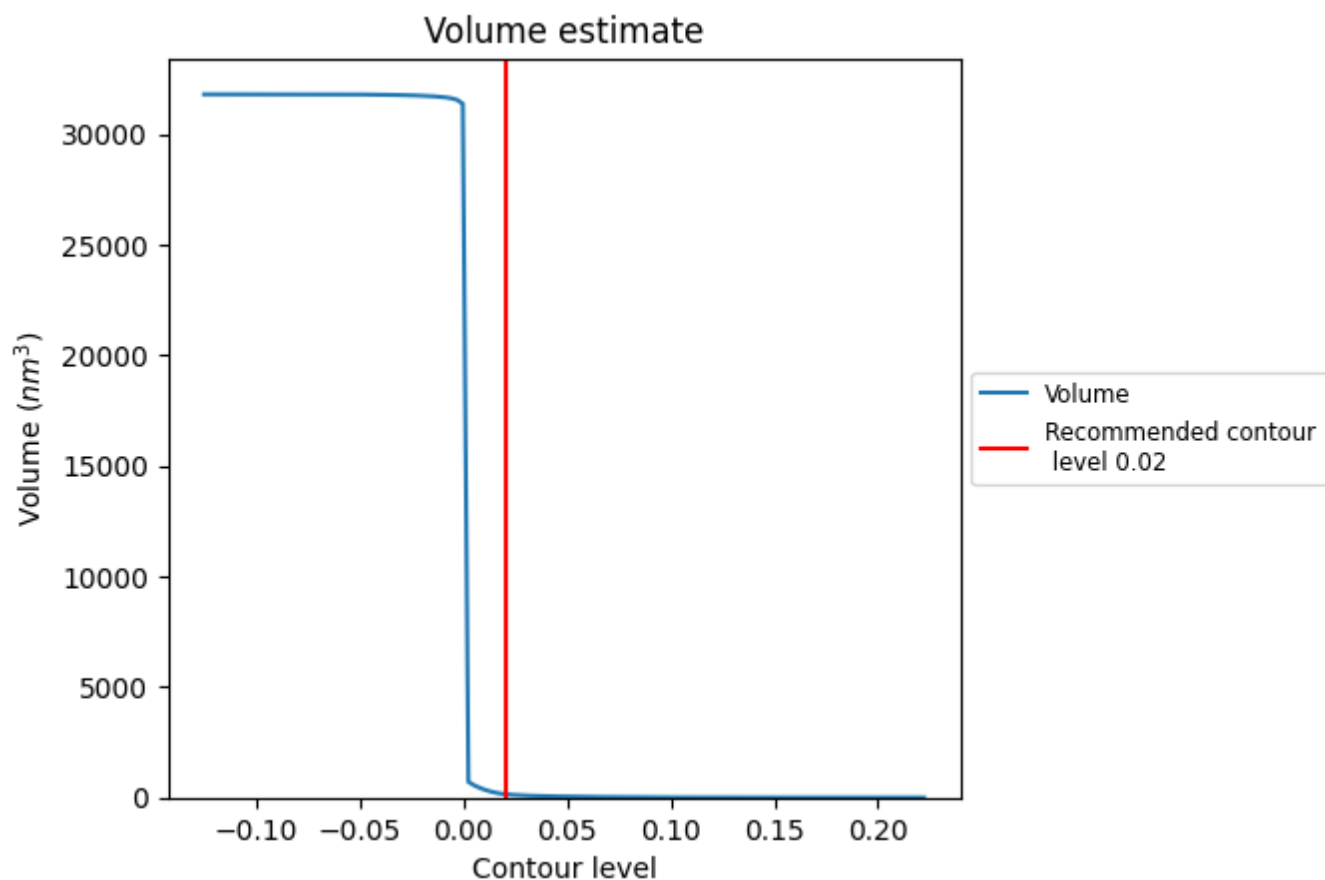
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

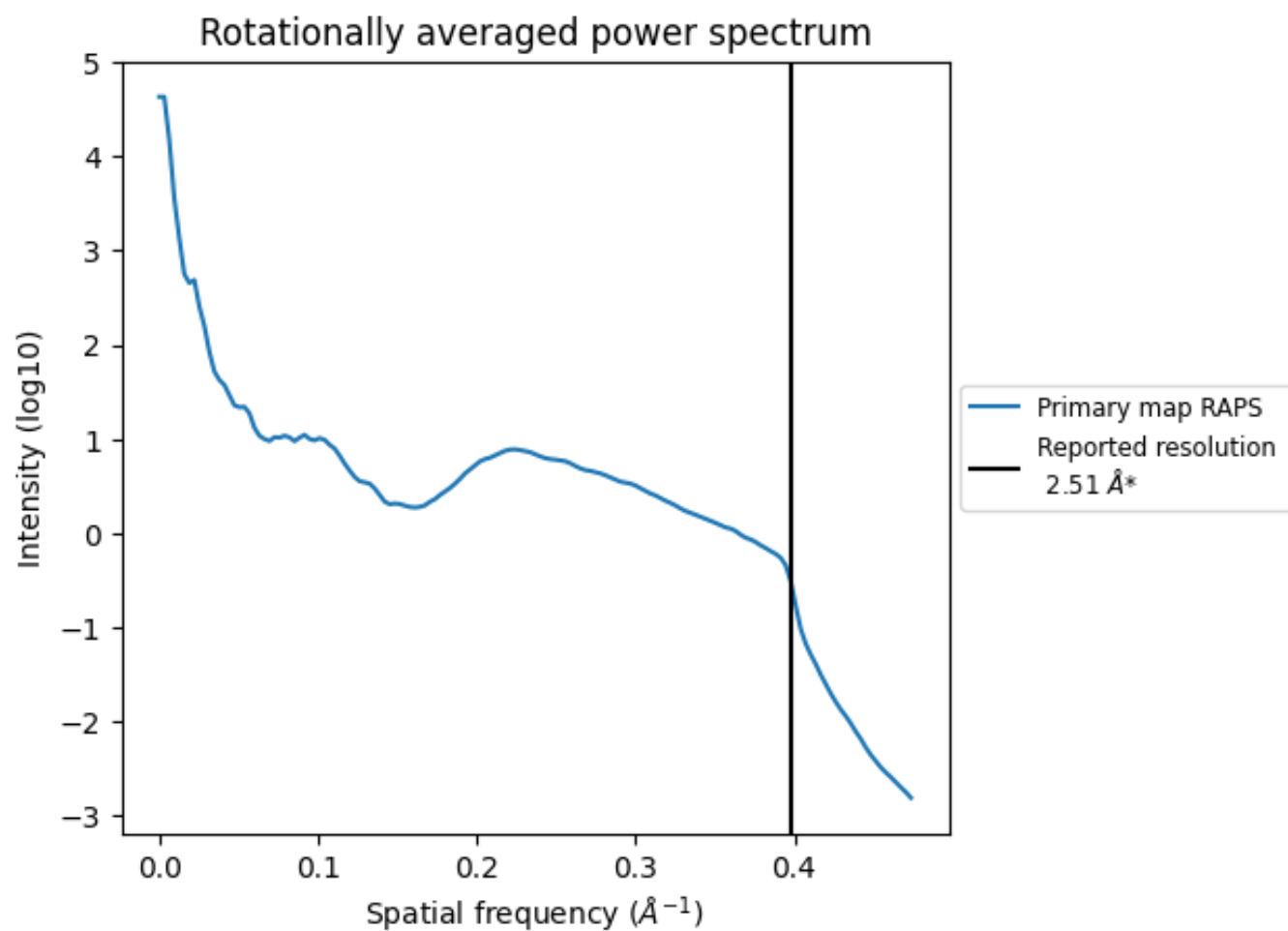
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

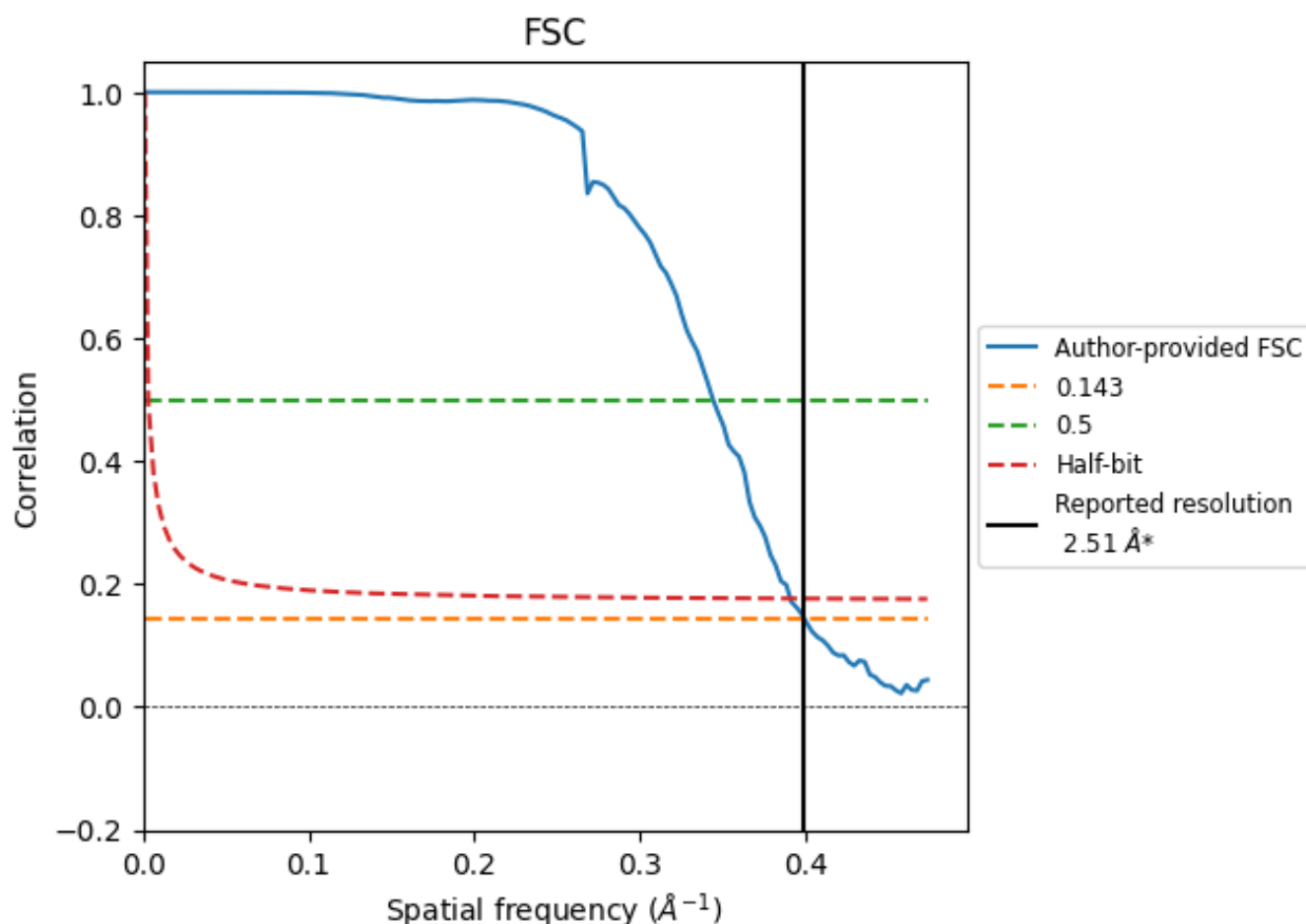


*Reported resolution corresponds to spatial frequency of 0.398 Å⁻¹

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 0.398 Å⁻¹

8.2 Resolution estimates [i](#)

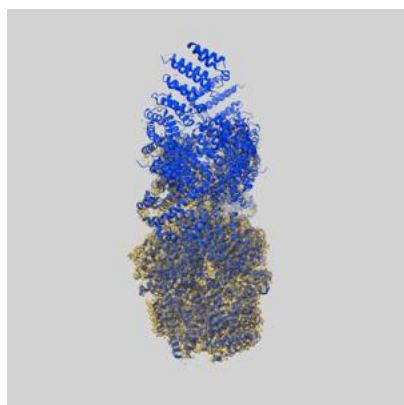
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.50	2.91	2.56
Unmasked-calculated*	-	-	-

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

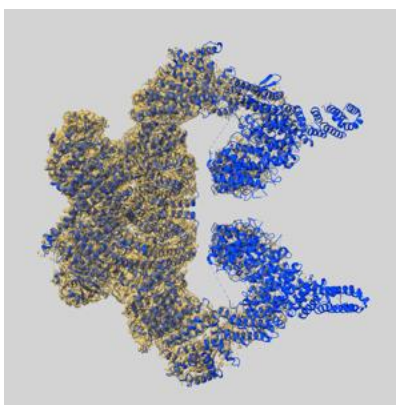
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25140 and PDB model 7SIC. Per-residue inclusion information can be found in section 3 on page 5.

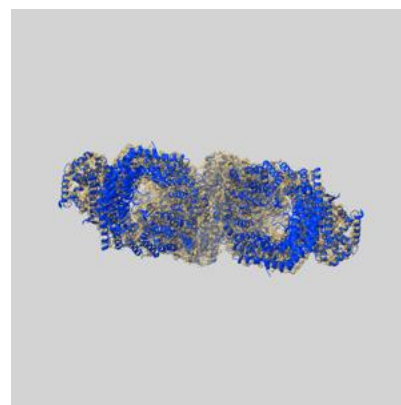
9.1 Map-model overlay [i](#)



X



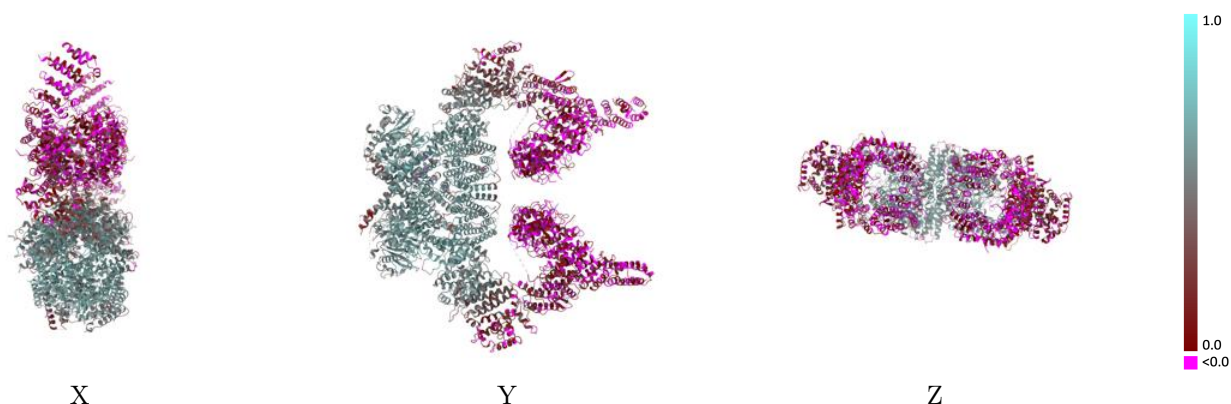
Y



Z

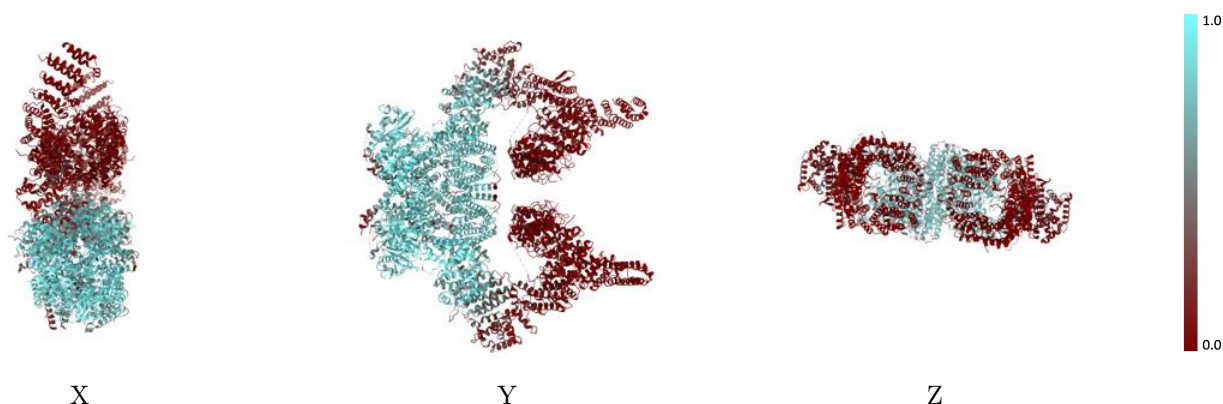
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



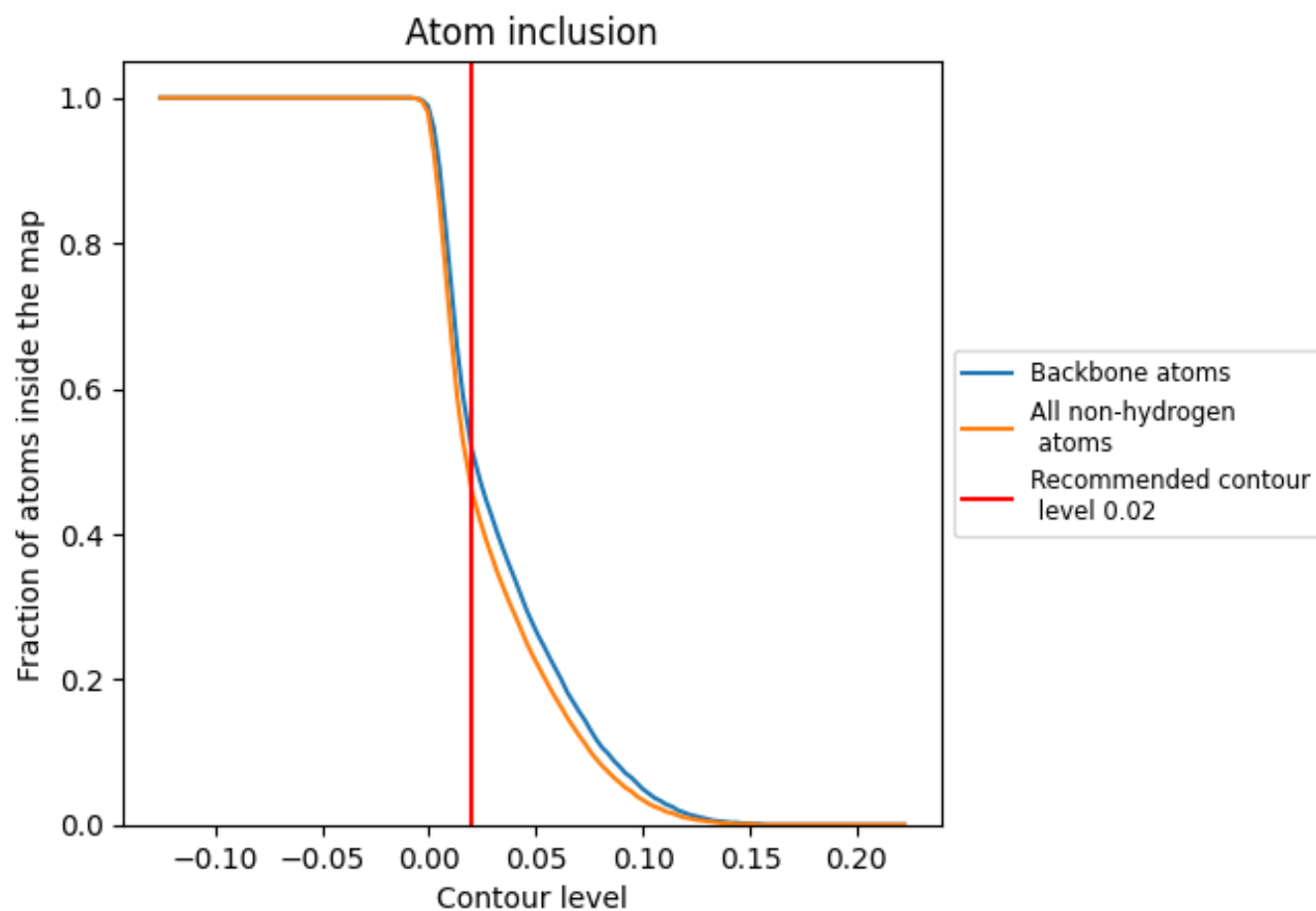
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 52% of all backbone atoms, 46% 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	0.4600	0.3400
A	0.4600	0.3400
B	0.4600	0.3400

