



Full wwPDB EM Validation Report ⓘ

Sep 1, 2025 – 02:02 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

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.dev126
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) : 2.45.1

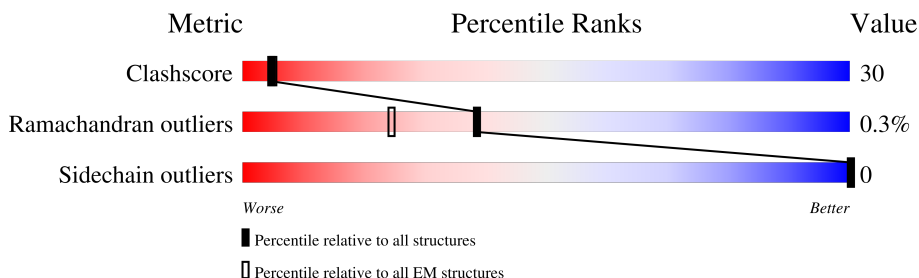
1 Overall quality at a glance

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 ≥ 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		

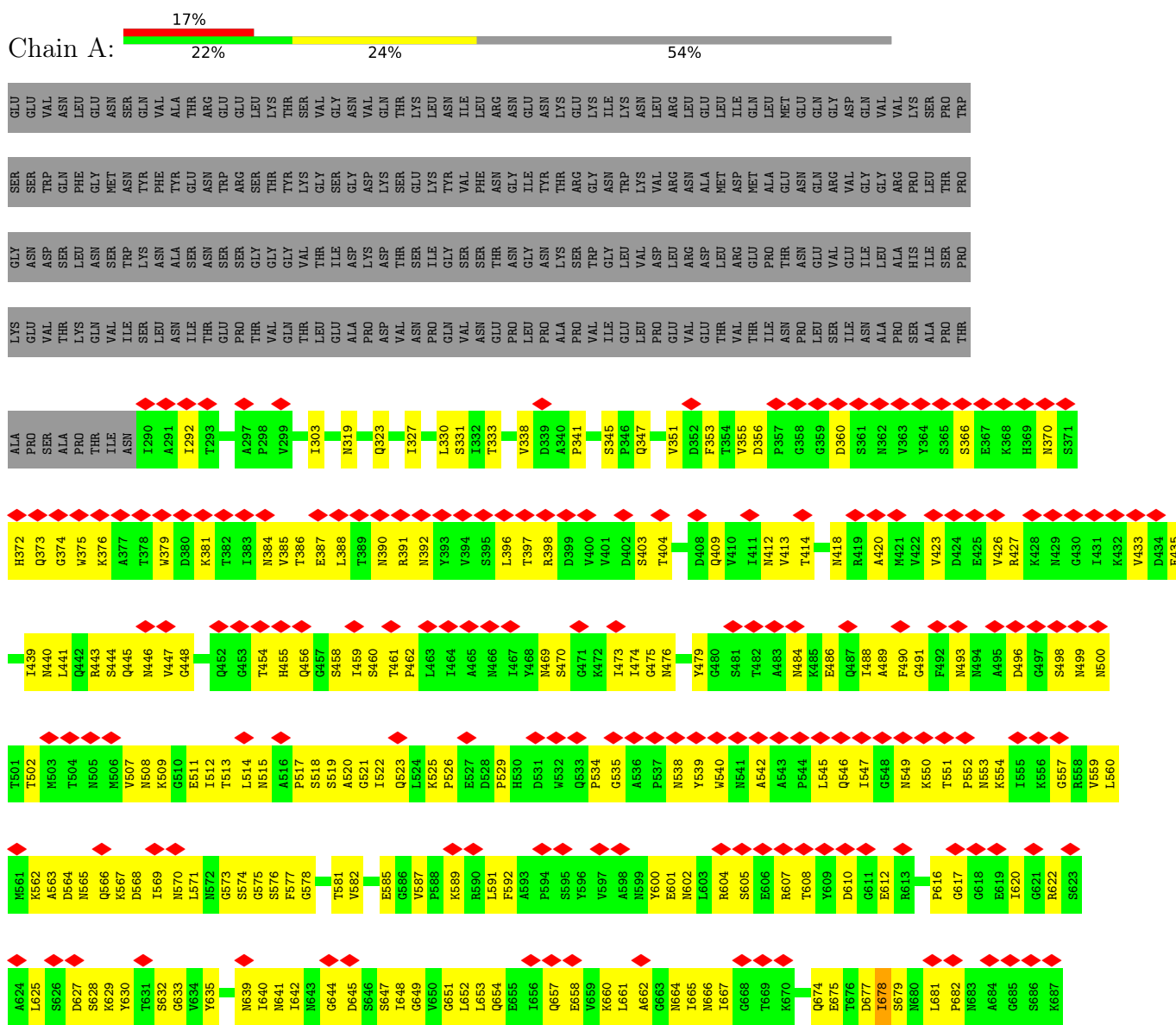
There are 20 discrepancies between the modelled and reference sequences:

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	K1481	N1485	S1486	G1487	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																											
K1410	V1411	D1412	T1417	G1418	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																											
S1340	K1341	T1342	T1343	N1344	T1345	G1346	T1347	G1348	T1349	K1350	G1351	I1354	V1355	K1356	E1357	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																														
K1410	V1411	D1412	T1417	G1418	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																											
I1276	Y1277	S1278	K1279	E1280	E1281	A1284	T1287	G1288	E1289	N1290	T1291	I1294	V1295	E1296	G1297	A1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	T1308	E1309	S1310	T1311	Q1312	A1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1321	G1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	I1332	G1333	I1335	M1336	G1337	E1338	K1339																											
T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	I1218	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	S1273	A1274	G1275																												
I1276	Y1277	S1278	K1279	E1280	E1281	A1284	T1287	G1288	E1289	N1290	T1291	I1294	V1295	E1296	G1297	A1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	T1308	E1309	S1310	T1311	Q1312	A1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1321	G1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	I1332	G1333	I1335	M1336	G1337	E1338	K1339																											
S1340	K1341	T1342	T1343	N1344	T1345	G1346	T1347	G1348	T1349	K1350	G1351	I1354	V1355	K1356	E1357	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																														
K1410	V1411	D1412	T1417	G1418	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																											
L1276	Y1277	S1278	K1279	E1280	E1281	A1284	T1287	G1288	E1289	N1290	T1291	I1294	V1295	E1296	G1297	A1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	T1308	E1309	S1310	T1311	Q1312	A1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1321	G1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	I1332	G1333	I1335	M1336	G1337	E1338	K1339																											
T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	I1218	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	S1273	A1274	G1275																												
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K1410	V1411	D1412	T1417	G1418	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																											
L1755	V1756	G1757	D1758	T1759	E1760	L1761	D1762	L1763	N1764	K1765	G1766	G1767	L1768	T1769	E1770	K1775	G1776	S1777	N1778	V1779	D1780	K1781	G1782	L1783	R1784	S1785	S1786	I1789	T1790	A1791	K1792	S1793	N1794	S1795	V1796	I1797	N1798	V1799	G1800	G1801	K1802	K1803	N1804	E1805	G1806	F1807	V1808	N1811	S1812	A1813	H1814	S1815	S1816	K1817	F1818	G1819																									
T1920	T1921	V1922	D1923	S1924	E1925	Y1927	D1930	K1931	T1932	H1933	H1934	G1935	K1936	N1939	E1940	G1941	I1942	I1943	N1944	G1945	S1946	S1947	D1948	E1949	S1950	K1951	G1952	F1953	N1954	A1955	S1956	K1957	G1958	N1959	S1960	S1961	K1962	S1963	S1964	V1969	K1970	K1971	D1972	G1973	N1974	S1975	S1976	N1977	I1978	N1979	A1980	P1981	E1982	E1983	L1984	A1985	N1986	S1987	S1988	K1989	G1990	T1991	T1992	I1995	Y1996	S1997	D1998	G1999	N1000	A1001	K1002	V1003	K1004	F1005	G1006	T1007	G1008	S1009	K1010	Q1011	L1012
S1885	F1886	S1889	G1890	T1891	I1892	E1893	V1894	T1895	E1896	S1897	K1898	K1899	K1900	N1901	K1902	A1903	V1904	V1905	L1906	D1907	G1908	T1909	S1910	A1911	S1912	N1913	K1914	I1915	N1916	F1917	T1918	N1919	T1920	G1921	G1922	N1923	N1926	T1927	S1928	D1929	N1930	N1931	N1932	T1933	N1934	L1935	D1936	G1937	N1940	I1941	G1942	I1943	Y1944	A1945	Q1946	G1947	N1948																								
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K1012	I1013	K1016	A1017	Y1021	A1022	D1024	P1025	T1026	K1027	F1028	N1029	M1030	T1031	F1032	K1033	I1034	E1035	S1036	G1037	K1038	T1039	L1040	D1041	E1042	E1043	L1044	G1045	K1046	N1047	S1048	T1049	F1050	G1051	L1052	L1053	N1054	G1055	M1056	M1057	T1058	V1059	N1060	N1061	S1062	P1063	L1064	L1065	S1066	K1067	Y1068	N1069	N1070	M1071	N1072	T1073	S1074																									
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A1138	G1139	L1140	I1141	A1142	T1146	G1147	F1148	F1149	T1150	S1151	V1152	A1153	K1154	N1155	N1156	G1157	T1158	T1162	I1163	D1164	D1165	K1166	G1167	T1168	G1169	Y1170	Y1171	T1172	S1173	A1174	N1175	G1176	E1177	L1178	S1179	N1180	G1181	T1182	T1183	T1184	M1185	Q1186	N1187	K1188	N1189	A1190	V1191	L1194	G1195	S1196	K1197	N1200	L1201	K1202	N1203																										
T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	I1218	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	S1273	A1274	G1275																												
I1276	Y1277	S1278	K1279	E1280	E1281	A1284	T1287	G1288	E1289	N1290	T1291	I1294	V1295	E1296	G1297	A1298	Q1299	A1302	G1303	I1304	Y1305	A1306	K1307	T1308	E1309	S1310	T1311	Q1312	A1313	T1314	T1315	Q1316	S1317	E1318	V1319	T1320	S1321	G1322	G1323	L1324	V1325	K1326	M1327	S1328	A1329	E1330	N1331	I1332	G1333	I1335	M1336	G1337	E1338	K1339																											
S1340	K1341	T1342	T1343	N1344	T1345	G1346	T1347	G1348	T1349	K1350	G1351	I1354	V1355	K1356	E1357	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	E																															





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

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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.

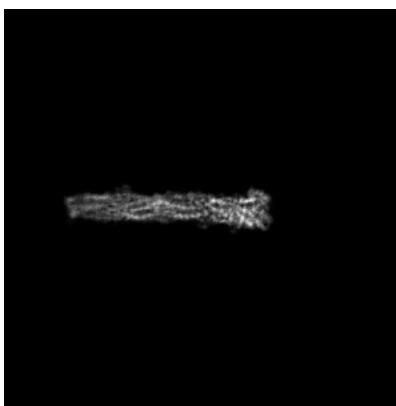
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

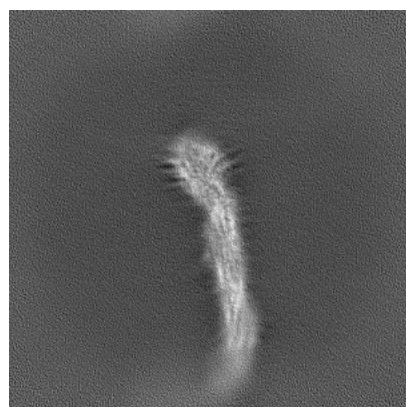


Y

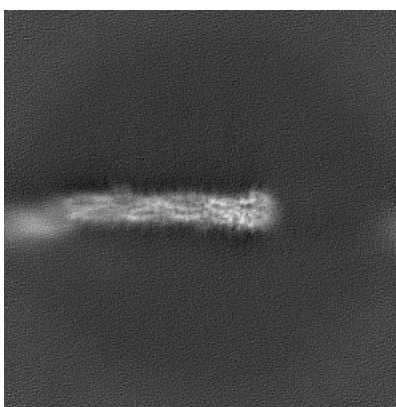


Z

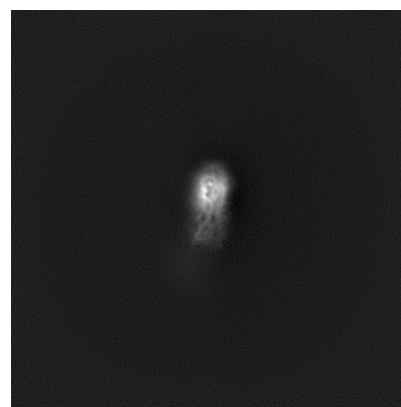
6.1.2 Raw map



X



Y

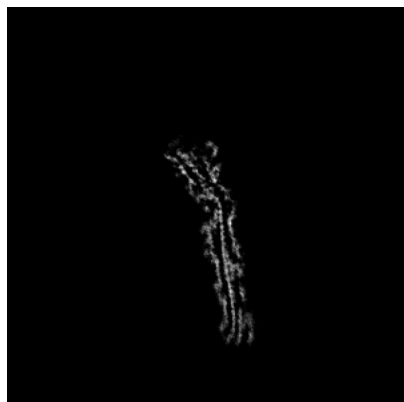


Z

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

6.2 Central slices [i](#)

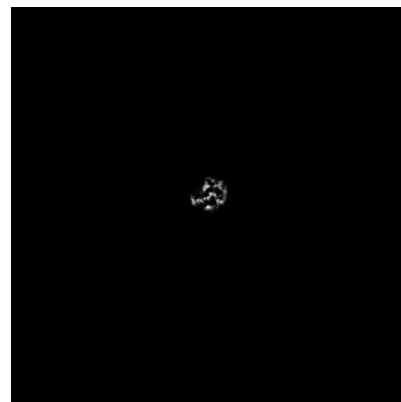
6.2.1 Primary map



X Index: 192

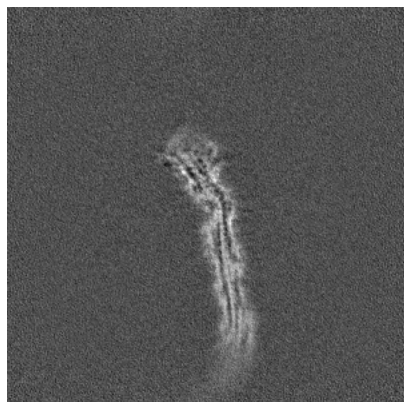


Y Index: 192



Z Index: 192

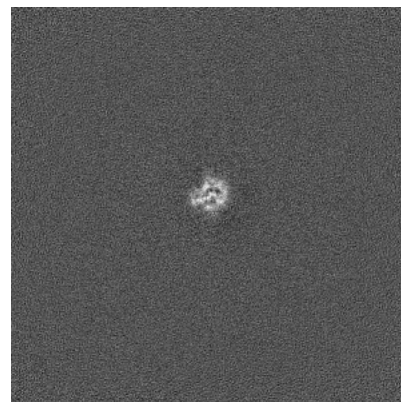
6.2.2 Raw map



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

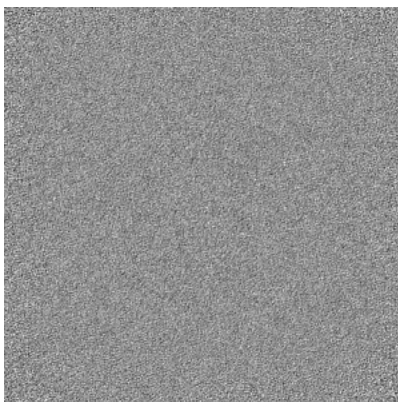


Z Index: 236

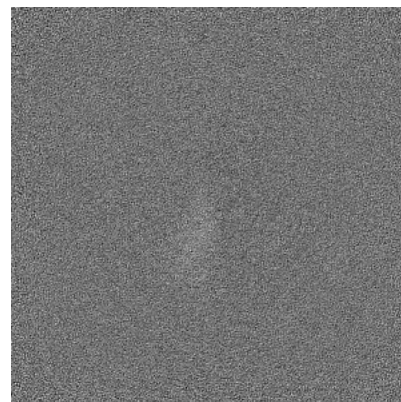
6.3.2 Raw map



X Index: 185



Y Index: 0

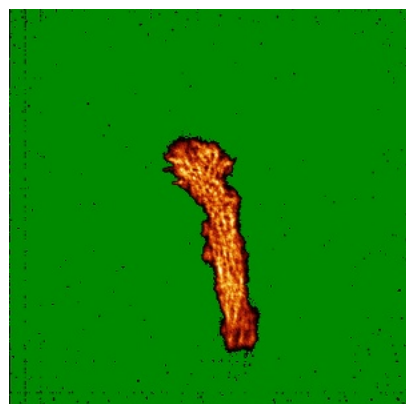


Z Index: 0

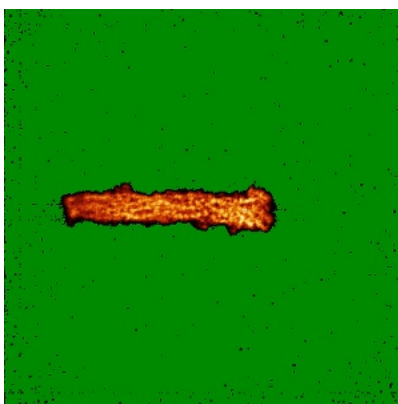
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

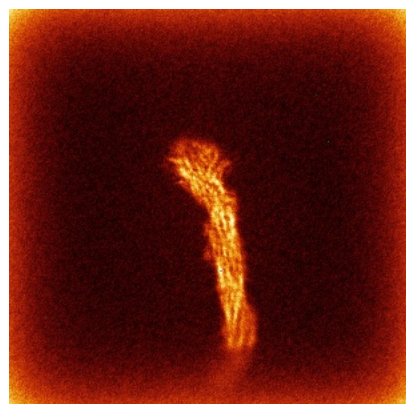


Y

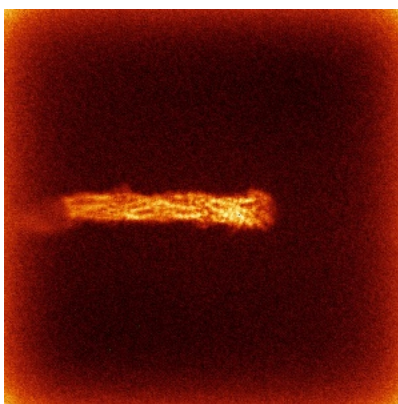


Z

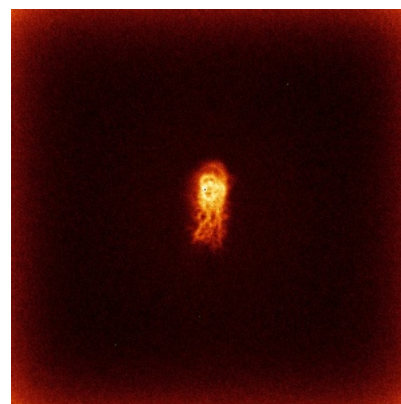
6.4.2 Raw map



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.

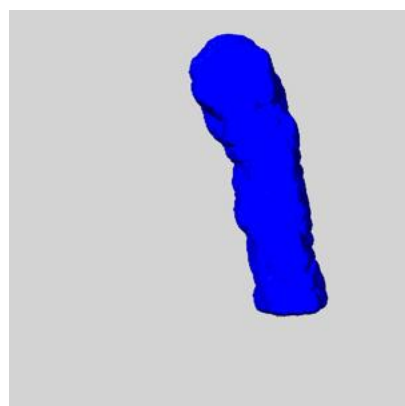
6.6 Mask visualisation [i](#)

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

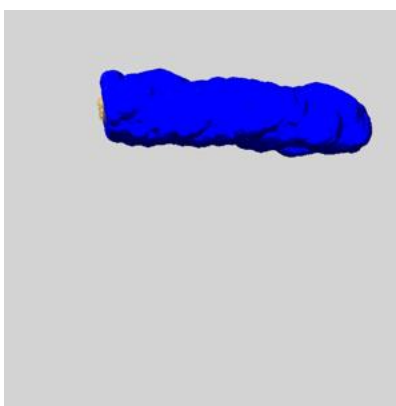
A mask typically either:

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

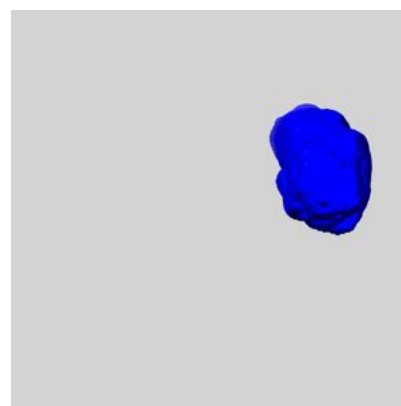
6.6.1 emd_53049_msk_1.map [i](#)



X



Y

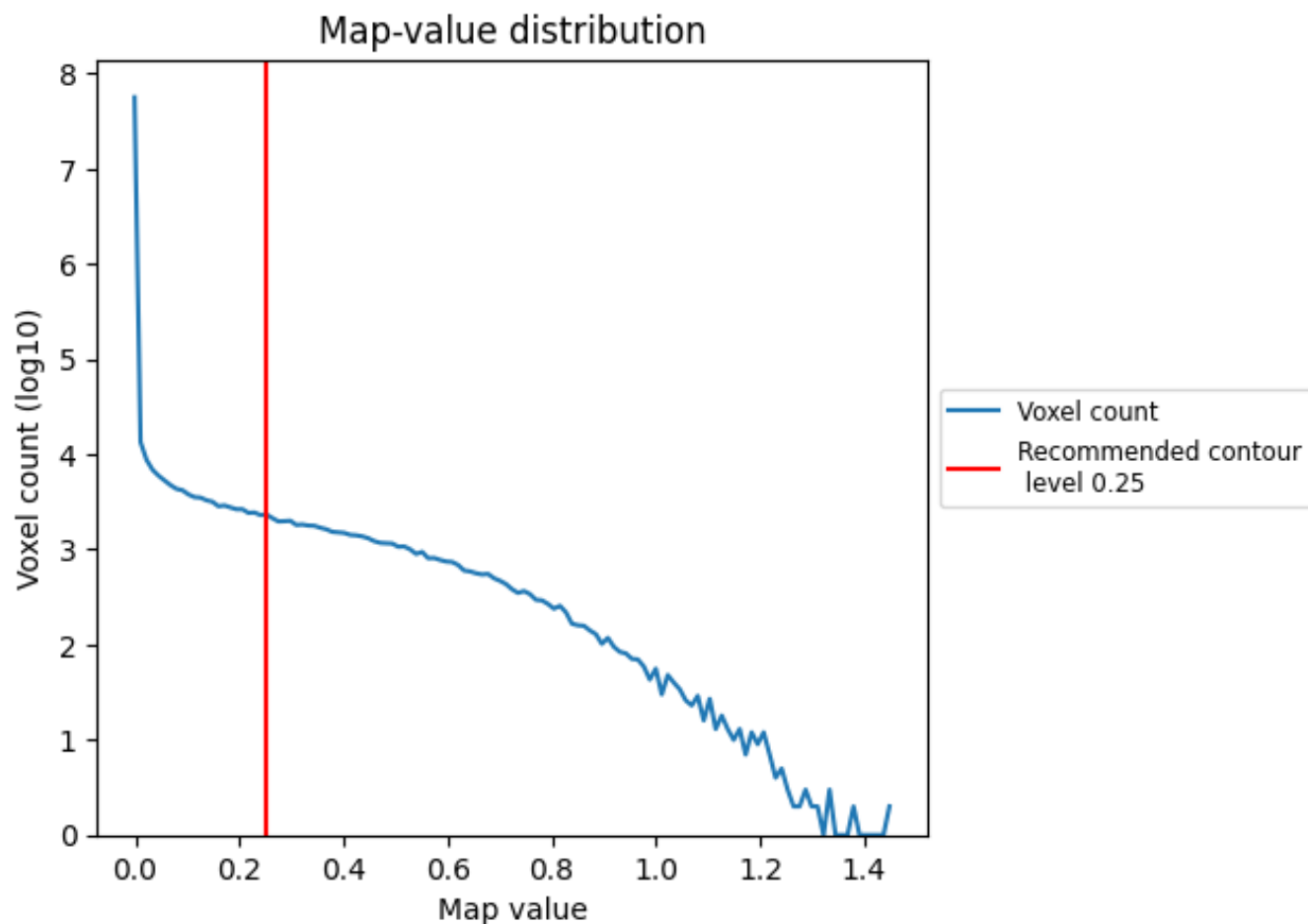


Z

7 Map analysis [i](#)

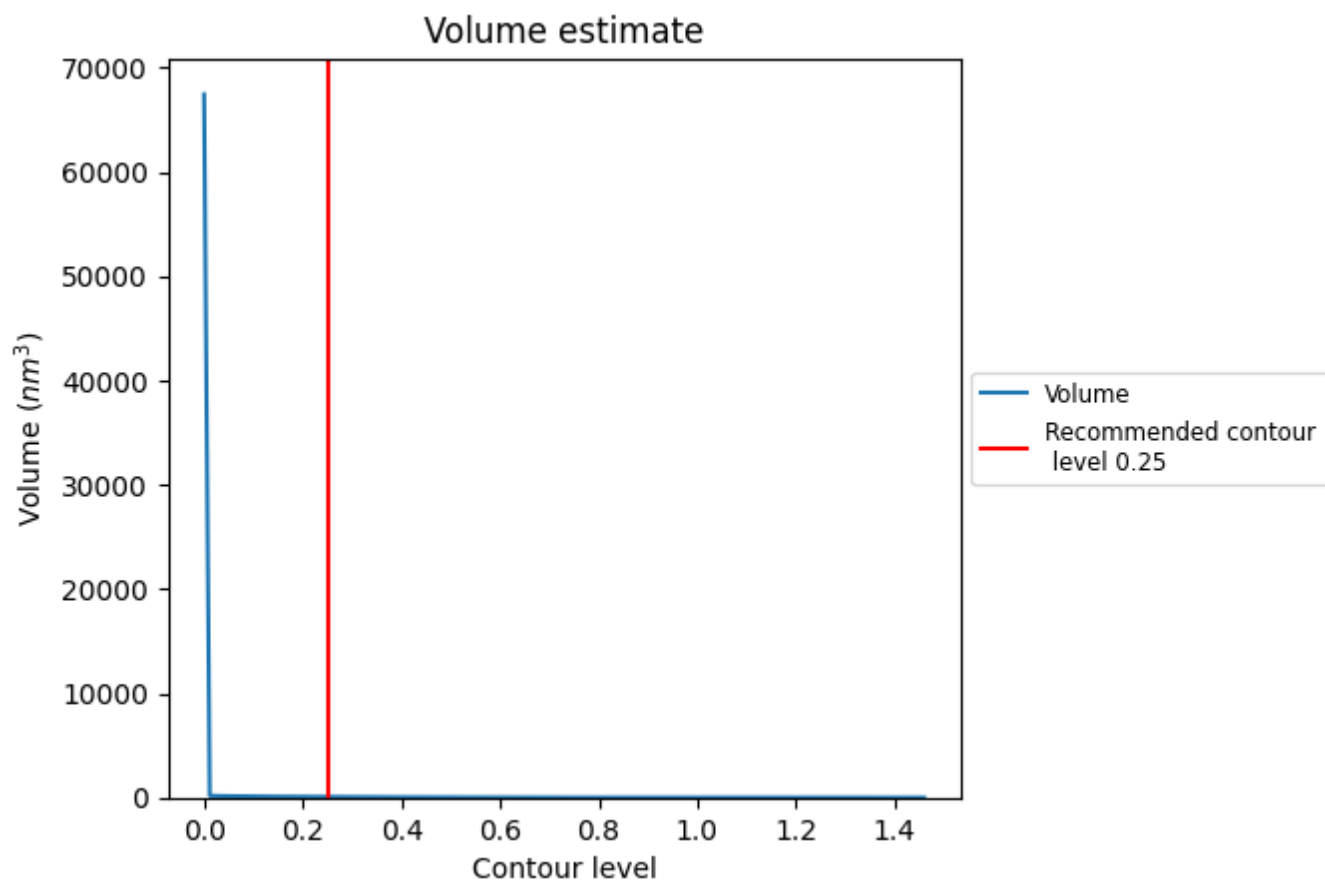
This section contains the results of statistical analysis of the map.

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.

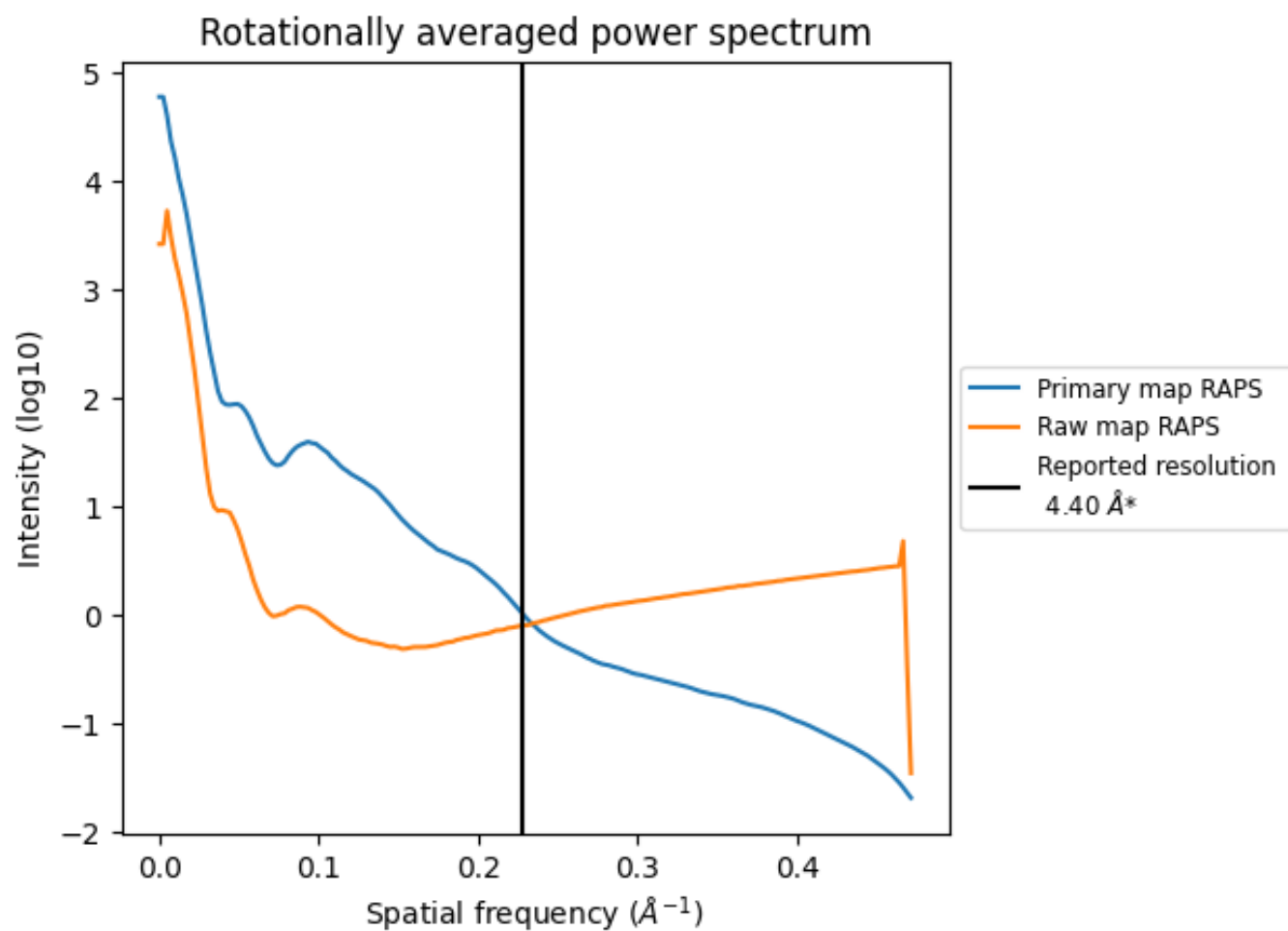
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm^3 ; 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 ⓘ

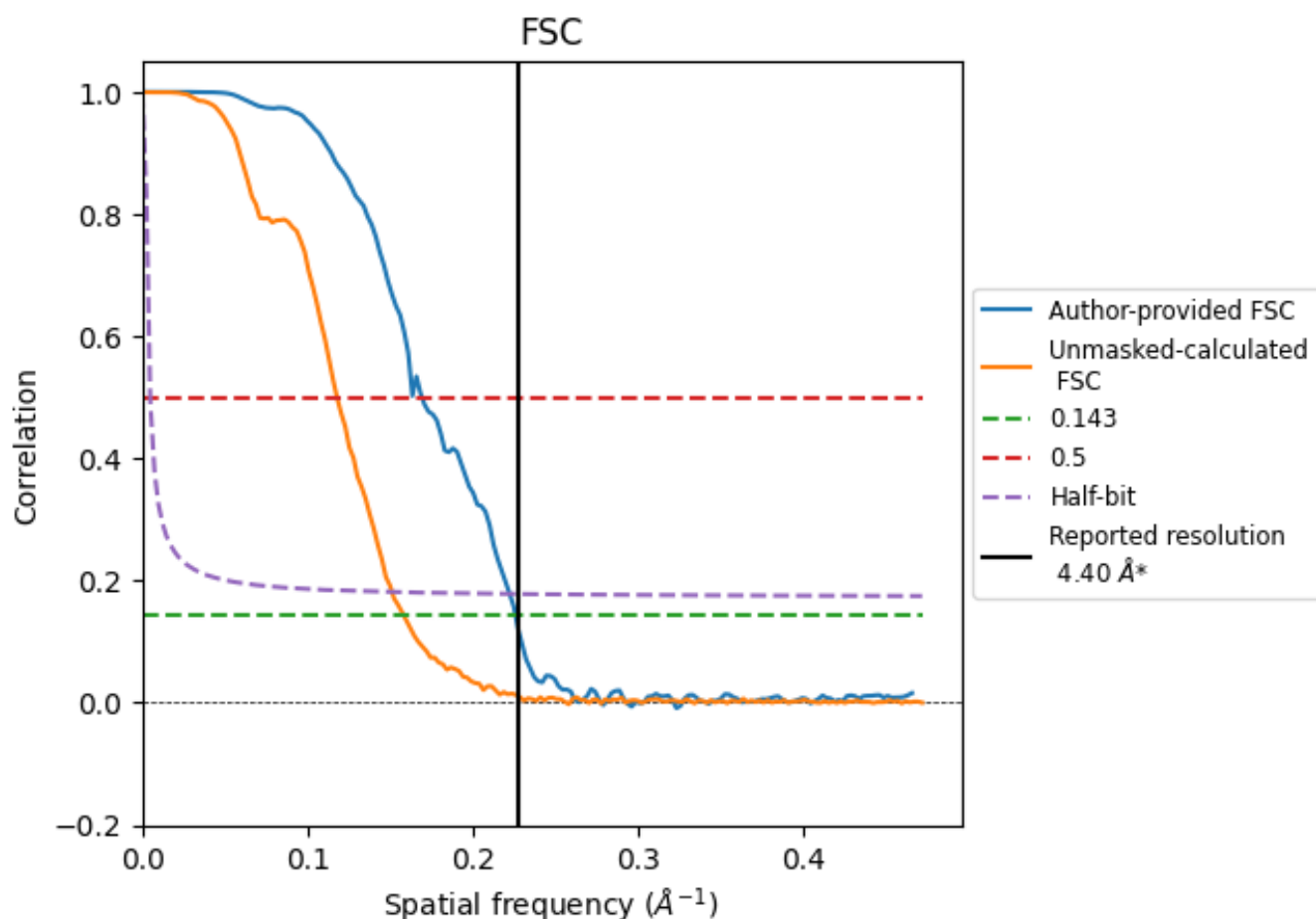


*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8.2 Resolution estimates [i](#)

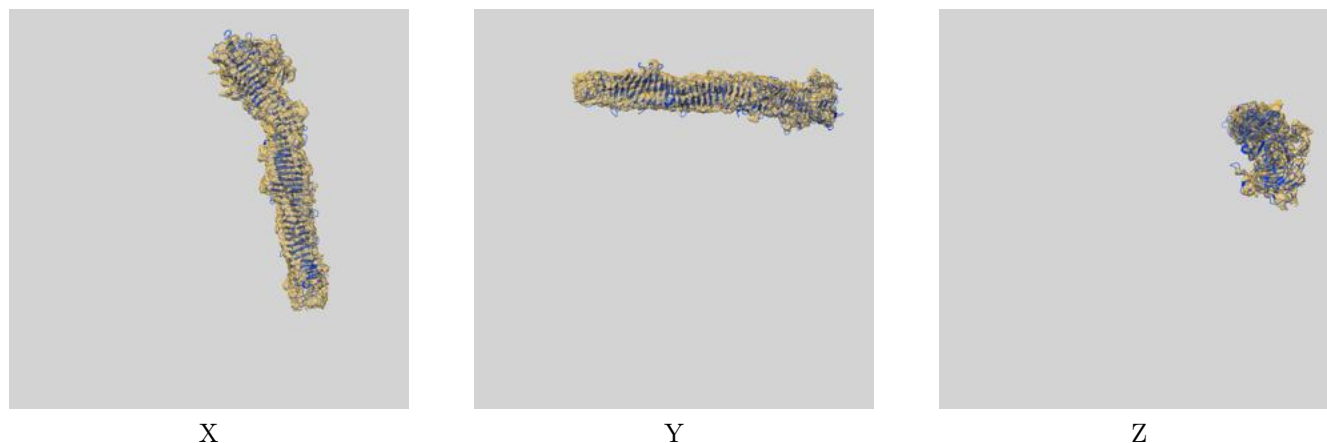
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.43	5.91	4.50
Unmasked-calculated*	6.33	8.49	6.62

*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](#)

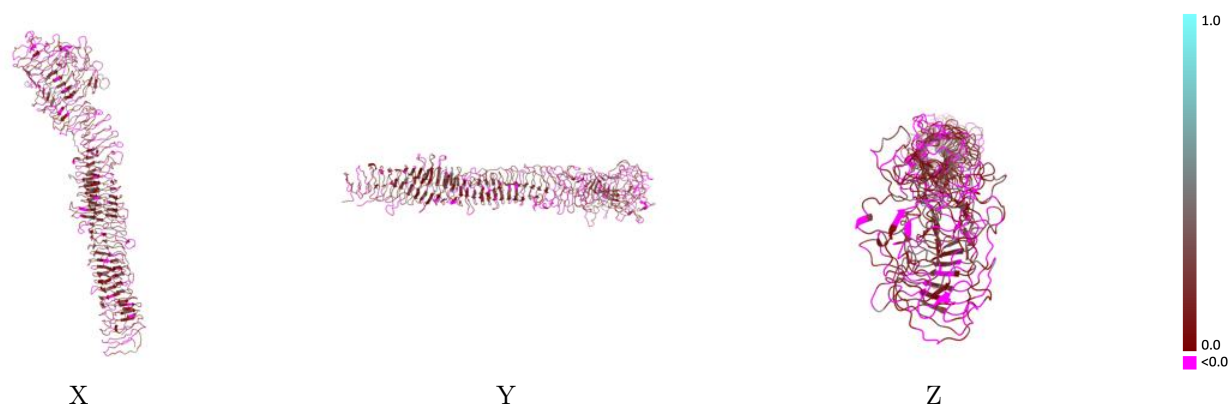
This section contains information regarding the fit between EMDB map EMD-53049 and PDB model 9QE7. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



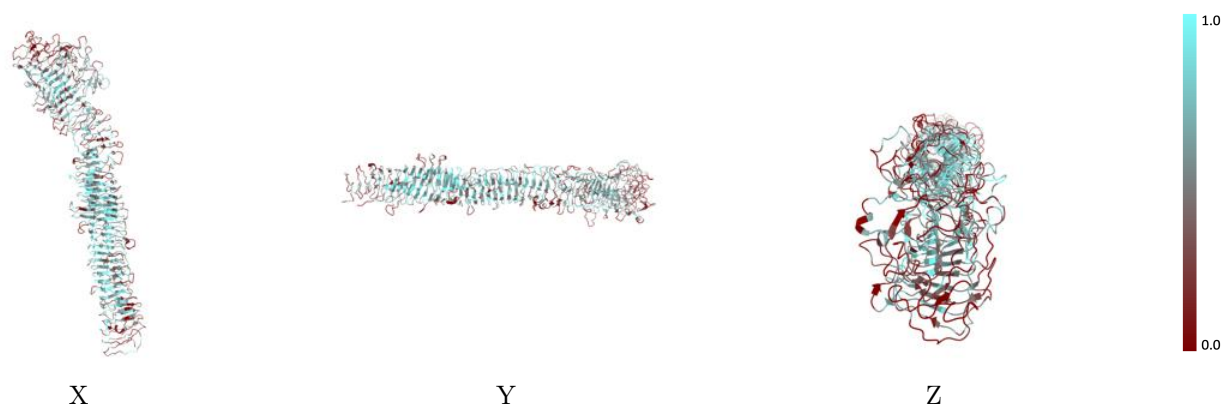
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



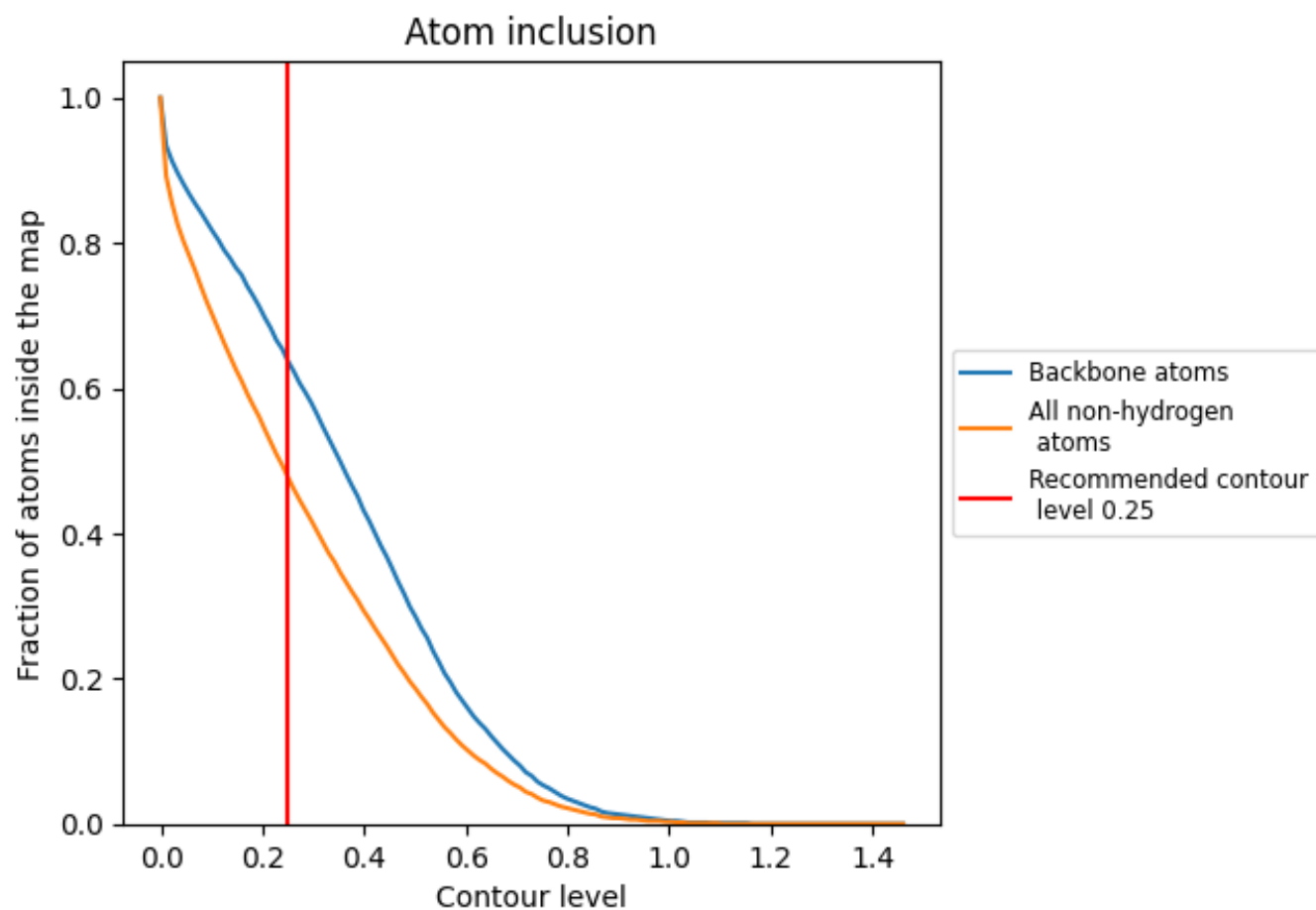
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

