



## Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 04:18 pm BST

PDB ID : 9QE7 / pdb\_00009qe7  
EMDB ID : EMD-53049  
Title : Membrane-distal part of extracellular domain of the Fap2 autotransporter adhesin from *Fusobacterium nucleatum* ATCC23726  
Authors : Schoepf, F.; Marongiu, G.L.; Milaj, K.; Sprink, T.; Kikhney, J.; Moter, A.; Roderer, D.  
Deposited on : 2025-03-07  
Resolution : 4.40 Å (reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

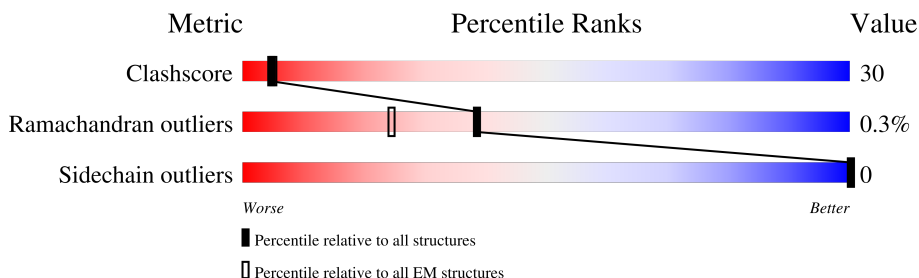
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	3250	<div> <div>17%</div> <div>22%</div> <div>24%</div> <div>54%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10826 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 Outer membrane autotransporter barrel domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1483	Total	C	N	O	S	0	0
			10826	6651	1867	2289	19		

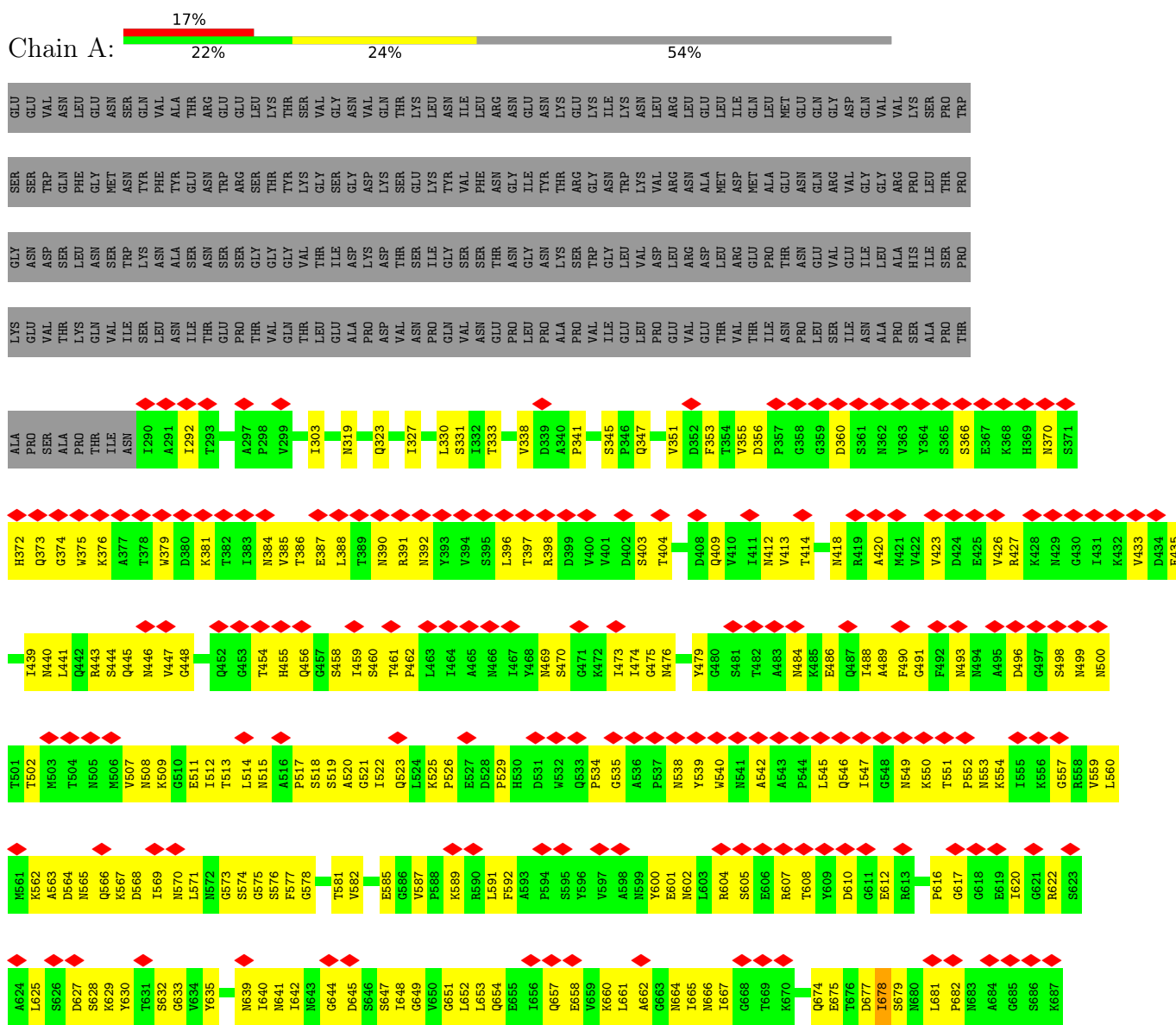
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3272	GLY	-	expression tag	UNP D5RBA4
A	3273	SER	-	expression tag	UNP D5RBA4
A	3274	ALA	-	expression tag	UNP D5RBA4
A	3275	HIS	-	expression tag	UNP D5RBA4
A	3276	HIS	-	expression tag	UNP D5RBA4
A	3277	HIS	-	expression tag	UNP D5RBA4
A	3278	HIS	-	expression tag	UNP D5RBA4
A	3279	HIS	-	expression tag	UNP D5RBA4
A	3280	HIS	-	expression tag	UNP D5RBA4
A	3281	HIS	-	expression tag	UNP D5RBA4
A	3282	HIS	-	expression tag	UNP D5RBA4
A	3283	SER	-	expression tag	UNP D5RBA4
A	3284	ALA	-	expression tag	UNP D5RBA4
A	3285	GLY	-	expression tag	UNP D5RBA4
A	3286	GLU	-	expression tag	UNP D5RBA4
A	3287	ASN	-	expression tag	UNP D5RBA4
A	3288	LEU	-	expression tag	UNP D5RBA4
A	3289	TYR	-	expression tag	UNP D5RBA4
A	3290	PHE	-	expression tag	UNP D5RBA4
A	3291	GLN	-	expression tag	UNP D5RBA4

### 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: Outer membrane autotransporter barrel domain protein



N1480	N1481	K1485	S1486	G1487	M1413	M1419	S1420	S1421	S1422	G1423	I1426	A1429	G1430	S1431	K1432	A1433	L1434	E1435	K1436	K1437	E1438	S1439	M1442	M1443	A1444	T1445	N1446	A1447	N1448	S1449	T1450	G1453	G1454	T1455	P1456	K1457	F1460	I1461	K1462	D1463	E1464	K1465	S1466	V1467	G1468	I1469	I1473	M1474	S1475	S1476	T1477	E1478	A1479	N1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	V1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	S1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548	K1340	K1341	T1342	T1343	N1344	T1345	G1346	T1347	G1348	T1349	K1350	G1351	I1354	V1355	K1356	K1357	K1358	S1359	I1362	L1363	V1364	T1365	N1366	E1367	S1368	I1371	N1372	S1373	G1374	R1375	I1376	S1377	L1378	S1381	S1382	I1383	S1384	A1385	S1386	S1387	D1388	G1389	L1390	V1391	G1392	V1395	S1399	N1403	D1404	A1405	E1408	I1409	T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	V1218	A1219	M1224	I1225	N1226	S1227	G1228	T1229	E1232	V1235	N1236	K1237	E1238	T1239	S1240	V1241	G1242	I1243	Y1244	T1248	S1249	I1250	S1251	S1252	V1253	S1254	K1255	N1256	K1258	N1259	E1260	G1261	T1262	I1263	E1264	I1265	K1266	A1267	D1268	G1269	D1270	L1271	K1272	G1273	S1274	G1275	I1276	Y1277	S1278	K1279	K1280	E1281	A1284	T1287	I1288	E1289	N1290	T1291	I1294	E1295	G1296	A1297	K1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	N1308	E1309	S1310	T1311	Q1312	N1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	S1332	I1333	G1334	I1335	M1336	G1337	E1338	K1339	T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	V1218	A1219	M1224	I1225	N1226	S1227	G1228	T1229	E1232	V1235	N1236	K1237	E1238	T1239	S1240	V1241	G1242	I1243	Y1244	T1248	S1249	I1250	S1251	S1252	V1253	S1254	K1255	N1256	K1258	N1259	E1260	G1261	T1262	I1263	E1264	I1265	K1266	A1267	D1268	G1269	D1270	L1271	K1272	G1273	S1274	G1275	I1276	Y1277	S1278	K1279	K1280	E1281	A1284	T1287	I1288	E1289	N1290	T1291	I1294	E1295	G1296	A1297	K1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	N1308	E1309	S1310	T1311	Q1312	N1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	S1332	I1333	G1334	I1335	M1336	G1337	E1338	K1339	T1137	N1138	N1139	N1140	N1141	N1142	N1143	N1144	N1145	N1146	N1147	N1148	N1149	N1150	N1151	N1152	N1153	N1154	N1155	N1156	N1157	N1158	T1162	N1163	I1164	D1165	K1166	G1167	I1168	G1169	I1170	Y1171	T1172	S1173	A1174	N1175	G1176	E1177	I1178	N1179	S1180	G1181	T1182	N1183	T1184	M1185	Q1186	N1187	K1188	N1189	A1190	V1191	L1194	G1195	S1196	K1197	N1200	L1201	K1202	N1203	N1137	N1138	N1139	N1140	N1141	N1142	N1143	N1144	N1145	N1146	N1147	N1148	N1149	N1150	N1151	N1152	N1153	N1154	N1155	N1156	N1157	N1158	T1162	N1163	I1164	D1165	K1166	G1167	I1168	G1169	I1170	Y1171	T1172	S1173	A1174	N1175	G1176	E1177	I1178	N1179	S1180	G1181	T1182	N1183	T1184	M1185	Q1186	N1187	K1188	N1189	A1190	V1191	L1194	G1195	S1196	K1197	N1200	L1201	K1202	N1203	D1075	K1076	I1077	N1078	I1079	V1080	S1081	F1082	G1083	E1084	L1088	F1089	A1090	A1091	T1092	S1093	K1094	A1095	K1096	L1099	D1100	E1101	D1102	Y1103	K1104	V1105	T1106	N1107	G1108	D1109	A1110	I1111	S1112	T1113	A1114	V1115	L1116	A1118	N1119	N1120	G1121	A1122	N1123	V1124	E1125	I1126	A1127	S1128	G1129	K1130	K1131	L1132	E1133	T1134	N1135	T1136	N1137	K1012	I1013	K1016	A1017	Y1021	A1022	D1024	P1025	T1026	K1027	F1028	N1029	M1030	T1031	F1032	K1033	I1034	E1035	S1036	G1037	K1038	T1039	L1040	D1041	E1043	L1044	G1045	K1046	N1047	S1048	T1049	F1050	G1051	L1052	L1053	N1054	M1056	M1057	T1058	V1059	N1061	S1062	P1063	L1064	L1065	S1066	K1067	Y1068	G1069	T1070	N1071	N1072	T1073	S1074	Y949	K950	V951	E952	H953	N954	G955	G956	I957	V958	K959	A960	K961	K962	D963	V964	I965	A966	F967	K970	D971	S972	T973	G974	N977	I978	N979	A980	P981	I982	E983	L984	A985	N986	S987	S988	K989	G990	T991	T992	I995	Y996	S997	D998	G999	N1000	A1001	K1002	V1003	K1004	F1005	G1006	T1007	G1008	S1009	K1010	L1011	S885	F886	S889	G890	T891	I892	E893	V894	T895	S896	A897	K898	H899	K899	K900	N901	K902	A903	V904	V905	L906	D907	G908	T909	S910	A911	S912	N913	K914	I915	F917	T918	N919	E983	L984	A985	N986	S987	S988	K989	G990	T991	T992	I995	Y996	S997	D998	G999	N1000	A1001	K1002	V1003	K1004	F1005	G1006	T1007	G1008	S1009	K1010	L1011	S885	F886	S889	G890	T891	I892	E893	V894	T895	S896	A897	K898	H899	K899	K900	N901	K902	A903	V904	V905	L906	D907	G908	T909	S910	A911	S912	N913	K914	I915	F917	T918	N919	E983	L984	A985	N986	S987	S988	K989	G990	T991	T992	I995	Y996	S997	D998	G999	N1000	A1001	K1002	V1003	K1004	F1005	G1006	T1007	G1008	S1009	K1010	L1011	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q946	E947	N948	T920	S921	G922	N923	N926	T927	S928	D929	N930	N931	N932	T933	N934	L935	D936	G937	N940	I941	G942	I943	Y944	A945	Q
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.460	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.19	0/10944	0.53	2/14805 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1376	ILE	N-CA-C	-5.26	106.30	111.88
1	A	678	ILE	N-CA-C	-5.09	106.70	111.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	ASP	Peptide

### 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	10826	0	10829	644	0
All	All	10826	0	10829	644	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 30.

All (644) 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:A:1126:ILE:HB	1:A:1155:ASN:HA	1.61	0.83
1:A:1235:VAL:HB	1:A:1265:ILE:HG23	1.59	0.82
1:A:882:LYS:HB3	1:A:909:THR:HA	1.62	0.81
1:A:1238:GLU:HB2	1:A:1272:LYS:HB3	1.64	0.78
1:A:439:ILE:HB	1:A:473:ILE:HG22	1.65	0.77
1:A:927:THR:HA	1:A:961:GLY:HA2	1.66	0.77
1:A:797:ILE:HD12	1:A:843:ILE:HG12	1.67	0.77
1:A:587:VAL:HG21	1:A:591:LEU:HD12	1.65	0.76
1:A:1104:LYS:HE3	1:A:1133:GLU:HB3	1.66	0.76
1:A:1030:ASN:O	1:A:1033:LYS:NZ	2.17	0.76
1:A:1383:ILE:HB	1:A:1436:LYS:HD2	1.67	0.76
1:A:1092:THR:HG22	1:A:1119:ASN:HB3	1.67	0.76
1:A:1280:LYS:NZ	1:A:1310:SER:OG	2.18	0.76
1:A:885:SER:HB2	1:A:919:ASN:HA	1.66	0.76
1:A:814:HIS:HA	1:A:827:TYR:HE1	1.51	0.75
1:A:984:LEU:O	1:A:1012:LYS:NZ	2.19	0.74
1:A:1011:LEU:HB3	1:A:1042:VAL:HG22	1.70	0.74
1:A:1079:ILE:O	1:A:1103:TYR:OH	2.04	0.74
1:A:1099:LEU:HD12	1:A:1132:LEU:HD23	1.68	0.74
1:A:427:ARG:HB2	1:A:454:THR:HG21	1.68	0.74
1:A:1453:GLY:HA2	1:A:1457:LYS:HE2	1.70	0.74
1:A:569:ILE:O	1:A:641:ASN:N	2.20	0.73
1:A:739:ASN:O	1:A:794:ASN:ND2	2.20	0.73
1:A:962:LYS:HB3	1:A:988:SER:HB3	1.68	0.73
1:A:627:ASP:OD2	1:A:629:LYS:NZ	2.21	0.72
1:A:1025:PRO:HA	1:A:1028:PHE:HB3	1.72	0.72
1:A:695:GLU:OE2	1:A:750:GLN:NE2	2.22	0.72
1:A:1769:VAL:HG22	1:A:1771:ASN:H	1.54	0.72
1:A:1419:MET:HB2	1:A:1442:MET:HA	1.71	0.71
1:A:1155:ASN:O	1:A:1180:SER:N	2.20	0.71
1:A:1374:GLY:O	1:A:1410:LYS:NZ	2.23	0.71
1:A:1123:ASN:ND2	1:A:1152:VAL:O	2.24	0.71
1:A:1598:ILE:HD13	1:A:1628:ALA:HA	1.74	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:LEU:H	1:A:1224:MET:HA	1.57	0.70
1:A:667:ILE:HB	1:A:744:LEU:HD13	1.74	0.70
1:A:1210:GLU:HA	1:A:1236:ASN:HB2	1.73	0.70
1:A:1454:ALA:HB2	1:A:1487:GLY:HA2	1.73	0.70
1:A:570:ASN:HA	1:A:641:ASN:HB2	1.73	0.69
1:A:1304:ILE:HG23	1:A:1336:MET:H	1.57	0.69
1:A:396:LEU:HD12	1:A:423:VAL:HG22	1.74	0.69
1:A:674:GLN:HB2	1:A:691:LYS:HA	1.74	0.69
1:A:1395:VAL:HG12	1:A:1421:SER:HA	1.74	0.69
1:A:1102:ASP:OD2	1:A:1104:LYS:NZ	2.24	0.69
1:A:1457:LYS:O	1:A:1488:THR:OG1	2.11	0.68
1:A:892:ILE:O	1:A:926:ASN:ND2	2.25	0.68
1:A:909:THR:HG21	1:A:912:SER:HB3	1.75	0.68
1:A:1442:MET:HB2	1:A:1469:ILE:HG22	1.75	0.68
1:A:856:ILE:HA	1:A:910:ASN:HD22	1.58	0.68
1:A:345:SER:O	1:A:347:GLN:NE2	2.27	0.68
1:A:384:ASN:O	1:A:392:ASN:ND2	2.27	0.68
1:A:1133:GLU:OE2	1:A:1162:THR:OG1	2.11	0.67
1:A:1140:LEU:HB3	1:A:1170:ILE:HG22	1.75	0.67
1:A:1066:SER:HA	1:A:1100:ASP:HA	1.75	0.67
1:A:1229:THR:HA	1:A:1261:GLY:HA2	1.76	0.67
1:A:1527:LYS:NZ	1:A:1558:GLU:OE2	2.28	0.67
1:A:951:VAL:HG11	1:A:967:PHE:HZ	1.60	0.67
1:A:303:ILE:HD11	1:A:1498:GLY:HA2	1.76	0.67
1:A:967:PHE:HB2	1:A:995:ILE:HA	1.75	0.67
1:A:514:LEU:HD13	1:A:519:SER:HB3	1.78	0.66
1:A:1496:LYS:HB3	1:A:1526:GLN:HE21	1.61	0.66
1:A:1551:GLY:O	1:A:1579:GLY:N	2.28	0.66
1:A:391:ARG:NH2	1:A:540:TRP:O	2.29	0.66
1:A:1094:LYS:NZ	1:A:1146:THR:OG1	2.29	0.66
1:A:665:ILE:HB	1:A:742:ILE:HA	1.77	0.66
1:A:1308:ASN:HD22	1:A:1339:LYS:HB2	1.60	0.66
1:A:1702:LEU:HG	1:A:1704:ASN:H	1.61	0.66
1:A:1604:ILE:HB	1:A:1636:ILE:HA	1.79	0.66
1:A:562:LYS:NZ	1:A:563:ALA:O	2.29	0.65
1:A:1042:VAL:HB	1:A:1079:ILE:HG23	1.78	0.65
1:A:1636:ILE:O	1:A:1661:THR:OG1	2.15	0.65
1:A:476:ASN:HA	1:A:515:ASN:HD22	1.59	0.65
1:A:750:GLN:HB3	1:A:803:LYS:HG3	1.78	0.65
1:A:1105:VAL:HG23	1:A:1136:THR:HG21	1.77	0.65
1:A:1162:THR:HG23	1:A:1186:GLN:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:THR:HA	1:A:1554:GLU:HB2	1.78	0.65
1:A:913:ASN:O	1:A:916:ASN:ND2	2.30	0.65
1:A:724:ARG:NH1	1:A:725:ASN:O	2.30	0.65
1:A:1572:ASN:HD22	1:A:1600:ASN:HA	1.62	0.64
1:A:649:GLY:N	1:A:698:VAL:O	2.31	0.64
1:A:1412:ASP:OD1	1:A:1436:LYS:NZ	2.29	0.64
1:A:840:GLU:OE2	1:A:862:LYS:NZ	2.31	0.64
1:A:744:LEU:HB2	1:A:799:VAL:HA	1.79	0.64
1:A:1129:GLY:O	1:A:1131:LYS:NZ	2.28	0.64
1:A:1256:ASN:HB2	1:A:1258:LYS:HE3	1.79	0.64
1:A:1679:THR:OG1	1:A:1681:LYS:NZ	2.31	0.64
1:A:604:ARG:HB3	1:A:763:LEU:HA	1.80	0.64
1:A:1165:ASP:OD1	1:A:1189:ASN:ND2	2.30	0.64
1:A:639:ASN:HA	1:A:664:ASN:HB2	1.80	0.64
1:A:855:MET:HB3	1:A:881:GLY:HA2	1.79	0.64
1:A:1688:GLY:H	1:A:1714:GLU:HG3	1.63	0.64
1:A:1069:LEU:HD23	1:A:1103:TYR:HA	1.79	0.63
1:A:758:ASP:OD2	1:A:857:LYS:NZ	2.31	0.63
1:A:1174:ALA:H	1:A:1197:LYS:HB3	1.63	0.63
1:A:1209:LEU:HD12	1:A:1235:VAL:HG22	1.79	0.63
1:A:1289:GLU:HG2	1:A:1320:THR:HG23	1.80	0.63
1:A:508:ASN:HB3	1:A:566:GLN:H	1.64	0.63
1:A:1525:ASN:O	1:A:1557:ASN:ND2	2.31	0.63
1:A:1163:ARG:NH1	1:A:1166:LYS:O	2.32	0.62
1:A:658:GLU:OE1	1:A:733:THR:N	2.32	0.62
1:A:1117:VAL:HG12	1:A:1141:ILE:HB	1.80	0.62
1:A:751:SER:O	1:A:805:TYR:N	2.32	0.62
1:A:848:ASP:HA	1:A:873:ALA:HB1	1.80	0.62
1:A:1461:ILE:HB	1:A:1491:ILE:HB	1.82	0.62
1:A:1700:SER:O	1:A:1725:SER:OG	2.17	0.62
1:A:475:GLY:O	1:A:515:ASN:N	2.29	0.62
1:A:1116:LEU:HG	1:A:1140:LEU:HD13	1.80	0.62
1:A:518:SER:N	1:A:574:SER:O	2.28	0.62
1:A:366:SER:OG	1:A:397:THR:O	2.19	0.61
1:A:1356:GLU:HG3	1:A:1357:LYS:H	1.65	0.61
1:A:815:SER:OG	1:A:834:HIS:ND1	2.29	0.61
1:A:1044:LEU:HD13	1:A:1082:PHE:HE1	1.65	0.61
1:A:1088:LEU:HB2	1:A:1115:VAL:O	2.00	0.61
1:A:385:VAL:O	1:A:414:THR:OG1	2.18	0.61
1:A:882:LYS:NZ	1:A:910:ASN:OD1	2.29	0.61
1:A:1088:LEU:HD13	1:A:1115:VAL:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:HB3	1:A:396:LEU:HA	1.81	0.61
1:A:1536:ASN:ND2	1:A:1538:SER:O	2.34	0.61
1:A:1747:ASP:OD2	1:A:1748:LYS:NZ	2.34	0.61
1:A:1172:THR:HB	1:A:1175:ALA:HB3	1.81	0.61
1:A:1217:VAL:HG13	1:A:1243:ILE:HA	1.82	0.60
1:A:1248:THR:HA	1:A:1281:GLU:HG3	1.83	0.60
1:A:758:ASP:OD1	1:A:786:SER:OG	2.19	0.60
1:A:812:SER:HB3	1:A:814:HIS:NE2	2.15	0.60
1:A:896:SER:O	1:A:899:LYS:NZ	2.33	0.60
1:A:1598:ILE:O	1:A:1629:THR:OG1	2.17	0.60
1:A:1671:MET:HB3	1:A:1694:ILE:HA	1.82	0.60
1:A:800:GLY:O	1:A:804:ASN:ND2	2.34	0.60
1:A:1263:ILE:HB	1:A:1294:ILE:HG22	1.84	0.60
1:A:1376:ILE:HD12	1:A:1409:ILE:HA	1.84	0.60
1:A:447:VAL:HG22	1:A:488:ILE:HD11	1.84	0.60
1:A:808:VAL:HG22	1:A:854:ALA:HB3	1.83	0.60
1:A:859:GLY:N	1:A:883:GLU:OE1	2.34	0.60
1:A:1226:ASN:HB2	1:A:1259:ASN:HA	1.84	0.60
1:A:1623:LEU:HD22	1:A:1654:LEU:HG	1.82	0.60
1:A:750:GLN:HA	1:A:804:ASN:HA	1.83	0.60
1:A:776:GLY:O	1:A:778:ASN:ND2	2.34	0.60
1:A:522:ILE:N	1:A:578:GLY:O	2.33	0.60
1:A:906:LEU:O	1:A:945:ALA:HB2	2.02	0.60
1:A:1179:ASN:HD21	1:A:1207:ILE:HD11	1.67	0.60
1:A:575:GLY:N	1:A:647:SER:OG	2.34	0.60
1:A:1178:GLU:HG2	1:A:1202:LYS:HB3	1.83	0.59
1:A:1304:ILE:HD11	1:A:1319:VAL:HG11	1.84	0.59
1:A:1434:LEU:HB3	1:A:1461:ILE:HG23	1.84	0.59
1:A:1508:SER:HB3	1:A:1537:GLU:HB2	1.84	0.59
1:A:1665:LYS:HB2	1:A:1668:ILE:HD13	1.84	0.59
1:A:642:ILE:HB	1:A:667:ILE:HA	1.84	0.59
1:A:752:ILE:HG13	1:A:805:TYR:HB2	1.83	0.59
1:A:724:ARG:HD2	1:A:725:ASN:O	2.02	0.59
1:A:1335:ILE:HB	1:A:1362:ILE:HA	1.85	0.59
1:A:763:LEU:HB2	1:A:781:ARG:HB3	1.85	0.59
1:A:576:SER:OG	1:A:577:PHE:N	2.34	0.59
1:A:807:PHE:O	1:A:853:PHE:HA	2.03	0.59
1:A:370:ASN:ND2	1:A:374:GLY:O	2.36	0.58
1:A:1327:MET:HE1	1:A:1356:GLU:HB3	1.85	0.58
1:A:1704:ASN:HD22	1:A:1730:ASN:HA	1.68	0.58
1:A:1013:ILE:HB	1:A:1044:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LEU:HB2	1:A:800:GLY:H	1.68	0.58
1:A:1572:ASN:ND2	1:A:1600:ASN:OD1	2.36	0.58
1:A:1654:LEU:HD22	1:A:1671:MET:HE1	1.85	0.58
1:A:1572:ASN:ND2	1:A:1599:ILE:O	2.36	0.58
1:A:370:ASN:OD1	1:A:373:GLN:NE2	2.34	0.58
1:A:714:LYS:HD2	1:A:724:ARG:HH12	1.68	0.58
1:A:806:GLY:N	1:A:851:VAL:O	2.25	0.58
1:A:1201:LEU:O	1:A:1225:ILE:N	2.36	0.58
1:A:1344:ASN:ND2	1:A:1375:ARG:O	2.34	0.58
1:A:898:LYS:O	1:A:899:LYS:NZ	2.37	0.57
1:A:1219:ALA:N	1:A:1244:TYR:O	2.36	0.57
1:A:815:SER:OG	1:A:817:LYS:NZ	2.31	0.57
1:A:1051:GLY:O	1:A:1090:TYR:N	2.37	0.57
1:A:1276:ILE:HG13	1:A:1304:ILE:HA	1.85	0.57
1:A:1050:PHE:CZ	1:A:1079:ILE:HB	2.40	0.57
1:A:744:LEU:HD23	1:A:799:VAL:HG12	1.86	0.57
1:A:1059:VAL:HG21	1:A:1095:ALA:HA	1.85	0.57
1:A:1702:LEU:O	1:A:1729:THR:OG1	2.22	0.57
1:A:666:ASN:OD1	1:A:743:SER:OG	2.22	0.57
1:A:1278:SER:C	1:A:1279:LYS:HD3	2.30	0.57
1:A:1747:ASP:HA	1:A:1770:LYS:HD3	1.85	0.57
1:A:1070:ASN:HA	1:A:1101:GLU:HB2	1.87	0.57
1:A:1141:ILE:HG23	1:A:1171:TYR:HD2	1.69	0.57
1:A:602:ASN:OD1	1:A:604:ARG:NH1	2.37	0.57
1:A:645:ASP:HA	1:A:694:VAL:HG23	1.86	0.57
1:A:746:GLU:O	1:A:802:LYS:NZ	2.33	0.56
1:A:1243:ILE:HB	1:A:1276:ILE:HG22	1.86	0.56
1:A:1259:ASN:ND2	1:A:1290:ASN:OD1	2.38	0.56
1:A:454:THR:HG22	1:A:456:GLN:H	1.69	0.56
1:A:1046:LYS:NZ	1:A:1084:GLU:O	2.35	0.56
1:A:493:ASN:HA	1:A:525:LYS:HD3	1.86	0.56
1:A:1021:TYR:CE1	1:A:1052:LEU:HD22	2.41	0.56
1:A:1530:VAL:HG13	1:A:1563:VAL:HA	1.86	0.56
1:A:567:LYS:HG3	1:A:568:ASP:H	1.71	0.56
1:A:554:LYS:HB2	1:A:610:ASP:HB2	1.88	0.56
1:A:585:GLU:O	1:A:602:ASN:ND2	2.37	0.56
1:A:1264:GLU:HA	1:A:1295:GLU:HB3	1.87	0.56
1:A:1462:LYS:O	1:A:1496:LYS:NZ	2.34	0.56
1:A:1322:SER:HA	1:A:1345:THR:HB	1.88	0.56
1:A:816:SER:HB3	1:A:825:LEU:HD11	1.88	0.56
1:A:1025:PRO:HG2	1:A:1059:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:ASN:OD1	1:A:1180:SER:OG	2.22	0.56
1:A:360:ASP:O	1:A:391:ARG:NH1	2.39	0.56
1:A:697:ALA:O	1:A:752:ILE:N	2.32	0.56
1:A:1265:ILE:HB	1:A:1296:VAL:HA	1.88	0.56
1:A:1325:VAL:N	1:A:1351:GLY:O	2.34	0.56
1:A:1607:GLU:O	1:A:1640:THR:OG1	2.18	0.56
1:A:1137:ASN:OD1	1:A:1163:ARG:NH1	2.39	0.56
1:A:1265:ILE:HD12	1:A:1296:VAL:HG22	1.88	0.56
1:A:977:ASN:OD1	1:A:979:ASN:ND2	2.39	0.55
1:A:1166:LYS:HD2	1:A:1189:ASN:HB3	1.88	0.55
1:A:882:LYS:O	1:A:909:THR:OG1	2.23	0.55
1:A:1288:ILE:HB	1:A:1319:VAL:HG12	1.86	0.55
1:A:479:TYR:HB2	1:A:484:ASN:HD21	1.71	0.55
1:A:770:GLU:HG3	1:A:827:TYR:HB3	1.89	0.55
1:A:1162:THR:O	1:A:1187:ASN:ND2	2.40	0.55
1:A:1574:GLY:HA3	1:A:1579:GLY:HA3	1.88	0.55
1:A:458:SER:OG	1:A:461:THR:OG1	2.14	0.55
1:A:1611:PRO:HD3	1:A:1640:THR:HG23	1.88	0.55
1:A:1338:GLU:OE1	1:A:1366:ASN:ND2	2.40	0.55
1:A:1674:ASP:OD1	1:A:1698:ASN:ND2	2.40	0.55
1:A:648:ILE:HD13	1:A:698:VAL:HB	1.88	0.55
1:A:1607:GLU:OE1	1:A:1608:ILE:N	2.40	0.55
1:A:1454:ALA:O	1:A:1457:LYS:NZ	2.39	0.55
1:A:734:GLU:HG2	1:A:735:THR:HG23	1.88	0.54
1:A:899:LYS:HE3	1:A:937:GLY:HA2	1.89	0.54
1:A:1289:GLU:OE2	1:A:1322:SER:N	2.36	0.54
1:A:681:LEU:HG	1:A:682:PRO:HD2	1.89	0.54
1:A:851:VAL:HG23	1:A:877:ILE:HG23	1.87	0.54
1:A:1423:GLY:N	1:A:1446:ASN:OD1	2.40	0.54
1:A:1600:ASN:HB3	1:A:1634:GLY:HA3	1.89	0.54
1:A:1044:LEU:HB2	1:A:1082:PHE:CD1	2.42	0.54
1:A:569:ILE:HB	1:A:640:ILE:HA	1.90	0.54
1:A:507:VAL:HA	1:A:566:GLN:HE21	1.73	0.54
1:A:553:ASN:OD1	1:A:554:LYS:N	2.39	0.54
1:A:1147:VAL:HG13	1:A:1148:GLY:H	1.71	0.54
1:A:385:VAL:HG11	1:A:420:ALA:HA	1.90	0.54
1:A:971:ASP:O	1:A:1000:ASN:HB2	2.07	0.54
1:A:1007:THR:HG23	1:A:1038:LYS:HA	1.89	0.54
1:A:1336:MET:HE3	1:A:1337:GLY:H	1.73	0.54
1:A:1263:ILE:O	1:A:1295:GLU:N	2.30	0.54
1:A:793:SER:HA	1:A:842:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:LYS:HE2	1:A:907:ASP:HB3	1.88	0.54
1:A:1154:LYS:HE3	1:A:1156:ASN:HD21	1.73	0.54
1:A:1382:SER:O	1:A:1384:SER:N	2.40	0.54
1:A:372:HIS:ND1	1:A:398:ARG:O	2.41	0.54
1:A:398:ARG:HH22	1:A:427:ARG:HH21	1.54	0.54
1:A:1209:LEU:HB2	1:A:1235:VAL:HA	1.89	0.54
1:A:1423:GLY:N	1:A:1447:ALA:HB2	2.23	0.54
1:A:1308:ASN:HB3	1:A:1339:LYS:HB2	1.88	0.53
1:A:1241:VAL:HG23	1:A:1274:ALA:HB3	1.91	0.53
1:A:1382:SER:C	1:A:1384:SER:H	2.16	0.53
1:A:1651:ASN:HA	1:A:1676:SER:HA	1.89	0.53
1:A:943:ILE:N	1:A:966:ALA:O	2.41	0.53
1:A:1024:ASP:OD2	1:A:1027:LYS:NZ	2.40	0.53
1:A:1324:LEU:HD21	1:A:1326:LYS:HD3	1.90	0.53
1:A:1621:ILE:O	1:A:1647:TYR:N	2.41	0.53
1:A:454:THR:O	1:A:502:THR:OG1	2.24	0.53
1:A:915:ILE:O	1:A:917:PHE:N	2.42	0.53
1:A:373:GLN:HE22	1:A:376:LYS:HA	1.72	0.53
1:A:500:ASN:HA	1:A:559:VAL:HA	1.91	0.53
1:A:1554:GLU:HG3	1:A:1556:LYS:HZ3	1.72	0.53
1:A:1195:GLY:HA3	1:A:1201:LEU:HD21	1.91	0.53
1:A:1357:LYS:HG2	1:A:1388:ASP:HA	1.90	0.53
1:A:833:HIS:HB3	1:A:834:HIS:CE1	2.43	0.53
1:A:1010:LYS:NZ	1:A:1043:GLU:OE1	2.33	0.53
1:A:1279:LYS:HA	1:A:1307:LYS:HB2	1.91	0.53
1:A:331:SER:HG	1:A:991:THR:HG1	1.55	0.53
1:A:476:ASN:HA	1:A:515:ASN:ND2	2.24	0.52
1:A:797:ILE:HB	1:A:843:ILE:HA	1.91	0.52
1:A:1271:GLY:N	1:A:1299:LYS:O	2.42	0.52
1:A:582:VAL:HA	1:A:653:LEU:HD12	1.90	0.52
1:A:1339:LYS:HG2	1:A:1366:ASN:HB3	1.92	0.52
1:A:1099:LEU:CD2	1:A:1126:ILE:HA	2.39	0.52
1:A:1306:ALA:H	1:A:1337:GLY:HA2	1.75	0.52
1:A:1530:VAL:HG11	1:A:1533:TYR:HD2	1.75	0.52
1:A:752:ILE:HA	1:A:805:TYR:O	2.08	0.52
1:A:1025:PRO:HD3	1:A:1055:GLY:HA2	1.91	0.52
1:A:549:ASN:OD1	1:A:551:THR:HG23	2.10	0.52
1:A:1084:GLU:OE2	1:A:1113:THR:OG1	2.19	0.52
1:A:376:LYS:HB3	1:A:379:TRP:NE1	2.25	0.52
1:A:752:ILE:HG21	1:A:755:LEU:HB2	1.92	0.52
1:A:1069:LEU:HD22	1:A:1103:TYR:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:GLU:O	1:A:1682:ASN:ND2	2.43	0.52
1:A:538:ASN:OD1	1:A:542:ALA:N	2.38	0.52
1:A:622:ARG:HB3	1:A:709:VAL:HG22	1.92	0.52
1:A:1168:ILE:HA	1:A:1191:VAL:HB	1.92	0.52
1:A:1364:VAL:HB	1:A:1368:SER:HB2	1.91	0.52
1:A:1473:ILE:HD11	1:A:1514:LEU:HB2	1.91	0.52
1:A:562:LYS:HZ1	1:A:635:TYR:HB3	1.73	0.51
1:A:907:ASP:CG	1:A:908:GLY:H	2.17	0.51
1:A:1243:ILE:N	1:A:1275:GLY:O	2.38	0.51
1:A:1433:ALA:HA	1:A:1460:PHE:O	2.09	0.51
1:A:1088:LEU:HD22	1:A:1115:VAL:HG13	1.91	0.51
1:A:1409:ILE:HD13	1:A:1432:ILE:HG13	1.93	0.51
1:A:1073:THR:HG22	1:A:1074:SER:H	1.75	0.51
1:A:1344:ASN:O	1:A:1374:GLY:HA3	2.10	0.51
1:A:1403:ASN:OD1	1:A:1429:ALA:N	2.43	0.51
1:A:1686:LEU:HD23	1:A:1691:ALA:HB1	1.93	0.51
1:A:330:LEU:HD13	1:A:1052:LEU:HD11	1.92	0.51
1:A:488:ILE:HG22	1:A:520:ALA:HB3	1.93	0.51
1:A:881:GLY:O	1:A:906:LEU:HA	2.11	0.51
1:A:1426:ILE:HD11	1:A:1449:VAL:HG22	1.93	0.51
1:A:617:GLY:O	1:A:654:GLN:NE2	2.44	0.51
1:A:950:LYS:HD3	1:A:977:ASN:HB2	1.92	0.51
1:A:459:ILE:HD13	1:A:719:ASN:HD21	1.76	0.51
1:A:797:ILE:HG22	1:A:799:VAL:HG13	1.93	0.51
1:A:1372:ASN:HB3	1:A:1376:ILE:HD11	1.92	0.51
1:A:412:ASN:HA	1:A:440:ASN:HB2	1.92	0.51
1:A:811:ASN:O	1:A:857:LYS:HG3	2.10	0.51
1:A:662:ALA:HA	1:A:740:GLY:HA3	1.92	0.50
1:A:1093:SER:H	1:A:1120:ASN:HB3	1.76	0.50
1:A:1590:ILE:N	1:A:1620:GLY:O	2.30	0.50
1:A:404:THR:HB	1:A:433:VAL:HB	1.93	0.50
1:A:589:LYS:HA	1:A:592:PHE:HB2	1.93	0.50
1:A:789:ILE:HB	1:A:807:PHE:HZ	1.76	0.50
1:A:387:GLU:HA	1:A:418:ASN:HB3	1.93	0.50
1:A:768:LEU:HB3	1:A:775:LYS:HB2	1.94	0.50
1:A:831:LYS:HA	1:A:836:LYS:HD3	1.94	0.50
1:A:521:GLY:N	1:A:577:PHE:O	2.32	0.50
1:A:604:ARG:HD2	1:A:762:ASP:O	2.12	0.50
1:A:742:ILE:HG23	1:A:797:ILE:HA	1.92	0.50
1:A:803:LYS:HB3	1:A:849:GLU:OE2	2.11	0.50
1:A:711:PRO:HD3	1:A:730:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:SER:OG	1:A:1540:HIS:ND1	2.40	0.50
1:A:1621:ILE:HB	1:A:1646:MET:HA	1.92	0.50
1:A:1118:ALA:HB3	1:A:1142:ALA:HA	1.93	0.50
1:A:1446:ASN:HB2	1:A:1479:ALA:HB3	1.94	0.50
1:A:1408:GLU:O	1:A:1410:LYS:NZ	2.33	0.50
1:A:857:LYS:HB3	1:A:911:ALA:HB3	1.93	0.50
1:A:1493:GLY:O	1:A:1557:ASN:ND2	2.44	0.49
1:A:356:ASP:HB2	1:A:388:LEU:HD13	1.95	0.49
1:A:550:LYS:NZ	1:A:601:GLU:OE1	2.45	0.49
1:A:844:ASN:OD1	1:A:870:LYS:HB2	2.12	0.49
1:A:996:TYR:HE1	1:A:1022:SER:HA	1.76	0.49
1:A:1513:LYS:HA	1:A:1544:GLU:HB3	1.92	0.49
1:A:1044:LEU:HB2	1:A:1082:PHE:HD1	1.77	0.49
1:A:909:THR:HB	1:A:915:ILE:HA	1.95	0.49
1:A:1118:ALA:N	1:A:1141:ILE:O	2.29	0.49
1:A:1327:MET:HG2	1:A:1354:ILE:HG23	1.93	0.49
1:A:1343:THR:HA	1:A:1371:ILE:HB	1.93	0.49
1:A:443:ARG:HB2	1:A:446:ASN:HD21	1.76	0.49
1:A:1013:ILE:HG23	1:A:1017:ALA:HB3	1.94	0.49
1:A:853:PHE:HB3	1:A:879:PHE:CD1	2.48	0.49
1:A:1503:TYR:HD1	1:A:1533:TYR:HB3	1.77	0.49
1:A:761:ILE:HB	1:A:783:LEU:HB3	1.95	0.49
1:A:1695:PHE:HA	1:A:1721:TYR:HB3	1.94	0.49
1:A:469:ASN:OD1	1:A:509:LYS:N	2.46	0.49
1:A:736:VAL:HB	1:A:789:ILE:HA	1.93	0.49
1:A:1342:ILE:O	1:A:1371:ILE:N	2.34	0.49
1:A:581:THR:OG1	1:A:652:LEU:HD12	2.13	0.49
1:A:803:LYS:HA	1:A:850:SER:HA	1.94	0.49
1:A:1178:GLU:HA	1:A:1202:LYS:O	2.13	0.49
1:A:1244:TYR:CE2	1:A:1279:LYS:HE3	2.48	0.49
1:A:1689:LYS:NZ	1:A:1716:GLU:OE1	2.33	0.49
1:A:667:ILE:O	1:A:745:GLY:N	2.25	0.48
1:A:1073:THR:O	1:A:1076:LYS:NZ	2.45	0.48
1:A:853:PHE:O	1:A:879:PHE:HA	2.13	0.48
1:A:856:ILE:HG23	1:A:857:LYS:HG2	1.95	0.48
1:A:893:GLU:OE2	1:A:926:ASN:ND2	2.46	0.48
1:A:1084:GLU:HG2	1:A:1108:GLY:HA3	1.94	0.48
1:A:1527:LYS:HD3	1:A:1557:ASN:ND2	2.28	0.48
1:A:658:GLU:CD	1:A:733:THR:H	2.22	0.48
1:A:970:LYS:NZ	1:A:998:ASP:OD2	2.45	0.48
1:A:1502:ILE:HB	1:A:1532:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:VAL:HA	1:A:566:GLN:NE2	2.29	0.48
1:A:777:SER:O	1:A:779:VAL:N	2.47	0.48
1:A:935:LEU:HD22	1:A:962:LYS:HB2	1.96	0.48
1:A:1392:GLY:N	1:A:1417:THR:O	2.39	0.48
1:A:475:GLY:N	1:A:513:THR:O	2.44	0.48
1:A:600:TYR:CZ	1:A:602:ASN:HB2	2.49	0.48
1:A:698:VAL:HG22	1:A:752:ILE:HB	1.95	0.48
1:A:951:VAL:HG22	1:A:953:HIS:HD1	1.78	0.48
1:A:1423:GLY:H	1:A:1447:ALA:HB2	1.79	0.48
1:A:1518:ASN:ND2	1:A:1549:ASN:OD1	2.46	0.48
1:A:1581:ILE:HG13	1:A:1605:LYS:NZ	2.29	0.48
1:A:1712:THR:OG1	1:A:1737:GLU:OE2	2.27	0.48
1:A:519:SER:H	1:A:576:SER:HB2	1.79	0.48
1:A:534:PRO:HA	1:A:547:ILE:HA	1.95	0.48
1:A:698:VAL:HG22	1:A:752:ILE:HD13	1.95	0.48
1:A:736:VAL:HB	1:A:789:ILE:HG12	1.96	0.48
1:A:1069:LEU:HD22	1:A:1103:TYR:CD1	2.49	0.48
1:A:1101:GLU:O	1:A:1131:LYS:N	2.37	0.48
1:A:905:VAL:HG13	1:A:944:TYR:HD2	1.78	0.47
1:A:940:ASN:HB2	1:A:964:VAL:HG22	1.96	0.47
1:A:1718:VAL:HG12	1:A:1742:ALA:HB3	1.95	0.47
1:A:386:THR:C	1:A:418:ASN:HD22	2.21	0.47
1:A:1277:TYR:CE2	1:A:1279:LYS:HD2	2.49	0.47
1:A:1552:LYS:HA	1:A:1579:GLY:H	1.80	0.47
1:A:1555:VAL:HB	1:A:1582:VAL:HA	1.94	0.47
1:A:715:ASP:O	1:A:724:ARG:HD3	2.15	0.47
1:A:1536:ASN:HD22	1:A:1567:LYS:HB3	1.79	0.47
1:A:441:LEU:HD11	1:A:448:GLY:HA2	1.96	0.47
1:A:1025:PRO:HB2	1:A:1063:PRO:HG3	1.95	0.47
1:A:1026:THR:HA	1:A:1061:ASN:O	2.14	0.47
1:A:1518:ASN:O	1:A:1551:GLY:N	2.47	0.47
1:A:323:GLN:HG2	1:A:1166:LYS:HB3	1.97	0.47
1:A:1074:SER:C	1:A:1076:LYS:H	2.21	0.47
1:A:1713:LYS:O	1:A:1738:LYS:NZ	2.48	0.47
1:A:475:GLY:HA3	1:A:514:LEU:HD23	1.96	0.47
1:A:644:GLY:HA2	1:A:679:SER:HB2	1.97	0.47
1:A:877:ILE:HD13	1:A:902:LYS:HB2	1.96	0.47
1:A:1194:LEU:HD13	1:A:1218:TYR:HB3	1.96	0.47
1:A:1243:ILE:HD12	1:A:1276:ILE:HG22	1.96	0.47
1:A:1291:THR:O	1:A:1350:LYS:NZ	2.42	0.47
1:A:1628:ALA:O	1:A:1655:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLY:N	1:A:546:GLN:O	2.48	0.47
1:A:571:LEU:HB2	1:A:642:ILE:HD13	1.96	0.47
1:A:1395:VAL:O	1:A:1422:SER:OG	2.25	0.47
1:A:661:LEU:O	1:A:739:ASN:N	2.39	0.47
1:A:1332:SER:O	1:A:1359:SER:HA	2.15	0.47
1:A:1403:ASN:OD1	1:A:1430:GLY:N	2.38	0.47
1:A:608:THR:OG1	1:A:612:GLU:O	2.24	0.47
1:A:737:GLU:OE2	1:A:792:LYS:HG2	2.15	0.47
1:A:982:ILE:HG21	1:A:1011:LEU:HD12	1.96	0.47
1:A:1073:THR:HG22	1:A:1074:SER:N	2.30	0.47
1:A:1421:SER:HB3	1:A:1444:ALA:HA	1.97	0.47
1:A:381:LYS:NZ	1:A:409:GLN:HE21	2.14	0.46
1:A:639:ASN:ND2	1:A:641:ASN:OD1	2.49	0.46
1:A:951:VAL:HG11	1:A:967:PHE:CZ	2.45	0.46
1:A:1016:LYS:HA	1:A:1047:ASN:O	2.15	0.46
1:A:1502:ILE:HG21	1:A:1516:VAL:HG21	1.96	0.46
1:A:1515:SER:OG	1:A:1546:ASP:OD2	2.31	0.46
1:A:375:TRP:H	1:A:403:SER:HB2	1.79	0.46
1:A:622:ARG:N	1:A:716:THR:OG1	2.49	0.46
1:A:754:ALA:HB3	1:A:807:PHE:CD1	2.50	0.46
1:A:953:HIS:HD2	1:A:980:ALA:HB3	1.79	0.46
1:A:1110:ALA:C	1:A:1137:ASN:HD22	2.23	0.46
1:A:1134:THR:O	1:A:1162:THR:N	2.44	0.46
1:A:1137:ASN:HA	1:A:1163:ARG:HD2	1.97	0.46
1:A:1152:VAL:HA	1:A:1176:ASN:O	2.15	0.46
1:A:1461:ILE:N	1:A:1490:ASP:O	2.38	0.46
1:A:1502:ILE:N	1:A:1531:GLY:O	2.48	0.46
1:A:882:LYS:HG3	1:A:910:ASN:ND2	2.31	0.46
1:A:953:HIS:NE2	1:A:978:ILE:HG23	2.31	0.46
1:A:1318:GLU:HA	1:A:1340:SER:HA	1.98	0.46
1:A:1513:LYS:HD3	1:A:1544:GLU:HA	1.97	0.46
1:A:1542:ASN:HD21	1:A:1597:GLU:HG2	1.80	0.46
1:A:512:ILE:HD13	1:A:569:ILE:HD13	1.98	0.46
1:A:783:LEU:HG	1:A:785:ARG:HD2	1.97	0.46
1:A:1006:GLY:HA2	1:A:1038:LYS:HB3	1.97	0.46
1:A:1169:GLY:N	1:A:1191:VAL:O	2.48	0.46
1:A:1593:LYS:N	1:A:1596:SER:OG	2.48	0.46
1:A:338:VAL:HG12	1:A:341:PRO:HD3	1.97	0.46
1:A:376:LYS:HB3	1:A:379:TRP:HE1	1.81	0.46
1:A:1033:LYS:HA	1:A:1067:LYS:NZ	2.31	0.46
1:A:1635:VAL:HA	1:A:1659:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1685:THR:HG22	1:A:1711:THR:HB	1.97	0.46
1:A:540:TRP:HA	1:A:545:LEU:HD21	1.97	0.46
1:A:962:LYS:HA	1:A:992:THR:HG22	1.97	0.46
1:A:526:PRO:HG3	1:A:620:ILE:HD11	1.98	0.46
1:A:649:GLY:HA3	1:A:699:GLY:HA2	1.98	0.46
1:A:355:VAL:H	1:A:493:ASN:ND2	2.13	0.46
1:A:879:PHE:HB2	1:A:904:VAL:HG23	1.97	0.46
1:A:1174:ALA:N	1:A:1197:LYS:HB3	2.30	0.46
1:A:1702:LEU:HG	1:A:1704:ASN:N	2.29	0.45
1:A:981:PRO:HA	1:A:1010:LYS:H	1.82	0.45
1:A:292:ILE:O	1:A:1721:TYR:OH	2.33	0.45
1:A:831:LYS:HA	1:A:836:LYS:CD	2.47	0.45
1:A:941:ILE:HD12	1:A:944:TYR:HB2	1.99	0.45
1:A:714:LYS:HB3	1:A:724:ARG:CZ	2.46	0.45
1:A:1147:VAL:O	1:A:1149:PHE:N	2.47	0.45
1:A:1184:THR:HG22	1:A:1208:GLU:HG2	1.99	0.45
1:A:1226:ASN:HD21	1:A:1243:ILE:HD11	1.82	0.45
1:A:1267:ALA:HB3	1:A:1298:GLN:CD	2.41	0.45
1:A:1716:GLU:HA	1:A:1740:THR:O	2.17	0.45
1:A:560:LEU:HB3	1:A:632:SER:OG	2.17	0.45
1:A:714:LYS:HD2	1:A:724:ARG:NH1	2.30	0.45
1:A:882:LYS:HD2	1:A:908:GLY:O	2.17	0.45
1:A:1308:ASN:H	1:A:1338:GLU:HB2	1.81	0.45
1:A:333:THR:O	1:A:1021:TYR:OH	2.22	0.45
1:A:617:GLY:HA3	1:A:785:ARG:HH12	1.81	0.45
1:A:1044:LEU:HD23	1:A:1048:SER:HB2	1.97	0.45
1:A:1154:LYS:HG3	1:A:1178:GLU:OE1	2.15	0.45
1:A:1726:LEU:HG	1:A:1727:LYS:HG2	1.99	0.45
1:A:1739:LYS:C	1:A:1740:THR:HG1	2.20	0.45
1:A:1043:GLU:C	1:A:1044:LEU:HD12	2.41	0.45
1:A:674:GLN:NE2	1:A:690:ASP:O	2.39	0.45
1:A:1336:MET:SD	1:A:1363:LEU:HB3	2.57	0.45
1:A:1469:ILE:HD11	1:A:1485:ASN:HD21	1.82	0.45
1:A:1742:ALA:HA	1:A:1765:ALA:O	2.16	0.45
1:A:710:LYS:HE2	1:A:730:LEU:HD13	1.99	0.45
1:A:798:ASN:HA	1:A:844:ASN:HB3	1.97	0.44
1:A:629:LYS:HE2	1:A:630:TYR:OH	2.17	0.44
1:A:784:LYS:HB3	1:A:814:HIS:HB3	1.99	0.44
1:A:330:LEU:HD21	1:A:1090:TYR:CD2	2.52	0.44
1:A:1280:LYS:HE2	1:A:1308:ASN:OD1	2.18	0.44
1:A:1669:VAL:HG22	1:A:1692:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:HIS:HA	1:A:827:TYR:CE1	2.41	0.44
1:A:1074:SER:HA	1:A:1076:LYS:NZ	2.33	0.44
1:A:1130:LYS:O	1:A:1158:THR:N	2.50	0.44
1:A:1588:ALA:HB1	1:A:1591:ILE:HD11	1.99	0.44
1:A:917:PHE:HE2	1:A:951:VAL:HA	1.82	0.44
1:A:1248:THR:OG1	1:A:1249:SER:N	2.49	0.44
1:A:1256:ASN:HA	1:A:1287:THR:O	2.18	0.44
1:A:569:ILE:N	1:A:639:ASN:O	2.38	0.44
1:A:903:ALA:H	1:A:941:ILE:HG12	1.82	0.44
1:A:1372:ASN:C	1:A:1408:GLU:H	2.25	0.44
1:A:1426:ILE:O	1:A:1450:THR:OG1	2.24	0.44
1:A:469:ASN:C	1:A:509:LYS:HB3	2.43	0.44
1:A:455:HIS:C	1:A:499:ASN:HB2	2.43	0.44
1:A:1162:THR:HG22	1:A:1187:ASN:ND2	2.33	0.44
1:A:1239:THR:N	1:A:1272:LYS:O	2.51	0.44
1:A:360:ASP:OD2	1:A:360:ASP:N	2.51	0.44
1:A:491:GLY:HA2	1:A:523:GLN:H	1.83	0.44
1:A:1279:LYS:HG3	1:A:1307:LYS:HG3	1.99	0.44
1:A:327:ILE:HG12	1:A:1117:VAL:HG21	1.99	0.43
1:A:526:PRO:HG2	1:A:654:GLN:HG2	1.98	0.43
1:A:1296:VAL:O	1:A:1328:SER:N	2.51	0.43
1:A:869:VAL:HG12	1:A:871:ASP:H	1.83	0.43
1:A:1437:LYS:HD2	1:A:1465:LYS:HE2	2.00	0.43
1:A:1448:ASN:N	1:A:1481:LYS:HE2	2.33	0.43
1:A:959:LYS:HB3	1:A:959:LYS:HE3	1.81	0.43
1:A:1308:ASN:O	1:A:1312:GLN:NE2	2.51	0.43
1:A:1454:ALA:HA	1:A:1488:THR:HG23	2.00	0.43
1:A:554:LYS:NZ	1:A:610:ASP:O	2.41	0.43
1:A:770:GLU:O	1:A:775:LYS:NZ	2.44	0.43
1:A:1547:VAL:HB	1:A:1570:VAL:HA	2.01	0.43
1:A:351:VAL:O	1:A:353:PHE:N	2.51	0.43
1:A:645:ASP:OD2	1:A:689:TYR:HB3	2.19	0.43
1:A:330:LEU:HD21	1:A:1090:TYR:CG	2.53	0.43
1:A:459:ILE:HD13	1:A:719:ASN:ND2	2.34	0.43
1:A:982:ILE:HG22	1:A:1010:LYS:O	2.19	0.43
1:A:1130:LYS:HA	1:A:1130:LYS:HD3	1.76	0.43
1:A:1422:SER:HA	1:A:1445:THR:O	2.19	0.43
1:A:1565:ALA:HB1	1:A:1568:TYR:HB2	2.00	0.43
1:A:1630:ASN:O	1:A:1657:GLU:HB3	2.18	0.43
1:A:573:GLY:O	1:A:644:GLY:HA3	2.19	0.43
1:A:1147:VAL:HG13	1:A:1148:GLY:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:SER:O	1:A:1307:LYS:N	2.47	0.43
1:A:1302:ALA:HB2	1:A:1333:ILE:HB	2.01	0.43
1:A:386:THR:OG1	1:A:390:ASN:HB3	2.19	0.43
1:A:473:ILE:HD12	1:A:489:ALA:HB1	2.01	0.43
1:A:1001:ALA:O	1:A:1031:THR:HA	2.19	0.43
1:A:423:VAL:HG12	1:A:426:VAL:HG21	2.00	0.43
1:A:508:ASN:ND2	1:A:565:ASN:OD1	2.30	0.43
1:A:987:SER:HB3	1:A:992:THR:HG23	2.00	0.43
1:A:1013:ILE:N	1:A:1043:GLU:O	2.41	0.43
1:A:1319:VAL:HG22	1:A:1340:SER:HB3	2.01	0.43
1:A:1411:VAL:O	1:A:1436:LYS:HG2	2.19	0.43
1:A:444:SER:HB3	1:A:486:GLU:HG2	2.01	0.43
1:A:863:SER:O	1:A:889:SER:N	2.52	0.43
1:A:1299:LYS:HB3	1:A:1331:ASN:HB3	2.00	0.43
1:A:1588:ALA:CB	1:A:1591:ILE:HD11	2.49	0.43
1:A:1699:SER:HA	1:A:1725:SER:HA	2.00	0.43
1:A:1065:LEU:HD11	1:A:1068:TYR:CE2	2.54	0.42
1:A:1405:ALA:O	1:A:1431:LYS:NZ	2.37	0.42
1:A:445:GLN:HG3	1:A:486:GLU:HG3	2.01	0.42
1:A:651:GLY:HA2	1:A:701:PHE:HB3	1.99	0.42
1:A:860:ASN:ND2	1:A:885:SER:O	2.47	0.42
1:A:949:TYR:OH	1:A:974:GLY:HA3	2.18	0.42
1:A:490:PHE:O	1:A:522:ILE:HA	2.20	0.42
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.52	0.42
1:A:1330:GLU:HB2	1:A:1357:LYS:HB2	2.01	0.42
1:A:1356:GLU:OE2	1:A:1357:LYS:NZ	2.53	0.42
1:A:1611:PRO:HB3	1:A:1616:ASP:O	2.19	0.42
1:A:496:ASP:OD2	1:A:539:TYR:OH	2.27	0.42
1:A:661:LEU:HB2	1:A:738:ILE:HG23	2.00	0.42
1:A:1178:GLU:OE2	1:A:1204:THR:OG1	2.38	0.42
1:A:1689:LYS:HE3	1:A:1690:LYS:HG3	2.02	0.42
1:A:517:PRO:HG2	1:A:677:ASP:HA	2.01	0.42
1:A:589:LYS:HD2	1:A:589:LYS:N	2.35	0.42
1:A:830:ASP:OD2	1:A:833:HIS:N	2.35	0.42
1:A:965:ILE:HG21	1:A:996:TYR:HB3	2.02	0.42
1:A:1088:LEU:HD21	1:A:1103:TYR:HD2	1.85	0.42
1:A:1099:LEU:HD12	1:A:1132:LEU:CD2	2.43	0.42
1:A:1239:THR:HG22	1:A:1272:LYS:HG2	2.00	0.42
1:A:1553:ILE:O	1:A:1581:ILE:HB	2.19	0.42
1:A:460:SER:O	1:A:625:LEU:HD22	2.19	0.42
1:A:562:LYS:HD2	1:A:633:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:TYR:CD1	1:A:660:LYS:HG3	2.54	0.42
1:A:719:ASN:HB2	1:A:723:ALA:HB3	2.01	0.42
1:A:1331:ASN:HA	1:A:1358:LYS:HB3	2.01	0.42
1:A:856:ILE:HG13	1:A:910:ASN:HB2	2.02	0.42
1:A:1248:THR:HG23	1:A:1250:ILE:H	1.85	0.42
1:A:413:VAL:HG12	1:A:420:ALA:HB2	2.01	0.42
1:A:435:PHE:O	1:A:470:SER:N	2.49	0.42
1:A:632:SER:O	1:A:657:GLN:HB3	2.19	0.42
1:A:839:ASN:O	1:A:864:SER:OG	2.29	0.42
1:A:1185:MET:SD	1:A:1185:MET:N	2.93	0.42
1:A:1367:GLU:H	1:A:1399:SER:CB	2.33	0.42
1:A:962:LYS:O	1:A:964:VAL:HG23	2.20	0.42
1:A:1251:SER:OG	1:A:1253:VAL:HG12	2.20	0.42
1:A:1437:LYS:NZ	1:A:1463:ASP:OD1	2.35	0.42
1:A:1694:ILE:HD13	1:A:1702:LEU:HD22	2.02	0.42
1:A:564:ASP:HA	1:A:635:TYR:O	2.20	0.41
1:A:792:LYS:HA	1:A:792:LYS:HD3	1.85	0.41
1:A:962:LYS:O	1:A:963:ASP:OD1	2.38	0.41
1:A:987:SER:OG	1:A:1017:ALA:HB2	2.20	0.41
1:A:1000:ASN:HB3	1:A:1027:LYS:HD2	2.01	0.41
1:A:1308:ASN:O	1:A:1339:LYS:HG3	2.20	0.41
1:A:1429:ALA:O	1:A:1457:LYS:HD2	2.19	0.41
1:A:605:SER:HB3	1:A:607:ARG:HH21	1.85	0.41
1:A:1082:PHE:HB2	1:A:1107:ASN:OD1	2.21	0.41
1:A:1344:ASN:HB3	1:A:1374:GLY:H	1.85	0.41
1:A:1496:LYS:O	1:A:1526:GLN:HG2	2.20	0.41
1:A:681:LEU:HD23	1:A:682:PRO:O	2.20	0.41
1:A:1467:VAL:HG11	1:A:1503:TYR:HB2	2.02	0.41
1:A:1691:ALA:O	1:A:1717:SER:OG	2.37	0.41
1:A:366:SER:HA	1:A:370:ASN:HB3	2.01	0.41
1:A:511:GLU:N	1:A:511:GLU:OE1	2.54	0.41
1:A:627:ASP:HB3	1:A:630:TYR:CD2	2.56	0.41
1:A:845:ILE:HB	1:A:869:VAL:HG22	2.02	0.41
1:A:1577:THR:O	1:A:1581:ILE:HD11	2.21	0.41
1:A:657:GLN:HE22	1:A:709:VAL:H	1.67	0.41
1:A:550:LYS:HG2	1:A:552:PRO:HD3	2.02	0.41
1:A:1010:LYS:HA	1:A:1010:LYS:HD2	1.86	0.41
1:A:1503:TYR:HE1	1:A:1533:TYR:HD1	1.67	0.41
1:A:1011:LEU:O	1:A:1042:VAL:HA	2.20	0.41
1:A:1096:LYS:NZ	1:A:1123:ASN:OD1	2.36	0.41
1:A:1136:THR:O	1:A:1163:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:THR:OG1	1:A:1281:GLU:OE2	2.26	0.41
1:A:1657:GLU:C	1:A:1682:ASN:HD22	2.28	0.41
1:A:370:ASN:O	1:A:373:GLN:HG3	2.20	0.41
1:A:529:PRO:HA	1:A:557:GLY:HA3	2.03	0.41
1:A:605:SER:C	1:A:616:PRO:HB3	2.46	0.41
1:A:660:LYS:HA	1:A:737:GLU:O	2.20	0.41
1:A:1025:PRO:HG3	1:A:1053:LEU:HD21	2.03	0.41
1:A:1115:VAL:HG23	1:A:1139:GLY:HA2	2.03	0.41
1:A:1259:ASN:HD22	1:A:1290:ASN:CG	2.29	0.41
1:A:1277:TYR:HA	1:A:1305:TYR:O	2.21	0.41
1:A:1366:ASN:N	1:A:1399:SER:OG	2.53	0.41
1:A:1532:ILE:H	1:A:1563:VAL:HG12	1.86	0.41
1:A:1294:ILE:HD11	1:A:1325:VAL:HG22	2.03	0.41
1:A:1558:GLU:HA	1:A:1584:ALA:HB1	2.03	0.41
1:A:744:LEU:CB	1:A:800:GLY:H	2.34	0.40
1:A:758:ASP:OD1	1:A:814:HIS:HD2	2.04	0.40
1:A:474:ILE:HA	1:A:513:THR:HB	2.02	0.40
1:A:545:LEU:HD23	1:A:545:LEU:HA	1.91	0.40
1:A:627:ASP:OD1	1:A:628:SER:N	2.54	0.40
1:A:1142:ALA:HB3	1:A:1172:THR:HG22	2.03	0.40
1:A:1252:SER:HA	1:A:1284:ALA:HB2	2.03	0.40
1:A:455:HIS:HD2	1:A:498:SER:HA	1.87	0.40
1:A:1050:PHE:CE1	1:A:1082:PHE:HZ	2.39	0.40
1:A:1309:GLU:OE2	1:A:1338:GLU:HG3	2.22	0.40
1:A:1497:THR:HB	1:A:1527:LYS:HB2	2.04	0.40
1:A:665:ILE:HG22	1:A:667:ILE:HD11	2.03	0.40
1:A:710:LYS:HB2	1:A:713:GLU:HB2	2.02	0.40
1:A:835:GLY:O	1:A:836:LYS:HD2	2.21	0.40
1:A:1243:ILE:HB	1:A:1276:ILE:HA	2.03	0.40
1:A:1585:LYS:NZ	1:A:1611:PRO:HA	2.37	0.40
1:A:462:PRO:HB2	1:A:630:TYR:HD1	1.86	0.40
1:A:635:TYR:HA	1:A:660:LYS:O	2.21	0.40
1:A:675:GLU:HB2	1:A:678:ILE:HD12	2.04	0.40
1:A:1131:LYS:HA	1:A:1158:THR:O	2.22	0.40
1:A:1224:MET:CE	1:A:1243:ILE:HD13	2.51	0.40
1:A:1686:LEU:HA	1:A:1686:LEU:HD12	1.87	0.40
1:A:1721:TYR:HE1	1:A:1723:SER:HB2	1.87	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	1481/3250 (46%)	1316 (89%)	160 (11%)	5 (0%)	37	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1383	ILE
1	A	319	ASN
1	A	778	ASN
1	A	1667	TYR
1	A	915	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1208/2632 (46%)	1208 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	A	440	ASN
1	A	500	ASN
1	A	533	GLN

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Mol	Chain	Res	Type
1	A	680	ASN
1	A	683	ASN
1	A	839	ASN
1	A	986	ASN
1	A	1047	ASN
1	A	1061	ASN
1	A	1203	ASN
1	A	1308	ASN
1	A	1572	ASN
1	A	1600	ASN
1	A	1664	ASN
1	A	1704	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](#)

There are no ligands in this entry.

### 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-53049. These allow visual inspection of the internal detail of the map and identification of artifacts.

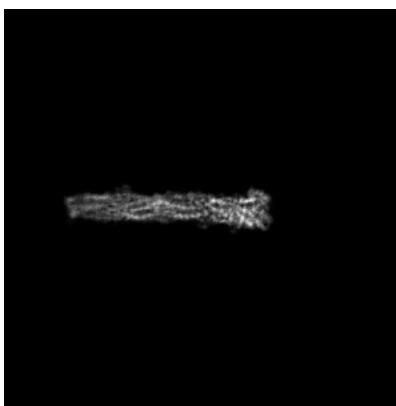
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

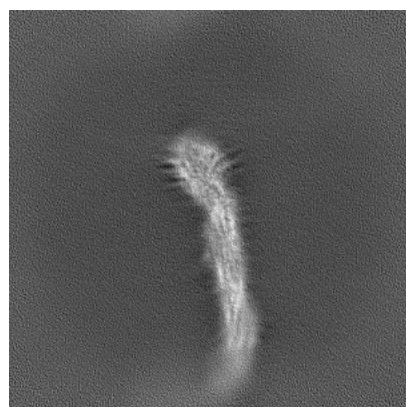


Y

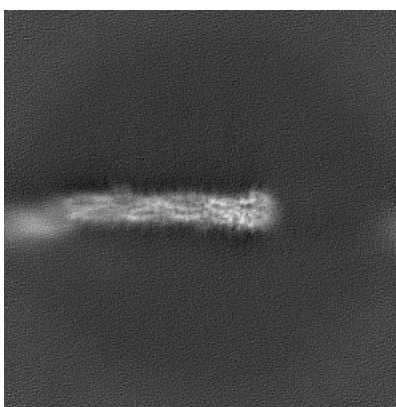


Z

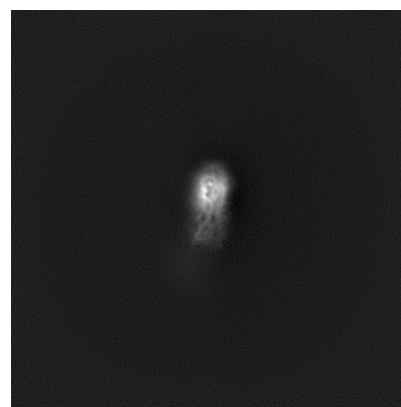
#### 6.1.2 Raw map



X



Y

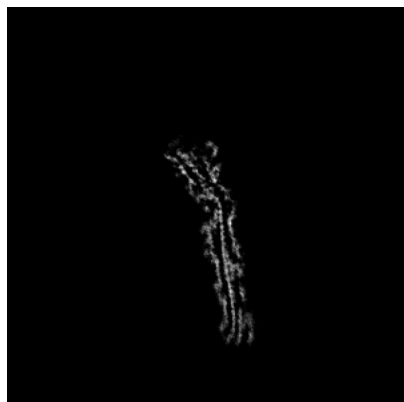


Z

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

## 6.2 Central slices [i](#)

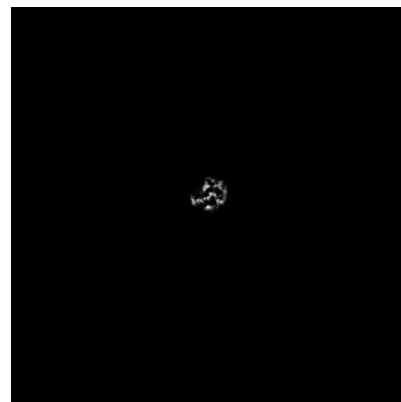
### 6.2.1 Primary map



X Index: 192

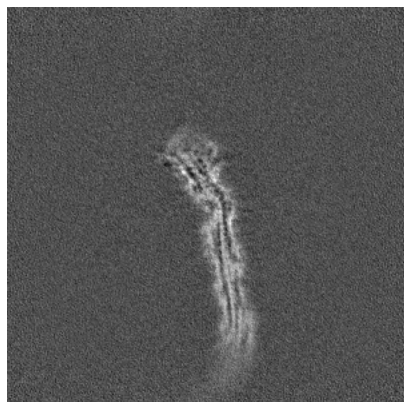


Y Index: 192



Z Index: 192

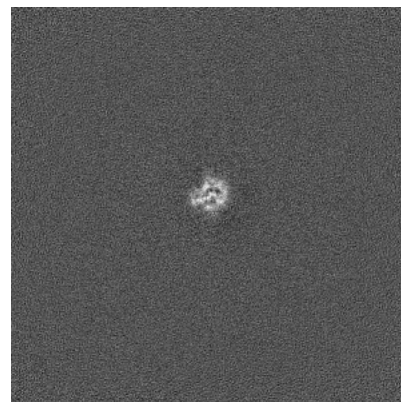
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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: 185



Y Index: 213

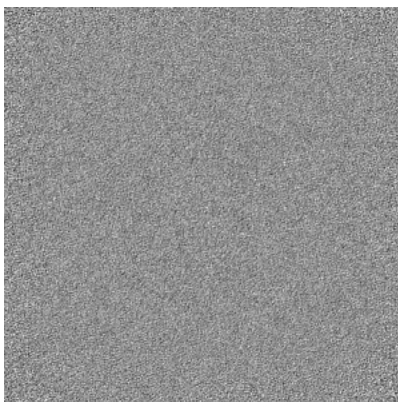


Z Index: 236

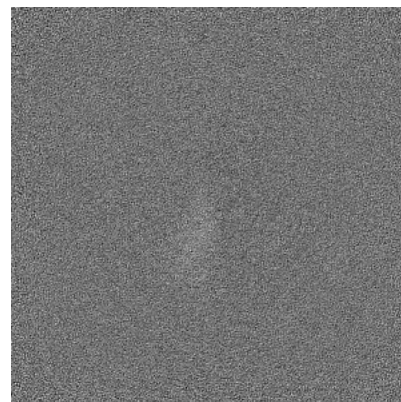
### 6.3.2 Raw map



X Index: 185



Y Index: 0



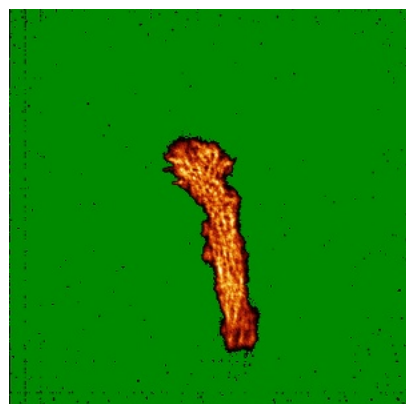
Z Index: 0

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

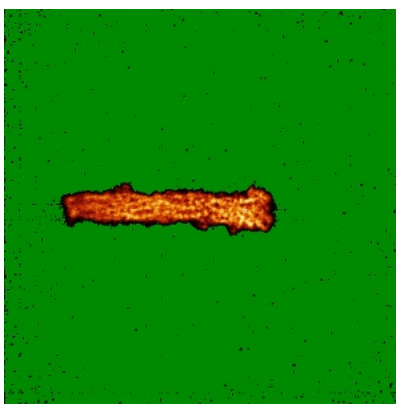


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

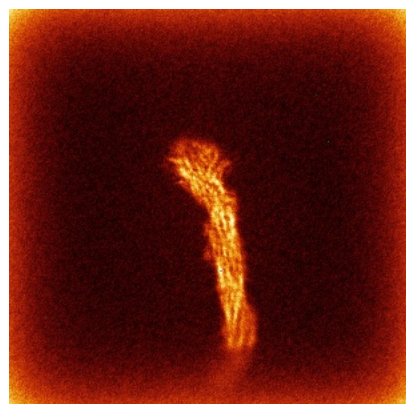


Y

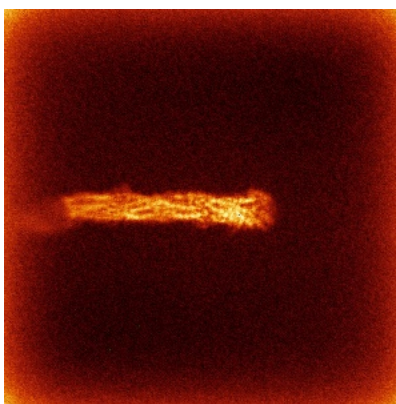


Z

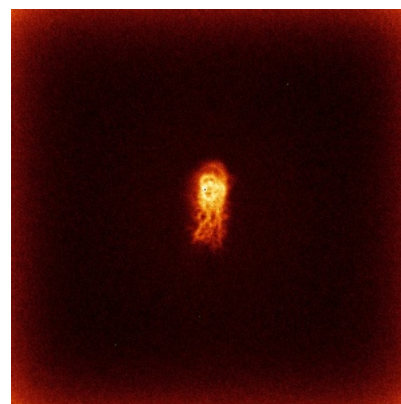
### 6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



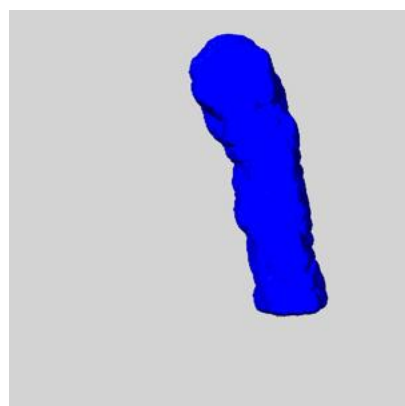
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

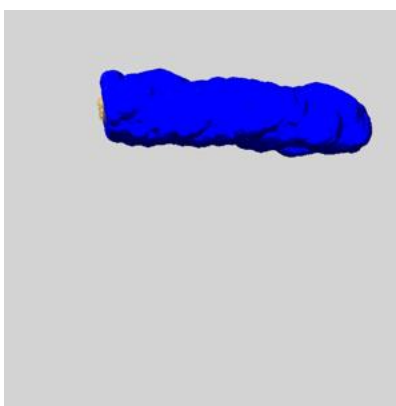
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

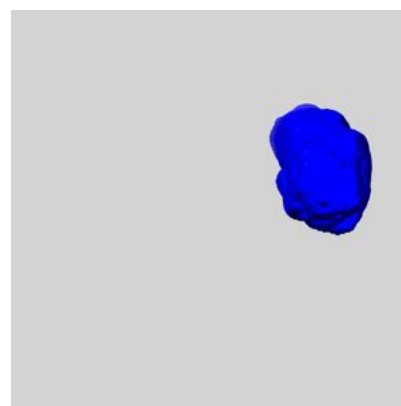
### 6.6.1 emd\_53049\_msk\_1.map [i](#)



X



Y

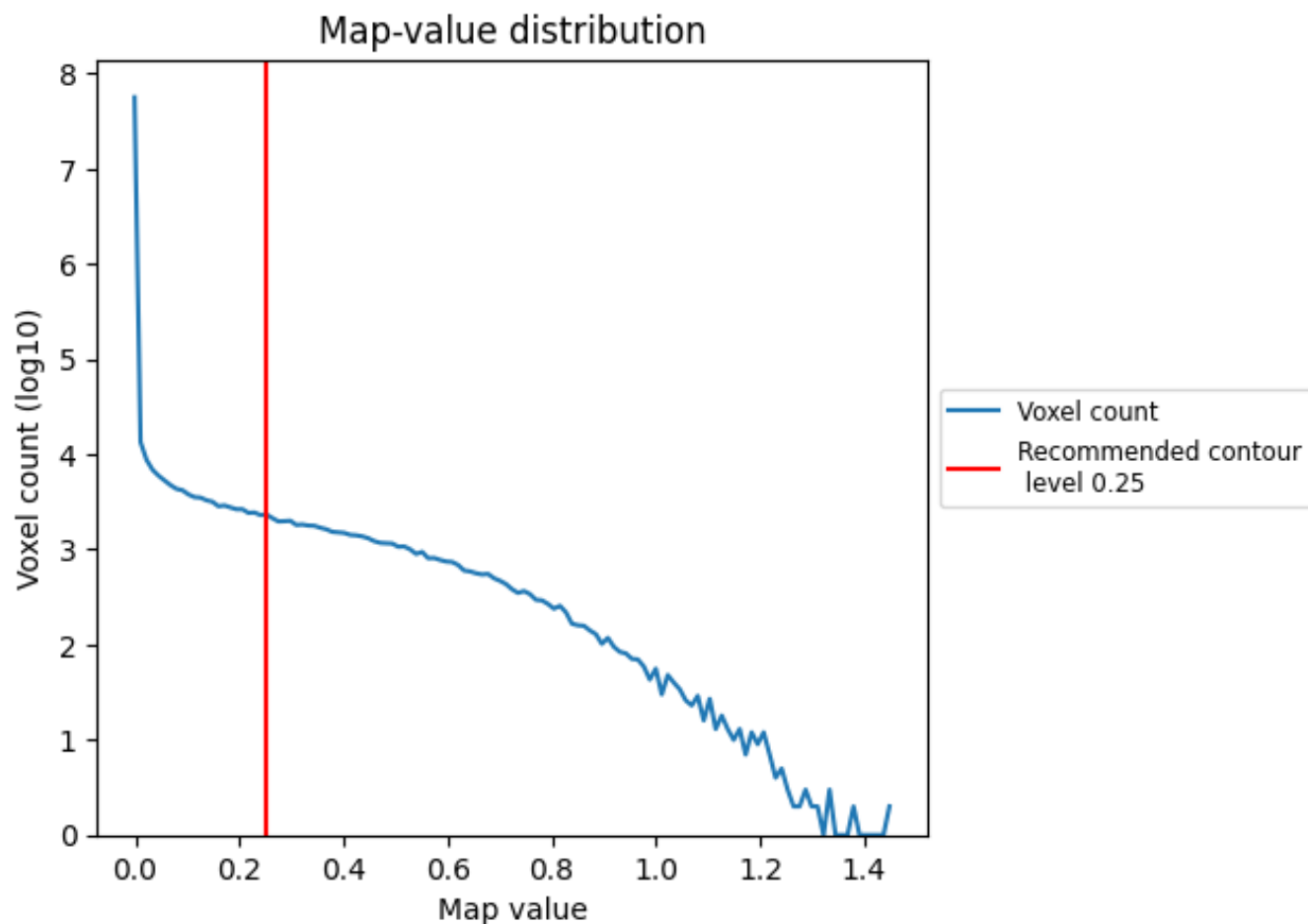


Z

## 7 Map analysis [i](#)

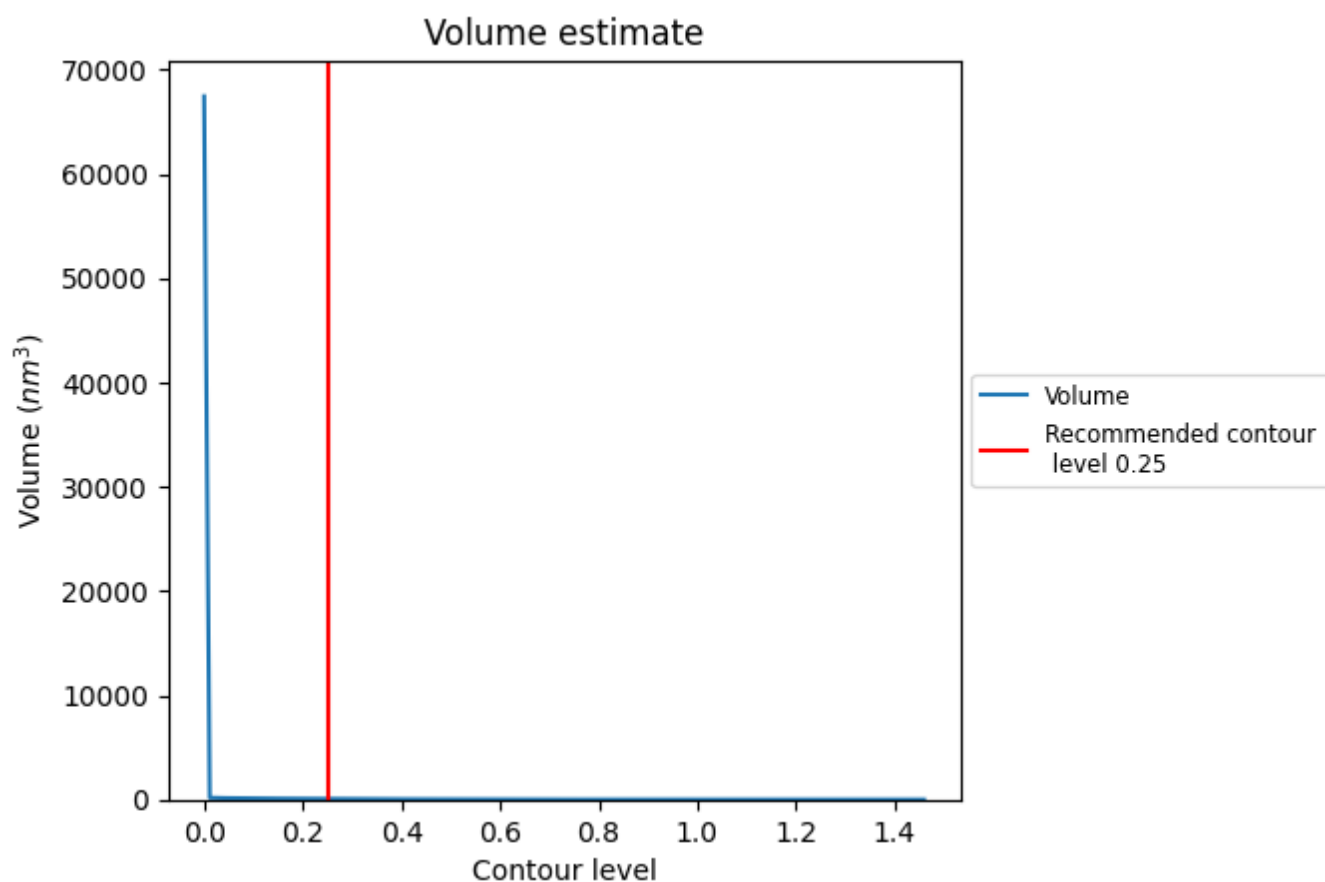
This section contains the results of statistical analysis of the map.

### 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.

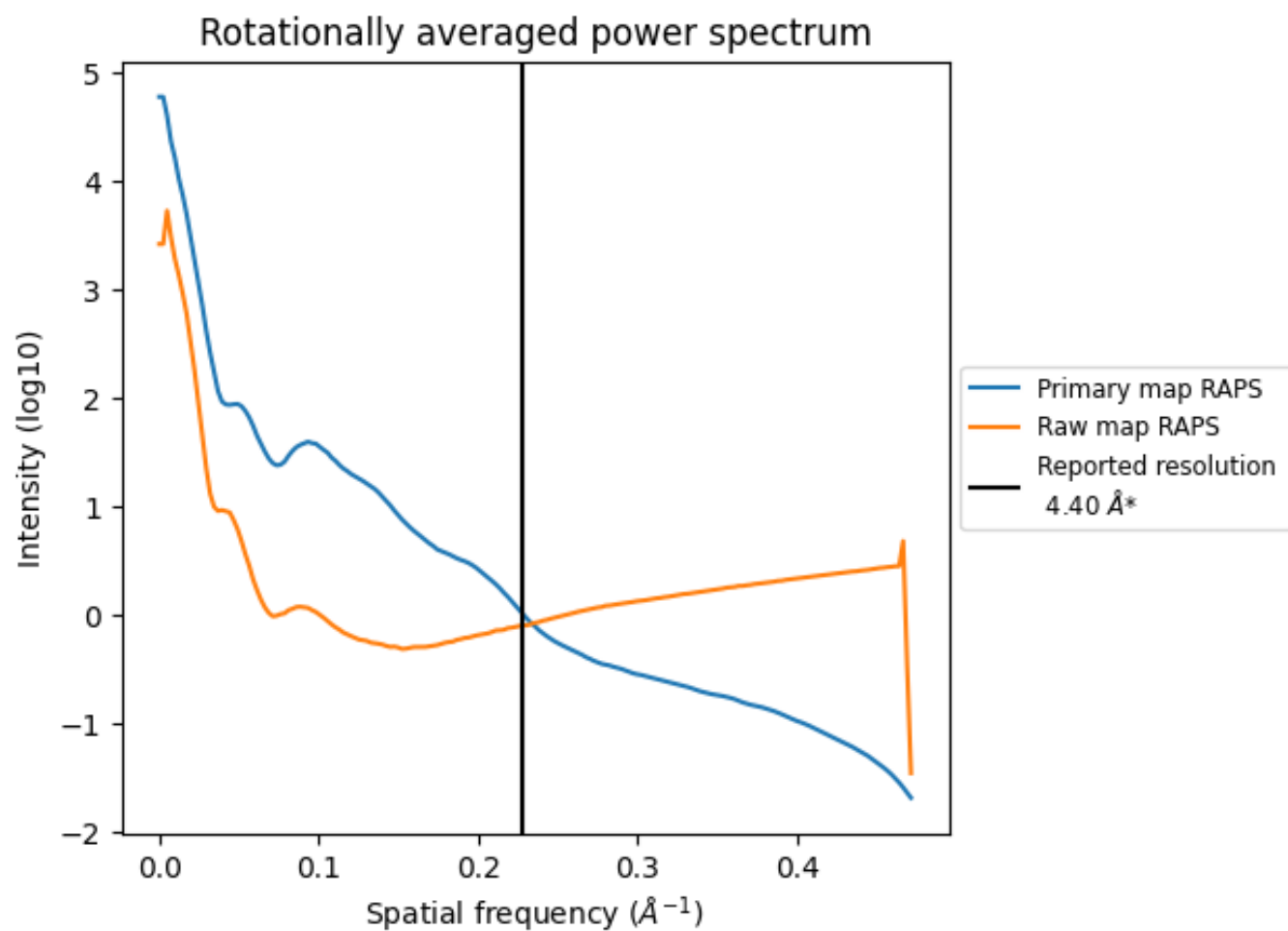
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm<sup>3</sup>; this corresponds to an approximate mass of 59 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 ⓘ

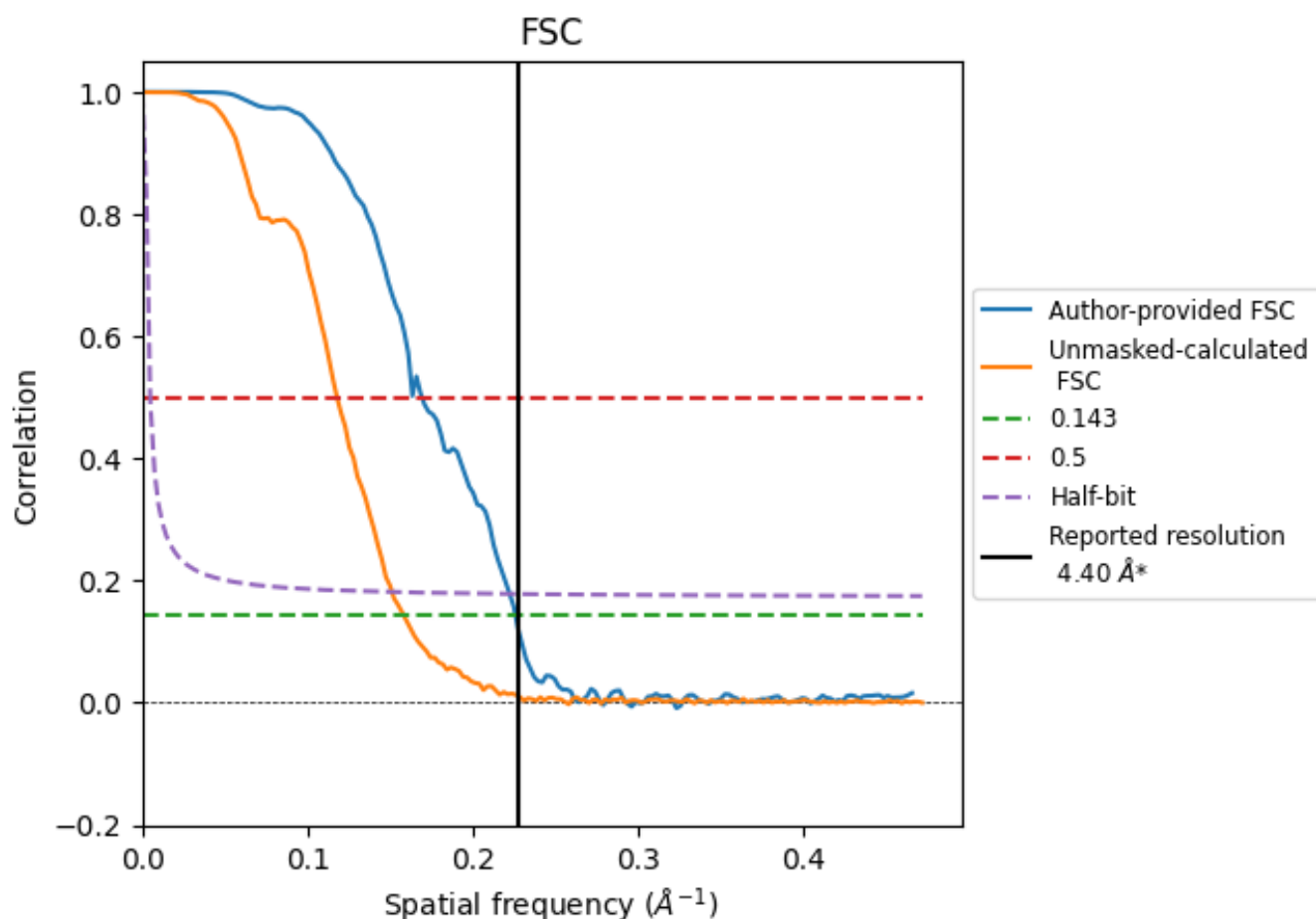


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

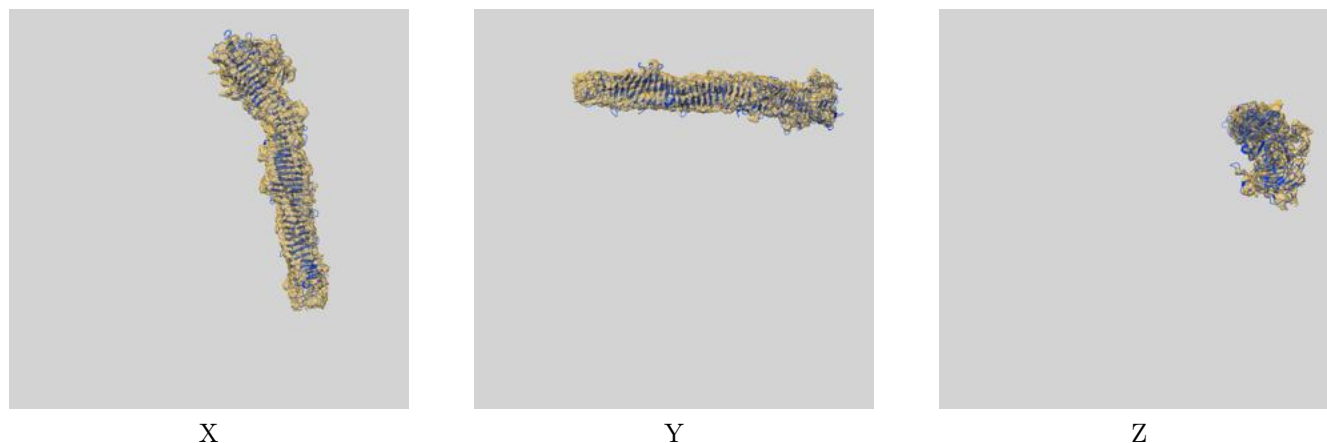
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.43	5.91	4.50
Unmasked-calculated*	6.33	8.49	6.62

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.33 differs from the reported value 4.4 by more than 10 %

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

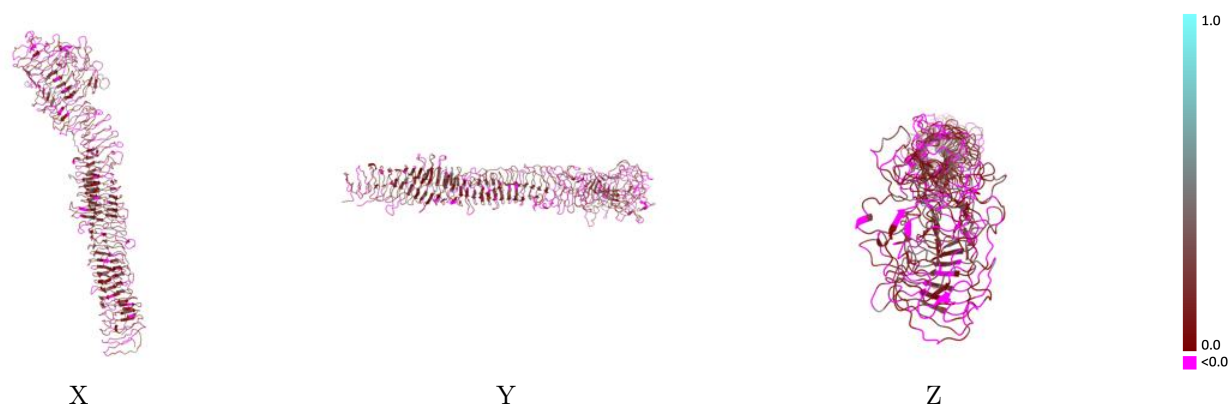
This section contains information regarding the fit between EMDB map EMD-53049 and PDB model 9QE7. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



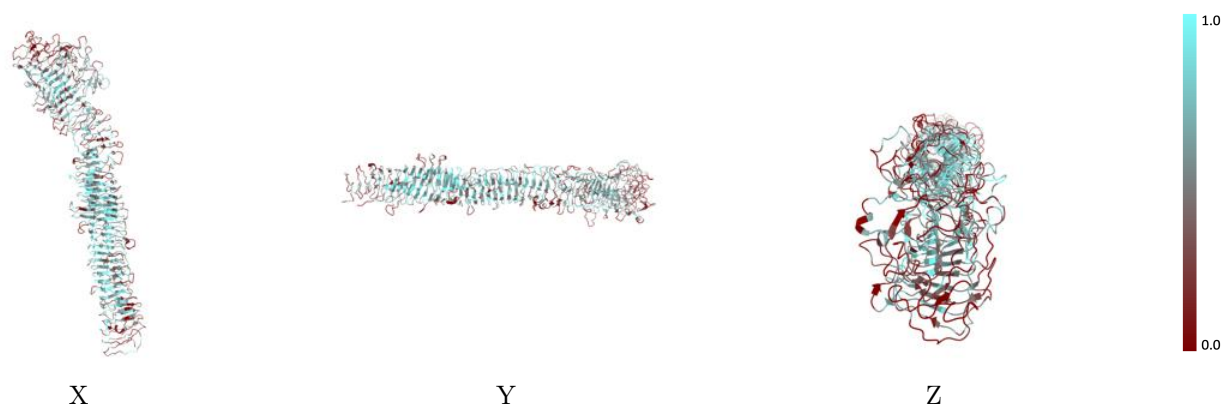
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

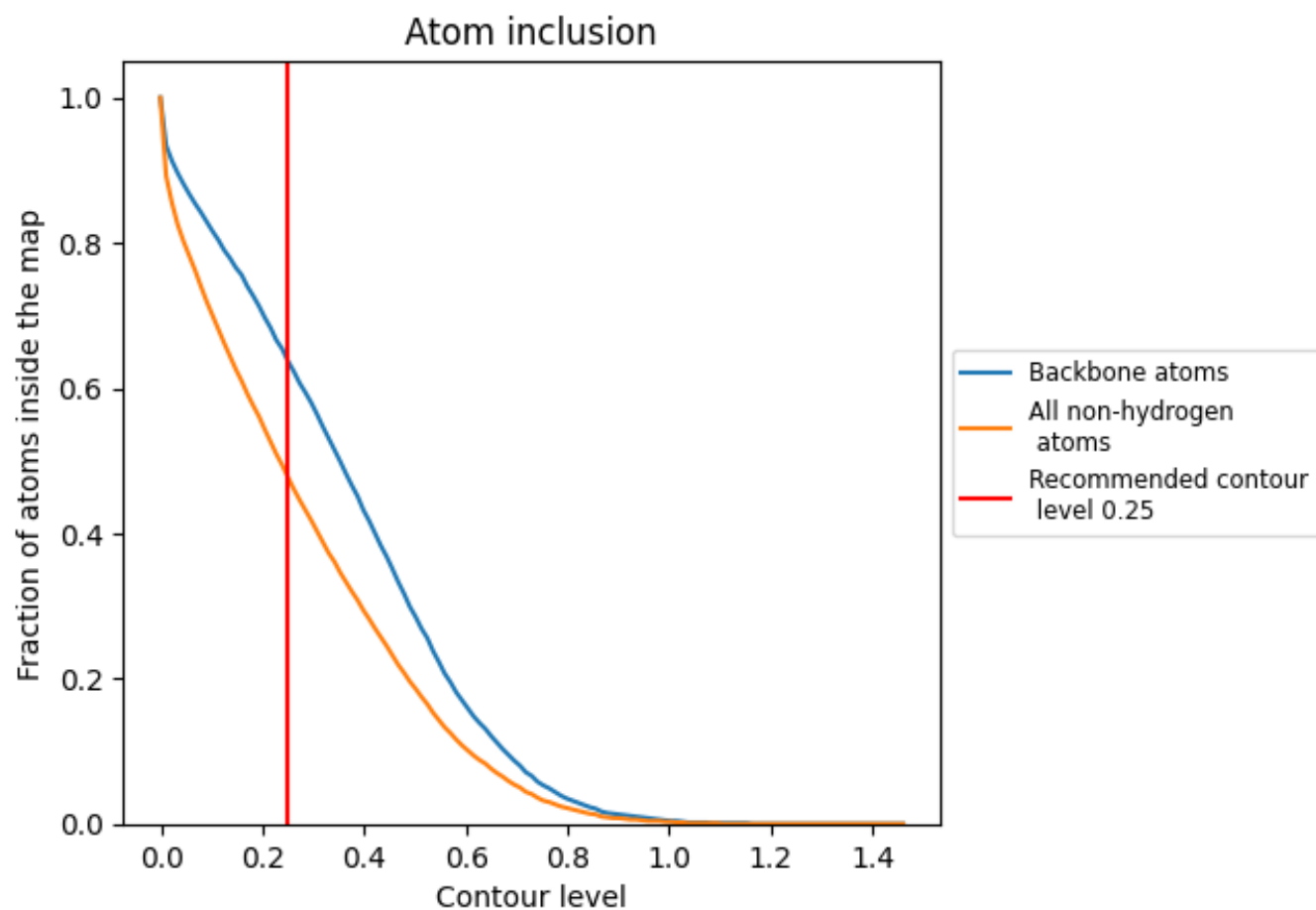
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.25).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4770	<div></div> 0.1180
A	<div></div> 0.4770	<div></div> 0.1180

