Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 03:12 am GMT

PDB ID	:	6RMH
EMDB ID	:	EMD-4937
Title	:	The Rigid-body refined model of the normal Huntingtin.
Authors	:	Jung, T.; Tamo, G.; Dal Perraro, M.; Hebert, H.; Song, J.
Deposited on	:	2019-05-06
Resolution	:	9.60 Å(reported)
Based on initial model	:	6EZ8

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 (i) 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 (i)) were used in the production of this report:

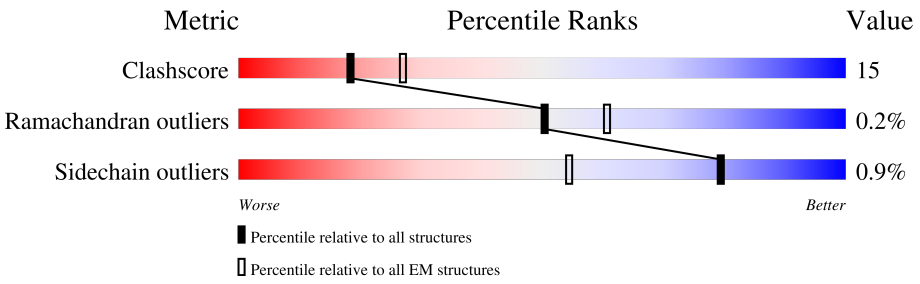
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

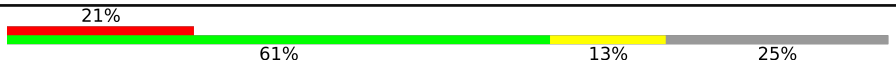
The reported resolution of this entry is 9.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	3142	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18465 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 Huntingtin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2353	18465	11842	3157	3347	119	0	0

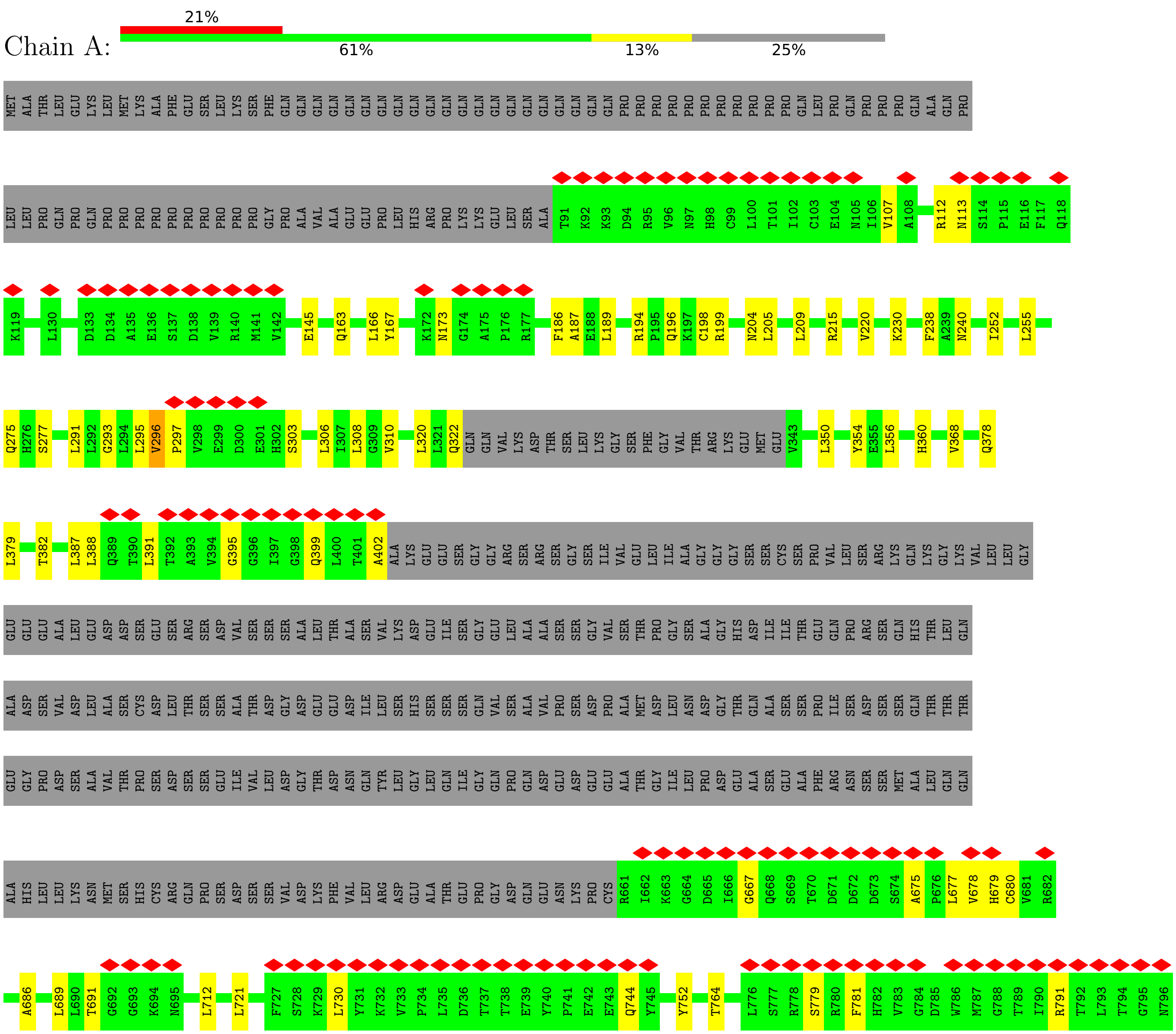
There are 2 discrepancies between the modelled and reference sequences:

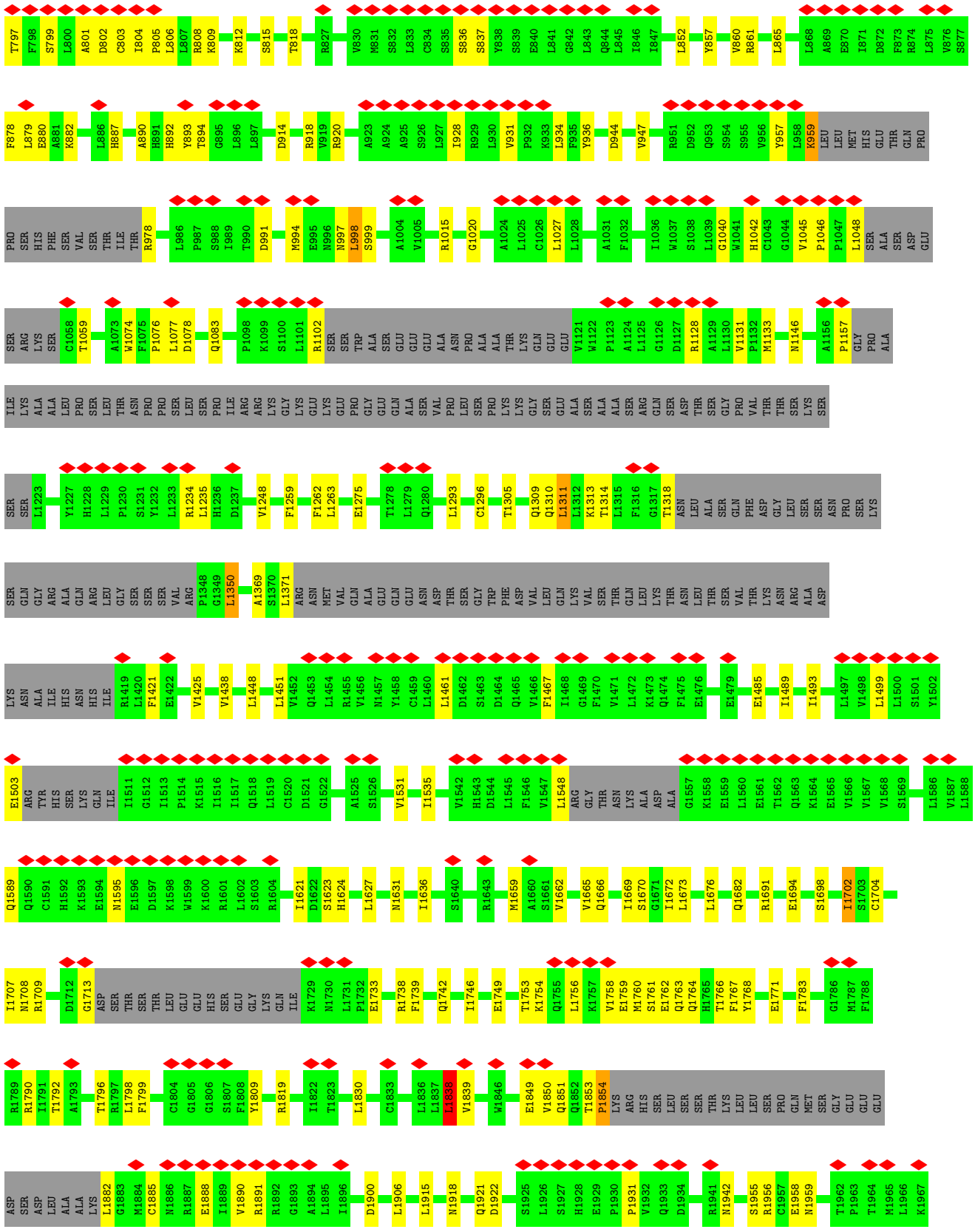
Chain	Residue	Modelled	Actual	Comment	Reference
A	1234	ARG	LYS	conflict	UNP P42858
A	2305	HIS	TYR	conflict	UNP P42858

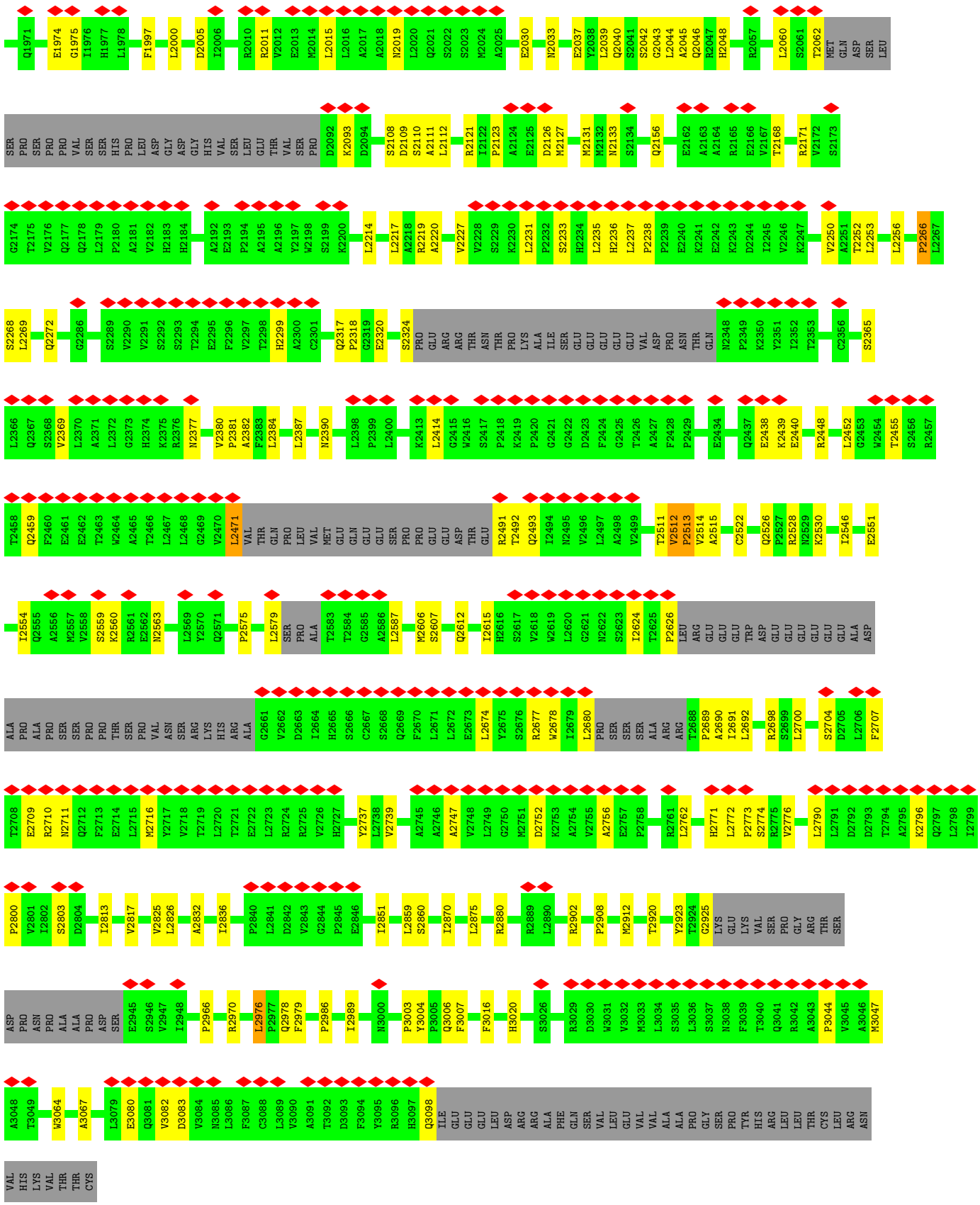
3 Residue-property plots (i)

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: Huntingtin




T797 F798 S799 L800 A801 D802 C803 I804 P805 L806 L807 R808 K809 K812 S815 T818 R827 V830 M831 S832 L833 C834 S835 S836 S837 Y838 S839 E840 L841 G842 L843 Q844 L845 I846 I847 L852 Y857 V860 R861 L865 L868 A869 E870 I871 D872 F873 R874 L875 V876 S877
F878 L879 E880 A881 K882 L886 H887 A890 H891 H892 Y893 T894 G895 L896 L897 D914 R918 V919 R920 A923 A924 A925 S926 L927 I928 R929 L930 V931 P932 K933 L934 F935 Y936 D944 V947 R951 D952 Q953 S954 S955 V956 Y957 L958 K959 LEU LEU MET HIS GLU THR GLN PRO
PRO SER HIS PHE SER VAL SER THR ILE THR R978 L986 P987 S988 I989 T990 D991 M994 E995 N996 N997 L998 S999 A1004 V1005 R1015 G1020 A1024 L1025 C1026 L1027 L1028 A1031 F1032 I1036 W1037 S1038 L1039 G1040 W1041 H1042 C1043 G1044 V1045 P1046 P1047 L1048 SER ALA SER ASP GLU
SER ARG LYS SER C1058 T1059 A1073 W1074 F1075 P1076 L1077 D1078 Q1083 P1098 K1099 S1100 L1101 R1102 SER SER TRP ALA SER GLU GLU GLU ALA ASN PRO ALA ALA THR LYS GLN GLU GLU V1121 W1122 P1123 A1124 L1125 G1126 D1127 R1128 A1129 L1130 V1131 P1132 M1133 N1146 A1156 P1157 GLY PRO ALA
ILE LYS ALA ALA LEU PRO SER LEU THR ASN PRO PRO SER LEU SER PRO ILE ARG ARG LYS GLY LYS GLU LYS GLU PRO GLY GLU GLN ALA SER VAL PRO LEU SER PRO LYS LYS GLY SER GLU ALA SER ALA ALA SER ARG GLN SER ASP THR SER GLY PRO VAL THR THR SER LYS SER
SER SER L1223 Y1227 H1228 L1229 P1230 S1231 Y1232 L1233 R1234 L1235 H1236 D1237 V1248 F1259 F1262 L1263 E1275 T1278 L1279 Q1280 L1293 C1296 T1305 Q1309 Q1310 L1311 L1312 K1313 T1314 L1315 F1316 G1317 T1318 ASN LEU ALA SER GLN PHE ASP GLY LEU SER SER ASN PRO SER LYS
SER GLN GLY ARG ALA GLN ARG LEU GLY SER SER SER VAL ARG P1348 G1349 L1350 A1369 S1370 L1371 ARG ASN MET VAL GLN GLN ALA GLU GLN GLU ASN ASP THR SER GLY TRP PHE ASP VAL LEU GLN GLN LYS VAL SER THR GLN LEU LYS THR ASN LEU THR SER VAL THR LYS ASN ARG ALA ASP
LYS ASN ALA ILE HIS ASN HIS ILE R1419 L1420 F1421 E1422 V1425 V1438 L1448 L1451 V1452 Q1453 L1454 R1455 V1456 N1457 Y1458 C1459 L1460 L1461 D1462 S1463 D1464 Q1465 V1466 F1467 I1468 G1469 F1470 V1471 L1472 K1473 Q1474 F1475 E1476 E1479 E1485 I1489 I1493 L1497 V1498 L1499 L1500 S1501 Y1502
E1503 ARG TYR HIS SER LYS GLN ILE I1511 G1512 I1513 P1514 K1515 I1516 I1517 Q1518 L1519 C1520 D1521 G1522 A1525 S1526 V1531 I1535 V1542 H1543 D1544 L1545 F1546 V1547 L1548 ARG GLY THR ASN LYS ALA ASP ALA G1557 K1558 E1559 L1560 E1561 T1562 Q1563 K1564 E1565 V1566 V1567 V1568 S1569 L1586 V1587 L1588
Q1589 Q1590 C1591 H1592 K1593 E1594 N1595 E1596 D1597 K1598 W1599 K1600 R1601 L1602 S1603 R1604 I1621 D1622 S1623 H1624 L1627 N1631 I1636 S1640 R1643 M1659 A1660 S1661 V1662 V1665 Q1666 I1669 S1670 G1671 I1672 L1673 L1676 Q1682 R1691 E1694 S1698 I1702 S1703 C1704
I1707 N1708 R1709 D1712 G1713 ASP SER THR SER THR LEU GLU GLU HIS SER GLU GLY LYS GLN ILE K1729 N1730 L1731 P1732 E1733 R1738 F1739 Q1742 I1746 E1749 T1753 K1754 Q1755 L1756 K1757 V1758 E1759 M1760 S1761 E1762 Q1763 Q1764 H1765 T1766 F1767 Y1768 E1771 F1783 G1786 M1787 F1788
R1789 R1790 I1791 T1792 A1793 T1796 R1797 L1798 F1799 C1804 G1805 G1806 S1807 F1808 Y1809 R1819 I1822 T1823 L1830 C1833 L1836 L1837 L1838 V1839 W1846 E1849 V1850 Q1851 Q1852 T1853 P1854 LYS ARG HIS SER LEU SER SER THR LYS LEU LEU SER PRO GLN MET SER GLY GLU GLU GLU
ASP SER ASP LEU ALA ALA LYS L1882 G1883 M1884 C1885 N1886 R1887 E1888 I1889 V1890 R1891 R1892 G1893 A1894 L1895 I1896 D1900 L1906 L1915 N1918 Q1921 D1922 S1925 L1926 S1927 H1928 E1929 P1930 P1931 V1932 Q1933 D1934 R1941 N1942 S1955 R1956 C1957 E1958 N1959 T1962 P1963 T1964 M1965 L1966 K1967


Q1971 E1974 G1975 I1976 H1977 L1978 F1997 L2000 D2005 I2006 R2010 R2011 V2012 E2013 M2014 L2015 L2016 A2017 A2018 N2019 L2020 Q2021 S2022 S2023 M2024 A2025 E2030 N2033 E2037 Y2038 L2039 Q2040 S2041 S2042 G2043 L2044 A2045 Q2046 R2047 H2048 R2057 L2060 S2061 T2062 MET GLN ASP SER LEU
SER PRO SER PRO PRO VAL SER SER HIS PRO LEU ASP GLY ASP GLY HIS VAL SER LEU GLU THR VAL SER PRO D2092 K2093 D2094 S2108 D2109 S2110 A2111 L2112 R2121 I2122 P2123 A2124 E2125 D2126 M2127 M2131 M2132 N2133 S2134 Q2156 E2162 A2163 A2164 R2165 E2166 V2167 T2168 R2171 V2172 S2173
G2174 T2175 V2176 Q2177 Q2178 L2179 P2180 A2181 V2182 H2183 H2184 A2192 E2193 P2194 A2195 A2196 Y2197 W2198 S2199 K2200 L2214 L2217 A2218 R2219 A2220 V2227 V2228 S2229 K2230 L2231 P2232 S2233 H2234 L2235 H2236 L2237 P2238 P2239 E2240 K2241 E2242 K2243 D2244 I2245 V2246 K2247 V2250 A2251 T2252 L2253 L2256 P2266 L2267
S2268 L2269 Q2272 G2286 S2289 V2290 V2291 S2292 S2293 T2294 E2295 F2296 V2297 T2298 H2299 A2300 C2301 Q2317 P2318 G2319 E2320 S2324 PRO GLU ARG ARG THR ASN THR PRO LYS ALA ILE SER GLU GLU GLU GLU GLU VAL ASP PRO ASN THR GLN N2348 P2349 K2350 Y2351 I2352 T2353 C2356 S2365
L2366 Q2367 S2368 V2369 L2370 A2371 L2372 G2373 H2374 K2375 R2376 N2377 V2380 P2381 A2382 F2383 L2384 L2387 N2390 L2398 P2399 L2400 K2413 L2414 G2415 W2416 S2417 P2418 K2419 P2420 G2421 G2422 D2423 F2424 G2425 T2426 A2427 F2428 P2429 E2434 Q2437 E2438 K2439 E2440 R2448 L2452 G2453 W2454 T2455 S2456 R2457
T2458 Q2459 F2460 E2461 E2462 T2463 W2464 A2465 T2466 L2467 L2468 G2469 V2470 L2471 VAL THR GLN PRO LEU VAL MET GLU GLN GLU GLU GLU SER PRO PRO GLU GLU ASP THR GLU R2491 T2492 Q2493 I2494 N2495 V2496 L2497 A2498 V2499 T2511 V2512 P2513 V2514 A2515 C2522 Q2526 P2527 R2528 N2529 K2530 I2546 E2551
I2554 Q2555 A2556 M2557 V2558 S2559 K2560 R2561 E2562 N2563 L2569 Y2570 Q2571 P2575 L2579 SER PRO ALA T2583 T2584 G2585 A2586 L2587 M2606 S2607 Q2612 I2615 H2616 S2617 V2618 W2619 L2620 G2621 N2622 S2623 I2624 T2625 P2626 LEU ARG GLU GLU GLU TRP ASP GLU GLU GLU GLU GLU GLU ALA ASP
ALA PRO ALA PRO SER SER SER PRO PRO THR SER PRO VAL ASN SER ARG LYS HIS ARG ALA G2661 V2662 D2663 I2664 H2665 S2666 C2667 S2668 Q2669 F2670 L2671 L2672 E2673 L2674 Y2675 S2676 R2677 W2678 I2679 L2680 PRO SER SER SER ALA ARG ARG T2688 P2689 A2690 I2691 L2692 R2698 S2699 L2700 S2704 D2705 L2706 F2707
T2708 E2709 R2710 N2711 Q2712 F2713 E2714 L2715 M2716 V2717 V2718 T2719 L2720 T2721 E2722 L2723 R2724 R2725 V2726 H2727 Y2737 L2738 V2739 A2745 A2746 A2747 V2748 L2749 G2750 M2751 D2752 K2753 A2754 V2755 A2756 E2757 P2758 R2761 L2762 H2771 L2772 P2773 S2774 R2775 V2776 L2790 L2791 D2792 D2793 T2794 A2795 K2796 Q2797 L2798 I2799
P2800 V2801 I2802 S2803 D2804 I2813 V2817 V2825 L2826 A2832 I2836 P2840 L2841 D2842 V2843 G2844 P2845 E2846 I2851 L2859 S2860 I2870 L2875 R2880 R2889 L2890 R2902 P2908 M2912 T2920 Y2923 T2924 G2925 LYS GLU LYS VAL SER PRO GLY ARG THR SER
ASP PRO ASN PRO ALA ALA PRO ASP SER E2945 S2946 V2947 I2948 P2966 R2970 L2976 P2977 Q2978 F2979 P2986 I2989 N3000 P3003 Y3004 P3005 Q3006 F3007 F3016 H3020 S3026 R3029 D3030 W3031 V3032 M3033 L3034 S3035 L3036 S3037 N3038 F3039 T3040 Q3041 R3042 A3043 P3044 V3045 A3046 M3047
A3048 T3049 W3064 A3067 L3079 E3080 Q3081 V3082 D3083 V3084 N3085 L3086 F3087 C3088 L3089 V3090 A3091 T3092 D3093 F3094 Y3095 R3096 H3097 Q3098 ILE GLU GLU GLU LEU ASP ARG ARG ALA PHE GLN SER VAL VAL LEU GLU VAL VAL ALA ALA PRO GLY SER PRO TYR HIS ARG LEU LEU THR CYS LEU ARG ASN
VAL HIS LYS VAL THR THR CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0117	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.52	20/18825 (0.1%)	0.66	27/25575 (0.1%)

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	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2925	GLY	C-O	-14.51	1.00	1.23
1	A	1713	GLY	C-O	-14.47	1.00	1.23
1	A	2680	LEU	C-O	-12.18	1.00	1.23
1	A	1503	GLU	C-O	-12.10	1.00	1.23
1	A	2471	LEU	C-O	-12.09	1.00	1.23
1	A	2062	THR	C-O	-12.08	1.00	1.23
1	A	1548	LEU	C-O	-12.08	1.00	1.23
1	A	3098	GLN	C-O	-12.07	1.00	1.23
1	A	322	GLN	C-O	-12.06	1.00	1.23
1	A	2324	SER	C-O	-12.06	1.00	1.23
1	A	1048	LEU	C-O	-12.06	1.00	1.23
1	A	402	ALA	C-O	-12.05	1.00	1.23
1	A	1102	ARG	C-O	-12.04	1.00	1.23
1	A	2579	LEU	C-O	-12.04	1.00	1.23
1	A	1318	THR	C-O	-12.03	1.00	1.23
1	A	1371	LEU	C-O	-12.03	1.00	1.23
1	A	959	LYS	C-O	-12.02	1.00	1.23
1	A	2626	PRO	C-O	-11.39	1.00	1.23
1	A	1854	PRO	C-O	-11.38	1.00	1.23
1	A	1157	PRO	C-O	-11.37	1.00	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1350	LEU	CA-CB-CG	7.76	133.16	115.30
1	A	2925	GLY	CA-C-O	-6.45	109.00	120.60
1	A	1713	GLY	CA-C-O	-6.44	109.00	120.60
1	A	852	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	1499	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	2015	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	1311	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	379	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	1048	LEU	CA-C-O	-5.35	108.86	120.10
1	A	2324	SER	CA-C-O	-5.32	108.93	120.10
1	A	1548	LEU	CA-C-O	-5.32	108.94	120.10
1	A	2062	THR	CA-C-O	-5.32	108.94	120.10
1	A	1102	ARG	CA-C-O	-5.31	108.94	120.10
1	A	2579	LEU	CA-C-O	-5.31	108.94	120.10
1	A	1503	GLU	CA-C-O	-5.30	108.98	120.10
1	A	2471	LEU	CA-C-O	-5.29	108.99	120.10
1	A	1371	LEU	CA-C-O	-5.29	108.99	120.10
1	A	2680	LEU	CA-C-O	-5.29	108.99	120.10
1	A	1318	THR	CA-C-O	-5.29	108.99	120.10
1	A	3098	GLN	CA-C-O	-5.29	108.99	120.10
1	A	402	ALA	CA-C-O	-5.28	109.01	120.10
1	A	959	LYS	CA-C-O	-5.27	109.03	120.10
1	A	322	GLN	CA-C-O	-5.25	109.08	120.10
1	A	2790	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	1915	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	998	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	865	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1045	VAL	Peptide
1	A	1314	THR	Peptide
1	A	1838	LEU	Peptide
1	A	2268	SER	Peptide
1	A	296	VAL	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	18465	0	18885	546	0
All	All	18465	0	18885	546	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 15.

All (546) 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:1676:LEU:HB3	1:A:1767:PHE:CZ	1.30	1.59
1:A:1702:ILE:HD12	1:A:1746:ILE:CD1	1.22	1.58
1:A:1662:VAL:CG1	1:A:1759:GLU:HB2	1.29	1.57
1:A:1854:PRO:HD2	1:A:2317:GLN:NE2	1.27	1.48
1:A:1627:LEU:CD1	1:A:1764:GLN:HA	1.44	1.47
1:A:1627:LEU:CD1	1:A:1764:GLN:CA	1.91	1.47
1:A:808:ARG:HG2	1:A:2691:ILE:CD1	1.46	1.45
1:A:1627:LEU:HD12	1:A:1764:GLN:N	1.20	1.45
1:A:2033:ASN:O	1:A:2110:SER:CB	1.67	1.42
1:A:1702:ILE:CD1	1:A:1746:ILE:CD1	1.93	1.41
1:A:1702:ILE:CD1	1:A:1746:ILE:HD13	1.45	1.41
1:A:801:ALA:CB	1:A:2439:LYS:NZ	1.87	1.38
1:A:1627:LEU:HD12	1:A:1764:GLN:CA	1.52	1.37
1:A:801:ALA:HB1	1:A:2439:LYS:NZ	1.33	1.37
1:A:882:LYS:HZ2	1:A:1882:LEU:N	1.17	1.37
1:A:1854:PRO:HD2	1:A:2317:GLN:CD	1.43	1.36
1:A:2046:GLN:HE22	1:A:3006:GLN:N	1.26	1.34
1:A:1676:LEU:CB	1:A:1767:PHE:HZ	1.43	1.29
1:A:1702:ILE:O	1:A:1746:ILE:HD11	1.20	1.28
1:A:2037:GLU:OE1	1:A:2112:LEU:HG	1.21	1.28
1:A:1662:VAL:CG1	1:A:1759:GLU:CB	2.12	1.27
1:A:1854:PRO:CD	1:A:2317:GLN:NE2	1.98	1.26
1:A:882:LYS:NZ	1:A:1882:LEU:N	1.84	1.25
1:A:1854:PRO:CD	1:A:2317:GLN:CD	2.05	1.25
1:A:2033:ASN:CB	1:A:2109:ASP:HA	1.66	1.24
1:A:894:THR:CG2	1:A:2776:VAL:HG21	1.68	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:GLN:NE2	1:A:3006:GLN:H	1.37	1.23
1:A:2033:ASN:O	1:A:2110:SER:HB2	1.25	1.20
1:A:2033:ASN:O	1:A:2110:SER:CA	1.89	1.20
1:A:1676:LEU:HD13	1:A:1771:GLU:CD	1.59	1.19
1:A:1627:LEU:CD1	1:A:1764:GLN:CG	2.19	1.19
1:A:1662:VAL:HG12	1:A:1759:GLU:CB	1.72	1.18
1:A:2033:ASN:O	1:A:2110:SER:N	1.74	1.18
1:A:801:ALA:CB	1:A:2439:LYS:HZ2	1.46	1.18
1:A:1676:LEU:CB	1:A:1767:PHE:CZ	2.20	1.17
1:A:1676:LEU:HD13	1:A:1771:GLU:CG	1.75	1.17
1:A:791:ARG:NH1	1:A:2414:LEU:HD21	1.59	1.16
1:A:802:ASP:OD2	1:A:2438:GLU:HG3	1.42	1.16
1:A:1853:THR:HG22	1:A:2317:GLN:CB	1.76	1.16
1:A:1704:CYS:SG	1:A:1809:TYR:CE1	2.39	1.15
1:A:1670:SER:HB3	1:A:1764:GLN:CD	1.67	1.15
1:A:1627:LEU:HD11	1:A:1764:GLN:CG	1.77	1.14
1:A:1702:ILE:HD13	1:A:1746:ILE:HD13	1.18	1.13
1:A:1666:GLN:N	1:A:1759:GLU:OE2	1.82	1.13
1:A:1670:SER:CB	1:A:1764:GLN:NE2	2.11	1.13
1:A:1627:LEU:HG	1:A:1764:GLN:HG3	1.23	1.11
1:A:1662:VAL:HG13	1:A:1759:GLU:HB2	1.33	1.11
1:A:2033:ASN:HB3	1:A:2109:ASP:CA	1.80	1.10
1:A:808:ARG:CG	1:A:2691:ILE:CD1	2.29	1.10
1:A:1350:LEU:HD11	1:A:1885:CYS:O	1.49	1.10
1:A:1669:ILE:CD1	1:A:1754:LYS:HZ2	1.65	1.10
1:A:2046:GLN:HB3	1:A:3003:PRO:O	1.52	1.09
1:A:1669:ILE:CD1	1:A:1754:LYS:NZ	2.16	1.09
1:A:882:LYS:HD2	1:A:1882:LEU:N	1.68	1.09
1:A:1670:SER:CB	1:A:1764:GLN:CD	2.21	1.08
1:A:801:ALA:CA	1:A:2439:LYS:NZ	2.15	1.08
1:A:812:LYS:CE	1:A:2691:ILE:HG13	1.81	1.07
1:A:1627:LEU:CD1	1:A:1764:GLN:N	2.09	1.07
1:A:1955:SER:O	1:A:2381:PRO:HB3	1.54	1.07
1:A:1673:LEU:HD21	1:A:1768:TYR:CA	1.83	1.06
1:A:882:LYS:CD	1:A:1882:LEU:N	2.19	1.06
1:A:1673:LEU:HD21	1:A:1768:TYR:HA	1.09	1.06
1:A:1670:SER:HB2	1:A:1764:GLN:NE2	1.71	1.05
1:A:1627:LEU:HD11	1:A:1764:GLN:HG2	1.33	1.05
1:A:1676:LEU:HD13	1:A:1771:GLU:OE2	1.57	1.04
1:A:1627:LEU:CG	1:A:1764:GLN:HG3	1.87	1.04
1:A:1854:PRO:C	1:A:2317:GLN:H	1.59	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:VAL:HG12	1:A:1759:GLU:HB2	1.22	1.04
1:A:1627:LEU:HD11	1:A:1764:GLN:HA	1.21	1.03
1:A:801:ALA:HA	1:A:2439:LYS:HZ1	1.20	1.03
1:A:812:LYS:HD3	1:A:2690:ALA:CA	1.87	1.03
1:A:1676:LEU:CD1	1:A:1771:GLU:HG2	1.87	1.03
1:A:804:ILE:N	1:A:2493:GLN:HE22	1.49	1.03
1:A:1631:ASN:ND2	1:A:1763:GLN:NE2	2.06	1.03
1:A:1627:LEU:HG	1:A:1764:GLN:CG	1.88	1.03
1:A:1702:ILE:CD1	1:A:1746:ILE:HD12	1.75	1.02
1:A:2043:GLY:H	1:A:2966:PRO:HB3	1.23	1.02
1:A:812:LYS:HD3	1:A:2690:ALA:HB3	1.39	1.02
1:A:1673:LEU:HB3	1:A:1767:PHE:HB3	1.35	1.02
1:A:1672:ILE:O	1:A:1771:GLU:OE2	1.78	1.02
1:A:959:LYS:C	1:A:1766:THR:HG21	1.79	1.02
1:A:1676:LEU:HD13	1:A:1771:GLU:HG2	1.38	1.01
1:A:1627:LEU:CG	1:A:1764:GLN:CG	2.38	1.00
1:A:812:LYS:HD3	1:A:2690:ALA:CB	1.91	1.00
1:A:801:ALA:CA	1:A:2439:LYS:HZ1	1.71	1.00
1:A:808:ARG:HG2	1:A:2691:ILE:HD11	1.02	1.00
1:A:1853:THR:HG22	1:A:2317:GLN:HB3	1.45	0.99
1:A:1627:LEU:HD11	1:A:1764:GLN:CB	1.92	0.99
1:A:1662:VAL:HG11	1:A:1759:GLU:HB2	1.44	0.99
1:A:2033:ASN:HB3	1:A:2109:ASP:HA	1.01	0.98
1:A:1627:LEU:HB2	1:A:1763:GLN:HB3	1.41	0.98
1:A:808:ARG:CG	1:A:2691:ILE:HD13	1.93	0.98
1:A:808:ARG:CG	1:A:2691:ILE:HD11	1.91	0.97
1:A:1854:PRO:CG	1:A:2317:GLN:NE2	2.27	0.97
1:A:894:THR:HG23	1:A:2776:VAL:HG21	1.45	0.97
1:A:1665:VAL:HG12	1:A:1754:LYS:HZ3	1.30	0.96
1:A:1627:LEU:HD12	1:A:1763:GLN:C	1.86	0.96
1:A:1676:LEU:HB3	1:A:1767:PHE:CE2	2.00	0.95
1:A:1958:GLU:CD	1:A:2381:PRO:C	2.24	0.95
1:A:2060:LEU:CD2	1:A:3080:GLU:OE1	2.14	0.95
1:A:1627:LEU:CD1	1:A:1764:GLN:CB	2.43	0.95
1:A:812:LYS:CD	1:A:2690:ALA:HB3	1.95	0.94
1:A:808:ARG:HG2	1:A:2691:ILE:HD13	1.46	0.94
1:A:1627:LEU:HD11	1:A:1764:GLN:CA	1.75	0.94
1:A:1676:LEU:CA	1:A:1767:PHE:HZ	1.80	0.94
1:A:2046:GLN:NE2	1:A:3006:GLN:HB2	1.83	0.94
1:A:1702:ILE:HD12	1:A:1746:ILE:HD12	0.96	0.93
1:A:2046:GLN:NE2	1:A:3006:GLN:CB	2.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1673:LEU:CD1	1:A:1767:PHE:CG	2.39	0.93
1:A:1669:ILE:HD11	1:A:1754:LYS:NZ	1.82	0.93
1:A:1702:ILE:O	1:A:1746:ILE:CD1	2.15	0.92
1:A:802:ASP:OD2	1:A:2438:GLU:CG	2.17	0.92
1:A:801:ALA:HB1	1:A:2439:LYS:CE	1.98	0.92
1:A:801:ALA:CB	1:A:2439:LYS:HZ1	1.80	0.91
1:A:1704:CYS:SG	1:A:1809:TYR:CD1	2.62	0.91
1:A:892:HIS:NE2	1:A:2698:ARG:NH1	2.18	0.91
1:A:1853:THR:CG2	1:A:2317:GLN:HB3	1.99	0.91
1:A:2037:GLU:OE1	1:A:2112:LEU:CG	2.16	0.90
1:A:2042:SER:HB3	1:A:2970:ARG:HH22	1.36	0.90
1:A:1854:PRO:HD2	1:A:2317:GLN:OE1	1.70	0.90
1:A:805:PRO:C	1:A:2493:GLN:HG3	1.81	0.90
1:A:1673:LEU:CD2	1:A:1768:TYR:HA	1.99	0.90
1:A:1854:PRO:HD2	1:A:2317:GLN:HE22	1.22	0.90
1:A:882:LYS:CE	1:A:1882:LEU:N	2.36	0.89
1:A:1624:HIS:HB2	1:A:1762:GLU:H	1.37	0.89
1:A:2037:GLU:HG3	1:A:2110:SER:CB	1.66	0.89
1:A:1666:GLN:HG3	1:A:1760:MET:HA	1.53	0.88
1:A:1627:LEU:HD13	1:A:1764:GLN:HA	1.56	0.88
1:A:791:ARG:NH1	1:A:2414:LEU:CD2	2.35	0.88
1:A:1704:CYS:HG	1:A:1809:TYR:HE1	1.16	0.88
1:A:1621:ILE:CG2	1:A:1764:GLN:HE21	1.85	0.88
1:A:1627:LEU:O	1:A:1763:GLN:CD	2.12	0.87
1:A:2043:GLY:N	1:A:2966:PRO:HB3	1.89	0.87
1:A:802:ASP:OD1	1:A:2439:LYS:CB	2.23	0.87
1:A:1627:LEU:CD1	1:A:1764:GLN:HG2	1.93	0.87
1:A:801:ALA:HB3	1:A:2440:GLU:HG3	1.55	0.86
1:A:1350:LEU:HG	1:A:1885:CYS:HB3	1.57	0.86
1:A:1631:ASN:ND2	1:A:1763:GLN:HE22	1.70	0.86
1:A:2043:GLY:H	1:A:2966:PRO:CB	1.87	0.86
1:A:803:CYS:C	1:A:2493:GLN:HE22	1.79	0.85
1:A:808:ARG:O	1:A:2691:ILE:HD11	1.75	0.85
1:A:1673:LEU:HD13	1:A:1767:PHE:CG	2.08	0.85
1:A:1670:SER:HB3	1:A:1764:GLN:OE1	1.76	0.85
1:A:1627:LEU:CD1	1:A:1763:GLN:C	2.43	0.85
1:A:2042:SER:HB3	1:A:2970:ARG:NH2	1.92	0.85
1:A:801:ALA:HB1	1:A:2439:LYS:HZ2	0.68	0.84
1:A:805:PRO:HB3	1:A:2493:GLN:CA	2.06	0.84
1:A:1662:VAL:HG13	1:A:1759:GLU:CG	2.07	0.84
1:A:1853:THR:HG22	1:A:2317:GLN:HB2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1665:VAL:HG12	1:A:1754:LYS:NZ	1.92	0.84
1:A:1621:ILE:HB	1:A:1764:GLN:HE22	1.43	0.83
1:A:812:LYS:CE	1:A:2691:ILE:CG1	2.56	0.83
1:A:1627:LEU:O	1:A:1763:GLN:NE2	2.12	0.83
1:A:805:PRO:HB3	1:A:2493:GLN:HA	1.61	0.83
1:A:1673:LEU:HD13	1:A:1767:PHE:CD2	2.14	0.83
1:A:1958:GLU:OE2	1:A:2381:PRO:HA	1.79	0.83
1:A:806:LEU:HD11	1:A:2491:ARG:N	1.93	0.82
1:A:1955:SER:O	1:A:2381:PRO:CB	2.26	0.82
1:A:1627:LEU:CG	1:A:1764:GLN:HG2	2.08	0.82
1:A:812:LYS:HE3	1:A:2691:ILE:HG13	1.58	0.82
1:A:1958:GLU:OE2	1:A:2381:PRO:C	2.17	0.82
1:A:957:TYR:CD1	1:A:1756:LEU:CD2	2.54	0.81
1:A:894:THR:HG21	1:A:2776:VAL:HG21	1.61	0.81
1:A:806:LEU:H	1:A:2493:GLN:NE2	1.78	0.81
1:A:1350:LEU:CG	1:A:1885:CYS:HB3	2.11	0.81
1:A:2046:GLN:HB3	1:A:3004:TYR:CA	2.07	0.81
1:A:894:THR:CG2	1:A:2776:VAL:CG2	2.57	0.81
1:A:1669:ILE:HD12	1:A:1754:LYS:NZ	1.93	0.81
1:A:1854:PRO:HG2	1:A:2317:GLN:NE2	1.96	0.81
1:A:801:ALA:CB	1:A:2439:LYS:CE	2.48	0.80
1:A:1665:VAL:HG11	1:A:1754:LYS:HE2	1.63	0.80
1:A:1673:LEU:CD1	1:A:1767:PHE:CD2	2.64	0.80
1:A:1631:ASN:HD21	1:A:1763:GLN:HE22	1.29	0.80
1:A:802:ASP:OD1	1:A:2439:LYS:N	2.14	0.80
1:A:1854:PRO:CD	1:A:2317:GLN:OE1	2.27	0.80
1:A:1627:LEU:HD13	1:A:1763:GLN:O	1.82	0.79
1:A:1621:ILE:HB	1:A:1764:GLN:NE2	1.97	0.78
1:A:1631:ASN:HD22	1:A:1763:GLN:NE2	1.81	0.78
1:A:1673:LEU:CB	1:A:1767:PHE:HB3	2.12	0.78
1:A:1662:VAL:CG1	1:A:1759:GLU:CG	2.60	0.78
1:A:1662:VAL:HG12	1:A:1759:GLU:CA	2.13	0.78
1:A:2060:LEU:HD22	1:A:3080:GLU:OE1	1.84	0.78
1:A:893:TYR:OH	1:A:2772:LEU:HB3	1.84	0.78
1:A:1670:SER:HB2	1:A:1764:GLN:CD	1.99	0.78
1:A:1853:THR:CG2	1:A:2317:GLN:CB	2.56	0.78
1:A:1665:VAL:CG1	1:A:1754:LYS:NZ	2.47	0.77
1:A:812:LYS:CD	1:A:2691:ILE:HG13	2.14	0.77
1:A:1704:CYS:H	1:A:1742:GLN:NE2	1.82	0.77
1:A:1676:LEU:CD2	1:A:1771:GLU:HG2	2.15	0.76
1:A:957:TYR:CD1	1:A:1756:LEU:HD21	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:GLN:HE22	1:A:3006:GLN:CA	1.98	0.76
1:A:1702:ILE:HD13	1:A:1746:ILE:HG21	1.67	0.76
1:A:1958:GLU:OE2	1:A:2381:PRO:CA	2.33	0.76
1:A:809:LYS:HD3	1:A:2492:THR:HG21	1.66	0.76
1:A:2060:LEU:HD21	1:A:3080:GLU:OE1	1.84	0.76
1:A:812:LYS:HD3	1:A:2690:ALA:N	2.01	0.76
1:A:806:LEU:CD1	1:A:2491:ARG:N	2.49	0.75
1:A:2046:GLN:O	1:A:3003:PRO:O	2.03	0.75
1:A:890:ALA:HB1	1:A:2737:TYR:HE2	1.51	0.75
1:A:1627:LEU:CD1	1:A:1764:GLN:HG3	2.03	0.75
1:A:2046:GLN:NE2	1:A:3006:GLN:N	2.10	0.75
1:A:1853:THR:C	1:A:2317:GLN:OE1	2.22	0.75
1:A:1662:VAL:HG13	1:A:1759:GLU:CB	1.96	0.74
1:A:802:ASP:OD1	1:A:2439:LYS:HB2	1.86	0.74
1:A:802:ASP:CG	1:A:2439:LYS:H	1.90	0.74
1:A:1854:PRO:N	1:A:2317:GLN:CD	2.41	0.74
1:A:1854:PRO:C	1:A:2317:GLN:HB2	2.09	0.73
1:A:2046:GLN:HB3	1:A:3003:PRO:C	2.08	0.73
1:A:812:LYS:CG	1:A:2690:ALA:HB3	2.19	0.73
1:A:809:LYS:HD3	1:A:2492:THR:CG2	2.19	0.73
1:A:1666:GLN:HG3	1:A:1760:MET:CA	2.14	0.73
1:A:809:LYS:CD	1:A:2492:THR:HG21	2.19	0.72
1:A:791:ARG:HH11	1:A:2414:LEU:CD2	2.03	0.72
1:A:1666:GLN:OE1	1:A:1759:GLU:HA	1.90	0.72
1:A:808:ARG:CD	1:A:2691:ILE:HD13	2.19	0.72
1:A:1676:LEU:CD1	1:A:1771:GLU:OE2	2.35	0.72
1:A:2030:GLU:HB2	1:A:2108:SER:OG	1.89	0.71
1:A:1627:LEU:HB2	1:A:1763:GLN:CB	2.18	0.71
1:A:2033:ASN:C	1:A:2110:SER:HB2	2.10	0.71
1:A:1672:ILE:HG22	1:A:1771:GLU:OE1	1.91	0.71
1:A:1854:PRO:N	1:A:2317:GLN:OE1	2.22	0.71
1:A:1631:ASN:HD21	1:A:1763:GLN:NE2	1.87	0.71
1:A:806:LEU:N	1:A:2493:GLN:NE2	2.36	0.70
1:A:1621:ILE:CG2	1:A:1764:GLN:NE2	2.53	0.70
1:A:812:LYS:HE3	1:A:2691:ILE:CG1	2.20	0.70
1:A:1676:LEU:CD1	1:A:1771:GLU:CG	2.54	0.70
1:A:2046:GLN:CB	1:A:3003:PRO:O	2.36	0.70
1:A:1621:ILE:CB	1:A:1764:GLN:NE2	2.55	0.70
1:A:2046:GLN:HB2	1:A:3004:TYR:CD1	2.26	0.70
1:A:892:HIS:CE1	1:A:2698:ARG:HH11	2.08	0.69
1:A:1076:PRO:HB2	1:A:1235:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1621:ILE:HG22	1:A:1764:GLN:HE21	1.57	0.69
1:A:804:ILE:N	1:A:2493:GLN:NE2	2.32	0.69
1:A:1676:LEU:HD22	1:A:1771:GLU:HG2	1.73	0.69
1:A:1704:CYS:SG	1:A:1809:TYR:HE1	1.99	0.68
1:A:1958:GLU:OE1	1:A:2381:PRO:C	2.28	0.68
1:A:1676:LEU:CA	1:A:1767:PHE:CZ	2.70	0.68
1:A:1669:ILE:HD11	1:A:1754:LYS:HZ1	1.58	0.68
1:A:1702:ILE:HD12	1:A:1746:ILE:HD11	1.63	0.68
1:A:1854:PRO:CG	1:A:2317:GLN:CD	2.60	0.68
1:A:882:LYS:HZ2	1:A:1882:LEU:CA	2.05	0.68
1:A:2046:GLN:HE21	1:A:3006:GLN:HB2	1.55	0.68
1:A:1662:VAL:O	1:A:1759:GLU:CD	2.13	0.67
1:A:812:LYS:HD2	1:A:2691:ILE:HG13	1.75	0.67
1:A:1666:GLN:HB2	1:A:1759:GLU:CG	2.24	0.67
1:A:1854:PRO:C	1:A:2320:GLU:OE1	2.33	0.67
1:A:2033:ASN:CB	1:A:2109:ASP:CA	2.56	0.67
1:A:890:ALA:HB1	1:A:2737:TYR:CE2	2.30	0.67
1:A:894:THR:N	1:A:2773:PRO:HB3	2.10	0.67
1:A:1854:PRO:C	1:A:2317:GLN:CB	2.63	0.67
1:A:801:ALA:CB	1:A:2440:GLU:HG3	2.24	0.67
1:A:1631:ASN:ND2	1:A:1763:GLN:HE21	1.93	0.67
1:A:799:SER:CB	1:A:2440:GLU:OE1	2.41	0.66
1:A:1631:ASN:HD22	1:A:1763:GLN:HE21	1.42	0.66
1:A:1673:LEU:CD2	1:A:1768:TYR:CA	2.68	0.66
1:A:809:LYS:HD3	1:A:2492:THR:OG1	1.96	0.66
1:A:1627:LEU:HD12	1:A:1764:GLN:CB	2.16	0.66
1:A:957:TYR:C	1:A:1762:GLU:OE2	2.35	0.65
1:A:791:ARG:CZ	1:A:2414:LEU:HD21	2.26	0.65
1:A:799:SER:HB2	1:A:2440:GLU:OE1	1.96	0.65
1:A:308:LEU:HD21	1:A:368:VAL:HA	1.80	0.64
1:A:1958:GLU:OE2	1:A:2380:VAL:O	2.14	0.64
1:A:808:ARG:O	1:A:2691:ILE:CD1	2.46	0.63
1:A:1621:ILE:O	1:A:1764:GLN:NE2	2.30	0.63
1:A:1676:LEU:CD1	1:A:1771:GLU:CD	2.53	0.63
1:A:893:TYR:OH	1:A:2772:LEU:CA	2.47	0.63
1:A:1665:VAL:CG1	1:A:1754:LYS:HE2	2.30	0.62
1:A:2060:LEU:CD1	1:A:3080:GLU:OE1	2.48	0.62
1:A:2832:ALA:HB1	1:A:2851:ILE:HD13	1.82	0.62
1:A:812:LYS:HD3	1:A:2690:ALA:C	2.10	0.61
1:A:1707:ILE:CD1	1:A:1746:ILE:HG12	2.31	0.61
1:A:2219:ARG:HH21	1:A:2269:LEU:HD11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1676:LEU:C	1:A:1767:PHE:CZ	2.73	0.61
1:A:2033:ASN:C	1:A:2110:SER:N	2.53	0.61
1:A:2037:GLU:HG3	1:A:2110:SER:HB3	1.75	0.61
1:A:2522:CYS:SG	1:A:2563:ASN:ND2	2.74	0.60
1:A:803:CYS:C	1:A:2493:GLN:NE2	2.52	0.60
1:A:1350:LEU:CD1	1:A:1885:CYS:HB3	2.32	0.60
1:A:2046:GLN:HB2	1:A:3004:TYR:CG	2.18	0.60
1:A:2046:GLN:HE22	1:A:3006:GLN:CB	2.05	0.60
1:A:878:PHE:HE1	1:A:1882:LEU:HB2	1.66	0.60
1:A:1707:ILE:HD11	1:A:1746:ILE:HG12	1.84	0.60
1:A:1854:PRO:HG2	1:A:2317:GLN:HG3	1.82	0.60
1:A:894:THR:HG21	1:A:2776:VAL:HG11	1.84	0.60
1:A:959:LYS:C	1:A:1766:THR:CG2	2.54	0.60
1:A:1669:ILE:HD12	1:A:1754:LYS:HZ3	1.66	0.60
1:A:1672:ILE:O	1:A:1767:PHE:HE2	1.85	0.60
1:A:1854:PRO:C	1:A:2317:GLN:N	2.42	0.60
1:A:2042:SER:CB	1:A:2970:ARG:NH2	2.64	0.60
1:A:1369:ALA:O	1:A:1682:GLN:NE2	2.34	0.60
1:A:861:ARG:NH1	1:A:914:ASP:OD1	2.36	0.59
1:A:928:ILE:HD11	1:A:1027:LEU:HB3	1.84	0.59
1:A:2233:SER:HA	1:A:2236:HIS:HD2	1.66	0.59
1:A:978:ARG:O	1:A:1313:LYS:NZ	2.35	0.59
1:A:1666:GLN:HB2	1:A:1759:GLU:HG3	1.84	0.59
1:A:1854:PRO:C	1:A:2317:GLN:HG3	2.22	0.59
1:A:893:TYR:OH	1:A:2772:LEU:CB	2.51	0.58
1:A:1958:GLU:CD	1:A:2381:PRO:O	2.40	0.58
1:A:173:ASN:OD1	1:A:215:ARG:NH2	2.35	0.58
1:A:1666:GLN:OE1	1:A:1759:GLU:CA	2.51	0.58
1:A:2030:GLU:O	1:A:2108:SER:OG	2.20	0.58
1:A:2033:ASN:HB2	1:A:2109:ASP:HA	1.73	0.58
1:A:1662:VAL:HG12	1:A:1759:GLU:CG	2.31	0.58
1:A:1676:LEU:C	1:A:1767:PHE:HZ	2.05	0.58
1:A:878:PHE:CE1	1:A:1882:LEU:HB2	2.39	0.58
1:A:1666:GLN:HB2	1:A:1759:GLU:CD	2.23	0.58
1:A:2448:ARG:O	1:A:2452:LEU:HB2	2.04	0.58
1:A:1489:ILE:HG12	1:A:1493:ILE:HG13	1.85	0.58
1:A:2060:LEU:HD22	1:A:3080:GLU:CD	2.24	0.58
1:A:2030:GLU:CA	1:A:2108:SER:OG	2.52	0.58
1:A:808:ARG:C	1:A:2691:ILE:HD11	2.23	0.58
1:A:920:ARG:HD2	1:A:1020:GLY:HA3	1.86	0.57
1:A:1673:LEU:HD21	1:A:1768:TYR:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1665:VAL:CG1	1:A:1754:LYS:CE	2.83	0.57
1:A:2624:ILE:HG21	1:A:2710:ARG:HB2	1.86	0.57
1:A:199:ARG:NH2	1:A:238:PHE:O	2.38	0.57
1:A:2272:GLN:HE21	1:A:2387:LEU:HD11	1.71	0.56
1:A:1676:LEU:HD22	1:A:1771:GLU:CG	2.34	0.56
1:A:2214:LEU:HD22	1:A:2252:THR:HG22	1.86	0.56
1:A:2511:THR:HB	1:A:2515:ALA:HA	1.87	0.56
1:A:689:LEU:HB2	1:A:752:TYR:HE2	1.70	0.56
1:A:2037:GLU:CD	1:A:2112:LEU:N	2.57	0.56
1:A:2256:LEU:HD13	1:A:2266:PRO:HG2	1.87	0.56
1:A:2365:SER:O	1:A:2369:VAL:N	2.37	0.56
1:A:1350:LEU:CD1	1:A:1885:CYS:O	2.39	0.55
1:A:1854:PRO:HG2	1:A:2317:GLN:HE21	1.69	0.55
1:A:1974:GLU:O	1:A:2011:ARG:NH1	2.39	0.55
1:A:1783:PHE:HB3	1:A:1838:LEU:HD22	1.87	0.55
1:A:808:ARG:HD2	1:A:2691:ILE:HD13	1.86	0.55
1:A:812:LYS:HG2	1:A:2690:ALA:HB3	1.88	0.55
1:A:857:TYR:HD2	1:A:860:VAL:HG23	1.71	0.55
1:A:1854:PRO:HG2	1:A:2317:GLN:CG	2.36	0.55
1:A:2037:GLU:CG	1:A:2110:SER:CB	2.47	0.55
1:A:2836:ILE:HD11	1:A:2851:ILE:HD12	1.89	0.55
1:A:1621:ILE:HG22	1:A:1764:GLN:NE2	2.18	0.55
1:A:1704:CYS:O	1:A:1708:ASN:ND2	2.40	0.55
1:A:686:ALA:HB2	1:A:730:LEU:HD11	1.90	0.54
1:A:2030:GLU:CB	1:A:2108:SER:OG	2.54	0.54
1:A:1854:PRO:HG2	1:A:2317:GLN:CD	2.27	0.54
1:A:293:GLY:HA2	1:A:296:VAL:HB	1.90	0.54
1:A:1900:ASP:HB2	1:A:1931:PRO:HB3	1.89	0.54
1:A:354:TYR:OH	1:A:680:CYS:SG	2.65	0.54
1:A:791:ARG:HH11	1:A:2414:LEU:CG	2.21	0.54
1:A:1704:CYS:CB	1:A:1809:TYR:CE1	2.91	0.54
1:A:882:LYS:CG	1:A:1882:LEU:N	2.72	0.53
1:A:1997:PHE:HB2	1:A:2000:LEU:HB2	1.90	0.53
1:A:1669:ILE:HD13	1:A:1754:LYS:HZ2	1.64	0.53
1:A:934:LEU:HD12	1:A:997:ASN:HB3	1.90	0.53
1:A:2044:LEU:HD12	1:A:2966:PRO:HG2	1.91	0.53
1:A:1275:GLU:OE2	1:A:1310:GLN:NE2	2.42	0.53
1:A:1704:CYS:HB2	1:A:1809:TYR:CD1	2.43	0.53
1:A:1733:GLU:HG2	1:A:1790:ARG:HB3	1.89	0.53
1:A:2709:GLU:HG2	1:A:2711:ASN:H	1.74	0.53
1:A:802:ASP:OD1	1:A:2439:LYS:HB3	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:VAL:HG12	1:A:1759:GLU:HA	1.88	0.53
1:A:1665:VAL:N	1:A:1759:GLU:OE2	2.41	0.53
1:A:1854:PRO:C	1:A:2317:GLN:CG	2.75	0.53
1:A:1958:GLU:OE1	1:A:2381:PRO:O	2.27	0.52
1:A:2817:VAL:HG11	1:A:2870:ILE:HG21	1.91	0.52
1:A:1749:GLU:O	1:A:1753:THR:OG1	2.28	0.52
1:A:1799:PHE:HD2	1:A:1839:VAL:HG11	1.75	0.52
1:A:1958:GLU:CD	1:A:2382:ALA:N	2.59	0.52
1:A:1975:GLY:HA2	1:A:2011:ARG:HH12	1.75	0.52
1:A:1350:LEU:HD11	1:A:1885:CYS:C	2.28	0.52
1:A:957:TYR:HD1	1:A:1756:LEU:HD21	1.72	0.52
1:A:1623:SER:C	1:A:1761:SER:OG	2.49	0.52
1:A:2615:ILE:HD13	1:A:2747:ALA:HB1	1.92	0.52
1:A:1672:ILE:O	1:A:1767:PHE:CE2	2.63	0.51
1:A:801:ALA:HA	1:A:2439:LYS:NZ	1.87	0.51
1:A:2551:GLU:HA	1:A:2554:ILE:HD12	1.92	0.51
1:A:1077:LEU:HD21	1:A:1234:ARG:HB3	1.92	0.51
1:A:808:ARG:CB	1:A:2691:ILE:CD1	2.87	0.51
1:A:2005:ASP:OD2	1:A:2048:HIS:ND1	2.44	0.51
1:A:808:ARG:C	1:A:2691:ILE:CD1	2.80	0.51
1:A:395:GLY:HA3	1:A:399:GLN:HE22	1.76	0.50
1:A:791:ARG:HH11	1:A:2414:LEU:HG	1.76	0.50
1:A:1666:GLN:OE1	1:A:1758:VAL:O	2.28	0.50
1:A:2033:ASN:HB3	1:A:2109:ASP:C	2.31	0.50
1:A:2046:GLN:HE22	1:A:3006:GLN:H	0.59	0.50
1:A:205:LEU:O	1:A:209:LEU:N	2.43	0.50
1:A:291:LEU:HB3	1:A:310:VAL:HG13	1.94	0.50
1:A:3080:GLU:H	1:A:3083:ASP:HB2	1.76	0.50
1:A:2046:GLN:HB3	1:A:3004:TYR:N	2.26	0.50
1:A:1350:LEU:HD11	1:A:1885:CYS:HB3	1.94	0.50
1:A:2384:LEU:HD23	1:A:2387:LEU:HD12	1.93	0.50
1:A:944:ASP:HB2	1:A:947:VAL:HG23	1.93	0.50
1:A:791:ARG:NH1	1:A:2414:LEU:CG	2.73	0.50
1:A:1702:ILE:HD13	1:A:1746:ILE:CD1	1.96	0.50
1:A:2704:SER:HA	1:A:2707:PHE:HD2	1.76	0.50
1:A:1918:ASN:HD21	1:A:2318:PRO:HD2	1.76	0.49
1:A:1083:GLN:HB3	1:A:1262:PHE:HD1	1.77	0.49
1:A:2530:LYS:O	1:A:2880:ARG:NH2	2.35	0.49
1:A:1906:LEU:HD12	1:A:1942:ASN:HD21	1.77	0.49
1:A:1627:LEU:HD12	1:A:1764:GLN:CG	2.29	0.49
1:A:1589:GLN:HE21	1:A:1636:ILE:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1704:CYS:CB	1:A:1742:GLN:HE21	2.26	0.49
1:A:1670:SER:OG	1:A:1764:GLN:NE2	2.44	0.49
1:A:1698:SER:O	1:A:1739:PHE:CE1	2.65	0.49
1:A:893:TYR:OH	1:A:2772:LEU:N	2.46	0.48
1:A:1665:VAL:C	1:A:1759:GLU:OE2	2.46	0.48
1:A:145:GLU:HB3	1:A:1248:VAL:HG13	1.95	0.48
1:A:2040:GLN:NE2	1:A:3006:GLN:OE1	2.46	0.48
1:A:296:VAL:HG22	1:A:297:PRO:HD3	1.96	0.48
1:A:2060:LEU:CD2	1:A:3080:GLU:CD	2.80	0.48
1:A:167:TYR:CZ	1:A:204:ASN:HB3	2.49	0.48
1:A:1421:PHE:O	1:A:1425:VAL:N	2.43	0.48
1:A:809:LYS:HD2	1:A:2492:THR:HG21	1.95	0.48
1:A:356:LEU:O	1:A:360:HIS:ND1	2.39	0.48
1:A:1958:GLU:OE2	1:A:2382:ALA:N	2.46	0.48
1:A:350:LEU:HB3	1:A:387:LEU:HD12	1.95	0.48
1:A:2365:SER:HB2	1:A:2369:VAL:HB	1.95	0.47
1:A:1704:CYS:CB	1:A:1809:TYR:CD1	2.97	0.47
1:A:2039:LEU:HB3	1:A:2045:ALA:HB2	1.94	0.47
1:A:2123:PRO:HG3	1:A:3064:TRP:HH2	1.79	0.47
1:A:252:ILE:HA	1:A:255:LEU:HD23	1.96	0.47
1:A:275:GLN:HE21	1:A:320:LEU:HD21	1.79	0.47
1:A:1531:VAL:HA	1:A:1535:ILE:HD12	1.95	0.47
1:A:1921:GLN:HG3	1:A:1956:ARG:HH11	1.79	0.47
1:A:2121:ARG:HH11	1:A:3067:ALA:HB2	1.79	0.47
1:A:1676:LEU:HD11	1:A:1771:GLU:HG2	1.89	0.47
1:A:2037:GLU:HG2	1:A:2111:ALA:HA	1.66	0.47
1:A:2471:LEU:HD22	1:A:2678:TRP:HH2	1.80	0.47
1:A:1078:ASP:OD1	1:A:1078:ASP:N	2.44	0.47
1:A:2046:GLN:NE2	1:A:3006:GLN:HB3	2.25	0.47
1:A:2813:ILE:HG22	1:A:2817:VAL:HG22	1.95	0.47
1:A:806:LEU:HD12	1:A:2491:ARG:N	2.26	0.47
1:A:991:ASP:HB3	1:A:994:MET:HB3	1.97	0.47
1:A:3044:PRO:HG2	1:A:3047:MET:HB3	1.96	0.47
1:A:1676:LEU:CD2	1:A:1767:PHE:CZ	2.98	0.47
1:A:2093:LYS:HG2	1:A:3064:TRP:HE1	1.80	0.47
1:A:2800:PRO:HA	1:A:2803:SER:HB3	1.97	0.47
1:A:166:LEU:HB3	1:A:186:PHE:CE1	2.50	0.47
1:A:1015:ARG:HG3	1:A:1074:TRP:HZ2	1.79	0.47
1:A:194:ARG:NH2	1:A:196:GLN:OE1	2.48	0.46
1:A:1448:LEU:HD23	1:A:1451:LEU:HD12	1.97	0.46
1:A:1662:VAL:HG13	1:A:1759:GLU:CD	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:CYS:SG	1:A:199:ARG:N	2.89	0.46
1:A:691:THR:O	1:A:744:GLN:NE2	2.48	0.46
1:A:894:THR:CG2	1:A:2776:VAL:HG11	2.45	0.46
1:A:2033:ASN:ND2	1:A:2108:SER:O	2.42	0.46
1:A:2920:THR:HA	1:A:2923:TYR:HB2	1.98	0.46
1:A:675:ALA:HB3	1:A:678:VAL:HG23	1.97	0.46
1:A:2231:LEU:HD13	1:A:2235:LEU:HB3	1.96	0.46
1:A:809:LYS:HD3	1:A:2492:THR:CB	2.45	0.46
1:A:1461:LEU:HD11	1:A:1467:PHE:HB3	1.97	0.46
1:A:1665:VAL:CA	1:A:1759:GLU:OE2	2.64	0.46
1:A:1042:HIS:HB2	1:A:1059:THR:HG21	1.97	0.46
1:A:2976:LEU:HA	1:A:2979:PHE:HB3	1.97	0.46
1:A:2986:PRO:HA	1:A:2989:ILE:HG12	1.98	0.46
1:A:836:SER:OG	1:A:837:SER:N	2.49	0.46
1:A:2739:VAL:HG22	1:A:2762:LEU:HD21	1.98	0.46
1:A:163:GLN:HE21	1:A:189:LEU:HB3	1.81	0.46
1:A:1670:SER:HB2	1:A:1764:GLN:CG	2.46	0.46
1:A:815:SER:HB2	1:A:818:THR:HG23	1.98	0.45
1:A:2526:GLN:N	1:A:2612:GLN:O	2.47	0.45
1:A:1666:GLN:CG	1:A:1760:MET:HA	2.36	0.45
1:A:1672:ILE:HG22	1:A:1771:GLU:CD	2.36	0.45
1:A:2607:SER:O	1:A:2612:GLN:NE2	2.48	0.45
1:A:2674:LEU:HD23	1:A:2677:ARG:HH21	1.82	0.45
1:A:931:VAL:HG11	1:A:998:LEU:HD23	1.97	0.45
1:A:2826:LEU:HD12	1:A:2870:ILE:HD13	1.99	0.45
1:A:2704:SER:HA	1:A:2707:PHE:CD2	2.51	0.45
1:A:2771:HIS:HB3	1:A:2774:SER:HB3	1.99	0.45
1:A:2860:SER:HA	1:A:2902:ARG:HD2	1.98	0.45
1:A:1438:VAL:HG21	1:A:1485:GLU:HB2	1.98	0.45
1:A:3080:GLU:HG3	1:A:3082:VAL:H	1.81	0.45
1:A:1259:PHE:O	1:A:1263:LEU:N	2.44	0.45
1:A:667:GLY:O	1:A:679:HIS:ND1	2.50	0.45
1:A:1891:ARG:NH2	1:A:1922:ASP:OD2	2.50	0.44
1:A:1819:ARG:HD2	1:A:1849:GLU:HG2	1.98	0.44
1:A:1621:ILE:HG21	1:A:1764:GLN:HE21	1.76	0.44
1:A:1659:MET:HB2	1:A:1665:VAL:HG22	1.99	0.44
1:A:2127:MET:O	1:A:2131:MET:N	2.50	0.44
1:A:1704:CYS:HB2	1:A:1809:TYR:CE1	2.52	0.44
1:A:2168:THR:HG23	1:A:2220:ALA:HB1	2.00	0.44
1:A:752:TYR:HB2	1:A:764:THR:HG21	1.99	0.44
1:A:999:SER:HB2	1:A:1040:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1595:ASN:OD1	1:A:1595:ASN:N	2.50	0.44
1:A:1673:LEU:HD23	1:A:1768:TYR:HD1	1.82	0.44
1:A:2455:THR:OG1	1:A:2459:GLN:OE1	2.31	0.44
1:A:2700:LEU:HD21	1:A:2716:MET:HG3	2.00	0.44
1:A:2859:LEU:HD13	1:A:2875:LEU:HD12	1.98	0.44
1:A:797:THR:HB	1:A:2438:GLU:OE1	2.17	0.44
1:A:187:ALA:HB1	1:A:230:LYS:HB2	1.99	0.43
1:A:378:GLN:NE2	1:A:382:THR:OG1	2.50	0.43
1:A:1305:THR:O	1:A:1309:GLN:N	2.47	0.43
1:A:1783:PHE:HA	1:A:1792:THR:HG22	2.00	0.43
1:A:2042:SER:CA	1:A:2970:ARG:NH2	2.80	0.43
1:A:801:ALA:CB	1:A:2439:LYS:HE3	2.18	0.43
1:A:2046:GLN:C	1:A:3003:PRO:O	2.57	0.43
1:A:2513:PRO:O	1:A:2515:ALA:N	2.51	0.43
1:A:1704:CYS:HB2	1:A:1742:GLN:HE21	1.83	0.43
1:A:2908:PRO:O	1:A:2912:MET:N	2.51	0.43
1:A:1918:ASN:OD1	1:A:2317:GLN:HG2	2.18	0.43
1:A:1293:LEU:HA	1:A:1296:CYS:HB3	2.00	0.43
1:A:1997:PHE:HD2	1:A:2000:LEU:HD22	1.82	0.43
1:A:295:LEU:HD22	1:A:356:LEU:HD11	2.00	0.43
1:A:712:LEU:HD13	1:A:764:THR:HG23	2.00	0.43
1:A:809:LYS:NZ	1:A:2492:THR:HG23	2.34	0.43
1:A:1738:ARG:HH21	1:A:1798:LEU:HD13	1.84	0.43
1:A:1665:VAL:CG1	1:A:1754:LYS:HZ1	2.31	0.43
1:A:805:PRO:CB	1:A:2493:GLN:CA	2.46	0.42
1:A:1311:LEU:HD12	1:A:1421:PHE:HZ	1.84	0.42
1:A:391:LEU:HB3	1:A:677:LEU:HG	2.01	0.42
1:A:1128:ARG:HE	1:A:1131:VAL:HG21	1.84	0.42
1:A:2030:GLU:HA	1:A:2108:SER:OG	2.19	0.42
1:A:2250:VAL:HG21	1:A:2299:HIS:HB3	1.99	0.42
1:A:1850:VAL:HG13	1:A:1851:GLN:HG3	2.00	0.42
1:A:107:VAL:HA	1:A:112:ARG:HH22	1.84	0.42
1:A:880:GLU:O	1:A:887:HIS:NE2	2.46	0.42
1:A:2060:LEU:HD22	1:A:3080:GLU:OE2	2.19	0.42
1:A:2563:ASN:HD21	1:A:2606:MET:HG3	1.85	0.42
1:A:1796:THR:HG22	1:A:1839:VAL:HG23	2.01	0.42
1:A:2546:ILE:HG12	1:A:2978:GLN:NE2	2.35	0.42
1:A:2559:SER:OG	1:A:2560:LYS:N	2.53	0.42
1:A:2575:PRO:HA	1:A:2587:LEU:HD21	2.00	0.42
1:A:2042:SER:CA	1:A:3007:PHE:CZ	3.03	0.42
1:A:2237:LEU:HA	1:A:2238:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:LEU:HD13	1:A:2452:LEU:HA	1.88	0.41
1:A:2817:VAL:HG13	1:A:2825:VAL:HG11	2.02	0.41
1:A:1830:LEU:HD21	1:A:1890:VAL:HA	2.01	0.41
1:A:2126:ASP:N	1:A:2126:ASP:OD1	2.53	0.41
1:A:2171:ARG:HG3	1:A:2217:LEU:HD11	2.03	0.41
1:A:3016:PHE:O	1:A:3020:HIS:ND1	2.47	0.41
1:A:779:SER:O	1:A:781:PHE:N	2.54	0.41
1:A:802:ASP:OD1	1:A:2439:LYS:CA	2.66	0.41
1:A:2689:PRO:HD2	1:A:2692:LEU:HD12	2.03	0.41
1:A:2752:ASP:O	1:A:2756:ALA:N	2.51	0.41
1:A:215:ARG:HD2	1:A:220:VAL:HG11	2.02	0.41
1:A:1853:THR:HG21	1:A:2317:GLN:HB3	1.98	0.41
1:A:303:SER:O	1:A:306:LEU:N	2.39	0.41
1:A:1851:GLN:HA	1:A:1891:ARG:HG3	2.02	0.41
1:A:2033:ASN:O	1:A:2110:SER:HB3	1.97	0.41
1:A:2033:ASN:HB3	1:A:2110:SER:N	2.36	0.41
1:A:2978:GLN:HE21	1:A:2978:GLN:HB3	1.69	0.41
1:A:809:LYS:CD	1:A:2492:THR:CG2	2.87	0.40
1:A:1673:LEU:CG	1:A:1767:PHE:HB3	2.40	0.40
1:A:808:ARG:CB	1:A:2691:ILE:HD13	2.47	0.40
1:A:1888:GLU:OE1	1:A:1891:ARG:NH1	2.47	0.40
1:A:2512:VAL:HG13	1:A:2513:PRO:HD2	2.03	0.40
1:A:879:LEU:HD23	1:A:879:LEU:HA	1.95	0.40
1:A:936:TYR:HD1	1:A:936:TYR:HA	1.78	0.40
1:A:388:LEU:HD21	1:A:721:LEU:HD22	2.03	0.40
1:A:2227:VAL:HG12	1:A:2231:LEU:HG	2.04	0.40
1:A:1665:VAL:HB	1:A:1759:GLU:CD	2.42	0.40
1:A:1691:ARG:HH11	1:A:1694:GLU:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2313/3142 (74%)	2162 (94%)	146 (6%)	5 (0%)	47 81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2514	VAL
1	A	277	SER
1	A	2513	PRO
1	A	1046	PRO
1	A	2266	PRO

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	2077/2767 (75%)	2058 (99%)	19 (1%)	78 87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	240	ASN
1	A	918	ARG
1	A	1133	MET
1	A	1146	ASN
1	A	1702	ILE
1	A	1709	ARG
1	A	1838	LEU
1	A	1959	ASN
1	A	2019	ASN
1	A	2133	ASN
1	A	2156	GLN
1	A	2253	LEU
1	A	2377	ASN
1	A	2390	ASN
1	A	2512	VAL

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Mol	Chain	Res	Type
1	A	2528	ARG
1	A	2796	LYS
1	A	2976	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	240	ASN
1	A	377	GLN
1	A	378	GLN
1	A	399	GLN
1	A	1091	ASN
1	A	1310	GLN
1	A	1492	ASN
1	A	1589	GLN
1	A	1631	ASN
1	A	1682	GLN
1	A	1708	ASN
1	A	1742	GLN
1	A	1764	GLN
1	A	1942	ASN
1	A	2019	ASN
1	A	2040	GLN
1	A	2046	GLN
1	A	2133	ASN
1	A	2137	ASN
1	A	2236	HIS
1	A	2555	GLN
1	A	2563	ASN
1	A	2612	GLN
1	A	2978	GLN
1	A	3071	HIS
1	A	3085	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

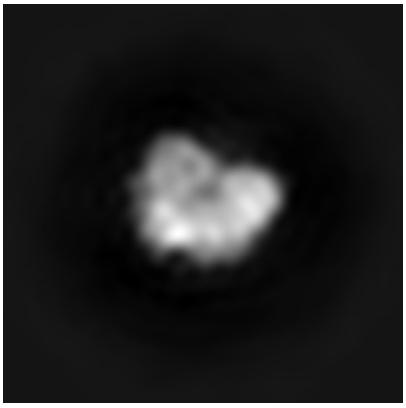
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4937. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

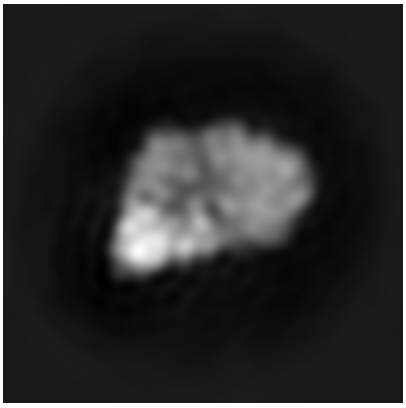
6.1 Orthogonal projections (i)

6.1.1 Primary map



X

Y



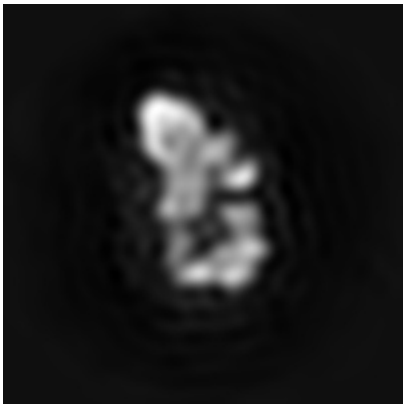
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 125



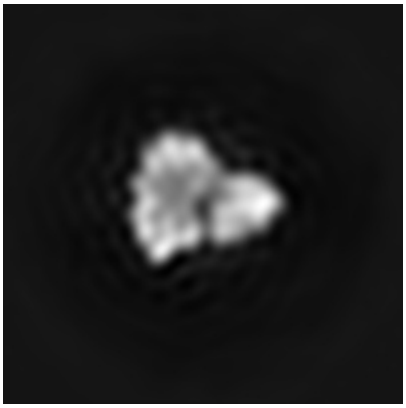
Y Index: 125

Z Index: 125

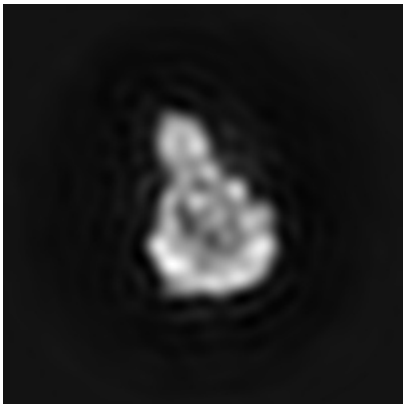
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

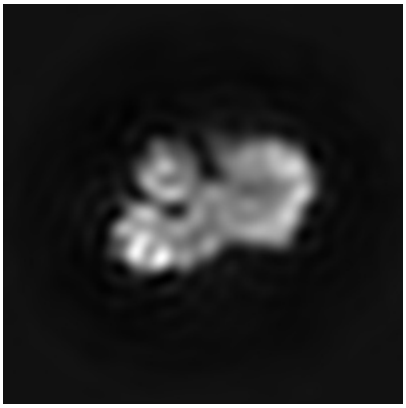
6.3.1 Primary map



X Index: 93



Y Index: 104

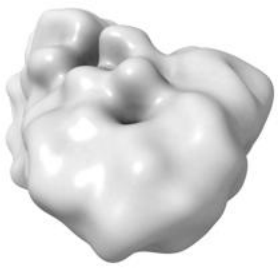


Z Index: 108

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

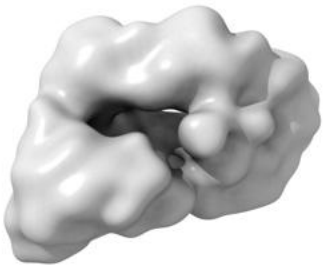
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

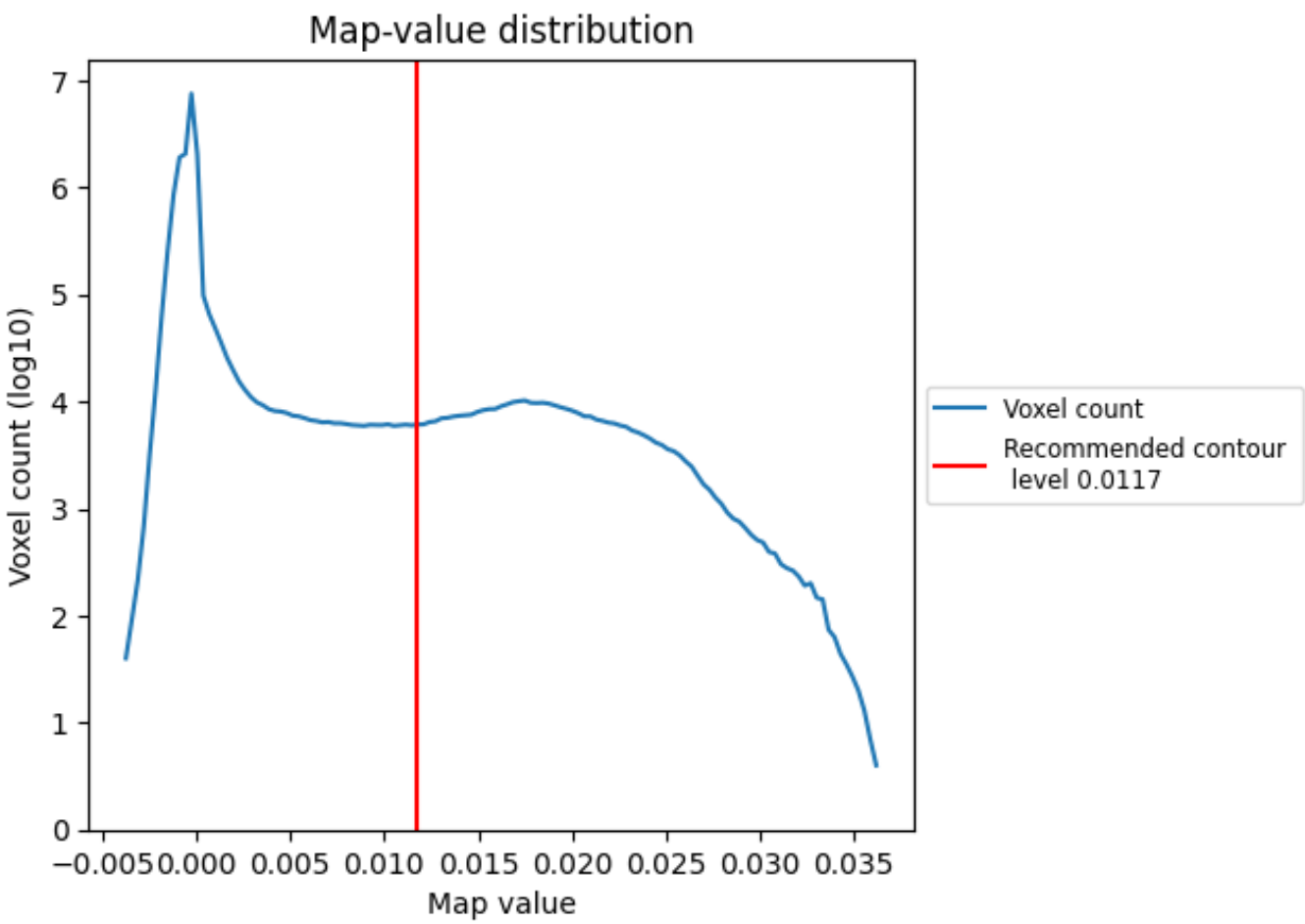
6.5 Mask visualisation (i)

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

7 Map analysis (i)

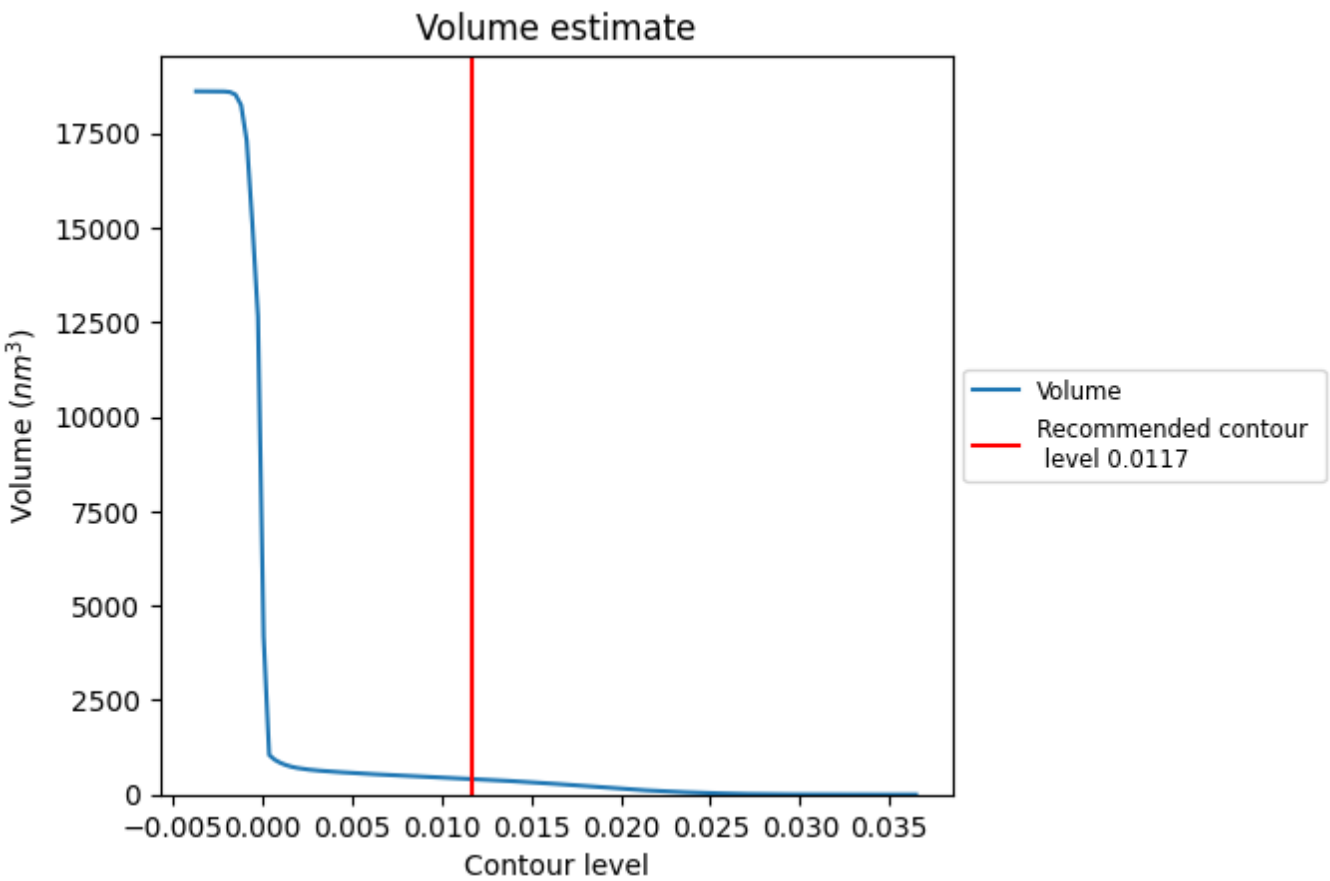
This section contains the results of statistical analysis of the map.

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.

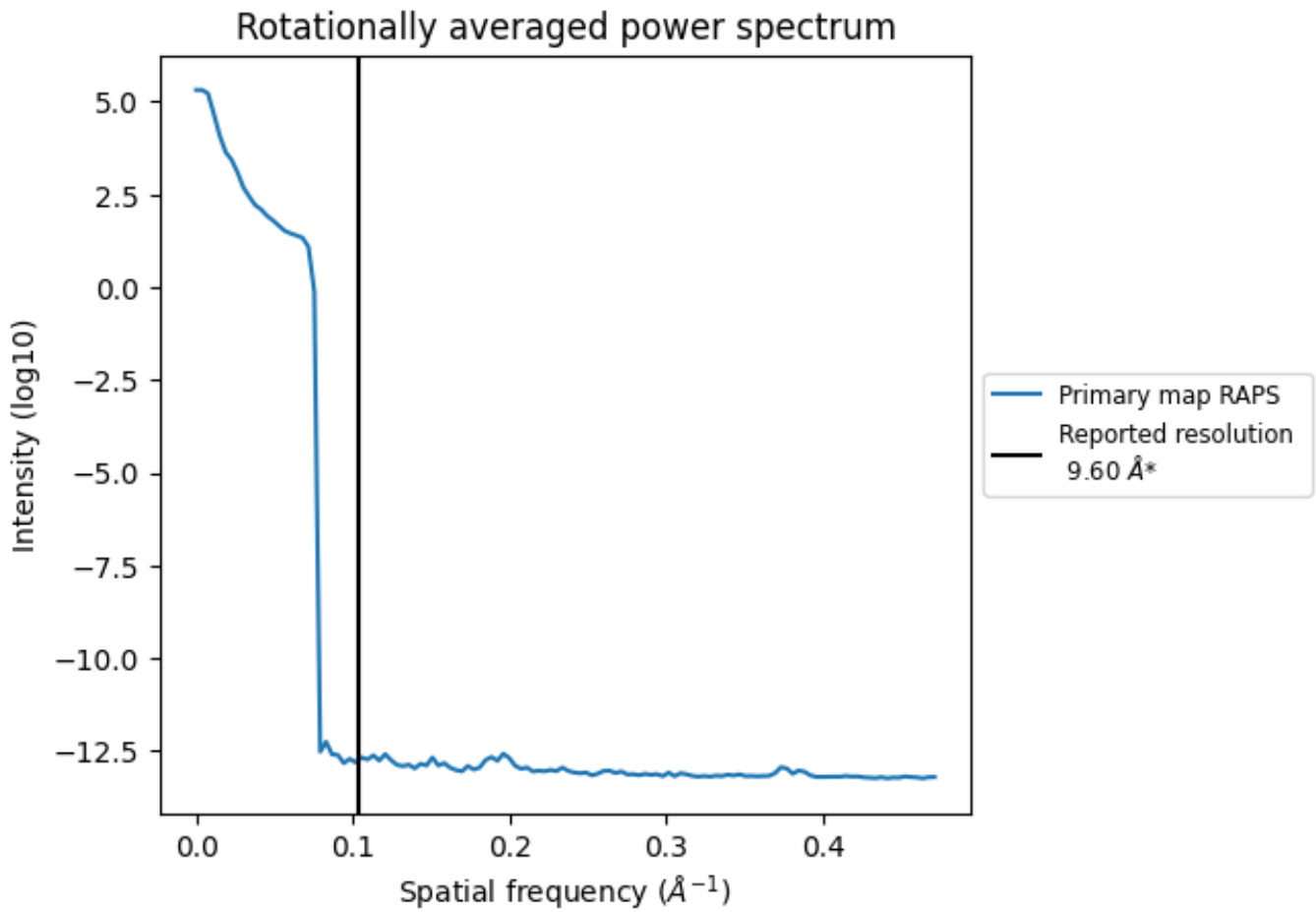
7.2 Volume estimate (i)



The volume at the recommended contour level is 411 nm^3; this corresponds to an approximate mass of 371 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 (i)

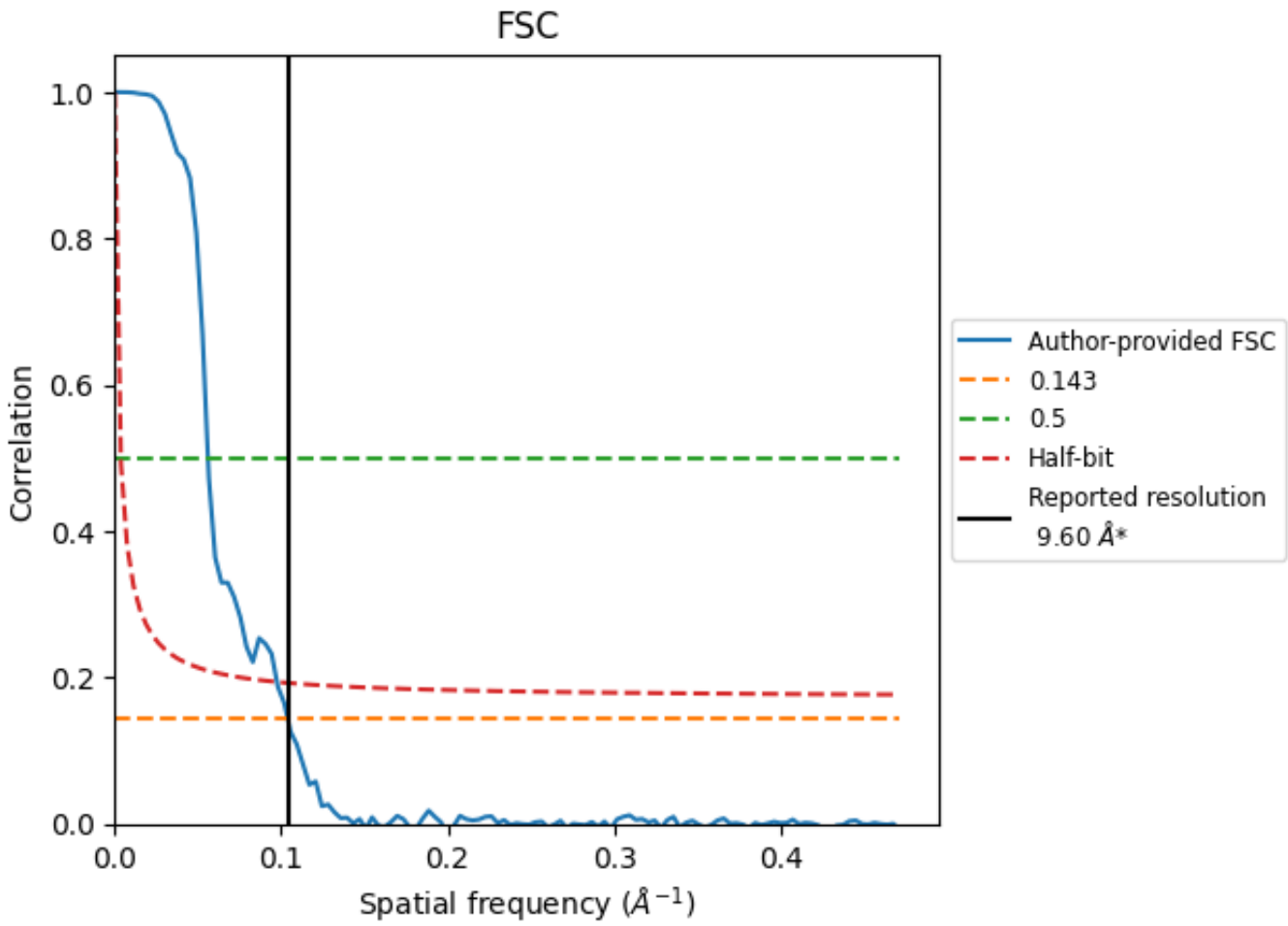


*Reported resolution corresponds to spatial frequency of 0.104 Å^{-1}

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 0.104 Å^{-1}

8.2 Resolution estimates (i)

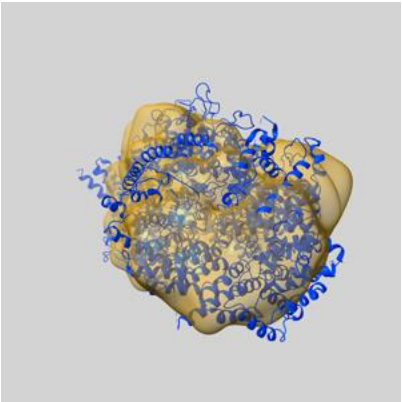
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.60	-	-
Author-provided FSC curve	9.62	17.83	10.25
Unmasked-calculated*	-	-	-

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

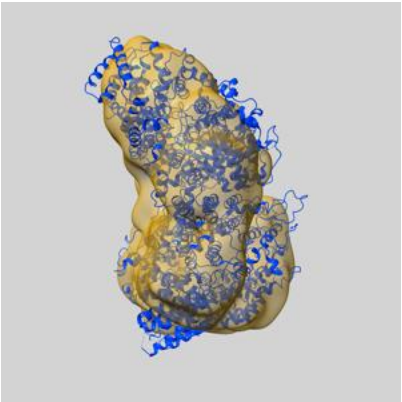
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4937 and PDB model 6RMH. Per-residue inclusion information can be found in section 3 on page 4.

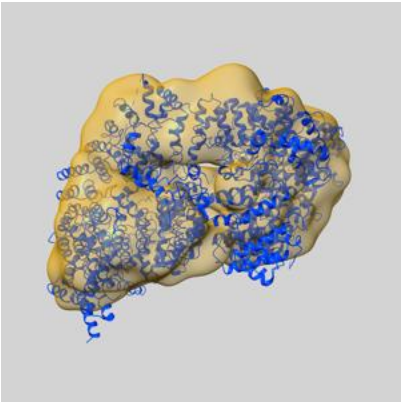
9.1 Map-model overlay (i)



X



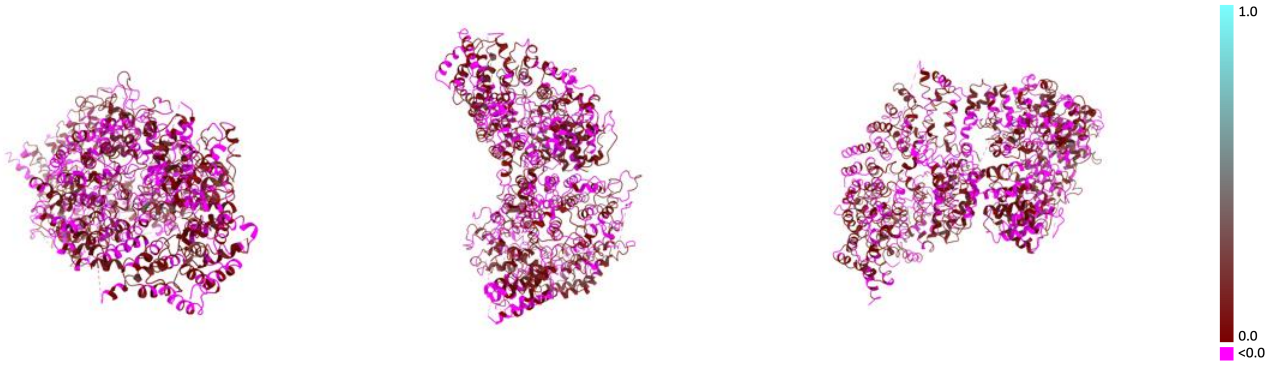
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117 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.

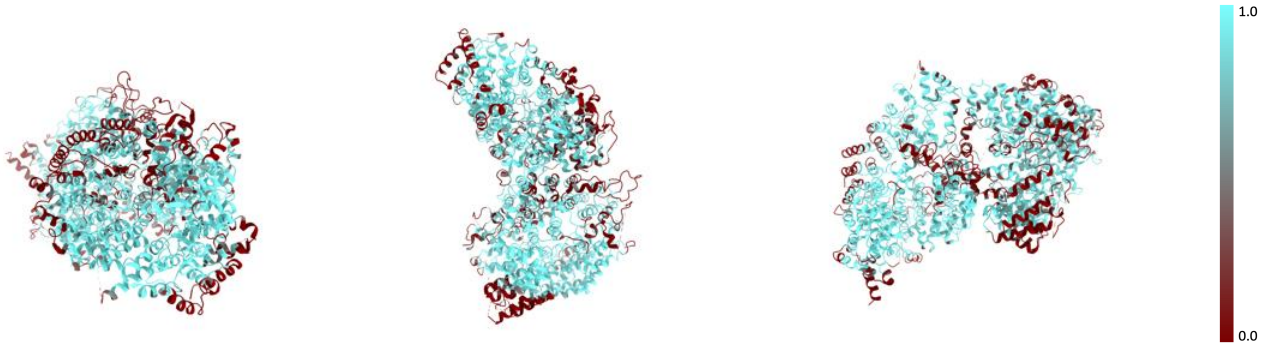
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

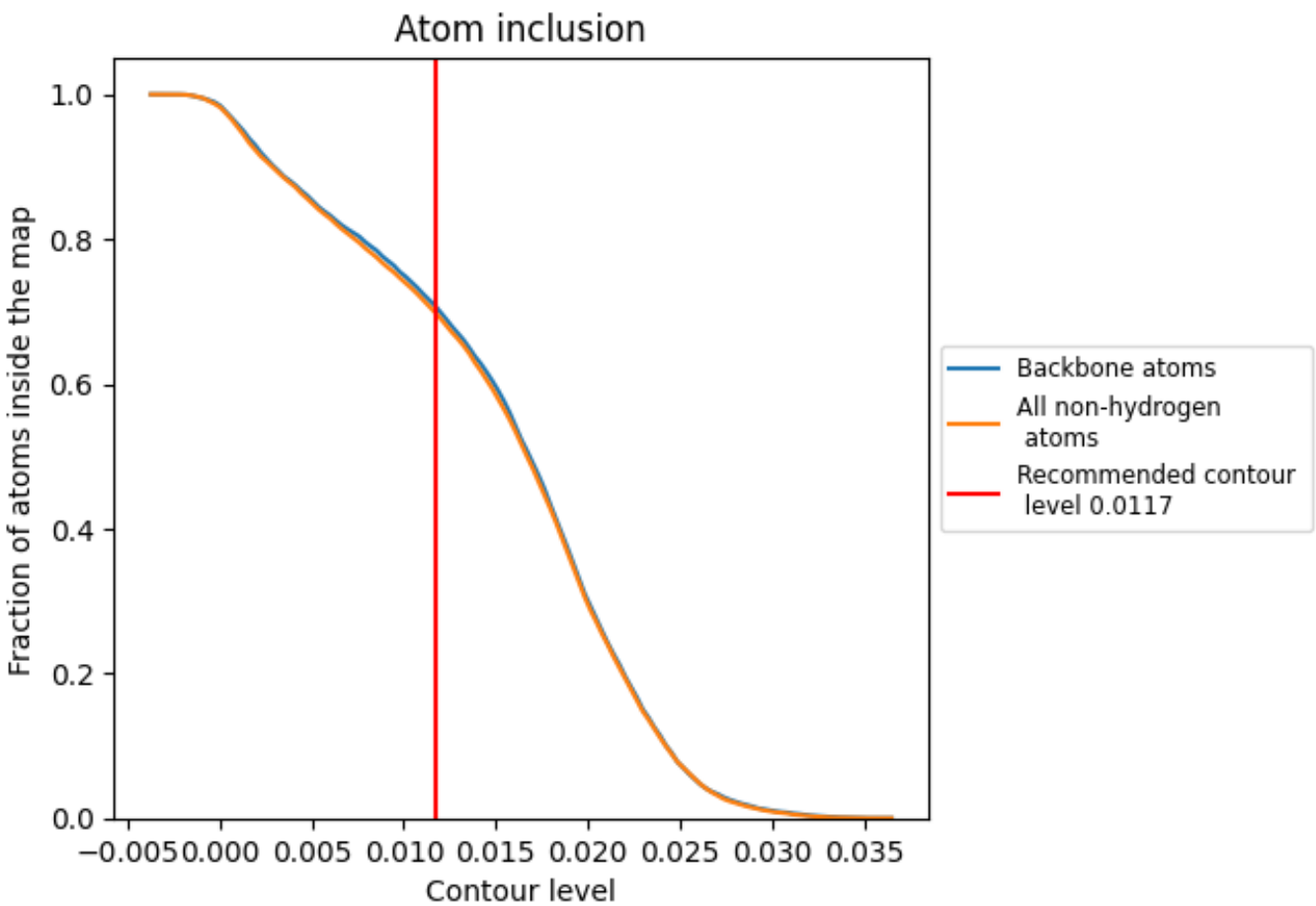
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0117).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0117) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6985	0.0260
A	0.6985	0.0260