



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:14 PM UTC

PDB ID : 8JB5 / pdb_00008jb5
EMDB ID : EMD-36141
Title : The cryo-EM structure of Paeniclostridium sordellii lethal toxin (TcsL)
Authors : Zhan, X.; Tao, L.
Deposited on : 2023-05-08
Resolution : 2.90 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

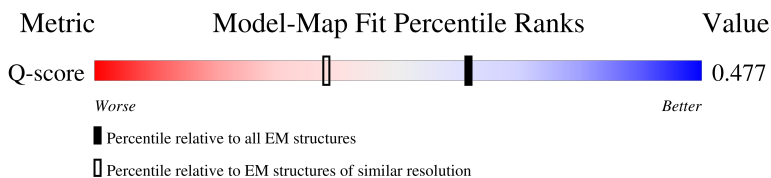
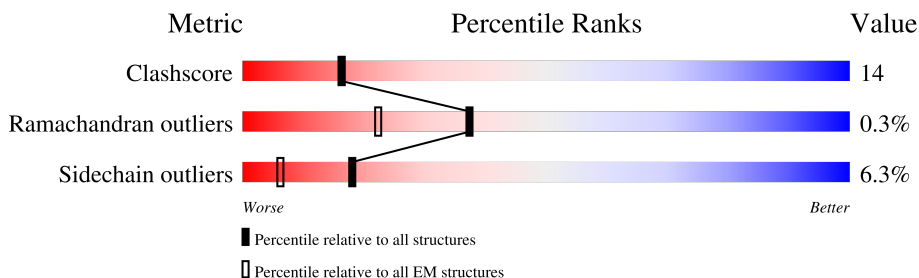
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	31% 69% 27% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19027 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	2355	Total	C	N	O	S	0	0
			19026	12183	3022	3774	47		

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

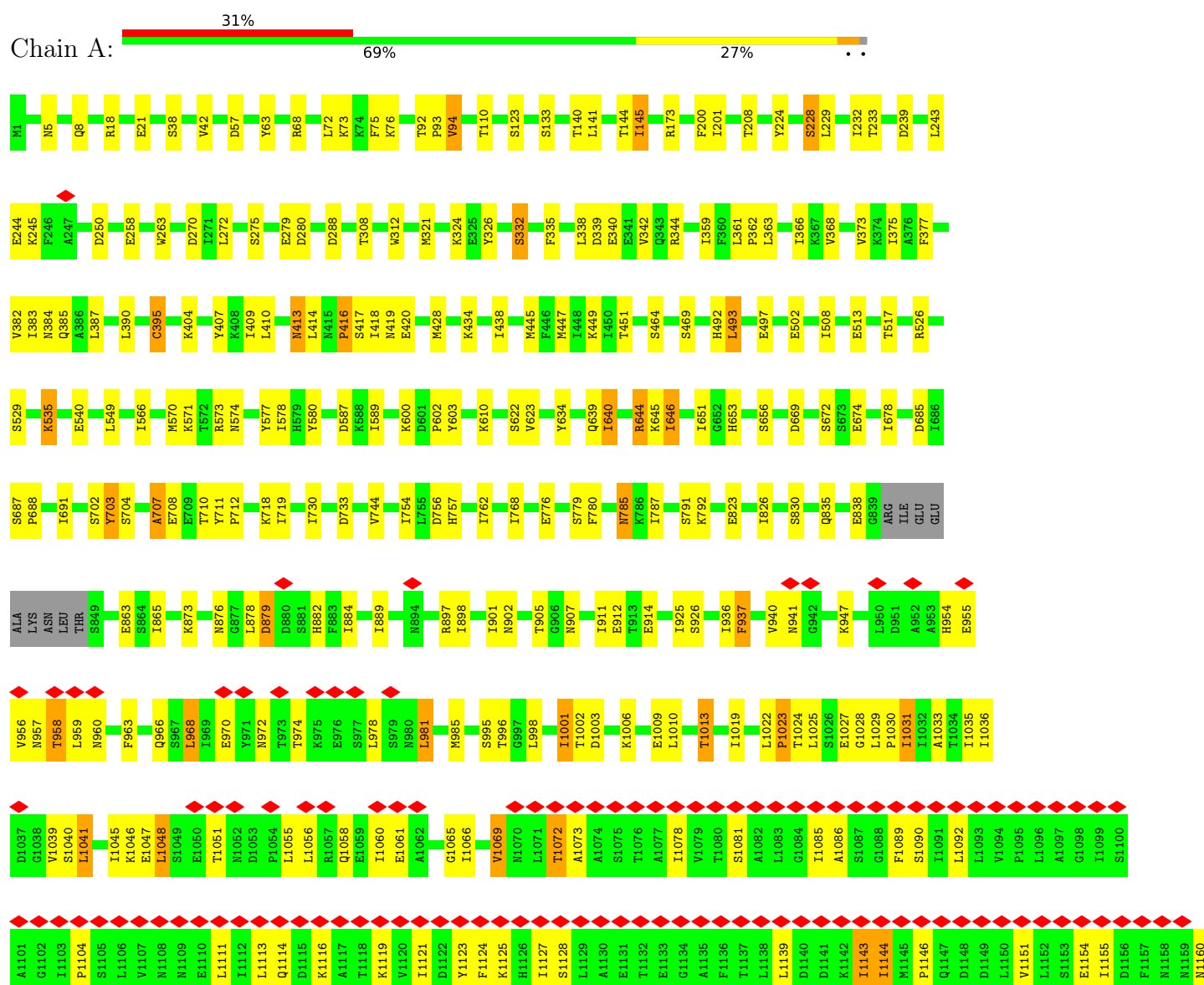
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



F2163	T2103	K2043	N1983	L1737	M1598	I1497	V1344	R1281	S1161
D2164	V2104	D2044	G1984	S1738	L1599	Y1498	V1345	Y1282	I1162
T2165	I2105	D2045	I1985	V1742	L1600	M1499	V1348	E1283	T1163
P2166	N2106	D2046	M1986	N1745	N1602	D1501	D1349	D1284	L1164
D2167	D2107	L2047	Q1987	I1751	F1603	S1502	M1350	T1285	G1165
G2168	C2108	G2048	T1988	I1761	F1604	N1503	V1351	M1286	K1166
Y2169	K2109	T2049	G1989	I1766	F1605	N1504	V1352	V1287	C1167
K2170	Y2110	E2050	T1914	S1756	D1608	L1505	K1353	E1168	E1168
T2171	Y2111	E2051	F1926	Q1761	T1609	F1506	I1415	I1169	I1169
A2173	D2112	E2053	I1927	P1762	M1610	I1507	K1354	W1170	W1170
P2174	D2114	L2054	G1928	Q1763	I1612	I1513	I1355	L1171	R1171
L2175	N2115	T2055	K1929	R1767	I1613	L1514	I1356	A1172	A1172
N2176	G2116	T2057	L1930	V1771	S1618	I1516	I1357	E1173	E1173
T2177	I2117	Y2057	D1933	F1772	E1623	K1521	D1360	G1174	G1174
V2178	R2118	N2058	I1936	D1775	L1624	G1522	E1361	G1175	G1175
D2179	Q2119	G2059	Y1937	T1776	K1628	D1523	I1362	S1176	S1176
N2180	L2120	T2060	Y1938	D1779	D1629	K1533	Q1363	G1177	G1177
O2181	G2121	D2061	A1945	D1787	P1634	D1534	K1364	H1178	H1178
I2182	F2122	N2062	A1946	D1791	Y1635	D1535	G1365	T1179	T1179
Y2183	I2123	F2063	E1947	V1795	F1636	D1536	E1366	L1180	L1180
G2184	T2124	N2064	E1948	K1795	Y1649	S1539	L1367	T1181	T1181
Q2185	I2125	G2065	K1950	L1540	V1650	L1540	I1368	D1182	D1182
A2186	N2126	K2066	L1951	S1541	G1651	S1541	E1369	D1183	D1183
V2187	D2127	T2067	L1952	I1797	G1652	T1543	E1370	I1184	I1184
K2188	L2128	Y2068	D1953	S1798	R1653	D1546	I1371	D1185	D1185
Y2189	I2129	F2069	E1954	T1799	L1656	D1547	L1372	H1186	H1186
S2190	F2130	D2070	D1955	F1800	L1662	T1547	L1373	F1187	F1187
G2191	Y2131	N2071	T1956	S1801	Y1662	N1548	S1373	F1188	F1188
L2192	D2132	I2072	Y1957	A1804	H1663	T1549	K1310	S1189	S1189
V2193	S2133	S2073	G1958	D1807	L1664	I1550	L1311	S1190	S1190
R2194	E2134	N2074	E1959	Y1812	G1668	I1552	L1376	P1191	P1191
V2195	S2135	T2075	E1960	E1813	I1670	N1553	I1377	S1192	S1192
N2196	Q2136	A2076	E1965	F1814	S1671	Y1556	E1378	I1193	I1193
E2197	K2137	F2077	L1967	N1821	D1686	L1557	D1379	T1194	T1194
D2198	I2138	G2078	L1968	N1831	R1687	G1561	I1382	Y1195	Y1195
V2199	E2139	G2079	K1969	N1840	V1692	K1573	I1383	R1196	R1196
Y2200	L2140	V2080	L1970	N1840	L1698	S1574	L1384	K1197	K1197
Y2201	G2141	G2081	H1971	T1870	L1714	A1575	L1385	P1198	P1198
F2202	Y2142	T2082	Q1972	S1876	I1719	T1578	N1386	W1199	W1199
G2203	Q2143	L2083	I1973	I1880	D1722	L1582	F1391	L1200	L1200
E2204	N2144	D2084	G1974	Y1880	I1726	F1585	Y1392	S1201	S1201
T2205	I2145	D2085	D1975	L1895	I1726	S1588	G1393	I1202	I1202
Y2206	N2146	G2086	N1976				D1394	Y1203	Y1203
K2207	G2147	S2087	K1977				E1397	D1204	D1204
L2208	N2148	T2088	Y1978					S1205	S1205
E2209	Y2149	Y2089	Y1979					L1206	L1206
T2210	F2150	F2090	D1981					F1207	F1207
G2211	Y2151	D2091	D1982					A1268	A1268
I2213	D2153	D2093						I1269	I1269
E2214	N2154	K2094						I1270	I1270
N2215	S2155	T2095						A1271	A1271
E2216	G2156	A2096						K1212	K1212
T2217	L2157	E2097						I1273	I1273
D2218	V2158	A2098						L1274	L1274
K2219	L2159	C2099						I1275	I1275
Y2220	I2160	G2101						T1276	T1276
Y2221	G2161	L2102						K1277	K1277
F2222	V2162							L1278	L1278
								K1279	K1279
								P1280	P1280

S2343	F2283	D2223
L2344	G2284	P2224
T2345	K2285	E2225
I2346	D2286	T2226
L2347	G2287	K2227
G2348	K2288	K2228
T2349	M2289	A2229
M2350	Q2290	Y2230
Y2351	I2291	K2231
Y2352	G2292	G2232
F2353	V2293	L2233
D2354	T2294	N2234
P2355	N2295	V2235
D2356	T2296	Y2236
T2357	P2297	D2237
A2358	D2298	Y2238
E2359	G2299	L2239
L2360	F2300	K2240
V2361	K2301	Y2241
V2362	Y2302	Y2242
S2363	F2303	F2243
E2364	A2304	D2244
HIS	H2305	E2245
HIS	Q2306	N2246
HIS	T2307	G2247
HIS	T2308	T2248
HIS	L2309	M2249
HIS	D2310	R2250
HIS	E2311	T2251
HIS	M2312	G2252
HIS	F2313	L2253
HIS	E2314	T2254
HIS	G2315	S2255
HIS	E2316	F2256
HIS	S2317	E2257
HIS	L2318	N2258
HIS	N2319	N2259
HIS	Y2320	N2260
HIS	T2321	Y2261
HIS	G2322	Y2262
HIS	F2323	F2263
HIS	L2324	N2264
HIS	D2325	E2265
HIS	L2326	D2266
HIS	D2327	G2267
HIS	G2328	K2268
HIS	K2329	M2269
HIS	R2330	Q2270
HIS	T2331	F2271
HIS	Y2332	G2272
HIS	F2333	Y2273
HIS	T2334	L2274
HIS	D2335	N2275
HIS	E2336	L2276
HIS	Y2337	K2277
HIS	L2338	D2278
HIS	A2339	K2279
HIS	A2340	N2280
HIS	T2341	F2281
HIS	G2342	Y2282

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229156	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	0.204	Depositor
Minimum map value	-0.099	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	321.752, 321.752, 321.752	wwPDB
Map dimensions	296, 296, 296	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

5.1 Standard geometry

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	0.43	1/19409 (0.0%)	0.61	4/26261 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	ILE	C-O	6.21	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	PRO	CA-N-CD	-13.11	93.65	112.00
1	A	1947	VAL	CA-C-N	5.88	132.77	121.54
1	A	1947	VAL	C-N-CA	5.88	132.77	121.54
1	A	1069	VAL	N-CA-C	-5.28	107.22	111.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	GLY	Peptide
1	A	1452	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19026	0	18584	534	0
2	A	1	0	0	0	0
All	All	19027	0	18584	534	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 (534) 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:1023:PRO:HG3	1:A:1649:TYR:CZ	1.49	1.48
1:A:1956:THR:HG23	1:A:1986:MET:N	1.21	1.45
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1023:PRO:CG	1:A:1649:TYR:CZ	2.18	1.26
1:A:1180:LEU:HD21	1:A:1185:ASP:OD1	1.34	1.22
1:A:1956:THR:HG21	1:A:1986:MET:CA	1.72	1.20
1:A:1022:LEU:HD22	1:A:1023:PRO:CD	1.72	1.20
1:A:1180:LEU:CD2	1:A:1185:ASP:HA	1.70	1.19
1:A:1956:THR:HG21	1:A:1986:MET:CB	1.74	1.18
1:A:1022:LEU:CD2	1:A:1023:PRO:HD3	1.74	1.17
1:A:1023:PRO:HG2	1:A:1649:TYR:CE2	1.79	1.17
1:A:1023:PRO:CG	1:A:1649:TYR:OH	1.93	1.16
1:A:1023:PRO:HG3	1:A:1649:TYR:OH	0.96	1.12
1:A:1956:THR:CG2	1:A:1986:MET:H	1.50	1.10
1:A:1956:THR:HG21	1:A:1986:MET:HB3	1.32	1.07
1:A:1023:PRO:CG	1:A:1649:TYR:CE2	2.37	1.05
1:A:1022:LEU:HD22	1:A:1023:PRO:HD3	1.07	1.05
1:A:1036:ILE:HG21	1:A:1521:LYS:HG2	1.35	1.05
1:A:1956:THR:CG2	1:A:1986:MET:CA	2.32	1.04
1:A:1956:THR:CG2	1:A:1986:MET:CB	2.34	1.04
1:A:1956:THR:HG22	1:A:1985:ILE:HG22	1.40	1.02
1:A:1180:LEU:HD23	1:A:1185:ASP:CA	1.90	1.01
1:A:1180:LEU:CD2	1:A:1185:ASP:CA	2.44	0.95
1:A:1180:LEU:HD21	1:A:1185:ASP:CG	1.90	0.95
1:A:1956:THR:CG2	1:A:1986:MET:HB3	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HD23	1:A:1185:ASP:HA	0.97	0.94
1:A:1180:LEU:CD2	1:A:1185:ASP:OD1	2.16	0.93
1:A:1023:PRO:HG3	1:A:1649:TYR:HH	1.27	0.92
1:A:1295:THR:HA	1:A:1322:SER:O	1.71	0.90
1:A:1505:LEU:O	1:A:1599:LEU:HD11	1.73	0.89
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.55	0.88
1:A:1956:THR:HG21	1:A:1986:MET:C	1.99	0.88
1:A:1534:ASP:O	1:A:1535:ASP:OD1	1.96	0.84
1:A:1025:LEU:HB3	1:A:1033:ALA:HB1	1.60	0.83
1:A:1180:LEU:CD2	1:A:1185:ASP:CG	2.54	0.81
1:A:589:ILE:HD13	1:A:757:HIS:HA	1.64	0.80
1:A:622:SER:HA	1:A:639:GLN:HE22	1.48	0.79
1:A:1956:THR:OG1	1:A:1986:MET:HB2	1.83	0.78
1:A:577:TYR:HB3	1:A:645:LYS:HB2	1.65	0.78
1:A:1036:ILE:HG21	1:A:1521:LYS:CG	2.14	0.77
1:A:1550:ILE:HG21	1:A:1605:PHE:HE1	1.47	0.77
1:A:1956:THR:OG1	1:A:1986:MET:CB	2.33	0.77
1:A:1507:ILE:O	1:A:1598:ASN:OD1	2.03	0.76
1:A:1795:LYS:O	1:A:1799:THR:OG1	2.03	0.76
1:A:754:ILE:HD12	1:A:754:ILE:O	1.86	0.76
1:A:2194:ARG:HG2	1:A:2199:VAL:HG12	1.67	0.75
1:A:1069:VAL:HG23	1:A:1461:PRO:HB3	1.69	0.75
1:A:1956:THR:CB	1:A:1986:MET:HB3	2.18	0.74
1:A:1956:THR:HG21	1:A:1986:MET:O	1.88	0.74
1:A:1041:LEU:HD23	1:A:1041:LEU:N	2.02	0.74
1:A:2128:ASN:HB3	1:A:2157:LEU:HD22	1.71	0.73
1:A:941:ASN:HD22	1:A:1056:LEU:HD13	1.54	0.73
1:A:1146:PRO:HD2	1:A:1221:VAL:HB	1.71	0.73
1:A:1956:THR:O	1:A:1985:ILE:HA	1.90	0.72
1:A:2088:THR:HG21	1:A:2118:ARG:HH21	1.55	0.72
1:A:589:ILE:CD1	1:A:757:HIS:HA	2.19	0.71
1:A:1031:ILE:HG22	1:A:1046:LYS:HD3	1.73	0.71
1:A:960:ASN:OD1	1:A:1652:ASN:ND2	2.20	0.70
1:A:1550:ILE:HB	1:A:1605:PHE:CD1	2.26	0.70
1:A:1737:LEU:HD13	1:A:1872:SER:HB2	1.74	0.69
1:A:1113:LEU:HG	1:A:1114:GLN:HG2	1.72	0.69
1:A:5:ASN:ND2	1:A:8:GLN:OE1	2.25	0.69
1:A:1022:LEU:HD22	1:A:1023:PRO:HD2	1.73	0.69
1:A:1772:PHE:HE1	1:A:1797:ILE:HD11	1.58	0.69
1:A:1025:LEU:HG	1:A:1612:ILE:HD13	1.75	0.68
1:A:1025:LEU:HD21	1:A:1635:TYR:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:GLU:HG3	1:A:787:ILE:HD12	1.76	0.68
1:A:1425:TYR:OH	1:A:1453:ASN:ND2	2.23	0.68
1:A:2123:ILE:O	1:A:2130:PHE:HB2	1.92	0.68
1:A:413:ASN:HD22	1:A:413:ASN:H	1.40	0.68
1:A:889:ILE:HG12	1:A:898:ILE:HG12	1.76	0.67
1:A:1180:LEU:CD2	1:A:1185:ASP:CB	2.72	0.67
1:A:2119:GLN:HG3	1:A:2123:ILE:HG13	1.76	0.67
1:A:1180:LEU:HD21	1:A:1185:ASP:CB	2.24	0.67
1:A:1952:LEU:HD12	1:A:1952:LEU:N	2.09	0.67
1:A:1408:ILE:HB	1:A:1446:LYS:HD2	1.76	0.67
1:A:1325:LEU:HD21	1:A:1334:ILE:HD12	1.77	0.67
1:A:792:LYS:HB2	1:A:835:GLN:HG3	1.77	0.66
1:A:1550:ILE:HG21	1:A:1605:PHE:CE1	2.30	0.66
1:A:1956:THR:O	1:A:1985:ILE:HG23	1.96	0.66
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.77	0.66
1:A:2017:TYR:HB2	1:A:2054:LEU:HD22	1.76	0.66
1:A:1025:LEU:HB3	1:A:1033:ALA:CB	2.26	0.66
1:A:2253:LEU:HG	1:A:2260:ASN:HD21	1.61	0.65
1:A:73:LYS:HD2	1:A:1726:ILE:HG23	1.78	0.65
1:A:2118:ARG:NH1	1:A:2135:SER:O	2.30	0.65
1:A:1089:PHE:HA	1:A:1092:LEU:HG	1.76	0.65
1:A:2111:TYR:HE1	1:A:2123:ILE:HB	1.61	0.65
1:A:1280:PRO:HB2	1:A:1282:TYR:HE1	1.61	0.64
1:A:879:ASP:N	1:A:879:ASP:OD1	2.31	0.64
1:A:577:TYR:HB3	1:A:645:LYS:CB	2.28	0.64
1:A:2244:ASP:HB3	1:A:2250:ARG:CZ	2.29	0.63
1:A:1111:LEU:H	1:A:1281:ARG:HH12	1.46	0.63
1:A:2174:PRO:O	1:A:2181:ASN:ND2	2.31	0.63
1:A:1197:LYS:NZ	1:A:1261:GLN:OE1	2.29	0.63
1:A:1368:ILE:HG23	1:A:1371:ILE:HB	1.80	0.62
1:A:956:VAL:HG21	1:A:1653:ARG:NE	2.14	0.62
1:A:2289:MET:HE2	1:A:2315:GLY:HA3	1.81	0.62
1:A:1003:ASP:HB3	1:A:1006:LYS:HE2	1.82	0.62
1:A:94:VAL:HG22	1:A:368:VAL:HG22	1.81	0.62
1:A:644:ARG:NH1	1:A:687:SER:O	2.32	0.62
1:A:754:ILE:HG23	1:A:768:ILE:HG12	1.79	0.62
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.82	0.62
1:A:623:VAL:H	1:A:639:GLN:HE22	1.47	0.62
1:A:1550:ILE:HB	1:A:1605:PHE:CE1	2.34	0.62
1:A:1960:ASN:HB3	1:A:1964:GLY:H	1.65	0.62
1:A:754:ILE:CG2	1:A:768:ILE:HG12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LEU:CD2	1:A:1023:PRO:CD	2.53	0.62
1:A:1550:ILE:CG2	1:A:1605:PHE:CE1	2.82	0.62
1:A:1505:LEU:O	1:A:1599:LEU:CD1	2.45	0.61
1:A:1314:TYR:HB2	1:A:1334:ILE:HD13	1.82	0.61
1:A:173:ARG:NH2	1:A:823:GLU:OE2	2.28	0.61
1:A:873:LYS:NZ	1:A:882:HIS:O	2.33	0.61
1:A:2043:LYS:H	1:A:2051:GLU:HG2	1.65	0.61
1:A:2282:TYR:H	1:A:2289:MET:HE1	1.64	0.61
1:A:1197:LYS:HG2	1:A:1198:PRO:HD2	1.83	0.60
1:A:57:ASP:OD1	1:A:76:LYS:NZ	2.33	0.60
1:A:1384:LEU:O	1:A:1387:HIS:HB2	2.01	0.60
1:A:1807:ASP:HB2	1:A:1812:TYR:HE2	1.67	0.60
1:A:243:LEU:HB3	1:A:245:LYS:HG2	1.84	0.60
1:A:1025:LEU:CD2	1:A:1635:TYR:CE1	2.85	0.60
1:A:1025:LEU:N	1:A:1025:LEU:HD22	2.16	0.60
1:A:1947:VAL:O	1:A:1959:PHE:HB2	2.01	0.60
1:A:1956:THR:CG2	1:A:1985:ILE:HG22	2.26	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	0.60
1:A:1575:ALA:HA	1:A:1578:THR:HG22	1.84	0.59
1:A:1495:ARG:HG2	1:A:1507:ILE:HG23	1.84	0.59
1:A:1239:GLY:H	1:A:1241:ARG:HH12	1.51	0.59
1:A:413:ASN:HD22	1:A:413:ASN:N	2.00	0.59
1:A:1956:THR:OG1	1:A:1986:MET:HB3	2.01	0.58
1:A:1354:ASN:O	1:A:1365:GLY:N	2.32	0.58
1:A:1296:ARG:HB2	1:A:1323:TYR:HD1	1.66	0.58
1:A:2273:TYR:HE2	1:A:2280:MET:HB3	1.68	0.58
1:A:1550:ILE:CG2	1:A:1605:PHE:HE1	2.17	0.58
1:A:1970:LEU:HD21	1:A:1977:LYS:HD3	1.84	0.58
1:A:1624:LEU:HD23	1:A:1634:PRO:HA	1.85	0.58
1:A:1128:SER:HB3	1:A:1250:LEU:HD22	1.84	0.58
1:A:540:GLU:OE2	1:A:540:GLU:HA	2.03	0.57
1:A:566:ILE:HD13	1:A:602:PRO:HB3	1.86	0.57
1:A:1447:ILE:O	1:A:1450:ILE:HG12	2.03	0.57
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.87	0.57
1:A:270:ASP:OD2	1:A:384:ASN:ND2	2.37	0.57
1:A:587:ASP:OD1	1:A:653:HIS:NE2	2.35	0.57
1:A:1113:LEU:HB2	1:A:1280:PRO:HD3	1.87	0.57
1:A:1956:THR:HG23	1:A:1986:MET:H	0.58	0.57
1:A:1956:THR:CB	1:A:1986:MET:CB	2.78	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:1144:ILE:HD11	1:A:1217:LYS:HB2	1.86	0.57
1:A:1327:LEU:HD23	1:A:1351:VAL:HG21	1.87	0.57
1:A:2244:ASP:HB3	1:A:2250:ARG:NE	2.19	0.57
1:A:1598:ASN:OD1	1:A:1598:ASN:N	2.33	0.56
1:A:451:THR:OG1	1:A:826:ILE:HD13	2.05	0.56
1:A:622:SER:HA	1:A:639:GLN:NE2	2.17	0.56
1:A:1348:VAL:HB	1:A:1351:VAL:HB	1.87	0.56
1:A:1139:LEU:HD23	1:A:1143:ILE:HD12	1.88	0.56
1:A:133:SER:OG	1:A:239:ASP:OD2	2.17	0.56
1:A:704:SER:HB3	1:A:776:GLU:OE2	2.06	0.56
1:A:1023:PRO:HG3	1:A:1649:TYR:CE2	2.12	0.56
1:A:1787:ASP:N	1:A:1787:ASP:OD1	2.37	0.56
1:A:1433:CYS:O	1:A:1437:ILE:HG12	2.06	0.56
1:A:1022:LEU:HD23	1:A:1023:PRO:HD3	1.82	0.56
1:A:1218:ASP:HA	1:A:1296:ARG:HH11	1.71	0.56
1:A:1329:PRO:HB3	1:A:1355:ILE:HG13	1.88	0.56
1:A:2320:TYR:HE1	1:A:2324:LEU:HB2	1.69	0.56
1:A:1168:GLU:HB3	1:A:1199:TRP:HB3	1.88	0.55
1:A:1334:ILE:HB	1:A:1389:ILE:HD12	1.87	0.55
1:A:1929:LYS:HE3	1:A:1936:ILE:HG23	1.87	0.55
1:A:1949:TRP:CZ2	1:A:1973:ILE:HG21	2.40	0.55
1:A:1104:PRO:HG2	1:A:1305:THR:HG21	1.87	0.55
1:A:2293:VAL:HG12	1:A:2300:PHE:HD2	1.72	0.55
1:A:1356:THR:HG22	1:A:1363:GLN:HB3	1.88	0.55
1:A:1956:THR:CG2	1:A:1986:MET:O	2.54	0.55
1:A:420:GLU:O	1:A:420:GLU:HG3	2.07	0.55
1:A:688:PRO:HG2	1:A:730:ILE:HD11	1.89	0.55
1:A:1086:ALA:O	1:A:1090:SER:OG	2.20	0.55
1:A:589:ILE:HD11	1:A:757:HIS:O	2.05	0.55
1:A:791:SER:HA	1:A:838:GLU:OE2	2.05	0.55
1:A:1258:TYR:HB3	1:A:1261:GLN:HB2	1.87	0.55
1:A:2276:ILE:HG22	1:A:2277:LYS:HG2	1.88	0.55
1:A:2043:LYS:HE2	1:A:2050:GLU:HA	1.88	0.55
1:A:1585:PHE:O	1:A:1588:SER:OG	2.22	0.54
1:A:1656:LEU:HD23	1:A:1692:VAL:HG13	1.88	0.54
1:A:998:LEU:HD12	1:A:1001:ILE:HD12	1.88	0.54
1:A:1375:LEU:HB2	1:A:1384:LEU:HD13	1.89	0.54
1:A:1381:LYS:NZ	1:A:1383:ILE:HD11	2.22	0.54
1:A:1719:ILE:HG12	1:A:1767:ARG:HD2	1.89	0.54
1:A:2300:PHE:HB3	1:A:2339:ALA:HB3	1.88	0.54
1:A:428:MET:HE1	1:A:451:THR:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:MET:HE3	1:A:449:LYS:HE3	1.87	0.54
1:A:2011:ILE:HD12	1:A:2020:PHE:HD2	1.72	0.54
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.54
1:A:954:HIS:O	1:A:954:HIS:ND1	2.40	0.54
1:A:995:SER:OG	1:A:996:THR:N	2.40	0.54
1:A:308:THR:HA	1:A:785:ASN:HD22	1.73	0.54
1:A:708:GLU:H	1:A:708:GLU:CD	2.13	0.54
1:A:145:ILE:HD12	1:A:263:TRP:HH2	1.73	0.54
1:A:707:ALA:O	1:A:710:THR:OG1	2.24	0.53
1:A:1045:ILE:HG12	1:A:1066:ILE:HD13	1.91	0.53
1:A:1876:SER:HB3	1:A:1880:ILE:HG13	1.90	0.53
1:A:258:GLU:OE1	1:A:407:TYR:OH	2.16	0.53
1:A:1030:PRO:HB2	1:A:1556:TYR:CZ	2.43	0.53
1:A:1291:LEU:HD21	1:A:1316:PHE:HD1	1.73	0.53
1:A:447:MET:O	1:A:451:THR:HG23	2.08	0.53
1:A:1989:GLY:H	1:A:2000:PHE:HB2	1.74	0.53
1:A:754:ILE:HD12	1:A:754:ILE:C	2.33	0.53
1:A:1251:LEU:HA	1:A:1254:ILE:HD12	1.90	0.53
1:A:963:PHE:HD2	1:A:1022:LEU:HD11	1.72	0.53
1:A:1371:ILE:HA	1:A:1374:LYS:NZ	2.24	0.53
1:A:610:LYS:HE3	1:A:674:GLU:OE2	2.09	0.52
1:A:711:TYR:HB3	1:A:712:PRO:HD3	1.91	0.52
1:A:733:ASP:OD1	1:A:733:ASP:N	2.38	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:CZ	2.87	0.52
1:A:2336:GLU:HG3	1:A:2338:ILE:HG22	1.91	0.52
1:A:1072:THR:HG22	1:A:1073:ALA:H	1.74	0.52
1:A:1171:ARG:HE	1:A:1261:GLN:HG2	1.74	0.52
1:A:2160:ILE:HA	1:A:2172:PHE:O	2.10	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:NH2	2.73	0.52
1:A:968:LEU:HD12	1:A:978:LEU:HD21	1.92	0.52
1:A:1324:SER:HB3	1:A:1345:VAL:HG23	1.91	0.52
1:A:1024:THR:HG22	1:A:1636:PHE:CD1	2.45	0.52
1:A:1061:GLU:O	1:A:1065:GLY:N	2.43	0.52
1:A:1249:LYS:NZ	1:A:1253:ARG:HE	2.09	0.51
1:A:1366:GLU:OE2	1:A:1449:HIS:NE2	2.43	0.51
1:A:1383:ILE:HA	1:A:1387:HIS:O	2.11	0.51
1:A:1996:LYS:HB3	1:A:2025:GLU:HG2	1.91	0.51
1:A:2223:ASP:HB2	1:A:2230:TYR:HE2	1.73	0.51
1:A:2142:TYR:OH	1:A:2167:ASP:OD2	2.21	0.51
1:A:1377:ILE:HD11	1:A:1420:LEU:HD23	1.92	0.51
1:A:2006:MET:HE3	1:A:2024:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:HD11	1:A:640:ILE:O	2.11	0.51
1:A:703:TYR:CD2	1:A:710:THR:HG21	2.45	0.51
1:A:756:ASP:HB2	1:A:762:ILE:HD12	1.93	0.51
1:A:438:ILE:O	1:A:438:ILE:HG13	2.10	0.51
1:A:1505:LEU:HG	1:A:1507:ILE:HD11	1.93	0.51
1:A:1540:LEU:HG	1:A:1542:PHE:HD1	1.75	0.51
1:A:1981:ASP:OD1	1:A:1985:ILE:N	2.41	0.51
1:A:2208:ILE:HD13	1:A:2227:LYS:HG2	1.93	0.51
1:A:623:VAL:H	1:A:639:GLN:NE2	2.06	0.51
1:A:1550:ILE:CB	1:A:1605:PHE:CE1	2.94	0.51
1:A:2177:THR:OG1	1:A:2181:ASN:ND2	2.31	0.51
1:A:1022:LEU:CB	1:A:1023:PRO:CD	2.89	0.51
1:A:2049:THR:HG22	1:A:2053:GLU:HB3	1.92	0.51
1:A:2242:TYR:HB2	1:A:2263:PHE:CZ	2.46	0.51
1:A:1968:LYS:HE2	1:A:1982:ASP:O	2.11	0.51
1:A:1976:ASN:HB3	1:A:2005:VAL:HG13	1.93	0.51
1:A:672:SER:OG	1:A:719:ILE:HG22	2.11	0.51
1:A:1383:ILE:HG12	1:A:1388:THR:HG22	1.93	0.51
1:A:1440:SER:HB3	1:A:1499:MET:SD	2.50	0.51
1:A:1957:TYR:HE1	1:A:1983:ASN:O	1.93	0.51
1:A:1154:GLU:HG2	1:A:1288:ARG:HB2	1.91	0.51
1:A:1981:ASP:OD1	1:A:1981:ASP:N	2.44	0.51
1:A:1367:LEU:HD21	1:A:1408:ILE:HG22	1.92	0.50
1:A:1354:ASN:N	1:A:1366:GLU:O	2.44	0.50
1:A:2264:ASN:OD1	1:A:2267:GLY:N	2.44	0.50
1:A:1495:ARG:HG2	1:A:1507:ILE:HD12	1.93	0.50
1:A:878:LEU:HD11	1:A:911:ILE:HD11	1.93	0.50
1:A:1628:LYS:HG3	1:A:1629:ASP:OD1	2.12	0.50
1:A:1906:LEU:HB2	1:A:1945:ALA:HB3	1.93	0.50
1:A:610:LYS:HE3	1:A:674:GLU:CD	2.37	0.50
1:A:1025:LEU:CD2	1:A:1025:LEU:N	2.75	0.50
1:A:1036:ILE:HB	1:A:1041:LEU:HD21	1.94	0.50
1:A:145:ILE:HD12	1:A:263:TRP:CH2	2.47	0.50
1:A:413:ASN:N	1:A:413:ASN:ND2	2.60	0.50
1:A:2011:ILE:HD12	1:A:2020:PHE:CD2	2.47	0.50
1:A:2058:ASN:HD21	1:A:2072:ILE:HA	1.77	0.50
1:A:383:ILE:HG12	1:A:385:GLN:HG3	1.93	0.49
1:A:513:GLU:O	1:A:517:THR:HG23	2.12	0.49
1:A:1151:VAL:HG12	1:A:1165:GLY:HA3	1.94	0.49
1:A:1171:ARG:HH21	1:A:1261:GLN:HG2	1.77	0.49
1:A:275:SER:O	1:A:279:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:VAL:HG23	1:A:390:LEU:HG	1.94	0.49
1:A:956:VAL:HG23	1:A:957:ASN:N	2.28	0.49
1:A:1085:ILE:HG13	1:A:1086:ALA:N	2.28	0.49
1:A:1375:LEU:HD12	1:A:1384:LEU:HB2	1.94	0.49
1:A:1956:THR:HG22	1:A:1985:ILE:CG2	2.26	0.49
1:A:1239:GLY:H	1:A:1241:ARG:NH1	2.09	0.49
1:A:2230:TYR:HD1	1:A:2234:ASN:HB3	1.78	0.49
1:A:2244:ASP:HB2	1:A:2250:ARG:NH2	2.27	0.49
1:A:21:GLU:HG2	1:A:63:TYR:CZ	2.48	0.49
1:A:1216:SER:O	1:A:1216:SER:OG	2.29	0.49
1:A:1369:GLU:OE1	1:A:1370:ASN:HB2	2.12	0.49
1:A:1124:PHE:HA	1:A:1127:ILE:HG12	1.95	0.49
1:A:1048:LEU:HD22	1:A:1066:ILE:HD11	1.94	0.49
1:A:1381:LYS:HD3	1:A:1390:ASN:HD22	1.77	0.48
1:A:1791:VAL:HG13	1:A:1795:LYS:HD2	1.94	0.48
1:A:21:GLU:OE2	1:A:68:ARG:NH2	2.37	0.48
1:A:1041:LEU:HD12	1:A:1045:ILE:HD11	1.94	0.48
1:A:1255:ARG:HH22	1:A:1259:GLU:HG2	1.79	0.48
1:A:2172:PHE:CE2	1:A:2186:ALA:HB2	2.48	0.48
1:A:549:LEU:HD11	1:A:589:ILE:HD12	1.96	0.48
1:A:1238:PRO:HG3	1:A:1271:ALA:HB1	1.94	0.48
1:A:1745:ASN:N	1:A:1745:ASN:OD1	2.46	0.48
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.14	0.48
1:A:1030:PRO:HB2	1:A:1556:TYR:OH	2.14	0.48
1:A:1303:ILE:O	1:A:1309:ARG:HD2	2.14	0.48
1:A:1385:ASN:O	1:A:1387:HIS:ND1	2.44	0.48
1:A:1041:LEU:HD23	1:A:1041:LEU:H	1.75	0.47
1:A:703:TYR:CD2	1:A:703:TYR:N	2.82	0.47
1:A:925:ILE:HG13	1:A:926:SER:N	2.28	0.47
1:A:940:VAL:HG21	1:A:1060:ILE:HA	1.96	0.47
1:A:974:THR:HG21	1:A:1664:LEU:H	1.80	0.47
1:A:1973:ILE:HD13	1:A:1978:TYR:HD2	1.79	0.47
1:A:1464:TYR:CE1	1:A:1466:ASP:HB2	2.50	0.47
1:A:1977:LYS:HD2	1:A:2006:MET:SD	2.55	0.47
1:A:1024:THR:HG22	1:A:1636:PHE:CE1	2.50	0.47
1:A:1967:LEU:HB3	1:A:1971:HIS:CD2	2.50	0.47
1:A:1195:TYR:HD2	1:A:1196:ARG:HD3	1.79	0.47
1:A:1502:SER:O	1:A:1505:LEU:HB2	2.15	0.47
1:A:1345:VAL:HG12	1:A:1403:SER:HB2	1.97	0.47
1:A:2243:PHE:CE2	1:A:2249:MET:HG3	2.50	0.47
1:A:1550:ILE:HD12	1:A:1605:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:O	1:A:144:THR:OG1	2.29	0.47
1:A:1168:GLU:O	1:A:1230:PHE:HB2	2.15	0.47
1:A:1170:TRP:CE2	1:A:1195:TYR:HB3	2.50	0.47
1:A:1427:ILE:HG13	1:A:1452:PHE:CE2	2.49	0.47
1:A:2317:SER:O	1:A:2317:SER:OG	2.32	0.47
1:A:375:ILE:HG12	1:A:383:ILE:O	2.15	0.46
1:A:902:ASN:CG	1:A:905:THR:HG22	2.39	0.46
1:A:905:THR:HG23	1:A:907:ASN:H	1.79	0.46
1:A:1947:VAL:O	1:A:1948:GLU:O	2.33	0.46
1:A:2264:ASN:HD21	1:A:2266:ASP:HB3	1.80	0.46
1:A:1205:VAL:HG13	1:A:1257:HIS:CD2	2.50	0.46
1:A:2129:ILE:O	1:A:2157:LEU:HA	2.15	0.46
1:A:2223:ASP:HB2	1:A:2230:TYR:CE2	2.49	0.46
1:A:2360:LEU:HG	1:A:2362:VAL:HG13	1.97	0.46
1:A:882:HIS:HA	1:A:901:ILE:O	2.16	0.46
1:A:1955:GLU:CG	1:A:1985:ILE:HD13	2.45	0.46
1:A:779:SER:OG	1:A:780:PHE:N	2.48	0.46
1:A:1307:GLN:O	1:A:1311:ASN:ND2	2.31	0.46
1:A:1738:SER:O	1:A:1840:ASN:ND2	2.43	0.46
1:A:1402:ILE:CG2	1:A:1418:ILE:HB	2.46	0.46
1:A:1452:PHE:HZ	1:A:1457:GLN:HB3	1.81	0.46
1:A:2177:THR:N	1:A:2181:ASN:OD1	2.43	0.46
1:A:2215:ASN:O	1:A:2217:THR:N	2.37	0.46
1:A:1543:THR:HG23	1:A:1551:LYS:HB3	1.96	0.46
1:A:1756:SER:HB2	1:A:1763:GLN:HB2	1.98	0.46
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.98	0.46
1:A:2151:TYR:HB2	1:A:2172:PHE:CZ	2.51	0.46
1:A:2242:TYR:HE1	1:A:2256:PHE:HB2	1.81	0.46
1:A:970:GLU:C	1:A:972:ASN:H	2.24	0.46
1:A:1036:ILE:CG2	1:A:1521:LYS:HG2	2.26	0.46
1:A:2289:MET:HE2	1:A:2315:GLY:CA	2.44	0.46
1:A:384:ASN:OD1	1:A:384:ASN:N	2.48	0.46
1:A:669:ASP:OD1	1:A:718:LYS:HE2	2.16	0.46
1:A:1125:LYS:HD3	1:A:1246:ASP:HB3	1.97	0.46
1:A:2050:GLU:N	1:A:2053:GLU:OE2	2.48	0.46
1:A:324:LYS:HE3	1:A:359:ILE:HD11	1.98	0.45
1:A:646:ILE:CG2	1:A:691:ILE:HG13	2.46	0.45
1:A:1546:ASP:OD2	1:A:1549:THR:OG1	2.27	0.45
1:A:1437:ILE:HD12	1:A:1497:ILE:HD12	1.98	0.45
1:A:2113:ASP:OD2	1:A:2117:ILE:HB	2.16	0.45
1:A:1371:ILE:HA	1:A:1374:LYS:HZ3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2090:TYR:O	1:A:2099:CYS:N	2.50	0.45
1:A:1761:GLN:O	1:A:1763:GLN:N	2.46	0.45
1:A:1179:THR:O	1:A:1180:LEU:HD23	2.17	0.45
1:A:229:LEU:O	1:A:233:THR:OG1	2.30	0.45
1:A:573:ARG:HD2	1:A:1804:ALA:O	2.17	0.45
1:A:1557:LEU:HB3	1:A:1561:GLY:HA3	1.98	0.45
1:A:1629:ASP:OD1	1:A:1629:ASP:N	2.50	0.45
1:A:1997:VAL:HB	1:A:2026:ARG:HB3	1.98	0.45
1:A:2170:LYS:HE3	1:A:2186:ALA:HB1	1.98	0.45
1:A:1009:GLU:O	1:A:1013:THR:OG1	2.35	0.45
1:A:2353:PHE:CZ	1:A:2360:LEU:HB2	2.51	0.45
1:A:623:VAL:N	1:A:639:GLN:HE22	2.12	0.45
1:A:1035:ILE:HB	1:A:1610:ASN:HD22	1.82	0.45
1:A:1533:LYS:O	1:A:1535:ASP:N	2.42	0.45
1:A:1957:TYR:CE1	1:A:1983:ASN:O	2.70	0.45
1:A:1352:VAL:O	1:A:1368:ILE:HG22	2.16	0.44
1:A:1979:TYR:HD1	1:A:1987:GLN:HB2	1.81	0.44
1:A:2092:ASP:N	1:A:2092:ASP:OD1	2.50	0.44
1:A:580:TYR:OH	1:A:634:TYR:HA	2.18	0.44
1:A:2299:GLY:HA3	1:A:2338:ILE:HD12	1.99	0.44
1:A:966:GLN:HE21	1:A:970:GLU:HG3	1.83	0.44
1:A:1036:ILE:HG21	1:A:1521:LYS:HE2	1.99	0.44
1:A:1081:SER:O	1:A:1085:ILE:HG23	2.17	0.44
1:A:876:ASN:N	1:A:876:ASN:HD22	2.16	0.44
1:A:1255:ARG:HA	1:A:1262:PHE:HB3	2.00	0.44
1:A:2277:LYS:HZ1	1:A:2313:PHE:HE1	1.66	0.44
1:A:2354:ASP:OD1	1:A:2355:PRO:HD2	2.17	0.44
1:A:332:SER:O	1:A:335:PHE:N	2.50	0.44
1:A:1025:LEU:CD2	1:A:1025:LEU:H	2.30	0.44
1:A:1047:GLU:O	1:A:1051:THR:OG1	2.29	0.44
1:A:1344:TRP:O	1:A:1402:ILE:HD12	2.17	0.44
1:A:1400:ARG:NH2	1:A:1421:VAL:HB	2.32	0.44
1:A:1959:PHE:HE1	1:A:1966:ALA:HB2	1.82	0.44
1:A:321:MET:SD	1:A:326:TYR:HB2	2.58	0.44
1:A:1025:LEU:HD23	1:A:1623:GLU:OE2	2.17	0.44
1:A:589:ILE:HD11	1:A:757:HIS:HA	1.99	0.44
1:A:1353:LYS:HA	1:A:1367:LEU:HA	2.00	0.44
1:A:2095:THR:HG23	1:A:2097:GLU:HG3	1.99	0.44
1:A:955:GLU:O	1:A:959:LEU:HG	2.17	0.44
1:A:1123:TYR:O	1:A:1127:ILE:HG23	2.17	0.44
1:A:1993:ILE:O	1:A:1996:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2195:VAL:HG12	1:A:2196:ASN:N	2.32	0.44
1:A:2230:TYR:CD1	1:A:2234:ASN:HB3	2.53	0.44
1:A:1376:ASN:ND2	1:A:1378:GLU:OE2	2.51	0.44
1:A:1686:ASP:OD1	1:A:1686:ASP:N	2.51	0.44
1:A:2254:ILE:HB	1:A:2263:PHE:HE2	1.82	0.44
1:A:2285:LYS:HA	1:A:2285:LYS:HD3	1.72	0.44
1:A:570:MET:HE2	1:A:570:MET:HA	2.00	0.43
1:A:674:GLU:O	1:A:678:ILE:HG13	2.18	0.43
1:A:1154:GLU:O	1:A:1155:ILE:HD13	2.18	0.43
1:A:1507:ILE:CG2	1:A:1598:ASN:HD21	2.31	0.43
1:A:1949:TRP:CE3	1:A:1958:TYR:HB2	2.53	0.43
1:A:1951:LEU:CD2	1:A:1956:THR:HA	2.48	0.43
1:A:377:PHE:CD2	1:A:502:GLU:HG3	2.53	0.43
1:A:1253:ARG:HD2	1:A:1257:HIS:HE1	1.83	0.43
1:A:2013:VAL:O	1:A:2016:LYS:HE2	2.18	0.43
1:A:2142:TYR:CD2	1:A:2166:PRO:HD2	2.53	0.43
1:A:2329:LYS:HE3	1:A:2360:LEU:H	1.82	0.43
1:A:308:THR:HA	1:A:785:ASN:ND2	2.34	0.43
1:A:1030:PRO:CB	1:A:1556:TYR:OH	2.66	0.43
1:A:1306:GLU:O	1:A:1310:LYS:HE2	2.19	0.43
1:A:1466:ASP:O	1:A:1469:THR:HB	2.18	0.43
1:A:1498:TYR:HB3	1:A:1501:ASP:O	2.19	0.43
1:A:1959:PHE:CE1	1:A:1966:ALA:HB2	2.53	0.43
1:A:2304:ALA:O	1:A:2315:GLY:N	2.52	0.43
1:A:414:LEU:HG	1:A:418:ILE:CD1	2.48	0.43
1:A:1022:LEU:HB3	1:A:1023:PRO:CD	2.48	0.43
1:A:1381:LYS:HZ2	1:A:1383:ILE:HD11	1.84	0.43
1:A:2185:GLN:NE2	1:A:2186:ALA:O	2.51	0.43
1:A:2235:VAL:HG22	1:A:2240:LYS:HG3	2.00	0.43
1:A:1123:TYR:OH	1:A:1228:ARG:NH2	2.52	0.43
1:A:1371:ILE:HG23	1:A:1372:LEU:HD22	2.00	0.43
1:A:1498:TYR:CE2	1:A:1500:PRO:HD2	2.54	0.43
1:A:577:TYR:HB2	1:A:645:LYS:O	2.18	0.43
1:A:1167:CYS:SG	1:A:1202:ILE:HD12	2.59	0.43
1:A:1515:ASP:OD1	1:A:1515:ASP:N	2.49	0.43
1:A:925:ILE:HD13	1:A:985:MET:HE1	1.99	0.43
1:A:1155:ILE:HB	1:A:1289:ILE:HD12	2.00	0.43
1:A:1427:ILE:HG13	1:A:1452:PHE:HE2	1.84	0.43
1:A:1459:TYR:OH	1:A:1522:GLY:O	2.25	0.43
1:A:1900:ILE:HD12	1:A:1909:PHE:CD2	2.54	0.43
1:A:1973:ILE:HB	1:A:1978:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2219:LYS:HE3	1:A:2249:MET:HB3	2.00	0.43
1:A:535:LYS:HB3	1:A:535:LYS:HE3	1.81	0.43
1:A:937:PHE:CD2	1:A:947:LYS:HB2	2.54	0.43
1:A:958:THR:OG1	1:A:959:LEU:N	2.51	0.43
1:A:1041:LEU:N	1:A:1041:LEU:CD2	2.73	0.43
1:A:968:LEU:HD12	1:A:968:LEU:HA	1.83	0.43
1:A:1212:LYS:HA	1:A:1212:LYS:HD3	1.76	0.43
1:A:1251:LEU:HD22	1:A:1264:TRP:CG	2.54	0.43
1:A:2178:VAL:HG21	1:A:2189:TYR:HB2	2.00	0.43
1:A:708:GLU:OE2	1:A:708:GLU:N	2.29	0.42
1:A:1116:LYS:NZ	1:A:1276:THR:OG1	2.42	0.42
1:A:1370:ASN:OD1	1:A:1373:SER:OG	2.24	0.42
1:A:1543:THR:HG22	1:A:1553:ASN:HD21	1.84	0.42
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.49	0.42
1:A:1742:VAL:HG12	1:A:1801:SER:HB2	2.00	0.42
1:A:2182:ILE:HB	1:A:2185:GLN:HB2	2.01	0.42
1:A:375:ILE:HG13	1:A:387:LEU:HD23	2.01	0.42
1:A:571:LYS:HA	1:A:600:LYS:O	2.19	0.42
1:A:1662:TYR:HD2	1:A:1670:ILE:HG23	1.85	0.42
1:A:224:TYR:O	1:A:228:SER:OG	2.33	0.42
1:A:250:ASP:HB2	1:A:404:LYS:HE2	2.02	0.42
1:A:1200:LEU:HD22	1:A:1258:TYR:CG	2.54	0.42
1:A:1513:LEU:HD23	1:A:1516:ILE:HD11	2.00	0.42
1:A:1650:VAL:O	1:A:1650:VAL:HG12	2.18	0.42
1:A:646:ILE:HG23	1:A:691:ILE:HG13	2.00	0.42
1:A:704:SER:HB3	1:A:776:GLU:CD	2.44	0.42
1:A:1306:GLU:HA	1:A:1309:ARG:HG3	2.02	0.42
1:A:1384:LEU:HD22	1:A:1404:LEU:HD21	2.01	0.42
1:A:2309:LEU:HD12	1:A:2309:LEU:HA	1.87	0.42
1:A:1036:ILE:CG2	1:A:1521:LYS:HE2	2.49	0.42
1:A:981:LEU:HA	1:A:981:LEU:HD12	1.78	0.42
1:A:1354:ASN:HB3	1:A:1365:GLY:HA3	2.00	0.42
1:A:1512:ASP:O	1:A:1514:LYS:HG3	2.19	0.42
1:A:1664:LEU:HD23	1:A:1669:ASN:O	2.20	0.42
1:A:2276:ILE:HB	1:A:2281:PHE:CE2	2.54	0.42
1:A:18:ARG:NH1	1:A:1668:GLY:O	2.53	0.42
1:A:578:ILE:HG12	1:A:640:ILE:HB	2.02	0.42
1:A:1169:ILE:HA	1:A:1230:PHE:HB2	2.02	0.42
1:A:312:TRP:HA	1:A:312:TRP:CE3	2.55	0.42
1:A:1114:GLN:OE1	1:A:1119:LYS:HB3	2.20	0.42
1:A:1236:TRP:CZ3	1:A:1273:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:ILE:HG22	1:A:912:GLU:O	2.20	0.41
1:A:1041:LEU:HD12	1:A:1045:ILE:CD1	2.50	0.41
1:A:1227:ASN:H	1:A:1285:THR:HG1	1.67	0.41
1:A:1958:TYR:HD1	1:A:1967:LEU:HD13	1.85	0.41
1:A:2226:THR:HG22	1:A:2228:LYS:HD3	2.00	0.41
1:A:1022:LEU:HB3	1:A:1023:PRO:HD2	2.02	0.41
1:A:2243:PHE:HE2	1:A:2249:MET:HG3	1.85	0.41
1:A:2259:ASN:HB2	1:A:2261:TYR:CE2	2.55	0.41
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.20	0.41
1:A:1264:TRP:CE2	1:A:1265:ARG:HD2	2.55	0.41
1:A:937:PHE:CE2	1:A:947:LYS:HB2	2.55	0.41
1:A:1086:ALA:HB2	1:A:1405:THR:OG1	2.20	0.41
1:A:1121:ILE:HD13	1:A:1248:THR:HG22	2.02	0.41
1:A:1329:PRO:HD3	1:A:1350:ASN:CG	2.45	0.41
1:A:2229:ALA:O	1:A:2231:LYS:HD2	2.20	0.41
1:A:416:PRO:HB2	1:A:434:LYS:HE2	2.03	0.41
1:A:1573:LYS:HD3	1:A:1687:ARG:HH22	1.84	0.41
1:A:1999:TYR:CE1	1:A:2011:ILE:HG21	2.56	0.41
1:A:2340:ALA:HB3	1:A:2353:PHE:CG	2.56	0.41
1:A:1582:LEU:HD21	1:A:1611:PHE:CD1	2.54	0.41
1:A:1608:ASP:OD1	1:A:1609:THR:N	2.52	0.41
1:A:2235:VAL:HG13	1:A:2240:LYS:HG3	2.02	0.41
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.85	0.41
1:A:2162:VAL:HG11	1:A:2200:TYR:HD2	1.85	0.41
1:A:280:ASP:N	1:A:280:ASP:OD1	2.54	0.41
1:A:340:GLU:O	1:A:344:ARG:HG3	2.21	0.41
1:A:493:LEU:HD22	1:A:497:GLU:OE1	2.20	0.41
1:A:1452:PHE:CZ	1:A:1457:GLN:HB3	2.56	0.41
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.73	0.41
1:A:93:PRO:HA	1:A:366:ILE:O	2.21	0.41
1:A:1406:PHE:CE1	1:A:1414:ILE:HB	2.56	0.41
1:A:1539:SER:HB2	1:A:1556:TYR:HB3	2.02	0.41
1:A:603:TYR:CD1	1:A:623:VAL:HG22	2.56	0.41
1:A:622:SER:CA	1:A:639:GLN:HE22	2.26	0.41
1:A:1253:ARG:HH11	1:A:1257:HIS:HE1	1.69	0.41
1:A:1550:ILE:HD12	1:A:1603:ILE:HG21	2.02	0.41
1:A:1973:ILE:HB	1:A:1978:TYR:HE2	1.85	0.41
1:A:1991:ILE:HD12	1:A:2000:PHE:CD2	2.56	0.41
1:A:2016:LYS:HB3	1:A:2053:GLU:CD	2.46	0.41
1:A:2223:ASP:O	1:A:2227:LYS:HA	2.21	0.41
1:A:2242:TYR:HB2	1:A:2263:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:CD1	1:A:602:PRO:HB3	2.48	0.40
1:A:1938:TYR:CE2	1:A:1952:LEU:HD23	2.56	0.40
1:A:2281:PHE:HD1	1:A:2289:MET:SD	2.45	0.40
1:A:72:LEU:O	1:A:75:PHE:HB3	2.22	0.40
1:A:1031:ILE:CG2	1:A:1046:LYS:HD3	2.48	0.40
1:A:1160:ASN:HA	1:A:1215:PHE:CE2	2.56	0.40
1:A:1195:TYR:CD2	1:A:1196:ARG:HD3	2.56	0.40
1:A:1286:ASN:OD1	1:A:1313:SER:HB2	2.21	0.40
1:A:1470:LYS:HE3	1:A:1470:LYS:HB2	1.99	0.40
1:A:2008:VAL:HG23	1:A:2021:GLY:O	2.21	0.40
1:A:363:LEU:HD22	1:A:366:ILE:HD11	2.02	0.40
1:A:1926:PHE:HE1	1:A:1930:LEU:HB2	1.86	0.40
1:A:1111:LEU:N	1:A:1281:ARG:HH12	2.13	0.40
1:A:2130:PHE:CD2	1:A:2132:PHE:HE2	2.40	0.40
1:A:1280:PRO:C	1:A:1281:ARG:HD2	2.46	0.40
1:A:1409:LEU:HB2	1:A:1412:ILE:HB	2.03	0.40
1:A:2174:PRO:HG2	1:A:2177:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2351/2372 (99%)	2210 (94%)	135 (6%)	6 (0%)	36 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	ALA
1	A	1948	GLU
1	A	1029	LEU
1	A	1762	PRO

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Mol	Chain	Res	Type
1	A	2342	GLY
1	A	1023	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2130/2146 (99%)	1995 (94%)	135 (6%)	16	45

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	42	VAL
1	A	92	THR
1	A	94	VAL
1	A	110	THR
1	A	123	SER
1	A	141	LEU
1	A	145	ILE
1	A	200	PHE
1	A	201	ILE
1	A	208	THR
1	A	228	SER
1	A	232	ILE
1	A	244	GLU
1	A	272	LEU
1	A	288	ASP
1	A	332	SER
1	A	338	LEU
1	A	339	ASP
1	A	342	VAL
1	A	382	VAL
1	A	395	CYS
1	A	410	LEU
1	A	413	ASN

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Mol	Chain	Res	Type
1	A	417	SER
1	A	419	ASN
1	A	464	SER
1	A	469	SER
1	A	492	HIS
1	A	493	LEU
1	A	508	ILE
1	A	529	SER
1	A	535	LYS
1	A	574	ASN
1	A	640	ILE
1	A	644	ARG
1	A	646	ILE
1	A	651	ILE
1	A	656	SER
1	A	685	ASP
1	A	702	SER
1	A	703	TYR
1	A	785	ASN
1	A	830	SER
1	A	863	GLU
1	A	865	ILE
1	A	879	ASP
1	A	884	ILE
1	A	897	ARG
1	A	914	GLU
1	A	936	ILE
1	A	937	PHE
1	A	958	THR
1	A	968	LEU
1	A	981	LEU
1	A	1001	ILE
1	A	1002	THR
1	A	1010	LEU
1	A	1013	THR
1	A	1019	ILE
1	A	1027	GLU
1	A	1031	ILE
1	A	1039	VAL
1	A	1040	SER
1	A	1041	LEU
1	A	1048	LEU

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Mol	Chain	Res	Type
1	A	1055	LEU
1	A	1058	GLN
1	A	1072	THR
1	A	1078	ILE
1	A	1143	ILE
1	A	1144	ILE
1	A	1167	CYS
1	A	1205	VAL
1	A	1213	ILE
1	A	1234	MET
1	A	1251	LEU
1	A	1285	THR
1	A	1297	SER
1	A	1305	THR
1	A	1324	SER
1	A	1327	LEU
1	A	1332	MET
1	A	1340	GLU
1	A	1368	ILE
1	A	1392	TYR
1	A	1418	ILE
1	A	1433	CYS
1	A	1447	ILE
1	A	1462	TYR
1	A	1515	ASP
1	A	1534	ASP
1	A	1543	THR
1	A	1547	THR
1	A	1576	LEU
1	A	1591	ILE
1	A	1598	ASN
1	A	1602	ASN
1	A	1613	ILE
1	A	1618	SER
1	A	1662	TYR
1	A	1671	SER
1	A	1698	LEU
1	A	1714	ILE
1	A	1726	ILE
1	A	1751	ILE
1	A	1771	VAL
1	A	1775	ASP

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Mol	Chain	Res	Type
1	A	1776	THR
1	A	1779	ASP
1	A	1795	LYS
1	A	1801	SER
1	A	1814	PHE
1	A	1821	ASN
1	A	1831	ASN
1	A	1870	THR
1	A	1895	LEU
1	A	1902	THR
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	2005	VAL
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 (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	8	GLN
1	A	35	HIS
1	A	53	ASN
1	A	58	ASN
1	A	97	ASN
1	A	106	GLN
1	A	139	ASN
1	A	169	ASN
1	A	222	ASN
1	A	413	ASN

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	639	GLN
1	A	732	GLN
1	A	741	GLN
1	A	785	ASN
1	A	795	HIS
1	A	876	ASN
1	A	907	ASN
1	A	941	ASN
1	A	949	ASN
1	A	972	ASN
1	A	988	GLN
1	A	1109	ASN
1	A	1257	HIS
1	A	1390	ASN
1	A	1453	ASN
1	A	1504	ASN
1	A	1520	ASN
1	A	1553	ASN
1	A	1593	ASN
1	A	1727	ASN
1	A	1731	ASN
1	A	1735	ASN
1	A	1761	GLN
1	A	1763	GLN
1	A	2032	ASN
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.

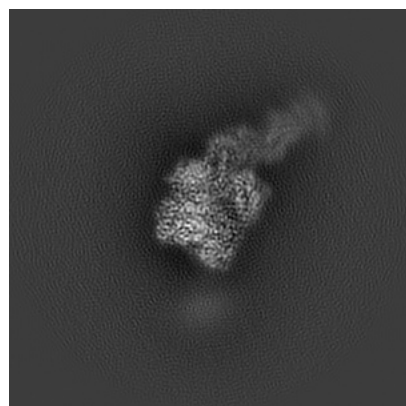
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36141. These allow visual inspection of the internal detail of the map and identification of artifacts.

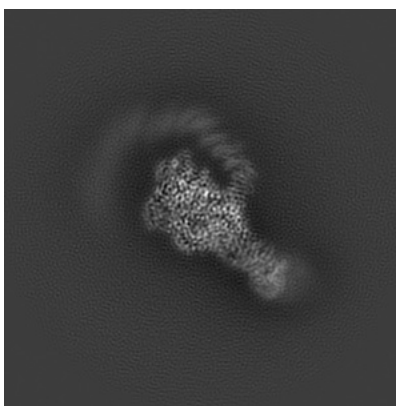
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

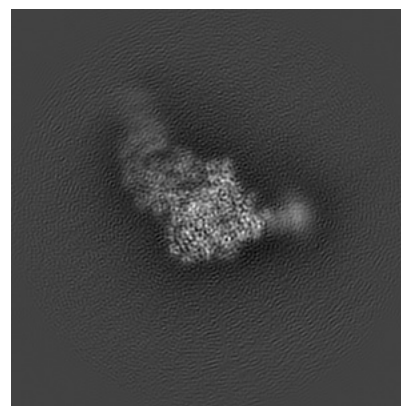
6.1.1 Primary map



X

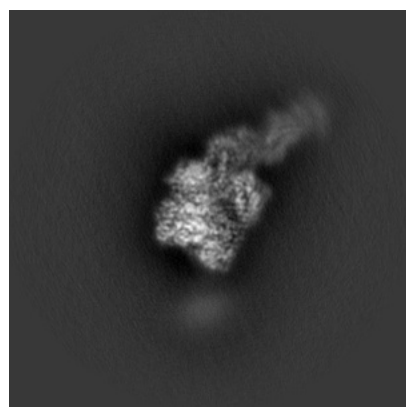


Y

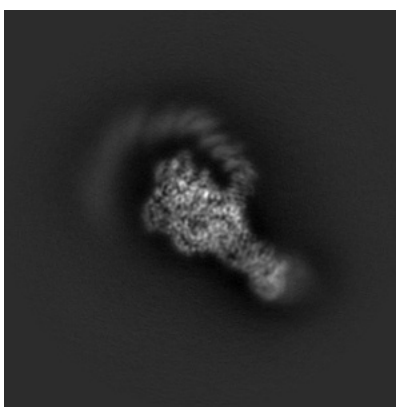


Z

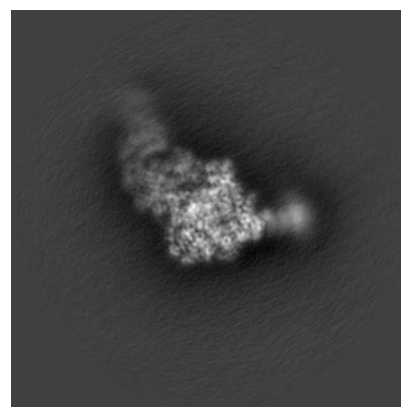
6.1.2 Raw map



X



Y

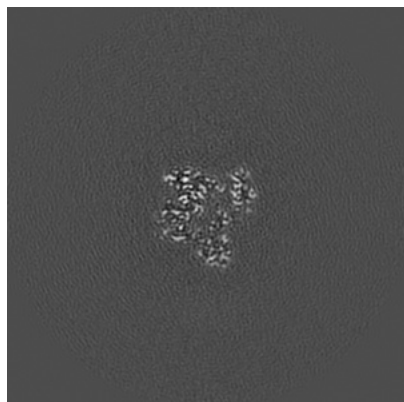


Z

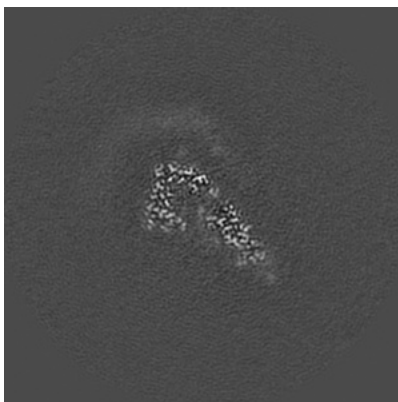
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

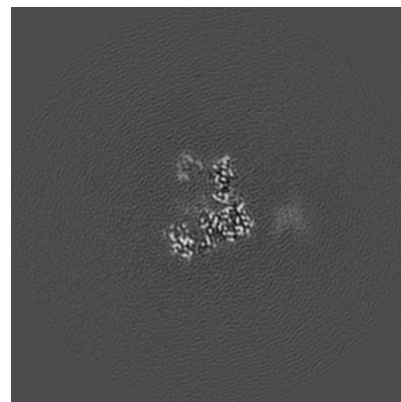
6.2.1 Primary map



X Index: 148

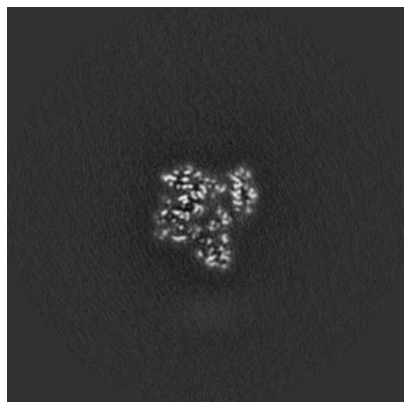


Y Index: 148

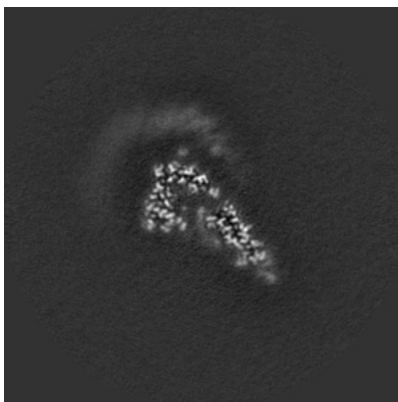


Z Index: 148

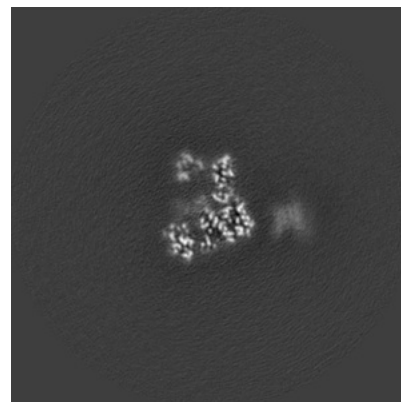
6.2.2 Raw map



X Index: 148



Y Index: 148

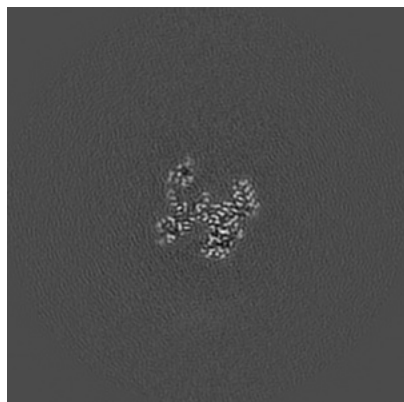


Z Index: 148

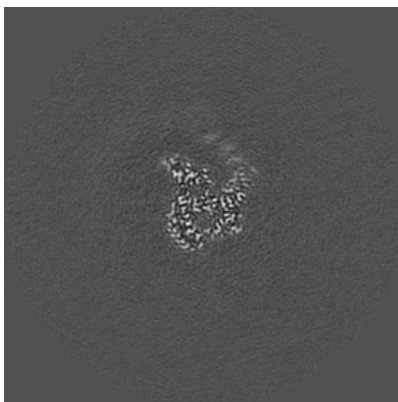
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

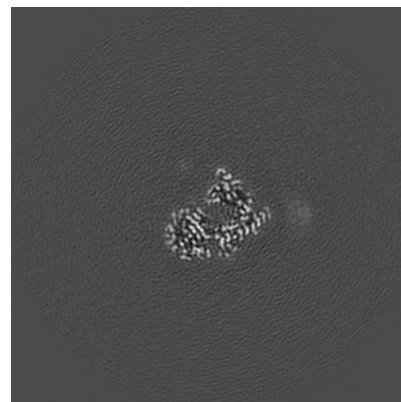
6.3.1 Primary map



X Index: 159

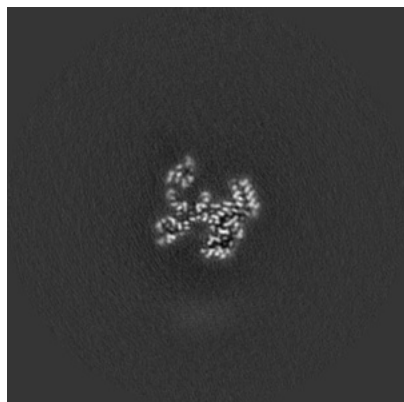


Y Index: 130

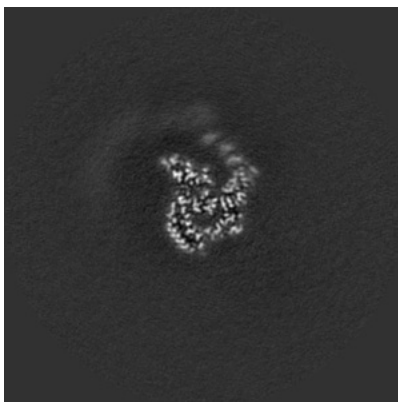


Z Index: 135

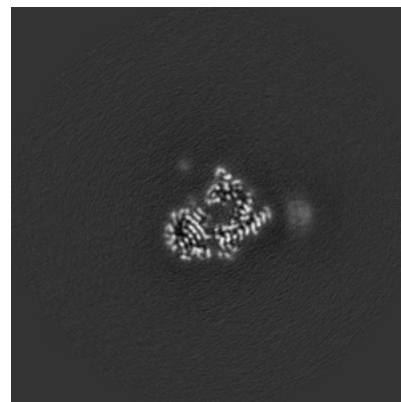
6.3.2 Raw map



X Index: 159



Y Index: 130

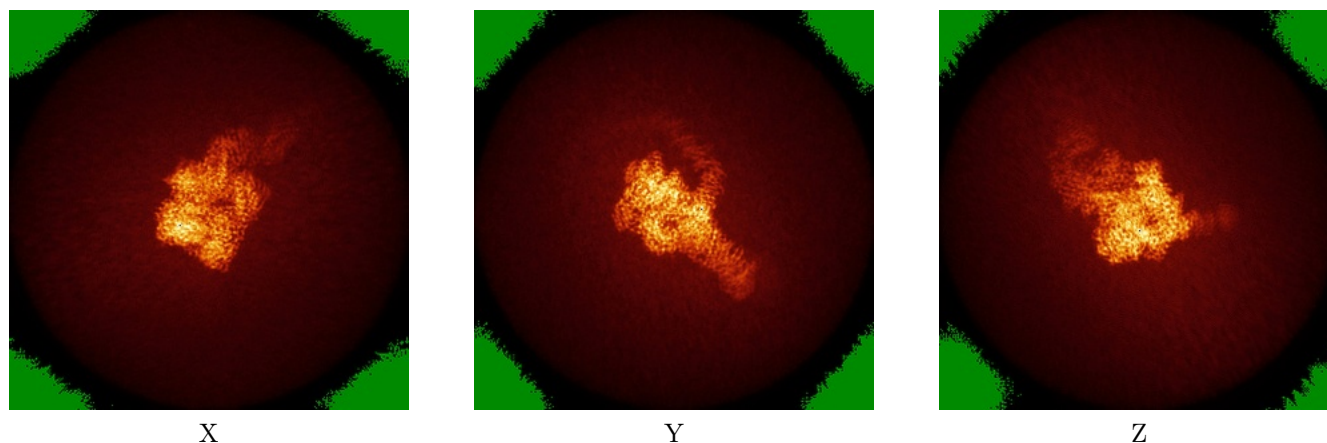


Z Index: 135

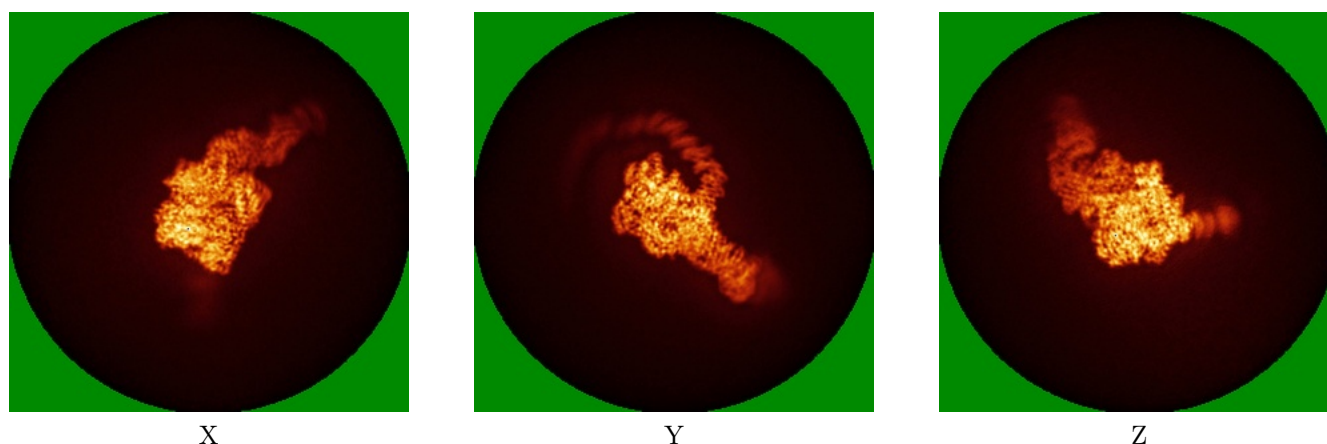
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

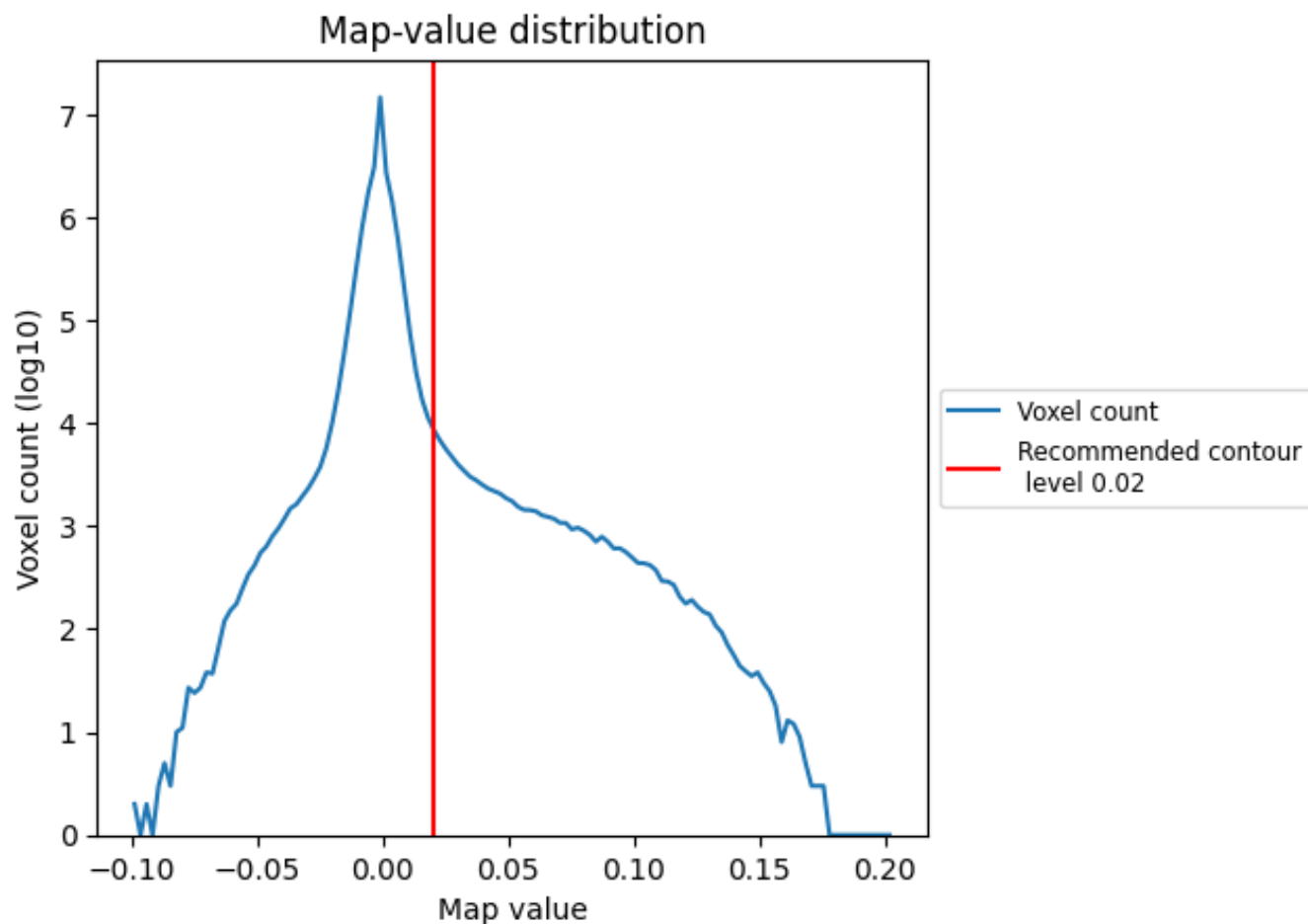
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

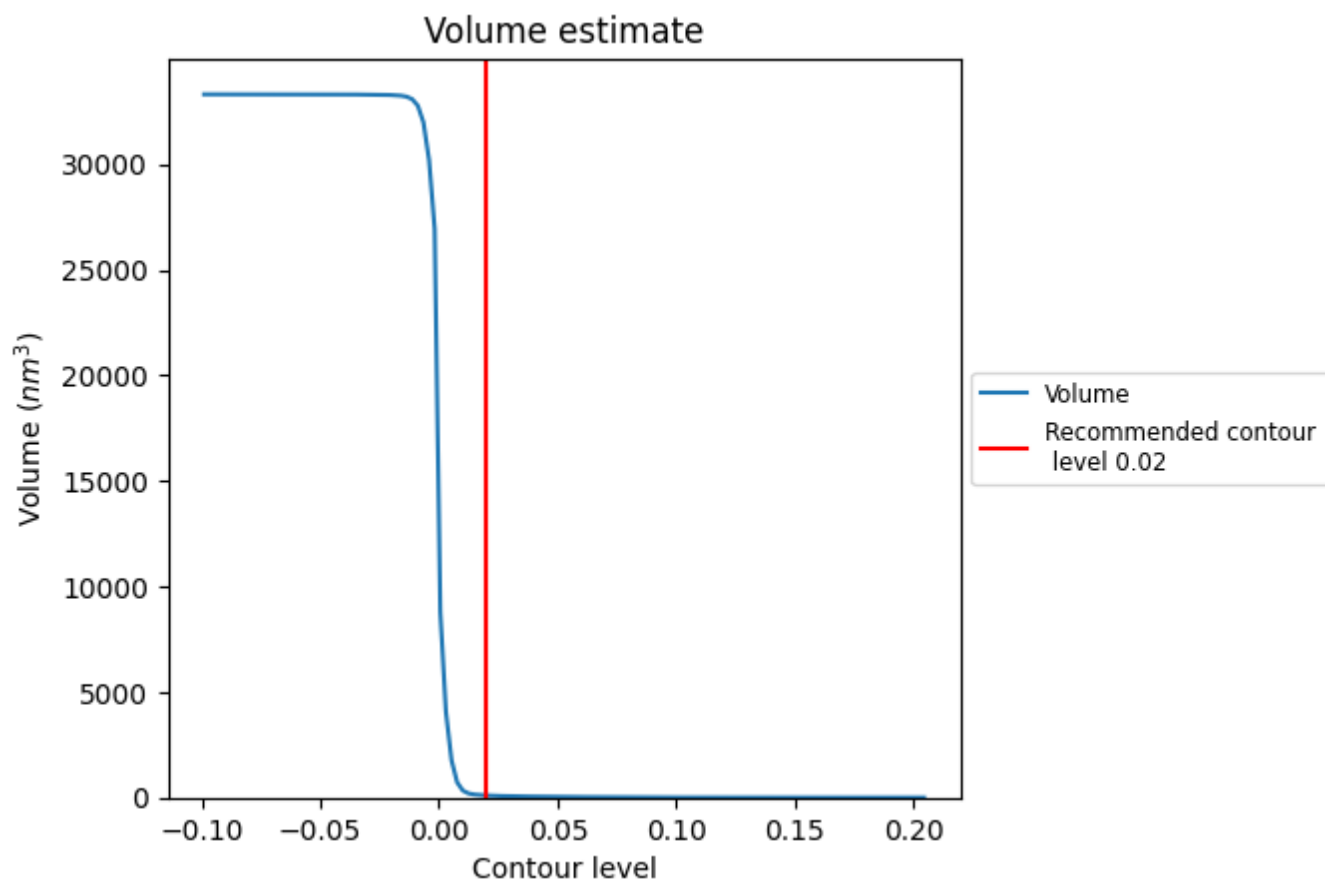
This section contains the results of statistical analysis of the map.

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.

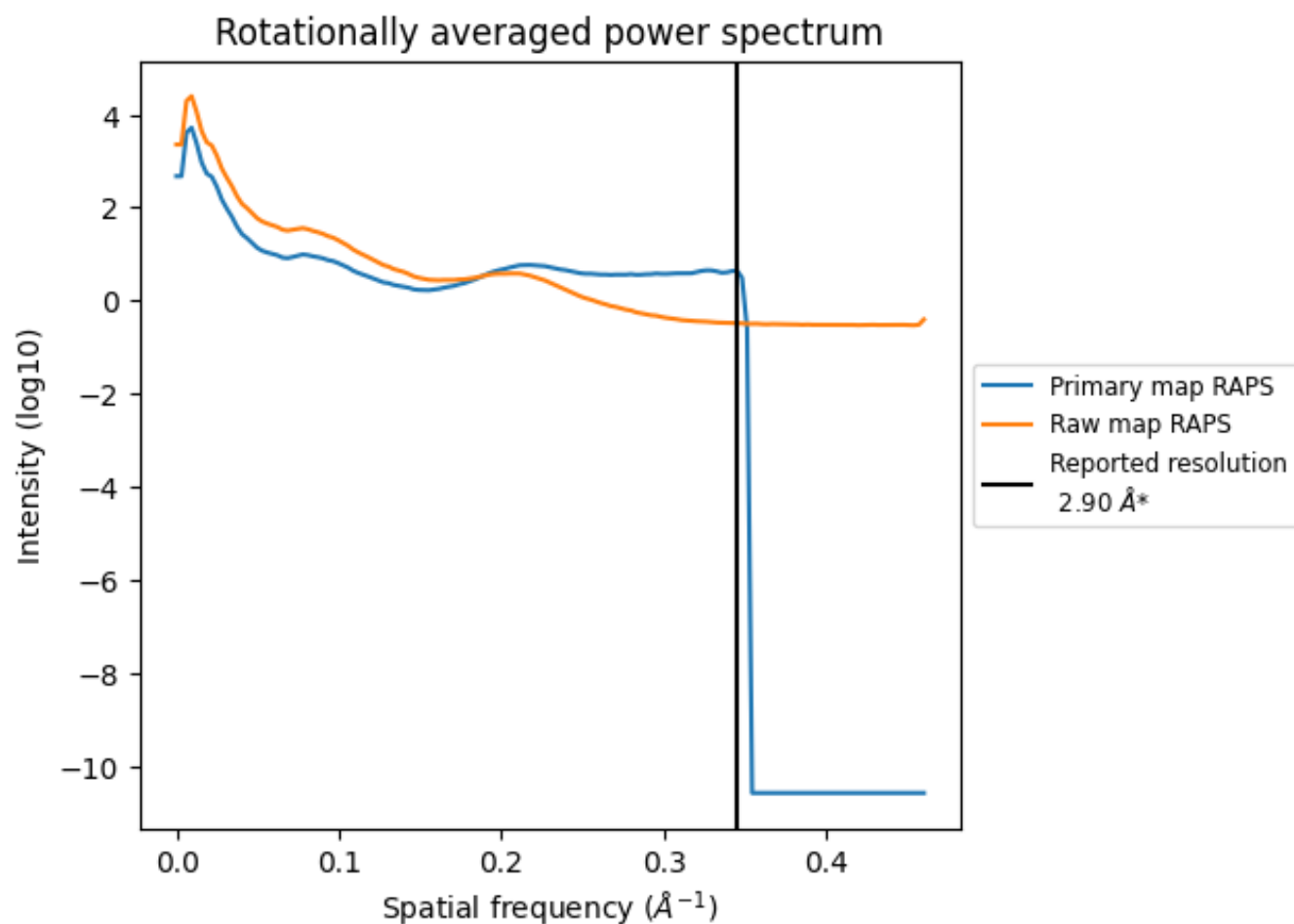
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

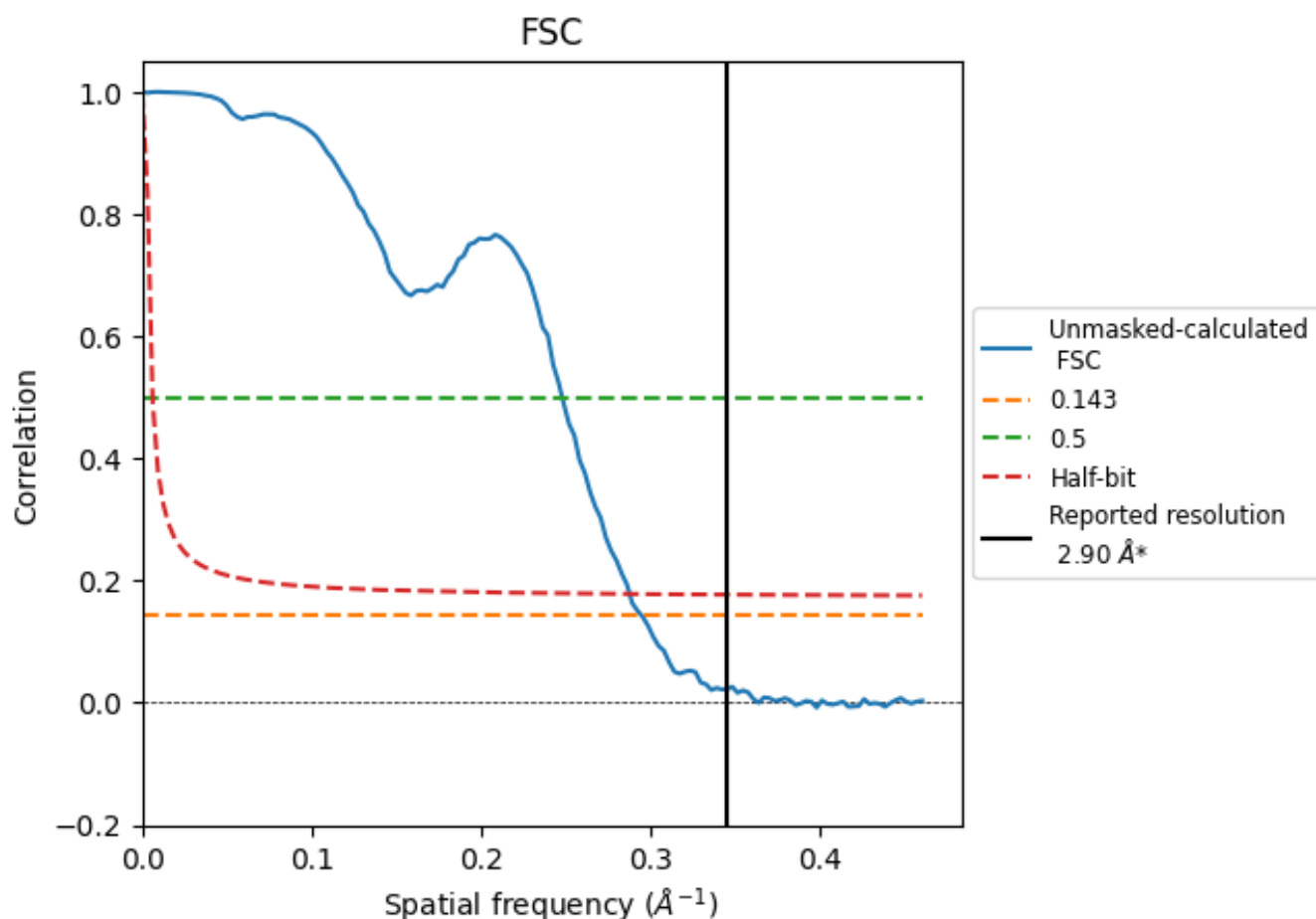


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

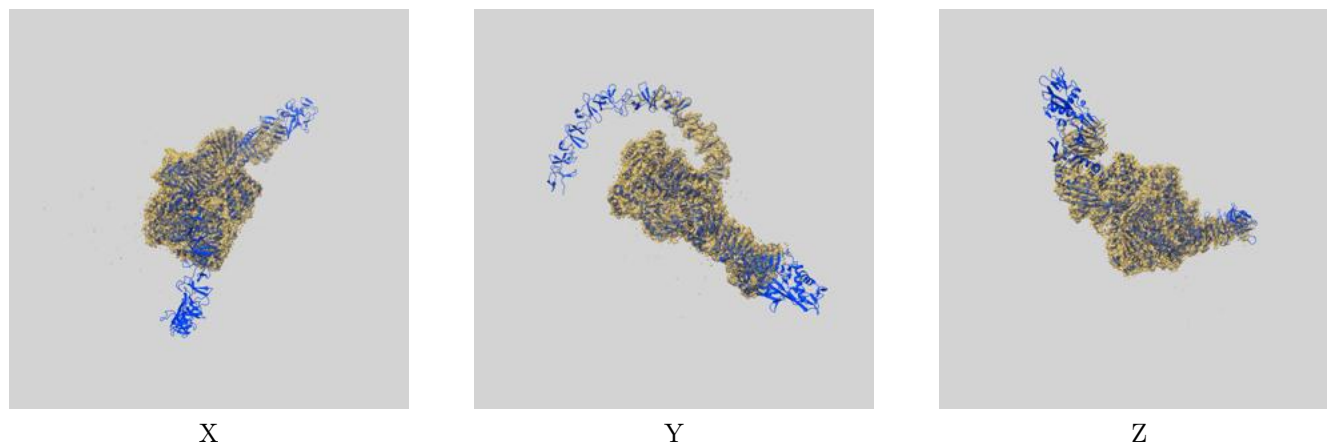
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.04	3.48

*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 3.40 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

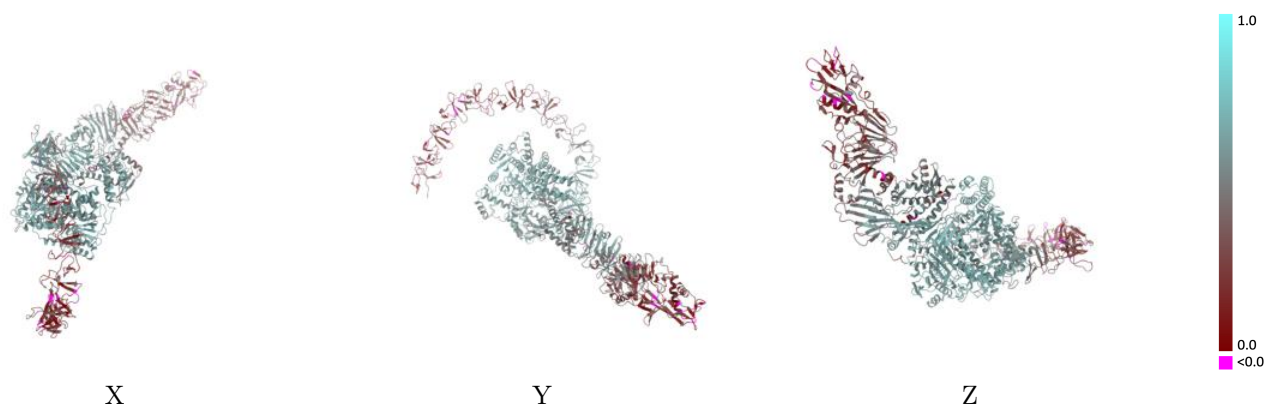
This section contains information regarding the fit between EMDB map EMD-36141 and PDB model 8JB5. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



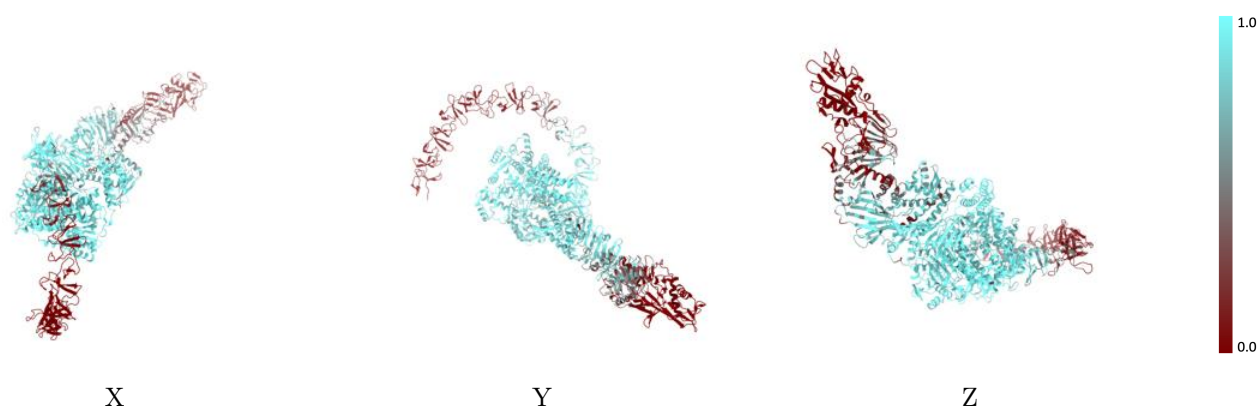
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



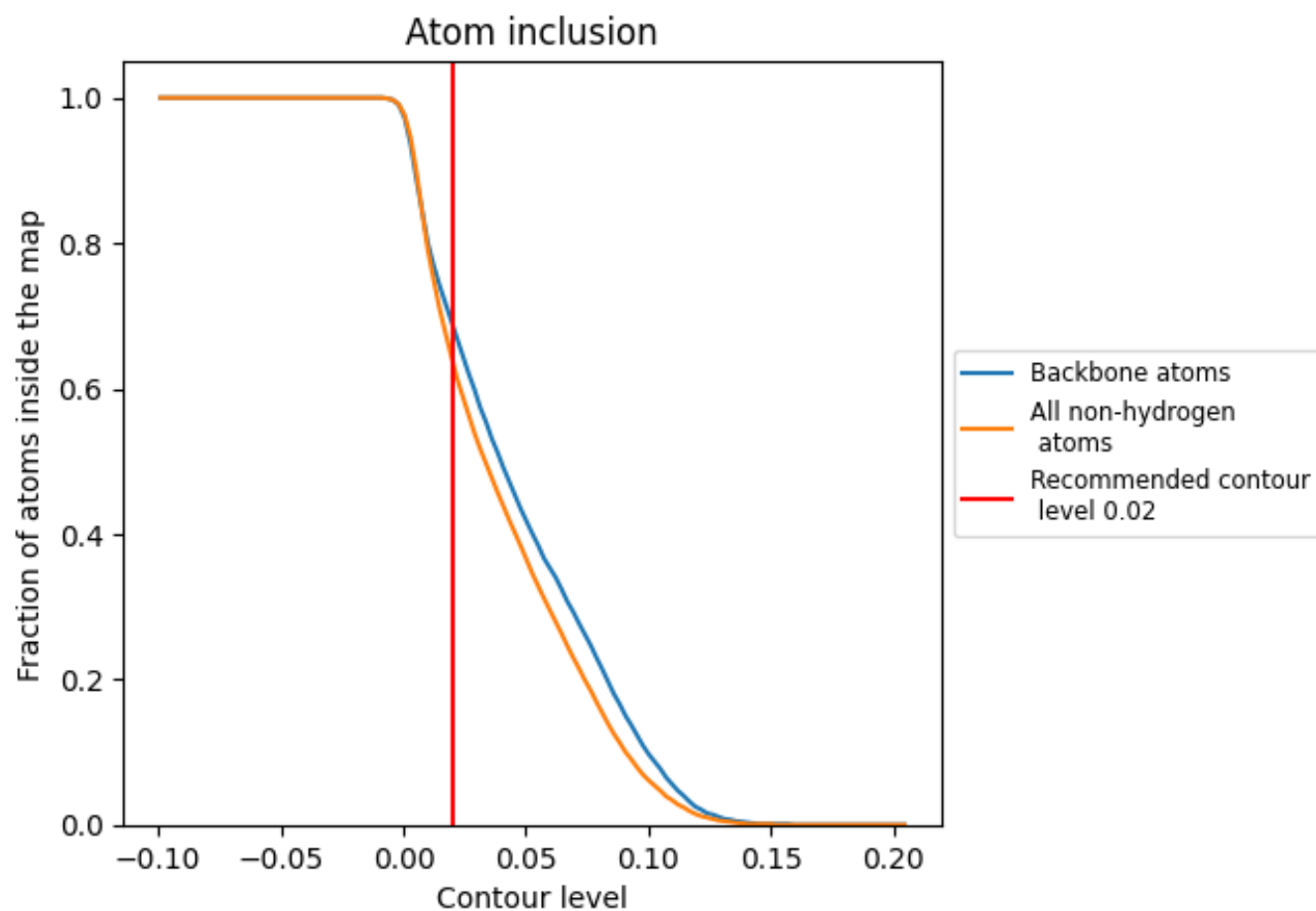
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.4770
A	0.6390	0.4770

