Full wwPDB EM Validation Report

May 29, 2024 – 12:20 PM JST

PDB ID	:	8IZL
EMDB ID	:	EMD-35864
Title	:	Structure of the Mumps Virus L Protein Bound by Phosphoprotein Tetramer
Authors	:	Li, T.H.; Shen, Q.T.
Deposited on	:	2023-04-07
Resolution	:	2.93 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:

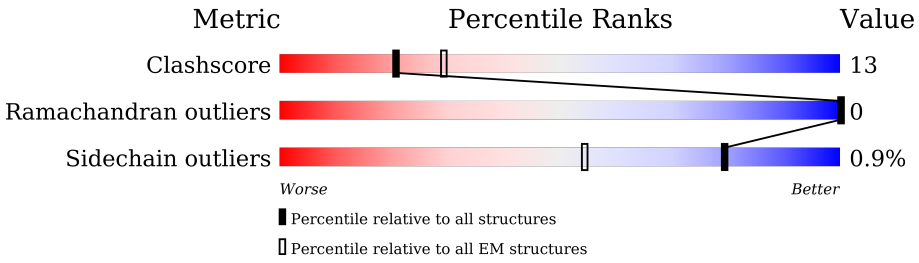
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.93 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	B	391	10% 8% 82%
1	C	391	12% 10% 77%
1	D	391	8% 7% 85%
1	E	391	8% 6% 85%
2	A	2261	67% 24% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18612 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	60	Total	C	N	O	S	0	0
			459	284	79	90	6		
1	E	58	Total	C	N	O	S	0	0
			440	272	76	87	5		
1	B	69	Total	C	N	O	S	0	0
			517	321	89	101	6		
1	C	91	Total	C	N	O	S	0	0
			680	420	119	135	6		

- Molecule 2 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2067	Total	C	N	O	S	0	0
			16514	10585	2805	3039	85		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

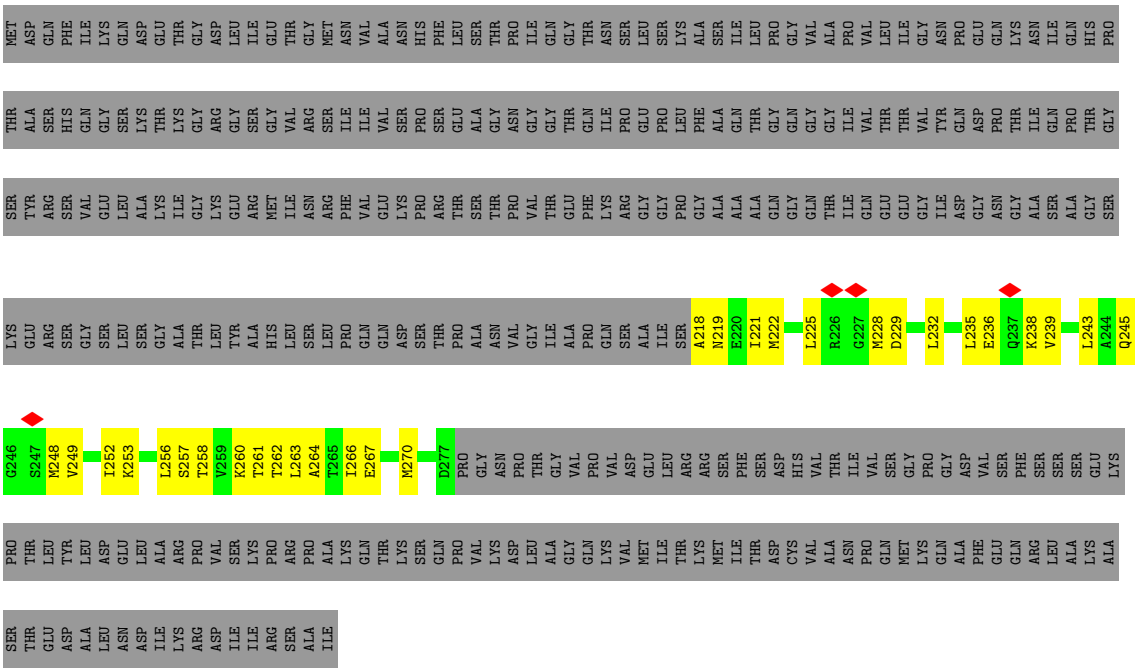
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

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.

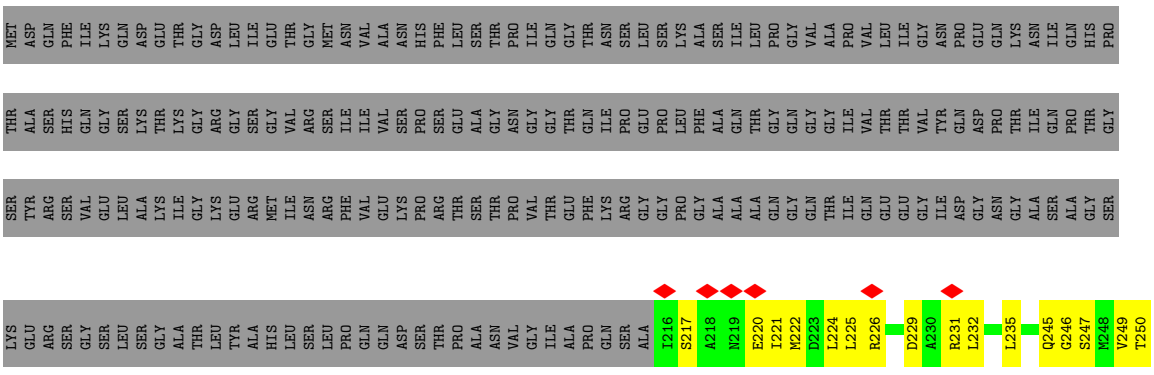
• Molecule 1: Phosphoprotein

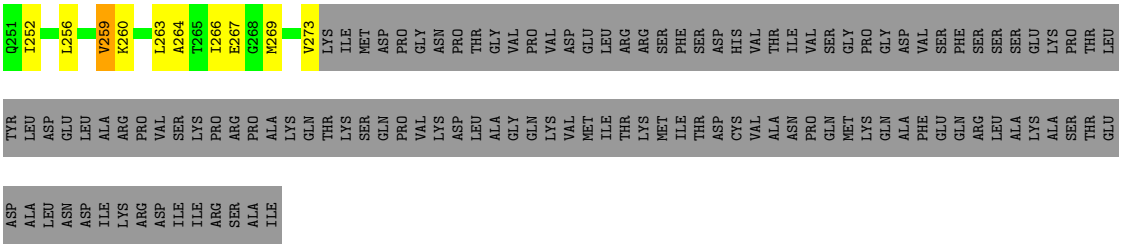
Chain D:



• Molecule 1: Phosphoprotein

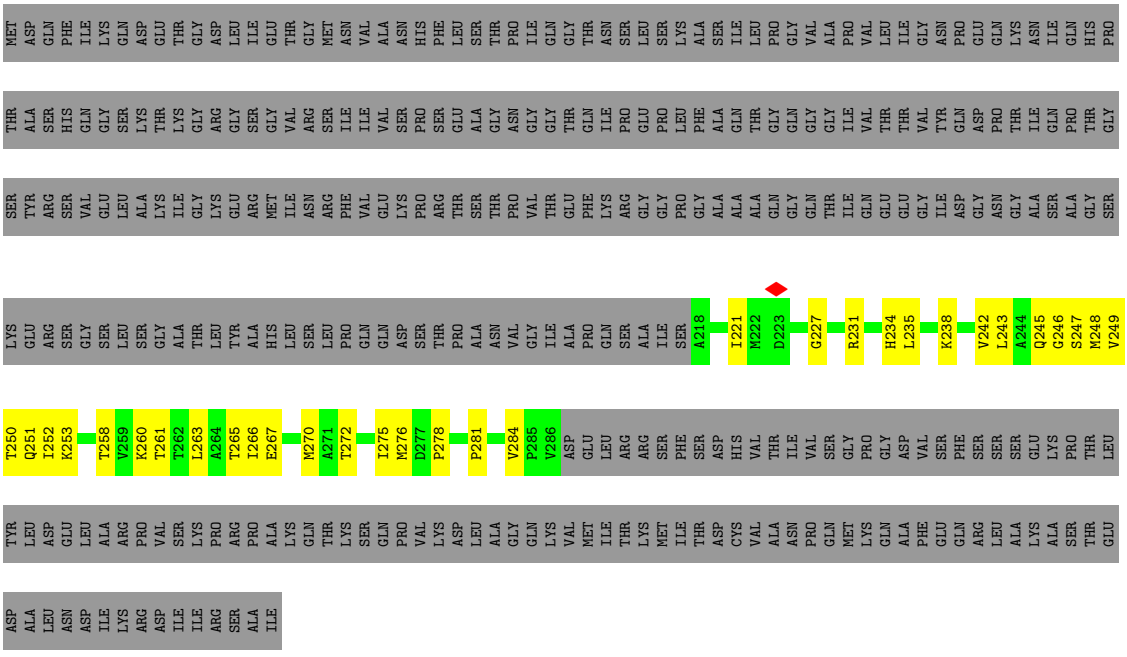
Chain E:





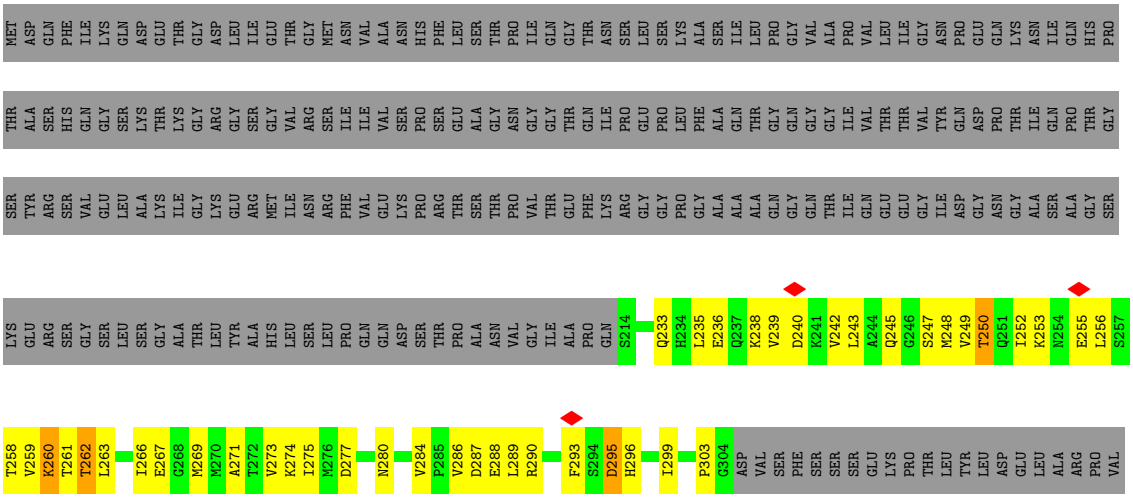
• Molecule 1: Phosphoprotein

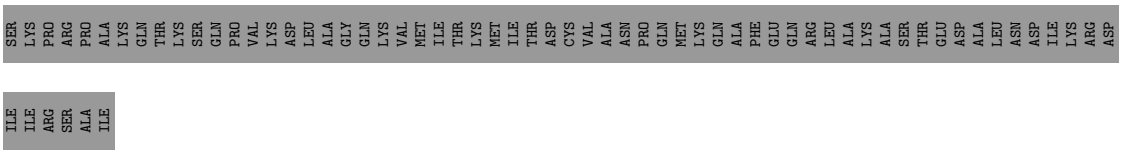
Chain B:



• Molecule 1: Phosphoprotein

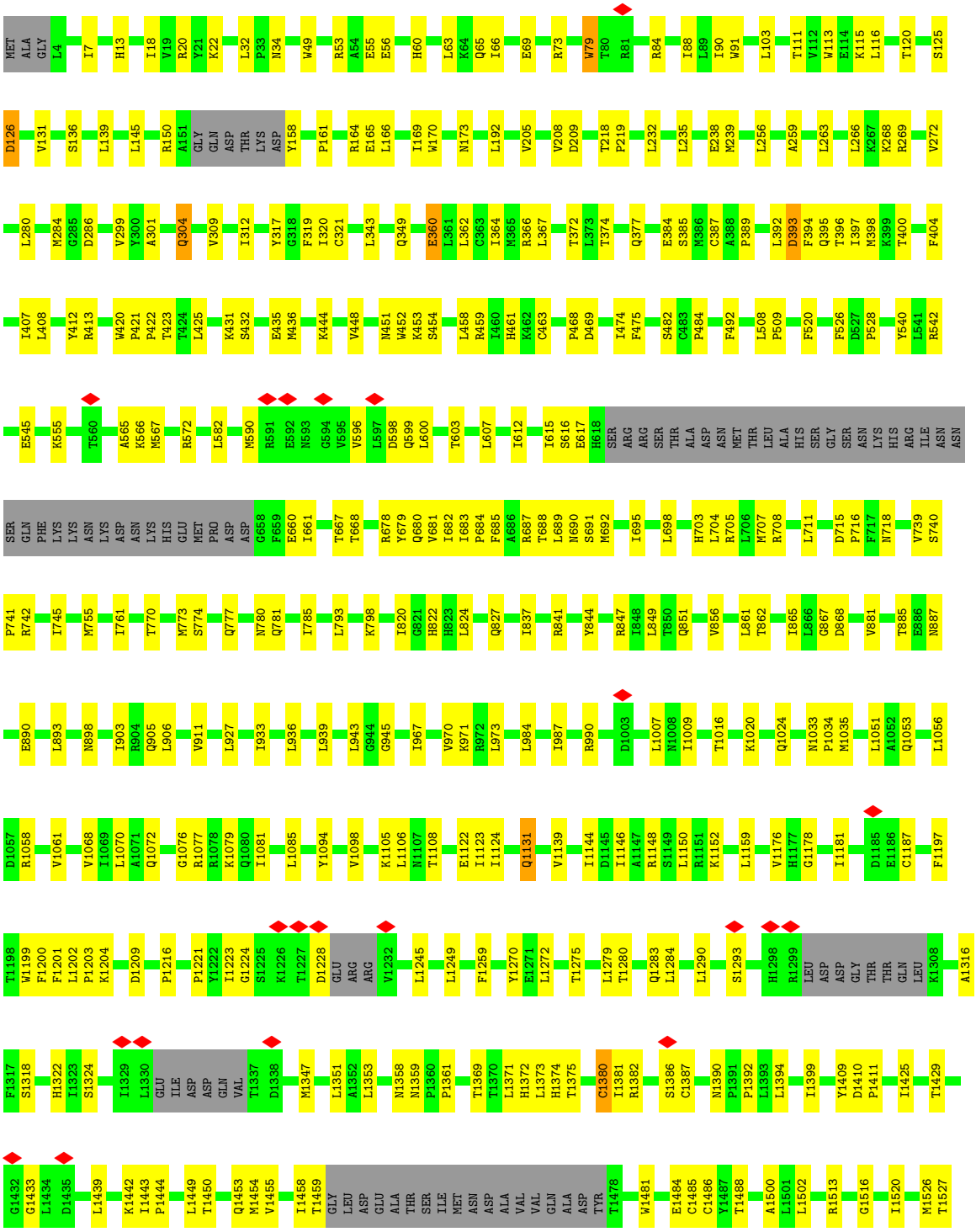
Chain C:

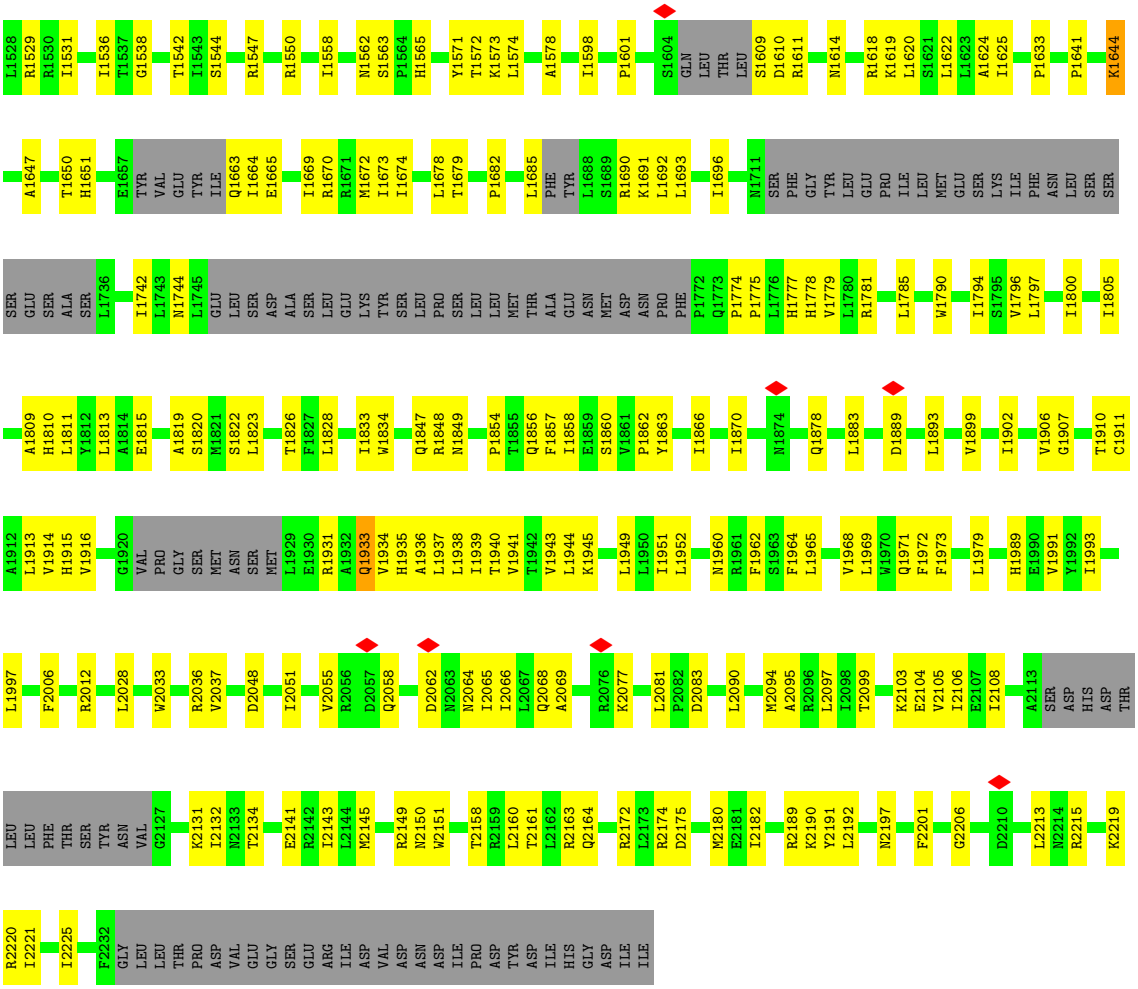




• Molecule 2: RNA-directed RNA polymerase L

Chain A:




L1528 R1529 R1530 I1531 I1536 T1537 G1538 T1542 I1543 S1544 R1547 R1550 I1558 N1562 S1563 P1564 H1565 Y1571 T1572 K1573 L1574 A1578 I1598 P1601 S1604 GLN LEU THR LEU S1609 D1610 R1611 N1614 R1618 K1619 L1620 S1621 L1622 L1623 A1624 I1625 P1633 P1641 K1644
A1647 T1650 H1651 E1657 TYR VAL GLU TYR ILE Q1663 I1664 E1665 I1669 R1670 R1671 M1672 I1673 I1674 L1678 T1679 P1682 L1685 PHE TYR L1688 S1689 R1690 K1691 L1692 L1693 I1696 N1711 SER PHE GLY TYR LEU GLU PRO ILE LEU MET GLU SER LYS ILE PHE ASN LEU SER SER
SER GLU SER ALA SER L1736 I1742 L1743 N1744 L1745 GLU LEU SER ASP ALA SER LEU GLU LYS TYR SER LEU PRO SER LEU LEU MET THR ALA GLU ASN MET ASP ASN PRO PHE P1772 Q1773 P1774 P1775 L1776 H1777 H1778 V1779 L1780 R1781 L1785 W1790 I1794 S1795 V1796 L1797 I1800 I1805
A1809 H1810 L1811 Y1812 L1813 A1814 E1815 A1819 S1820 W1821 S1822 L1823 T1826 F1827 L1828 I1833 W1834 Q1847 R1848 N1849 P1854 T1855 Q1856 F1857 I1858 E1859 S1860 V1861 P1862 Y1863 I1866 I1870 N1874 Q1878 L1883 D1889 L1893 V1899 I1902 V1906 G1907 T1910 C1911
A1912 L1913 V1914 H1915 V1916 G1920 VAL PRO GLY SER MET ASN SER MET L1929 E1930 R1931 A1932 Q1933 V1934 H1935 A1936 L1937 L1938 I1939 T1940 V1941 T1942 V1943 L1944 K1945 L1949 L1950 I1951 L1952 N1960 R1961 F1962 S1963 F1964 L1965 V1968 L1969 W1970 Q1971 F1972 F1973 L1979 H1989 E1990 V1991 Y1992 I1993
L1997 F2006 R2012 L2028 W2033 R2036 V2037 D2048 I2051 V2055 R2056 D2057 Q2058 D2062 N2063 N2064 I2065 I2066 L2067 Q2068 A2069 R2076 K2077 L2081 P2082 D2083 L2090 M2094 A2095 R2096 L2097 I2098 T2099 K2103 E2104 V2105 I2106 E2107 I2108 A2113 SER ASP HIS ASP THR
LEU LEU PHE THR SER TYR ASN VAL G2127 K2131 I2132 N2133 T2134 E2141 R2142 I2143 L2144 M2145 R2149 N2150 W2151 T2158 R2159 L2160 T2161 L2162 R2163 Q2164 R2172 L2173 R2174 D2175 M2180 E2181 I2182 R2189 K2190 Y2191 L2192 N2197 F2201 G2206 D2210 L2213 N2214 R2215 K2219
R2220 I2221 I2225 F2232 GLY LEU LEU THR PRO ASP VAL GLU GLY SER GLU ARG ILE ASP VAL ASP ASN ASP ILE PRO ASP TYR ASP ILE HIS GLY ASP ILE ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	438014	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.500	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.53, 0.53, 0.53	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	B	0.41	0/520	0.66	0/701
1	C	0.40	0/686	0.58	0/926
1	D	0.39	0/459	0.62	0/614
1	E	0.48	0/440	0.65	0/590
2	A	0.31	0/16861	0.52	0/22897
All	All	0.32	0/18966	0.53	0/25728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	517	0	545	51	0
1	C	680	0	702	58	0
1	D	459	0	487	35	0
1	E	440	0	466	40	0
2	A	16514	0	16753	395	0
3	A	2	0	0	0	0
All	All	18612	0	18953	503	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 13.

All (503) 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)
2:A:1290:LEU:CD2	2:A:1691:LYS:HE3	1.65	1.26
1:D:256:LEU:HD11	1:C:256:LEU:HD23	1.14	1.11
1:D:256:LEU:CD1	1:C:256:LEU:HD23	1.85	1.07
2:A:1290:LEU:HD21	2:A:1691:LYS:CE	1.86	1.05
2:A:2090:LEU:HD13	2:A:2150:ASN:HD22	1.20	1.03
2:A:1290:LEU:HD21	2:A:1691:LYS:HE3	1.00	0.98
1:C:271:ALA:O	2:A:395:GLN:HB2	1.68	0.93
1:D:256:LEU:HD11	1:C:256:LEU:CD2	1.99	0.91
1:D:253:LYS:HD3	1:C:252:ILE:HG22	1.55	0.87
1:C:303:PRO:HG2	2:A:459:ARG:HB2	1.53	0.87
2:A:1290:LEU:CD2	2:A:1691:LYS:CE	2.50	0.83
2:A:1324:SER:OG	2:A:1849:ASN:HB2	1.79	0.82
1:E:259:VAL:HG22	1:B:263:LEU:HD22	1.61	0.81
2:A:2090:LEU:HD13	2:A:2150:ASN:ND2	1.96	0.80
2:A:1914:VAL:HG11	2:A:1940:THR:HG22	1.66	0.77
2:A:136:SER:HB2	2:A:145:LEU:HB3	1.67	0.77
1:E:259:VAL:HG23	1:B:260:LYS:CE	2.14	0.76
1:E:259:VAL:HG23	1:B:260:LYS:HE2	1.67	0.76
1:C:280:ASN:HB3	2:A:387:CYS:HB3	1.67	0.75
2:A:777:GLN:HG2	2:A:780:ASN:O	1.87	0.74
2:A:1624:ALA:HB2	2:A:1651:HIS:NE2	2.01	0.74
2:A:1502:LEU:HB3	2:A:1622:LEU:HD11	1.69	0.74
2:A:841:ARG:HH12	2:A:887:ASN:HD21	1.36	0.73
2:A:1558:ILE:HD12	2:A:1574:LEU:HD22	1.70	0.72
2:A:2105:VAL:HG13	2:A:2132:ILE:HD12	1.70	0.72
1:B:249:VAL:O	1:B:252:ILE:HG22	1.89	0.72
1:D:263:LEU:HD21	1:C:259:VAL:HG13	1.72	0.71
2:A:1176:VAL:HG12	2:A:1375:THR:HG22	1.74	0.70
1:D:263:LEU:CD2	1:C:259:VAL:HG13	2.21	0.69
2:A:360:GLU:HG3	2:A:851:GLN:HA	1.74	0.69
1:E:256:LEU:O	1:E:259:VAL:HG12	1.93	0.69
1:D:266:ILE:HG22	1:C:266:ILE:HD13	1.76	0.68
2:A:1810:HIS:HB2	2:A:1833:ILE:HD13	1.74	0.68
1:C:239:VAL:HA	1:C:242:VAL:HG22	1.77	0.67
2:A:111:THR:O	2:A:115:LYS:HG2	1.93	0.67
2:A:615:ILE:HD11	2:A:661:ILE:HG22	1.76	0.67
2:A:703:HIS:O	2:A:707:MET:HG2	1.94	0.67
2:A:1902:ILE:O	2:A:1906:VAL:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1529:ARG:HD3	2:A:1573:LYS:HZ3	1.61	0.66
2:A:715:ASP:HB3	2:A:718:ASN:HB2	1.78	0.66
2:A:1811:LEU:HB3	2:A:1914:VAL:HG22	1.77	0.66
2:A:615:ILE:HD12	2:A:660:GLU:HG2	1.79	0.65
2:A:20:ARG:HB2	2:A:372:THR:HB	1.78	0.65
2:A:1061:VAL:HG21	2:A:1159:LEU:HD22	1.77	0.65
2:A:1200:PHE:HB2	2:A:1371:LEU:HB3	1.79	0.65
2:A:2090:LEU:HD11	2:A:2094:MET:HE2	1.79	0.65
2:A:2158:THR:HA	2:A:2161:THR:HG22	1.79	0.65
2:A:1123:ILE:HG13	2:A:1124:ILE:HG23	1.79	0.64
2:A:13:HIS:NE2	2:A:862:THR:O	2.26	0.64
2:A:425:LEU:HD23	2:A:458:LEU:HD13	1.79	0.64
2:A:469:ASP:HB3	2:A:528:PRO:HG2	1.79	0.64
2:A:280:LEU:O	2:A:284:MET:HG3	1.99	0.63
2:A:235:LEU:HA	2:A:239:MET:HE2	1.80	0.63
1:E:259:VAL:HG22	1:B:263:LEU:CD2	2.29	0.63
2:A:2104:GLU:O	2:A:2108:ILE:HG12	1.99	0.63
2:A:1202:LEU:HB3	2:A:1369:THR:HG22	1.81	0.62
2:A:1520:ILE:HD11	2:A:1625:ILE:HG22	1.80	0.62
1:B:276:MET:O	2:A:680:GLN:HG2	1.99	0.62
2:A:881:VAL:HG11	2:A:898:ASN:HB2	1.80	0.62
2:A:1866:ILE:HD11	2:A:1878:GLN:HB2	1.81	0.62
2:A:1550:ARG:HH22	2:A:1858:ILE:HD12	1.64	0.62
2:A:1777:HIS:HD2	2:A:1781:ARG:HH21	1.48	0.62
2:A:1056:LEU:HD22	2:A:1061:VAL:HG13	1.82	0.62
2:A:55:GLU:HG3	2:A:56:GLU:HG3	1.81	0.62
1:E:273:VAL:CG2	1:B:270:MET:CE	2.78	0.61
1:C:284:VAL:O	2:A:739:VAL:HG11	1.99	0.61
2:A:820:ILE:HG13	2:A:822:HIS:HD2	1.66	0.61
2:A:1785:LEU:HD23	2:A:1785:LEU:H	1.64	0.61
1:E:256:LEU:HD22	1:E:259:VAL:CG1	2.30	0.61
1:B:227:GLY:O	1:B:231:ARG:HG2	2.00	0.61
2:A:1531:ILE:HD11	2:A:1536:ILE:HD12	1.83	0.61
2:A:1790:TRP:HB2	2:A:1823:LEU:HD13	1.83	0.61
2:A:2172:ARG:HD2	2:A:2174:ARG:HH22	1.66	0.61
2:A:319:PHE:HE2	2:A:827:GLN:HG3	1.66	0.61
2:A:301:ALA:HB2	2:A:320:ILE:HD12	1.83	0.60
2:A:1813:LEU:HD23	2:A:1916:VAL:HG22	1.83	0.60
1:E:266:ILE:CD1	1:B:266:ILE:HG22	2.32	0.60
2:A:1858:ILE:HA	2:A:1863:TYR:HD2	1.66	0.60
2:A:1290:LEU:HD22	2:A:1691:LYS:HE3	1.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:PHE:H	2:A:1034:PRO:HG2	1.66	0.60
1:D:257:SER:O	1:D:261:THR:HG23	2.02	0.60
2:A:268:LYS:O	2:A:272:VAL:HG23	2.02	0.60
2:A:1359:ASN:HB3	2:A:1361:PRO:HD2	1.83	0.60
2:A:1481:TRP:H	2:A:1542:THR:HG22	1.66	0.60
2:A:520:PHE:O	2:A:1033:ASN:ND2	2.34	0.59
2:A:1203:PRO:HB2	2:A:1216:PRO:HG3	1.84	0.59
2:A:2048:ASP:HA	2:A:2163:ARG:HH12	1.67	0.59
1:E:273:VAL:HG21	1:B:270:MET:CE	2.32	0.59
1:C:284:VAL:CG1	1:C:288:GLU:HB2	2.32	0.59
2:A:2180:MET:N	2:A:2180:MET:SD	2.74	0.59
2:A:492:PHE:HA	2:A:716:PRO:HA	1.85	0.59
2:A:1318:SER:HB2	2:A:1351:LEU:HD22	1.86	0.58
2:A:715:ASP:OD2	2:A:718:ASN:ND2	2.37	0.58
2:A:1870:ILE:HD12	2:A:1870:ILE:H	1.67	0.58
2:A:139:LEU:HB3	2:A:1353:LEU:HD11	1.85	0.58
2:A:678:ARG:O	2:A:681:VAL:HG12	2.03	0.58
2:A:1558:ILE:HD11	2:A:1578:ALA:HB2	1.85	0.57
2:A:695:ILE:HG21	2:A:698:LEU:HB2	1.86	0.57
2:A:1663:GLN:HG2	2:A:1664:ILE:HG23	1.86	0.57
2:A:1790:TRP:CD1	2:A:2066:ILE:HD12	2.39	0.57
1:B:276:MET:HA	2:A:683:ILE:HG21	1.86	0.57
2:A:451:ASN:HD21	2:A:454:SER:HB2	1.70	0.57
2:A:1790:TRP:O	2:A:1794:ILE:HG12	2.03	0.57
2:A:2095:ALA:HA	2:A:2182:ILE:HD13	1.86	0.57
1:B:249:VAL:O	1:B:250:THR:C	2.43	0.57
2:A:2160:LEU:O	2:A:2164:GLN:HG2	2.05	0.57
2:A:113:TRP:HB2	2:A:911:VAL:HG11	1.85	0.57
2:A:1425:ILE:HD12	2:A:1682:PRO:CB	2.35	0.57
2:A:1670:ARG:O	2:A:1674:ILE:HG12	2.05	0.57
2:A:847:ARG:NH2	2:A:1209:ASP:OD1	2.38	0.57
2:A:906:LEU:HD23	2:A:933:ILE:HG23	1.86	0.57
2:A:1439:LEU:HA	2:A:1442:LYS:HD2	1.86	0.57
2:A:484:PRO:HB3	2:A:545:GLU:HG3	1.85	0.56
2:A:1936:ALA:O	2:A:1940:THR:HG23	2.05	0.56
2:A:1068:VAL:O	2:A:1072:GLN:HG2	2.04	0.56
2:A:150:ARG:O	2:A:158:TYR:N	2.39	0.56
2:A:2051:ILE:HG21	2:A:2163:ARG:HD2	1.88	0.56
2:A:847:ARG:HG2	2:A:1316:ALA:HA	1.87	0.56
2:A:943:LEU:HB3	2:A:987:ILE:HD13	1.88	0.56
2:A:1425:ILE:HD12	2:A:1682:PRO:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1822:SER:O	2:A:1826:THR:HG23	2.06	0.56
2:A:1484:GLU:HG3	2:A:1693:LEU:HD22	1.87	0.56
1:B:276:MET:HG2	2:A:683:ILE:CG2	2.36	0.56
1:B:272:THR:O	1:B:275:ILE:HG13	2.05	0.56
2:A:384:GLU:HG3	2:A:385:SER:N	2.20	0.55
2:A:1571:TYR:HA	2:A:1574:LEU:HB2	1.88	0.55
2:A:374:THR:HB	2:A:377:GLN:HG3	1.88	0.55
2:A:1380:CYS:O	2:A:1382:ARG:HG2	2.06	0.55
2:A:1937:LEU:HD22	2:A:1969:LEU:HD21	1.88	0.55
2:A:1915:HIS:HA	2:A:1951:ILE:HG23	1.87	0.55
1:B:266:ILE:HD11	1:C:267:GLU:CA	2.36	0.55
1:C:273:VAL:HG23	2:A:394:PHE:HB2	1.88	0.55
2:A:366:ARG:NH2	2:A:555:LYS:O	2.40	0.55
2:A:1598:ILE:HD11	2:A:1619:LYS:HD2	1.87	0.55
2:A:2090:LEU:HD11	2:A:2094:MET:CE	2.36	0.55
2:A:319:PHE:CE2	2:A:827:GLN:HG3	2.41	0.55
1:E:273:VAL:CG2	1:B:270:MET:HE2	2.37	0.55
1:C:266:ILE:O	1:C:269:MET:HG2	2.07	0.55
2:A:1486:CYS:SG	2:A:1547:ARG:NH2	2.79	0.55
2:A:451:ASN:ND2	2:A:454:SER:HB2	2.22	0.54
1:D:248:MET:HE1	1:E:250:THR:HA	1.89	0.54
2:A:1199:TRP:CD2	2:A:1849:ASN:OD1	2.61	0.54
2:A:2215:ARG:O	2:A:2219:LYS:HG3	2.08	0.54
1:D:219:ASN:O	1:D:222:MET:HG2	2.08	0.54
1:E:256:LEU:HD22	1:E:259:VAL:HG12	1.90	0.54
2:A:1279:LEU:HB3	2:A:1283:GLN:HG3	1.89	0.54
2:A:2083:ASP:OD1	2:A:2083:ASP:N	2.36	0.54
2:A:841:ARG:NH2	2:A:849:LEU:O	2.39	0.54
1:E:231:ARG:O	1:E:235:LEU:HG	2.07	0.54
1:E:247:SER:O	1:E:250:THR:HG22	2.08	0.54
2:A:1775:PRO:HB2	2:A:1778:HIS:HD2	1.72	0.54
2:A:1664:ILE:HG13	2:A:1665:GLU:HG3	1.90	0.53
2:A:205:VAL:HG22	2:A:218:THR:HG22	1.89	0.53
2:A:1826:THR:HG21	2:A:2069:ALA:HA	1.89	0.53
1:D:253:LYS:HE3	1:C:255:GLU:OE1	2.08	0.53
2:A:1272:LEU:O	2:A:1275:THR:OG1	2.22	0.53
2:A:1685:LEU:O	2:A:1690:ARG:NH1	2.42	0.53
2:A:1070:LEU:O	2:A:1076:GLY:HA3	2.09	0.53
1:B:275:ILE:HG22	1:C:299:ILE:HD11	1.90	0.53
2:A:423:THR:HB	2:A:458:LEU:HD11	1.91	0.53
2:A:1516:GLY:O	2:A:1520:ILE:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1854:PRO:HG2	2:A:1857:PHE:HB3	1.91	0.53
2:A:400:THR:HG23	2:A:685:PHE:HZ	1.74	0.53
2:A:1620:LEU:HD22	2:A:1644:LYS:HE2	1.89	0.53
1:E:273:VAL:HG21	1:B:270:MET:HE3	1.91	0.53
1:C:249:VAL:O	1:C:252:ILE:HG13	2.09	0.53
2:A:169:ILE:HD11	2:A:259:ALA:HB2	1.90	0.53
1:C:274:LYS:NZ	2:A:393:ASP:CG	2.63	0.52
2:A:1259:PHE:HA	2:A:1390:ASN:OD1	2.08	0.52
2:A:1815:GLU:OE2	2:A:1820:SER:HB2	2.10	0.52
2:A:1913:LEU:HD13	2:A:1949:LEU:HD23	1.92	0.52
2:A:1796:VAL:HG11	2:A:1951:ILE:HD12	1.91	0.52
1:B:284:VAL:HG11	2:A:691:SER:HB2	1.92	0.52
2:A:1678:LEU:HD13	2:A:1679:THR:N	2.24	0.52
2:A:761:ILE:HG21	2:A:774:SER:HB3	1.91	0.52
1:D:225:LEU:HD21	1:E:225:LEU:HD13	1.90	0.52
2:A:1053:GLN:HG2	2:A:1394:LEU:HD22	1.92	0.52
2:A:1280:THR:HG22	2:A:1283:GLN:HG2	1.92	0.52
1:D:235:LEU:O	1:D:238:LYS:HG2	2.09	0.52
1:B:251:GLN:NE2	1:C:253:LYS:HE3	2.25	0.52
2:A:1790:TRP:CE3	2:A:1819:ALA:HB1	2.45	0.52
2:A:1952:LEU:HB3	2:A:1993:ILE:HB	1.92	0.52
2:A:422:PRO:HB2	2:A:461:HIS:HB2	1.91	0.52
1:E:269:MET:HE2	1:B:270:MET:O	2.09	0.52
2:A:432:SER:O	2:A:436:MET:HG3	2.10	0.52
2:A:603:THR:HG23	2:A:1223:ILE:HD12	1.91	0.52
2:A:2094:MET:HG2	2:A:2143:ILE:HD12	1.92	0.52
2:A:770:THR:HG21	2:A:785:ILE:HG23	1.91	0.51
1:C:235:LEU:HA	1:C:238:LYS:HD2	1.92	0.51
2:A:397:ILE:HG12	2:A:681:VAL:HG23	1.92	0.51
1:E:259:VAL:CG1	1:E:260:LYS:N	2.74	0.51
2:A:1455:VAL:HG21	2:A:1500:ALA:HB3	1.93	0.51
2:A:1529:ARG:HH11	2:A:1573:LYS:HZ1	1.57	0.51
2:A:2141:GLU:O	2:A:2145:MET:HG3	2.10	0.51
1:E:256:LEU:HD22	1:E:259:VAL:HG11	1.93	0.51
1:B:281:PRO:HD2	1:C:293:PHE:HB2	1.91	0.51
1:D:221:ILE:O	1:D:225:LEU:HD22	2.11	0.51
2:A:2099:THR:HG22	2:A:2192:LEU:CD1	2.41	0.51
2:A:508:LEU:HD13	2:A:509:PRO:HD2	1.93	0.51
1:C:296:HIS:CE1	2:A:540:TYR:CE1	2.99	0.50
1:D:253:LYS:HD3	1:C:252:ILE:CG2	2.34	0.50
2:A:309:VAL:HB	2:A:312:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1823:LEU:HD11	2:A:2065:ILE:HG22	1.92	0.50
2:A:63:LEU:O	2:A:66:ILE:HG22	2.11	0.50
2:A:1678:LEU:HD13	2:A:1679:THR:H	1.76	0.50
1:B:250:THR:O	1:B:251:GLN:C	2.50	0.50
1:B:250:THR:O	1:B:253:LYS:N	2.44	0.50
2:A:2090:LEU:CD1	2:A:2094:MET:HE2	2.41	0.50
1:C:247:SER:O	1:C:250:THR:HG22	2.12	0.49
2:A:596:VAL:HG23	2:A:598:ASP:H	1.77	0.49
2:A:688:THR:O	2:A:692:MET:HG3	2.12	0.49
2:A:612:ILE:HD11	2:A:773:MET:SD	2.53	0.49
2:A:1051:LEU:HD13	2:A:1399:ILE:HD11	1.94	0.49
2:A:2215:ARG:HH11	2:A:2219:LYS:HZ1	1.61	0.49
1:E:217:SER:O	1:E:221:ILE:HG12	2.11	0.49
1:D:235:LEU:O	1:D:239:VAL:HG12	2.13	0.49
1:E:266:ILE:HD11	1:B:270:MET:HB2	1.95	0.49
1:C:296:HIS:CE1	2:A:540:TYR:HE1	2.31	0.49
2:A:393:ASP:N	2:A:393:ASP:OD1	2.45	0.49
2:A:1742:ILE:HG22	2:A:1979:LEU:HB2	1.93	0.49
1:B:275:ILE:HD13	2:A:687:ARG:HD3	1.94	0.49
2:A:582:LEU:HD21	2:A:689:LEU:HD13	1.94	0.49
2:A:53:ARG:HD3	2:A:60:HIS:HE1	1.77	0.49
2:A:1178:GLY:HA2	2:A:1373:LEU:HA	1.95	0.49
2:A:1197:PHE:HE2	2:A:1199:TRP:HB2	1.78	0.49
2:A:1809:ALA:HB3	2:A:1911:CYS:HB3	1.93	0.49
1:C:275:ILE:N	2:A:392:LEU:O	2.46	0.49
1:C:280:ASN:H	2:A:387:CYS:HA	1.78	0.49
1:E:266:ILE:HD13	1:B:266:ILE:HG22	1.94	0.49
1:B:249:VAL:O	1:B:252:ILE:N	2.46	0.49
1:D:228:MET:HG2	1:E:229:ASP:OD1	2.13	0.48
1:D:245:GLN:HA	1:D:248:MET:HB3	1.95	0.48
1:D:266:ILE:CG2	1:C:266:ILE:HD13	2.43	0.48
1:E:266:ILE:HD12	1:B:267:GLU:HA	1.94	0.48
2:A:2213:LEU:HD13	2:A:2221:ILE:HD12	1.95	0.48
1:E:235:LEU:HD22	1:B:235:LEU:HD12	1.95	0.48
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.44	0.48
2:A:1609:SER:OG	2:A:1610:ASP:N	2.42	0.48
1:B:278:PRO:HG3	2:A:679:TYR:CD2	2.47	0.48
2:A:103:LEU:HD22	2:A:208:VAL:HG11	1.94	0.48
2:A:1199:TRP:CE2	2:A:1849:ASN:OD1	2.66	0.48
2:A:1563:SER:OG	2:A:1565:HIS:O	2.31	0.48
2:A:1144:ILE:O	2:A:1148:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:LEU:O	1:E:267:GLU:HG3	2.14	0.48
2:A:88:ILE:HD12	2:A:232:LEU:HD23	1.95	0.48
2:A:740:SER:OG	2:A:742:ARG:NH1	2.46	0.48
1:C:258:THR:O	1:C:262:THR:HG22	2.13	0.48
1:C:260:LYS:HE3	1:C:260:LYS:HB3	1.43	0.48
2:A:126:ASP:OD1	2:A:126:ASP:N	2.45	0.48
2:A:412:TYR:CG	2:A:421:PRO:HG3	2.48	0.48
2:A:990:ARG:NH1	2:A:1009:ILE:HD13	2.28	0.48
2:A:166:LEU:HD21	2:A:893:LEU:HD11	1.95	0.48
2:A:299:VAL:HG11	2:A:362:LEU:HG	1.95	0.48
2:A:321:CYS:HB3	2:A:343:LEU:HD21	1.95	0.48
2:A:1007:LEU:HD11	2:A:1150:LEU:HD21	1.95	0.48
1:D:260:LYS:NZ	1:D:264:ALA:HB2	2.28	0.48
2:A:69:GLU:O	2:A:73:ARG:HG2	2.14	0.48
2:A:1181:ILE:HD11	2:A:1187:CYS:HB2	1.96	0.48
2:A:413:ARG:HD2	2:A:420:TRP:CD1	2.49	0.47
2:A:599:GLN:O	2:A:603:THR:HG22	2.14	0.47
2:A:1805:ILE:HD11	2:A:1828:LEU:HB3	1.97	0.47
2:A:394:PHE:O	2:A:398:MET:HG2	2.14	0.47
1:C:275:ILE:HG21	2:A:680:GLN:HB3	1.97	0.47
1:C:286:VAL:HG22	1:C:290:ARG:HG3	1.95	0.47
2:A:936:LEU:HB2	2:A:1124:ILE:HD13	1.97	0.47
2:A:1449:LEU:HD12	2:A:1685:LEU:HB3	1.96	0.47
2:A:683:ILE:CG2	2:A:684:PRO:HD3	2.45	0.47
1:C:233:GLN:O	1:C:236:GLU:HG3	2.14	0.47
2:A:1024:GLN:HG2	2:A:1085:LEU:HB2	1.96	0.47
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.82	0.47
2:A:1228:ASP:N	2:A:1228:ASP:OD1	2.48	0.47
2:A:1601:PRO:O	2:A:1611:ARG:NH2	2.48	0.47
2:A:1834:TRP:CG	2:A:1906:VAL:HG12	2.50	0.47
1:C:273:VAL:HG23	2:A:394:PHE:CB	2.44	0.46
2:A:865:ILE:HD13	2:A:868:ASP:H	1.80	0.46
2:A:2192:LEU:H	2:A:2197:ASN:ND2	2.12	0.46
2:A:967:ILE:HG21	2:A:1146:ILE:HB	1.97	0.46
2:A:1538:GLY:O	2:A:1542:THR:HG23	2.15	0.46
1:B:258:THR:HA	1:B:261:THR:HG22	1.97	0.46
2:A:1200:PHE:HZ	2:A:1347:MET:HA	1.81	0.46
2:A:125:SER:OG	2:A:164:ARG:N	2.49	0.46
2:A:165:GLU:O	2:A:169:ILE:HG23	2.15	0.46
1:D:249:VAL:O	1:D:252:ILE:HG22	2.16	0.46
1:B:278:PRO:HG3	2:A:679:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1692:LEU:O	2:A:1696:ILE:HG13	2.16	0.46
2:A:1899:VAL:HG21	2:A:1935:HIS:CD2	2.51	0.46
1:D:249:VAL:HA	1:D:252:ILE:HG22	1.98	0.46
2:A:668:THR:HB	2:A:781:GLN:HG2	1.96	0.46
1:E:220:GLU:O	1:E:224:LEU:HG	2.15	0.46
2:A:116:LEU:HD22	2:A:927:LEU:HD23	1.97	0.46
2:A:2151:TRP:CD2	2:A:2225:ILE:HD12	2.51	0.46
1:E:249:VAL:O	1:E:252:ILE:HG22	2.17	0.46
1:B:238:LYS:HB3	1:C:239:VAL:HG21	1.97	0.46
1:B:266:ILE:HD11	1:C:267:GLU:HA	1.97	0.46
1:C:260:LYS:HZ2	1:C:261:THR:HG23	1.81	0.46
2:A:1245:LEU:O	2:A:1249:LEU:HG	2.16	0.46
2:A:1536:ILE:HG21	2:A:1572:THR:HG23	1.97	0.46
2:A:1779:VAL:HG21	2:A:2051:ILE:HD11	1.98	0.45
1:D:229:ASP:HA	1:D:232:LEU:HB3	1.98	0.45
2:A:600:LEU:HD11	2:A:1224:GLY:HA3	1.98	0.45
2:A:1122:GLU:HG2	2:A:1123:ILE:HG23	1.97	0.45
1:C:303:PRO:HG2	2:A:459:ARG:CB	2.37	0.45
1:E:264:ALA:HA	1:E:267:GLU:OE1	2.15	0.45
2:A:1152:LYS:HE2	2:A:1152:LYS:HB2	1.78	0.45
2:A:1386:SER:OG	2:A:1387:CYS:N	2.48	0.45
2:A:1744:ASN:OD1	2:A:1744:ASN:N	2.49	0.45
2:A:2174:ARG:HD3	2:A:2206:GLY:HA2	1.97	0.45
2:A:1513:ARG:HH21	2:A:1633:PRO:HG2	1.82	0.45
2:A:1647:ALA:HA	2:A:1650:THR:HG22	1.98	0.45
2:A:2033:TRP:O	2:A:2037:VAL:HG22	2.17	0.45
2:A:2055:VAL:HB	2:A:2058:GLN:HE21	1.81	0.45
1:B:250:THR:OG1	1:B:251:GLN:N	2.50	0.45
2:A:407:ILE:HG21	2:A:590:MET:HE3	1.98	0.45
2:A:705:ARG:NH1	2:A:708:ARG:HB2	2.32	0.45
2:A:1544:SER:HB2	2:A:1848:ARG:HH11	1.82	0.45
2:A:1847:GLN:O	2:A:1848:ARG:NE	2.49	0.45
2:A:1962:PHE:HZ	2:A:1991:VAL:HG11	1.81	0.45
2:A:2172:ARG:HB2	2:A:2175:ASP:OD2	2.17	0.45
2:A:1409:TYR:HD2	2:A:1411:PRO:HD3	1.82	0.45
2:A:2192:LEU:H	2:A:2197:ASN:HD22	1.64	0.45
2:A:704:LEU:HD22	2:A:708:ARG:HH21	1.82	0.45
2:A:705:ARG:HD2	2:A:705:ARG:HA	1.70	0.45
2:A:1058:ARG:HD3	2:A:1392:PRO:HA	1.99	0.45
2:A:2097:LEU:HD12	2:A:2143:ILE:HD11	1.98	0.45
2:A:2191:TYR:O	2:A:2192:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:MET:O	1:E:226:ARG:HG2	2.17	0.45
2:A:53:ARG:HD3	2:A:60:HIS:CE1	2.52	0.45
2:A:1449:LEU:O	2:A:1453:GLN:HG3	2.17	0.45
1:C:280:ASN:H	2:A:387:CYS:CA	2.30	0.44
2:A:366:ARG:HG3	2:A:366:ARG:HH11	1.81	0.44
2:A:1937:LEU:O	2:A:1941:VAL:HG23	2.17	0.44
2:A:2215:ARG:HD3	2:A:2219:LYS:HZ2	1.81	0.44
1:C:296:HIS:NE2	2:A:540:TYR:HE1	2.14	0.44
2:A:616:SER:OG	2:A:617:GLU:N	2.51	0.44
2:A:690:ASN:HB3	2:A:695:ILE:O	2.18	0.44
2:A:1797:LEU:HD13	2:A:1800:ILE:HD11	1.98	0.44
2:A:1856:GLN:O	2:A:1860:SER:OG	2.34	0.44
1:B:234:HIS:O	1:B:238:LYS:HG2	2.17	0.44
1:C:295:ASP:HA	2:A:542:ARG:HH21	1.82	0.44
2:A:79:TRP:N	2:A:79:TRP:HE3	2.15	0.44
2:A:2189:ARG:HG3	2:A:2191:TYR:O	2.17	0.44
2:A:131:VAL:HG21	2:A:973:LEU:HD23	1.99	0.44
2:A:1199:TRP:CZ2	2:A:1201:PHE:HB2	2.53	0.44
2:A:1558:ILE:HG23	2:A:1574:LEU:HD22	2.00	0.44
2:A:1690:ARG:H	2:A:1690:ARG:HD3	1.82	0.44
1:D:236:GLU:HA	1:D:239:VAL:HG12	1.99	0.44
2:A:395:GLN:HG3	2:A:452:TRP:CH2	2.53	0.44
1:C:245:GLN:O	1:C:249:VAL:HG23	2.17	0.44
2:A:1935:HIS:HA	2:A:1938:LEU:CD2	2.47	0.44
2:A:2182:ILE:HG21	2:A:2201:PHE:HZ	1.83	0.44
1:C:277:ASP:O	2:A:389:PRO:HA	2.17	0.44
2:A:431:LYS:O	2:A:435:GLU:HG3	2.18	0.44
2:A:269:ARG:HA	2:A:349:GLN:HG3	1.99	0.44
2:A:890:GLU:HG3	2:A:1359:ASN:ND2	2.32	0.44
2:A:1774:PRO:HA	2:A:1775:PRO:HD3	1.88	0.44
2:A:32:LEU:HD11	2:A:66:ILE:HG23	1.99	0.43
1:D:243:LEU:HD21	1:C:238:LYS:HB3	1.98	0.43
2:A:412:TYR:CE2	2:A:463:CYS:HB3	2.53	0.43
2:A:2182:ILE:HG21	2:A:2201:PHE:CZ	2.53	0.43
1:D:270:MET:HG2	1:C:269:MET:HG3	2.00	0.43
2:A:1077:ARG:O	2:A:1081:ILE:HG13	2.18	0.43
2:A:1964:PHE:O	2:A:1968:VAL:HG12	2.18	0.43
2:A:2062:ASP:O	2:A:2066:ILE:HG12	2.18	0.43
1:D:258:THR:O	1:D:262:THR:HG22	2.18	0.43
2:A:301:ALA:HB1	2:A:317:TYR:HA	2.00	0.43
2:A:366:ARG:HG3	2:A:366:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:408:LEU:HD12	2:A:692:MET:HE1	2.01	0.43
1:C:240:ASP:O	1:C:243:LEU:HG	2.19	0.43
2:A:7:ILE:HD11	2:A:1106:LEU:HD12	1.99	0.43
2:A:1204:LYS:HE2	2:A:1889:ASP:OD1	2.18	0.43
2:A:1443:ILE:HG23	2:A:1488:THR:HA	2.01	0.43
2:A:1960:ASN:OD1	2:A:1960:ASN:N	2.51	0.43
2:A:1614:ASN:O	2:A:1618:ARG:HG3	2.19	0.43
2:A:2028:LEU:HD23	2:A:2028:LEU:HA	1.92	0.43
2:A:22:LYS:NZ	2:A:238:GLU:OE1	2.40	0.43
2:A:65:GLN:OE1	2:A:65:GLN:HA	2.19	0.43
2:A:192:LEU:HB3	2:A:219:PRO:HG3	2.00	0.43
2:A:1562:ASN:HD21	2:A:2220:ARG:HG2	1.83	0.43
2:A:286:ASP:OD2	2:A:372:THR:OG1	2.36	0.43
2:A:304:GLN:O	2:A:304:GLN:HG3	2.19	0.43
2:A:1016:THR:O	2:A:1020:LYS:HG3	2.19	0.43
2:A:1144:ILE:HB	2:A:1382:ARG:NH2	2.34	0.43
2:A:1945:LYS:HB2	2:A:1945:LYS:HE2	1.68	0.43
2:A:169:ILE:O	2:A:173:ASN:HB2	2.18	0.43
2:A:1094:TYR:CZ	2:A:1098:VAL:HG11	2.54	0.43
2:A:2103:LYS:HB2	2:A:2103:LYS:HE3	1.81	0.43
1:D:249:VAL:HB	1:C:248:MET:CE	2.48	0.42
2:A:73:ARG:HH12	2:A:209:ASP:HB2	1.84	0.42
2:A:590:MET:SD	2:A:755:MET:HG2	2.59	0.42
2:A:1372:HIS:HB3	2:A:1374:HIS:CD2	2.54	0.42
2:A:1669:ILE:O	2:A:1672:MET:HG2	2.19	0.42
2:A:1931:ARG:HD3	2:A:1935:HIS:HE1	1.84	0.42
2:A:2064:ASN:O	2:A:2068:GLN:HG3	2.18	0.42
1:D:229:ASP:O	1:D:232:LEU:HB3	2.20	0.42
2:A:161:PRO:HG2	2:A:893:LEU:HD13	2.01	0.42
2:A:268:LYS:HE3	2:A:268:LYS:HB2	1.84	0.42
2:A:2221:ILE:O	2:A:2225:ILE:HG12	2.18	0.42
2:A:393:ASP:O	2:A:397:ILE:HG13	2.19	0.42
2:A:565:ALA:HB3	2:A:745:ILE:HG21	2.01	0.42
1:D:232:LEU:HB2	1:E:232:LEU:HD11	2.01	0.42
2:A:120:THR:HG22	2:A:903:ILE:HD13	2.00	0.42
2:A:939:LEU:HB3	2:A:945:GLY:HA3	2.02	0.42
2:A:1598:ILE:HB	2:A:1678:LEU:HD22	2.02	0.42
2:A:1641:PRO:O	2:A:1644:LYS:HG2	2.19	0.42
2:A:1669:ILE:HD13	2:A:1669:ILE:HA	1.86	0.42
2:A:1857:PHE:HE1	2:A:1862:PRO:HB2	1.84	0.42
2:A:1972:PHE:HD1	2:A:1973:PHE:CD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:GLY:HA2	1:E:249:VAL:HG12	2.00	0.42
1:E:273:VAL:HG21	1:B:270:MET:HE2	2.01	0.42
1:B:266:ILE:CD1	1:C:267:GLU:HA	2.49	0.42
1:C:274:LYS:HZ2	2:A:393:ASP:CG	2.22	0.42
2:A:34:ASN:HA	2:A:88:ILE:HG21	2.00	0.42
2:A:482:SER:N	2:A:567:MET:O	2.36	0.42
2:A:1485:CYS:HA	2:A:1488:THR:HG22	2.02	0.42
2:A:1939:ILE:O	2:A:1943:VAL:HG22	2.19	0.42
2:A:53:ARG:HG2	2:A:60:HIS:ND1	2.34	0.42
2:A:90:ILE:HG22	2:A:91:TRP:H	1.85	0.42
2:A:1105:LYS:HA	2:A:1108:THR:HG22	2.02	0.42
2:A:1796:VAL:O	2:A:1800:ILE:HG12	2.20	0.42
1:B:246:GLY:O	1:B:247:SER:C	2.58	0.42
1:B:246:GLY:O	1:B:249:VAL:N	2.52	0.42
1:B:281:PRO:HB2	1:C:296:HIS:HA	2.00	0.42
1:C:296:HIS:HE2	2:A:540:TYR:HE1	1.68	0.42
2:A:844:TYR:HD2	2:A:847:ARG:HH21	1.68	0.42
1:E:235:LEU:HD13	1:B:235:LEU:HD12	2.02	0.42
1:B:221:ILE:HD12	1:B:221:ILE:H	1.85	0.42
1:B:247:SER:O	1:B:248:MET:C	2.58	0.42
2:A:861:LEU:O	2:A:905:GLN:NE2	2.52	0.42
2:A:1079:LYS:HB3	2:A:1079:LYS:HE2	1.77	0.42
2:A:1293:SER:O	2:A:1293:SER:OG	2.32	0.42
2:A:1458:ILE:HG13	2:A:1459:THR:N	2.34	0.42
2:A:1502:LEU:HD23	2:A:1502:LEU:HA	1.87	0.42
2:A:1670:ARG:HA	2:A:1673:ILE:HD12	2.01	0.42
2:A:1931:ARG:O	2:A:1935:HIS:ND1	2.53	0.42
2:A:2081:LEU:HB2	2:A:2149:ARG:HG2	2.02	0.42
1:D:225:LEU:HD21	1:E:225:LEU:HB3	2.01	0.42
2:A:596:VAL:HG23	2:A:598:ASP:N	2.35	0.42
2:A:667:THR:HG21	2:A:837:ILE:HB	2.01	0.42
2:A:867:GLY:H	2:A:1016:THR:HG22	1.83	0.42
2:A:2131:LYS:HA	2:A:2134:THR:HG22	2.02	0.42
1:C:284:VAL:HB	1:C:289:LEU:HD21	2.01	0.41
2:A:1443:ILE:HB	2:A:1444:PRO:HD3	2.02	0.41
2:A:1450:THR:O	2:A:1454:MET:HG3	2.20	0.41
2:A:1558:ILE:HD13	2:A:1558:ILE:HA	1.93	0.41
2:A:1933:GLN:O	2:A:1937:LEU:HG	2.19	0.41
2:A:2106:ILE:HG13	2:A:2191:TYR:CE1	2.55	0.41
1:E:246:GLY:O	1:E:249:VAL:HG12	2.19	0.41
2:A:572:ARG:HA	2:A:572:ARG:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1131:GLN:H	2:A:1131:GLN:HG2	1.44	0.41
2:A:1933:GLN:HE21	2:A:1965:LEU:HD11	1.84	0.41
2:A:1934:VAL:HG23	2:A:2006:PHE:HE2	1.84	0.41
1:B:276:MET:HG2	2:A:683:ILE:HG21	2.02	0.41
1:C:275:ILE:O	2:A:392:LEU:N	2.53	0.41
1:C:286:VAL:O	1:C:287:ASP:C	2.58	0.41
2:A:1197:PHE:HB3	2:A:1374:HIS:ND1	2.35	0.41
2:A:256:LEU:HD22	2:A:856:VAL:HG21	2.02	0.41
2:A:1201:PHE:HB3	2:A:1322:HIS:HB2	2.02	0.41
2:A:2190:LYS:HA	2:A:2190:LYS:HD2	1.82	0.41
2:A:824:LEU:HD23	2:A:824:LEU:HA	1.86	0.41
2:A:1443:ILE:HG12	2:A:1696:ILE:HD13	2.01	0.41
1:D:218:ALA:O	1:D:221:ILE:HG22	2.20	0.41
1:B:246:GLY:O	1:B:249:VAL:HB	2.21	0.41
2:A:970:VAL:HG11	2:A:984:LEU:HD13	2.02	0.41
2:A:1033:ASN:HB3	2:A:1035:MET:O	2.21	0.41
1:E:259:VAL:HG12	1:E:260:LYS:N	2.36	0.41
2:A:18:ILE:HG22	2:A:372:THR:HA	2.03	0.41
2:A:79:TRP:HE3	2:A:79:TRP:H	1.68	0.41
2:A:468:PRO:HB2	2:A:528:PRO:HB2	2.03	0.41
2:A:679:TYR:HA	2:A:682:ILE:HG13	2.03	0.41
2:A:1429:THR:O	2:A:1433:GLY:HA2	2.21	0.41
1:E:259:VAL:CG2	1:B:263:LEU:CD2	2.98	0.41
1:B:242:VAL:HA	1:B:245:GLN:CD	2.41	0.41
2:A:404:PHE:CE1	2:A:755:MET:HE3	2.56	0.41
2:A:711:LEU:HG	2:A:741:PRO:HG3	2.03	0.41
2:A:1527:THR:O	2:A:1531:ILE:HG23	2.20	0.41
2:A:1944:LEU:HB2	2:A:1997:LEU:HD22	2.03	0.41
1:C:280:ASN:H	2:A:387:CYS:C	2.24	0.41
2:A:79:TRP:HB2	2:A:84:ARG:HB3	2.02	0.41
2:A:263:LEU:HD12	2:A:266:LEU:HD12	2.03	0.41
2:A:364:ILE:HA	2:A:367:LEU:HG	2.02	0.41
2:A:474:ILE:HG13	2:A:475:PHE:N	2.36	0.41
2:A:540:TYR:HD1	2:A:540:TYR:H	1.68	0.41
2:A:1270:TYR:HA	2:A:1284:LEU:CD2	2.51	0.41
2:A:1813:LEU:HD12	2:A:1893:LEU:HD21	2.03	0.40
2:A:1971:GLN:OE1	2:A:2012:ARG:HD3	2.21	0.40
2:A:2077:LYS:HE3	2:A:2077:LYS:HB3	1.79	0.40
1:D:267:GLU:HB3	1:C:266:ILE:HD11	2.03	0.40
1:B:265:THR:HG21	2:A:453:LYS:HD3	2.03	0.40
2:A:396:THR:O	2:A:400:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:444:LYS:O	2:A:448:VAL:HG23	2.21	0.40
2:A:683:ILE:HG23	2:A:684:PRO:HD3	2.03	0.40
2:A:793:LEU:O	2:A:798:LYS:NZ	2.46	0.40
2:A:1907:GLY:O	2:A:1910:THR:OG1	2.38	0.40
2:A:482:SER:HB2	2:A:566:LYS:HG3	2.04	0.40
2:A:881:VAL:O	2:A:885:THR:HG23	2.21	0.40
2:A:971:LYS:HD2	2:A:1139:VAL:O	2.21	0.40
2:A:1526:MET:HE3	2:A:1526:MET:HB3	1.88	0.40
2:A:1989:HIS:H	2:A:2036:ARG:HH21	1.69	0.40
1:D:225:LEU:CD2	1:E:225:LEU:HD13	2.51	0.40
1:D:228:MET:SD	1:E:232:LEU:HD13	2.61	0.40
2:A:49:TRP:HB2	2:A:53:ARG:NH2	2.37	0.40
2:A:607:LEU:HD13	2:A:1221:PRO:HD2	2.03	0.40
2:A:1883:LEU:HD13	2:A:1902:ILE:HG12	2.03	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	B	67/391 (17%)	64 (96%)	3 (4%)	0	100	100
1	C	89/391 (23%)	85 (96%)	4 (4%)	0	100	100
1	D	58/391 (15%)	58 (100%)	0	0	100	100
1	E	56/391 (14%)	56 (100%)	0	0	100	100
2	A	2039/2261 (90%)	1991 (98%)	48 (2%)	0	100	100
All	All	2309/3825 (60%)	2254 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	59/324 (18%)	59 (100%)	0	100 100
1	C	78/324 (24%)	73 (94%)	5 (6%)	17 43
1	D	52/324 (16%)	52 (100%)	0	100 100
1	E	50/324 (15%)	48 (96%)	2 (4%)	31 62
2	A	1858/2037 (91%)	1846 (99%)	12 (1%)	86 95
All	All	2097/3333 (63%)	2078 (99%)	19 (1%)	79 92

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

Mol	Chain	Res	Type
1	E	245	GLN
1	E	259	VAL
1	C	250	THR
1	C	260	LYS
1	C	262	THR
1	C	263	LEU
1	C	295	ASP
2	A	79	TRP
2	A	126	ASP
2	A	170	TRP
2	A	304	GLN
2	A	360	GLU
2	A	393	ASP
2	A	1131	GLN
2	A	1358	ASN
2	A	1380	CYS
2	A	1381	ILE
2	A	1644	LYS
2	A	1933	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	251	GLN
1	B	233	GLN
2	A	451	ASN
2	A	887	ASN
2	A	1778	HIS
2	A	1933	GLN
2	A	2011	ASN
2	A	2150	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

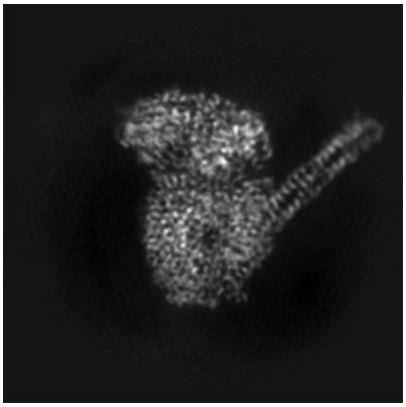
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35864. These allow visual inspection of the internal detail of the map and identification of artifacts.

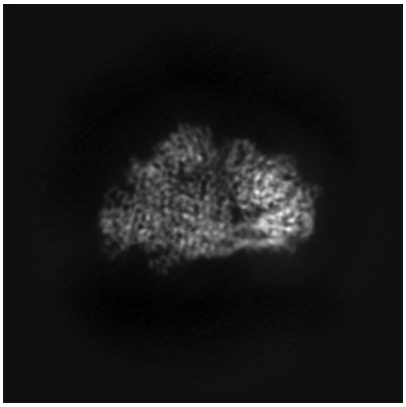
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

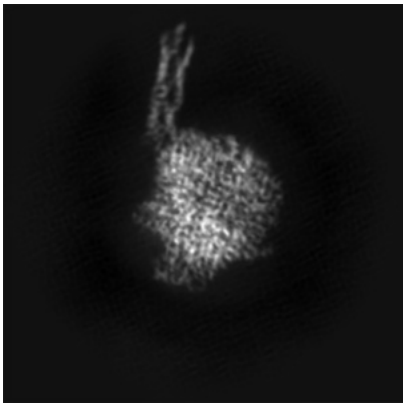
6.1.1 Primary map



X



Y



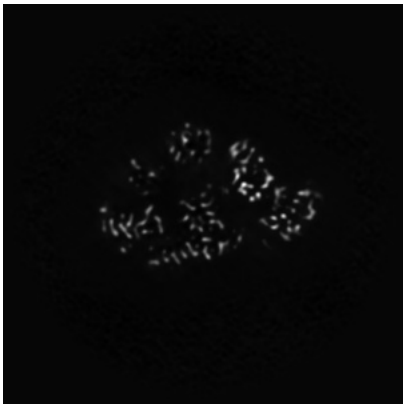
Z

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

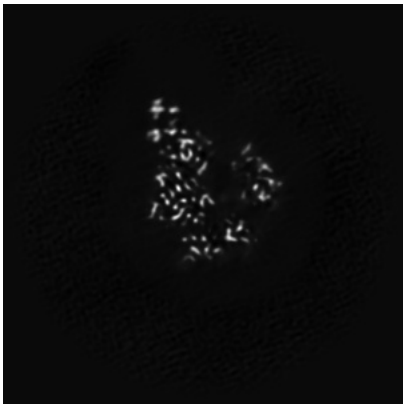
6.2 Central slices

6.2.1 Primary map

X Index: 220



Y Index: 220

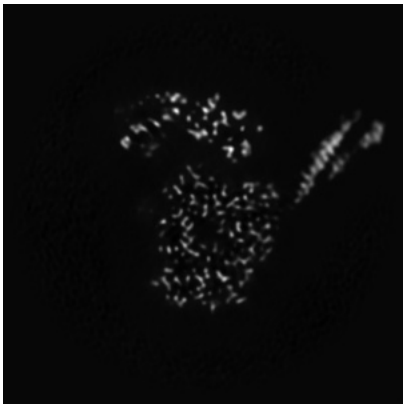


Z Index: 220

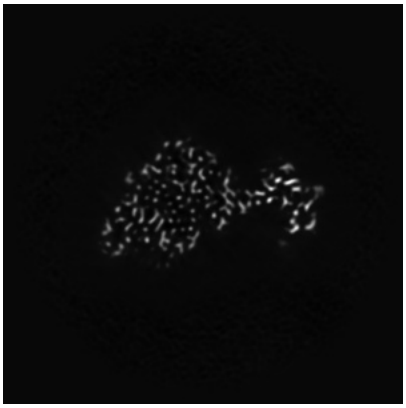
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

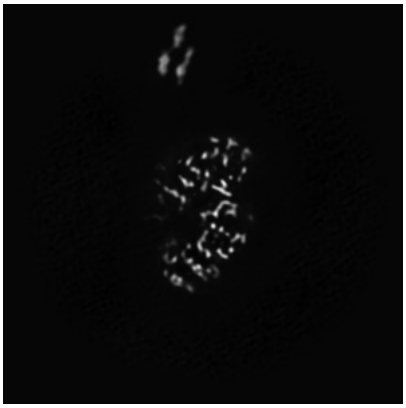
6.3.1 Primary map



X Index: 194



Y Index: 189

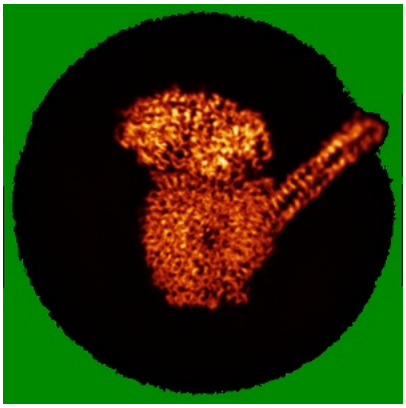


Z Index: 290

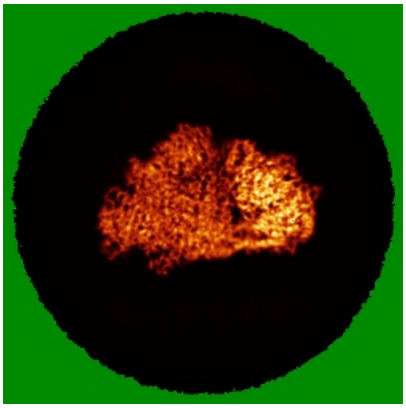
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

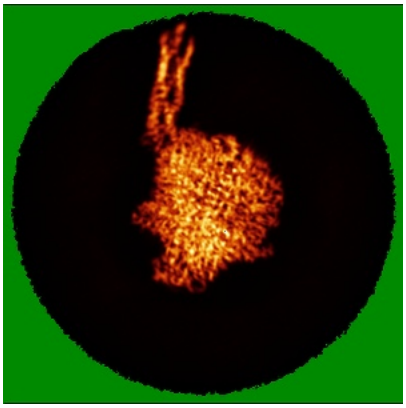
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

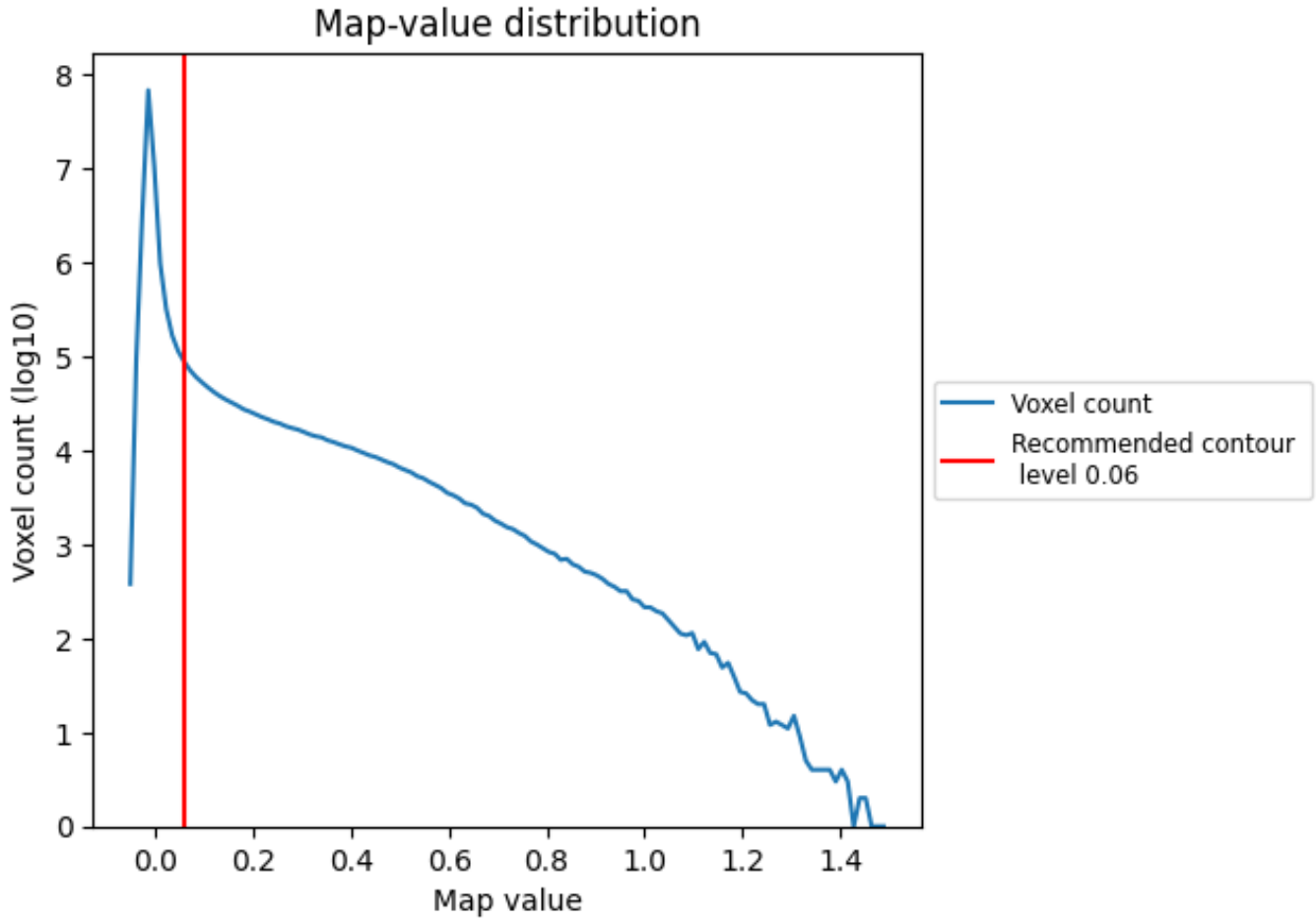
6.6 Mask visualisation (i)

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

7 Map analysis

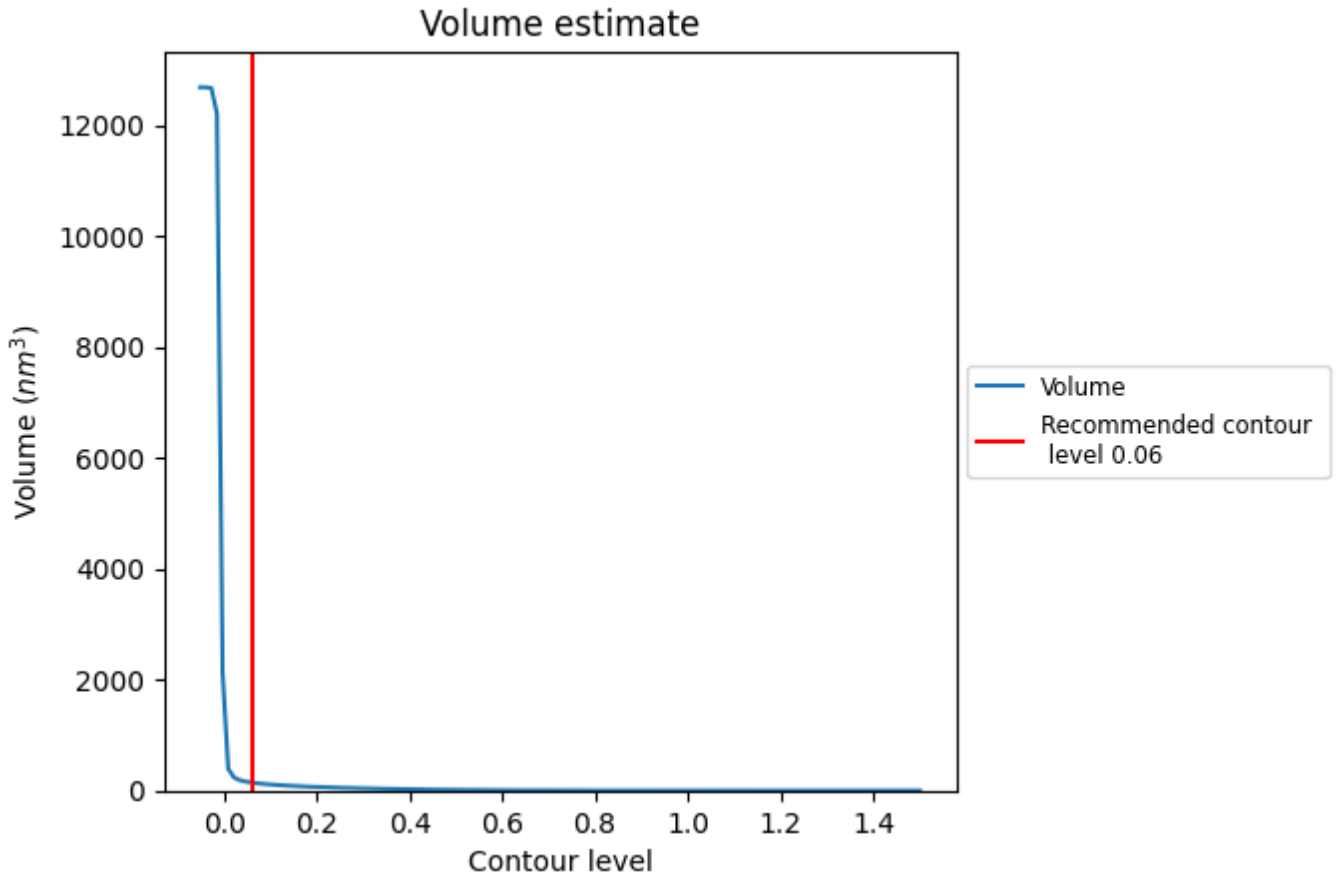
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

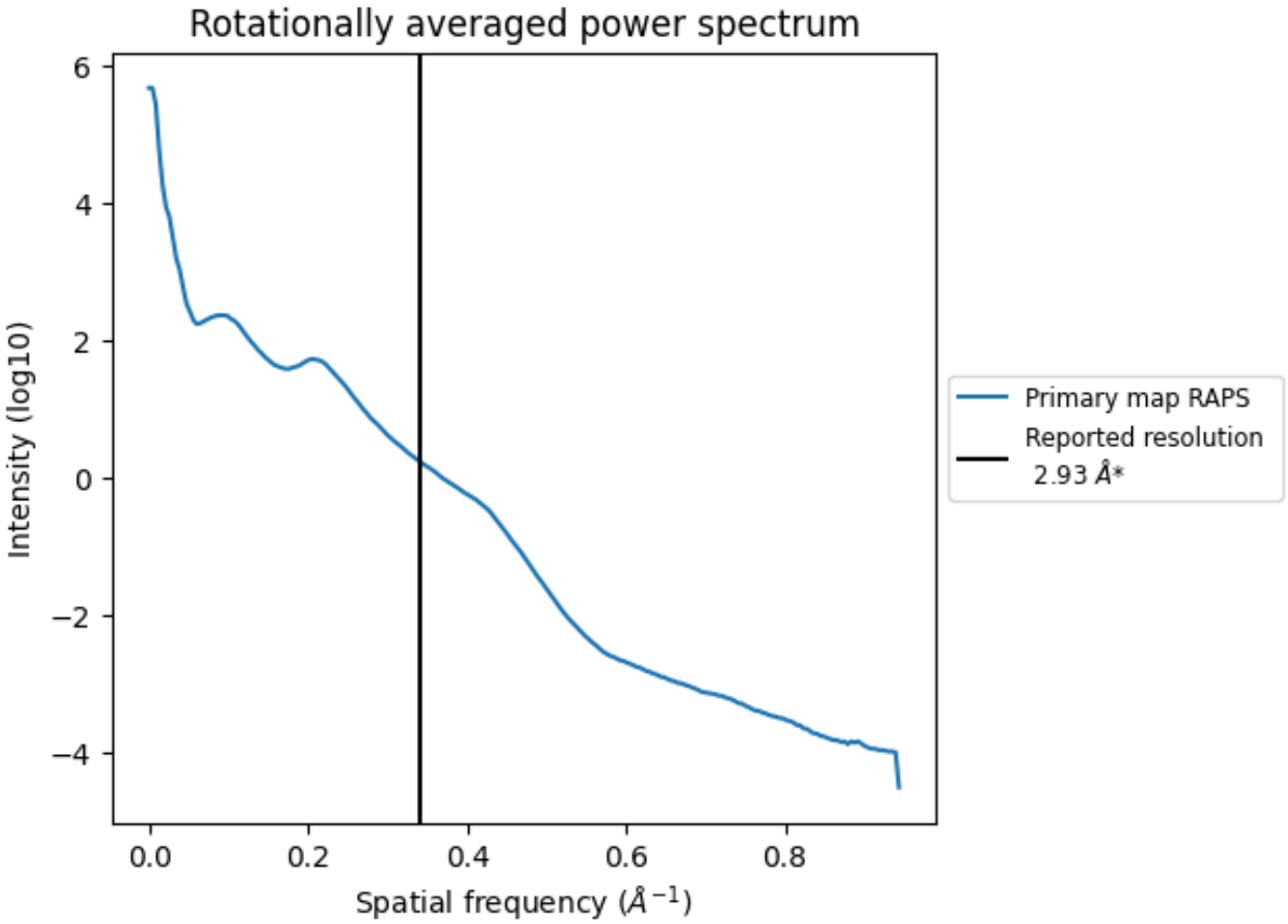
7.2 Volume estimate (i)



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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)

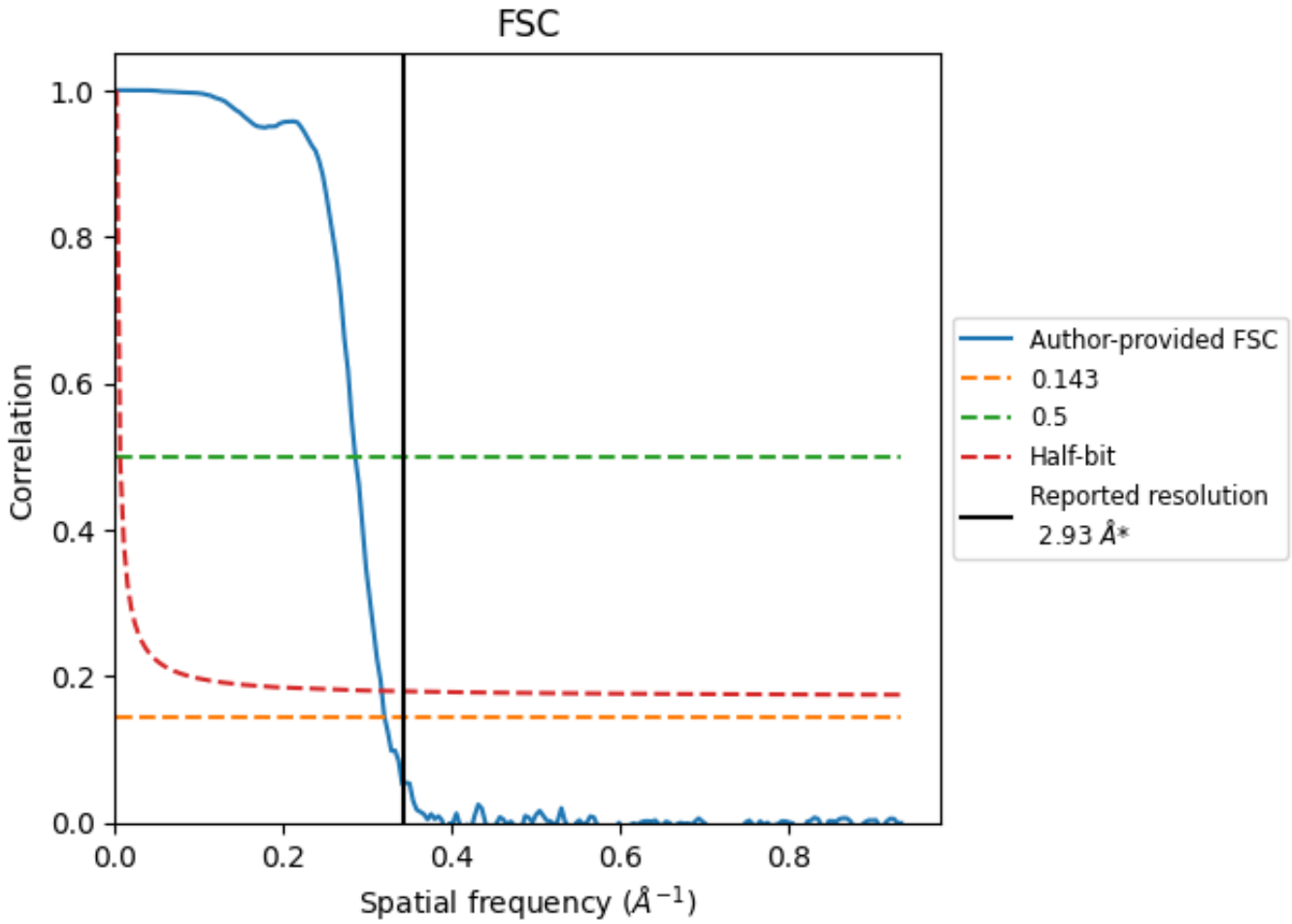


*Reported resolution corresponds to spatial frequency of 0.341 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

8.2 Resolution estimates (i)

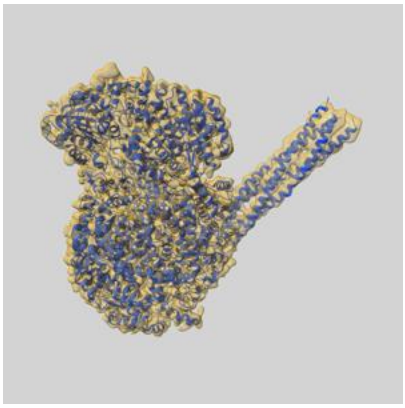
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	3.13	3.51	3.16
Unmasked-calculated*	-	-	-

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

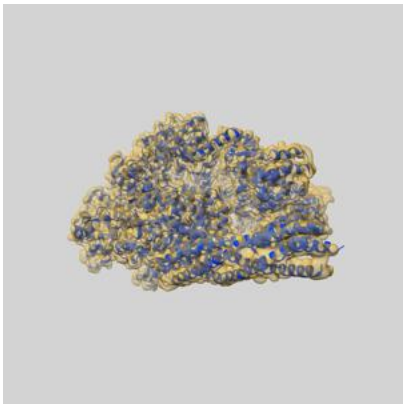
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35864 and PDB model 8IZL. Per-residue inclusion information can be found in section 3 on page 4.

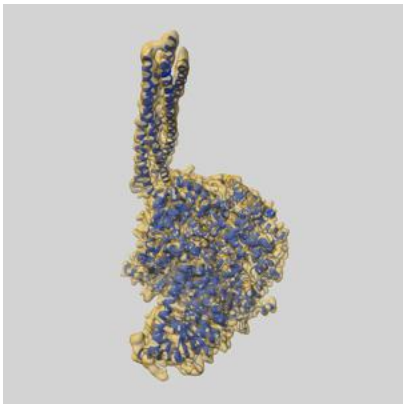
9.1 Map-model overlay



X



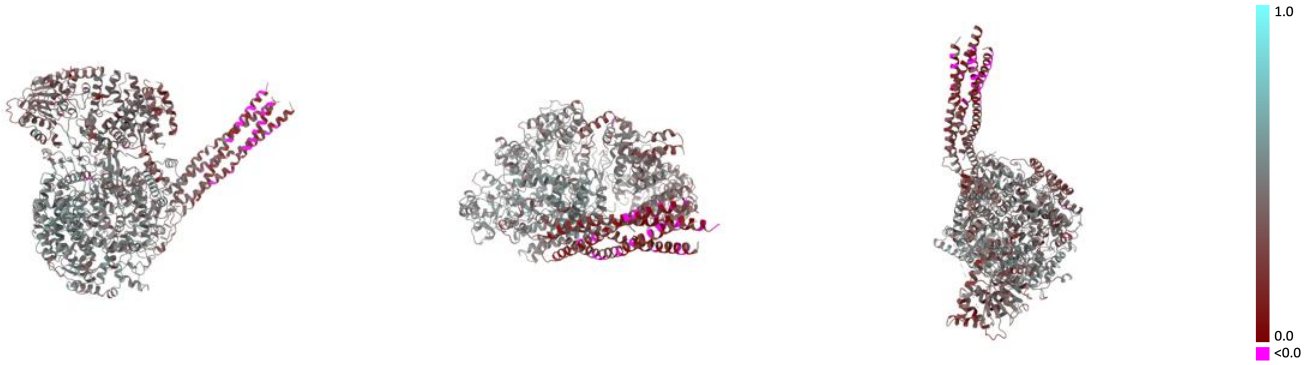
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

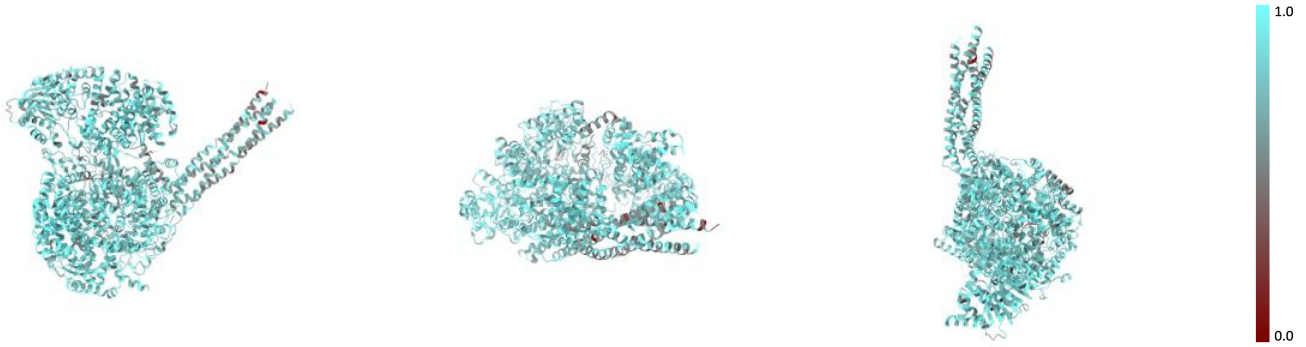
9.2 Q-score mapped to coordinate model (i)



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.

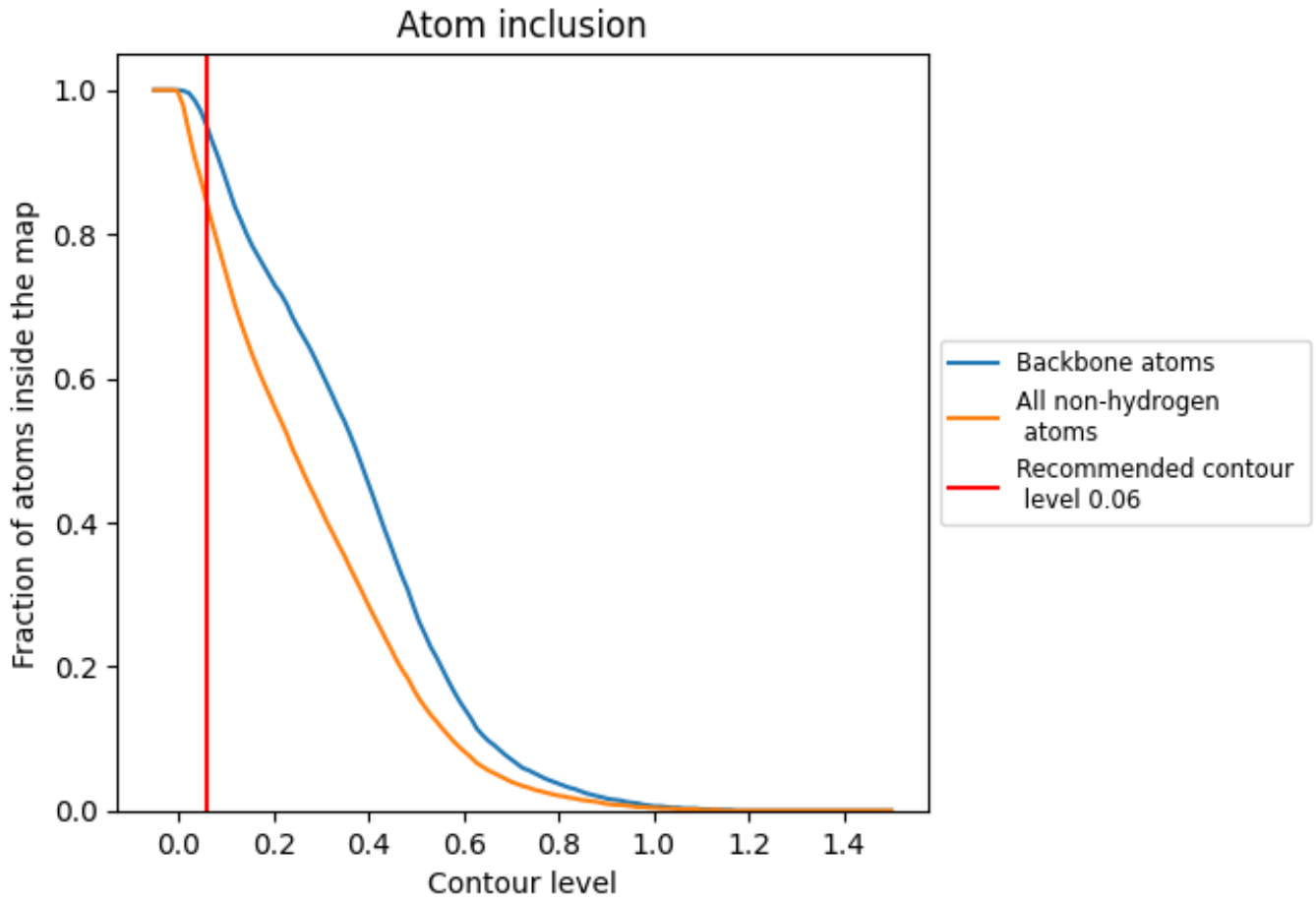
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.4200
A	0.8590	0.4450
B	0.7660	0.2650
C	0.7320	0.2430
D	0.6770	0.1700
E	0.6810	0.1670