



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:40 PM UTC

PDB ID : 8X2I / pdb_00008x2i
EMDB ID : EMD-38011
Title : Cryo-EM structure of the TcsL at pH 5.0 in its open conformation
Authors : Zhan, X.; Tao, L.
Deposited on : 2023-11-09
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

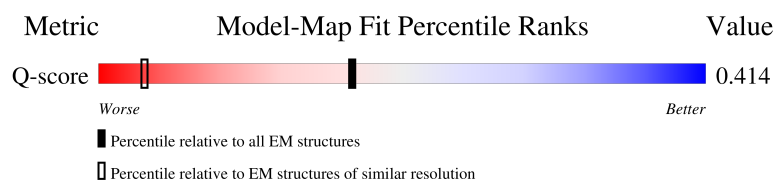
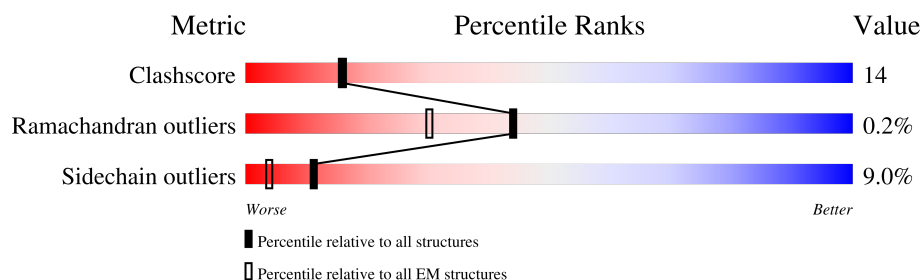
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	2372	25% 64% 29% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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 Cytotoxin-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2303	Total	C	N	O	S	0	0
			18644	11942	2959	3697	46		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2365	HIS	-	expression tag	UNP T0D3N5
A	2366	HIS	-	expression tag	UNP T0D3N5
A	2367	HIS	-	expression tag	UNP T0D3N5
A	2368	HIS	-	expression tag	UNP T0D3N5
A	2369	HIS	-	expression tag	UNP T0D3N5
A	2370	HIS	-	expression tag	UNP T0D3N5
A	2371	HIS	-	expression tag	UNP T0D3N5
A	2372	HIS	-	expression tag	UNP T0D3N5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

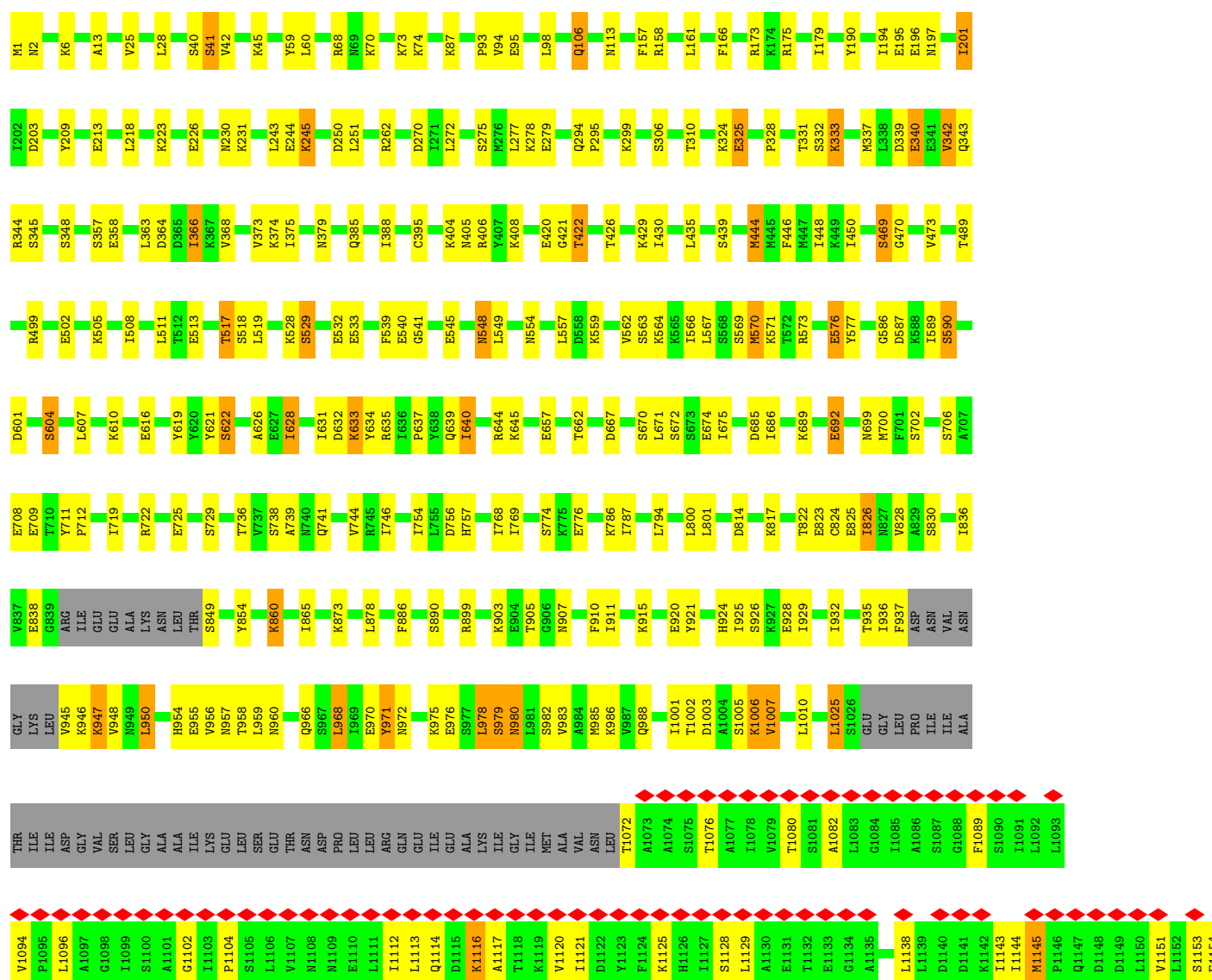
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytotoxin-L

Chain A: 



Q2119	G2059	Y1999	L1930	Y1838	P1711	M1593	P1500	S1422	K1353	L1278	K1217	T1155
L2120	I2060	F2000	M1931	D1841	M1712	I1594	M1503	K1423	M1354	K1279	D1218	D1156
G2121	L2061	M2001	I1932	S1842	Y1713	M1598	N1504	S1424	T1355	P1280	L1219	F1157
F2122	N2062	N2002	Y1936	L1843	C1715	M1610	L1505	Y1425	T1356	R1281	M1220	N1158
T2123	F2063	D2003	Y1937	K1847	P1716	E1717	S1510	I1427	I1357	Y1282	V1221	M1159
L2124	G2064	G2004	Y1938		E1717				E1358	E1283	N1224	M1160
L2125	G2065	V2005	Y1947	N1851	D1722	I1613	D1512	S1430	S1359	D1284	A1225	S1161
N2126	K2066	G2006	I1948	I1854	I1726	G1615	L1513	G1431	D1360	T1288	P1226	T1162
L2127	I2067	Q2007	K1949		I1726	S1616	K1514	N1432	E1361	I1289	N1227	T1163
N2128	K2068	V2008	K1950		K1729	M1617	D1515	C1433	I1362	N1290	R1228	G1165
F2069	G2009	V2009	L1951	F1857	K1729	S1618	M1516	M1434	I1362	L1291	G1166	K1166
L2129	F2069	G2010	L1952	T1858	L1737		R1517	K1435	Q1363	F1230	C1167	C1167
F2130	D2070	Y2010	D1953	K1864	L1737	Q1621	G1522	L1436	E1366			
Y2131	D2071	I2011	D1954		Y1741	L1624	D1523	I1437	L1367	G1293	G1231	E1168
F2132	I2072	E2012	E1955	F1867	Y1741		V1524	E1438	I1368	N1294	Y1232	T1169
S2133	S2073	V2013	T1956		S1748	K1628		N1439	E1369	T1295	E1233	M1170
S2134	N2074	N2014	Y1957	S1872	D1749			S1440	M1370	R1296	M1234	R1171
E2134	Y1958	G2015	F1959		I1751	P1634	M1530	S1441	L1371	I1299	G1235	A1172
S2135	T2075	K2016	M1960	S1876	I1751		F1531	D1442	L1372	V1300	W1236	E1173
G2136	A2076	Y2017	P1961	I1877	A1754	K1638	F1532	I1443	S1373		T1237	G1174
K2137	V2077	F2018	K1962			K1639	D1534	Q1444	L1375	I1303	P1238	G1175
T2138	G2078	Y2019	T1963	I1880	E1758	K1640	D1535	Q1445	M1376	T1304	G1239	S1176
E2139	G2079	F2020	G1964	K1885		I1641	M1536	K1446		T1305	F1240	G1177
L2140	W2080	F2020	E1965	D1886	M1770	K1642		I1447		E1306	R1241	H1178
G2141	G2081	G2021	A1966	Y1887	F1771	E1643	S1539	D1448		Q1307	R1241	H1178
G2141	Y1958	K2022	L1967	Y1888	F1772	T1644	L1540	I1449		I1308	S1242	T1179
Y2142	T2082	N2023	K1968	Y1646		S1645	F1542	I1450	G1451	I1309	L1243	L1180
Q2143	L2083	G2024	G1969	T1647	D1779			G1451	T1383	K1309	D1244	T1181
N2144	D2084	E2025	I1894		S1782	G1651	T1547	F1452	L1384	R1310	D1245	D1182
L2145	D2085	R2026	L1895			M1652		N1453	M1385	K1311	N1246	D1183
N2146	G2086	Q2027	V1899		V1791	K1653	L1552	G1454	H1387	L1312	G1247	I1184
G2147	S2087	L2028	G1972		K1795	Q1654	Y1556	H1455	T1388			T1185
T2088	T2088	G2029	I1973	D1975	I1796	M1655		K1457	I1389	F1316	T1248	D1186
Y2089	Y2089	V2030	D1975		I1797		E1559	K1458	M1390	Y1317	K1249	H1187
Y2149	Y2090	F2031	N1976	L1906	F1800	S1661	L1566	I1460	G1318	L1251	K1250	F1188
F2150	Y2091	N2032	K1907	K1907	S1801	Y1662		P1461	S1319		D1252	S1189
T2151	D2092	N2033	Y1908	Y1909	Q1679		N1570	Y1462	I1395	S1322	R1253	S1190
L2152	D2093	T2033	F1911	F1911	L1682		K1573	S1463	N1396	Y1323	I1254	P1191
D2153	N2094	T2034	G1912	G1912	Y1683		S1574	I1465	E1397	S1324	R1255	S1192
E2154	D2094	D2035	G1913	G1913	G1684		A1575	D1466	M1399	L1325	D1256	I1193
S2155	T2095	G2036	T1914	T1914	G1808			N1467	R1400	S1326		T1194
G2156	A2096	F2037	G1984	L1915	Y1812	R1687	T1578		S1403	H1257	Y1257	T1194
L2157	E2097	K2038	I1985		S1818	K1691	L1582	Y1471	L1404	Y1258		Y1195
Y2158	A2098	F2039	M1986	E1920		V1692	M1583	Y1477	D1335	E1259	R1196	R1196
L2159	C2099	F2040	Q1987	G1921	Y1823	I1693		S1478	F1406	G1260	K1197	K1197
T2160	I2100	G2041	T1988	E1922			L1586	K1479	S1407	Q1261	P1198	P1198
G2161	G2101	F2042	G1989	S1923	M1827	L1698		K1480	I1408	F1262	W1199	W1199
V2162	L2102	K2043	F1990	V1924			S1588	F1484	L1409	Y1263	L1200	L1200
F2163	T2103	D2044	I1991	N1925	M1831	T1706	I1589	E1491	M1413	W1264	S1201	S1201
D2164	Y2104	D2045	F1992	F1926		P1707	N1590	I1414	R1265	I1202	I1202	I1202
T2165	I2105	D2046	I1993	I1927	L1836		T1591	I1415	I1266	Y1203	D1204	V1205
P2166	N2106	L2047	H1994	G1928	I1837	K1710	I1592	N1496	I1276	F1267	A1268	V1206
D2167	D2107	G2048	D1995					I1497			F1269	L1206
G2168	K2109	T2049	K1996								I1270	N1207
Y2169	Y2110	E2050	V1997	K1929							A1271	I1208
K2170	Y2111	E2051	F1998									I1208
Y2171	F2112	G2052										K1212
F2172	D2113	E2053										I1213
A2173	L2054	T2055										D1272
P2174	D2114	T2056										A1273
L2175	N2115	L2056										I1274
G2116	G2116	Y2057										I1275
N2176	I2117	N2058										T1276
T2177	R2118											S1216
V2178												



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1045888	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.371	Depositor
Minimum map value	-8.281	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/19023	0.57	2/25734 (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	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1947	VAL	CA-C-N	5.87	132.75	121.54
1	A	1947	VAL	C-N-CA	5.87	132.75	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1511	LYS	Peptide
1	A	364	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	18644	0	18175	530	0
2	A	1	0	0	0	0
All	All	18645	0	18175	530	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 14.

All (530) 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:1956:THR:HG23	1:A:1986:MET:N	1.21	1.51
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1956:THR:HG21	1:A:1986:MET:CA	1.71	1.19
1:A:1956:THR:HG21	1:A:1986:MET:CB	1.74	1.18
1:A:1956:THR:CG2	1:A:1986:MET:CB	2.34	1.05
1:A:1956:THR:CG2	1:A:1986:MET:H	1.50	1.04
1:A:1956:THR:HG22	1:A:1985:ILE:HG22	1.40	1.03
1:A:1956:THR:HG21	1:A:1986:MET:HB3	1.32	1.03
1:A:1956:THR:CG2	1:A:1986:MET:CA	2.32	1.03
1:A:699:ASN:H	1:A:741:GLN:HE21	1.12	0.95
1:A:1956:THR:CG2	1:A:1986:MET:HB3	1.96	0.94
1:A:1956:THR:HG21	1:A:1986:MET:C	1.99	0.88
1:A:1356:THR:HG23	1:A:1363:GLN:HB3	1.59	0.84
1:A:1591:ILE:HG22	1:A:1592:LYS:HD2	1.64	0.79
1:A:1154:GLU:HG3	1:A:1163:THR:HG22	1.65	0.79
1:A:1573:LYS:HA	1:A:1687:ARG:HH12	1.47	0.78
1:A:1956:THR:OG1	1:A:1986:MET:HB2	1.83	0.77
1:A:1956:THR:OG1	1:A:1986:MET:CB	2.33	0.77
1:A:1326:SER:HA	1:A:1347:ASP:HB3	1.65	0.76
1:A:1082:ALA:HB1	1:A:1405:THR:HG21	1.68	0.76
1:A:957:ASN:HA	1:A:960:ASN:HB2	1.68	0.76
1:A:2194:ARG:HG2	1:A:2199:VAL:HG12	1.67	0.75
1:A:1628:LYS:H	1:A:1628:LYS:HD2	1.51	0.74
1:A:2128:ASN:HB3	1:A:2157:LEU:HD22	1.70	0.73
1:A:499:ARG:NH1	1:A:502:GLU:OE1	2.22	0.73
1:A:1827:ASN:ND2	1:A:1831:ASN:O	2.22	0.72
1:A:1956:THR:HG21	1:A:1986:MET:O	1.88	0.72
1:A:1956:THR:CB	1:A:1986:MET:HB3	2.18	0.72
1:A:1956:THR:O	1:A:1985:ILE:HA	1.90	0.71
1:A:2088:THR:HG21	1:A:2118:ARG:HH21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1791:VAL:HG13	1:A:1795:LYS:HD2	1.72	0.71
1:A:1570:ASN:O	1:A:1687:ARG:NH2	2.24	0.70
1:A:1464:TYR:HB3	1:A:1471:TYR:HB2	1.71	0.70
1:A:1334:ILE:HB	1:A:1389:ILE:HG23	1.75	0.69
1:A:1427:ILE:HD13	1:A:1452:PHE:HE2	1.57	0.69
1:A:1345:VAL:HA	1:A:1403:SER:O	1.93	0.69
1:A:1233:GLU:HB3	1:A:1277:LYS:HB2	1.74	0.68
1:A:2123:ILE:O	1:A:2130:PHE:HB2	1.92	0.68
1:A:1952:LEU:HD12	1:A:1952:LEU:N	2.09	0.68
1:A:1427:ILE:O	1:A:1457:GLN:NE2	2.19	0.67
1:A:924:HIS:O	1:A:928:GLU:HG3	1.93	0.67
1:A:2017:TYR:HB2	1:A:2054:LEU:HD22	1.76	0.67
1:A:1128:SER:HB2	1:A:1250:LEU:HG	1.77	0.67
1:A:1371:ILE:HG23	1:A:1372:LEU:HD22	1.74	0.67
1:A:2119:GLN:HG3	1:A:2123:ILE:HG13	1.76	0.67
1:A:1353:LYS:HA	1:A:1367:LEU:HA	1.76	0.66
1:A:1348:VAL:HG21	1:A:1404:LEU:HD13	1.77	0.66
1:A:1956:THR:O	1:A:1985:ILE:HG23	1.95	0.65
1:A:2118:ARG:NH1	1:A:2135:SER:O	2.30	0.65
1:A:1307:GLN:O	1:A:1311:ASN:ND2	2.22	0.64
1:A:2253:LEU:HG	1:A:2260:ASN:HD21	1.61	0.64
1:A:294:GLN:NE2	1:A:357:SER:O	2.30	0.64
1:A:1899:VAL:HG11	1:A:1937:TYR:CE1	2.32	0.64
1:A:295:PRO:O	1:A:299:LYS:HE3	1.98	0.64
1:A:2111:TYR:HE1	1:A:2123:ILE:HB	1.61	0.64
1:A:1096:LEU:HD11	1:A:1357:ILE:HD11	1.79	0.63
1:A:1184:ILE:HD12	1:A:1265:ARG:HB3	1.79	0.63
1:A:2174:PRO:O	1:A:2181:ASN:ND2	2.31	0.63
1:A:921:TYR:CZ	1:A:925:ILE:HG21	2.33	0.63
1:A:1827:ASN:HD21	1:A:1831:ASN:HB2	1.63	0.63
1:A:1218:ASP:HB2	1:A:1296:ARG:HA	1.80	0.63
1:A:2282:TYR:H	1:A:2289:MET:HE1	1.64	0.63
1:A:1737:LEU:HD13	1:A:1872:SER:HB2	1.82	0.62
1:A:985:MET:HE2	1:A:985:MET:HA	1.81	0.62
1:A:2244:ASP:HB3	1:A:2250:ARG:CZ	2.29	0.62
1:A:1290:ASN:HA	1:A:1317:TYR:HB3	1.82	0.62
1:A:559:LYS:O	1:A:563:SER:OG	2.14	0.62
1:A:1960:ASN:HB3	1:A:1964:GLY:H	1.65	0.62
1:A:2289:MET:HE2	1:A:2315:GLY:HA3	1.82	0.62
1:A:1405:THR:HG22	1:A:1415:ILE:HG12	1.81	0.62
1:A:421:GLY:O	1:A:426:THR:HB	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:SER:HB2	1:A:1345:VAL:HG23	1.82	0.62
1:A:1143:ILE:HG23	1:A:1219:LEU:HG	1.82	0.61
1:A:622:SER:HA	1:A:639:GLN:HE22	1.64	0.61
1:A:1295:THR:HA	1:A:1322:SER:O	2.00	0.61
1:A:1003:ASP:HB3	1:A:1006:LYS:HB2	1.80	0.61
1:A:2043:LYS:H	1:A:2051:GLU:HG2	1.65	0.61
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.82	0.61
1:A:1170:TRP:O	1:A:1232:TYR:OH	2.12	0.60
1:A:769:ILE:HG21	1:A:824:CYS:HB3	1.82	0.60
1:A:1181:THR:O	1:A:1184:ILE:HG22	2.01	0.60
1:A:1316:PHE:HE2	1:A:1334:ILE:HG23	1.65	0.60
1:A:250:ASP:HB3	1:A:404:LYS:HE2	1.83	0.60
1:A:324:LYS:O	1:A:325:GLU:HG2	2.02	0.60
1:A:1001:ILE:HD12	1:A:1010:LEU:HD13	1.84	0.60
1:A:1956:THR:CB	1:A:1986:MET:CB	2.78	0.60
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.25	0.60
1:A:1968:LYS:O	1:A:1971:HIS:NE2	2.33	0.60
1:A:1955:GLU:HG2	1:A:1985:ILE:HD13	1.84	0.59
1:A:1956:THR:OG1	1:A:1986:MET:HB3	2.01	0.59
1:A:1587:GLU:HA	1:A:1592:LYS:HD3	1.84	0.59
1:A:1818:SER:HB2	1:A:1823:TYR:CE1	2.37	0.59
1:A:1970:LEU:HD21	1:A:1977:LYS:HD3	1.84	0.58
1:A:854:TYR:CE1	1:A:960:ASN:HB3	2.37	0.58
1:A:1947:VAL:O	1:A:1959:PHE:HB2	2.01	0.58
1:A:959:LEU:HB2	1:A:1651:GLY:HA3	1.85	0.58
1:A:1772:PHE:CE1	1:A:1797:ILE:HD11	2.39	0.58
1:A:1915:LEU:CD2	1:A:1925:ASN:O	2.51	0.58
1:A:158:ARG:HG3	1:A:539:PHE:HE1	1.68	0.58
1:A:637:PRO:HD2	1:A:640:ILE:HD11	1.84	0.58
1:A:966:GLN:O	1:A:970:GLU:HB3	2.03	0.58
1:A:1153:SER:HB2	1:A:1163:THR:HG23	1.85	0.58
1:A:1496:ASN:O	1:A:1505:LEU:HA	2.03	0.58
1:A:979:SER:HA	1:A:982:SER:HB3	1.85	0.58
1:A:2244:ASP:HB3	1:A:2250:ARG:NE	2.19	0.58
1:A:631:ILE:HD12	1:A:637:PRO:HG3	1.86	0.58
1:A:2320:TYR:HE1	1:A:2324:LEU:HB2	1.69	0.57
1:A:1858:THR:HB	1:A:1867:PHE:HE2	1.70	0.57
1:A:1956:THR:HG23	1:A:1986:MET:H	0.58	0.57
1:A:2273:TYR:HE2	1:A:2280:MET:HB3	1.68	0.57
1:A:1640:LYS:HE2	1:A:1643:GLU:HA	1.86	0.57
1:A:2188:LYS:HB3	1:A:2206:TYR:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:LYS:HE2	1:A:1536:MET:HE3	1.87	0.57
1:A:173:ARG:NH2	1:A:823:GLU:OE2	2.34	0.57
1:A:528:LYS:NZ	1:A:545:GLU:OE2	2.33	0.57
1:A:577:TYR:HB3	1:A:645:LYS:HB2	1.87	0.57
1:A:1748:SER:HB2	1:A:1770:ASN:HA	1.86	0.57
1:A:1929:LYS:HE3	1:A:1936:ILE:HG23	1.87	0.57
1:A:196:GLU:HG3	1:A:197:ASN:N	2.20	0.57
1:A:540:GLU:HG2	1:A:541:GLY:H	1.70	0.57
1:A:702:SER:HB3	1:A:776:GLU:HB2	1.86	0.57
1:A:529:SER:O	1:A:533:GLU:HG3	2.04	0.56
1:A:1511:LYS:HG2	1:A:1512:ASP:OD1	2.05	0.56
1:A:1908:TYR:O	1:A:1923:SER:HA	2.05	0.56
1:A:1908:TYR:CE2	1:A:1930:LEU:HD21	2.40	0.56
1:A:1348:VAL:HG23	1:A:1406:PHE:HB3	1.86	0.56
1:A:921:TYR:CE1	1:A:925:ILE:HD13	2.40	0.56
1:A:1385:ASN:O	1:A:1387:HIS:ND1	2.34	0.56
1:A:2300:PHE:HB3	1:A:2339:ALA:HB3	1.88	0.56
1:A:60:LEU:HD13	1:A:73:LYS:HE2	1.87	0.56
1:A:1437:ILE:HD12	1:A:1497:ILE:HD12	1.87	0.56
1:A:1899:VAL:HG11	1:A:1937:TYR:CZ	2.40	0.56
1:A:1956:THR:CG2	1:A:1985:ILE:HG22	2.26	0.56
1:A:1292:ASP:OD1	1:A:1296:ARG:NH1	2.26	0.56
1:A:1949:TRP:CZ2	1:A:1973:ILE:HG21	2.40	0.56
1:A:1864:LYS:HE3	1:A:1895:LEU:HD13	1.87	0.56
1:A:1956:THR:CG2	1:A:1986:MET:O	2.54	0.56
1:A:310:THR:HG23	1:A:511:LEU:HD13	1.87	0.56
1:A:1154:GLU:HA	1:A:1288:ARG:O	2.06	0.56
1:A:1345:VAL:HG12	1:A:1403:SER:HB3	1.87	0.55
1:A:1586:LEU:HD21	1:A:1613:ILE:HD11	1.88	0.55
1:A:2276:ILE:HG22	1:A:2277:LYS:HG2	1.88	0.55
1:A:1303:ILE:HB	1:A:1309:ARG:HG2	1.88	0.55
1:A:1151:VAL:HG12	1:A:1165:GLY:HA3	1.88	0.55
1:A:545:GLU:HB2	1:A:757:HIS:CD2	2.41	0.55
1:A:1346:ILE:HG22	1:A:1348:VAL:HG13	1.87	0.55
1:A:1515:ASP:HB3	1:A:1530:ASN:ND2	2.22	0.55
1:A:562:VAL:O	1:A:566:ILE:HG13	2.07	0.55
1:A:2293:VAL:HG12	1:A:2300:PHE:HD2	1.72	0.55
1:A:955:GLU:O	1:A:959:LEU:HG	2.07	0.55
1:A:2011:ILE:HD12	1:A:2020:PHE:HD2	1.72	0.55
1:A:1316:PHE:HB2	1:A:1336:LEU:HD23	1.89	0.54
1:A:2043:LYS:HE2	1:A:2050:GLU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:GLU:HG3	1:A:787:ILE:HD12	1.89	0.54
1:A:814:ASP:OD2	1:A:814:ASP:N	2.37	0.54
1:A:968:LEU:HG	1:A:985:MET:HG3	1.90	0.54
1:A:1185:ASP:HB2	1:A:1265:ARG:O	2.07	0.54
1:A:1425:TYR:O	1:A:1456:HIS:NE2	2.36	0.54
1:A:1166:LYS:HD2	1:A:1227:ASN:HB3	1.90	0.54
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.54
1:A:559:LYS:NZ	1:A:628:ILE:O	2.35	0.53
1:A:1168:GLU:HB2	1:A:1229:VAL:HA	1.90	0.53
1:A:1432:ASN:OD1	1:A:1435:LYS:N	2.30	0.53
1:A:420:GLU:HG3	1:A:430:ILE:HD13	1.91	0.53
1:A:226:GLU:OE1	1:A:230:ASN:ND2	2.39	0.53
1:A:1514:LYS:N	1:A:1530:ASN:O	2.39	0.53
1:A:1638:LYS:HG3	1:A:1647:THR:HG23	1.90	0.53
1:A:1714:ILE:HG13	1:A:1716:PRO:HD3	1.89	0.53
1:A:1512:ASP:OD1	1:A:1512:ASP:N	2.41	0.53
1:A:2223:ASP:HB2	1:A:2230:TYR:HE2	1.73	0.53
1:A:1316:PHE:CE2	1:A:1334:ILE:HG23	2.43	0.53
1:A:1448:ASP:OD1	1:A:1477:TYR:OH	2.25	0.53
1:A:692:GLU:HG2	1:A:736:THR:HB	1.90	0.53
1:A:719:ILE:HA	1:A:722:ARG:HE	1.73	0.53
1:A:1125:LYS:HG3	1:A:1247:GLY:HA3	1.91	0.53
1:A:1698:LEU:HD12	1:A:1726:ILE:HG13	1.89	0.53
1:A:1334:ILE:HB	1:A:1389:ILE:HD12	1.91	0.53
1:A:672:SER:HB3	1:A:722:ARG:NH2	2.24	0.53
1:A:1264:TRP:HE1	1:A:1265:ARG:HH21	1.56	0.53
1:A:1996:LYS:HB3	1:A:2025:GLU:HG2	1.91	0.53
1:A:1989:GLY:H	1:A:2000:PHE:HB2	1.73	0.53
1:A:587:ASP:OD2	1:A:590:SER:OG	2.21	0.52
1:A:980:ASN:N	1:A:980:ASN:OD1	2.41	0.52
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.91	0.52
1:A:1624:LEU:HD23	1:A:1634:PRO:HA	1.91	0.52
1:A:573:ARG:HG2	1:A:1806:SER:O	2.09	0.52
1:A:633:LYS:HE2	1:A:634:TYR:CE1	2.44	0.52
1:A:1340:GLU:HB2	1:A:1396:ASN:HD21	1.74	0.52
1:A:175:ARG:O	1:A:179:ILE:HG13	2.09	0.52
1:A:1847:LYS:O	1:A:1851:ASN:N	2.39	0.52
1:A:1336:LEU:HD12	1:A:1338:LEU:HD23	1.92	0.52
1:A:1221:VAL:HG22	1:A:1299:ILE:HG23	1.90	0.52
1:A:2160:ILE:HA	1:A:2172:PHE:O	2.10	0.52
1:A:1575:ALA:HA	1:A:1578:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1796:ILE:O	1:A:1800:PHE:HB2	2.10	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:CZ	2.87	0.52
1:A:2049:THR:HG22	1:A:2053:GLU:HB3	1.92	0.51
1:A:1510:SER:OG	1:A:1511:LYS:O	2.27	0.51
1:A:1540:LEU:HD11	1:A:1552:LEU:HD22	1.92	0.51
1:A:1957:TYR:HE1	1:A:1983:ASN:O	1.93	0.51
1:A:196:GLU:HG3	1:A:197:ASN:H	1.74	0.51
1:A:2336:GLU:HG3	1:A:2338:ILE:HG22	1.91	0.51
1:A:975:LYS:O	1:A:976:GLU:HG2	2.11	0.51
1:A:1120:VAL:HG13	1:A:1278:LEU:HD11	1.92	0.51
1:A:2242:TYR:HB2	1:A:2263:PHE:CZ	2.46	0.51
1:A:513:GLU:O	1:A:517:THR:HG23	2.09	0.51
1:A:549:LEU:HD11	1:A:589:ILE:HD12	1.92	0.51
1:A:621:TYR:HD2	1:A:628:ILE:HG13	1.76	0.51
1:A:1264:TRP:NE1	1:A:1265:ARG:HE	2.08	0.51
1:A:1976:ASN:HB3	1:A:2005:VAL:HG13	1.93	0.51
1:A:2244:ASP:CB	1:A:2250:ARG:NH2	2.73	0.51
1:A:13:ALA:O	1:A:68:ARG:NH1	2.44	0.51
1:A:1444:GLN:HA	1:A:1447:ILE:HG22	1.93	0.51
1:A:1968:LYS:HE2	1:A:1982:ASP:O	2.11	0.51
1:A:1116:LYS:O	1:A:1120:VAL:HG23	2.11	0.51
1:A:1559:GLU:OE1	1:A:1618:SER:OG	2.27	0.51
1:A:576:GLU:HB2	1:A:577:TYR:CD1	2.46	0.51
1:A:979:SER:O	1:A:983:VAL:HG22	2.11	0.51
1:A:1117:ALA:O	1:A:1121:ILE:HD12	2.10	0.51
1:A:1292:ASP:O	1:A:1323:TYR:OH	2.24	0.51
1:A:966:GLN:HE21	1:A:970:GLU:HB2	1.76	0.50
1:A:2177:THR:OG1	1:A:2181:ASN:ND2	2.31	0.50
1:A:1586:LEU:O	1:A:1591:ILE:HB	2.11	0.50
1:A:1400:ARG:NH2	1:A:1421:VAL:HB	2.26	0.50
1:A:2011:ILE:HD12	1:A:2020:PHE:CD2	2.47	0.50
1:A:1497:ILE:HG12	1:A:1505:LEU:HB2	1.93	0.50
1:A:1291:LEU:O	1:A:1319:SER:OG	2.22	0.50
1:A:1459:TYR:OH	1:A:1522:GLY:O	2.27	0.50
1:A:2177:THR:N	1:A:2181:ASN:OD1	2.43	0.50
1:A:340:GLU:O	1:A:344:ARG:HG2	2.12	0.50
1:A:1251:LEU:HD13	1:A:1264:TRP:CZ2	2.46	0.50
1:A:1352:VAL:HG13	1:A:1371:ILE:HG12	1.93	0.50
1:A:2244:ASP:HB2	1:A:2250:ARG:NH2	2.27	0.50
1:A:2006:MET:HE3	1:A:2024:GLY:HA3	1.92	0.50
1:A:1981:ASP:N	1:A:1981:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:O	1:A:194:ILE:HG13	2.12	0.49
1:A:700:MET:HB3	1:A:739:ALA:HB1	1.94	0.49
1:A:2264:ASN:OD1	1:A:2267:GLY:N	2.45	0.49
1:A:1327:LEU:HD13	1:A:1346:ILE:HG23	1.94	0.49
1:A:1807:ASP:HB2	1:A:1812:TYR:HE2	1.77	0.49
1:A:1104:PRO:HA	1:A:1112:ILE:O	2.13	0.49
1:A:886:PHE:HB2	1:A:988:GLN:HE22	1.77	0.49
1:A:1238:PRO:HG3	1:A:1271:ALA:HB1	1.94	0.49
1:A:1582:LEU:O	1:A:1586:LEU:HG	2.13	0.49
1:A:722:ARG:HA	1:A:725:GLU:HG2	1.94	0.49
1:A:1169:ILE:HG23	1:A:1232:TYR:HE2	1.77	0.49
1:A:2208:ILE:HD13	1:A:2227:LYS:HG2	1.93	0.49
1:A:557:LEU:HD22	1:A:607:LEU:HD23	1.95	0.49
1:A:2172:PHE:CE2	1:A:2186:ALA:HB2	2.48	0.49
1:A:2215:ASN:O	1:A:2217:THR:N	2.37	0.49
1:A:106:GLN:NE2	1:A:231:LYS:HD3	2.28	0.48
1:A:1956:THR:HG22	1:A:1985:ILE:CG2	2.26	0.48
1:A:2058:ASN:HD21	1:A:2072:ILE:HA	1.77	0.48
1:A:2230:TYR:HD1	1:A:2234:ASN:HB3	1.77	0.48
1:A:1144:ILE:HD11	1:A:1217:LYS:HD2	1.95	0.48
1:A:1113:LEU:HB2	1:A:1280:PRO:HD3	1.94	0.48
1:A:1352:VAL:HG13	1:A:1371:ILE:HG21	1.95	0.48
1:A:1981:ASP:OD1	1:A:1985:ILE:N	2.41	0.48
1:A:1348:VAL:HB	1:A:1351:VAL:HB	1.96	0.48
1:A:1437:ILE:HD11	1:A:1484:PHE:CE2	2.47	0.48
1:A:959:LEU:HB2	1:A:1651:GLY:CA	2.43	0.48
1:A:1076:THR:O	1:A:1080:THR:HG23	2.13	0.48
1:A:921:TYR:O	1:A:925:ILE:HG12	2.14	0.48
1:A:1901:ASN:HA	1:A:1906:LEU:HA	1.96	0.48
1:A:635:ARG:NH2	1:A:685:ASP:OD1	2.47	0.47
1:A:1154:GLU:HG3	1:A:1163:THR:CG2	2.39	0.47
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.14	0.47
1:A:838:GLU:HA	1:A:838:GLU:OE1	2.13	0.47
1:A:2289:MET:HE2	1:A:2315:GLY:CA	2.44	0.47
1:A:956:VAL:HG23	1:A:957:ASN:H	1.79	0.47
1:A:1439:ASN:OD1	1:A:1442:ASP:HB3	2.14	0.47
1:A:1542:PHE:HB3	1:A:1552:LEU:HD23	1.94	0.47
1:A:1967:LEU:HB3	1:A:1971:HIS:CD2	2.50	0.47
1:A:2317:SER:O	1:A:2317:SER:OG	2.32	0.47
1:A:41:SER:O	1:A:45:LYS:HG3	2.13	0.47
1:A:1610:ASN:OD1	1:A:1610:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:PRO:HD2	1:A:1654:GLN:NE2	2.30	0.47
1:A:2129:ILE:O	1:A:2157:LEU:HA	2.15	0.47
1:A:1292:ASP:OD1	1:A:1292:ASP:N	2.46	0.47
1:A:1409:LEU:HD11	1:A:1446:LYS:HG3	1.97	0.47
1:A:801:LEU:HD13	1:A:828:VAL:HB	1.97	0.47
1:A:1169:ILE:HD12	1:A:1202:ILE:HD11	1.97	0.47
1:A:1327:LEU:HD22	1:A:1348:VAL:HG12	1.96	0.47
1:A:1439:ASN:O	1:A:1443:ILE:HG13	2.15	0.47
1:A:1977:LYS:HD2	1:A:2006:MET:SD	2.55	0.47
1:A:2243:PHE:CE2	1:A:2249:MET:HG3	2.50	0.47
1:A:1156:ASP:OD1	1:A:1290:ASN:ND2	2.48	0.47
1:A:1167:CYS:HB2	1:A:1203:TYR:CD2	2.50	0.47
1:A:1458:LYS:HE3	1:A:1458:LYS:HB3	1.55	0.47
1:A:1973:ILE:HD13	1:A:1978:TYR:HD2	1.79	0.47
1:A:689:LYS:HD3	1:A:729:SER:HB2	1.97	0.47
1:A:970:GLU:C	1:A:972:ASN:H	2.23	0.47
1:A:1480:LYS:HG3	1:A:1500:PRO:HD3	1.97	0.47
1:A:1838:TYR:CE1	1:A:1843:LEU:HB2	2.50	0.47
1:A:270:ASP:HB3	1:A:469:SER:HB2	1.96	0.46
1:A:1691:LYS:NZ	1:A:1717:GLU:OE2	2.44	0.46
1:A:2242:TYR:HE1	1:A:2256:PHE:HB2	1.81	0.46
1:A:2264:ASN:HD21	1:A:2266:ASP:HB3	1.80	0.46
1:A:754:ILE:HG23	1:A:768:ILE:HG12	1.97	0.46
1:A:1354:ASN:N	1:A:1366:GLU:O	2.44	0.46
1:A:1371:ILE:HG22	1:A:1450:ILE:HD12	1.96	0.46
1:A:2113:ASP:OD2	1:A:2117:ILE:HB	2.16	0.46
1:A:2151:TYR:HB2	1:A:2172:PHE:CZ	2.51	0.46
1:A:1512:ASP:HA	1:A:1514:LYS:HZ2	1.78	0.46
1:A:822:THR:O	1:A:826:ILE:HD12	2.15	0.46
1:A:1380:ASN:HB3	1:A:1391:PHE:O	2.16	0.46
1:A:201:ILE:HD11	1:A:203:ASP:HB2	1.97	0.46
1:A:960:ASN:ND2	1:A:1652:ASN:HA	2.31	0.46
1:A:2360:LEU:HG	1:A:2362:VAL:HG13	1.97	0.46
1:A:1947:VAL:O	1:A:1948:GLU:O	2.33	0.46
1:A:2215:ASN:C	1:A:2217:THR:H	2.23	0.46
1:A:278:LYS:HD3	1:A:279:GLU:OE1	2.16	0.46
1:A:935:THR:O	1:A:947:LYS:HB3	2.16	0.46
1:A:2170:LYS:HE3	1:A:2186:ALA:HB1	1.98	0.46
1:A:1997:VAL:HB	1:A:2026:ARG:HB3	1.98	0.45
1:A:1310:LYS:HE2	1:A:1310:LYS:HB2	1.68	0.45
1:A:1396:ASN:N	1:A:1399:ASN:OD1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1979:TYR:HD1	1:A:1987:GLN:HB2	1.81	0.45
1:A:243:LEU:HB3	1:A:245:LYS:H	1.81	0.45
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.77	0.45
1:A:1452:PHE:HE1	1:A:1460:ILE:HD11	1.81	0.45
1:A:1741:TYR:CE1	1:A:1754:ALA:HB2	2.50	0.45
1:A:1750:LEU:HD12	1:A:1751:ILE:H	1.82	0.45
1:A:2142:TYR:OH	1:A:2167:ASP:OD2	2.21	0.45
1:A:2353:PHE:CZ	1:A:2360:LEU:HB2	2.51	0.45
1:A:324:LYS:C	1:A:325:GLU:HG2	2.42	0.45
1:A:1679:GLN:O	1:A:1712:ASN:ND2	2.47	0.45
1:A:2223:ASP:HB2	1:A:2230:TYR:CE2	2.49	0.45
1:A:1:MET:HE3	1:A:2:ASN:H	1.81	0.45
1:A:294:GLN:HG3	1:A:358:GLU:O	2.16	0.45
1:A:899:ARG:HB2	1:A:910:PHE:CE1	2.52	0.45
1:A:2095:THR:HG23	1:A:2097:GLU:HG3	1.99	0.45
1:A:2354:ASP:OD1	1:A:2355:PRO:HD2	2.17	0.45
1:A:554:ASN:OD1	1:A:586:GLY:HA3	2.17	0.45
1:A:1372:LEU:HD23	1:A:1450:ILE:HG21	1.99	0.45
1:A:610:LYS:HE3	1:A:674:GLU:OE2	2.17	0.45
1:A:873:LYS:HG2	1:A:878:LEU:HB2	1.99	0.45
1:A:1171:ARG:HG3	1:A:1194:THR:HB	1.98	0.45
1:A:1264:TRP:HB2	1:A:1275:ILE:HG13	1.99	0.45
1:A:1640:LYS:HE3	1:A:1661:SER:CB	2.47	0.45
1:A:1895:LEU:HD21	1:A:1921:GLY:HA3	1.97	0.45
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.98	0.45
1:A:1374:LYS:HD2	1:A:1385:ASN:H	1.82	0.45
1:A:1408:ILE:HD12	1:A:1409:LEU:HD12	1.99	0.45
1:A:1908:TYR:HE2	1:A:1932:ILE:HD11	1.82	0.45
1:A:2254:ILE:HB	1:A:2263:PHE:HE2	1.82	0.45
1:A:70:LYS:HG3	1:A:1698:LEU:HD11	1.98	0.45
1:A:374:LYS:HB2	1:A:388:ILE:HB	1.99	0.45
1:A:1230:PHE:CE2	1:A:1280:PRO:HB3	2.51	0.45
1:A:1655:ASN:HB3	1:A:1693:ILE:CD1	2.47	0.45
1:A:1959:PHE:HE1	1:A:1966:ALA:HB2	1.82	0.45
1:A:1993:ILE:O	1:A:1996:LYS:HB2	2.17	0.45
1:A:936:ILE:HG13	1:A:946:LYS:HG3	1.99	0.44
1:A:1885:LYS:HE3	1:A:1922:GLU:OE2	2.17	0.44
1:A:1296:ARG:O	1:A:1323:TYR:HA	2.18	0.44
1:A:1400:ARG:O	1:A:1420:LEU:HG	2.17	0.44
1:A:1432:ASN:O	1:A:1436:LEU:N	2.51	0.44
1:A:2090:TYR:O	1:A:2099:CYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ASP:OD2	1:A:587:ASP:N	2.45	0.44
1:A:406:ARG:HG2	1:A:446:PHE:CE2	2.52	0.44
1:A:93:PRO:HA	1:A:366:ILE:O	2.17	0.44
1:A:2299:GLY:HA3	1:A:2338:ILE:HD12	1.99	0.44
1:A:540:GLU:HG2	1:A:541:GLY:N	2.32	0.44
1:A:936:ILE:HG13	1:A:946:LYS:CD	2.47	0.44
1:A:2092:ASP:N	1:A:2092:ASP:OD1	2.50	0.44
1:A:2185:GLN:NE2	1:A:2186:ALA:O	2.51	0.44
1:A:1113:LEU:O	1:A:1114:GLN:NE2	2.51	0.44
1:A:1155:ILE:HB	1:A:1289:ILE:HG23	1.99	0.44
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.99	0.44
1:A:1533:LYS:O	1:A:1535:ASP:N	2.44	0.44
1:A:505:LYS:HB2	1:A:505:LYS:HE2	1.60	0.44
1:A:978:LEU:HD23	1:A:982:SER:HB2	2.00	0.44
1:A:1001:ILE:HG22	1:A:1007:VAL:HG23	1.99	0.44
1:A:1955:GLU:CG	1:A:1985:ILE:HD13	2.45	0.44
1:A:2195:VAL:HG12	1:A:2196:ASN:N	2.32	0.44
1:A:2329:LYS:HE3	1:A:2360:LEU:H	1.82	0.44
1:A:1164:LEU:HG	1:A:1203:TYR:CD2	2.53	0.44
1:A:1291:LEU:HD23	1:A:1323:TYR:CG	2.52	0.44
1:A:1513:LEU:HA	1:A:1513:LEU:HD12	1.72	0.44
1:A:1959:PHE:CE1	1:A:1966:ALA:HB2	2.53	0.44
1:A:2235:VAL:HG22	1:A:2240:LYS:HG3	2.00	0.44
1:A:570:MET:HE2	1:A:570:MET:HB2	1.83	0.43
1:A:1218:ASP:O	1:A:1296:ARG:HG3	2.18	0.43
1:A:1296:ARG:NH1	1:A:1296:ARG:HB2	2.33	0.43
1:A:1531:TYR:CD1	1:A:1594:ILE:HD13	2.53	0.43
1:A:1706:THR:HA	1:A:1707:PRO:HD3	1.83	0.43
1:A:2285:LYS:HD3	1:A:2285:LYS:HA	1.72	0.43
1:A:429:LYS:HA	1:A:429:LYS:HD2	1.81	0.43
1:A:622:SER:O	1:A:626:ALA:N	2.51	0.43
1:A:1405:THR:HG22	1:A:1415:ILE:HG23	1.99	0.43
1:A:2178:VAL:HG21	1:A:2189:TYR:HB2	2.00	0.43
1:A:2219:LYS:HE3	1:A:2249:MET:HB3	2.01	0.43
1:A:936:ILE:HG13	1:A:946:LYS:HD2	2.00	0.43
1:A:1089:PHE:HD2	1:A:1299:ILE:HD13	1.83	0.43
1:A:1145:MET:HB3	1:A:1145:MET:HE2	1.64	0.43
1:A:1316:PHE:N	1:A:1335:ASP:O	2.47	0.43
1:A:1949:TRP:CE3	1:A:1958:TYR:HB2	2.53	0.43
1:A:1957:TYR:CE1	1:A:1983:ASN:O	2.70	0.43
1:A:2050:GLU:N	1:A:2053:GLU:OE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1973:ILE:HB	1:A:1978:TYR:CE2	2.53	0.43
1:A:2142:TYR:CD2	1:A:2166:PRO:HD2	2.53	0.43
1:A:2226:THR:HG22	1:A:2228:LYS:HD3	2.00	0.43
1:A:2304:ALA:O	1:A:2315:GLY:N	2.52	0.43
1:A:1951:LEU:CD2	1:A:1956:THR:HA	2.48	0.43
1:A:2013:VAL:O	1:A:2016:LYS:HE2	2.18	0.43
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.76	0.43
1:A:1171:ARG:NH1	1:A:1197:LYS:HD3	2.33	0.43
1:A:1413:ASN:OD1	1:A:1430:SER:HB2	2.18	0.43
1:A:87:LYS:HB3	1:A:87:LYS:HE3	1.75	0.43
1:A:333:LYS:H	1:A:333:LYS:HD2	1.84	0.43
1:A:569:SER:O	1:A:571:LYS:HD2	2.19	0.43
1:A:1166:LYS:HD3	1:A:1228:ARG:O	2.19	0.43
1:A:1368:ILE:HG13	1:A:1371:ILE:HB	2.00	0.43
1:A:1908:TYR:CE1	1:A:1910:ALA:HB2	2.54	0.43
1:A:2182:ILE:HB	1:A:2185:GLN:HB2	2.01	0.43
1:A:209:TYR:CZ	1:A:213:GLU:HG3	2.54	0.43
1:A:333:LYS:O	1:A:337:MET:HG3	2.19	0.43
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.86	0.43
1:A:1025:LEU:HD23	1:A:1621:GLN:OE1	2.18	0.43
1:A:640:ILE:H	1:A:640:ILE:HG12	1.62	0.43
1:A:2177:THR:HG1	1:A:2181:ASN:HD21	1.61	0.43
1:A:1416:ILE:HD12	1:A:1427:ILE:HG13	2.01	0.43
1:A:1652:ASN:OD1	1:A:1652:ASN:N	2.52	0.43
1:A:706:SER:HB3	1:A:709:GLU:CG	2.49	0.42
1:A:1533:LYS:HG3	1:A:1590:ASN:HB2	2.01	0.42
1:A:1432:ASN:HA	1:A:1464:TYR:CE2	2.55	0.42
1:A:1679:GLN:O	1:A:1682:LEU:HB2	2.19	0.42
1:A:1952:LEU:N	1:A:1952:LEU:CD1	2.80	0.42
1:A:1909:PHE:HB3	1:A:1921:GLY:O	2.19	0.42
1:A:860:LYS:HA	1:A:860:LYS:HD3	1.69	0.42
1:A:2230:TYR:CD1	1:A:2234:ASN:HB3	2.53	0.42
1:A:2273:TYR:CE2	1:A:2280:MET:HB3	2.52	0.42
1:A:209:TYR:CE2	1:A:213:GLU:HG3	2.54	0.42
1:A:971:TYR:HH	1:A:1662:TYR:HD1	1.68	0.42
1:A:1299:ILE:HG13	1:A:1300:VAL:N	2.35	0.42
1:A:339:ASP:O	1:A:343:GLN:HG3	2.19	0.42
1:A:886:PHE:HB2	1:A:988:GLN:NE2	2.34	0.42
1:A:972:ASN:ND2	1:A:986:LYS:HD3	2.34	0.42
1:A:1515:ASP:HB3	1:A:1530:ASN:HD21	1.83	0.42
1:A:1729:LYS:HB2	1:A:1729:LYS:HE2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2259:ASN:HB2	1:A:2261:TYR:CE2	2.55	0.42
1:A:548:ASN:OD1	1:A:548:ASN:N	2.53	0.42
1:A:1376:ASN:HB2	1:A:1383:ILE:HB	2.01	0.42
1:A:1415:ILE:O	1:A:1416:ILE:HD13	2.19	0.42
1:A:1912:ALA:N	1:A:1920:GLU:HB3	2.34	0.42
1:A:2243:PHE:HE2	1:A:2249:MET:HG3	1.85	0.42
1:A:444:MET:HE3	1:A:444:MET:HB3	1.71	0.42
1:A:1234:MET:H	1:A:1234:MET:HG2	1.62	0.42
1:A:1369:GLU:OE2	1:A:1370:ASN:HB2	2.20	0.42
1:A:1432:ASN:ND2	1:A:1464:TYR:OH	2.39	0.42
1:A:1253:ARG:HH11	1:A:1253:ARG:HG3	1.83	0.42
1:A:1359:SER:O	1:A:1359:SER:OG	2.36	0.42
1:A:601:ASP:OD2	1:A:604:SER:OG	2.38	0.42
1:A:1383:ILE:HA	1:A:1387:HIS:O	2.20	0.42
1:A:2174:PRO:HG2	1:A:2177:THR:HG21	2.02	0.42
1:A:2229:ALA:O	1:A:2231:LYS:HD2	2.20	0.42
1:A:566:ILE:HG23	1:A:571:LYS:NZ	2.35	0.41
1:A:905:THR:HG23	1:A:907:ASN:H	1.84	0.41
1:A:1025:LEU:HD12	1:A:1556:TYR:HE2	1.84	0.41
1:A:1224:ASN:N	1:A:1224:ASN:OD1	2.52	0.41
1:A:1230:PHE:HE2	1:A:1280:PRO:HB3	1.83	0.41
1:A:1352:VAL:HG21	1:A:1406:PHE:CD2	2.55	0.41
1:A:1876:SER:HB2	1:A:1880:ILE:HG13	2.00	0.41
1:A:1889:PHE:CE1	1:A:1895:LEU:HB2	2.55	0.41
1:A:711:TYR:HB3	1:A:712:PRO:HD3	2.02	0.41
1:A:955:GLU:CD	1:A:955:GLU:H	2.28	0.41
1:A:1407:SER:HA	1:A:1413:ASN:HA	2.03	0.41
1:A:6:LYS:HE3	1:A:28:LEU:HB3	2.02	0.41
1:A:244:GLU:CD	1:A:244:GLU:H	2.28	0.41
1:A:157:PHE:CD2	1:A:166:PHE:CE2	3.08	0.41
1:A:294:GLN:HG3	1:A:358:GLU:C	2.45	0.41
1:A:2242:TYR:HB2	1:A:2263:PHE:CE1	2.56	0.41
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.20	0.41
1:A:635:ARG:HH21	1:A:685:ASP:CG	2.28	0.41
1:A:1200:LEU:HD22	1:A:1258:TYR:CD1	2.56	0.41
1:A:1228:ARG:HB3	1:A:1282:TYR:CE1	2.55	0.41
1:A:2235:VAL:HG13	1:A:2240:LYS:HG3	2.02	0.41
1:A:2309:LEU:HD12	1:A:2309:LEU:HA	1.87	0.41
1:A:95:GLU:H	1:A:95:GLU:CD	2.27	0.41
1:A:339:ASP:HB2	1:A:342:VAL:HG22	2.03	0.41
1:A:557:LEU:HD23	1:A:619:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:ASP:HA	1:A:1390:ASN:O	2.19	0.41
1:A:1991:ILE:HD12	1:A:2000:PHE:CD2	2.56	0.41
1:A:2276:ILE:HB	1:A:2281:PHE:CE2	2.54	0.41
1:A:2340:ALA:HB3	1:A:2353:PHE:CG	2.55	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.90	0.41
1:A:1556:TYR:OH	1:A:1616:SER:OG	2.30	0.41
1:A:1926:PHE:HE1	1:A:1930:LEU:HB2	1.86	0.41
1:A:98:LEU:HD21	1:A:363:LEU:HD11	2.02	0.41
1:A:1212:LYS:HD2	1:A:1212:LYS:HA	1.69	0.41
1:A:1423:LYS:HD3	1:A:1423:LYS:HA	1.87	0.41
1:A:1566:LEU:HD22	1:A:1684:GLY:HA3	2.02	0.41
1:A:1854:ILE:HD13	1:A:1854:ILE:HA	1.93	0.41
1:A:1999:TYR:CE1	1:A:2011:ILE:HG21	2.56	0.41
1:A:333:LYS:HD2	1:A:333:LYS:N	2.36	0.41
1:A:1102:GLY:HA3	1:A:1114:GLN:HE22	1.85	0.41
1:A:1241:ARG:HD3	1:A:1267:PHE:HZ	1.86	0.41
1:A:1316:PHE:CE2	1:A:1334:ILE:HD12	2.56	0.41
1:A:1464:TYR:CZ	1:A:1466:ASP:HB2	2.56	0.41
1:A:1491:GLU:HG2	1:A:1511:LYS:HA	2.03	0.41
1:A:2198:ASP:OD1	1:A:2198:ASP:N	2.48	0.41
1:A:921:TYR:O	1:A:925:ILE:HG23	2.21	0.41
1:A:1642:LYS:O	1:A:1643:GLU:HB2	2.20	0.41
1:A:589:ILE:HD11	1:A:757:HIS:HA	2.04	0.40
1:A:925:ILE:HG13	1:A:926:SER:N	2.35	0.40
1:A:1241:ARG:HE	1:A:1241:ARG:HB2	1.68	0.40
1:A:1296:ARG:HB2	1:A:1296:ARG:CZ	2.52	0.40
1:A:2090:TYR:CZ	1:A:2105:ILE:HG12	2.57	0.40
1:A:470:GLY:O	1:A:473:VAL:HG22	2.21	0.40
1:A:950:LEU:H	1:A:950:LEU:HD22	1.85	0.40
1:A:1973:ILE:HB	1:A:1978:TYR:HE2	1.86	0.40
1:A:331:THR:HB	1:A:333:LYS:HD2	2.03	0.40
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.83	0.40
1:A:671:LEU:O	1:A:675:ILE:HG13	2.22	0.40
1:A:954:HIS:C	1:A:956:VAL:N	2.78	0.40
1:A:1184:ILE:HG12	1:A:1267:PHE:CD1	2.56	0.40
1:A:1353:LYS:HB3	1:A:1353:LYS:HE2	1.87	0.40
1:A:2006:MET:HE3	1:A:2024:GLY:CA	2.51	0.40
1:A:113:ASN:ND2	1:A:328:PRO:HD2	2.37	0.40
1:A:1143:ILE:HG12	1:A:1219:LEU:HD23	2.03	0.40
1:A:1938:TYR:CE2	1:A:1952:LEU:HD23	2.56	0.40
1:A:2016:LYS:HB3	1:A:2053:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2291:ILE:HA	1:A:2303:PHE:O	2.21	0.40
1:A:59:TYR:CD1	1:A:59:TYR:C	3.00	0.40
1:A:925:ILE:O	1:A:929:ILE:HG13	2.22	0.40
1:A:955:GLU:O	1:A:958:THR:HB	2.21	0.40
1:A:1089:PHE:CE2	1:A:1299:ILE:HB	2.57	0.40
1:A:1196:ARG:H	1:A:1196:ARG:HG2	1.74	0.40
1:A:1958:TYR:HD1	1:A:1967:LEU:HD13	1.85	0.40
1:A:2008:VAL:HG23	1:A:2021:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2295/2372 (97%)	2163 (94%)	128 (6%)	4 (0%)	43 63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1948	GLU
1	A	633	LYS
1	A	2342	GLY
1	A	422	THR

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	2088/2146 (97%)	1901 (91%)	187 (9%)	9 19

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	40	SER
1	A	41	SER
1	A	42	VAL
1	A	74	LYS
1	A	94	VAL
1	A	106	GLN
1	A	161	LEU
1	A	195	GLU
1	A	201	ILE
1	A	223	LYS
1	A	245	LYS
1	A	251	LEU
1	A	272	LEU
1	A	275	SER
1	A	306	SER
1	A	325	GLU
1	A	332	SER
1	A	333	LYS
1	A	340	GLU
1	A	342	VAL
1	A	345	SER
1	A	348	SER
1	A	366	ILE
1	A	368	VAL
1	A	375	ILE
1	A	379	ASN
1	A	385	GLN
1	A	405	ASN
1	A	408	LYS
1	A	422	THR
1	A	439	SER
1	A	444	MET
1	A	448	ILE
1	A	450	ILE
1	A	469	SER
1	A	489	THR
1	A	508	ILE

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Mol	Chain	Res	Type
1	A	517	THR
1	A	518	SER
1	A	519	LEU
1	A	529	SER
1	A	532	GLU
1	A	548	ASN
1	A	564	LYS
1	A	567	LEU
1	A	570	MET
1	A	576	GLU
1	A	590	SER
1	A	604	SER
1	A	616	GLU
1	A	622	SER
1	A	628	ILE
1	A	632	ASP
1	A	640	ILE
1	A	644	ARG
1	A	657	GLU
1	A	662	THR
1	A	667	ASP
1	A	670	SER
1	A	686	ILE
1	A	692	GLU
1	A	738	SER
1	A	746	ILE
1	A	756	ASP
1	A	774	SER
1	A	786	LYS
1	A	800	LEU
1	A	817	LYS
1	A	825	GLU
1	A	826	ILE
1	A	830	SER
1	A	836	ILE
1	A	849	SER
1	A	860	LYS
1	A	865	ILE
1	A	890	SER
1	A	903	LYS
1	A	911	ILE
1	A	915	LYS

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Mol	Chain	Res	Type
1	A	920	GLU
1	A	932	ILE
1	A	937	PHE
1	A	945	VAL
1	A	947	LYS
1	A	948	VAL
1	A	950	LEU
1	A	968	LEU
1	A	971	TYR
1	A	978	LEU
1	A	979	SER
1	A	980	ASN
1	A	1002	THR
1	A	1005	SER
1	A	1006	LYS
1	A	1007	VAL
1	A	1025	LEU
1	A	1072	THR
1	A	1094	VAL
1	A	1116	LYS
1	A	1129	LEU
1	A	1138	LEU
1	A	1145	MET
1	A	1161	SER
1	A	1166	LYS
1	A	1167	CYS
1	A	1169	ILE
1	A	1181	THR
1	A	1197	LYS
1	A	1212	LYS
1	A	1214	ASP
1	A	1228	ARG
1	A	1243	LEU
1	A	1250	LEU
1	A	1251	LEU
1	A	1270	ILE
1	A	1299	ILE
1	A	1310	LYS
1	A	1327	LEU
1	A	1345	VAL
1	A	1356	THR
1	A	1362	ILE

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Mol	Chain	Res	Type
1	A	1390	ASN
1	A	1397	GLU
1	A	1403	SER
1	A	1407	SER
1	A	1409	LEU
1	A	1423	LYS
1	A	1434	MET
1	A	1435	LYS
1	A	1462	TYR
1	A	1465	ILE
1	A	1478	SER
1	A	1512	ASP
1	A	1516	ILE
1	A	1517	ARG
1	A	1524	VAL
1	A	1539	SER
1	A	1541	SER
1	A	1547	THR
1	A	1582	LEU
1	A	1583	MET
1	A	1588	SER
1	A	1591	ILE
1	A	1610	ASN
1	A	1614	SER
1	A	1616	SER
1	A	1618	SER
1	A	1641	ILE
1	A	1645	SER
1	A	1647	THR
1	A	1653	ARG
1	A	1662	TYR
1	A	1682	LEU
1	A	1698	LEU
1	A	1710	LYS
1	A	1714	ILE
1	A	1722	ASP
1	A	1748	SER
1	A	1758	GLU
1	A	1779	ASP
1	A	1782	SER
1	A	1801	SER
1	A	1836	LEU

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Mol	Chain	Res	Type
1	A	1841	ASP
1	A	1842	SER
1	A	1857	PHE
1	A	1877	ILE
1	A	1885	LYS
1	A	1887	TYR
1	A	1894	ILE
1	A	1914	THR
1	A	1927	ILE
1	A	1947	VAL
1	A	1952	LEU
1	A	1955	GLU
1	A	1963	THR
1	A	1988	THR
1	A	1992	THR
1	A	1995	ASP
1	A	2037	PHE
1	A	2078	VAL
1	A	2181	ASN
1	A	2192	LEU
1	A	2235	VAL
1	A	2259	ASN
1	A	2362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	ASN
1	A	58	ASN
1	A	106	GLN
1	A	117	GLN
1	A	302	ASN
1	A	380	ASN
1	A	419	ASN
1	A	487	ASN
1	A	553	GLN
1	A	579	HIS
1	A	639	GLN
1	A	699	ASN
1	A	741	GLN
1	A	757	HIS

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Mol	Chain	Res	Type
1	A	876	ASN
1	A	924	HIS
1	A	960	ASN
1	A	988	GLN
1	A	1114	GLN
1	A	1126	HIS
1	A	1178	HIS
1	A	1207	ASN
1	A	1257	HIS
1	A	1290	ASN
1	A	1333	ASN
1	A	1396	ASN
1	A	1444	GLN
1	A	1520	ASN
1	A	1530	ASN
1	A	1548	ASN
1	A	1598	ASN
1	A	1654	GLN
1	A	1663	HIS
1	A	1669	ASN
1	A	1676	ASN
1	A	1704	ASN
1	A	1727	ASN
1	A	1733	ASN
1	A	1763	GLN
1	A	1789	GLN
1	A	2058	ASN
1	A	2146	ASN
1	A	2260	ASN
1	A	2319	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

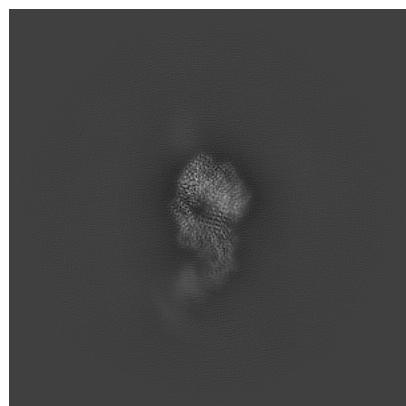
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38011. These allow visual inspection of the internal detail of the map and identification of artifacts.

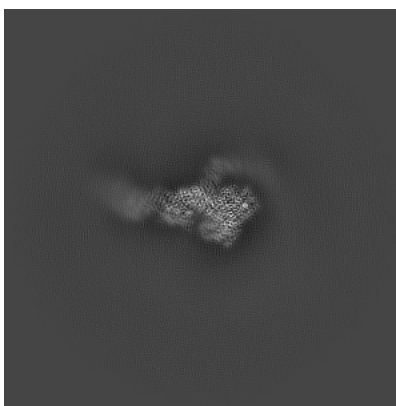
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

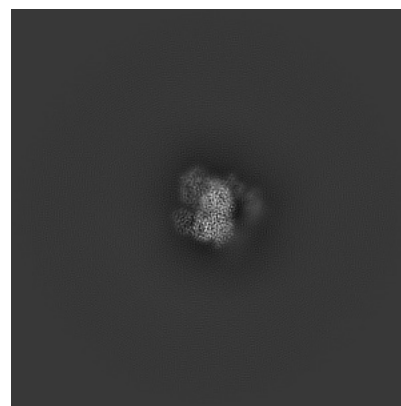
6.1.1 Primary map



X

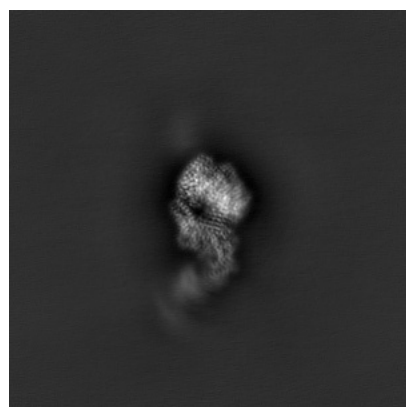


Y

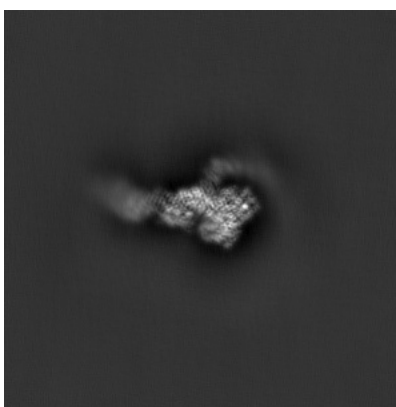


Z

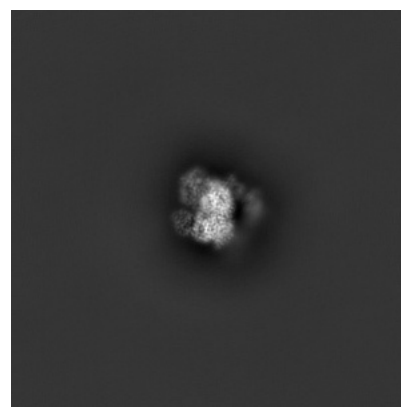
6.1.2 Raw map



X



Y

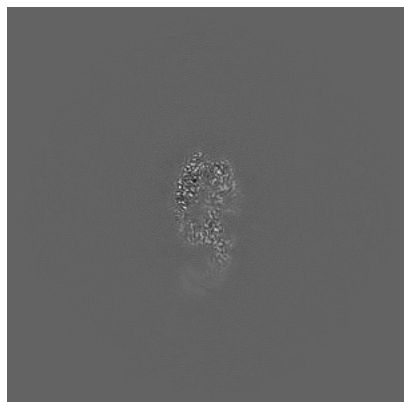


Z

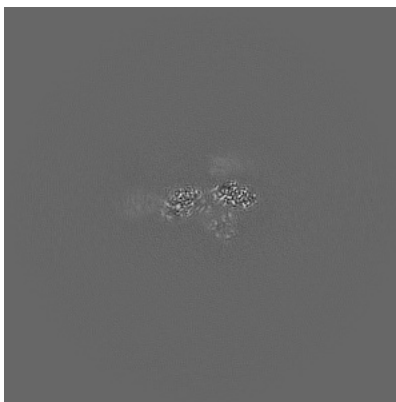
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

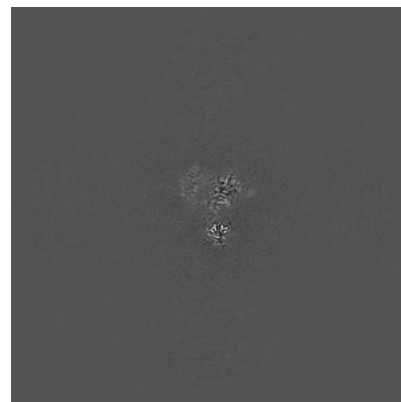
6.2.1 Primary map



X Index: 200

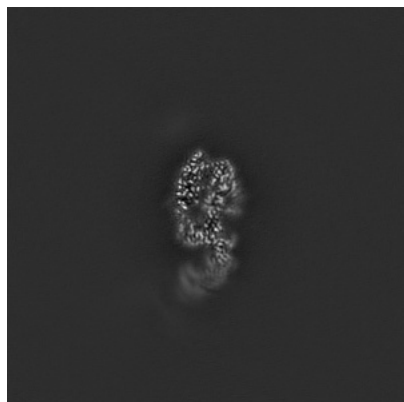


Y Index: 200

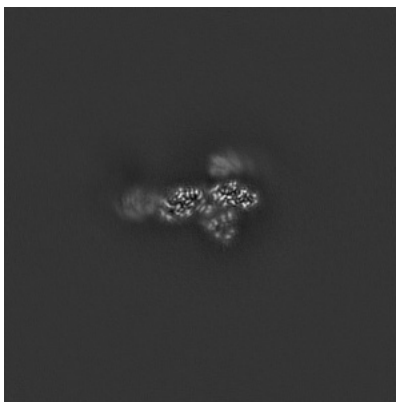


Z Index: 200

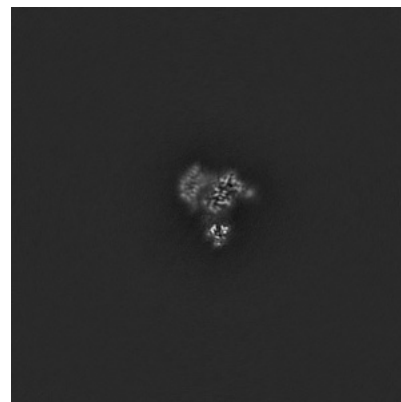
6.2.2 Raw map



X Index: 200



Y Index: 200

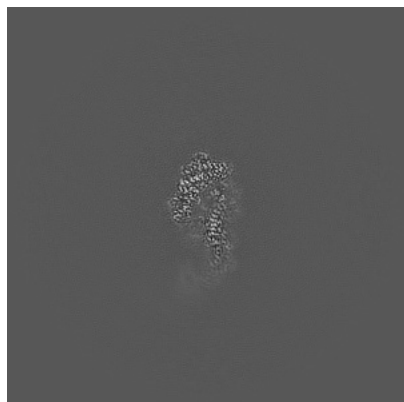


Z Index: 200

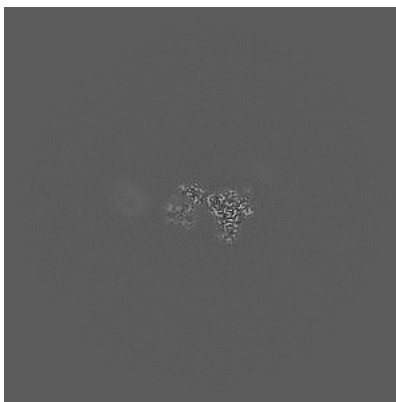
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

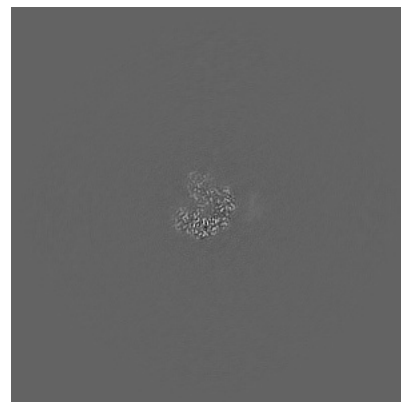
6.3.1 Primary map



X Index: 204

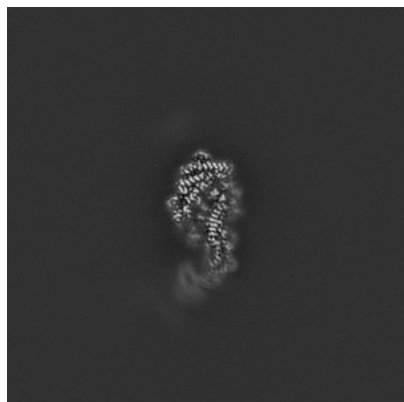


Y Index: 182

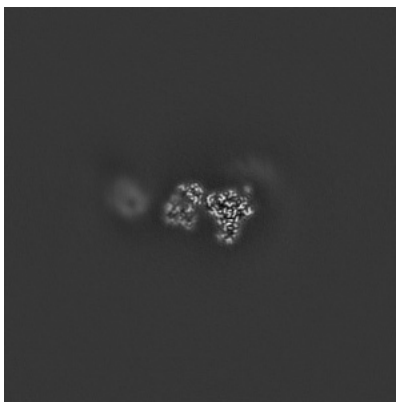


Z Index: 226

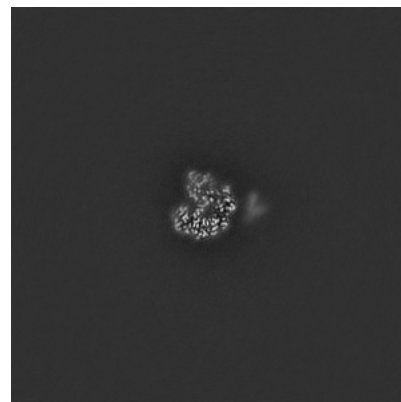
6.3.2 Raw map



X Index: 204



Y Index: 182

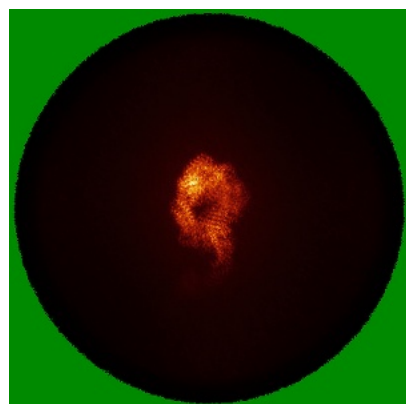


Z Index: 226

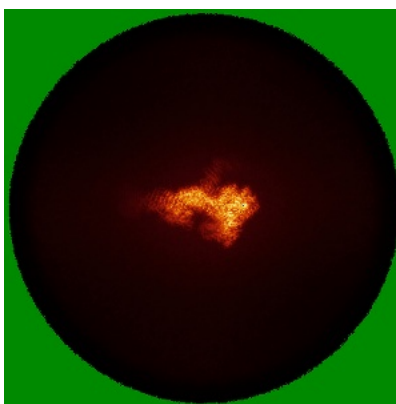
The images above show the largest variance slices of the map in three orthogonal directions.

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

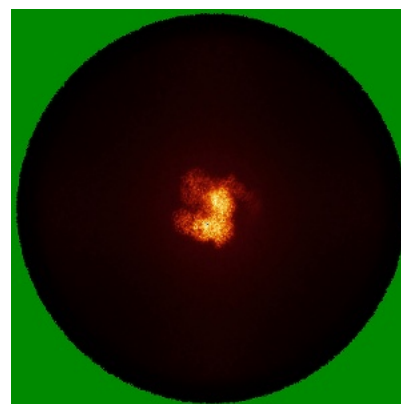
6.4.1 Primary map



X

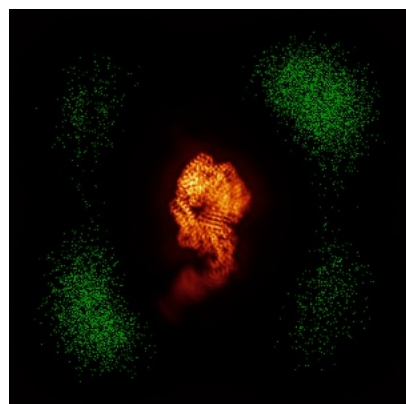


Y

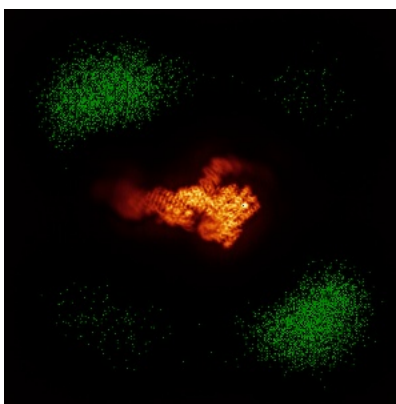


Z

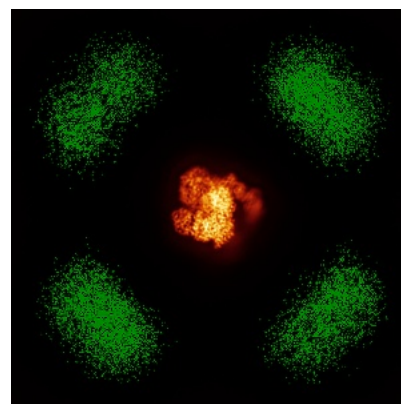
6.4.2 Raw map



X



Y

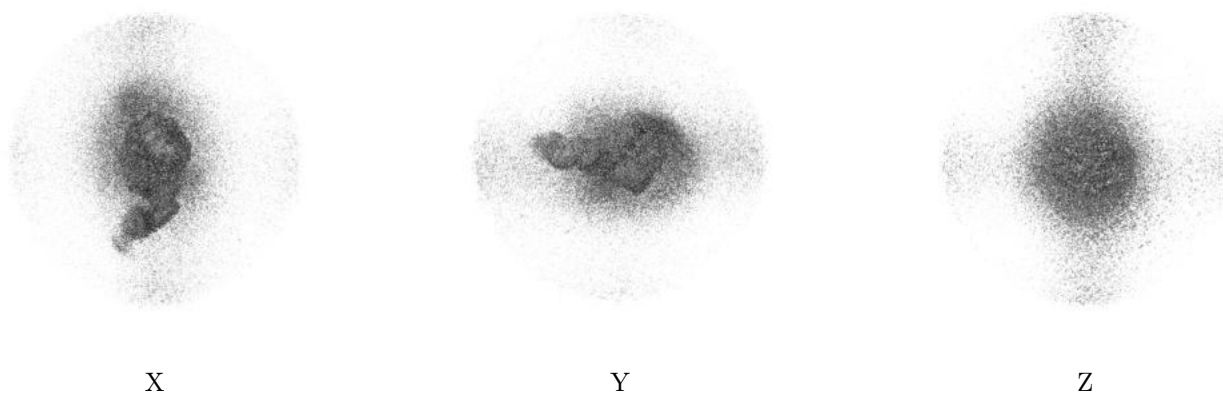


Z

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.

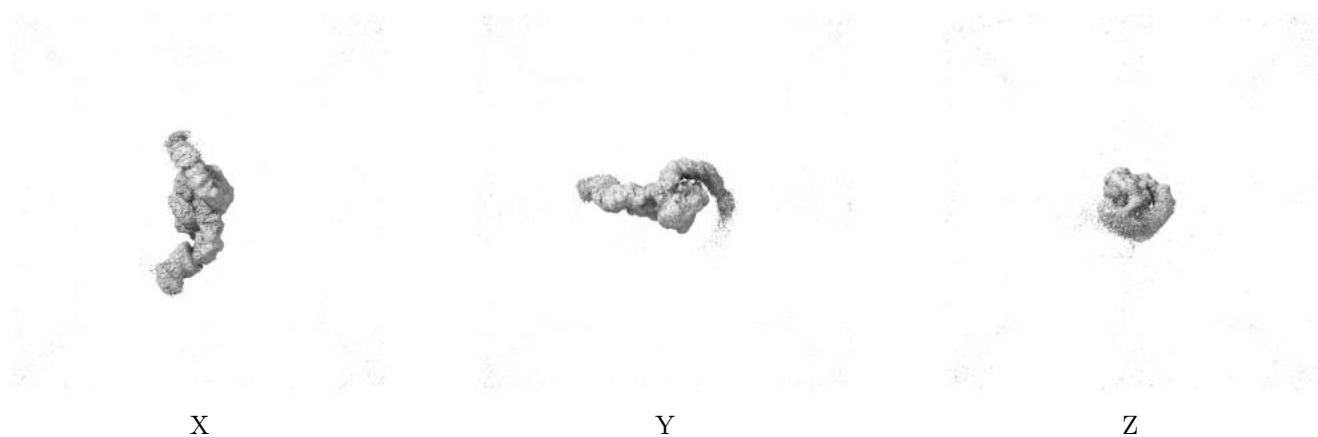
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

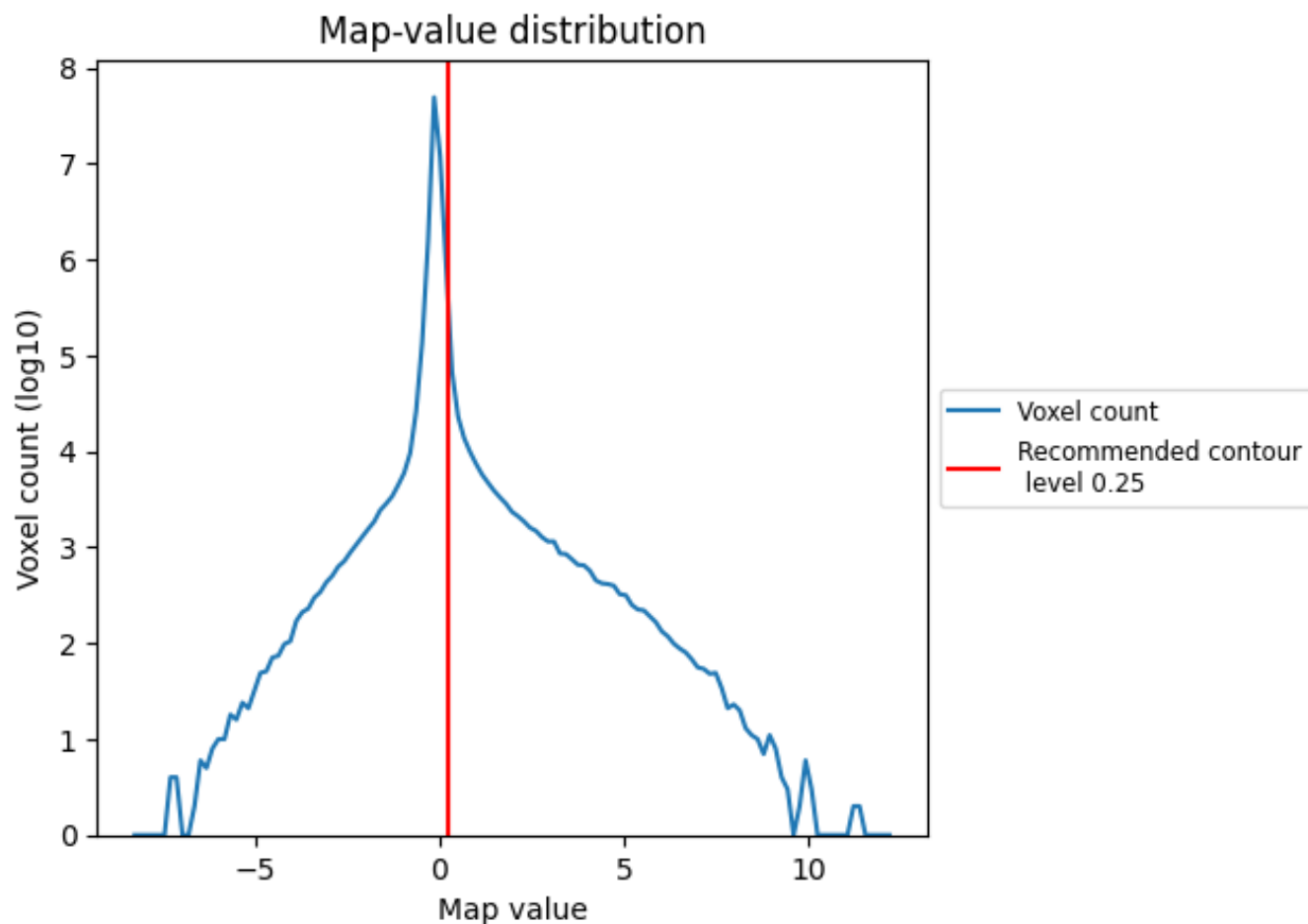
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

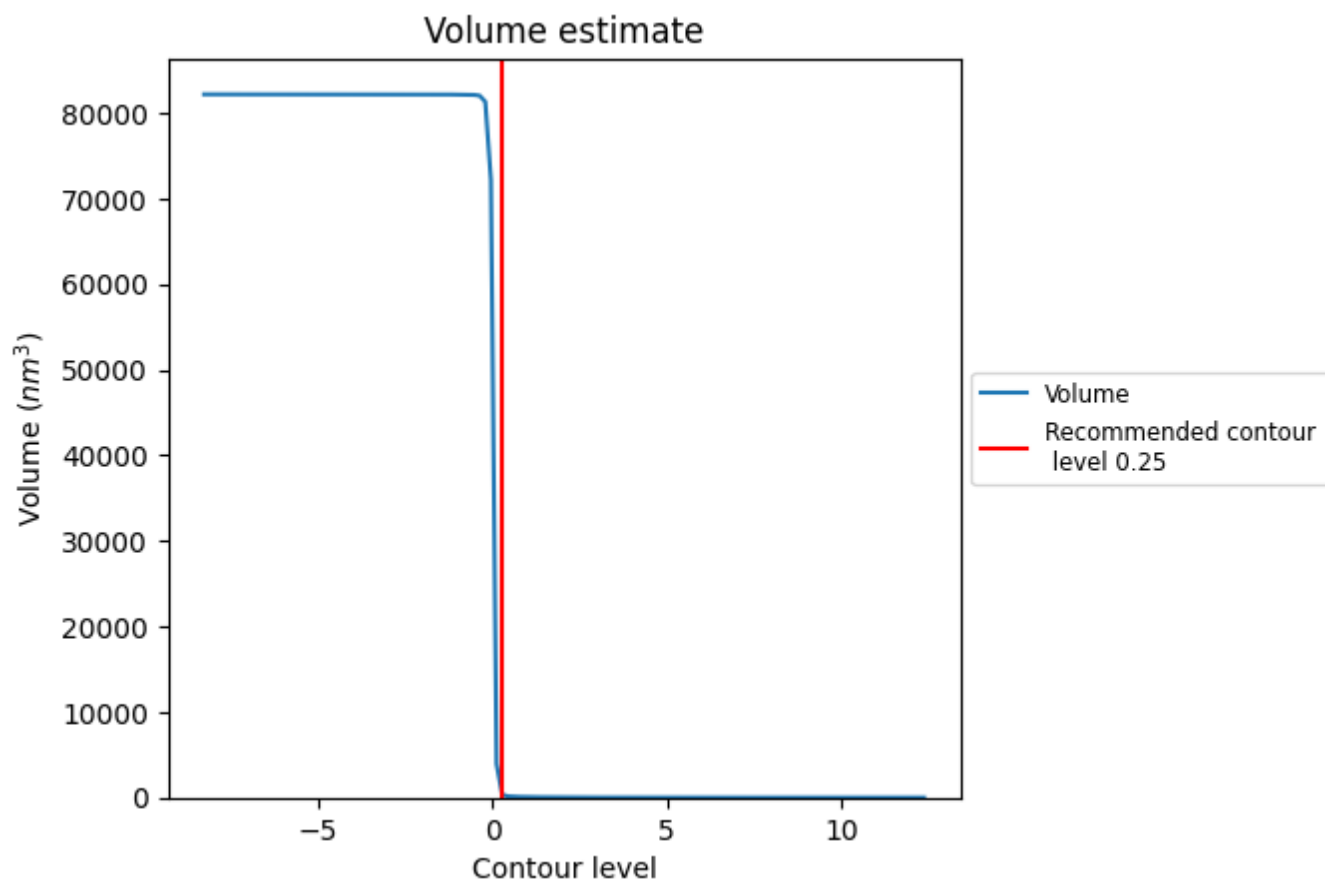
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

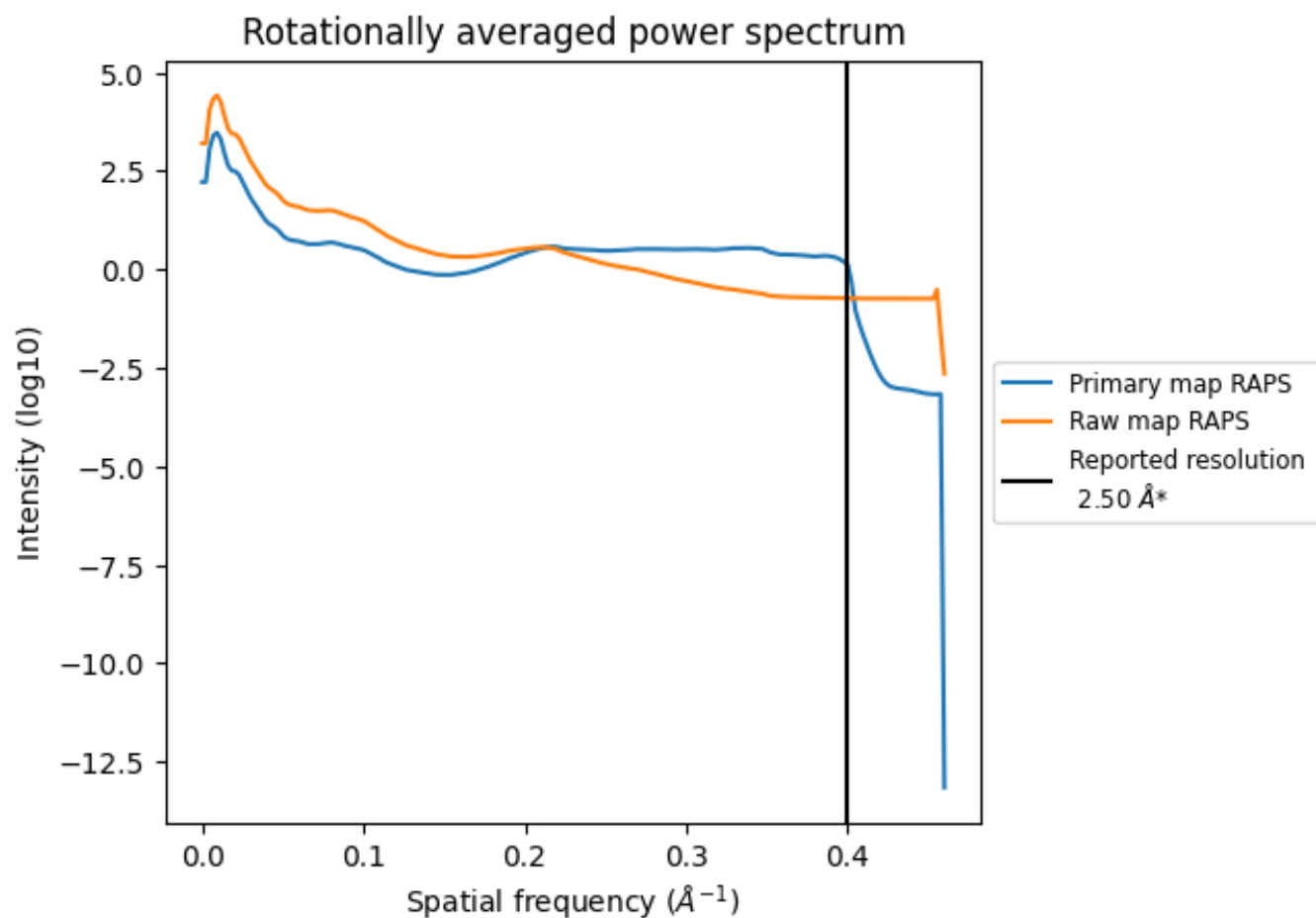
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm^3 ; this corresponds to an approximate mass of 724 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 ⓘ

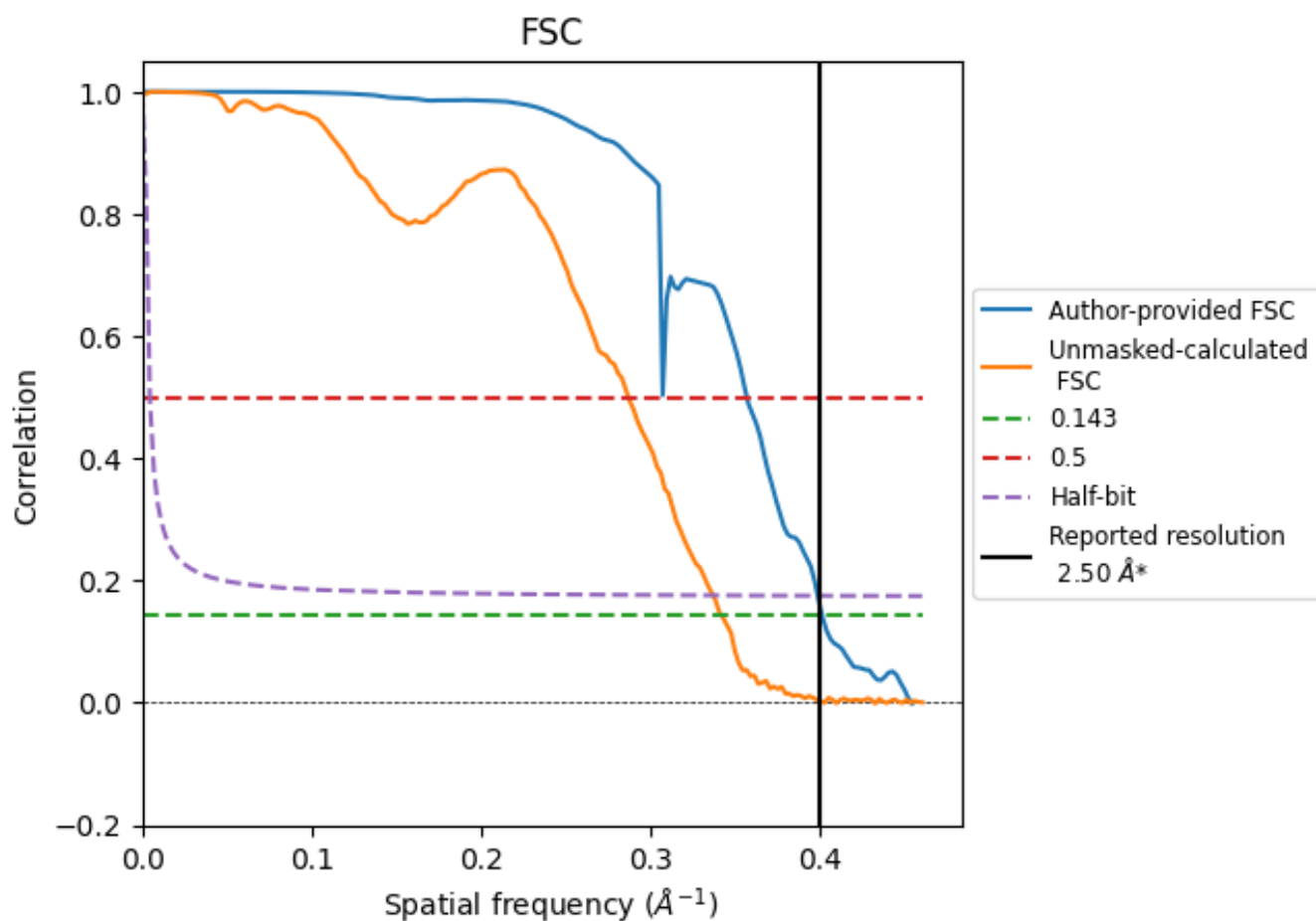


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

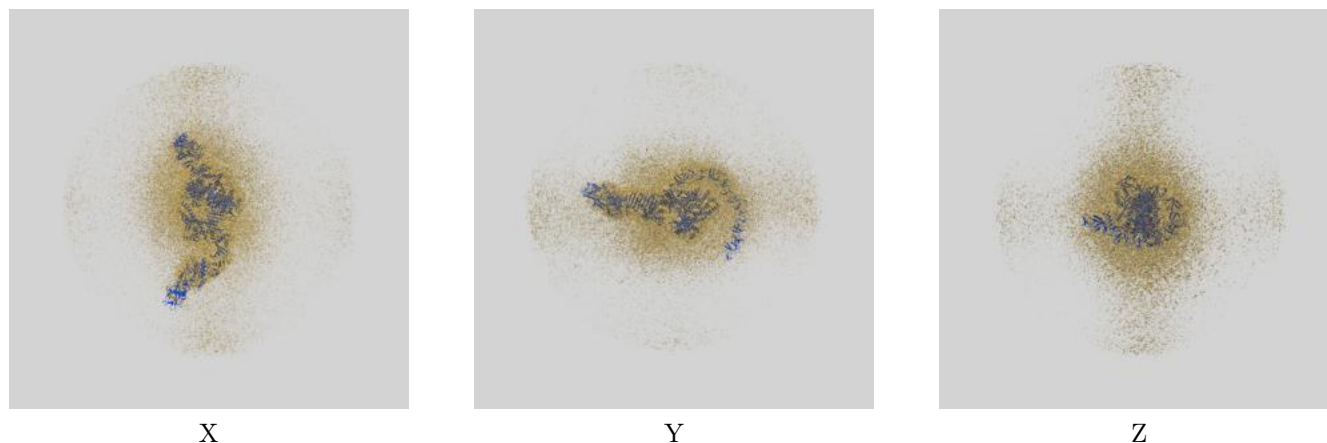
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.80	2.51
Unmasked-calculated*	2.93	3.49	2.97

*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 2.93 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

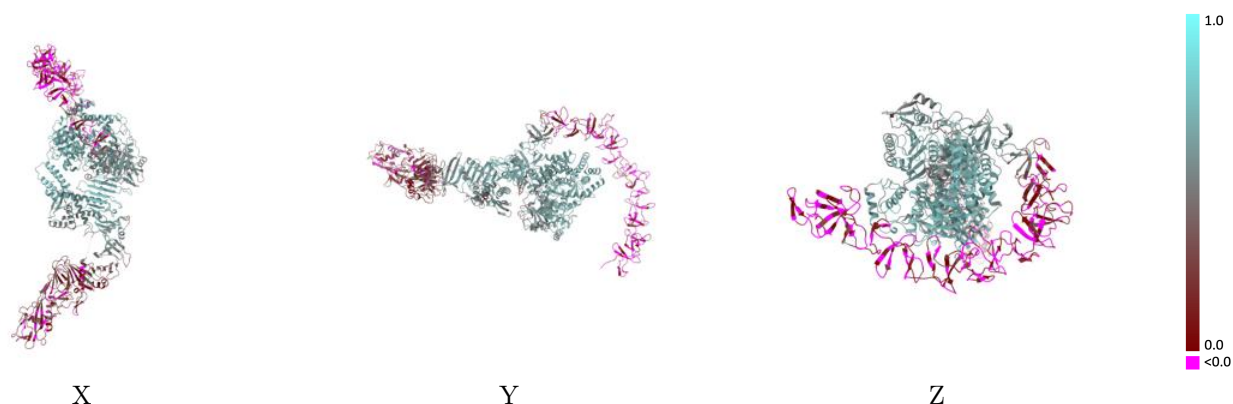
This section contains information regarding the fit between EMDB map EMD-38011 and PDB model 8X2I. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



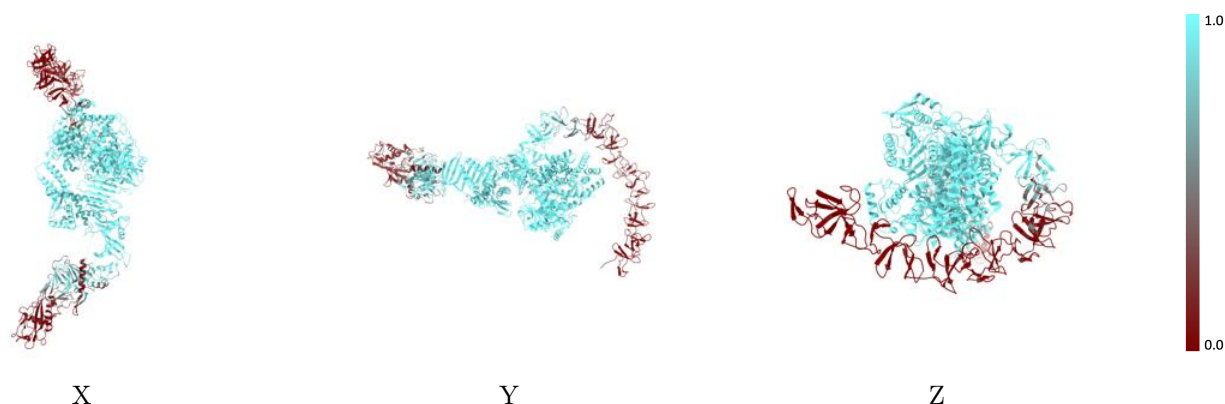
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



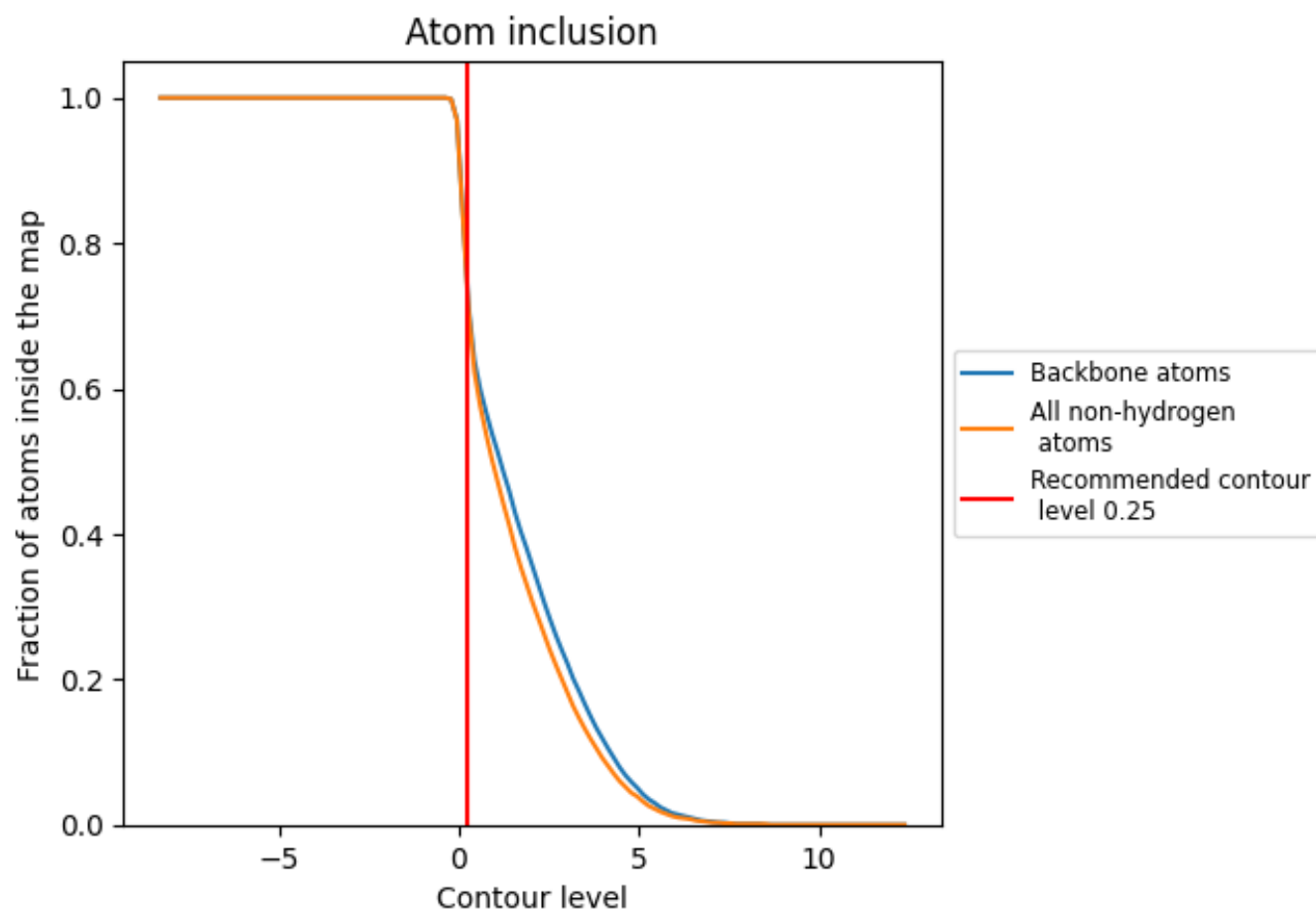
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 72% 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	0.7210	0.4140
A	0.7210	0.4140

