Full wwPDB EM Validation Report ⓘ

Sep 4, 2024 – 04:20 PM EDT

PDB ID	:	9C47
EMDB ID	:	EMD-45176
Title	:	TRRAP module of the human TIP60 complex
Authors	:	Yang, Z.; Mameri, A.; Florez Ariza, A.J.; Cote, J.; Nogales, E.
Deposited on	:	2024-06-03
Resolution	:	3.40 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:

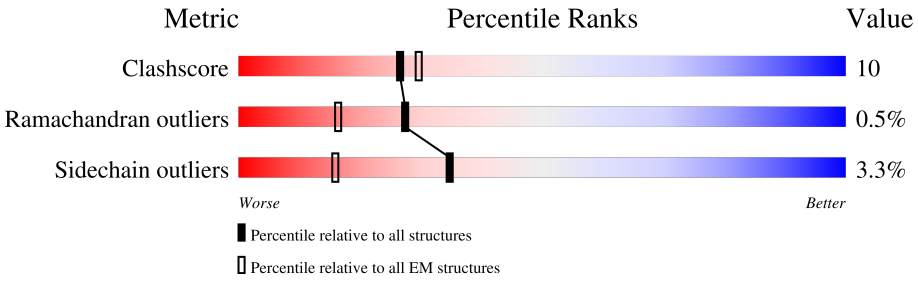
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	3859	9% 60% 19% 20%
2	G	3159	96%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 52167 atoms, of which 26380 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 Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	3079	50044	15891	25317	4263	4390	183	0	0

- Molecule 2 is a protein called E1A-binding protein p400.

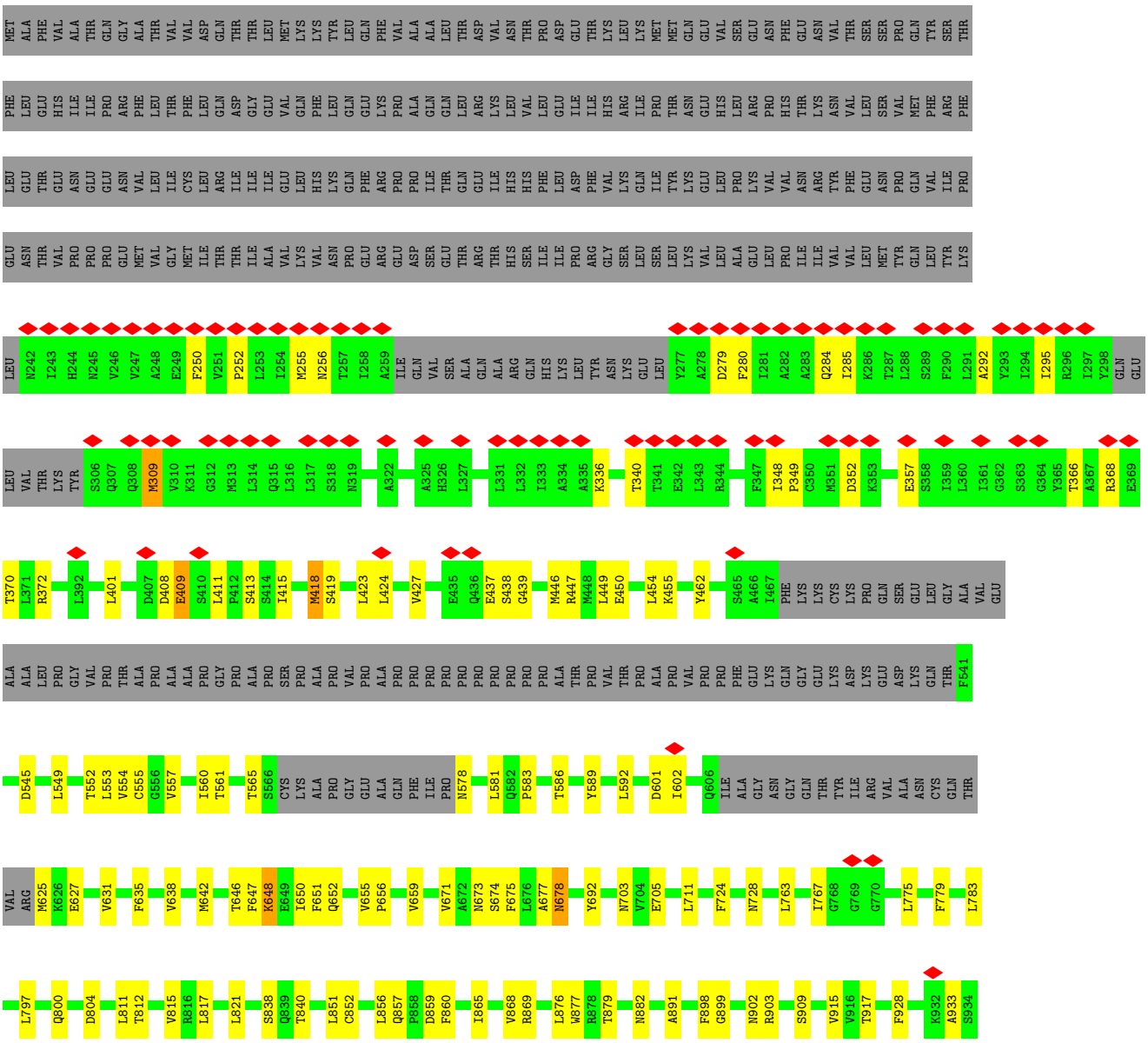
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	G	133	2123	669	1063	186	201	4	0	0

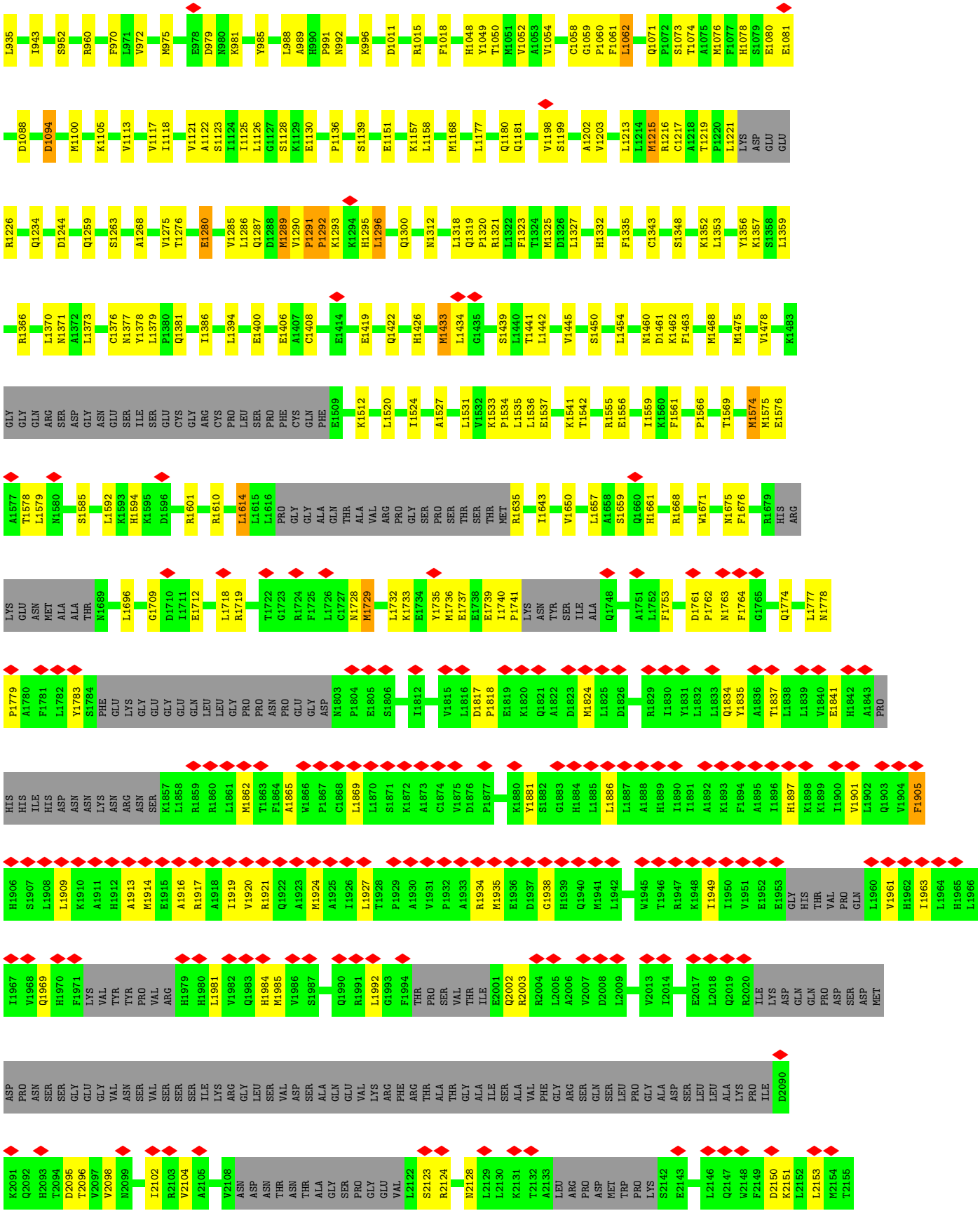
3 Residue-property plots (i)

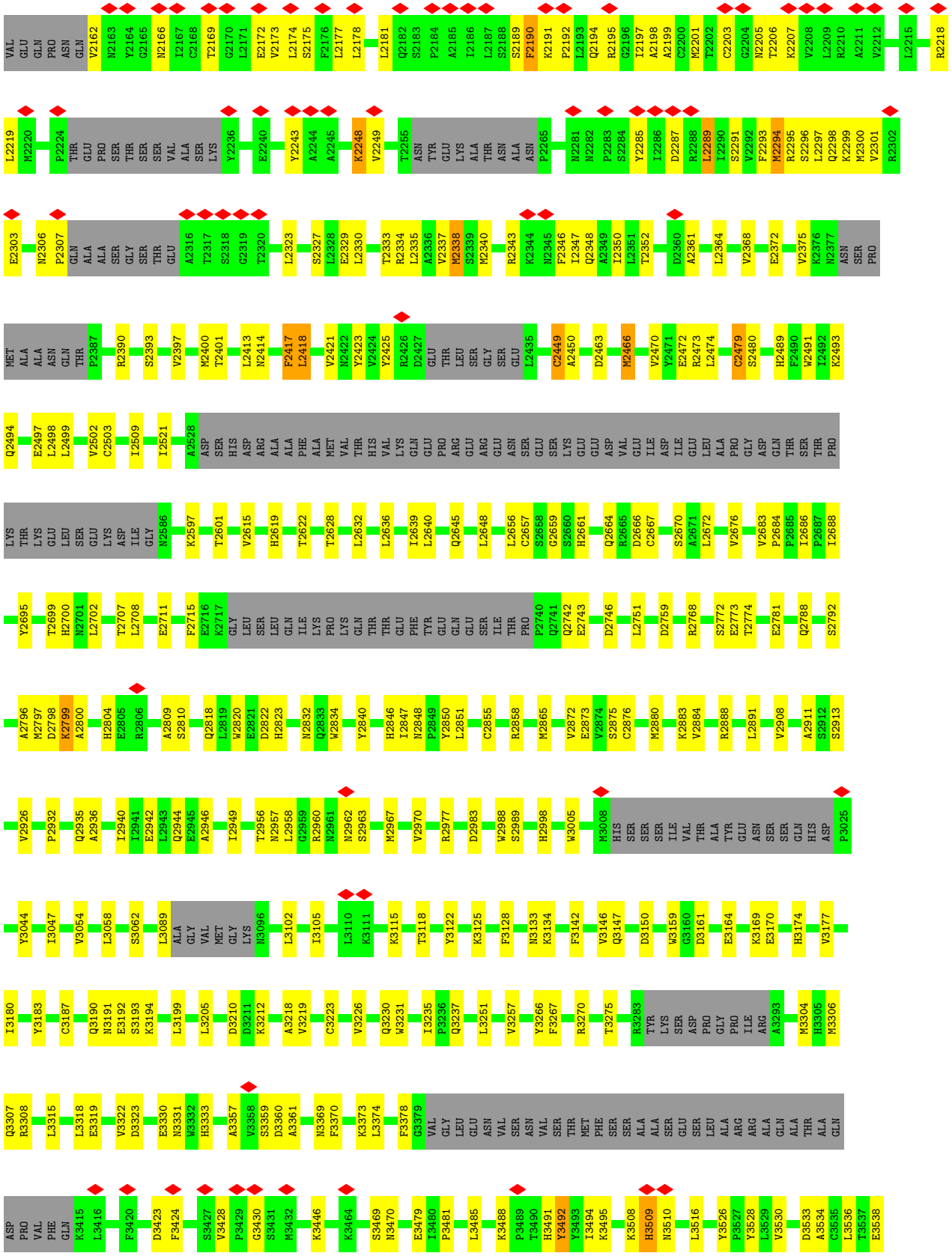
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

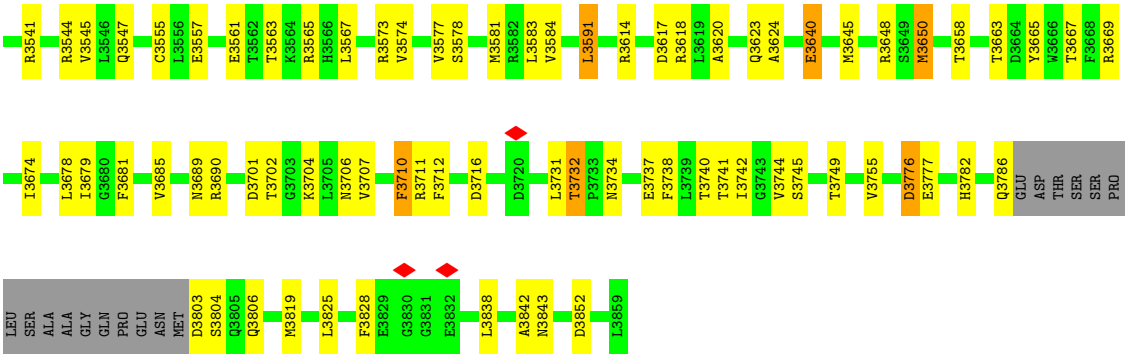
- Molecule 1: Transformation/transcription domain-associated protein

Chain C:



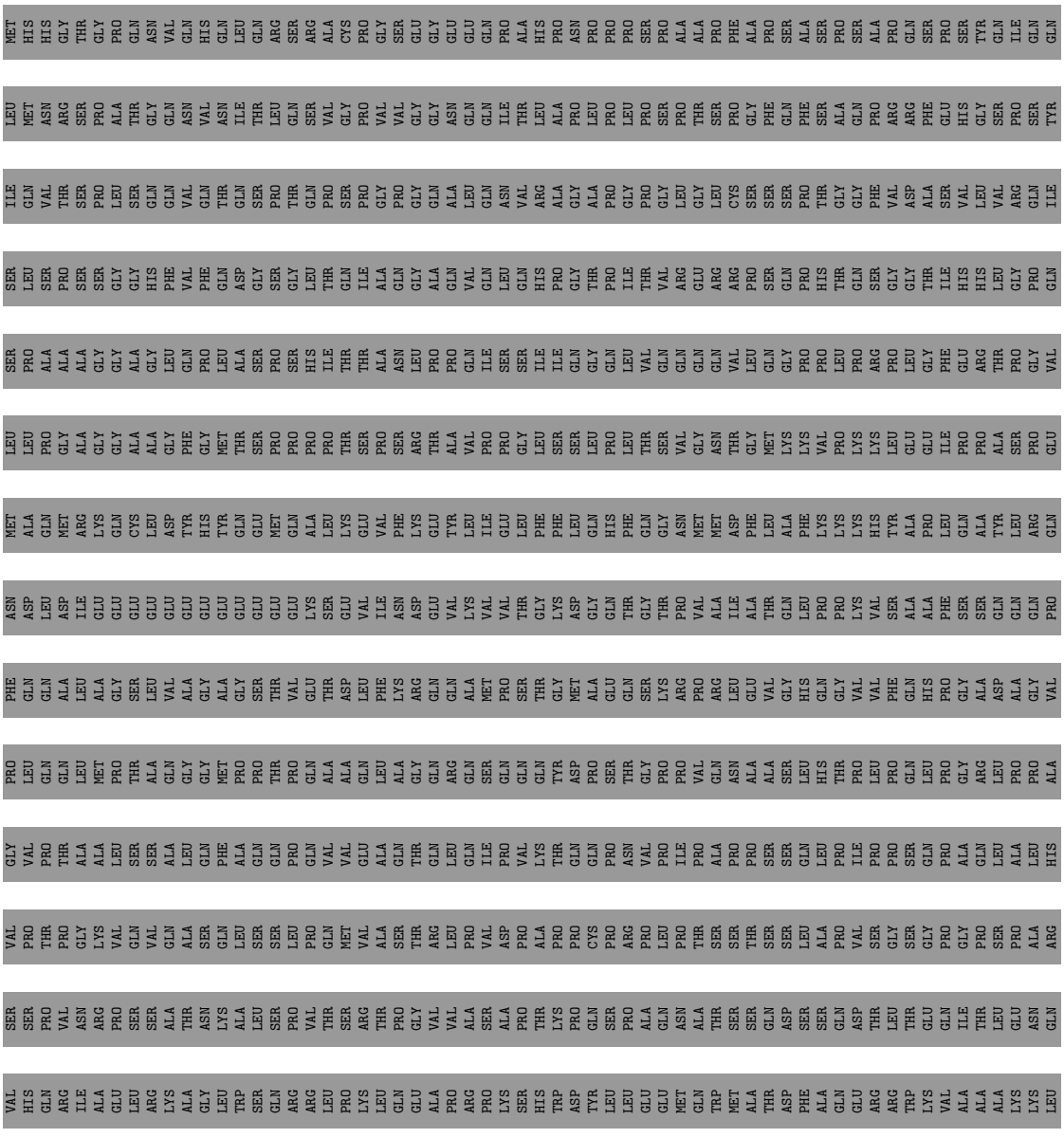

L935 I943 S952 R960 F970 L971 V972 M975 E978 D979 N980 K981 Y985 L988 A989 H990 P991 N992 K996 D1011 R1015 F1018 H1048 Y1049 T1050 M1051 V1052 A1053 V1054 C1058 G1059 P1060 F1061 L1062 Q1071 P1072 S1073 T1074 A1075 M1076 F1077 H1078 S1079 E1080 E1081
D1088 D1094 M1100 K1105 V1113 V1117 I1118 V1121 A1122 S1123 I1124 I1125 L1126 G1127 S1128 K1129 E1130 P1136 S1139 E1151 K1157 L1158 M1168 L1177 Q1180 Q1181 V1198 S1199 A1202 V1203 L1213 L1214 M1215 R1216 C1217 A1218 T1219 P1220 L1221 LYS ASP GLU GLU
R1226 Q1234 D1244 Q1259 S1263 A1268 V1275 T1276 E1280 V1285 L1286 Q1287 D1288 M1289 V1290 P1291 P1292 K1293 K1294 H1295 L1296 Q1300 N1312 L1318 Q1319 P1320 R1321 L1322 F1323 T1324 M1325 D1326 L1327 H1332 F1335 C1343 S1348 K1352 L1353 Y1356 K1357 S1358 L1359
R1366 L1370 N1371 A1372 L1373 C1376 N1377 Y1378 L1379 P1380 Q1381 I1386 L1394 E1400 E1406 A1407 C1408 E1414 E1419 Q1422 H1426 M1433 L1434 G1435 S1439 L1440 T1441 L1442 V1445 S1450 L1454 N1460 D1461 K1462 F1463 M1468 M1475 V1478 K1483
GLY GLY GLN ARG SER ASP GLY ASN GLU SER ILE SER GLU CYS GLY ARG CYS PRO LEU SER PRO PHE CYS GLN PHE E1509 K1512 L1520 I1524 A1527 L1531 V1532 K1533 P1534 L1535 L1536 E1537 K1541 T1542 R1555 E1556 I1559 K1560 F1561 P1566 T1569 M1574 M1575 E1576
A1577 T1578 L1579 N1580 S1585 L1592 K1593 H1594 K1595 D1596 R1601 R1610 L1614 L1615 L1616 PRO GLY GLY ALA GLN THR ALA VAL ARG PRO GLY SER PRO SER THR SER THR MET R1635 I1643 V1650 L1657 A1658 S1659 Q1660 H1661 R1668 W1671 N1675 F1676 R1679 HIS ARG
LYS GLU ASN MET ALA ALA THR N1689 L1696 G1709 D1710 I1711 E1712 L1718 R1719 T1722 G1723 R1724 F1725 L1726 C1727 N1728 M1729 L1732 K1733 E1734 Y1735 M1736 E1737 E1738 E1739 I1740 P1741 LYS ASN TYR SER ILE ALA Q1748 A1751 L1752 F1753 D1761 P1762 N1763 F1764 G1765 Q1774 L1777 N1778
P1779 A1780 F1781 L1782 Y1783 S1784 PHE GLU LYS GLY GLU GLY GLU GLN LEU LEU GLY PRO PRO ASN PRO GLU GLY ASP N1803 P1804 E1805 S1806 I1812 V1815 L1816 D1817 P1818 E1819 K1820 Q1821 A1822 D1823 M1824 L1825 D1826 R1829 I1830 Y1831 L1832 L1833 Q1834 Y1835 A1836 T1837 L1838 L1839 V1840 E1841 H1842 A1843 PRO
HIS HIS ILE HIS ASP ASN ASN LYS ASN ARG ASN SER K1857 L1858 R1859 R1860 L1861 M1862 T1863 F1864 A1865 W1866 P1867 C1868 L1869 L1870 S1871 K1872 A1873 C1874 V1875 D1876 P1877 K1880 Y1881 S1882 G1883 H1884 L1885 L1886 L1887 A1888 H1889 I1890 I1891 A1892 K1893 F1894 A1895 I1896 H1897 K1898 K1899 I1900 V1901 L1902 Q1903 V1904 F1905
H1906 S1907 L1908 L1909 K1910 A1911 H1912 A1913 M1914 E1915 A1916 R1917 A1918 I1919 V1920 R1921 Q1922 A1923 M1924 A1925 I1926 L1927 T1928 P1929 A1930 V1931 P1932 A1933 R1934 M1935 E1936 D1937 G1938 H1939 Q1940 M1941 L1942 W1945 T1946 R1947 K1948 I1949 I1950 V1951 E1952 E1953 GLY HIS THR VAL PRO GLN L1960 V1961 H1962 I1963 L1964 H1965 L1966
I1967 V1968 Q1969 H1970 F1971 LYS VAL TYR TYR PRO VAL ARG H1979 H1980 L1981 V1982 Q1983 H1984 M1985 V1986 S1987 Q1990 R1991 L1992 G1993 F1994 THR PRO SER VAL THR ILE E2001 Q2002 R2003 R2004 L2005 A2006 V2007 D2008 L2009 V2013 I2014 E2017 L2018 Q2019 R2020 ILE LYS ASP GLN GLN PRO ASP SER ASP MET
ASP PRO ASN SER SER GLY GLU GLY VAL ASN SER VAL SER SER SER ILE LYS ARG GLY LEU SER VAL ASP SER ALA GLN GLU VAL LYS ARG PHE ARG THR ALA THR GLY ALA ILE SER ALA VAL PHE GLY ARG SER GLN SER LEU PRO GLY ALA ASP SER LEU LEU ALA LYS PRO ILE D2090
K2091 Q2092 H2093 T2094 D2095 T2096 V2097 V2098 N2099 I2102 R2103 V2104 A2105 V2106 ASN ASP ASN THR ASN THR ALA GLY SER PRO GLY GLU VAL L2122 S2123 R2124 N2128 L2129 L2130 K2131 T2132 A2133 LEU ARG PRO ASP MET TRP PRO LYS S2142 E2143 L2146 Q2147 W2148 F2149 D2150 K2151 L2152 L2153 M2154 T2155

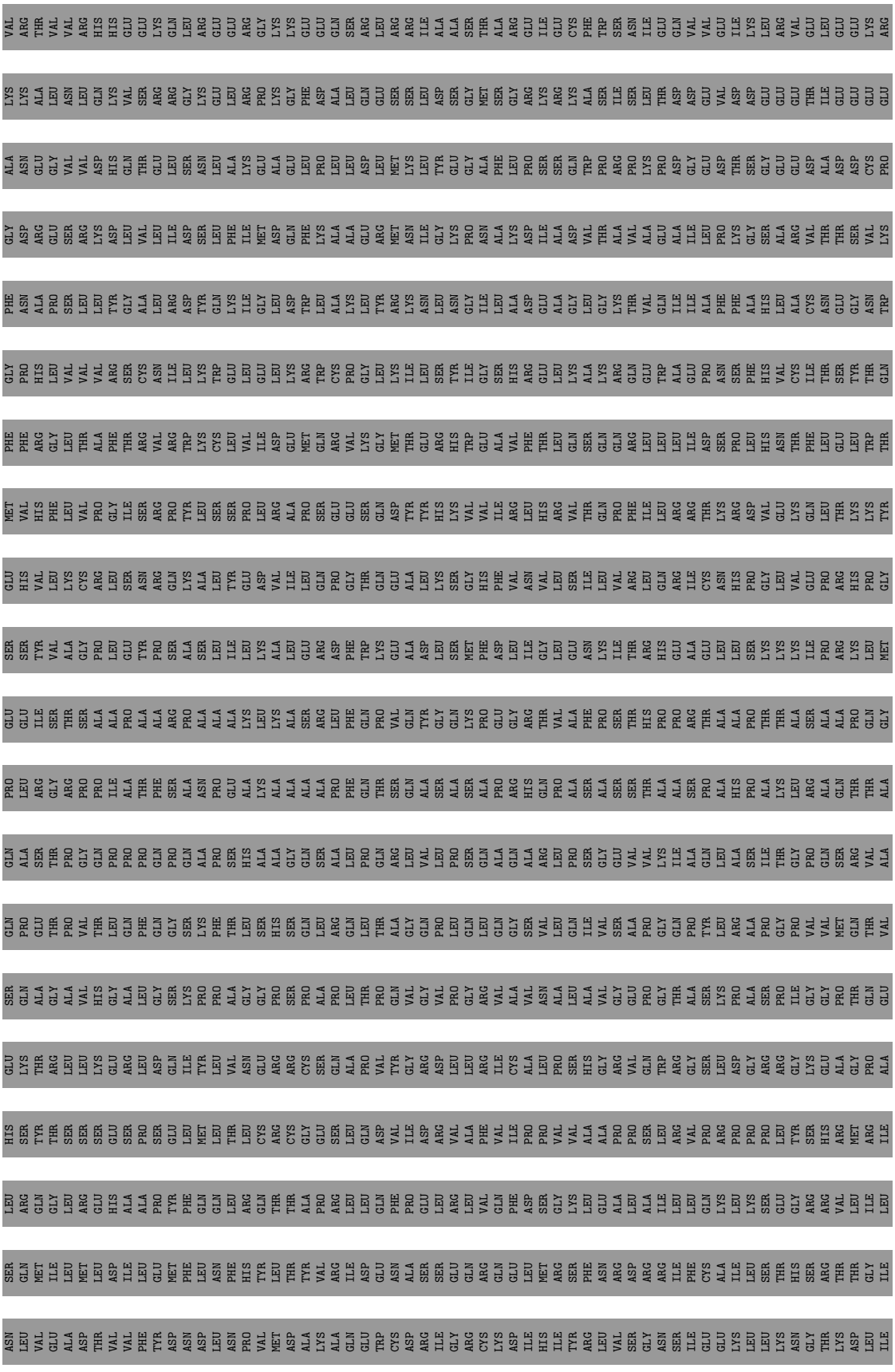


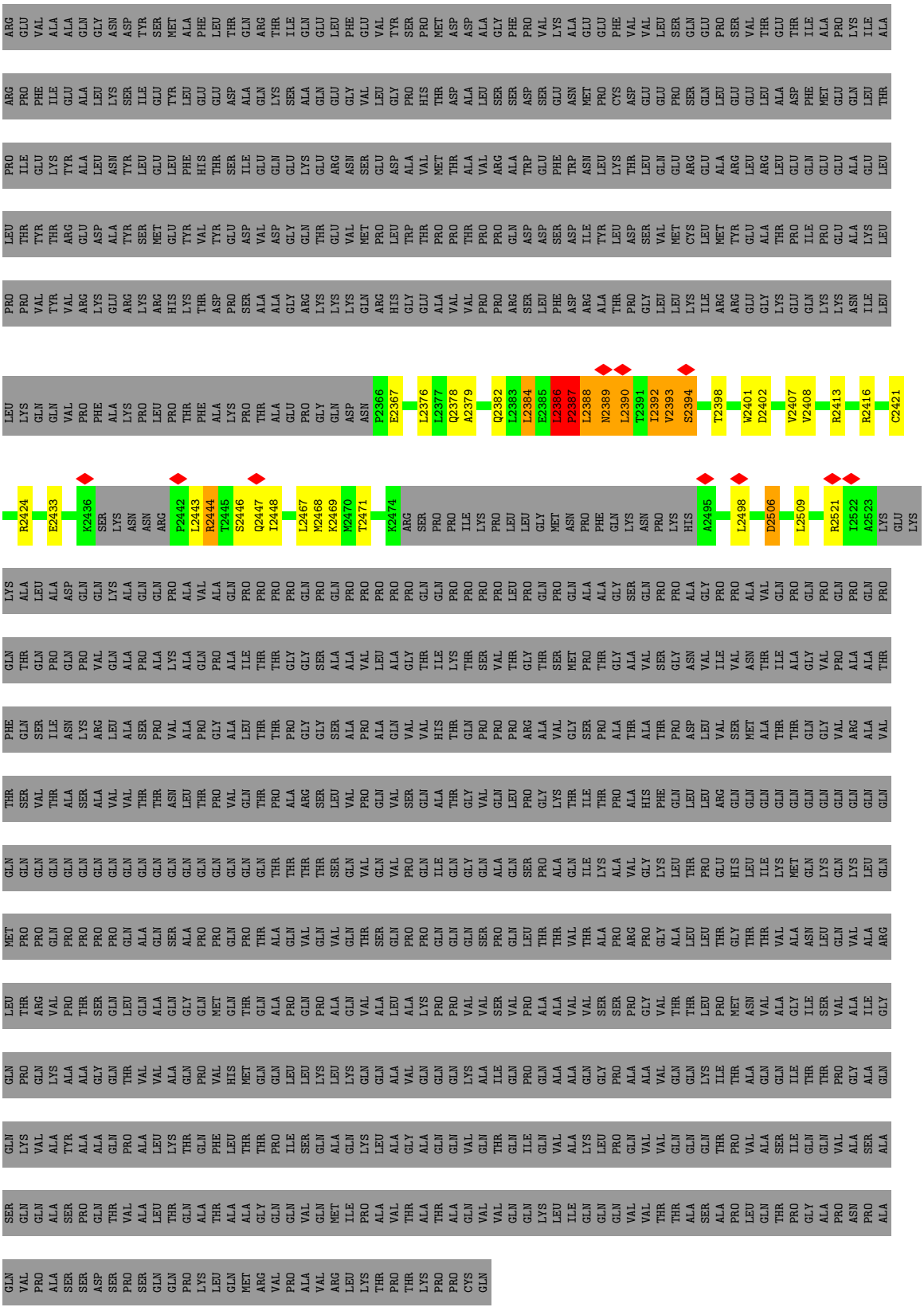


• Molecule 2: E1A-binding protein p400

Chain G: 96%




VAL ARG THR VAL VAL ARG HIS HIS GLU GLU GLU LYS LYS GLN LEU ARG GLU GLU GLU ARG GLY LYS LYS GLU GLU GLN SER ARG LEU ARG ARG ILE ALA ALA SER THR ALA ARG GLU ILE GLU CYS PHE TRP SER ASN ILE GLU GLN VAL VAL GLU ILE LYS LEU ARG VAL GLU ARG GLU LYS ARG
LYS LYS ALA LEU ASN LEU GLN LYS VAL SER ARG ARG GLY LYS GLU LEU ARG PRO LYS GLY PHE ASP ALA LEU GLN GLU SER SER LEU ASP SER GLY MET SER GLY ARG LYS ARG LYS ALA SER ILE SER LEU THR ASP ASP GLU VAL ASP ASP GLU GLU GLU THR ILE GLU GLU GLU
ALA ASN GLU GLY VAL VAL ASP HIS GLN THR GLU LEU SER ASN LEU ALA LYS GLU ALA GLU LEU PRO LEU LEU ASP HIS GLN LEU MET LYS LEU TYR GLU GLY ALA PHE LEU PRO SER SER ALA GLN TRP PRO ARG PRO LYS PRO ASP GLY GLU ASP THR SER GLY GLU GLU GLU ASP ALA ASP ASP CYS PRO
GLY ASP ARG GLU SER ARG LYS ASP LEU VAL LEU ILE ASP SER LEU PHE ILE MET ASP GLN PHE LYS ALA ALA GLU ARG GLU LEU ASP ARG MET ASN ILE GLY LYS PRO ASN ALA LYS ASP VAL THR ALA VAL ALA GLU ALA ILE LEU PRO LYS GLY SER ALA ARG VAL THR THR SER VAL LYS
PHE ASN ALA PRO SER LEU LEU TYR GLY ALA LEU ARG ASP GLU ALA LYS LEU TYR ARG LYS ASN LEU ASN GLY LYS THR VAL ILE LEU LEU ALA ASP GLU ALA GLY LEU GLY LYS THR VAL GLN ILE ILE ALA PHE PHE HIS LEU ALA CYS ASN GLU SER ASN TRP
GLY PRO HIS LEU VAL VAL ARG SER CYS ASN ILE LEU GLU LEU LYS ILE TRP GLU LEU GLU LEU LYS ARG TRP CYS PRO GLY LEU TYR ARG LYS ILE LEU SER TYR ILE GLY SER HIS ARG GLU LEU LYS ALA GLY GLN GLU TRP ALA GLU PRO ASN SER PHE HIS VAL CYS ILE THR SER TYR THR GLN
PHE PHE ARG GLY LEU THR ARG VAL ARG PHE THR ARG TRP LYS CYS LEU VAL ILE ASP GLU MET GLN ARG VAL LYS GLY MET THR GLU ARG HIS TRP GLU ALA VAL PHE THR LEU GLN SER GLN GLN ARG LEU LEU LEU ASP SER PRO LEU HIS ASN THR PHE LEU GLU LEU LEU THR
MET VAL HIS PHE LEU VAL PRO GLY ILE SER ARG PRO TYR LEU SER SER PRO LEU ARG ALA PRO SER GLU GLU SER GLN ASP TYR TYR HIS LYS VAL VAL ILE ARG LEU HIS ARG VAL THR GLN PRO PHE ILE LEU ARG ARG THR LYS ARG ASP VAL GLU LYS LEU LYS LYS TYR
GLU HIS VAL LEU LYS CYS ARG LEU SER ASN ARG GLN LYS ALA LEU TYR GLU ASP VAL ILE LEU GLN PRO GLY THR GLN GLU ALA LEU LYS SER GLY HIS PHE VAL ASN VAL LEU SER ILE LEU VAL ARG LEU GLN ARG ILE CYS ASN HIS PRO GLY LEU VAL GLU PRO ARG HIS PRO GLY
SER SER TYR VAL ALA GLY PRO LEU GLU TYR PRO SER ALA SER LEU ILE LEU LYS ALA LEU GLU ARG ASP PHE TRP LYS GLU ALA ASP LEU SER MET PHE ASP LEU GLU ILE GLY LEU GLU ASN LYS ILE THR ARG HIS GLU ALA GLU LEU LEU SER LYS LYS LYS ILE PRO ARG LYS LEU MET
GLU GLU ILE SER THR SER ALA ALA PRO ALA ALA ALA LYS LEU LYS LYS ALA SER ARG LEU PHE GLN PRO VAL GLN TYR GLY GLN LYS PRO GLU GLY ARG THR VAL ALA PHE PRO PRO SER THR HIS PRO PRO ARG THR ALA GLU ALA GLU LEU SER LYS THR THR ALA SER ALA PRO GLN GLY
PRO LEU ARG GLY ARG PRO PRO ILE ALA THR PHE SER ALA ASN PRO GLU ALA LYS ALA ALA GLY GLN ALA ALA PRO PHE GLN THR SER GLN ALA SER ALA ALA SER ALA SER SER THR ALA ALA SER PRO ALA HIS PRO THR LYS LEU ARG ALA SER GLN ALA
GLN ALA SER THR PRO GLY GLN PRO PRO GLN GLN PRO GLN ALA PRO SER HIS ALA ALA GLY GLN ALA LEU PRO GLN ARG LEU VAL LEU PRO SER GLN ALA GLN ALA ARG LEU PRO SER GLY GLU VAL VAL LYS ILE ALA GLN LEU ARG ALA SER ILE THR GLY PRO VAL MET GLN THR VAL
GLN PRO GLU THR PRO VAL THR LEU GLN PHE GLN GLY SER LYS PHE THR LEU SER HIS SER GLN LEU ARG GLN LEU THR ALA GLY GLN PRO LEU GLN LEU GLN GLN GLY SER VAL LEU ARG GLN ALA VAL SER ALA PRO GLY GLN PRO TYR LEU ARG ALA PRO GLY PRO VAL GLY ALA
SER GLN ALA GLY ALA LEU GLY GLY SER LYS PRO PRO ALA GLY GLY PRO GLY PRO ALA ALA PRO PRO LEU THR PRO GLN VAL GLY VAL PRO GLY ARG VAL ALA ASN ALA LEU ALA VAL GLY GLU PRO GLY THR ALA SER LYS PRO ALA SER PRO ILE GLY PRO VAL GLY GLY PRO GLN GLU
GLU LYS THR ARG LEU LEU TYR LEU VAL ASN GLU ARG CYS SER GLN ALA PRO VAL TYR GLY ARG ASP LEU LEU ARG ILE CYS ALA LEU PRO SER HIS GLY ARG VAL GLN TRP ARG GLY SER LEU ASP GLY LYS GLU ALA LEU PRO ARG GLY ARG
HIS SER TYR THR SER SER SER GLU SER GLN LEU SER GLN ASP VAL ILE ASP ARG VAL ALA ILE ASP ARG PRO VAL VAL PHE VAL ILE PRO PRO VAL ALA ALA PRO SER LEU ARG VAL PRO ARG PRO PRO LEU TYR SER HIS ARG MET ARG ILE
LEU ARG GLN GLY LEU HIS ALA ALA PRO TYR PHE GLN CYS THR ALA PRO ARG LEU GLU LEU ARG LEU LEU GLN PHE PRO GLU LEU ARG LEU VAL PHE ASP SER GLY LYS LEU GLU ALA LEU GLU LEU LEU GLN LYS LEU LYS SER GLU GLY ARG ARG VAL LEU ILE LEU
SER GLN MET ILE LEU MET PHE LEU ASN PHE HIS TYR LEU THR ARG GLN GLU ASP ILE ASP GLU GLN ARG GLN GLU LEU MET ARG SER PHE GLU ALA ILE LEU GLU SER THR HIS SER ARG THR THR GLY ILE
ASN LEU VAL GLU ALA ASP THR VAL ALA GLN GLU TRP CYS ASP ARG ILE GLY ARG CYS LYS ASP ILE HIS ILE TYR ARG LEU VAL SER GLY ASN SER ILE GLU GLU LYS LEU LEU LYS ASN GLY THR LYS ASP LEU ILE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Q2382
L2383
L2384
E2385
L2386
P2387
L2388
N2389
L2390
T2391
I2392
V2393
S2394
T2398
W2401
D2402
V2407
V2408
R2413
R2416
C2421

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23442	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.397	Depositor
Minimum map value	-1.369	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.451	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.24	0/25236	0.46	1/34128 (0.0%)
2	G	0.65	2/1081 (0.2%)	0.57	0/1468
All	All	0.27	2/26317 (0.0%)	0.46	1/35596 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2387	PRO	N-CD	16.70	1.71	1.47
2	G	2386	LEU	C-N	8.85	1.51	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1291	PRO	N-CA-C	-5.41	98.02	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	2444	ARG	Sidechain

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	C	24727	25317	25273	480	0
2	G	1060	1063	1062	39	0
All	All	25787	26380	26335	511	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 10.

All (511) 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:G:2387:PRO:N	2:G:2387:PRO:CD	1.71	1.45
2:G:2433:GLU:O	2:G:2444:ARG:NH1	1.83	1.10
1:C:3578:SER:OG	1:C:3581:MET:N	2.08	0.86
2:G:2378:GLN:NE2	2:G:2382:GLN:OE1	2.09	0.86
1:C:1574:MET:HE3	1:C:1579:LEU:HD11	1.62	0.81
1:C:2832:ASN:ND2	1:C:3044:TYR:OH	2.13	0.81
1:C:3617:ASP:OD1	1:C:3618:ARG:N	2.15	0.79
1:C:3544:ARG:NE	1:C:3776:ASP:OD2	2.15	0.79
1:C:2743:GLU:OE1	1:C:2743:GLU:N	2.16	0.79
1:C:1400:GLU:N	1:C:1400:GLU:OE1	2.14	0.78
1:C:3745:SER:O	1:C:3749:THR:OG1	1.99	0.78
1:C:2293:PHE:O	1:C:2296:SER:OG	2.01	0.78
1:C:446:MET:O	1:C:449:LEU:N	2.15	0.78
1:C:366:THR:O	1:C:370:THR:OG1	1.99	0.78
1:C:2335:LEU:O	1:C:2337:VAL:HG23	1.84	0.78
1:C:1381:GLN:N	1:C:1381:GLN:OE1	2.17	0.77
1:C:2348:GLN:O	1:C:2352:THR:OG1	2.01	0.77
1:C:450:GLU:N	1:C:450:GLU:OE2	2.18	0.77
1:C:411:LEU:HB3	1:C:415:ILE:HD11	1.67	0.76
1:C:1594:HIS:O	1:C:1601:ARG:NH2	2.18	0.76
1:C:2818:GLN:NE2	1:C:2822:ASP:OD1	2.18	0.76
1:C:2189:SER:O	1:C:2191:LYS:N	2.19	0.75
1:C:1136:PRO:O	1:C:1139:SER:OG	2.04	0.74
1:C:1217:CYS:O	1:C:1234:GLN:NE2	2.19	0.74
1:C:2303:GLU:O	1:C:2306:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2400:MET:SD	1:C:2401:THR:N	2.60	0.74
1:C:1168:MET:O	1:C:1216:ARG:NH1	2.20	0.74
1:C:627:GLU:N	1:C:627:GLU:OE1	2.20	0.74
1:C:1100:MET:O	1:C:1105:LYS:NZ	2.20	0.74
1:C:898:PHE:O	1:C:902:ASN:ND2	2.21	0.73
2:G:2376:LEU:HD22	2:G:2408:VAL:HG11	1.71	0.73
1:C:2393:SER:O	1:C:2397:VAL:HG12	1.88	0.73
1:C:565:THR:HG1	1:C:578:ASN:N	1.86	0.73
1:C:3508:LYS:O	1:C:3510:ASN:N	2.22	0.72
2:G:2367:GLU:O	2:G:2416:ARG:NH2	2.22	0.72
1:C:1081:GLU:N	1:C:1081:GLU:OE1	2.22	0.72
1:C:2788:GLN:OE1	1:C:2788:GLN:N	2.22	0.72
1:C:3701:ASP:OD1	1:C:3702:THR:N	2.23	0.71
1:C:2334:ARG:NE	1:C:2334:ARG:O	2.24	0.71
1:C:561:THR:HG22	1:C:589:TYR:OH	1.92	0.70
1:C:3574:VAL:HG22	1:C:3584:VAL:HG23	1.72	0.69
1:C:651:PHE:O	1:C:655:VAL:N	2.24	0.69
1:C:763:LEU:O	1:C:767:ILE:HG22	1.92	0.69
1:C:3357:ALA:O	1:C:3623:GLN:NE2	2.25	0.69
1:C:2699:THR:HG1	1:C:2700:HIS:HD1	1.41	0.69
1:C:705:GLU:OE1	1:C:705:GLU:N	2.26	0.69
1:C:3479:GLU:OE2	1:C:3495:LYS:NZ	2.18	0.69
1:C:673:ASN:OD1	1:C:674:SER:N	2.27	0.68
1:C:2472:GLU:N	1:C:2472:GLU:OE1	2.25	0.68
1:C:2873:GLU:OE2	1:C:2888:ARG:NE	2.27	0.68
1:C:2479:CYS:SG	1:C:2480:SER:N	2.66	0.68
1:C:1735:TYR:O	1:C:1739:GLU:N	2.26	0.67
1:C:2474:LEU:CD1	1:C:2640:LEU:HD11	2.25	0.67
1:C:557:VAL:HG21	1:C:592:LEU:HD11	1.77	0.67
1:C:2338:MET:SD	1:C:2338:MET:N	2.68	0.67
1:C:1215:MET:O	1:C:1219:THR:OG1	2.09	0.67
1:C:437:GLU:OE1	1:C:439:GLY:N	2.28	0.66
1:C:1668:ARG:NH1	1:C:1712:GLU:OE1	2.28	0.66
2:G:2443:LEU:HD22	2:G:2447:GLN:HB2	1.76	0.66
1:C:2935:GLN:NE2	1:C:2983:ASP:OD1	2.30	0.65
1:C:1373:LEU:HD22	1:C:1386:ILE:HG22	1.78	0.65
1:C:1737:GLU:N	1:C:1737:GLU:OE1	2.30	0.65
1:C:724:PHE:O	1:C:728:ASN:ND2	2.29	0.65
1:C:2414:ASN:O	1:C:2418:LEU:HD12	1.97	0.65
1:C:2798:ASP:OD2	2:G:2469:LYS:NZ	2.30	0.65
1:C:2172:GLU:O	1:C:2175:SER:OG	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1671:TRP:O	1:C:1719:ARG:NH1	2.30	0.64
2:G:2384:LEU:HD13	2:G:2393:VAL:HG23	1.79	0.64
1:C:3360:ASP:OD1	1:C:3361:ALA:N	2.31	0.64
1:C:2340:MET:SD	1:C:2343:ARG:N	2.71	0.64
1:C:3359:SER:N	1:C:3623:GLN:OE1	2.31	0.64
1:C:1048:HIS:O	1:C:1052:VAL:HG23	1.98	0.63
1:C:3838:LEU:O	1:C:3842:ALA:N	2.32	0.63
1:C:1376:CYS:SG	1:C:1379:LEU:HD12	2.37	0.63
1:C:2497:GLU:OE1	1:C:2619:HIS:NE2	2.32	0.63
1:C:1198:VAL:HG11	1:C:1203:VAL:HG22	1.81	0.62
1:C:309:MET:SD	1:C:309:MET:N	2.72	0.62
1:C:2150:ASP:OD1	1:C:2151:LYS:N	2.33	0.62
1:C:2285:TYR:CD2	1:C:2289:LEU:HD21	2.34	0.62
1:C:372:ARG:NH2	1:C:411:LEU:HD11	2.13	0.62
1:C:2197:ILE:O	1:C:2197:ILE:HG22	1.99	0.62
2:G:2386:LEU:HB3	2:G:2387:PRO:CD	2.29	0.62
1:C:2489:HIS:O	1:C:2664:GLN:NE2	2.33	0.62
1:C:583:PRO:O	1:C:586:THR:OG1	2.16	0.62
1:C:3681:PHE:CE2	1:C:3685:VAL:HG21	2.35	0.62
1:C:3707:VAL:HG21	1:C:3710:PHE:CE2	2.34	0.62
1:C:1433:MET:O	1:C:1439:SER:OG	2.13	0.61
1:C:3577:VAL:HG23	1:C:3577:VAL:O	2.00	0.61
1:C:3190:GLN:OE1	1:C:3191:ASN:N	2.32	0.61
1:C:3142:PHE:O	1:C:3146:VAL:HG12	2.00	0.61
1:C:1729:MET:SD	1:C:1729:MET:N	2.72	0.61
1:C:1442:LEU:O	1:C:1512:LYS:NZ	2.34	0.61
1:C:1576:GLU:HA	1:C:1579:LEU:HD12	1.83	0.61
1:C:3481:PRO:O	1:C:3528:TYR:OH	2.10	0.61
1:C:1370:LEU:HA	1:C:1373:LEU:HD12	1.82	0.61
1:C:3538:GLU:OE1	1:C:3711:ARG:NH1	2.34	0.61
1:C:3614:ARG:NE	1:C:3645:MET:SD	2.74	0.60
1:C:1295:HIS:O	1:C:1296:LEU:C	2.40	0.60
1:C:409:GLU:N	1:C:409:GLU:OE1	2.35	0.60
1:C:2299:LYS:NZ	1:C:2303:GLU:OE1	2.34	0.60
1:C:1199:SER:OG	1:C:1202:ALA:N	2.31	0.60
1:C:3782:HIS:O	1:C:3786:GLN:N	2.34	0.60
1:C:427:VAL:HG11	1:C:560:ILE:HG22	1.82	0.60
1:C:2491:TRP:NE1	1:C:2664:GLN:OE1	2.32	0.59
1:C:252:PRO:O	1:C:256:ASN:ND2	2.35	0.59
1:C:1650:VAL:HG21	1:C:1657:LEU:HD12	1.85	0.59
1:C:783:LEU:HD11	1:C:815:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2880:MET:O	1:C:2883:LYS:N	2.35	0.59
1:C:1054:VAL:HG11	1:C:1125:ILE:HD13	1.84	0.59
1:C:3731:LEU:O	1:C:3732:THR:HG22	2.03	0.59
1:C:1015:ARG:NH1	1:C:1088:ASP:OD1	2.36	0.59
1:C:1286:LEU:HG	1:C:1290:VAL:HG23	1.85	0.58
1:C:1454:LEU:H	1:C:1454:LEU:HD23	1.68	0.58
1:C:423:LEU:O	1:C:427:VAL:HG13	2.03	0.58
1:C:549:LEU:O	1:C:552:THR:OG1	2.21	0.58
1:C:1105:LYS:HD2	1:C:1158:LEU:HD23	1.86	0.58
1:C:1325:MET:O	1:C:1379:LEU:HD11	2.04	0.57
1:C:2942:GLU:OE2	1:C:2977:ARG:NH1	2.37	0.57
1:C:3210:ASP:OD1	1:C:3212:LYS:N	2.37	0.57
1:C:348:ILE:HG23	1:C:349:PRO:HD3	1.86	0.57
1:C:2708:LEU:HD11	1:C:3665:TYR:CD1	2.39	0.57
1:C:877:TRP:CE3	1:C:2926:VAL:HG21	2.40	0.57
1:C:2095:ASP:OD1	1:C:2096:THR:N	2.38	0.57
1:C:1221:LEU:O	1:C:1226:ARG:NH1	2.38	0.57
1:C:2169:THR:O	1:C:2173:VAL:HG22	2.04	0.57
1:C:3494:ILE:N	1:C:3494:ILE:HD12	2.19	0.57
1:C:2194:GLN:O	1:C:2198:ALA:N	2.38	0.57
1:C:2851:LEU:HD12	1:C:2851:LEU:O	2.04	0.56
2:G:2387:PRO:O	2:G:2388:LEU:C	2.44	0.56
1:C:2759:ASP:N	1:C:2759:ASP:OD1	2.39	0.56
1:C:3803:ASP:O	1:C:3804:SER:OG	2.15	0.56
1:C:1080:GLU:N	1:C:1080:GLU:OE1	2.37	0.56
1:C:1419:GLU:N	1:C:1419:GLU:OE1	2.38	0.56
1:C:1475:MET:HE2	1:C:1542:THR:HG21	1.87	0.56
2:G:2388:LEU:HD21	2:G:2401:TRP:HH2	1.70	0.56
2:G:2388:LEU:HD21	2:G:2401:TRP:CH2	2.40	0.56
1:C:2840:TYR:HB2	2:G:2471:THR:HG21	1.88	0.56
1:C:3266:TYR:OH	1:C:3319:GLU:OE1	2.12	0.56
1:C:2463:ASP:OD1	1:C:2473:ARG:NH2	2.37	0.56
1:C:2474:LEU:HD13	1:C:2640:LEU:HD11	1.86	0.56
1:C:2361:ALA:HA	1:C:2364:LEU:HD23	1.87	0.55
1:C:711:LEU:HD12	1:C:711:LEU:O	2.07	0.55
1:C:3237:GLN:OE1	1:C:3547:GLN:NE2	2.38	0.55
1:C:3689:ASN:OD1	1:C:3690:ARG:N	2.40	0.55
1:C:3275:THR:HG23	1:C:3536:LEU:HD11	1.88	0.55
1:C:357:GLU:OE1	1:C:401:LEU:HD23	2.07	0.55
1:C:1897:HIS:O	1:C:1901:VAL:HG23	2.07	0.55
1:C:3331:ASN:OD1	1:C:3333:HIS:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1061:PHE:C	1:C:1062:LEU:HD23	2.27	0.54
1:C:1774:GLN:OE1	1:C:1774:GLN:HA	2.07	0.54
1:C:3177:VAL:HG23	1:C:3218:ALA:CB	2.37	0.54
2:G:2386:LEU:HB3	2:G:2387:PRO:HD3	1.90	0.54
1:C:557:VAL:HG21	1:C:592:LEU:CD1	2.37	0.54
1:C:1353:LEU:O	1:C:1357:LYS:N	2.41	0.54
1:C:1343:CYS:O	1:C:1366:ARG:NH2	2.40	0.54
1:C:2201:MET:O	1:C:2205:ASN:N	2.40	0.54
1:C:671:VAL:O	1:C:675:PHE:N	2.40	0.54
1:C:909:SER:OG	1:C:3704:LYS:NZ	2.41	0.54
1:C:1121:VAL:O	1:C:1125:ILE:HG22	2.08	0.54
1:C:2169:THR:O	1:C:2173:VAL:HG13	2.07	0.54
1:C:279:ASP:OD1	1:C:280:PHE:N	2.40	0.54
1:C:979:ASP:OD2	1:C:2521:ILE:HD12	2.08	0.54
2:G:2389:ASN:O	2:G:2390:LEU:C	2.44	0.54
1:C:554:VAL:HG21	1:C:631:VAL:HG23	1.89	0.54
1:C:2364:LEU:HD22	1:C:2364:LEU:H	1.71	0.54
1:C:3742:ILE:HD12	1:C:3742:ILE:N	2.22	0.54
1:C:1181:GLN:NE2	1:C:1244:ASP:OD2	2.41	0.54
1:C:2683:VAL:HG22	1:C:2684:PRO:HD3	1.89	0.54
1:C:2962:ASN:OD1	1:C:2963:SER:N	2.41	0.54
1:C:2742:GLN:N	1:C:2743:GLU:OE1	2.41	0.54
1:C:2949:ILE:HD13	1:C:2967:MET:SD	2.47	0.53
1:C:2124:ARG:NH1	1:C:2128:ASN:OD1	2.41	0.53
1:C:3226:VAL:HG13	1:C:3226:VAL:O	2.06	0.53
1:C:775:LEU:O	1:C:779:PHE:N	2.41	0.53
1:C:1373:LEU:CD2	1:C:1386:ILE:HG22	2.37	0.53
1:C:635:PHE:O	1:C:638:VAL:HG12	2.09	0.53
1:C:1113:VAL:O	1:C:1117:VAL:HG23	2.09	0.53
1:C:1913:ALA:O	1:C:1917:ARG:N	2.39	0.53
2:G:2376:LEU:HD11	2:G:2421:CYS:SG	2.48	0.53
1:C:1180:GLN:NE2	1:C:1217:CYS:SG	2.81	0.53
1:C:2203:CYS:O	1:C:2207:LYS:NZ	2.42	0.52
1:C:3267:PHE:CE1	1:C:3318:LEU:HD22	2.44	0.52
1:C:1901:VAL:HG11	1:C:1935:MET:HE1	1.91	0.52
1:C:1592:LEU:O	1:C:1601:ARG:NH1	2.42	0.52
1:C:2418:LEU:HD12	1:C:2418:LEU:H	1.74	0.52
1:C:2640:LEU:O	1:C:2645:GLN:NE2	2.43	0.52
1:C:2676:VAL:HG11	1:C:2702:LEU:HD22	1.92	0.52
1:C:3275:THR:HG23	1:C:3536:LEU:CD1	2.39	0.52
1:C:1198:VAL:HG11	1:C:1203:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLN:HE22	1:C:285:ILE:HD13	1.75	0.52
1:C:2781:GLU:OE2	1:C:2823:HIS:ND1	2.42	0.52
1:C:3423:ASP:OD1	1:C:3424:PHE:N	2.41	0.52
1:C:1659:SER:O	1:C:1661:HIS:ND1	2.40	0.52
1:C:3146:VAL:HG11	1:C:3159:TRP:CZ3	2.45	0.52
2:G:2392:ILE:HD11	2:G:2398:THR:HA	1.91	0.52
1:C:401:LEU:HD22	1:C:401:LEU:H	1.74	0.51
1:C:1259:GLN:O	1:C:1263:SER:N	2.37	0.51
1:C:1535:LEU:HD12	1:C:1536:LEU:N	2.25	0.51
1:C:1292:PRO:HG2	1:C:1335:PHE:CG	2.45	0.51
1:C:1377:ASN:OD1	1:C:1378:TYR:N	2.44	0.51
1:C:450:GLU:O	1:C:454:LEU:HD23	2.11	0.51
1:C:1078:HIS:N	1:C:1088:ASP:OD2	2.39	0.51
1:C:2449:CYS:SG	1:C:2450:ALA:N	2.83	0.51
1:C:2661:HIS:CD2	1:C:2672:LEU:HD13	2.45	0.51
2:G:2384:LEU:HD13	2:G:2393:VAL:CG2	2.41	0.51
1:C:2499:LEU:O	1:C:2502:VAL:HG12	2.10	0.51
1:C:2872:VAL:O	1:C:2876:CYS:N	2.43	0.51
1:C:446:MET:O	1:C:450:GLU:OE2	2.29	0.51
1:C:1556:GLU:OE2	1:C:1594:HIS:NE2	2.41	0.51
1:C:2285:TYR:CE2	1:C:2289:LEU:HD21	2.46	0.51
1:C:3544:ARG:NH1	1:C:3777:GLU:OE1	2.40	0.51
1:C:3618:ARG:NH1	1:C:3640:GLU:OE2	2.43	0.51
1:C:292:ALA:O	1:C:295:ILE:HD11	2.11	0.50
1:C:408:ASP:HB3	1:C:411:LEU:HD13	1.93	0.50
1:C:601:ASP:OD1	1:C:602:ILE:N	2.42	0.50
1:C:2375:VAL:HG21	1:C:2417:PHE:CE1	2.46	0.50
1:C:1460:ASN:OD1	1:C:1462:LYS:N	2.44	0.50
1:C:1834:GLN:O	1:C:1837:THR:OG1	2.28	0.50
1:C:3648:ARG:O	1:C:3734:ASN:ND2	2.45	0.50
1:C:800:GLN:NE2	1:C:804:ASP:OD1	2.45	0.50
1:C:2908:VAL:HG21	1:C:2944:GLN:HB2	1.93	0.50
1:C:1325:MET:N	1:C:1378:TYR:OH	2.38	0.50
1:C:2494:GLN:OE1	1:C:2494:GLN:N	2.44	0.50
1:C:2865:MET:HG3	1:C:2891:LEU:HD21	1.93	0.50
1:C:2946:ALA:HB1	1:C:2998:HIS:NE2	2.27	0.50
1:C:3306:MET:SD	1:C:3307:GLN:N	2.85	0.50
1:C:418:MET:SD	1:C:419:SER:N	2.84	0.50
1:C:2153:LEU:HD22	1:C:2199:ALA:HB3	1.93	0.50
1:C:3330:GLU:OE1	1:C:3330:GLU:N	2.39	0.50
1:C:592:LEU:C	1:C:592:LEU:HD23	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2834:TRP:HZ3	1:C:2855:CYS:HG	1.58	0.50
1:C:1394:LEU:HD23	1:C:1394:LEU:O	2.12	0.50
1:C:581:LEU:H	1:C:646:THR:HG21	1.77	0.49
1:C:952:SER:O	1:C:960:ARG:NH2	2.45	0.49
1:C:1461:ASP:OD1	1:C:1462:LYS:N	2.44	0.49
1:C:1555:ARG:O	1:C:1559:ILE:HG23	2.12	0.49
1:C:1862:MET:CE	1:C:1865:ALA:HB3	2.41	0.49
1:C:2298:GLN:OE1	1:C:2298:GLN:N	2.45	0.49
1:C:811:LEU:O	1:C:812:THR:OG1	2.29	0.49
1:C:1916:ALA:O	1:C:1920:VAL:HG22	2.12	0.49
1:C:3267:PHE:CZ	1:C:3318:LEU:HD22	2.47	0.49
1:C:1527:ALA:HB1	1:C:1531:LEU:HD21	1.93	0.49
1:C:3193:SER:OG	1:C:3194:LYS:N	2.44	0.49
1:C:3133:ASN:OD1	1:C:3134:LYS:N	2.45	0.49
1:C:1981:LEU:O	1:C:1984:HIS:N	2.45	0.49
1:C:2798:ASP:OD1	1:C:2799:LYS:N	2.45	0.49
1:C:3270:ARG:CZ	1:C:3322:VAL:HG11	2.42	0.49
1:C:3494:ILE:HG21	1:C:3526:TYR:HE2	1.78	0.49
1:C:1290:VAL:HG11	1:C:1323:PHE:CB	2.42	0.49
1:C:1934:ARG:O	1:C:1938:GLY:N	2.46	0.49
1:C:2949:ILE:HD11	1:C:2970:VAL:CG1	2.42	0.49
1:C:1061:PHE:O	1:C:1062:LEU:O	2.29	0.49
1:C:3533:ASP:OD1	1:C:3534:ALA:N	2.44	0.49
1:C:933:ALA:HB1	1:C:2639:ILE:HD12	1.94	0.48
1:C:2659:GLY:N	2:G:2398:THR:O	2.42	0.48
1:C:3058:LEU:O	1:C:3062:SER:OG	2.24	0.48
1:C:821:LEU:HD11	1:C:856:LEU:HD11	1.94	0.48
1:C:1348:SER:O	1:C:1352:LYS:N	2.45	0.48
1:C:1921:ARG:NH2	1:C:1924:MET:SD	2.87	0.48
1:C:2466:MET:CE	1:C:2498:LEU:HD22	2.43	0.48
1:C:2291:SER:OG	1:C:2295:ARG:NH1	2.42	0.48
1:C:3177:VAL:HG23	1:C:3218:ALA:HB2	1.94	0.48
1:C:3428:VAL:O	1:C:3430:GLY:N	2.45	0.48
1:C:1531:LEU:HD11	1:C:1561:PHE:CE2	2.49	0.48
1:C:1058:CYS:SG	1:C:1126:LEU:HD11	2.53	0.48
2:G:2393:VAL:O	2:G:2394:SER:C	2.52	0.48
1:C:671:VAL:O	1:C:675:PHE:HB2	2.13	0.48
1:C:3650:MET:HA	1:C:3650:MET:CE	2.43	0.48
1:C:1610:ARG:O	1:C:1614:LEU:HD12	2.14	0.48
1:C:2695:TYR:CE1	1:C:2699:THR:HG21	2.48	0.48
1:C:3187:CYS:SG	1:C:3199:LEU:HD22	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3054:VAL:HG11	1:C:3089:LEU:HD23	1.96	0.47
1:C:1865:ALA:HB2	1:C:1886:LEU:HD22	1.97	0.47
1:C:3663:THR:O	1:C:3667:THR:HG22	2.14	0.47
1:C:3685:VAL:CG2	1:C:3825:LEU:HD21	2.43	0.47
1:C:1422:GLN:O	1:C:1426:HIS:ND1	2.47	0.47
1:C:2174:LEU:O	1:C:2178:LEU:HD12	2.14	0.47
1:C:2346:PHE:O	1:C:2350:ILE:N	2.46	0.47
1:C:3322:VAL:HG22	1:C:3577:VAL:HG21	1.95	0.47
1:C:427:VAL:HG11	1:C:560:ILE:CG2	2.44	0.47
1:C:2683:VAL:CG2	1:C:2684:PRO:HD3	2.44	0.47
1:C:2205:ASN:OD1	1:C:2206:THR:N	2.47	0.47
1:C:655:VAL:N	1:C:656:PRO:HD2	2.30	0.47
1:C:1675:ASN:OD1	1:C:1675:ASN:N	2.43	0.47
1:C:3492:TYR:O	1:C:3492:TYR:CD1	2.68	0.47
1:C:1276:THR:O	1:C:1280:GLU:N	2.48	0.47
1:C:1356:TYR:HB3	1:C:1359:LEU:HD12	1.96	0.47
1:C:3679:ILE:HG23	1:C:3707:VAL:HG21	1.96	0.47
1:C:1862:MET:HE3	1:C:1865:ALA:HB3	1.97	0.47
1:C:557:VAL:O	1:C:561:THR:HG23	2.14	0.47
1:C:991:PRO:O	1:C:992:ASN:HB3	2.15	0.47
1:C:2711:GLU:OE2	1:C:3669:ARG:NH2	2.38	0.47
1:C:3102:LEU:HA	1:C:3105:ILE:HG22	1.97	0.47
1:C:3146:VAL:O	1:C:3150:ASP:N	2.47	0.47
1:C:2988:TRP:CE2	1:C:3047:ILE:HD13	2.50	0.47
1:C:3054:VAL:HG12	1:C:3058:LEU:CD2	2.45	0.47
1:C:336:LYS:O	1:C:340:THR:HG23	2.15	0.46
1:C:659:VAL:HG11	1:C:692:TYR:HE2	1.80	0.46
1:C:1151:GLU:O	1:C:1157:LYS:NZ	2.40	0.46
1:C:797:LEU:HD23	1:C:797:LEU:H	1.81	0.46
1:C:1454:LEU:HD23	1:C:1454:LEU:N	2.30	0.46
1:C:1671:TRP:CE3	1:C:1696:LEU:HD22	2.51	0.46
2:G:2392:ILE:HG23	2:G:2392:ILE:O	2.15	0.46
1:C:2956:THR:O	1:C:2960:ARG:NH2	2.48	0.46
1:C:3561:GLU:O	1:C:3565:ARG:NH1	2.49	0.46
1:C:411:LEU:N	1:C:411:LEU:HD12	2.30	0.46
1:C:3223:CYS:O	1:C:3226:VAL:HG12	2.16	0.46
1:C:1061:PHE:O	1:C:1062:LEU:HD23	2.14	0.46
1:C:1614:LEU:HD12	1:C:1614:LEU:H	1.81	0.46
1:C:2197:ILE:O	1:C:2197:ILE:CG2	2.64	0.46
1:C:1992:LEU:O	1:C:2002:GLN:NE2	2.47	0.46
1:C:2774:THR:OG1	1:C:2820:TRP:NE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3716:ASP:OD1	1:C:3716:ASP:N	2.49	0.46
1:C:2421:VAL:HG12	1:C:2421:VAL:O	2.16	0.46
1:C:2414:ASN:O	1:C:2417:PHE:N	2.49	0.46
1:C:1015:ARG:NH2	1:C:1094:ASP:OD2	2.49	0.45
1:C:1071:GLN:O	1:C:1073:SER:N	2.47	0.45
1:C:1122:ALA:HA	1:C:1125:ILE:HG22	1.99	0.45
1:C:1286:LEU:CG	1:C:1290:VAL:HG23	2.45	0.45
1:C:3150:ASP:OD2	2:G:2521:ARG:NH2	2.49	0.45
2:G:2443:LEU:HD22	2:G:2447:GLN:CB	2.44	0.45
1:C:859:ASP:OD1	1:C:860:PHE:N	2.50	0.45
1:C:1168:MET:SD	1:C:1213:LEU:HA	2.56	0.45
1:C:851:LEU:C	1:C:851:LEU:HD12	2.37	0.45
1:C:868:VAL:HG22	1:C:868:VAL:O	2.16	0.45
1:C:3054:VAL:HG11	1:C:3089:LEU:CD2	2.47	0.45
1:C:3530:VAL:HG22	1:C:3583:LEU:CD2	2.45	0.45
1:C:1566:PRO:HA	1:C:1569:THR:HG22	1.99	0.45
1:C:462:TYR:CD1	1:C:462:TYR:N	2.82	0.45
1:C:2294:MET:HG3	1:C:2347:ILE:HD11	1.99	0.45
1:C:2337:VAL:HG12	1:C:2337:VAL:O	2.16	0.45
1:C:424:LEU:HD21	1:C:555:CYS:HB3	1.98	0.45
1:C:642:MET:CE	1:C:650:ILE:HD12	2.47	0.45
1:C:917:THR:HG23	1:C:917:THR:O	2.17	0.45
1:C:1268:ALA:HB2	1:C:1275:VAL:HG22	1.99	0.45
1:C:1475:MET:O	1:C:1478:VAL:HG12	2.17	0.45
1:C:3744:VAL:O	1:C:3749:THR:HG23	2.16	0.45
1:C:348:ILE:N	1:C:349:PRO:HD2	2.32	0.45
1:C:1327:LEU:HD13	1:C:1379:LEU:HD13	1.98	0.45
1:C:1643:ILE:HD13	1:C:1643:ILE:N	2.32	0.45
1:C:3741:THR:OG1	1:C:3742:ILE:HD12	2.16	0.45
1:C:1290:VAL:O	1:C:1312:ASN:OD1	2.35	0.45
1:C:1537:GLU:O	1:C:1541:LYS:N	2.39	0.45
1:C:2104:VAL:HG21	1:C:2123:SER:HB3	1.98	0.45
1:C:2368:VAL:CG2	1:C:2413:LEU:HD22	2.47	0.45
1:C:865:ILE:O	1:C:869:ARG:N	2.50	0.44
1:C:1318:LEU:O	1:C:1321:ARG:N	2.50	0.44
1:C:1441:THR:O	1:C:1445:VAL:HG22	2.16	0.44
1:C:3567:LEU:HD13	1:C:3755:VAL:HG23	2.00	0.44
1:C:3737:GLU:HA	1:C:3740:THR:HG23	1.99	0.44
1:C:1048:HIS:CE1	1:C:2521:ILE:HD11	2.51	0.44
1:C:2699:THR:OG1	1:C:2700:HIS:ND1	2.34	0.44
1:C:838:SER:OG	1:C:840:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2162:VAL:O	1:C:2166:ASN:ND2	2.51	0.44
1:C:3690:ARG:NH2	1:C:3852:ASP:OD2	2.42	0.44
1:C:455:LYS:CG	1:C:553:LEU:HD21	2.48	0.44
1:C:2177:LEU:O	1:C:2181:LEU:HG	2.16	0.44
1:C:2177:LEU:HD22	1:C:2218:ARG:NH2	2.32	0.44
1:C:2375:VAL:HG21	1:C:2417:PHE:HE1	1.81	0.44
1:C:2699:THR:HG1	1:C:2700:HIS:CE1	2.32	0.44
1:C:1295:HIS:O	1:C:1296:LEU:O	2.36	0.44
1:C:1533:LYS:HB3	1:C:1534:PRO:HD3	2.00	0.44
1:C:2181:LEU:HD21	1:C:2218:ARG:HG2	1.99	0.44
1:C:2493:LYS:HE3	1:C:2622:THR:HG22	2.00	0.44
1:C:642:MET:HE1	1:C:650:ILE:HD12	1.99	0.44
1:C:3678:LEU:CD1	1:C:3755:VAL:HG21	2.47	0.44
2:G:2506:ASP:N	2:G:2506:ASP:OD1	2.49	0.44
1:C:678:ASN:OD1	1:C:678:ASN:C	2.56	0.44
1:C:3235:ILE:HD11	1:C:3257:VAL:HG11	2.00	0.44
1:C:3266:TYR:CD1	1:C:3315:LEU:HD12	2.52	0.44
1:C:3731:LEU:HD23	1:C:3843:ASN:HB3	1.99	0.44
1:C:879:THR:HG23	1:C:891:ALA:HB1	2.00	0.44
1:C:2327:SER:HA	1:C:2330:LEU:HD23	1.99	0.44
2:G:2384:LEU:CD1	2:G:2393:VAL:HG23	2.46	0.44
1:C:2189:SER:O	1:C:2192:PRO:HD2	2.18	0.43
1:C:1817:ASP:N	1:C:1818:PRO:CD	2.81	0.43
1:C:2707:THR:HG22	1:C:2751:LEU:HD13	2.01	0.43
1:C:988:LEU:HG	1:C:1125:ILE:HD11	2.00	0.43
1:C:1774:GLN:OE1	1:C:1777:LEU:HD22	2.18	0.43
1:C:1319:GLN:N	1:C:1320:PRO:CD	2.82	0.43
1:C:3530:VAL:HG22	1:C:3583:LEU:HD21	1.99	0.43
1:C:1291:PRO:HB3	1:C:1332:HIS:NE2	2.34	0.43
1:C:1579:LEU:O	1:C:1585:SER:OG	2.37	0.43
1:C:2368:VAL:HG23	1:C:2413:LEU:HD22	2.01	0.43
1:C:2686:ILE:O	1:C:2688:ILE:HD12	2.18	0.43
1:C:2809:ALA:O	1:C:2810:SER:OG	2.25	0.43
1:C:3169:LYS:O	1:C:3170:GLU:HG2	2.18	0.43
1:C:1736:MET:SD	1:C:1736:MET:N	2.91	0.43
1:C:3199:LEU:HD12	1:C:3231:TRP:CZ3	2.54	0.43
1:C:2707:THR:CG2	1:C:2751:LEU:HD13	2.48	0.43
1:C:3115:LYS:O	1:C:3118:THR:OG1	2.36	0.43
1:C:3147:GLN:OE1	2:G:2509:LEU:HD13	2.19	0.43
1:C:3578:SER:OG	1:C:3581:MET:O	2.27	0.43
1:C:413:SER:OG	1:C:545:ASP:OD2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1059:GLY:N	1:C:1060:PRO:HD3	2.34	0.43
1:C:3488:LYS:O	1:C:3488:LYS:HG3	2.17	0.43
1:C:1778:ASN:HB2	1:C:1779:PRO:HD3	2.01	0.43
1:C:3509:HIS:CG	1:C:3510:ASN:N	2.87	0.43
2:G:2379:ALA:HB2	2:G:2407:VAL:HG11	2.01	0.43
1:C:1824:MET:SD	1:C:1824:MET:N	2.91	0.42
1:C:2656:LEU:HD23	1:C:2672:LEU:HD11	2.01	0.42
1:C:1475:MET:CE	1:C:1542:THR:HG21	2.48	0.42
1:C:2911:ALA:CB	1:C:2940:ILE:HD11	2.49	0.42
1:C:3161:ASP:OD1	1:C:3183:TYR:OH	2.29	0.42
1:C:3304:MET:O	1:C:3308:ARG:N	2.50	0.42
1:C:673:ASN:O	1:C:677:ALA:HB2	2.19	0.42
1:C:2958:LEU:HD11	1:C:3005:TRP:HB2	2.00	0.42
1:C:3516:LEU:HD22	1:C:3530:VAL:HG23	2.00	0.42
1:C:3561:GLU:H	1:C:3561:GLU:CD	2.22	0.42
2:G:2384:LEU:HD11	2:G:2392:ILE:HA	2.01	0.42
2:G:2393:VAL:HG12	2:G:2394:SER:N	2.34	0.42
1:C:2323:LEU:HD12	1:C:2323:LEU:O	2.18	0.42
1:C:3541:ARG:NH2	1:C:3712:PHE:O	2.52	0.42
1:C:817:LEU:HD23	1:C:817:LEU:H	1.85	0.42
1:C:1293:LYS:HA	1:C:1293:LYS:HD2	1.92	0.42
1:C:1371:ASN:ND2	1:C:1408:CYS:SG	2.93	0.42
1:C:1909:LEU:HA	1:C:1963:ILE:HD13	2.01	0.42
1:C:2297:LEU:O	1:C:2301:VAL:N	2.52	0.42
1:C:3591:LEU:H	1:C:3591:LEU:HD23	1.83	0.42
1:C:1718:LEU:HD11	1:C:1764:PHE:CZ	2.54	0.42
1:C:1761:ASP:O	1:C:1763:ASN:ND2	2.52	0.42
1:C:2932:PRO:O	1:C:2936:ALA:N	2.51	0.42
1:C:3192:GLU:N	1:C:3230:GLN:OE1	2.53	0.42
2:G:2387:PRO:HG2	2:G:2390:LEU:HD12	2.02	0.42
2:G:2384:LEU:HD12	2:G:2388:LEU:O	2.18	0.42
1:C:446:MET:O	1:C:447:ARG:C	2.58	0.42
1:C:1406:GLU:OE2	1:C:1450:SER:OG	2.36	0.42
1:C:1524:ILE:HG23	1:C:1524:ILE:O	2.20	0.42
1:C:1728:ASN:HD21	1:C:1732:LEU:HD13	1.85	0.42
2:G:2398:THR:O	2:G:2398:THR:OG1	2.37	0.42
1:C:992:ASN:O	1:C:996:LYS:N	2.34	0.42
1:C:1289:MET:O	1:C:1290:VAL:C	2.59	0.42
1:C:2329:GLU:O	1:C:2333:THR:N	2.46	0.42
1:C:2800:ALA:O	1:C:2804:HIS:ND1	2.42	0.42
1:C:2880:MET:O	1:C:2884:VAL:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3741:THR:CB	1:C:3742:ILE:HD12	2.50	0.42
1:C:2628:THR:O	1:C:2632:LEU:N	2.52	0.42
1:C:2847:ILE:HG22	1:C:2848:ASN:N	2.35	0.42
1:C:2949:ILE:HD11	1:C:2970:VAL:HG13	2.02	0.42
2:G:2467:LEU:O	2:G:2471:THR:HG23	2.20	0.42
1:C:1434:LEU:HD21	1:C:1463:PHE:CD1	2.55	0.41
1:C:2474:LEU:HB3	1:C:2648:LEU:HD11	2.02	0.41
1:C:2957:ASN:OD1	1:C:2957:ASN:N	2.50	0.41
1:C:1050:THR:OG1	1:C:1118:ILE:HG22	2.20	0.41
1:C:1052:VAL:HG22	1:C:2521:ILE:HG13	2.01	0.41
1:C:1740:ILE:HB	1:C:1741:PRO:HD3	2.02	0.41
1:C:1865:ALA:O	1:C:1869:LEU:N	2.52	0.41
1:C:2248:LYS:HE3	1:C:2249:VAL:HG13	2.01	0.41
1:C:2773:GLU:HB2	1:C:2796:ALA:HB2	2.02	0.41
1:C:554:VAL:HG23	1:C:555:CYS:N	2.36	0.41
1:C:2846:HIS:O	2:G:2413:ARG:NH1	2.51	0.41
1:C:3122:TYR:CZ	2:G:2498:LEU:HD21	2.56	0.41
1:C:3369:ASN:O	1:C:3373:LYS:N	2.48	0.41
1:C:565:THR:OG1	1:C:578:ASN:N	2.50	0.41
1:C:817:LEU:HD23	1:C:817:LEU:N	2.36	0.41
1:C:935:LEU:HD11	1:C:2636:LEU:HB3	2.02	0.41
1:C:1292:PRO:HG2	1:C:1335:PHE:CD1	2.55	0.41
1:C:1881:TYR:HB2	1:C:1919:ILE:HG21	2.02	0.41
1:C:1949:ILE:HG21	1:C:1961:VAL:HG12	2.03	0.41
1:C:2206:THR:O	1:C:2207:LYS:CG	2.68	0.41
1:C:899:GLY:O	1:C:903:ARG:NH2	2.53	0.41
1:C:1177:LEU:HD13	1:C:1234:GLN:HA	2.00	0.41
1:C:1905:PHE:CD1	1:C:1927:LEU:HD21	2.55	0.41
1:C:3370:PHE:O	1:C:3374:LEU:N	2.54	0.41
1:C:3491:HIS:O	1:C:3492:TYR:C	2.58	0.41
1:C:3731:LEU:O	1:C:3732:THR:O	2.39	0.41
1:C:1128:SER:OG	1:C:1130:GLU:OE2	2.32	0.41
1:C:2098:VAL:HG12	1:C:2102:ILE:CD1	2.51	0.41
1:C:2797:MET:HE1	2:G:2468:MET:SD	2.60	0.41
1:C:3574:VAL:CG2	1:C:3584:VAL:HG23	2.47	0.41
1:C:915:VAL:HG23	1:C:915:VAL:O	2.21	0.41
1:C:2850:TYR:CE1	1:C:2872:VAL:HG23	2.56	0.41
1:C:3105:ILE:HD11	1:C:3125:LYS:HB2	2.02	0.41
2:G:2384:LEU:HD11	2:G:2392:ILE:CA	2.51	0.41
1:C:985:TYR:O	1:C:989:ALA:N	2.52	0.41
1:C:1575:MET:O	1:C:1578:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2497:GLU:HB2	1:C:2615:VAL:HG13	2.03	0.41
1:C:2773:GLU:CB	1:C:2796:ALA:HB2	2.51	0.41
1:C:3509:HIS:CG	1:C:3510:ASN:H	2.38	0.41
1:C:3557:GLU:O	1:C:3563:THR:OG1	2.37	0.41
1:C:928:PHE:HE1	1:C:2503:CYS:HG	1.64	0.41
1:C:1290:VAL:HB	1:C:1291:PRO:HD3	2.03	0.41
1:C:1520:LEU:O	1:C:1520:LEU:HD23	2.20	0.41
1:C:2597:LYS:O	1:C:2601:THR:HG23	2.22	0.41
1:C:3485:LEU:HD12	1:C:3573:ARG:HG3	2.04	0.41
2:G:2443:LEU:HB3	2:G:2448:ILE:HG23	2.02	0.41
1:C:438:SER:O	1:C:438:SER:OG	2.38	0.40
1:C:648:LYS:O	1:C:652:GLN:HG2	2.20	0.40
1:C:876:LEU:O	1:C:879:THR:HG22	2.21	0.40
1:C:2219:LEU:HD11	1:C:2243:TYR:CD1	2.56	0.40
1:C:3545:VAL:HG11	1:C:3710:PHE:O	2.21	0.40
1:C:3620:ALA:O	1:C:3624:ALA:N	2.46	0.40
1:C:1709:GLY:O	1:C:1712:GLU:N	2.48	0.40
1:C:2300:MET:C	1:C:2300:MET:SD	3.00	0.40
1:C:3180:ILE:HG21	1:C:3219:VAL:HG23	2.03	0.40
1:C:255:MET:HG3	1:C:256:ASN:H	1.86	0.40
1:C:1917:ARG:HA	1:C:1920:VAL:HG22	2.03	0.40
1:C:2306:ASN:N	1:C:2307:PRO:CD	2.84	0.40
1:C:2368:VAL:O	1:C:2372:GLU:N	2.51	0.40
1:C:3491:HIS:CD2	1:C:3491:HIS:H	2.38	0.40
1:C:972:VAL:HG23	1:C:2509:ILE:HG21	2.03	0.40
1:C:1018:PHE:HE1	1:C:1049:TYR:HH	1.66	0.40
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.54	0.40
1:C:2858:ARG:NH1	1:C:2989:SER:OG	2.55	0.40
1:C:3567:LEU:CD2	1:C:3674:ILE:HG23	2.52	0.40
1:C:3658:THR:O	1:C:3658:THR:HG22	2.21	0.40
2:G:2433:GLU:O	2:G:2444:ARG:CZ	2.62	0.40
1:C:943:ILE:HD11	1:C:970:PHE:CB	2.51	0.40
1:C:1074:THR:O	1:C:1074:THR:HG22	2.21	0.40
1:C:2470:VAL:HG22	1:C:2502:VAL:HG11	2.04	0.40
1:C:2746:ASP:OD1	1:C:2768:ARG:NH1	2.45	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	C	3015/3859 (78%)	2824 (94%)	179 (6%)	12 (0%)	30 60
2	G	127/3159 (4%)	114 (90%)	9 (7%)	4 (3%)	3 18
All	All	3142/7018 (45%)	2938 (94%)	188 (6%)	16 (0%)	27 54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1062	LEU
1	C	2190	PHE
1	C	2449	CYS
1	C	3509	HIS
2	G	2393	VAL
1	C	678	ASN
1	C	1296	LEU
2	G	2386	LEU
2	G	2387	PRO
2	G	2388	LEU
1	C	1292	PRO
1	C	857	GLN
1	C	981	LYS
1	C	1285	VAL
1	C	1762	PRO
1	C	3732	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	2742/3423 (80%)	2658 (97%)	84 (3%)	35 60
2	G	119/2663 (4%)	109 (92%)	10 (8%)	9 29
All	All	2861/6086 (47%)	2767 (97%)	94 (3%)	35 58

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	250	PHE
1	C	309	MET
1	C	352	ASP
1	C	368	ARG
1	C	409	GLU
1	C	418	MET
1	C	625	MET
1	C	647	PHE
1	C	648	LYS
1	C	703	ASN
1	C	852	CYS
1	C	882	ASN
1	C	975	MET
1	C	1011	ASP
1	C	1076	MET
1	C	1094	ASP
1	C	1123	SER
1	C	1215	MET
1	C	1280	GLU
1	C	1287	GLN
1	C	1289	MET
1	C	1300	GLN
1	C	1433	MET
1	C	1468	MET
1	C	1574	MET
1	C	1614	LEU
1	C	1635	ARG
1	C	1676	PHE
1	C	1729	MET
1	C	1733	LYS
1	C	1753	PHE
1	C	1783	TYR
1	C	1835	TYR
1	C	1841	GLU
1	C	1905	PHE

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Mol	Chain	Res	Type
1	C	1914	MET
1	C	1969	GLN
1	C	1985	MET
1	C	2003	ARG
1	C	2190	PHE
1	C	2195	ARG
1	C	2248	LYS
1	C	2289	LEU
1	C	2294	MET
1	C	2338	MET
1	C	2390	ARG
1	C	2417	PHE
1	C	2418	LEU
1	C	2423	TYR
1	C	2425	TYR
1	C	2466	MET
1	C	2479	CYS
1	C	2657	CYS
1	C	2666	ASP
1	C	2667	CYS
1	C	2670	SER
1	C	2715	PHE
1	C	2772	SER
1	C	2792	SER
1	C	2799	LYS
1	C	2875	SER
1	C	2913	SER
1	C	3128	PHE
1	C	3164	GLU
1	C	3174	HIS
1	C	3205	LEU
1	C	3251	LEU
1	C	3323	ASP
1	C	3378	PHE
1	C	3446	LYS
1	C	3469	SER
1	C	3470	ASN
1	C	3492	TYR
1	C	3555	CYS
1	C	3591	LEU
1	C	3640	GLU
1	C	3650	MET

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Mol	Chain	Res	Type
1	C	3706	ASN
1	C	3710	PHE
1	C	3738	PHE
1	C	3776	ASP
1	C	3806	GLN
1	C	3819	MET
1	C	3828	PHE
2	G	2384	LEU
2	G	2386	LEU
2	G	2389	ASN
2	G	2390	LEU
2	G	2392	ILE
2	G	2394	SER
2	G	2402	ASP
2	G	2424	ARG
2	G	2446	SER
2	G	2506	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	284	GLN
1	C	405	ASN
1	C	425	ASN
1	C	652	GLN
1	C	801	HIS
1	C	836	ASN
1	C	855	ASN
1	C	920	GLN
1	C	1005	HIS
1	C	1078	HIS
1	C	1287	GLN
1	C	1312	ASN
1	C	1328	ASN
1	C	1371	ASN
1	C	1443	ASN
1	C	1652	ASN
1	C	1707	ASN
1	C	1728	ASN
1	C	1763	ASN
1	C	1803	ASN
1	C	2166	ASN

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Mol	Chain	Res	Type
1	C	2377	ASN
1	C	2464	ASN
1	C	2832	ASN
1	C	2928	HIS
1	C	2935	GLN
1	C	3088	GLN
1	C	3435	HIS
1	C	3474	GLN
2	G	2378	GLN
2	G	2382	GLN
2	G	2427	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

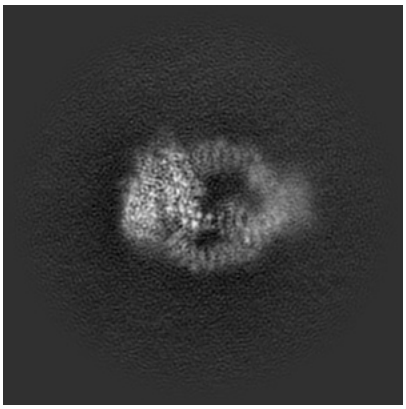
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45176. These allow visual inspection of the internal detail of the map and identification of artifacts.

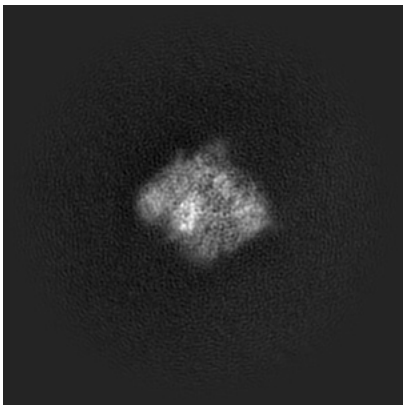
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

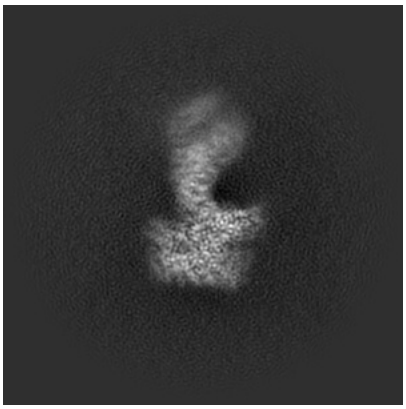
6.1.1 Primary map



X

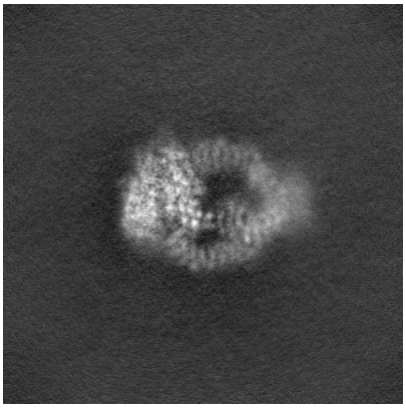


Y

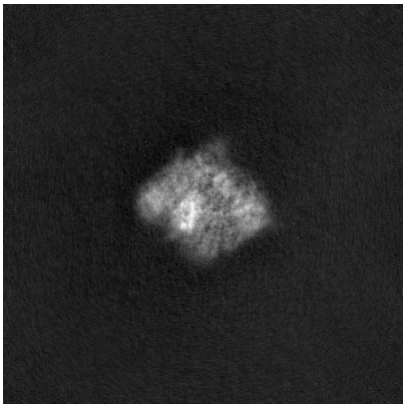


Z

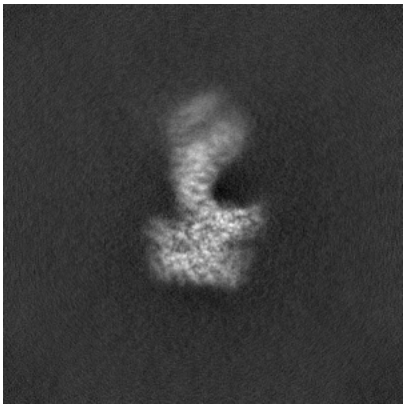
6.1.2 Raw map



X



Y

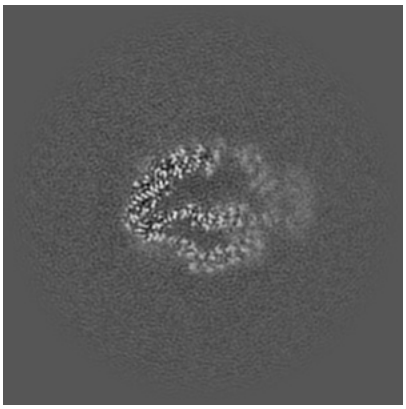


Z

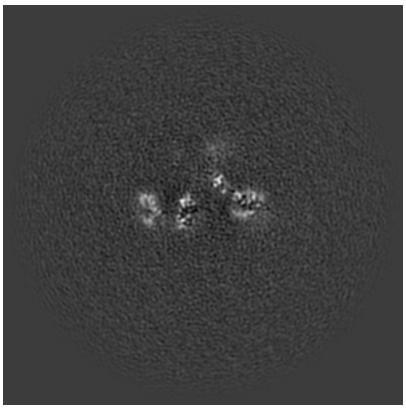
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

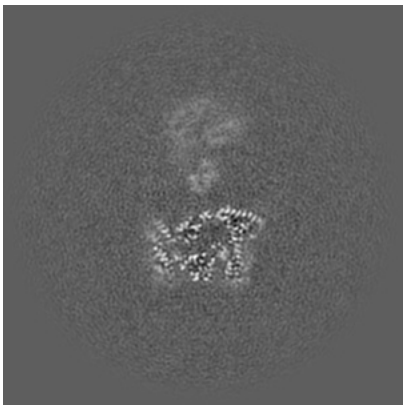
6.2.1 Primary map



X Index: 180

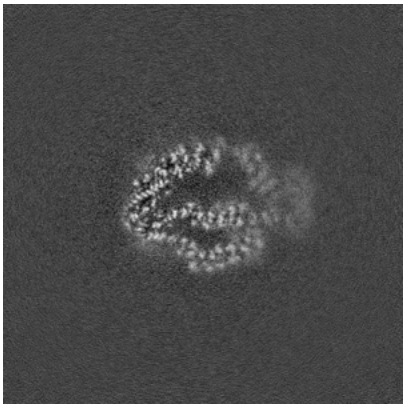


Y Index: 180

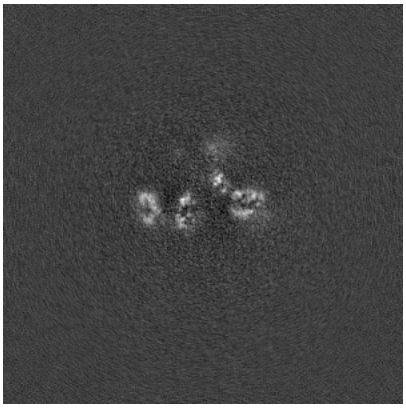


Z Index: 180

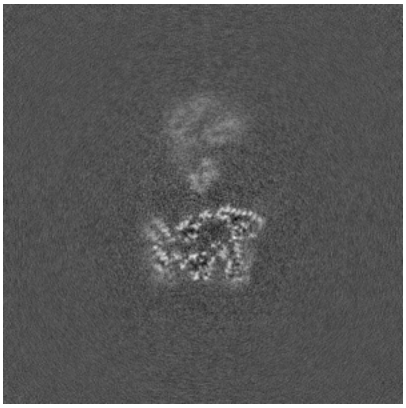
6.2.2 Raw map



X Index: 180



Y Index: 180

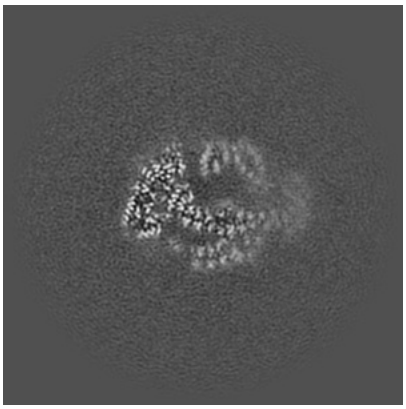


Z Index: 180

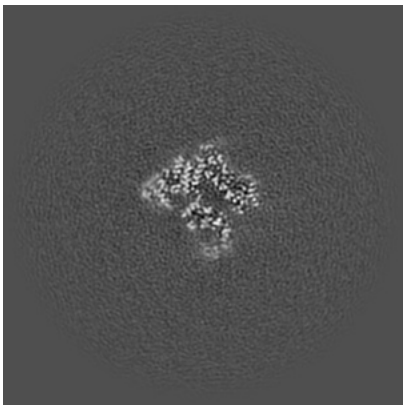
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

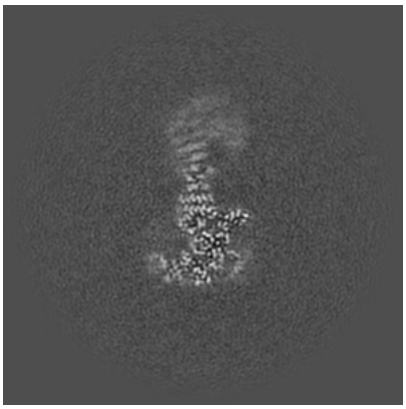
6.3.1 Primary map



X Index: 173

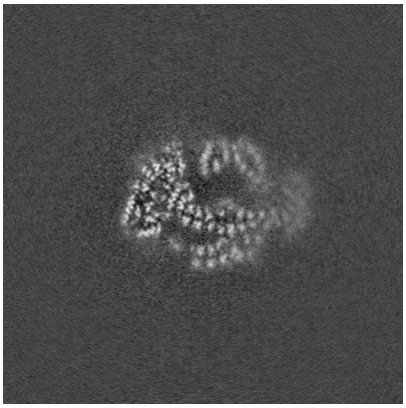


Y Index: 162

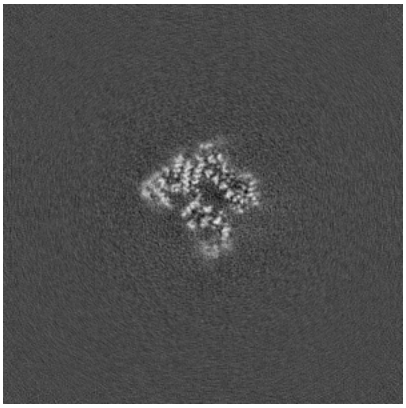


Z Index: 170

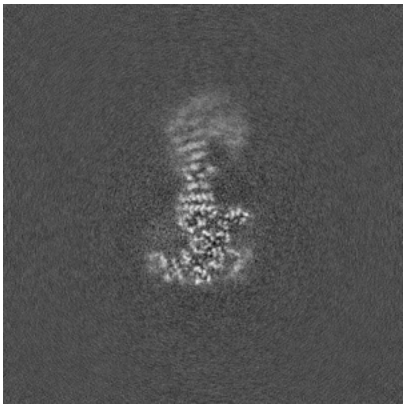
6.3.2 Raw map



X Index: 173



Y Index: 162

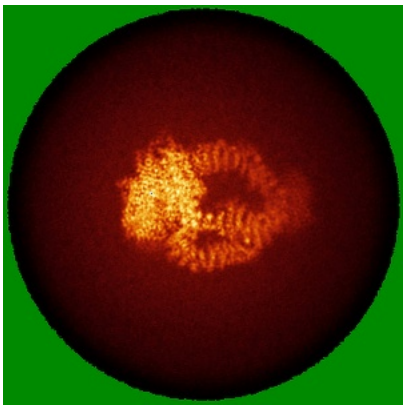


Z Index: 170

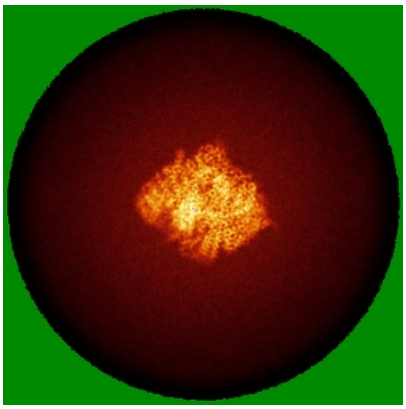
The images above show the largest variance slices of the map in three orthogonal directions.

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

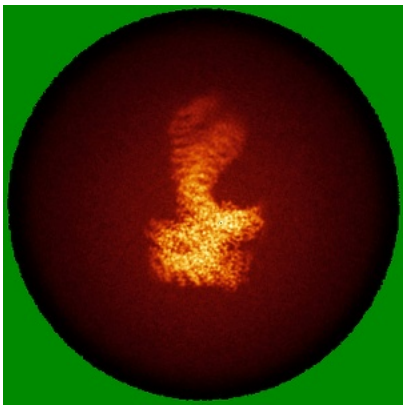
6.4.1 Primary map



X

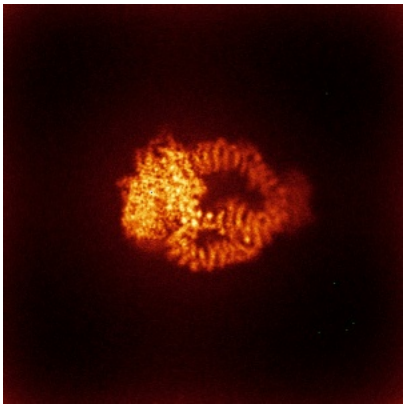


Y

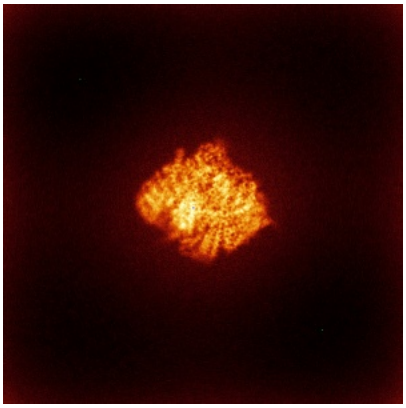


Z

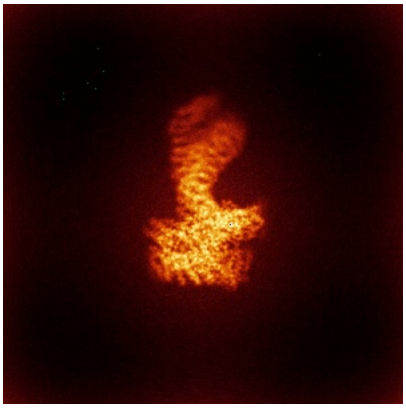
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.451. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

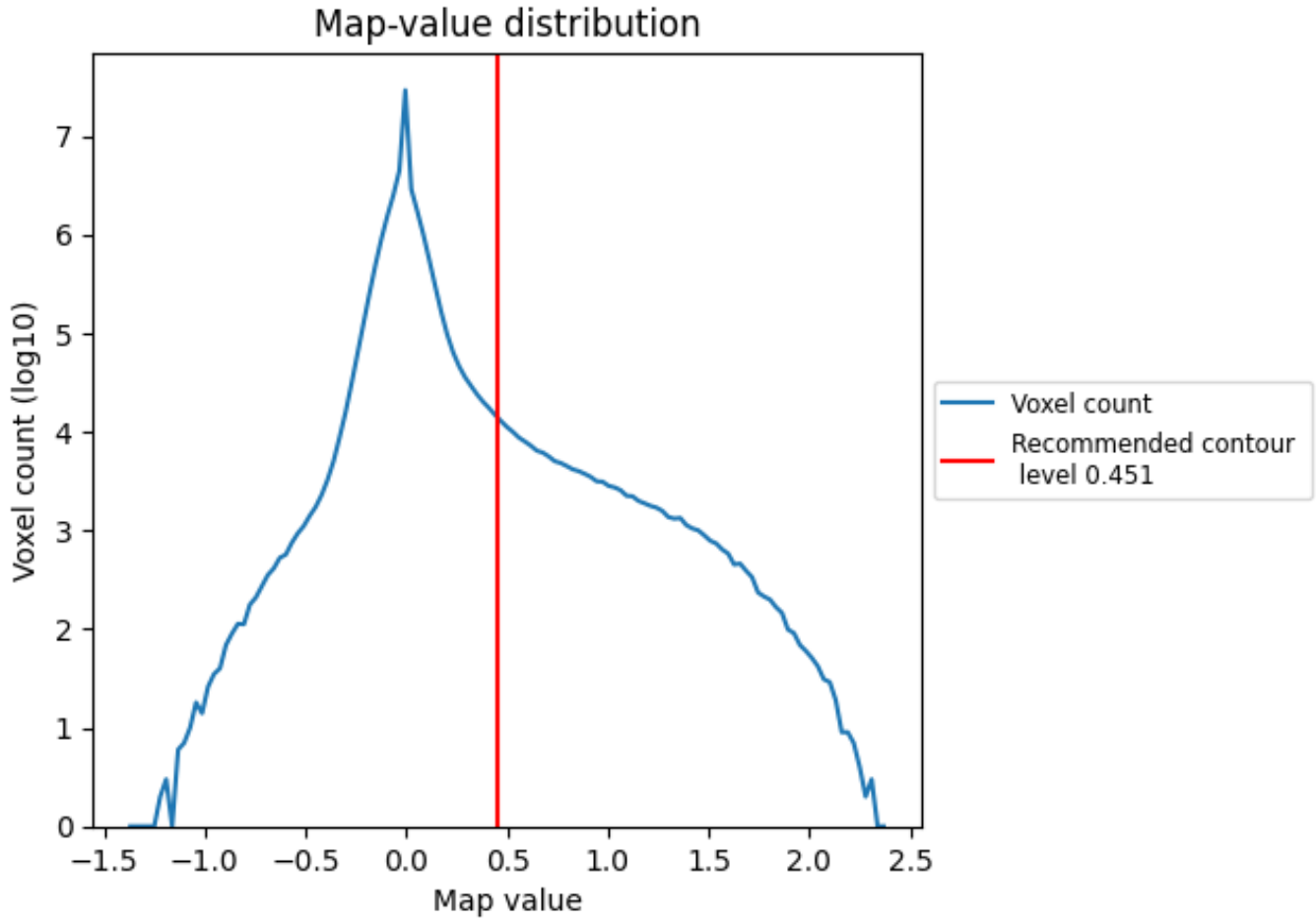
6.6 Mask visualisation (i)

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

7 Map analysis

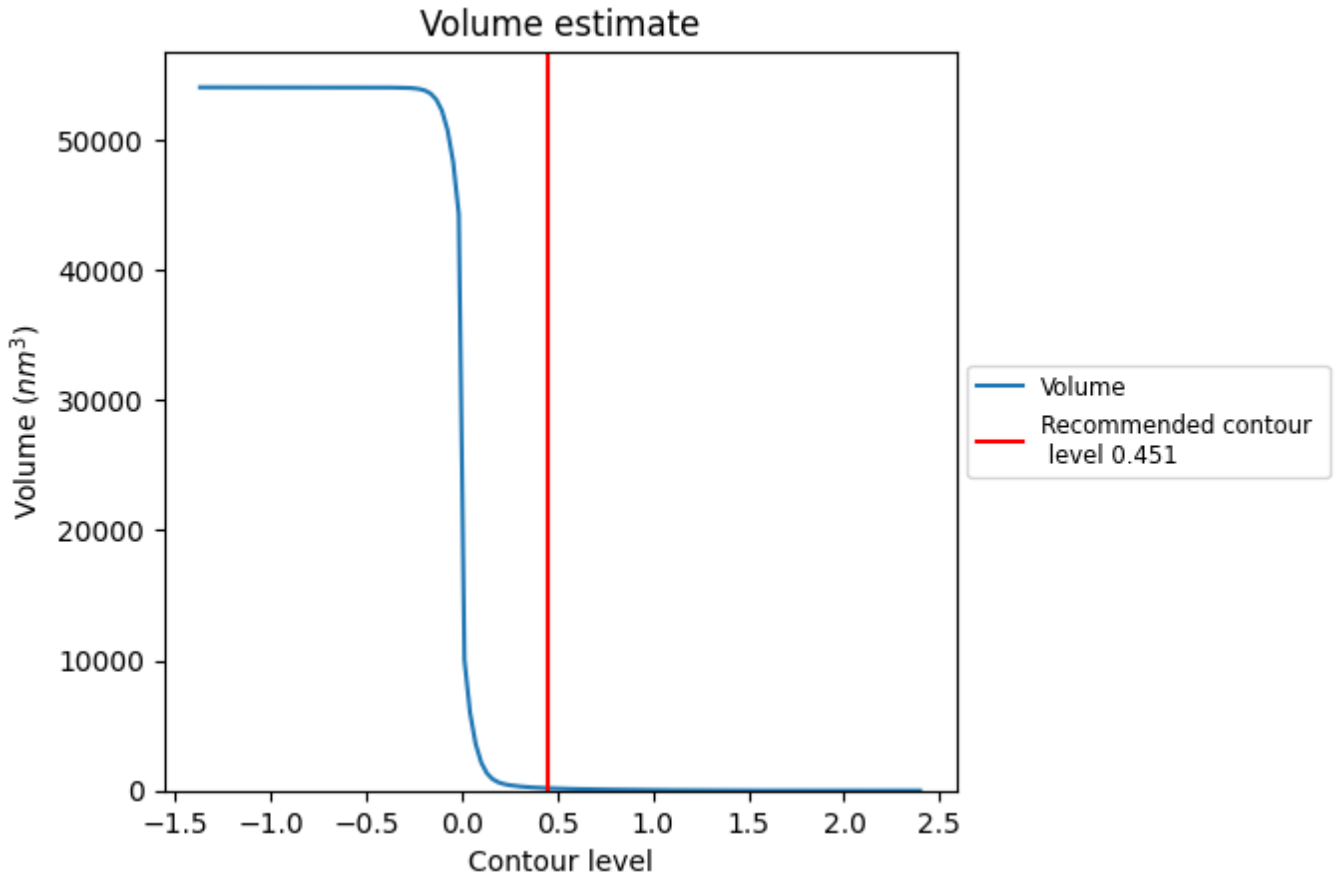
This section contains the results of statistical analysis of the map.

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.

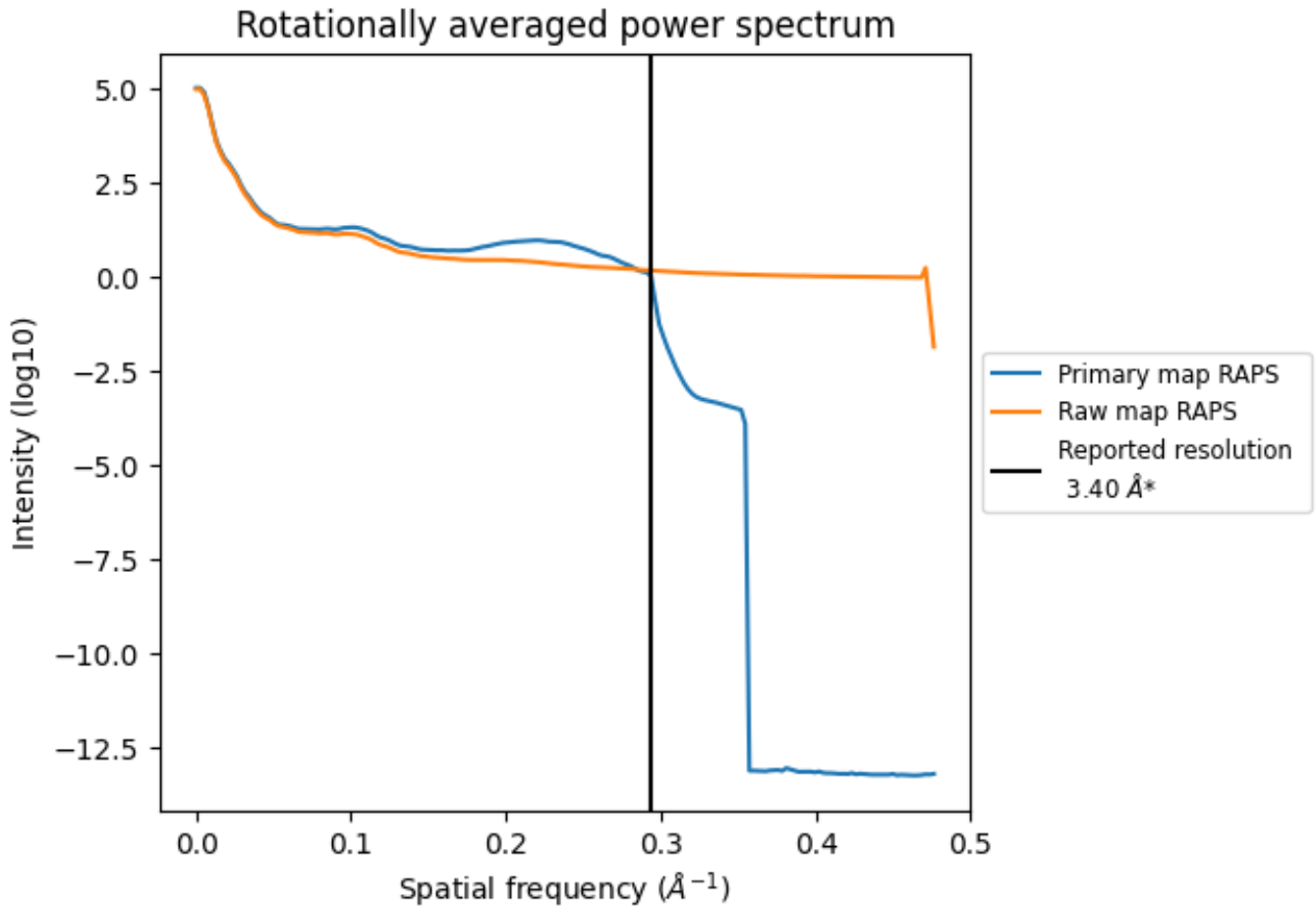
7.2 Volume estimate (i)



The volume at the recommended contour level is 182 nm^3; this corresponds to an approximate mass of 164 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)

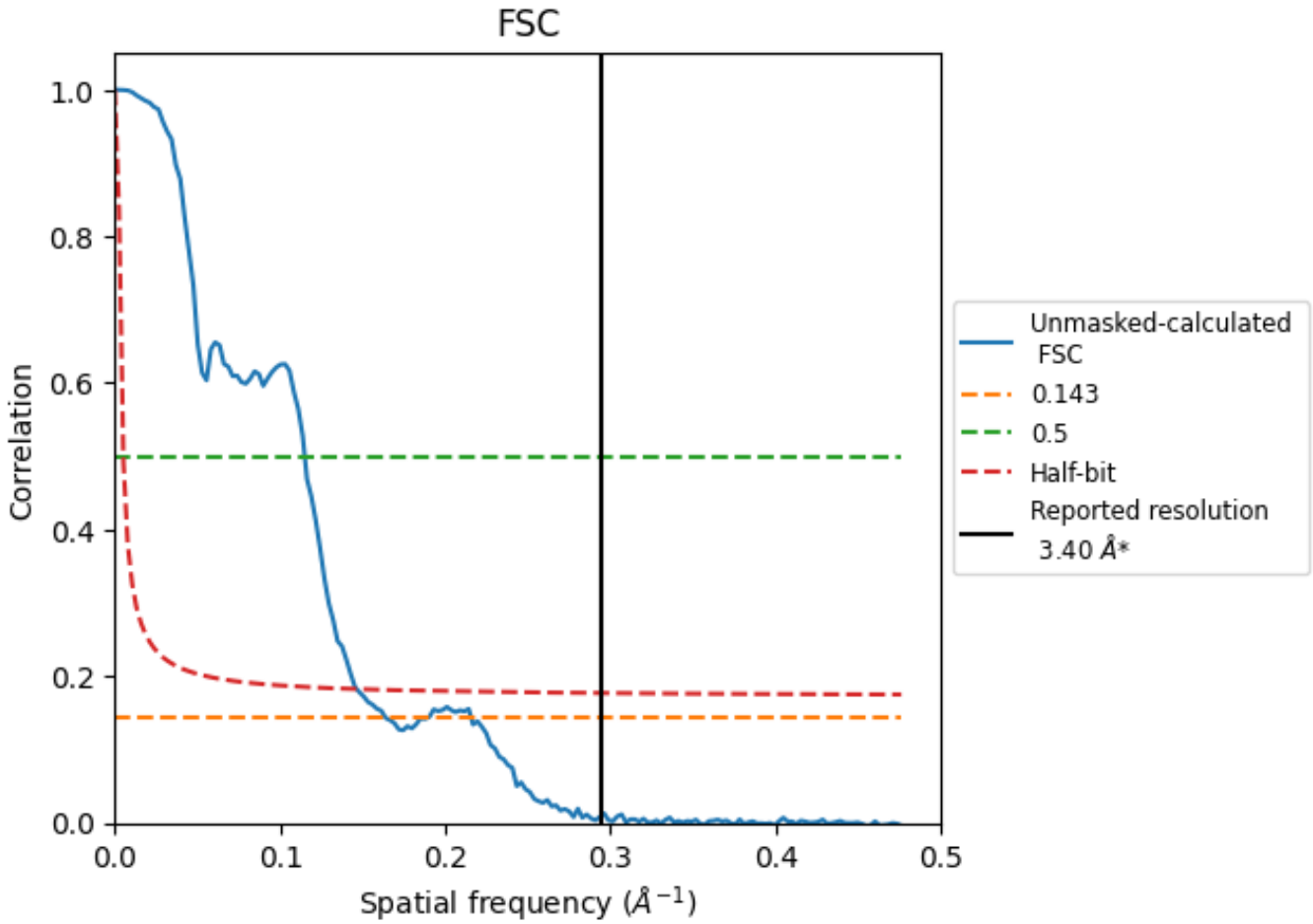


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

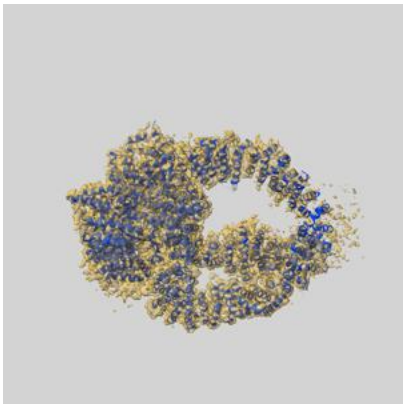
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.10	8.70	6.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.10 differs from the reported value 3.4 by more than 10 %

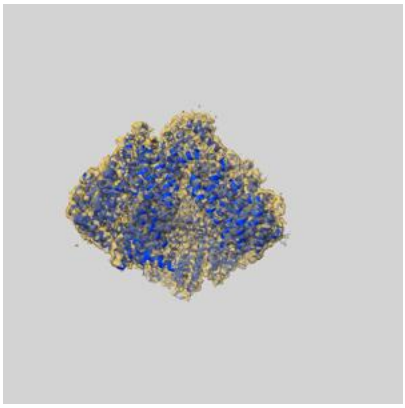
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45176 and PDB model 9C47. Per-residue inclusion information can be found in section 3 on page 4.

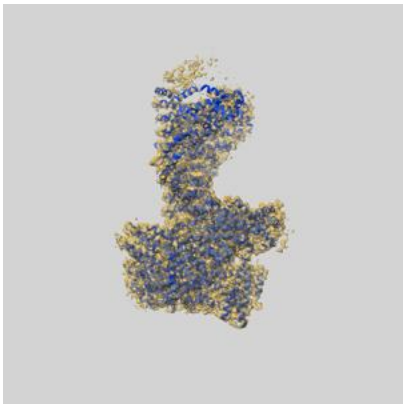
9.1 Map-model overlay



X



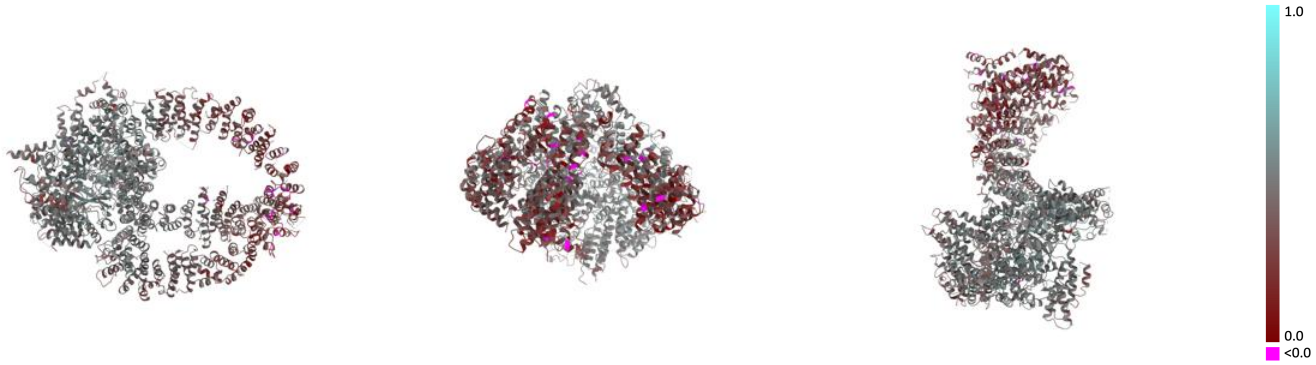
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.451 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.

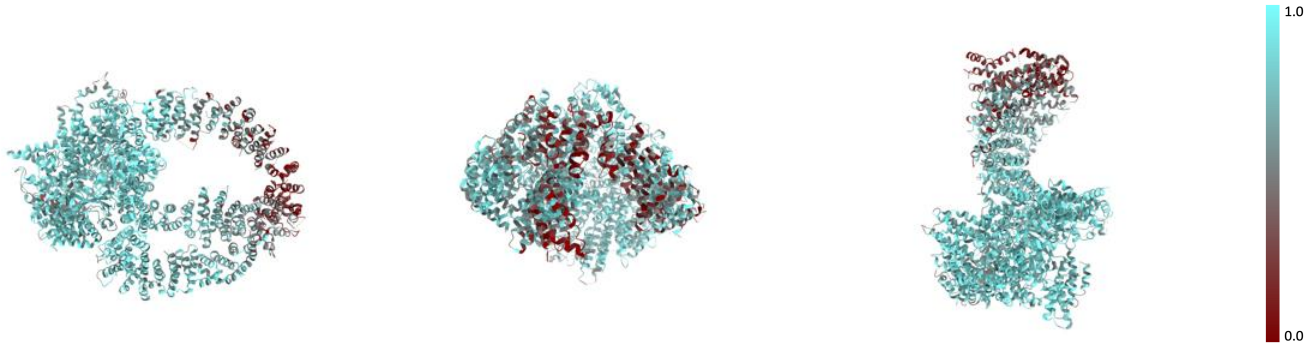
9.2 Q-score mapped to coordinate model (i)



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.

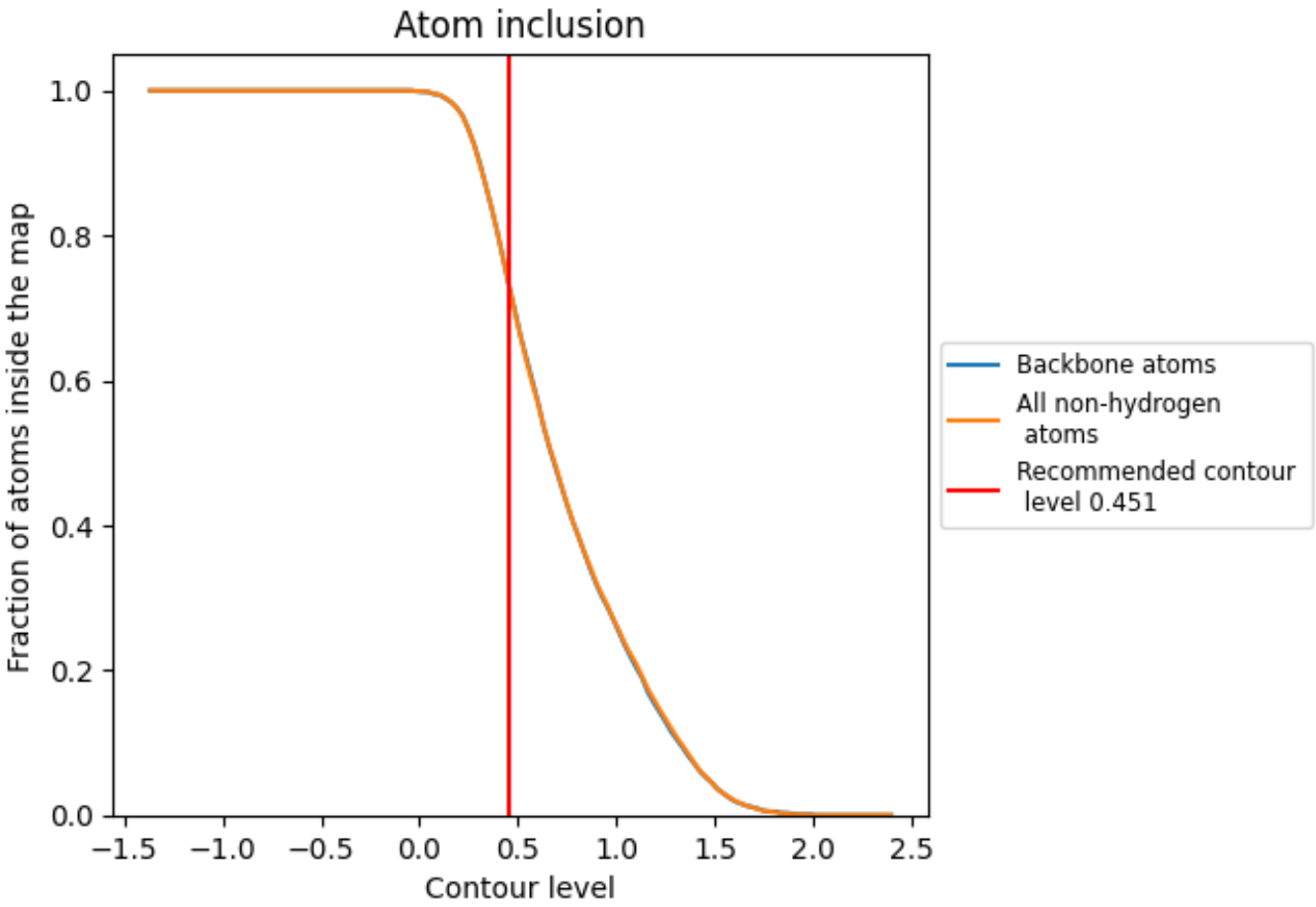
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.451).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 74% 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 (0.451) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.4200
C	0.7460	0.4200
G	0.7250	0.4210