Full wwPDB EM Validation Report ⓘ

Apr 19, 2025 – 07:29 am BST

PDB ID	:	8RD4 / pdb_00008rd4
EMDB ID	:	EMD-19065
Title	:	Telomeric RAP1:DNA-PK complex
Authors	:	Eickhoff, P.; Fisher, C.E.L.; Inian, O.; Guettler, S.; Douglas, M.E.
Deposited on	:	2023-12-07
Resolution	:	3.58 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:

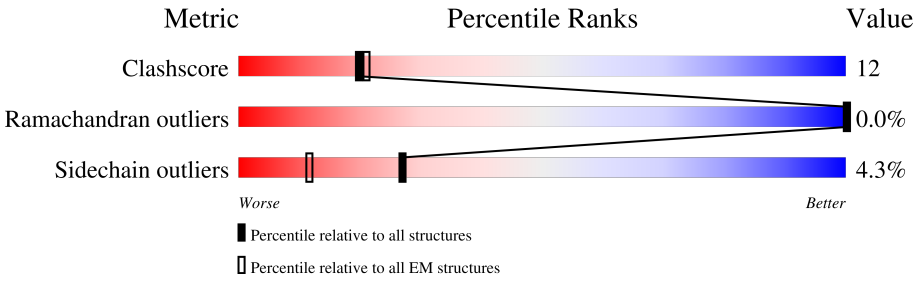
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.58 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	A	4128	7% 61% 25% • 13%
2	D	399	• 27% 12% • 60%
3	E	609	• 64% 27% • 8%
4	F	732	• 52% 22% • 24%
5	X	100	6% 20% 21% 59%
6	Y	100	5% 16% 25% 59%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40711 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3597	28855	18531	4885	5250	189	0	0

- Molecule 2 is a protein called Telomeric repeat-binding factor 2-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	158	1232	770	223	235	4	0	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	560	4522	2891	764	847	20	0	0

- Molecule 4 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	553	4421	2820	747	831	23	0	0

- Molecule 5 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	X	41	842	401	154	246	41	0	0

- Molecule 6 is a DNA chain called DNA (41-MER).

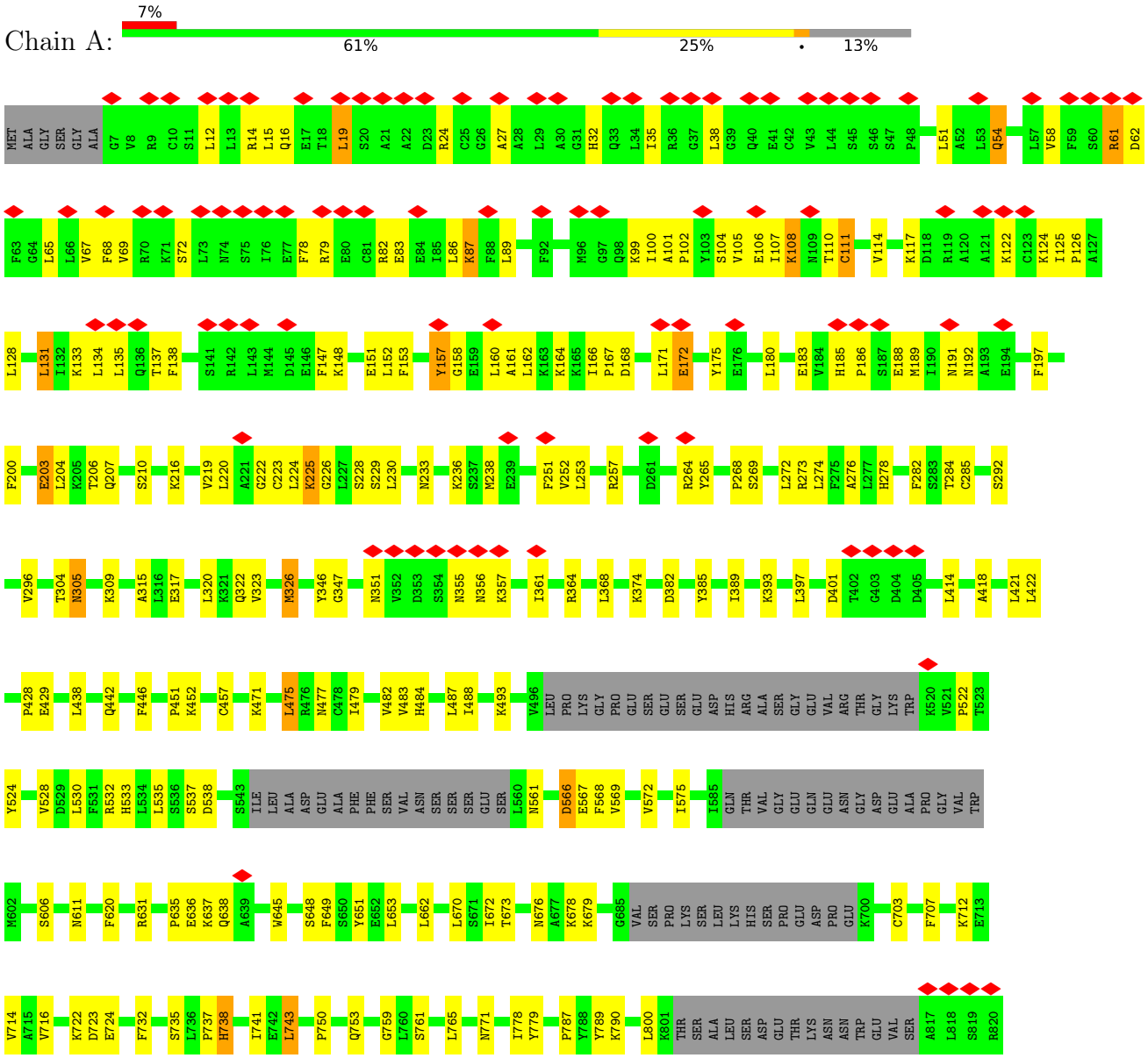
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	Y	41	839	400	152	246	41	0	0

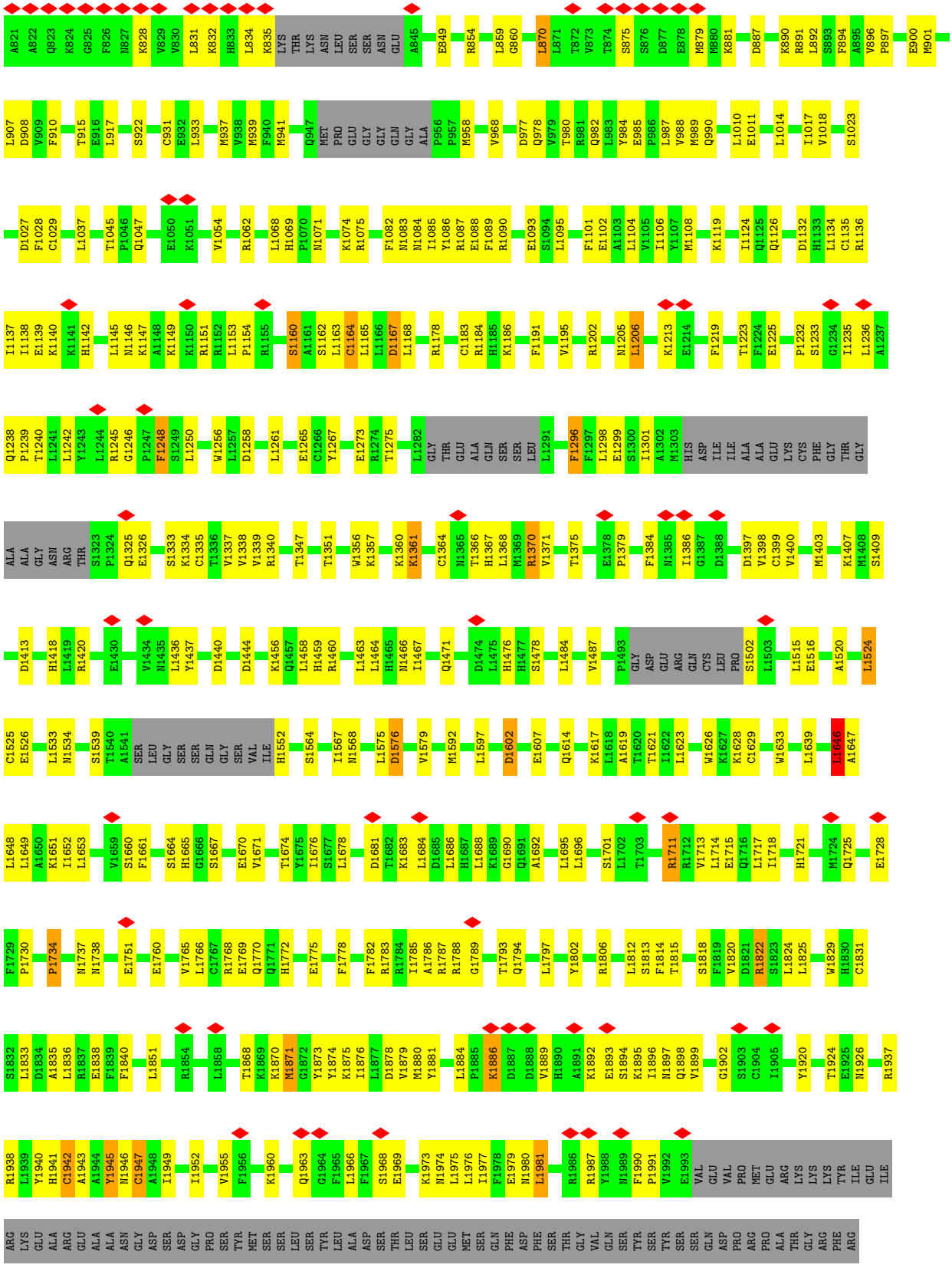
3 Residue-property plots (i)

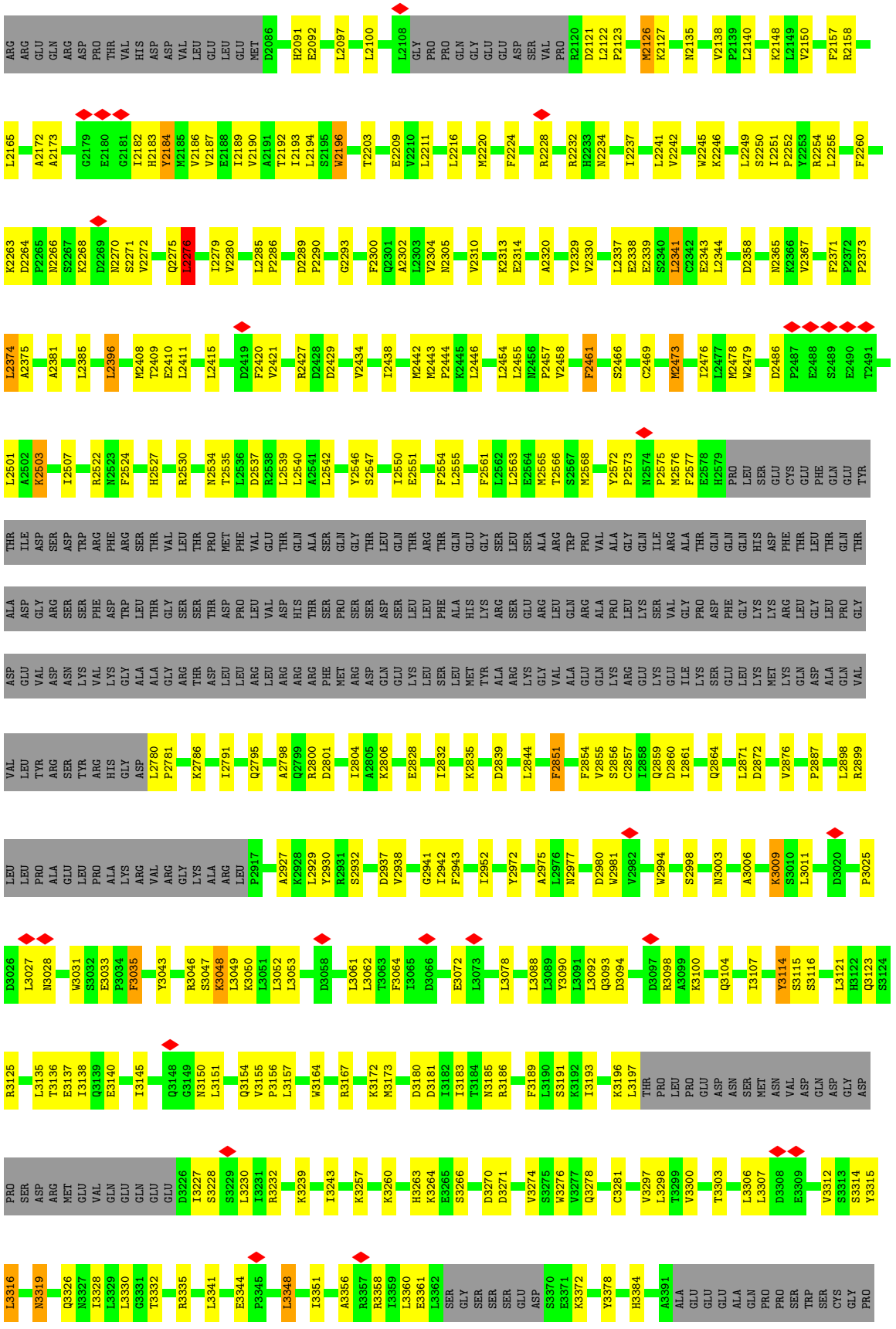
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

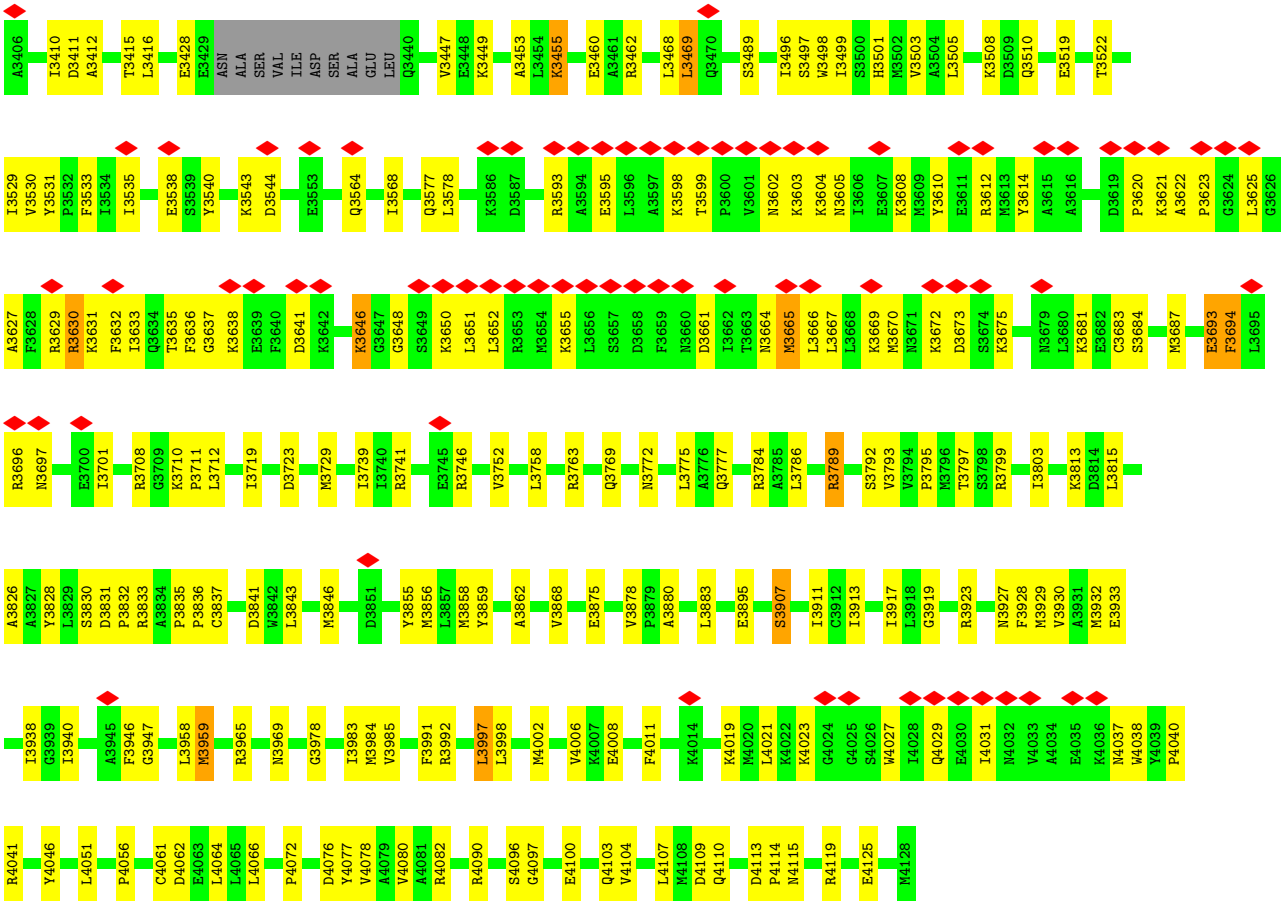
- Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain A:



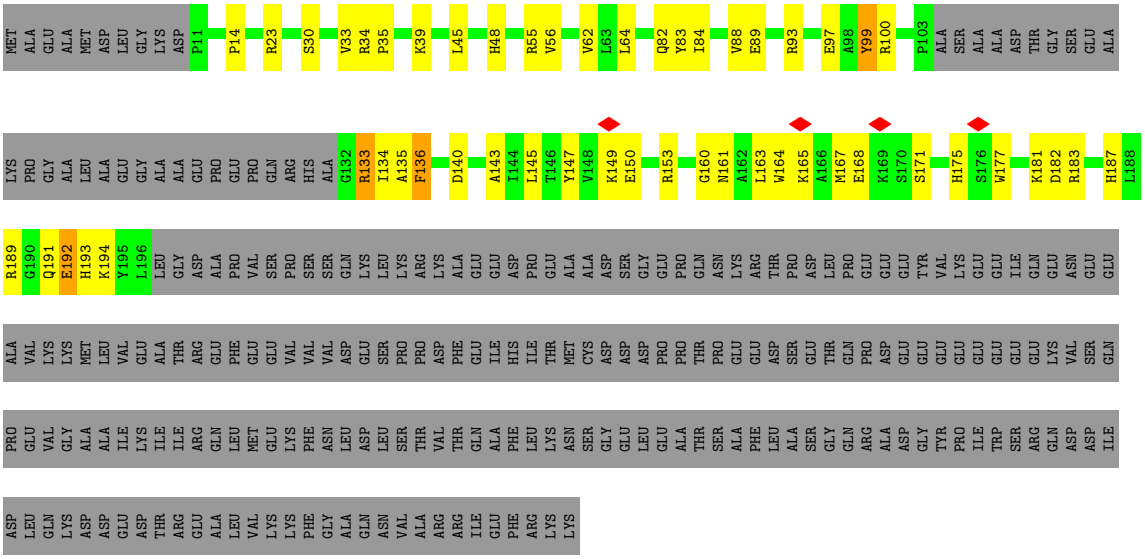

A821 A822 Q823 K824 G825 F826 N827 K828 V829 V830 L831 K832 H833 L834 K835 LYS THR LYS ASN LEU SER ASN GLU A845 E849 R854 L859 G860 L870 L871 T872 V873 T874 S875 S876 D877 E878 M879 M880 K881 D887 K890 R891 L892 S893 F894 A895 V896 P897 E900 M901
L907 D908 V909 F910 T915 E916 L917 S922 C931 E932 L933 M937 V938 M939 F940 M941 Q947 MET PRO GLU GLY GLY GLN GLY ALA P956 P957 M958 V968 D977 Q978 V979 T980 R981 Q982 L983 Y984 E985 P986 L987 V988 M989 Q990 L1010 E1011 L1014 I1017 V1018 S1023
D1027 F1028 C1029 L1037 T1045 P1046 Q1047 E1050 K1051 V1054 R1062 L1068 H1069 P1070 N1071 K1074 R1075 F1082 N1083 N1084 I1085 Y1086 R1087 E1088 F1089 R1090 E1093 S1094 L1095 F1101 E1102 A1103 L1104 V1105 I1106 Y1107 M1108 K1119 I1124 Q1125 Q1126 D1132 H1133 L1134 C1135 R1136
I1137 I1138 E1139 K1140 K1141 H1142 L1145 N1146 K1147 A1148 K1149 K1150 R1151 R1152 L1153 P1154 R1155 S1160 A1161 S1162 L1163 C1164 L1165 L1166 D1167 L1168 R1178 C1183 R1184 H1185 K1186 F1191 V1195 R1202 N1205 L1206 K1213 E1214 F1219 T1223 F1224 E1225 P1232 S1233 G1234 I1235 L1236 A1237
Q1238 P1239 T1240 L1241 L1242 Y1243 L1244 R1245 G1246 P1247 F1248 S1249 L1250 W1256 L1257 D1258 L1261 E1265 C1266 Y1267 E1273 R1274 T1275 L1282 GLY THR GLU ALA GLN SER SER LEU L1291 F1296 F1297 L1298 E1299 S1300 I1301 A1302 M1303 HIS ASP ILE ILE ALA ALA GLU LYS CYS PHE GLY THR GLY
ALA ALA GLY ASN ARG THR S1323 P1324 Q1325 E1326 S1333 K1334 C1335 T1336 V1337 V1338 V1339 R1340 T1347 T1351 W1356 K1357 K1360 K1361 C1364 N1365 T1366 H1367 L1368 M1369 R1370 V1371 T1375 E1378 P1379 F1384 N1385 I1386 G1387 D1388 D1397 V1398 C1399 V1400 M1403 K1407 M1408 S1409
D1413 H1418 L1419 R1420 E1430 V1434 N1435 L1436 Y1437 D1440 D1444 K1456 Q1457 L1458 H1459 R1460 L1463 L1464 H1465 N1466 I1467 Q1471 D1474 L1475 H1476 H1477 S1478 L1484 V1487 P1493 GLY ASP GLU ARG GLN CYS LEU PRO S1502 L1503 L1515 E1516 A1520 L1524
C1525 E1526 L1533 N1534 S1539 T1540 A1541 SER LEU GLY SER SER GLN GLY SER VAL ILE H1552 S1564 I1567 N1568 L1575 D1576 V1579 M1592 L1597 D1602 E1607 Q1614 K1617 L1618 A1619 T1620 T1621 I1622 L1623 W1626 K1627 K1628 C1629 W1633 L1639 L1646 A1647
L1648 L1649 A1650 K1651 I1652 L1653 V1659 S1660 F1661 S1664 H1665 G1666 S1667 E1670 V1671 T1674 Y1675 I1676 S1677 L1678 D1681 T1682 K1683 L1684 D1685 L1686 H1687 L1688 K1689 G1690 Q1691 A1692 L1695 L1696 S1701 L1702 T1703 R1711 R1712 V1713 L1714 E1715 Q1716 L1717 I1718 H1721 M1724 Q1725 E1728
F1729 P1730 P1734 N1737 N1738 E1751 E1760 V1765 L1766 C1767 R1768 E1769 Q1770 Q1771 H1772 E1775 F1778 F1782 R1783 R1784 I1785 A1786 R1787 R1788 G1789 T1793 Q1794 L1797 Y1802 R1806 L1812 S1813 F1814 T1815 S1818 F1819 V1820 D1821 R1822 S1823 L1824 L1825 W1829 H1830 C1831
S1832 L1833 D1834 A1835 L1836 R1837 E1838 F1839 F1840 L1851 R1854 L1858 T1868 K1869 K1870 M1871 G1872 Y1873 Y1874 K1875 I1876 L1877 D1878 V1879 M1880 Y1881 L1884 P1885 K1886 D1887 D1888 V1889 H1890 A1891 K1892 E1893 S1894 K1895 I1896 N1897 Q1898 V1899 G1902 S1903 C1904 I1905 Y1920 T1924 E1925 N1926 R1937
R1938 L1939 Y1940 H1941 C1942 A1943 A1944 Y1945 N1946 C1947 A1948 I1949 I1952 V1955 F1956 K1960 Q1963 G1964 F1965 L1966 F1967 S1968 E1969 K1973 N1974 L1975 L1976 I1977 F1978 E1979 N1980 L1981 R1986 R1987 Y1988 N1989 F1990 P1991 V1992 E1993 VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE
ARG LYS GLU ALA ARG GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER SER LEU SER TYR LEU ALA ASP SER THR LEU SER GLU GLU MET SER GLN PHE ASP PHE SER THR GLY VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG





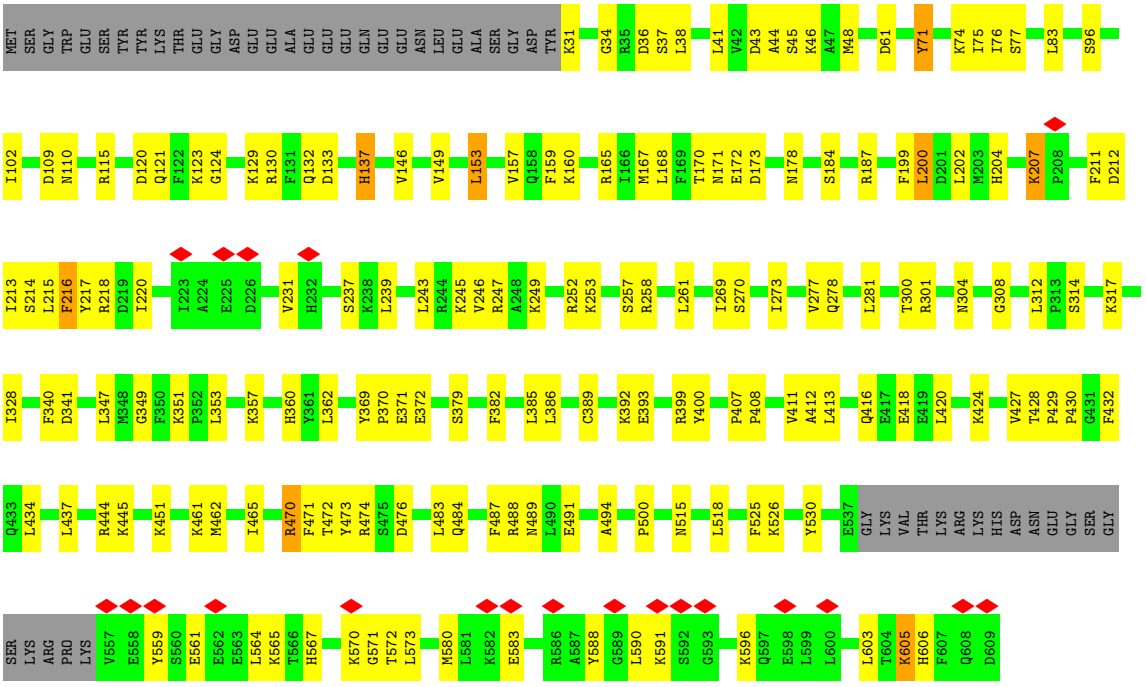
• Molecule 2: Telomeric repeat-binding factor 2-interacting protein 1

Chain D:



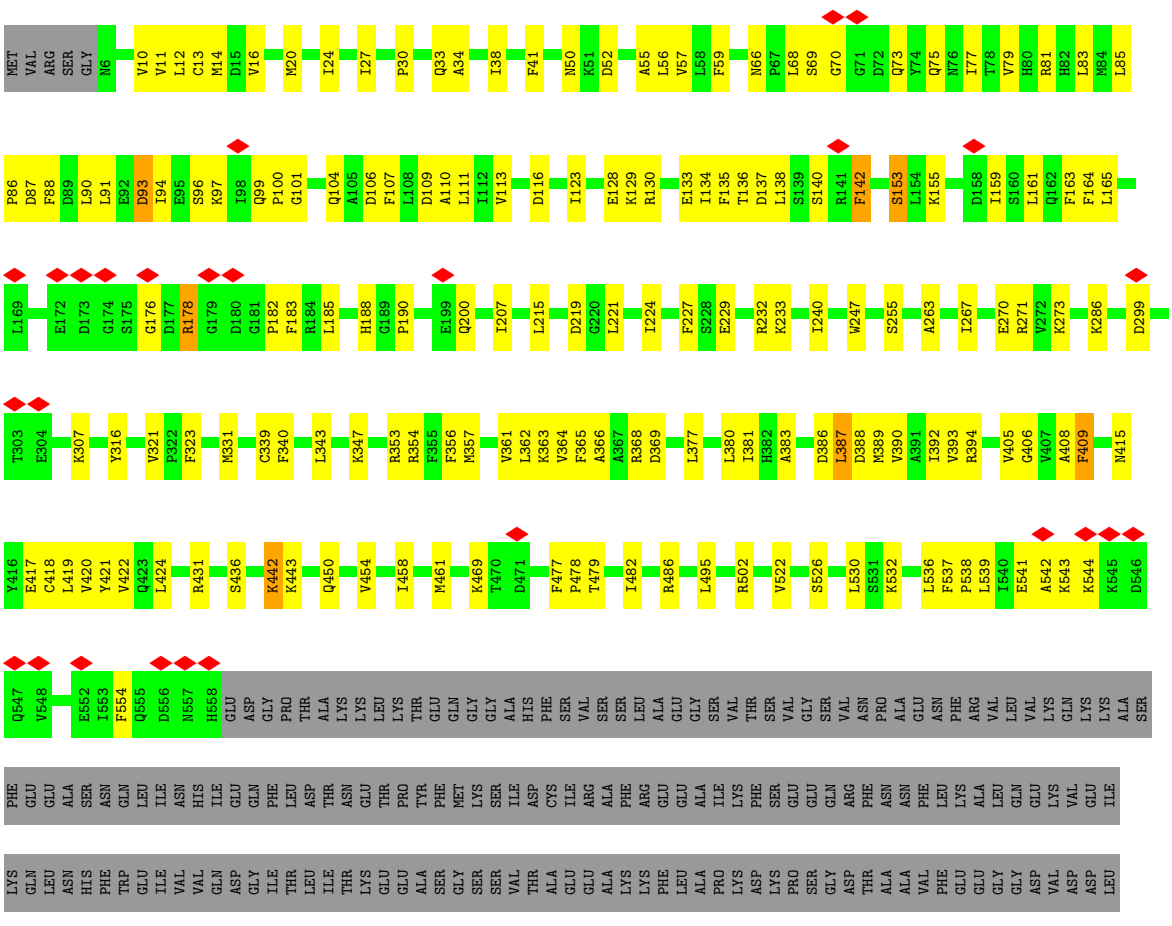
• Molecule 3: X-ray repair cross-complementing protein 6

Chain E:

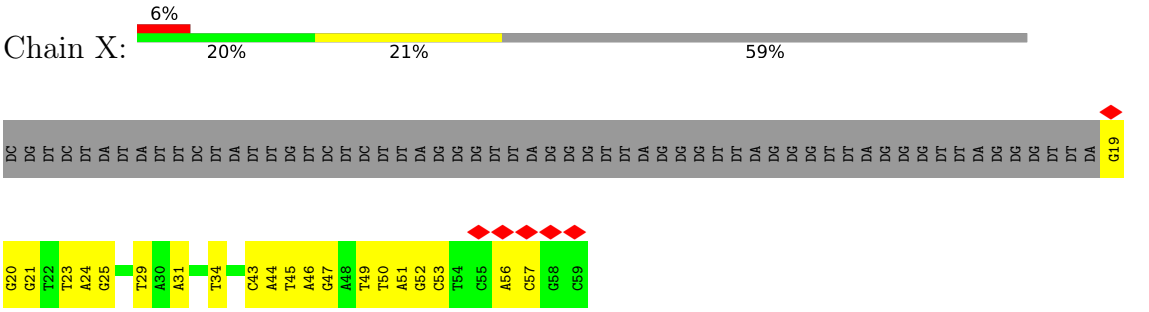


• Molecule 4: X-ray repair cross-complementing protein 5

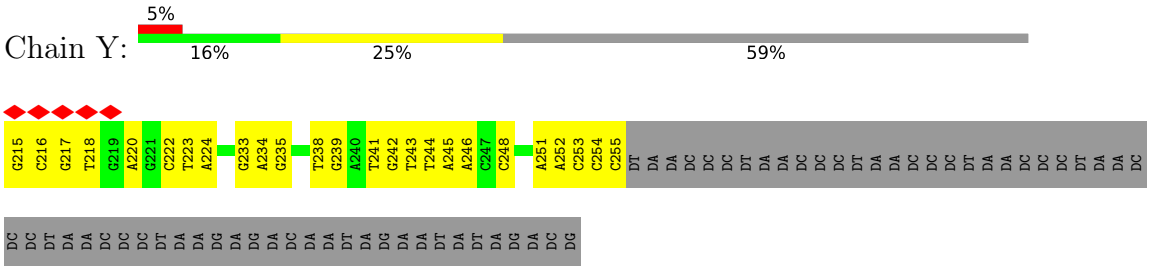
Chain F:



• Molecule 5: DNA (41-MER)



• Molecule 6: DNA (41-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	526885	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	57.506	Depositor
Minimum map value	-30.445	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.084	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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	A	0.26	0/29447	0.52	7/39776 (0.0%)
2	D	0.28	0/1257	0.57	0/1699
3	E	0.30	0/4609	0.52	0/6202
4	F	0.30	0/4511	0.52	1/6084 (0.0%)
5	X	0.57	0/944	0.91	0/1455
6	Y	0.60	0/940	0.93	0/1448
All	All	0.29	0/41708	0.55	8/56664 (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	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1734	PRO	CA-N-CD	-8.25	99.95	111.50
1	A	2374	LEU	CA-CB-CG	6.97	131.32	115.30
4	F	387	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	2276	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	1991	PRO	CA-N-CD	-5.70	103.52	111.50
1	A	1646	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	3316	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	326	MET	CA-CB-CG	5.26	122.24	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	183	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28855	0	29332	698	0
2	D	1232	0	1217	39	0
3	E	4522	0	4607	124	0
4	F	4421	0	4445	125	0
5	X	842	0	463	21	0
6	Y	839	0	463	22	0
All	All	40711	0	40527	991	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 12.

All (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:TYR:HH	1:A:1502:SER:N	1.47	1.12
1:A:2374:LEU:HD12	1:A:2375:ALA:H	1.37	0.88
1:A:1976:LEU:HD12	1:A:1979:GLU:HB3	1.57	0.86
3:E:411:VAL:HG11	3:E:434:LEU:HG	1.56	0.85
4:F:387:LEU:HD12	4:F:388:ASP:H	1.44	0.82
1:A:606:SER:HB3	1:A:1023:SER:HB2	1.64	0.80
1:A:86:LEU:HA	1:A:89:LEU:HB2	1.63	0.79
4:F:130:ARG:HB2	4:F:159:ILE:HG22	1.65	0.79
3:E:470:ARG:NH1	4:F:389:MET:SD	2.58	0.77
1:A:131:LEU:O	1:A:135:LEU:HB3	1.85	0.75
1:A:1245:ARG:HD2	1:A:1246:GLY:H	1.50	0.75
3:E:252:ARG:HD3	3:E:253:LYS:H	1.52	0.74
1:A:2871:LEU:HD22	1:A:2876:VAL:HG23	1.71	0.73
1:A:2234:ASN:HA	1:A:2237:ILE:HD12	1.70	0.73
3:E:413:LEU:HB3	3:E:432:PHE:HD2	1.54	0.73
4:F:93:ASP:HA	4:F:96:SER:HB3	1.70	0.73
1:A:111:CYS:SG	1:A:133:LYS:NZ	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1783:ARG:HG2	1:A:1787:ARG:HH21	1.54	0.72
1:A:3603:LYS:O	1:A:3605:ASN:ND2	2.23	0.72
3:E:207:LYS:NZ	3:E:211:PHE:O	2.20	0.72
4:F:363:LYS:HG2	4:F:420:VAL:HG12	1.72	0.72
3:E:170:THR:HG22	3:E:172:GLU:H	1.54	0.71
1:A:160:LEU:HD21	3:E:312:LEU:HG	1.72	0.71
1:A:1833:LEU:HD23	1:A:1835:ALA:H	1.55	0.71
3:E:77:SER:HB2	3:E:249:LYS:HB3	1.70	0.71
1:A:15:LEU:HD11	1:A:65:LEU:HD21	1.72	0.70
5:X:20:DG:H2"	5:X:21:DG:H5"	1.72	0.70
4:F:50:ASN:ND2	4:F:52:ASP:OD2	2.24	0.70
1:A:1298:LEU:HD13	1:A:1364:CYS:HB3	1.74	0.69
1:A:1225:GLU:HB3	1:A:1232:PRO:HD2	1.74	0.69
3:E:515:ASN:ND2	4:F:255:SER:OG	2.25	0.69
1:A:3646:LYS:HA	1:A:3650:LYS:HD3	1.74	0.68
1:A:3710:LYS:HD2	1:A:3711:PRO:HD2	1.74	0.68
1:A:3052:LEU:HD22	1:A:3092:LEU:HD21	1.76	0.68
1:A:1602:ASP:OD1	1:A:1651:LYS:NZ	2.27	0.68
1:A:3650:LYS:HG3	1:A:3651:LEU:HD22	1.75	0.68
3:E:561:GLU:HG3	3:E:565:LYS:HD2	1.76	0.67
1:A:1949:ILE:HD12	1:A:2100:LEU:HD22	1.77	0.67
3:E:213:ILE:HG23	3:E:231:VAL:HG13	1.75	0.67
4:F:85:LEU:HD12	4:F:86:PRO:HD2	1.75	0.67
4:F:66:ASN:HB3	4:F:69:SER:HB2	1.77	0.67
1:A:2540:LEU:HD21	1:A:2832:ILE:HG23	1.77	0.67
3:E:570:LYS:HG3	3:E:572:THR:HG23	1.75	0.67
4:F:486:ARG:NH2	6:Y:235:DG:OP1	2.25	0.67
1:A:1876:ILE:O	1:A:1880:MET:HG2	1.94	0.67
2:D:133:ARG:NH2	5:X:29:DT:O2	2.27	0.67
1:A:148:LYS:NZ	1:A:185:HIS:O	2.26	0.66
3:E:317:LYS:HB2	3:E:328:ILE:HD11	1.76	0.66
1:A:3462:ARG:O	1:A:3498:TRP:NE1	2.27	0.66
3:E:252:ARG:HD3	3:E:253:LYS:N	2.10	0.66
1:A:158:GLY:HA2	1:A:161:ALA:HB3	1.76	0.66
4:F:68:LEU:HG	4:F:70:GLY:H	1.60	0.66
4:F:339:CYS:SG	4:F:394:ARG:NH1	2.69	0.66
1:A:1539:SER:HG	1:A:1552:HIS:HD1	1.38	0.65
2:D:97:GLU:OE1	2:D:97:GLU:N	2.30	0.65
1:A:1868:THR:HA	1:A:1871:MET:HG3	1.79	0.65
1:A:3048:LYS:HB3	1:A:3061:LEU:HD11	1.78	0.64
3:E:407:PRO:HG3	4:F:486:ARG:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:55:ALA:HB2	4:F:83:LEU:HD22	1.80	0.64
2:D:135:ALA:HB3	2:D:175:HIS:HB3	1.79	0.64
4:F:73:GLN:O	4:F:75:GLN:NE2	2.30	0.64
4:F:138:LEU:HD11	4:F:165:LEU:HD22	1.78	0.64
1:A:1010:LEU:HD22	1:A:1054:VAL:HG13	1.80	0.64
4:F:16:VAL:HB	4:F:101:GLY:H	1.61	0.64
1:A:2381:ALA:O	1:A:2385:LEU:HD12	1.98	0.64
1:A:1132:ASP:HB3	1:A:1136:ARG:HH21	1.63	0.64
1:A:3831:ASP:O	1:A:3833:ARG:N	2.28	0.64
2:D:164:TRP:HZ2	2:D:181:LYS:HE2	1.62	0.63
3:E:214:SER:HB3	3:E:218:ARG:HD3	1.80	0.63
1:A:1261:LEU:HD13	1:A:1337:VAL:HG22	1.80	0.63
1:A:1018:VAL:HG21	1:A:1074:LYS:HA	1.81	0.63
1:A:3630:ARG:HG2	1:A:3633:ILE:H	1.62	0.63
1:A:828:LYS:HA	1:A:831:LEU:HD23	1.80	0.63
1:A:1018:VAL:HG21	1:A:1074:LYS:HD3	1.81	0.63
1:A:2550:ILE:HG13	1:A:2550:ILE:O	1.98	0.63
3:E:489:ASN:ND2	4:F:331:MET:O	2.30	0.63
4:F:381:ILE:HD11	4:F:417:GLU:HB3	1.80	0.63
1:A:268:PRO:O	1:A:272:LEU:HD22	1.99	0.63
1:A:901:MET:SD	1:A:2535:THR:OG1	2.56	0.63
2:D:167:MET:HA	2:D:171:SER:HB2	1.81	0.63
1:A:887:ASP:OD2	1:A:891:ARG:NH1	2.32	0.62
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.72	0.62
1:A:2249:LEU:HG	1:A:2250:SER:HB2	1.80	0.62
3:E:427:VAL:HG23	3:E:428:THR:HG23	1.81	0.62
1:A:3499:ILE:HD11	1:A:3529:ILE:HD13	1.81	0.62
3:E:392:LYS:HG3	4:F:458:ILE:HD11	1.79	0.62
6:Y:241:DT:H2"	6:Y:242:DG:C8	2.35	0.62
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.81	0.62
1:A:1775:GLU:OE2	1:A:1822:ARG:NH1	2.32	0.62
4:F:386:ASP:OD1	4:F:387:LEU:N	2.33	0.62
3:E:36:ASP:OD1	3:E:37:SER:N	2.32	0.62
4:F:479:THR:HA	4:F:482:ILE:HD12	1.80	0.62
1:A:3326:GLN:O	1:A:3330:LEU:HG	2.00	0.62
3:E:588:TYR:OH	3:E:606:HIS:NE2	2.18	0.62
1:A:3630:ARG:HB3	1:A:3633:ILE:HG22	1.82	0.62
1:A:1119:LYS:HD3	1:A:1124:ILE:HD11	1.81	0.62
1:A:1145:LEU:O	1:A:1147:LYS:NZ	2.33	0.62
1:A:3878:VAL:HG23	1:A:3965:ARG:HH21	1.65	0.62
1:A:2828:GLU:O	1:A:2832:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3598:LYS:HG3	1:A:3599:THR:HG23	1.82	0.62
1:A:1400:VAL:HG11	1:A:1460:ARG:HD2	1.81	0.62
1:A:1851:LEU:HA	1:A:1870:LYS:HE3	1.81	0.62
1:A:3009:LYS:HE2	1:A:3009:LYS:HA	1.82	0.62
1:A:3319:ASN:O	1:A:3319:ASN:ND2	2.24	0.62
1:A:3693:GLU:HB3	1:A:3696:ARG:HD2	1.81	0.61
1:A:723:ASP:OD1	1:A:724:GLU:N	2.33	0.61
1:A:2272:VAL:O	1:A:2276:LEU:HD12	2.00	0.61
3:E:596:LYS:NZ	5:X:31:DA:OP1	2.33	0.61
4:F:24:ILE:HG13	4:F:27:ILE:HD13	1.82	0.61
1:A:134:LEU:HD23	1:A:180:LEU:HD13	1.83	0.61
1:A:1017:ILE:HG12	1:A:1029:CYS:HB3	1.82	0.61
1:A:4038:TRP:HD1	1:A:4040:PRO:HG3	1.66	0.61
1:A:2941:GLY:HA3	1:A:3978:GLY:HA2	1.81	0.61
1:A:1734:PRO:O	1:A:1738:ASN:N	2.23	0.61
1:A:1938:ARG:NH2	1:A:2092:GLU:OE1	2.34	0.61
1:A:172:GLU:HB2	1:A:222:GLY:HA3	1.83	0.61
1:A:533:HIS:O	1:A:537:SER:OG	2.19	0.61
3:E:304:ASN:HD22	3:E:308:GLY:HA2	1.65	0.61
2:D:45:LEU:HD23	2:D:88:VAL:HG21	1.83	0.61
4:F:140:SER:O	4:F:200:GLN:NE2	2.33	0.61
1:A:897:PRO:O	1:A:2566:THR:OG1	2.19	0.60
1:A:1219:PHE:O	1:A:1223:THR:OG1	2.17	0.60
5:X:24:DA:H2'	5:X:25:DG:C8	2.36	0.60
1:A:1768:ARG:HA	1:A:1815:THR:HG22	1.83	0.60
3:E:413:LEU:HD22	3:E:432:PHE:HB3	1.83	0.60
4:F:59:PHE:HA	4:F:77:ILE:HA	1.84	0.60
1:A:1725:GLN:HB3	1:A:1728:GLU:HB2	1.83	0.60
1:A:3708:ARG:NH2	1:A:3769:GLN:OE1	2.34	0.60
4:F:541:GLU:HB3	4:F:543:LYS:HG2	1.81	0.60
1:A:879:MET:SD	1:A:879:MET:N	2.75	0.60
1:A:2937:ASP:OD1	1:A:3784:ARG:NH2	2.32	0.60
5:X:50:DT:H2"	5:X:51:DA:C8	2.37	0.60
1:A:984:TYR:HA	1:A:987:LEU:HB3	1.83	0.60
1:A:1892:LYS:HA	1:A:1896:ILE:HD13	1.83	0.60
1:A:2252:PRO:HB2	1:A:2255:LEU:HB3	1.83	0.60
2:D:164:TRP:HA	2:D:167:MET:HG2	1.84	0.60
1:A:3303:THR:O	1:A:3307:LEU:N	2.28	0.60
1:A:105:VAL:HA	1:A:147:PHE:HE1	1.66	0.60
1:A:304:THR:HG22	1:A:305:ASN:H	1.67	0.60
1:A:3100:LYS:O	1:A:3104:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ILE:O	2:D:88:VAL:HG23	2.02	0.59
1:A:2242:VAL:HA	1:A:2245:TRP:HB3	1.84	0.59
3:E:157:VAL:HG12	3:E:159:PHE:H	1.68	0.59
4:F:368:ARG:HG3	4:F:369:ASP:H	1.68	0.59
1:A:3508:LYS:NZ	1:A:3510:GLN:OE1	2.34	0.59
4:F:155:LYS:HE2	4:F:215:LEU:HD11	1.83	0.59
1:A:131:LEU:O	1:A:135:LEU:CB	2.50	0.59
1:A:1191:PHE:O	1:A:1195:VAL:HG23	2.02	0.59
1:A:175:TYR:HB3	1:A:200:PHE:HE1	1.68	0.59
1:A:1102:GLU:HA	1:A:1154:PRO:HB3	1.85	0.59
1:A:3538:GLU:OE2	1:A:3797:THR:OG1	2.21	0.59
3:E:215:LEU:O	3:E:217:TYR:N	2.29	0.59
4:F:362:LEU:HB2	4:F:421:TYR:HB3	1.85	0.59
1:A:3843:LEU:HD23	1:A:3858:MET:HG3	1.84	0.59
1:A:269:SER:OG	1:A:273:ARG:NH2	2.35	0.58
1:A:566:ASP:HB2	1:A:645:TRP:HE1	1.67	0.58
1:A:3603:LYS:HA	1:A:3655:LYS:HZ1	1.67	0.58
3:E:444:ARG:HH22	4:F:270:GLU:HB2	1.68	0.58
1:A:3630:ARG:HG3	1:A:3632:PHE:H	1.68	0.58
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.36	0.58
1:A:253:LEU:HD11	1:A:257:ARG:HH21	1.67	0.58
5:X:56:DA:H2"	5:X:57:DC:H5"	1.86	0.58
3:E:369:TYR:OH	4:F:436:SER:O	2.16	0.58
1:A:1665:HIS:CD2	1:A:1667:SER:H	2.21	0.58
1:A:2844:LEU:HD12	1:A:2871:LEU:HD21	1.86	0.58
1:A:493:LYS:HE2	1:A:522:PRO:HG2	1.85	0.58
1:A:292:SER:O	1:A:296:VAL:HG22	2.02	0.57
1:A:1881:TYR:HE1	1:A:1889:VAL:HG21	1.68	0.57
1:A:2980:ASP:HB3	1:A:2981:TRP:HE3	1.69	0.57
1:A:3006:ALA:HB3	1:A:3257:LYS:HD2	1.86	0.57
1:A:3140:GLU:OE2	1:A:3164:TRP:NE1	2.32	0.57
1:A:3263:HIS:O	1:A:3266:SER:OG	2.22	0.57
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.36	0.57
1:A:1976:LEU:O	1:A:1980:ASN:ND2	2.38	0.57
1:A:1420:ARG:NH2	1:A:1466:ASN:O	2.37	0.57
1:A:1897:ASN:HA	1:A:1902:GLY:HA2	1.87	0.57
1:A:3455:LYS:NZ	1:A:3489:SER:OG	2.37	0.57
3:E:462:MET:HG2	4:F:380:LEU:HA	1.87	0.57
1:A:1407:LYS:HD3	1:A:1463:LEU:HD22	1.87	0.57
1:A:2857:CYS:O	1:A:2861:ILE:HG12	2.04	0.57
1:A:3469:LEU:HD11	1:A:3505:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1681:ASP:OD2	1:A:1683:LYS:NZ	2.33	0.57
1:A:1836:LEU:HD21	1:A:1884:LEU:HD21	1.87	0.57
1:A:2547:SER:O	1:A:2547:SER:OG	2.21	0.57
1:A:778:ILE:HG22	1:A:779:TYR:HD1	1.69	0.57
1:A:1233:SER:HA	1:A:1236:LEU:HG	1.87	0.57
1:A:3793:VAL:HG22	1:A:3803:ILE:HG22	1.86	0.57
1:A:1619:ALA:O	1:A:1623:LEU:HD22	2.05	0.57
1:A:3358:ARG:NH1	1:A:3361:GLU:OE1	2.38	0.57
1:A:3627:ALA:HA	1:A:3629:ARG:HH12	1.70	0.57
4:F:188:HIS:CE1	4:F:478:PRO:HD2	2.39	0.57
2:D:55:ARG:HG2	2:D:56:VAL:HG13	1.87	0.56
1:A:1167:ASP:N	1:A:1167:ASP:OD1	2.33	0.56
3:E:200:LEU:HD11	3:E:220:ILE:HG22	1.87	0.56
6:Y:217:DG:H2'	6:Y:218:DT:H71	1.87	0.56
1:A:662:LEU:HD23	1:A:662:LEU:H	1.70	0.56
1:A:1202:ARG:HH21	1:A:1206:LEU:HD12	1.71	0.56
1:A:1652:ILE:HG13	1:A:1653:LEU:N	2.20	0.56
1:A:1684:LEU:HD21	1:A:1688:LEU:HD21	1.85	0.56
1:A:1734:PRO:HA	1:A:1737:ASN:HB2	1.87	0.56
1:A:2268:LYS:O	1:A:2271:SER:OG	2.20	0.56
1:A:2458:VAL:HG21	1:A:2476:ILE:HD11	1.87	0.56
1:A:2952:ILE:HG12	1:A:2975:ALA:HB2	1.86	0.56
1:A:3410:ILE:HG13	1:A:3453:ALA:HB1	1.86	0.56
2:D:164:TRP:CZ2	2:D:181:LYS:HE2	2.40	0.56
1:A:168:ASP:OD2	1:A:168:ASP:N	2.35	0.56
1:A:2241:LEU:O	1:A:2245:TRP:N	2.38	0.56
4:F:163:PHE:HB2	4:F:224:ILE:HG22	1.87	0.56
1:A:568:PHE:O	1:A:572:VAL:HG23	2.06	0.56
1:A:941:MET:HB2	1:A:958:MET:HE1	1.85	0.56
1:A:3946:PHE:HZ	1:A:4002:MET:HB3	1.71	0.56
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.38	0.56
1:A:2263:LYS:N	1:A:2263:LYS:HD3	2.21	0.56
1:A:4061:CYS:SG	1:A:4078:VAL:HG23	2.46	0.56
1:A:24:ARG:HH22	1:A:27:ALA:HB3	1.71	0.56
1:A:1963:GLN:O	1:A:1968:SER:OG	2.24	0.56
3:E:420:LEU:HD21	3:E:424:LYS:HA	1.88	0.56
1:A:1301:ILE:HD13	1:A:1371:VAL:HG12	1.86	0.56
1:A:1617:LYS:O	1:A:1621:THR:OG1	2.21	0.56
1:A:2575:PRO:HD3	1:A:2786:LYS:HA	1.88	0.56
1:A:3531:TYR:O	1:A:3535:ILE:HG12	2.06	0.56
1:A:2563:LEU:HD12	1:A:2795:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3815:LEU:HD22	1:A:3930:VAL:HG11	1.87	0.56
2:D:182:ASP:OD2	6:Y:248:DC:N4	2.39	0.56
4:F:263:ALA:HB2	4:F:364:VAL:HG12	1.88	0.56
1:A:3028:ASN:H	1:A:3031:TRP:HD1	1.52	0.55
3:E:385:LEU:O	3:E:389:CYS:HB2	2.06	0.55
1:A:86:LEU:HD11	1:A:125:ILE:HG12	1.88	0.55
1:A:186:PRO:HA	1:A:189:MET:HB2	1.88	0.55
1:A:1942:CYS:O	1:A:1946:ASN:ND2	2.39	0.55
3:E:474:ARG:HH21	3:E:476:ASP:HB3	1.70	0.55
4:F:81:ARG:HH11	4:F:90:LEU:HD13	1.72	0.55
1:A:3826:ALA:O	1:A:3830:SER:OG	2.19	0.55
1:A:2216:LEU:O	1:A:2220:MET:HG3	2.07	0.55
1:A:2434:VAL:O	1:A:2438:ILE:HG12	2.07	0.55
4:F:91:LEU:HA	4:F:94:ILE:HG12	1.88	0.55
1:A:3684:SER:HB3	1:A:3687:MET:HB2	1.89	0.55
2:D:33:VAL:HB	2:D:39:LYS:HG3	1.88	0.55
3:E:149:VAL:O	3:E:153:LEU:HD12	2.06	0.55
3:E:204:HIS:CE1	3:E:212:ASP:HB2	2.41	0.55
1:A:978:GLN:NE2	1:A:982:GLN:OE1	2.39	0.55
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.88	0.55
2:D:140:ASP:OD1	2:D:140:ASP:N	2.39	0.55
1:A:1273:GLU:HG3	1:A:1275:THR:HG23	1.88	0.55
1:A:2123:PRO:HA	1:A:2127:LYS:HB2	1.89	0.55
1:A:2461:PHE:HB3	1:A:2473:MET:CE	2.37	0.55
4:F:13:CYS:SG	4:F:110:ALA:HB1	2.47	0.55
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.40	0.55
1:A:1711:ARG:NH1	1:A:1760:GLU:OE2	2.38	0.55
4:F:90:LEU:O	4:F:94:ILE:HG23	2.06	0.55
1:A:2461:PHE:HB3	1:A:2473:MET:HE1	1.88	0.54
1:A:3011:LEU:HD22	1:A:3047:SER:HB3	1.87	0.54
1:A:3356:ALA:O	1:A:3360:LEU:HB2	2.07	0.54
4:F:267:ILE:HD12	4:F:267:ILE:H	1.72	0.54
6:Y:215:DG:N3	6:Y:215:DG:H2'	2.22	0.54
1:A:2339:GLU:O	1:A:2343:GLU:HG2	2.07	0.54
1:A:631:ARG:HG3	1:A:672:ILE:HD11	1.89	0.54
1:A:1265:GLU:OE1	1:A:1340:ARG:NE	2.39	0.54
1:A:3530:VAL:HG11	1:A:3568:ILE:HG21	1.89	0.54
2:D:145:LEU:HD21	2:D:187:HIS:NE2	2.22	0.54
3:E:412:ALA:HB2	3:E:437:LEU:HD11	1.89	0.54
4:F:409:PHE:HD2	4:F:420:VAL:HG23	1.71	0.54
1:A:1714:LEU:HD12	1:A:1717:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3758:LEU:HB2	1:A:3795:PRO:HB3	1.88	0.54
1:A:3828:TYR:HE1	1:A:3835:PRO:HG2	1.72	0.54
3:E:252:ARG:HH11	3:E:253:LYS:H	1.55	0.54
1:A:3608:LYS:HG3	1:A:3612:ARG:HH22	1.72	0.54
3:E:567:HIS:O	3:E:571:GLY:N	2.34	0.54
3:E:71:TYR:O	3:E:75:ILE:HG22	2.08	0.54
4:F:526:SER:HB2	4:F:530:LEU:HD23	1.90	0.54
1:A:87:LYS:HE3	1:A:124:LYS:HG2	1.89	0.54
1:A:1623:LEU:HA	1:A:1626:TRP:HD1	1.72	0.54
1:A:3031:TRP:HE1	1:A:3064:PHE:HE1	1.55	0.54
1:A:87:LYS:HD2	1:A:128:LEU:HD13	1.90	0.53
1:A:931:CYS:O	1:A:984:TYR:OH	2.23	0.53
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.42	0.53
1:A:1364:CYS:HB2	1:A:1368:LEU:H	1.72	0.53
1:A:3049:LEU:O	1:A:3053:LEU:HD12	2.08	0.53
1:A:3630:ARG:HD2	1:A:3683:CYS:HB3	1.90	0.53
1:A:3665:MET:H	1:A:3665:MET:CE	2.21	0.53
3:E:245:LYS:HD2	3:E:247:ARG:HH21	1.72	0.53
3:E:491:GLU:OE1	4:F:316:TYR:OH	2.23	0.53
1:A:79:ARG:O	1:A:82:ARG:NH2	2.41	0.53
4:F:104:GLN:OE1	4:F:140:SER:OG	2.24	0.53
1:A:1047:GLN:OE1	1:A:1047:GLN:N	2.33	0.53
1:A:1147:LYS:HD2	1:A:1149:LYS:HE3	1.90	0.53
1:A:1623:LEU:HA	1:A:1626:TRP:CD1	2.43	0.53
4:F:153:SER:O	4:F:153:SER:OG	2.25	0.53
1:A:162:LEU:HD23	3:E:301:ARG:HB3	1.90	0.53
1:A:2304:VAL:HG11	1:A:2344:LEU:HG	1.91	0.53
2:D:140:ASP:HA	2:D:143:ALA:HB3	1.91	0.53
4:F:128:GLU:HG2	4:F:129:LYS:HE3	1.89	0.53
5:X:43:DC:H2"	5:X:44:DA:H8	1.73	0.53
1:A:635:PRO:O	1:A:638:GLN:NE2	2.41	0.53
1:A:1772:HIS:N	1:A:1775:GLU:OE1	2.41	0.53
4:F:133:GLU:HG2	4:F:164:PHE:HE1	1.74	0.53
5:X:19:DG:H22	6:Y:255:DC:H2"	1.73	0.53
1:A:3992:ARG:HD3	1:A:4100:GLU:HG2	1.90	0.53
6:Y:252:DA:H2"	6:Y:253:DC:OP2	2.08	0.53
1:A:228:SER:HB3	1:A:274:LEU:HD12	1.91	0.53
1:A:1101:PHE:HD1	1:A:1168:LEU:HD22	1.72	0.53
1:A:1296:PHE:O	1:A:1299:GLU:N	2.40	0.53
1:A:1437:TYR:OH	1:A:1502:SER:N	2.29	0.53
2:D:134:ILE:HD13	3:E:596:LYS:HZ3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:81:ARG:HD2	4:F:90:LEU:HD13	1.90	0.53
1:A:1104:LEU:O	1:A:1108:MET:HG2	2.09	0.53
1:A:2189:ILE:O	1:A:2193:ILE:HG12	2.09	0.53
1:A:1239:PRO:HD3	1:A:1256:TRP:CD2	2.44	0.52
1:A:1245:ARG:CD	1:A:1246:GLY:H	2.20	0.52
1:A:3661:ASP:O	1:A:3664:ASN:ND2	2.42	0.52
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.91	0.52
4:F:347:LYS:HA	4:F:389:MET:HA	1.91	0.52
1:A:72:SER:OG	1:A:82:ARG:NH1	2.36	0.52
3:E:43:ASP:OD1	3:E:44:ALA:N	2.42	0.52
1:A:418:ALA:O	1:A:422:LEU:HD12	2.09	0.52
1:A:446:PHE:CG	1:A:530:LEU:HD22	2.45	0.52
1:A:3666:LEU:O	1:A:3670:MET:HG2	2.09	0.52
1:A:442:GLN:HE21	1:A:457:CYS:HB2	1.75	0.52
1:A:487:LEU:HD11	1:A:568:PHE:HE1	1.73	0.52
1:A:1487:VAL:HG11	1:A:1515:LEU:HD22	1.92	0.52
1:A:2572:TYR:N	1:A:2573:PRO:HD3	2.25	0.52
1:A:2798:ALA:HA	1:A:2804:ILE:HG23	1.92	0.52
1:A:3274:VAL:O	1:A:3278:GLN:HG3	2.10	0.52
1:A:3564:GLN:OE1	1:A:3564:GLN:N	2.42	0.52
6:Y:253:DC:H5'	6:Y:253:DC:C6	2.44	0.52
1:A:3859:TYR:HE2	1:A:4080:VAL:HG11	1.74	0.52
3:E:357:LYS:HD2	3:E:360:HIS:HE1	1.74	0.52
4:F:106:ASP:OD2	4:F:109:ASP:N	2.41	0.52
5:X:49:DT:H2"	5:X:50:DT:H5"	1.91	0.52
1:A:1793:THR:O	1:A:1797:LEU:HG	2.10	0.52
1:A:2091:HIS:O	1:A:2091:HIS:ND1	2.42	0.52
1:A:3786:LEU:HD21	1:A:3983:ILE:HD12	1.92	0.52
2:D:193:HIS:CD2	2:D:194:LYS:HD3	2.44	0.52
3:E:461:LYS:O	3:E:465:ILE:HG13	2.09	0.52
4:F:10:VAL:HB	4:F:240:ILE:HD11	1.92	0.52
4:F:107:PHE:HE1	4:F:134:ILE:HG21	1.75	0.52
1:A:743:LEU:HD12	1:A:743:LEU:H	1.74	0.52
1:A:1893:GLU:OE1	1:A:1893:GLU:N	2.40	0.52
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	1.91	0.52
3:E:484:GLN:OE1	3:E:488:ARG:NH1	2.43	0.52
4:F:91:LEU:H	4:F:91:LEU:HD23	1.75	0.52
1:A:892:LEU:HD13	1:A:908:ASP:HB3	1.92	0.52
1:A:1238:GLN:HG2	1:A:1296:PHE:HB3	1.92	0.52
1:A:3460:GLU:OE2	1:A:3460:GLU:N	2.27	0.52
1:A:1960:LYS:O	1:A:1963:GLN:NE2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3578:LEU:HD23	1:A:3752:VAL:HG21	1.91	0.51
1:A:566:ASP:OD1	1:A:567:GLU:N	2.44	0.51
1:A:2365:ASN:OD1	1:A:2396:LEU:HD23	2.10	0.51
1:A:3855:TYR:HA	1:A:3858:MET:HB3	1.91	0.51
2:D:189:ARG:HD3	2:D:194:LYS:HG3	1.92	0.51
3:E:386:LEU:HB2	3:E:432:PHE:HE1	1.75	0.51
1:A:14:ARG:HD3	1:A:38:LEU:HD11	1.91	0.51
1:A:1238:GLN:O	1:A:1240:THR:N	2.39	0.51
1:A:2503:LYS:O	1:A:2507:ILE:HG13	2.11	0.51
1:A:2860:ASP:OD1	1:A:2864:GLN:NE2	2.43	0.51
1:A:479:ILE:O	1:A:483:VAL:HG22	2.10	0.51
1:A:990:GLN:HG3	1:A:2781:PRO:HA	1.92	0.51
1:A:3307:LEU:HD21	1:A:3330:LEU:HD23	1.92	0.51
1:A:2780:LEU:N	1:A:2781:PRO:HD2	2.25	0.51
1:A:3693:GLU:OE2	1:A:3694:PHE:N	2.43	0.51
3:E:347:LEU:HD23	3:E:349:GLY:H	1.75	0.51
1:A:2358:ASP:OD1	1:A:2358:ASP:N	2.43	0.51
1:A:3772:ASN:HA	1:A:3775:LEU:HB2	1.92	0.51
1:A:16:GLN:N	1:A:16:GLN:OE1	2.44	0.51
1:A:3648:GLY:O	1:A:3652:LEU:HB3	2.11	0.51
3:E:341:ASP:OD2	3:E:399:ARG:NH2	2.41	0.51
3:E:357:LYS:HD2	3:E:360:HIS:CE1	2.46	0.51
4:F:405:VAL:HG23	4:F:424:LEU:HB2	1.93	0.51
1:A:2172:ALA:HB2	1:A:2189:ILE:HG21	1.92	0.51
3:E:304:ASN:OD1	3:E:304:ASN:N	2.44	0.51
4:F:461:MET:HG2	4:F:522:VAL:HG13	1.92	0.51
1:A:385:TYR:CE1	1:A:389:ILE:HD11	2.45	0.51
1:A:2280:VAL:O	1:A:2285:LEU:HB2	2.11	0.51
1:A:2565:MET:O	1:A:2568:MET:HG3	2.11	0.51
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.44	0.51
1:A:985:GLU:O	1:A:989:MET:HG2	2.11	0.50
1:A:1045:THR:OG1	1:A:1047:GLN:OE1	2.17	0.50
1:A:1347:THR:O	1:A:1351:THR:HG22	2.11	0.50
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.44	0.50
1:A:1335:CYS:HA	1:A:1338:VAL:HG22	1.93	0.50
1:A:2158:ARG:HG2	1:A:2196:TRP:HE3	1.77	0.50
5:X:44:DA:H2'	5:X:45:DT:C6	2.46	0.50
1:A:2289:ASP:N	1:A:2290:PRO:HD3	2.26	0.50
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.11	0.50
3:E:109:ASP:OD1	3:E:110:ASN:N	2.41	0.50
1:A:117:LYS:HE3	4:F:299:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3602:ASN:HD21	1:A:3605:ASN:HB2	1.76	0.50
1:A:1646:LEU:HD21	1:A:1688:LEU:HB2	1.94	0.50
1:A:1661:PHE:H	1:A:1665:HIS:HB2	1.77	0.50
1:A:1952:ILE:O	1:A:1955:VAL:HG12	2.12	0.50
1:A:2421:VAL:HG13	1:A:2457:PRO:HG3	1.94	0.50
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.92	0.50
1:A:939:MET:HE1	1:A:987:LEU:HD13	1.94	0.50
1:A:3332:THR:HA	1:A:3335:ARG:HG2	1.94	0.50
2:D:163:LEU:H	2:D:165:LYS:HE2	1.76	0.50
5:X:19:DG:H2"	5:X:20:DG:H5"	1.92	0.50
1:A:122:LYS:CB	1:A:167:PRO:HG2	2.42	0.50
1:A:2260:PHE:HA	1:A:2270:ASN:HA	1.93	0.50
3:E:132:GLN:HE22	3:E:137:HIS:CE1	2.30	0.50
4:F:20:MET:SD	4:F:30:PRO:HB2	2.52	0.50
1:A:651:TYR:HE1	1:A:1386:ILE:HD11	1.77	0.50
1:A:2183:HIS:HA	1:A:2186:VAL:HG22	1.94	0.50
1:A:4046:TYR:HE2	1:A:4066:LEU:HD22	1.76	0.50
4:F:97:LYS:NZ	4:F:99:GLN:O	2.35	0.50
1:A:3701:ILE:HB	1:A:3719:ILE:HG23	1.94	0.50
3:E:473:TYR:HB2	4:F:392:ILE:HD11	1.94	0.50
1:A:197:PHE:HE2	1:A:236:LYS:HZ3	1.60	0.49
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.41	0.49
1:A:2446:LEU:HD11	1:A:2454:LEU:HD12	1.94	0.49
3:E:120:ASP:HB2	3:E:123:LYS:HE2	1.94	0.49
4:F:178:ARG:HG3	4:F:182:PRO:HB3	1.94	0.49
1:A:638:GLN:HG3	1:A:679:LYS:HG2	1.93	0.49
1:A:2337:LEU:HG	1:A:2341:LEU:HD11	1.94	0.49
1:A:3157:LEU:HD11	1:A:3193:ILE:HG21	1.93	0.49
4:F:364:VAL:HG23	4:F:419:LEU:HB2	1.94	0.49
1:A:265:TYR:N	5:X:53:DC:OP1	2.41	0.49
1:A:3316:LEU:HD12	1:A:3316:LEU:O	2.12	0.49
4:F:461:MET:HG3	4:F:526:SER:HB3	1.94	0.49
1:A:771:ASN:OD1	1:A:854:ARG:NH1	2.43	0.49
1:A:1235:ILE:O	1:A:1235:ILE:HG13	2.13	0.49
1:A:108:LYS:NZ	1:A:151:GLU:OE2	2.34	0.49
1:A:678:LYS:HD2	1:A:737:PRO:HA	1.94	0.49
1:A:984:TYR:HD1	1:A:987:LEU:HD23	1.77	0.49
1:A:1364:CYS:O	1:A:1367:HIS:ND1	2.39	0.49
1:A:2546:TYR:OH	1:A:2551:GLU:OE2	2.24	0.49
1:A:787:PRO:O	1:A:790:LYS:NZ	2.34	0.49
1:A:1068:LEU:HG	1:A:1106:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.85	0.49
1:A:3416:LEU:HD23	1:A:3449:LYS:HG3	1.93	0.49
3:E:41:LEU:HB3	3:E:168:LEU:HD12	1.95	0.49
3:E:473:TYR:CZ	4:F:424:LEU:HD13	2.48	0.49
1:A:220:LEU:HA	1:A:223:CYS:HB3	1.95	0.49
1:A:1139:GLU:OE2	1:A:1140:LYS:NZ	2.45	0.49
1:A:1399:CYS:O	1:A:1403:MET:HG2	2.12	0.49
1:A:1973:LYS:HB2	1:A:1975:LEU:HG	1.95	0.49
3:E:61:ASP:OD2	3:E:124:GLY:N	2.41	0.49
1:A:364:ARG:O	1:A:368:LEU:HG	2.12	0.49
1:A:1205:ASN:HB3	1:A:1275:THR:HA	1.95	0.49
1:A:2473:MET:O	1:A:2476:ILE:HG12	2.12	0.49
1:A:3746:ARG:HG3	1:A:3746:ARG:HH11	1.77	0.49
1:A:4038:TRP:CD1	1:A:4040:PRO:HG3	2.45	0.49
2:D:33:VAL:HG22	2:D:64:LEU:HB2	1.95	0.49
3:E:278:GLN:NE2	6:Y:233:DG:OP2	2.28	0.49
1:A:2121:ASP:HA	1:A:2126:MET:HE3	1.94	0.49
1:A:3846:MET:SD	1:A:3862:ALA:HB2	2.52	0.49
1:A:126:PRO:C	1:A:128:LEU:H	2.15	0.48
1:A:538:ASP:N	1:A:538:ASP:OD1	2.45	0.48
1:A:636:GLU:HA	1:A:638:GLN:NE2	2.28	0.48
1:A:636:GLU:O	1:A:637:LYS:HG2	2.13	0.48
6:Y:222:DC:H2”	6:Y:223:DT:C6	2.48	0.48
1:A:414:LEU:HD11	1:A:438:LEU:HG	1.95	0.48
1:A:2190:VAL:O	1:A:2194:LEU:HD12	2.13	0.48
3:E:204:HIS:HB3	3:E:237:SER:OG	2.13	0.48
4:F:469:LYS:HA	4:F:469:LYS:HD3	1.61	0.48
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.49	0.48
1:A:3239:LYS:O	1:A:3243:ILE:HG12	2.13	0.48
1:A:3739:ILE:HG22	1:A:3739:ILE:O	2.12	0.48
3:E:34:GLY:HA2	3:E:160:LYS:HB2	1.95	0.48
4:F:377:LEU:O	4:F:381:ILE:HG23	2.13	0.48
1:A:922:SER:O	1:A:922:SER:OG	2.30	0.48
1:A:1820:VAL:HG12	1:A:1824:LEU:HD23	1.94	0.48
1:A:2189:ILE:O	1:A:2192:THR:OG1	2.25	0.48
1:A:3025:PRO:O	1:A:3027:LEU:N	2.46	0.48
4:F:136:THR:OG1	4:F:137:ASP:N	2.47	0.48
1:A:1202:ARG:HB3	1:A:1206:LEU:HD11	1.95	0.48
1:A:3114:TYR:HE1	1:A:3125:ARG:HH21	1.62	0.48
1:A:252:VAL:HG11	1:A:274:LEU:HD22	1.96	0.48
1:A:800:LEU:O	1:A:3115:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:SER:OG	1:A:1162:SER:O	2.32	0.48
1:A:1926:ASN:HD21	1:A:1974:ASN:HB3	1.79	0.48
4:F:450:GLN:HB3	4:F:537:PHE:CZ	2.49	0.48
1:A:122:LYS:HB2	1:A:167:PRO:HG2	1.96	0.48
1:A:1379:PRO:O	1:A:1384:PHE:HB2	2.14	0.48
1:A:2929:LEU:O	1:A:2932:SER:OG	2.29	0.48
4:F:219:ASP:OD1	4:F:219:ASP:N	2.47	0.48
1:A:896:VAL:HG23	1:A:2791:ILE:HD11	1.96	0.48
1:A:1366:THR:HB	1:A:1418:HIS:CE1	2.49	0.48
1:A:1633:TRP:CE2	1:A:1674:THR:HG22	2.48	0.48
3:E:465:ILE:HG23	3:E:518:LEU:HD11	1.96	0.48
1:A:3298:LEU:HD21	1:A:3351:ILE:HG12	1.95	0.48
1:A:110:THR:O	1:A:114:VAL:HG23	2.14	0.47
1:A:162:LEU:HA	3:E:300:THR:O	2.14	0.47
1:A:1093:GLU:O	1:A:1095:LEU:HD12	2.14	0.47
1:A:3181:ASP:O	1:A:3185:ASN:ND2	2.47	0.47
2:D:35:PRO:HB2	3:E:500:PRO:HD3	1.96	0.47
3:E:273:ILE:HD13	3:E:400:TYR:HE1	1.78	0.47
1:A:1607:GLU:OE1	1:A:1614:GLN:NE2	2.47	0.47
1:A:1878:ASP:HB3	1:A:1947:CYS:HA	1.96	0.47
1:A:1943:ALA:HA	1:A:1946:ASN:HD22	1.79	0.47
1:A:2173:ALA:HB3	1:A:2211:LEU:HD12	1.96	0.47
1:A:2300:PHE:O	1:A:2304:VAL:HG12	2.14	0.47
1:A:2980:ASP:HB3	1:A:2981:TRP:CE3	2.49	0.47
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.96	0.47
1:A:1676:ILE:HG23	1:A:1713:VAL:HG21	1.96	0.47
1:A:2250:SER:C	1:A:2251:ILE:HD12	2.35	0.47
1:A:3050:LYS:NZ	1:A:3180:ASP:OD1	2.47	0.47
1:A:4082:ARG:HD2	1:A:4082:ARG:HA	1.63	0.47
3:E:38:LEU:HD11	3:E:167:MET:SD	2.54	0.47
6:Y:233:DG:H2"	6:Y:234:DA:C8	2.50	0.47
1:A:61:ARG:HA	1:A:67:VAL:HG11	1.95	0.47
1:A:171:LEU:HB2	1:A:219:VAL:HG22	1.97	0.47
1:A:471:LYS:HD2	1:A:475:LEU:HD21	1.96	0.47
1:A:83:GLU:CD	1:A:124:LYS:HD3	2.35	0.47
1:A:133:LYS:HA	1:A:137:THR:OG1	2.15	0.47
1:A:183:GLU:HA	1:A:233:ASN:ND2	2.30	0.47
1:A:561:ASN:N	1:A:561:ASN:OD1	2.47	0.47
1:A:1366:THR:O	1:A:1370:ARG:NE	2.37	0.47
1:A:158:GLY:HA3	1:A:162:LEU:HG	1.96	0.47
1:A:3875:GLU:OE2	1:A:3965:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:111:LEU:HD11	4:F:161:LEU:HD11	1.95	0.47
1:A:12:LEU:HA	1:A:16:GLN:OE1	2.15	0.47
1:A:148:LYS:HZ1	1:A:188:GLU:HB3	1.80	0.47
1:A:1238:GLN:CG	1:A:1296:PHE:HB3	2.44	0.47
1:A:1459:HIS:CE1	1:A:1520:ALA:HB1	2.49	0.47
1:A:1686:LEU:HD11	1:A:1721:HIS:HB3	1.97	0.47
1:A:1920:TYR:O	1:A:1924:THR:OG1	2.22	0.47
1:A:2310:VAL:HG23	1:A:2310:VAL:O	2.15	0.47
1:A:3411:ASP:O	1:A:3415:THR:OG1	2.30	0.47
4:F:57:VAL:HG12	4:F:79:VAL:HG13	1.97	0.47
4:F:307:LYS:HD2	4:F:307:LYS:O	2.14	0.47
1:A:1069:HIS:O	1:A:1075:ARG:NH1	2.48	0.47
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.97	0.47
4:F:366:ALA:HA	4:F:377:LEU:HD23	1.97	0.47
1:A:984:TYR:CD1	1:A:987:LEU:HD23	2.50	0.47
1:A:3137:GLU:OE1	1:A:3167:ARG:NH2	2.48	0.47
1:A:3595:GLU:O	1:A:3599:THR:OG1	2.22	0.47
2:D:168:GLU:OE2	2:D:177:TRP:HA	2.15	0.47
1:A:347:GLY:O	1:A:351:ASN:ND2	2.48	0.47
1:A:915:THR:HG23	1:A:968:VAL:HG11	1.96	0.47
1:A:566:ASP:O	1:A:569:VAL:HG12	2.14	0.46
1:A:1789:GLY:O	1:A:1794:GLN:NE2	2.48	0.46
1:A:1938:ARG:NH1	1:A:1981:LEU:O	2.39	0.46
1:A:2135:ASN:O	1:A:2138:VAL:HG12	2.16	0.46
1:A:2203:THR:HA	1:A:2209:GLU:HG3	1.96	0.46
1:A:3917:ILE:HG13	1:A:3991:PHE:HD2	1.79	0.46
3:E:129:LYS:NZ	3:E:133:ASP:OD2	2.47	0.46
4:F:11:VAL:HG22	4:F:55:ALA:HB3	1.97	0.46
4:F:97:LYS:HD2	4:F:97:LYS:HA	1.69	0.46
1:A:1648:LEU:O	1:A:1652:ILE:HG23	2.15	0.46
1:A:1875:LYS:HA	1:A:1878:ASP:OD2	2.14	0.46
1:A:2276:LEU:HA	1:A:2279:ILE:HG12	1.98	0.46
1:A:2466:SER:OG	1:A:2469:CYS:SG	2.57	0.46
1:A:2994:TRP:O	1:A:2998:SER:OG	2.29	0.46
1:A:3281:CYS:SG	1:A:3307:LEU:HD22	2.55	0.46
2:D:136:PHE:HD2	6:Y:246:DA:H5"	1.80	0.46
1:A:282:PHE:HB3	1:A:285:CYS:SG	2.55	0.46
1:A:1456:LYS:HD3	1:A:1516:GLU:HG2	1.96	0.46
2:D:193:HIS:HD2	2:D:194:LYS:HD3	1.80	0.46
1:A:12:LEU:O	1:A:16:GLN:HB2	2.16	0.46
1:A:1014:LEU:HD23	1:A:1014:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1653:LEU:HD12	1:A:1695:LEU:HD23	1.96	0.46
1:A:3789:ARG:HB3	1:A:3938:ILE:HG22	1.97	0.46
4:F:343:LEU:HD21	4:F:394:ARG:HB2	1.98	0.46
1:A:1765:VAL:HG23	1:A:1768:ARG:HH12	1.81	0.46
1:A:2938:VAL:O	1:A:2942:ILE:HG23	2.15	0.46
1:A:3155:VAL:HG12	1:A:3156:PRO:HD3	1.98	0.46
1:A:3669:LYS:HA	1:A:3672:LYS:HD3	1.96	0.46
3:E:237:SER:O	3:E:239:LEU:N	2.47	0.46
1:A:1670:GLU:O	1:A:1674:THR:HG23	2.16	0.46
1:A:1688:LEU:O	1:A:1692:ALA:N	2.41	0.46
1:A:1945:TYR:O	1:A:1949:ILE:HG12	2.15	0.46
1:A:2330:VAL:HG13	1:A:2338:GLU:HB2	1.97	0.46
1:A:2443:MET:HA	1:A:2446:LEU:HD12	1.97	0.46
1:A:4056:PRO:HG3	1:A:4107:LEU:HD12	1.96	0.46
4:F:361:VAL:HG22	4:F:422:VAL:HG12	1.98	0.46
1:A:1239:PRO:O	1:A:1245:ARG:HD3	2.15	0.46
1:A:225:LYS:HA	1:A:228:SER:OG	2.16	0.46
1:A:487:LEU:HB3	1:A:575:ILE:HD11	1.98	0.46
1:A:881:LYS:HG2	1:A:3933:GLU:OE1	2.16	0.46
1:A:1766:LEU:HD22	1:A:1778:PHE:CD1	2.50	0.46
1:A:3917:ILE:HG13	1:A:3991:PHE:CD2	2.51	0.46
3:E:270:SER:OG	3:E:371:GLU:OE2	2.30	0.46
1:A:19:LEU:H	1:A:19:LEU:HD23	1.81	0.46
1:A:2121:ASP:HB2	1:A:2127:LYS:HZ3	1.81	0.46
3:E:173:ASP:HB3	3:E:204:HIS:CE1	2.50	0.46
4:F:142:PHE:CZ	4:F:207:ILE:HD11	2.51	0.46
6:Y:222:DC:H2"	6:Y:223:DT:C5	2.51	0.46
1:A:203:GLU:HG3	1:A:204:LEU:H	1.80	0.46
1:A:207:GLN:OE1	1:A:216:LYS:N	2.33	0.46
1:A:220:LEU:HD11	4:F:554:PHE:HE2	1.81	0.46
1:A:1245:ARG:HD2	1:A:1246:GLY:N	2.27	0.46
1:A:2266:ASN:OD1	1:A:2266:ASN:N	2.48	0.46
1:A:2575:PRO:O	1:A:2576:MET:HG3	2.16	0.46
1:A:3959:MET:SD	1:A:3959:MET:N	2.87	0.46
2:D:149:LYS:HE3	2:D:149:LYS:HB3	1.79	0.46
4:F:12:LEU:HB2	4:F:56:LEU:HD13	1.98	0.46
4:F:409:PHE:CD2	4:F:420:VAL:HG23	2.49	0.46
1:A:1949:ILE:HD13	1:A:1966:LEU:HD22	1.98	0.45
1:A:2245:TRP:NE1	1:A:2249:LEU:O	2.49	0.45
3:E:278:GLN:HB3	4:F:431:ARG:HH21	1.81	0.45
3:E:494:ALA:HB2	4:F:321:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:603:LEU:HD23	3:E:603:LEU:HA	1.82	0.45
1:A:166:ILE:HD12	1:A:166:ILE:H	1.81	0.45
1:A:2275:GLN:O	1:A:2279:ILE:HG12	2.16	0.45
5:X:24:DA:N1	6:Y:251:DA:N6	2.64	0.45
1:A:1238:GLN:HA	1:A:1256:TRP:CE2	2.51	0.45
1:A:1539:SER:HG	1:A:1552:HIS:CG	2.29	0.45
1:A:1678:LEU:HD23	1:A:1678:LEU:HA	1.84	0.45
1:A:1926:ASN:ND2	1:A:1974:ASN:HB3	2.32	0.45
1:A:3543:LYS:HA	1:A:3543:LYS:HD3	1.76	0.45
1:A:3610:TYR:CZ	1:A:3614:TYR:HE2	2.35	0.45
3:E:261:LEU:HB3	3:E:269:ILE:HG12	1.98	0.45
3:E:353:LEU:HD23	3:E:353:LEU:HA	1.81	0.45
3:E:416:GLN:NE2	3:E:429:PRO:O	2.49	0.45
4:F:532:LYS:O	4:F:536:LEU:HB2	2.16	0.45
1:A:204:LEU:HB3	1:A:251:PHE:CE2	2.52	0.45
1:A:479:ILE:HA	1:A:482:VAL:HG12	1.98	0.45
1:A:2851:PHE:HB3	1:A:2854:PHE:HB3	1.97	0.45
1:A:3078:LEU:HD12	1:A:3078:LEU:HA	1.82	0.45
1:A:3763:ARG:NE	1:A:4008:GLU:OE1	2.39	0.45
1:A:87:LYS:HA	1:A:128:LEU:HD21	1.98	0.45
1:A:355:ASN:OD1	1:A:357:LYS:N	2.35	0.45
1:A:2320:ALA:HB1	1:A:2367:VAL:HG23	1.97	0.45
1:A:2855:VAL:O	1:A:2859:GLN:HG3	2.16	0.45
4:F:34:ALA:HB2	4:F:227:PHE:CE2	2.52	0.45
4:F:364:VAL:CG2	4:F:419:LEU:HB2	2.46	0.45
1:A:428:PRO:O	1:A:429:GLU:HG2	2.16	0.45
1:A:1178:ARG:O	1:A:1184:ARG:NH1	2.49	0.45
1:A:3632:PHE:O	1:A:3636:PHE:N	2.35	0.45
2:D:134:ILE:HD13	3:E:596:LYS:NZ	2.32	0.45
2:D:193:HIS:CE1	4:F:128:GLU:HA	2.52	0.45
1:A:1818:SER:OG	1:A:1822:ARG:NE	2.46	0.45
1:A:3011:LEU:HD21	1:A:3043:TYR:HB3	1.99	0.45
1:A:3997:LEU:H	1:A:3997:LEU:HD12	1.81	0.45
3:E:102:ILE:HD12	3:E:146:VAL:HB	1.98	0.45
3:E:588:TYR:CE2	3:E:590:LEU:HB2	2.51	0.45
1:A:148:LYS:NZ	1:A:188:GLU:HB3	2.32	0.45
1:A:750:PRO:HA	1:A:753:GLN:HG2	1.99	0.45
1:A:1628:LYS:HD3	1:A:1628:LYS:HA	1.77	0.45
1:A:3637:GLY:HA2	1:A:3641:ASP:HB3	1.98	0.45
1:A:1812:LEU:HG	1:A:1814:PHE:H	1.82	0.45
2:D:160:GLY:HA2	5:X:23:DT:H71	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:46:DA:H2"	5:X:47:DG:C8	2.52	0.45
1:A:1990:PHE:HD2	1:A:2182:ILE:HG21	1.82	0.45
1:A:3499:ILE:O	1:A:3503:VAL:HG23	2.17	0.45
1:A:3620:PRO:HB3	1:A:3641:ASP:HB2	1.98	0.45
1:A:3622:ALA:N	1:A:3623:PRO:HD2	2.32	0.45
1:A:3919:GLY:HA3	1:A:3947:GLY:N	2.31	0.45
2:D:161:ASN:OD1	2:D:177:TRP:HH2	2.00	0.45
3:E:74:LYS:HD3	3:E:83:LEU:HD11	1.98	0.45
4:F:27:ILE:HA	4:F:183:PHE:CE2	2.51	0.45
4:F:113:VAL:HA	4:F:116:ASP:OD2	2.17	0.45
1:A:54:GLN:O	1:A:58:VAL:HG12	2.16	0.44
1:A:134:LEU:H	1:A:138:PHE:HD2	1.65	0.44
1:A:875:SER:HA	1:A:879:MET:HB2	2.00	0.44
1:A:1471:GLN:O	1:A:1478:SER:N	2.39	0.44
1:A:2408:MET:HE2	1:A:2411:LEU:HG	1.99	0.44
1:A:2539:LEU:HA	1:A:2542:LEU:HD12	1.99	0.44
1:A:3449:LYS:HA	1:A:3449:LYS:HD2	1.74	0.44
2:D:145:LEU:HD21	2:D:187:HIS:CE1	2.51	0.44
1:A:1250:LEU:HD21	1:A:1326:GLU:HB3	1.97	0.44
1:A:3154:GLN:HG3	1:A:3227:ILE:HD11	1.99	0.44
3:E:312:LEU:C	3:E:314:SER:H	2.20	0.44
1:A:1661:PHE:CE1	1:A:1671:VAL:HG11	2.52	0.44
1:A:1924:THR:HG22	1:A:1977:ILE:HG12	1.99	0.44
3:E:340:PHE:HB2	3:E:408:PRO:HD3	1.99	0.44
1:A:180:LEU:O	1:A:183:GLU:HG3	2.17	0.44
1:A:1715:GLU:HA	1:A:1718:ILE:HG22	2.00	0.44
1:A:3878:VAL:O	1:A:3965:ARG:NH2	2.51	0.44
4:F:87:ASP:OD1	4:F:88:PHE:N	2.50	0.44
1:A:1873:TYR:O	1:A:1876:ILE:HG13	2.17	0.44
1:A:2871:LEU:HD23	1:A:2872:ASP:N	2.33	0.44
1:A:4096:SER:OG	1:A:4097:GLY:N	2.51	0.44
3:E:362:LEU:HD23	3:E:362:LEU:HA	1.72	0.44
4:F:91:LEU:HD12	4:F:495:LEU:HD22	1.99	0.44
1:A:224:LEU:C	1:A:226:GLY:H	2.20	0.44
1:A:446:PHE:CD2	1:A:530:LEU:HD22	2.52	0.44
1:A:732:PHE:O	1:A:735:SER:OG	2.31	0.44
1:A:1539:SER:OG	1:A:1552:HIS:ND1	2.34	0.44
1:A:2527:HIS:HB3	1:A:2530:ARG:HH11	1.83	0.44
1:A:3880:ALA:HB1	1:A:3969:ASN:HD22	1.82	0.44
1:A:3923:ARG:HB3	1:A:3928:PHE:HE1	1.82	0.44
3:E:31:LYS:HD2	3:E:31:LYS:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:188:HIS:O	4:F:190:PRO:HD2	2.17	0.44
6:Y:220:DA:H5'	6:Y:220:DA:C8	2.52	0.44
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.81	0.44
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.50	0.44
1:A:1525:CYS:SG	1:A:1526:GLU:N	2.91	0.44
1:A:1696:LEU:HD23	1:A:1696:LEU:HA	1.86	0.44
1:A:1987:ARG:HH12	1:A:2140:LEU:HB3	1.82	0.44
1:A:2254:ARG:CZ	1:A:2293:GLY:HA2	2.48	0.44
1:A:2887:PRO:HB2	1:A:3895:GLU:HA	1.99	0.44
1:A:3107:ILE:HG13	1:A:3135:LEU:HD12	1.99	0.44
1:A:3602:ASN:OD1	1:A:3605:ASN:ND2	2.50	0.44
3:E:411:VAL:CG1	3:E:434:LEU:HG	2.39	0.44
1:A:714:VAL:HG11	1:A:732:PHE:HE2	1.82	0.44
1:A:738:HIS:ND1	1:A:741:ILE:O	2.51	0.44
1:A:1360:LYS:HG3	1:A:1361:LYS:HE3	1.99	0.44
1:A:1484:LEU:HD12	1:A:1524:LEU:HD22	2.00	0.44
1:A:1533:LEU:HD23	1:A:1592:MET:HG3	2.00	0.44
1:A:2150:VAL:HA	1:A:2157:PHE:HE2	1.83	0.44
1:A:2314:GLU:OE2	1:A:2314:GLU:N	2.50	0.44
1:A:3137:GLU:OE2	1:A:3186:ARG:NE	2.44	0.44
6:Y:238:DT:H2"	6:Y:239:DG:C8	2.53	0.44
1:A:355:ASN:OD1	1:A:356:ASN:N	2.51	0.43
1:A:393:LYS:HA	1:A:397:LEU:HB2	2.00	0.43
1:A:910:PHE:HB3	1:A:2804:ILE:HD11	1.99	0.43
1:A:1937:ARG:O	1:A:1941:HIS:ND1	2.51	0.43
1:A:3929:MET:HB2	1:A:3938:ILE:HG13	2.00	0.43
3:E:369:TYR:CG	3:E:370:PRO:HD2	2.53	0.43
3:E:372:GLU:OE2	3:E:379:SER:OG	2.26	0.43
1:A:100:ILE:HD12	1:A:100:ILE:O	2.17	0.43
1:A:152:LEU:HD21	1:A:192:ASN:CG	2.38	0.43
1:A:990:GLN:NE2	1:A:2781:PRO:O	2.51	0.43
1:A:1134:LEU:O	1:A:1137:ILE:HG22	2.18	0.43
1:A:2806:LYS:NZ	1:A:2856:SER:OG	2.44	0.43
1:A:3297:VAL:HA	1:A:3300:VAL:HG22	2.00	0.43
1:A:3638:LYS:HA	1:A:3638:LYS:HD3	1.62	0.43
2:D:14:PRO:HB2	2:D:48:HIS:CE1	2.54	0.43
3:E:76:ILE:HD11	3:E:487:PHE:CE1	2.53	0.43
4:F:273:LYS:HE2	4:F:273:LYS:HB2	1.86	0.43
1:A:484:HIS:CE1	1:A:488:ILE:HD11	2.53	0.43
1:A:834:LEU:O	1:A:835:LYS:HG2	2.19	0.43
1:A:1088:GLU:C	1:A:1090:ARG:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:LEU:HD12	1:A:1154:PRO:HD2	2.00	0.43
1:A:1357:LYS:HD2	1:A:1357:LYS:HA	1.80	0.43
1:A:3033:GLU:O	1:A:3035:PHE:N	2.51	0.43
1:A:3341:LEU:HD13	1:A:3348:LEU:HD13	2.00	0.43
1:A:3913:ILE:HB	1:A:3984:MET:HG2	2.00	0.43
1:A:4103:GLN:O	1:A:4107:LEU:HD13	2.19	0.43
2:D:147:TYR:HE2	2:D:167:MET:SD	2.41	0.43
3:E:45:SER:OG	3:E:46:LYS:N	2.51	0.43
1:A:361:ILE:HD12	1:A:361:ILE:HA	1.87	0.43
1:A:1368:LEU:HA	1:A:1371:VAL:HG22	2.00	0.43
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.18	0.43
1:A:3985:VAL:HG23	1:A:4104:VAL:HG11	1.99	0.43
1:A:4046:TYR:CZ	1:A:4062:ASP:HB3	2.54	0.43
4:F:299:ASP:OD1	4:F:299:ASP:N	2.50	0.43
1:A:101:ALA:N	1:A:102:PRO:HD3	2.33	0.43
1:A:1071:ASN:HB3	1:A:1074:LYS:HB2	2.01	0.43
1:A:2302:ALA:HA	1:A:2305:ASN:ND2	2.33	0.43
3:E:472:THR:O	3:E:472:THR:OG1	2.31	0.43
1:A:1135:CYS:HA	1:A:1138:ILE:HG22	2.01	0.43
1:A:1375:THR:HA	1:A:1379:PRO:HB3	2.00	0.43
1:A:3145:ILE:HD13	1:A:3145:ILE:HA	1.87	0.43
1:A:3260:LYS:HA	1:A:3260:LYS:HD3	1.59	0.43
1:A:4021:LEU:HD21	1:A:4029:GLN:HB3	1.99	0.43
4:F:340:PHE:CE1	4:F:393:VAL:HG11	2.53	0.43
1:A:104:SER:O	1:A:107:ILE:HG22	2.18	0.43
1:A:200:PHE:HE2	1:A:230:LEU:HD13	1.84	0.43
1:A:645:TRP:O	1:A:649:PHE:HB2	2.19	0.43
1:A:849:GLU:H	1:A:849:GLU:CD	2.19	0.43
1:A:1400:VAL:HG21	1:A:1460:ARG:HE	1.84	0.43
1:A:1575:LEU:HG	1:A:1576:ASP:OD1	2.19	0.43
1:A:1639:LEU:HD22	1:A:1684:LEU:HD13	2.01	0.43
1:A:1938:ARG:HG3	1:A:1981:LEU:HA	2.01	0.43
1:A:2302:ALA:HA	1:A:2305:ASN:HD21	1.84	0.43
1:A:2313:LYS:H	1:A:2313:LYS:HG2	1.53	0.43
1:A:2898:LEU:HD23	1:A:2898:LEU:HA	1.86	0.43
1:A:3090:TYR:HE2	1:A:3098:ARG:HE	1.67	0.43
1:A:3832:PRO:HB3	1:A:3837:CYS:SG	2.59	0.43
2:D:30:SER:O	2:D:62:VAL:N	2.51	0.43
3:E:362:LEU:HD21	4:F:267:ILE:HG22	2.00	0.43
1:A:1802:TYR:CZ	1:A:1806:ARG:HD2	2.54	0.43
1:A:3348:LEU:H	1:A:3348:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3681:LYS:NZ	1:A:3723:ASP:O	2.50	0.43
3:E:247:ARG:HH12	3:E:488:ARG:CZ	2.32	0.43
4:F:176:GLY:HA2	4:F:178:ARG:HH21	1.83	0.43
1:A:3183:ILE:HD13	1:A:3183:ILE:HA	1.87	0.43
1:A:3330:LEU:HD12	1:A:3384:HIS:CD2	2.54	0.43
1:A:3498:TRP:HE3	1:A:3501:HIS:CD2	2.36	0.43
1:A:3859:TYR:HB3	1:A:4076:ASP:OD1	2.19	0.43
3:E:370:PRO:HD3	3:E:382:PHE:CE2	2.54	0.43
3:E:483:LEU:HD12	3:E:487:PHE:CZ	2.54	0.43
3:E:567:HIS:HA	3:E:570:LYS:HB3	2.01	0.43
4:F:532:LYS:HB2	4:F:532:LYS:HE2	1.84	0.43
1:A:649:PHE:O	1:A:653:LEU:HG	2.19	0.43
1:A:890:LYS:HE3	1:A:890:LYS:HB2	1.81	0.43
1:A:987:LEU:O	1:A:987:LEU:HD12	2.18	0.43
1:A:2427:ARG:HD2	1:A:2427:ARG:HA	1.82	0.43
1:A:2801:ASP:OD1	1:A:2804:ILE:HG22	2.18	0.43
1:A:3312:VAL:O	1:A:3314:SER:N	2.51	0.43
1:A:3344:GLU:HB2	1:A:3348:LEU:HD11	2.01	0.43
1:A:3508:LYS:HE2	1:A:3508:LYS:HB2	1.87	0.43
3:E:216:PHE:CG	3:E:216:PHE:O	2.71	0.43
3:E:580:MET:O	3:E:583:GLU:HG3	2.19	0.43
4:F:221:LEU:HD23	4:F:221:LEU:HA	1.82	0.43
5:X:43:DC:H2"	5:X:44:DA:C8	2.53	0.43
1:A:393:LYS:O	1:A:397:LEU:HB2	2.19	0.42
1:A:451:PRO:O	1:A:452:LYS:HB3	2.19	0.42
1:A:524:TYR:O	1:A:528:VAL:HG13	2.18	0.42
1:A:977:ASP:HB3	1:A:980:THR:HB	2.01	0.42
1:A:1751:GLU:HA	1:A:1785:ILE:HG22	2.01	0.42
1:A:2246:LYS:HZ2	1:A:2285:LEU:HG	1.84	0.42
1:A:2534:ASN:HB3	1:A:2537:ASP:HB2	2.00	0.42
1:A:3608:LYS:HG3	1:A:3612:ARG:NH2	2.34	0.42
1:A:3631:LYS:O	1:A:3635:THR:OG1	2.26	0.42
3:E:187:ARG:HG2	3:E:220:ILE:HD11	2.00	0.42
3:E:580:MET:HA	3:E:583:GLU:HG3	2.02	0.42
4:F:185:LEU:HA	4:F:185:LEU:HD12	1.68	0.42
6:Y:243:DT:H2'	6:Y:244:DT:H72	2.01	0.42
1:A:164:LYS:NZ	1:A:167:PRO:HD3	2.34	0.42
1:A:670:LEU:HA	1:A:673:THR:HG22	2.00	0.42
1:A:765:LEU:HA	1:A:765:LEU:HD12	1.82	0.42
1:A:1701:SER:O	1:A:1701:SER:OG	2.36	0.42
1:A:3868:VAL:HG23	1:A:4114:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:605:LYS:HD2	3:E:606:HIS:N	2.34	0.42
4:F:38:ILE:HD11	4:F:135:PHE:CE1	2.53	0.42
4:F:542:ALA:O	4:F:544:LYS:NZ	2.42	0.42
1:A:1326:GLU:OE1	1:A:1326:GLU:N	2.49	0.42
1:A:2522:ARG:HG3	1:A:2561:PHE:HE1	1.82	0.42
1:A:3028:ASN:HA	1:A:3031:TRP:HB2	2.02	0.42
1:A:3197:LEU:HD23	1:A:3197:LEU:HA	1.81	0.42
1:A:3276:TRP:HZ3	1:A:3306:LEU:HD21	1.84	0.42
2:D:167:MET:SD	2:D:167:MET:N	2.92	0.42
3:E:437:LEU:HD13	4:F:479:THR:HG21	2.00	0.42
3:E:559:TYR:CD1	3:E:564:LEU:HD11	2.54	0.42
1:A:1444:ASP:OD1	1:A:1444:ASP:N	2.48	0.42
1:A:1456:LYS:HB3	1:A:1456:LYS:HE3	1.68	0.42
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.67	0.42
1:A:1876:ILE:HA	1:A:1879:VAL:HG12	2.01	0.42
1:A:1894:SER:O	1:A:1898:GLN:HG2	2.19	0.42
1:A:3154:GLN:NE2	1:A:3227:ILE:HG12	2.35	0.42
1:A:322:GLN:O	1:A:326:MET:SD	2.77	0.42
1:A:1458:LEU:HD21	1:A:1467:ILE:HD13	2.01	0.42
1:A:1770:GLN:HA	1:A:1770:GLN:OE1	2.19	0.42
1:A:2122:LEU:H	1:A:2126:MET:HE3	1.85	0.42
3:E:487:PHE:O	3:E:491:GLU:HG2	2.20	0.42
4:F:229:GLU:HG2	4:F:233:LYS:HD2	2.02	0.42
5:X:45:DT:H2"	5:X:46:DA:C8	2.55	0.42
1:A:2341:LEU:HD12	1:A:2341:LEU:H	1.85	0.42
3:E:48:MET:HA	3:E:171:ASN:ND2	2.35	0.42
6:Y:216:DC:H1'	6:Y:217:DG:C8	2.55	0.42
1:A:204:LEU:HB3	1:A:251:PHE:HE2	1.85	0.42
1:A:238:MET:HG2	1:A:284:THR:HG22	2.02	0.42
1:A:1011:GLU:OE1	1:A:1062:ARG:NH1	2.53	0.42
1:A:1886:LYS:H	1:A:1886:LYS:HG2	1.61	0.42
1:A:3121:LEU:HD12	1:A:3121:LEU:HA	1.81	0.42
1:A:3927:ASN:O	1:A:3940:ILE:HG12	2.20	0.42
2:D:82:GLN:HA	2:D:82:GLN:OE1	2.18	0.42
3:E:243:LEU:O	3:E:246:VAL:HG13	2.20	0.42
3:E:428:THR:O	3:E:428:THR:OG1	2.28	0.42
6:Y:223:DT:H2"	6:Y:224:DA:C8	2.55	0.42
1:A:206:THR:O	1:A:210:SER:HB2	2.19	0.42
1:A:1238:GLN:NE2	1:A:1296:PHE:H	2.18	0.42
1:A:1245:ARG:HA	1:A:1248:PHE:HE1	1.84	0.42
1:A:2443:MET:N	1:A:2444:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2455:LEU:HD23	1:A:2501:LEU:HD23	2.02	0.42
1:A:2800:ARG:HD3	1:A:2800:ARG:HA	1.76	0.42
1:A:3360:LEU:HD12	1:A:3360:LEU:HA	1.94	0.42
1:A:3813:LYS:NZ	1:A:4125:GLU:OE2	2.53	0.42
1:A:3835:PRO:N	1:A:3836:PRO:HD2	2.35	0.42
1:A:4019:LYS:HB3	1:A:4019:LYS:HE3	1.85	0.42
3:E:121:GLN:O	3:E:130:ARG:NH2	2.51	0.42
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.84	0.42
1:A:276:ALA:HB2	1:A:315:ALA:HA	2.02	0.42
1:A:638:GLN:OE1	1:A:676:ASN:HA	2.20	0.42
1:A:933:LEU:O	1:A:937:MET:HG3	2.20	0.42
1:A:2454:LEU:HD23	1:A:2454:LEU:HA	1.80	0.42
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.84	0.42
1:A:3605:ASN:O	1:A:3608:LYS:HG2	2.18	0.42
1:A:3673:ASP:HB2	1:A:3675:LYS:HE3	2.02	0.42
3:E:168:LEU:HB3	3:E:202:LEU:HB3	2.01	0.42
1:A:106:GLU:OE1	1:A:106:GLU:N	2.33	0.42
1:A:157:TYR:CG	1:A:157:TYR:O	2.73	0.42
1:A:228:SER:O	1:A:229:SER:HB2	2.20	0.42
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.88	0.42
1:A:2478:MET:HG2	1:A:2524:PHE:CE1	2.55	0.42
4:F:107:PHE:HD2	4:F:142:PHE:HZ	1.67	0.42
4:F:383:ALA:O	4:F:387:LEU:HB3	2.20	0.42
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	2.01	0.41
1:A:3519:GLU:O	1:A:3522:THR:HG22	2.20	0.41
4:F:406:GLY:HA3	4:F:421:TYR:CE1	2.55	0.41
1:A:67:VAL:C	1:A:69:VAL:H	2.23	0.41
1:A:1142:HIS:NE2	1:A:1146:ASN:OD1	2.53	0.41
1:A:1567:ILE:H	1:A:1567:ILE:HG12	1.63	0.41
1:A:1969:GLU:HG3	1:A:1975:LEU:O	2.20	0.41
1:A:3503:VAL:HG11	1:A:3533:PHE:HA	2.02	0.41
4:F:12:LEU:HD11	4:F:41:PHE:CE2	2.54	0.41
4:F:155:LYS:HD2	4:F:159:ILE:HG12	2.02	0.41
1:A:894:PHE:HB2	1:A:907:LEU:HG	2.03	0.41
1:A:2097:LEU:HD12	1:A:2097:LEU:HA	1.80	0.41
1:A:2438:ILE:O	1:A:2442:MET:HG2	2.20	0.41
1:A:3228:SER:C	1:A:3230:LEU:H	2.22	0.41
1:A:3630:ARG:CG	1:A:3633:ILE:H	2.31	0.41
1:A:3856:MET:CE	1:A:4072:PRO:HG2	2.51	0.41
1:A:3917:ILE:HD12	1:A:4051:LEU:HD13	2.03	0.41
3:E:526:LYS:O	3:E:530:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:123:ILE:HD12	4:F:123:ILE:H	1.85	0.41
1:A:1820:VAL:O	1:A:1825:LEU:HD23	2.21	0.41
1:A:3372:LYS:HE3	1:A:3372:LYS:HB2	1.80	0.41
2:D:83:TYR:HB2	2:D:99:TYR:HD2	1.86	0.41
4:F:247:TRP:CE3	4:F:263:ALA:HB3	2.56	0.41
1:A:108:LYS:HD3	1:A:147:PHE:HD1	1.86	0.41
1:A:264:ARG:NH1	5:X:52:DG:H4'	2.36	0.41
1:A:1661:PHE:HE1	1:A:1671:VAL:HG11	1.85	0.41
3:E:420:LEU:HD21	3:E:424:LYS:HD3	2.03	0.41
3:E:572:THR:OG1	3:E:573:LEU:N	2.52	0.41
4:F:408:ALA:HA	4:F:420:VAL:O	2.19	0.41
1:A:51:LEU:H	1:A:51:LEU:HD12	1.85	0.41
1:A:1684:LEU:HD11	1:A:1688:LEU:HD21	2.02	0.41
1:A:1937:ARG:HD2	1:A:1937:ARG:HA	1.90	0.41
1:A:3984:MET:HB3	1:A:4104:VAL:HG21	2.03	0.41
4:F:390:VAL:HG23	4:F:409:PHE:HA	2.03	0.41
1:A:917:LEU:HD23	1:A:917:LEU:HA	1.89	0.41
1:A:1186:LYS:HD3	1:A:1186:LYS:HA	1.70	0.41
1:A:1334:LYS:HB3	1:A:1334:LYS:HE3	1.81	0.41
1:A:1646:LEU:HD12	1:A:1647:ALA:N	2.36	0.41
1:A:2443:MET:HE3	1:A:2479:TRP:HB3	2.02	0.41
1:A:3577:GLN:OE1	1:A:3577:GLN:HA	2.21	0.41
3:E:165:ARG:HA	3:E:199:PHE:O	2.20	0.41
3:E:178:ASN:OD1	3:E:178:ASN:N	2.51	0.41
4:F:454:VAL:O	4:F:458:ILE:HG23	2.21	0.41
1:A:759:GLY:C	1:A:761:SER:H	2.24	0.41
1:A:4031:ILE:HD12	1:A:4031:ILE:HA	1.89	0.41
2:D:23:ARG:HA	2:D:93:ARG:HH12	1.86	0.41
3:E:48:MET:HE3	3:E:48:MET:O	2.21	0.41
4:F:33:GLN:HG2	4:F:185:LEU:HD11	2.03	0.41
4:F:134:ILE:HD13	4:F:163:PHE:CE1	2.56	0.41
4:F:286:LYS:HE3	4:F:286:LYS:HB3	1.82	0.41
4:F:369:ASP:OD1	4:F:369:ASP:N	2.53	0.41
1:A:32:HIS:HA	1:A:35:ILE:HG12	2.02	0.41
1:A:125:ILE:HB	1:A:126:PRO:HD3	2.02	0.41
1:A:236:LYS:HD2	1:A:236:LYS:HA	1.94	0.41
1:A:320:LEU:HA	1:A:323:VAL:HG12	2.02	0.41
1:A:651:TYR:CE1	1:A:1386:ILE:HD11	2.56	0.41
1:A:859:LEU:HD11	1:A:870:LEU:HD13	2.02	0.41
1:A:988:VAL:HG11	1:A:1028:PHE:HZ	1.86	0.41
1:A:1366:THR:O	1:A:1370:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1782:PHE:HA	1:A:1785:ILE:HG12	2.03	0.41
1:A:1783:ARG:O	1:A:1787:ARG:HG2	2.20	0.41
1:A:1786:ALA:HB1	1:A:1831:CYS:O	2.21	0.41
1:A:2409:THR:OG1	1:A:2410:GLU:N	2.54	0.41
1:A:3062:LEU:HD21	1:A:3093:GLN:HG3	2.02	0.41
1:A:3151:LEU:HD11	1:A:3196:LYS:HB2	2.02	0.41
1:A:3172:LYS:HE2	1:A:3172:LYS:HB2	1.89	0.41
1:A:3351:ILE:HD12	1:A:3351:ILE:HA	1.93	0.41
2:D:191:GLN:O	2:D:192:GLU:HB2	2.21	0.41
3:E:171:ASN:C	3:E:171:ASN:OD1	2.59	0.41
3:E:215:LEU:HD23	3:E:215:LEU:HA	1.74	0.41
3:E:261:LEU:HD23	3:E:269:ILE:HD11	2.02	0.41
3:E:418:GLU:HB2	3:E:430:PRO:HB3	2.03	0.41
4:F:12:LEU:HD11	4:F:41:PHE:HE2	1.86	0.41
4:F:356:PHE:CZ	4:F:409:PHE:HZ	2.39	0.41
4:F:365:PHE:HA	4:F:418:CYS:HB2	2.03	0.41
5:X:34:DT:H6	5:X:34:DT:H5'	1.86	0.41
6:Y:245:DA:C2	6:Y:246:DA:C6	3.08	0.41
1:A:257:ARG:HD3	1:A:296:VAL:HG11	2.03	0.41
1:A:860:GLY:HA3	1:A:3136:THR:OG1	2.20	0.41
1:A:900:GLU:N	1:A:900:GLU:OE1	2.54	0.41
1:A:1086:TYR:CE1	1:A:1087:ARG:HG3	2.56	0.41
1:A:1579:VAL:HG21	1:A:1621:THR:HG21	2.03	0.41
1:A:2184:TYR:O	1:A:2187:VAL:HG12	2.21	0.41
1:A:2551:GLU:HA	1:A:2554:PHE:HB2	2.02	0.41
1:A:4006:VAL:HG23	1:A:4011:PHE:HE2	1.86	0.41
2:D:150:GLU:OE1	2:D:150:GLU:N	2.54	0.41
3:E:249:LYS:HB3	3:E:249:LYS:HE2	1.91	0.41
4:F:34:ALA:O	4:F:38:ILE:HG12	2.20	0.41
1:A:532:ARG:HA	1:A:535:LEU:HD23	2.02	0.40
1:A:1339:VAL:HG13	1:A:1398:VAL:HG21	2.02	0.40
1:A:1686:LEU:O	1:A:1690:GLY:N	2.50	0.40
1:A:3088:LEU:O	1:A:3092:LEU:HB2	2.21	0.40
1:A:3883:LEU:HD12	1:A:3883:LEU:HA	1.84	0.40
3:E:392:LYS:C	3:E:393:GLU:HG3	2.42	0.40
1:A:832:LYS:NZ	6:Y:218:DT:H3'	2.37	0.40
1:A:1597:LEU:HD23	1:A:1597:LEU:HA	1.92	0.40
1:A:1893:GLU:CD	1:A:1894:SER:H	2.24	0.40
1:A:2148:LYS:HD2	1:A:2148:LYS:HA	1.95	0.40
1:A:2286:PRO:HB3	1:A:2329:TYR:CZ	2.56	0.40
1:A:3264:LYS:HE2	1:A:3264:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3911:ILE:HD11	1:A:3928:PHE:CE2	2.56	0.40
3:E:202:LEU:HD21	3:E:217:TYR:HB3	2.03	0.40
5:X:34:DT:H5'	5:X:34:DT:C6	2.55	0.40
1:A:446:PHE:HD2	1:A:457:CYS:HG	1.68	0.40
1:A:1037:LEU:HD12	1:A:1037:LEU:HA	1.80	0.40
1:A:1242:LEU:HA	1:A:1242:LEU:HD23	1.80	0.40
1:A:1649:LEU:HD12	1:A:1649:LEU:HA	1.90	0.40
1:A:1878:ASP:OD1	1:A:1879:VAL:N	2.54	0.40
1:A:1895:LYS:O	1:A:1899:VAL:HG23	2.20	0.40
1:A:2228:ARG:HH21	1:A:2232:ARG:HD3	1.85	0.40
1:A:2415:LEU:HD13	1:A:2420:PHE:CD2	2.56	0.40
1:A:3496:ILE:H	1:A:3496:ILE:HG12	1.72	0.40
1:A:3623:PRO:HD3	1:A:3629:ARG:NH2	2.37	0.40
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.45	0.40
3:E:451:LYS:HZ3	4:F:415:ASN:C	2.25	0.40
4:F:442:LYS:HE2	4:F:442:LYS:HB2	1.78	0.40
1:A:712:LYS:O	1:A:716:VAL:HG13	2.22	0.40
1:A:1788:ARG:HA	1:A:1788:ARG:HD2	1.79	0.40
1:A:2835:LYS:NZ	1:A:2839:ASP:OD2	2.54	0.40
1:A:3593:ARG:NH1	1:A:3661:ASP:OD1	2.52	0.40
1:A:3681:LYS:HD2	1:A:3687:MET:HB3	2.03	0.40
1:A:4037:ASN:OD1	1:A:4037:ASN:N	2.55	0.40
3:E:277:VAL:HG22	4:F:357:MET:SD	2.61	0.40
4:F:229:GLU:HG3	4:F:232:ARG:NH2	2.37	0.40
1:A:1463:LEU:HD12	1:A:1463:LEU:HA	1.93	0.40
1:A:3003:ASN:HD21	1:A:3046:ARG:CZ	2.34	0.40
1:A:3621:LYS:HD2	1:A:3621:LYS:HA	1.78	0.40
1:A:4023:LYS:HE3	1:A:4023:LYS:HB2	1.88	0.40
1:A:4040:PRO:HD2	1:A:4041:ARG:NH1	2.37	0.40
5:X:43:DC:C2	5:X:44:DA:N7	2.89	0.40
6:Y:253:DC:H1'	6:Y:254:DC:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3557/4128 (86%)	3192 (90%)	365 (10%)	0	100	100
2	D	154/399 (39%)	132 (86%)	21 (14%)	1 (1%)	22	55
3	E	556/609 (91%)	513 (92%)	43 (8%)	0	100	100
4	F	551/732 (75%)	493 (90%)	58 (10%)	0	100	100
All	All	4818/5868 (82%)	4330 (90%)	487 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	192	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3218/3671 (88%)	3072 (96%)	146 (4%)	23	53
2	D	133/336 (40%)	126 (95%)	7 (5%)	19	48
3	E	507/548 (92%)	488 (96%)	19 (4%)	29	58
4	F	496/649 (76%)	479 (97%)	17 (3%)	32	60
All	All	4354/5204 (84%)	4165 (96%)	189 (4%)	27	54

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	54	GLN
1	A	61	ARG
1	A	62	ASP
1	A	68	PHE
1	A	78	PHE
1	A	87	LYS

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Mol	Chain	Res	Type
1	A	108	LYS
1	A	111	CYS
1	A	131	LEU
1	A	153	PHE
1	A	157	TYR
1	A	172	GLU
1	A	191	ASN
1	A	203	GLU
1	A	225	LYS
1	A	278	HIS
1	A	305	ASN
1	A	309	LYS
1	A	317	GLU
1	A	346	TYR
1	A	374	LYS
1	A	382	ASP
1	A	401	ASP
1	A	475	LEU
1	A	477	ASN
1	A	566	ASP
1	A	611	ASN
1	A	620	PHE
1	A	648	SER
1	A	703	CYS
1	A	707	PHE
1	A	722	LYS
1	A	738	HIS
1	A	743	LEU
1	A	789	TYR
1	A	870	LEU
1	A	1084	ASN
1	A	1089	PHE
1	A	1160	SER
1	A	1164	CYS
1	A	1167	ASP
1	A	1206	LEU
1	A	1213	LYS
1	A	1248	PHE
1	A	1258	ASP
1	A	1267	TYR
1	A	1296	PHE
1	A	1325	GLN

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Mol	Chain	Res	Type
1	A	1333	SER
1	A	1356	TRP
1	A	1361	LYS
1	A	1370	ARG
1	A	1397	ASP
1	A	1409	SER
1	A	1436	LEU
1	A	1476	HIS
1	A	1524	LEU
1	A	1534	ASN
1	A	1576	ASP
1	A	1602	ASP
1	A	1629	CYS
1	A	1646	LEU
1	A	1660	SER
1	A	1664	SER
1	A	1711	ARG
1	A	1730	PRO
1	A	1813	SER
1	A	1822	ARG
1	A	1829	TRP
1	A	1838	GLU
1	A	1840	PHE
1	A	1871	MET
1	A	1886	LYS
1	A	1942	CYS
1	A	1945	TYR
1	A	1947	CYS
1	A	1981	LEU
1	A	2126	MET
1	A	2165	LEU
1	A	2184	TYR
1	A	2196	TRP
1	A	2224	PHE
1	A	2264	ASP
1	A	2276	LEU
1	A	2341	LEU
1	A	2396	LEU
1	A	2429	ASP
1	A	2461	PHE
1	A	2473	MET
1	A	2486	ASP

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Mol	Chain	Res	Type
1	A	2503	LYS
1	A	2577	PHE
1	A	2851	PHE
1	A	2899	ARG
1	A	2930	TYR
1	A	2943	PHE
1	A	2972	TYR
1	A	2977	ASN
1	A	3009	LYS
1	A	3035	PHE
1	A	3048	LYS
1	A	3072	GLU
1	A	3094	ASP
1	A	3114	TYR
1	A	3116	SER
1	A	3123	GLN
1	A	3150	ASN
1	A	3173	MET
1	A	3191	SER
1	A	3232	ARG
1	A	3270	ASP
1	A	3271	ASP
1	A	3315	TYR
1	A	3319	ASN
1	A	3348	LEU
1	A	3378	TYR
1	A	3428	GLU
1	A	3455	LYS
1	A	3469	LEU
1	A	3497	SER
1	A	3540	TYR
1	A	3544	ASP
1	A	3604	LYS
1	A	3625	LEU
1	A	3630	ARG
1	A	3646	LYS
1	A	3665	MET
1	A	3667	LEU
1	A	3693	GLU
1	A	3694	PHE
1	A	3697	ASN
1	A	3712	LEU

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Mol	Chain	Res	Type
1	A	3729	MET
1	A	3741	ARG
1	A	3777	GLN
1	A	3789	ARG
1	A	3792	SER
1	A	3799	ARG
1	A	3841	ASP
1	A	3907	SER
1	A	3932	MET
1	A	3959	MET
1	A	3997	LEU
1	A	4027	TRP
1	A	4109	ASP
2	D	34	ARG
2	D	89	GLU
2	D	99	TYR
2	D	100	ARG
2	D	133	ARG
2	D	136	PHE
2	D	153	ARG
3	E	71	TYR
3	E	96	SER
3	E	115	ARG
3	E	137	HIS
3	E	153	LEU
3	E	184	SER
3	E	200	LEU
3	E	207	LYS
3	E	216	PHE
3	E	257	SER
3	E	258	ARG
3	E	281	LEU
3	E	351	LYS
3	E	445	LYS
3	E	470	ARG
3	E	471	PHE
3	E	525	PHE
3	E	591	LYS
3	E	605	LYS
4	F	14	MET
4	F	93	ASP
4	F	100	PRO

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Mol	Chain	Res	Type
4	F	142	PHE
4	F	153	SER
4	F	178	ARG
4	F	271	ARG
4	F	323	PHE
4	F	353	ARG
4	F	354	ARG
4	F	409	PHE
4	F	442	LYS
4	F	443	LYS
4	F	477	PHE
4	F	502	ARG
4	F	538	PRO
4	F	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1946	ASN
1	A	2795	GLN
2	D	48	HIS
3	E	137	HIS
3	E	204	HIS
3	E	360	HIS
3	E	515	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.

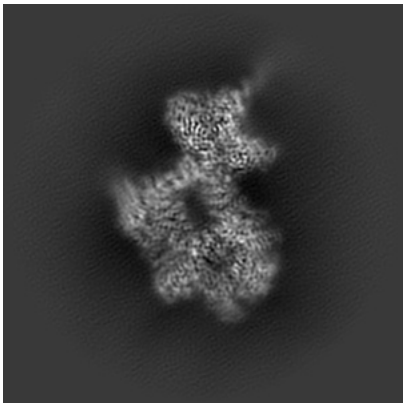
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19065. These allow visual inspection of the internal detail of the map and identification of artifacts.

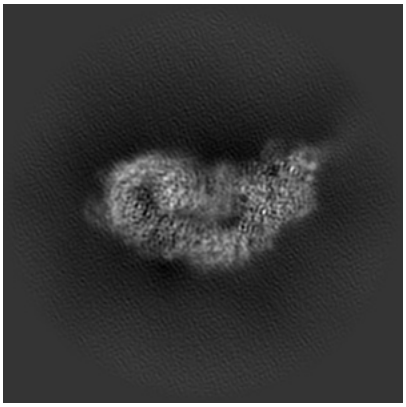
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

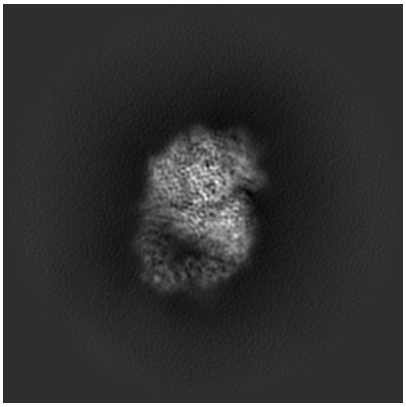
6.1.1 Primary map



X



Y

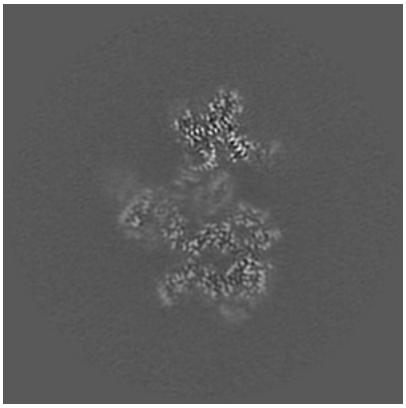


Z

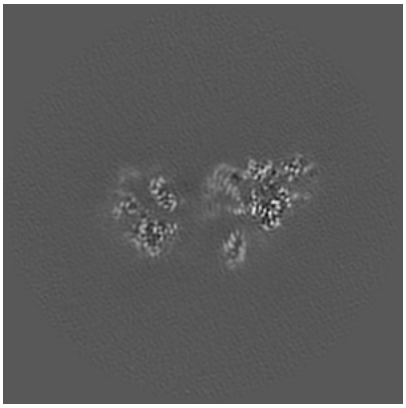
The images above show the map projected in three orthogonal directions.

6.2 Central slices

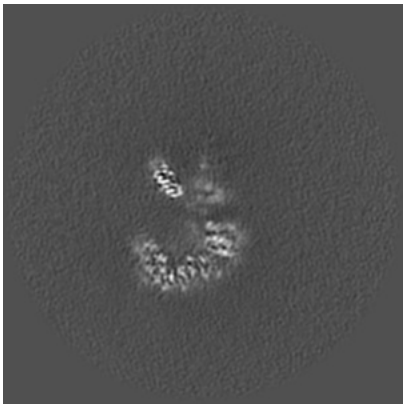
6.2.1 Primary map



X Index: 192



Y Index: 192

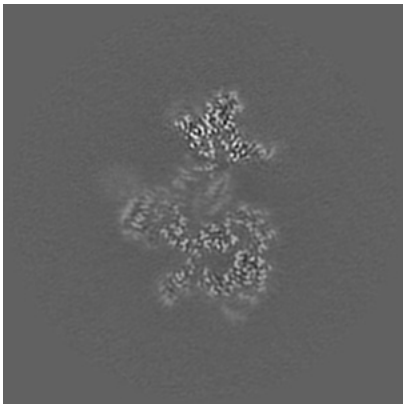


Z Index: 192

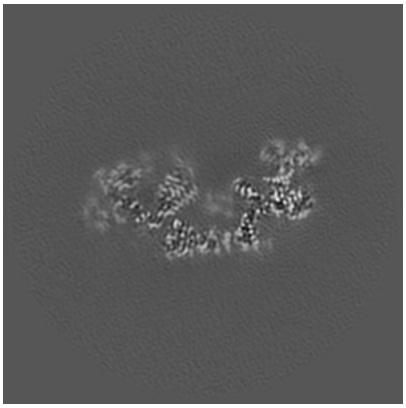
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

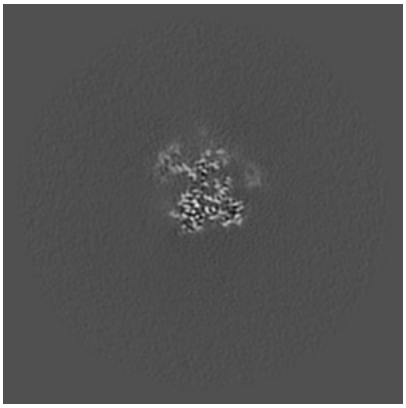
6.3.1 Primary map



X Index: 194



Y Index: 217

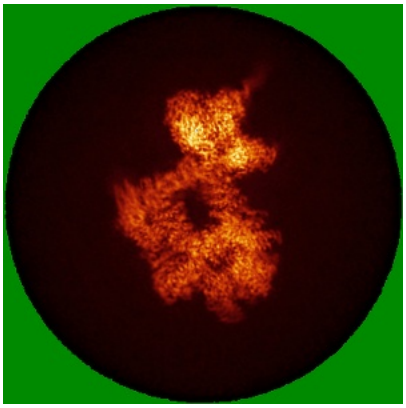


Z Index: 251

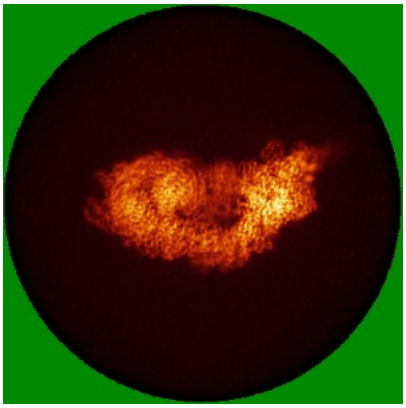
The images above show the largest variance slices of the map in three orthogonal directions.

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

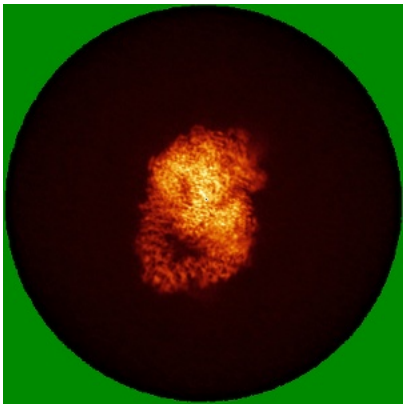
6.4.1 Primary map



X



Y

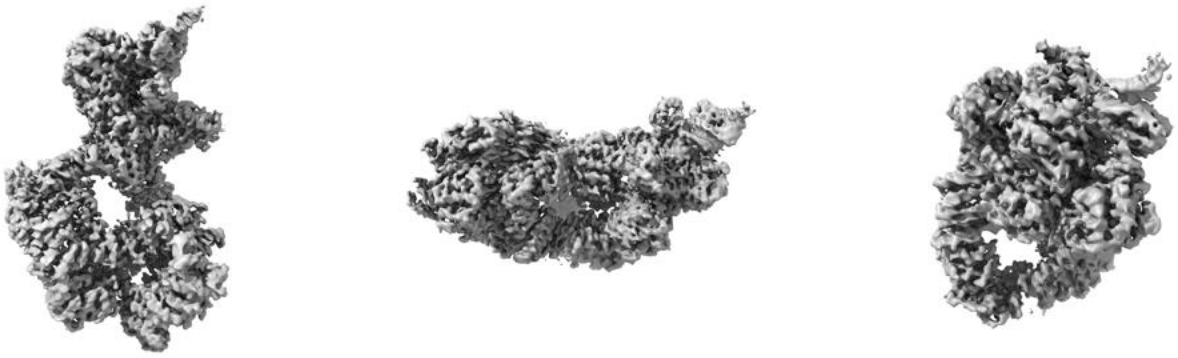


Z

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 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

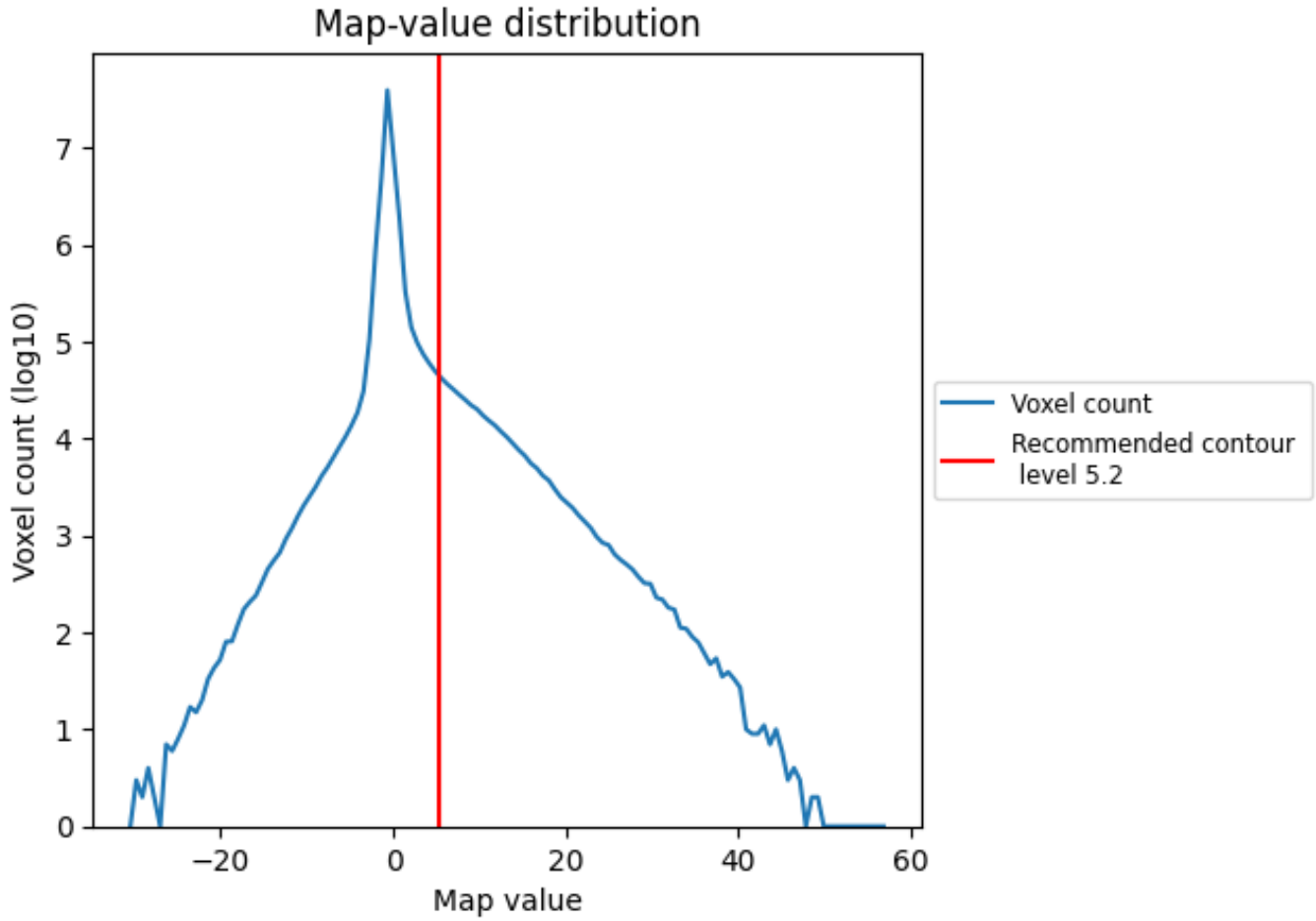
6.6 Mask visualisation (i)

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

7 Map analysis

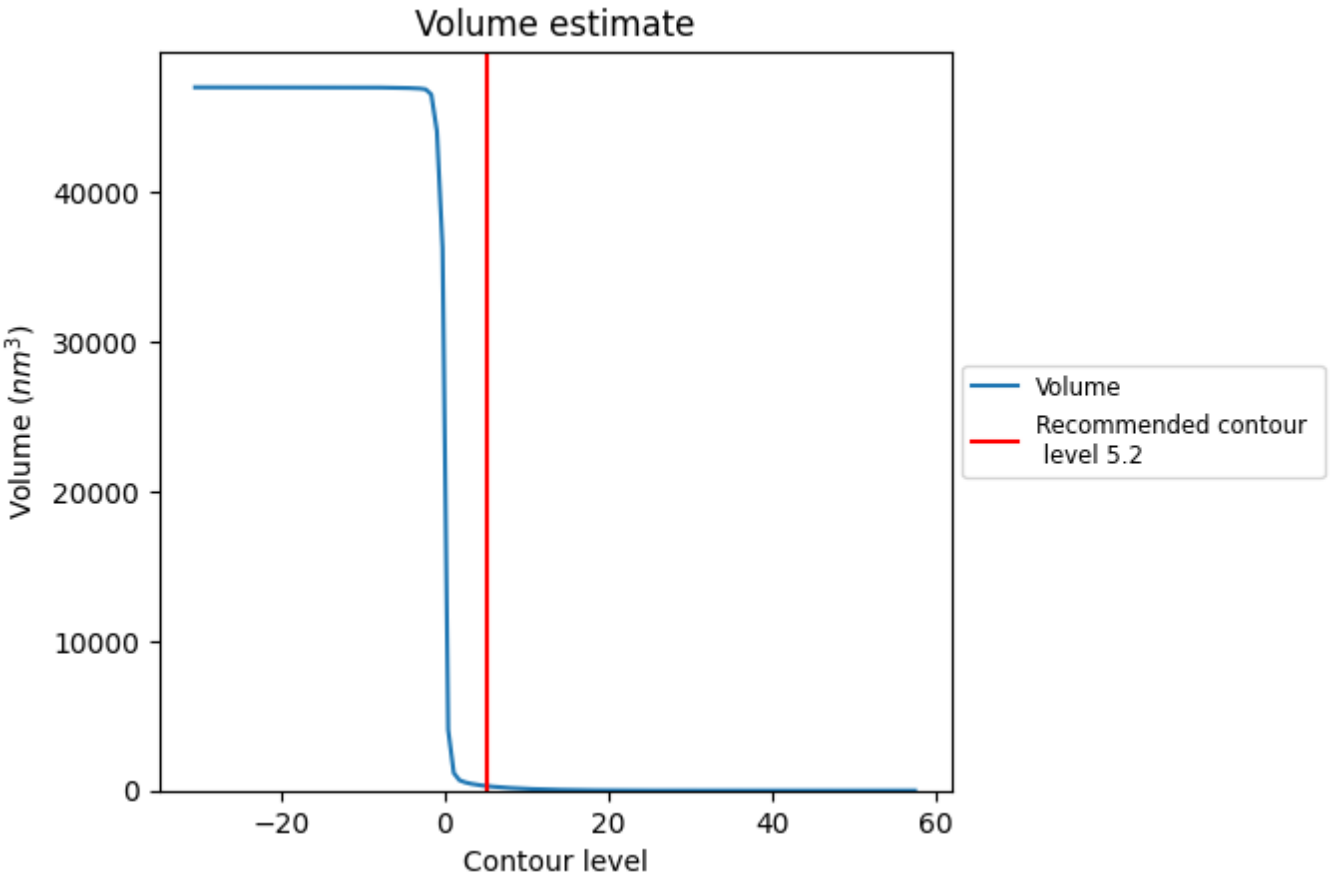
This section contains the results of statistical analysis of the map.

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.

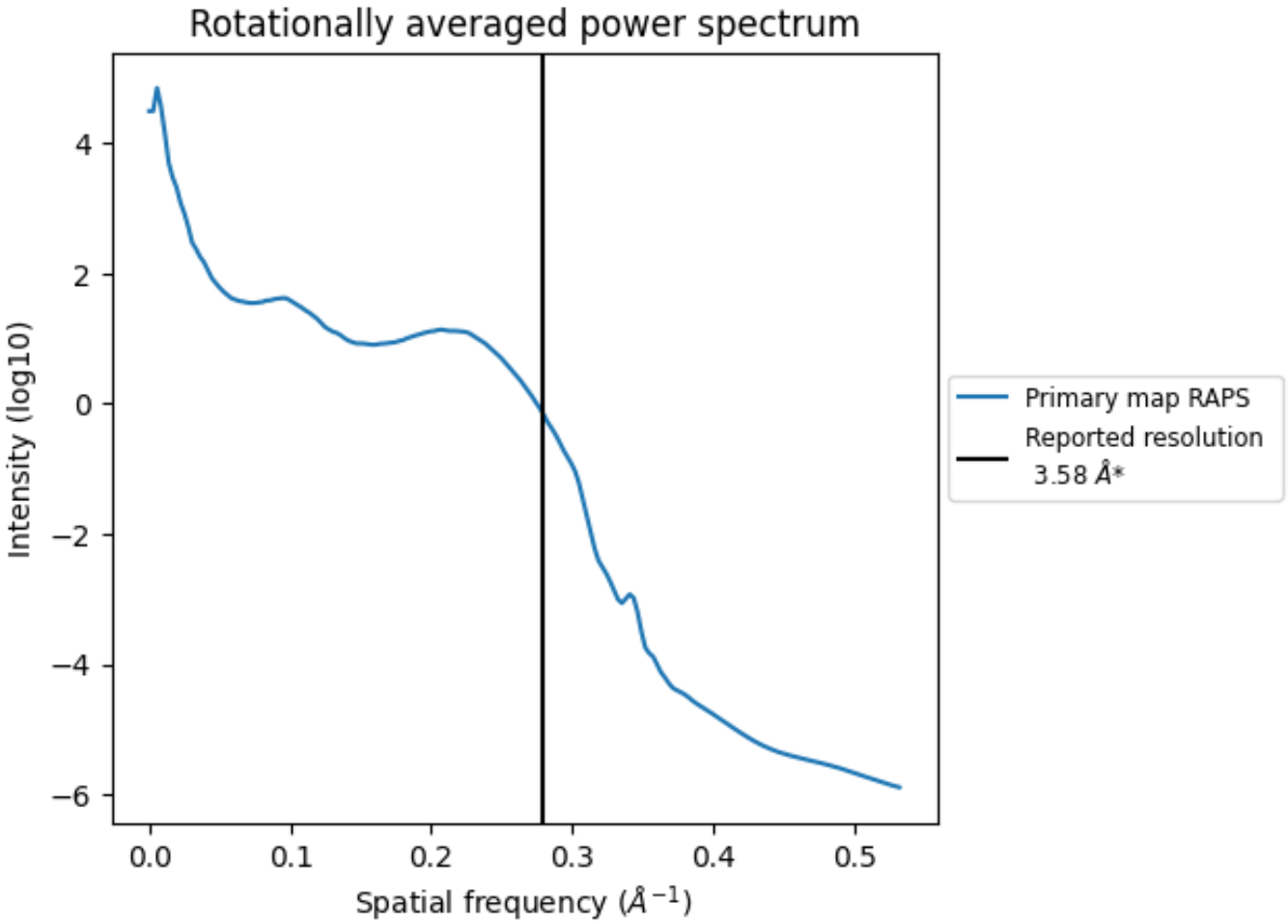
7.2 Volume estimate



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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 0.279 Å^{-1}

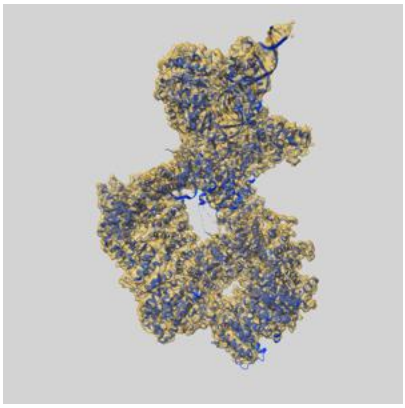
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

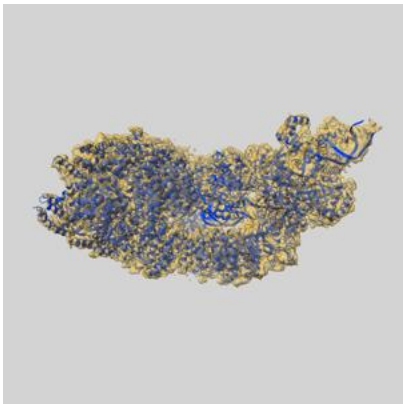
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19065 and PDB model 8RD4. Per-residue inclusion information can be found in section 3 on page 4.

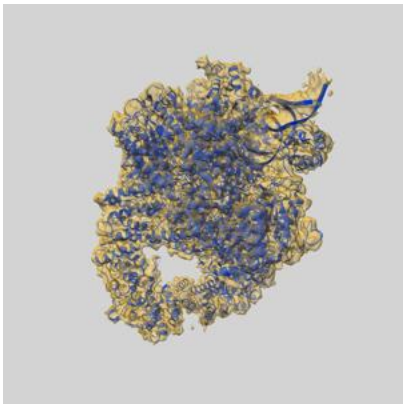
9.1 Map-model overlay



X



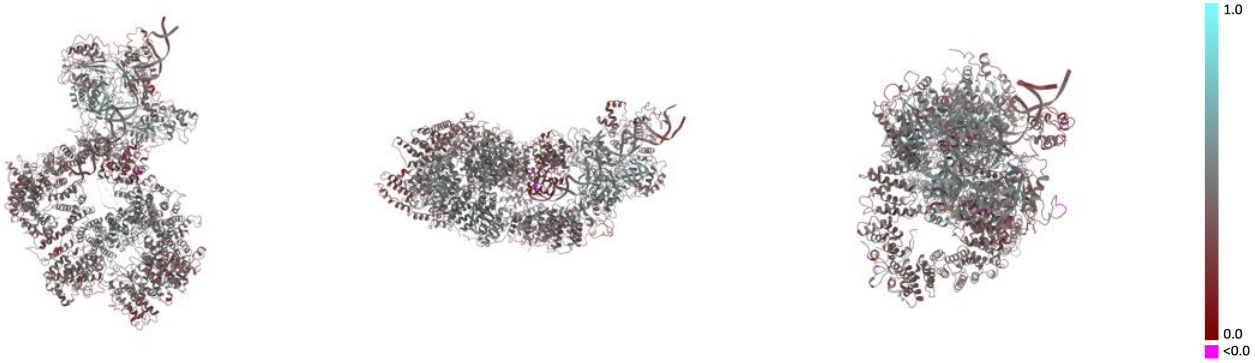
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2 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.

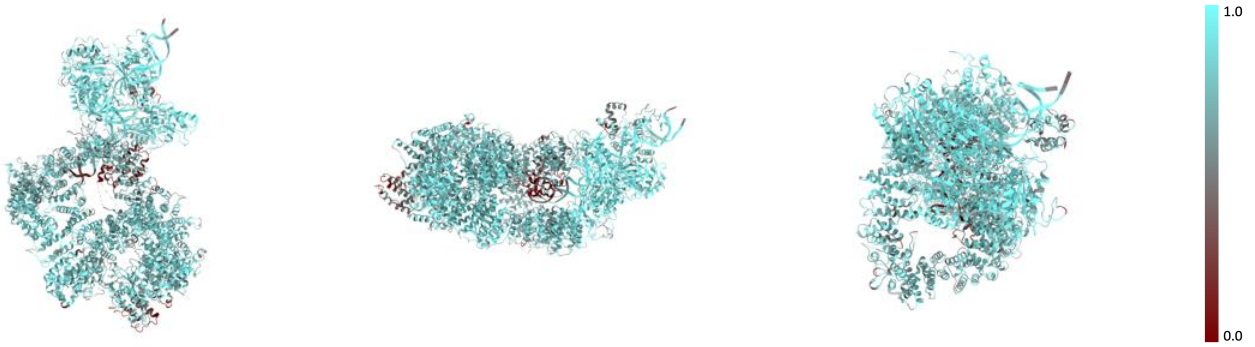
9.2 Q-score mapped to coordinate model (i)



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.

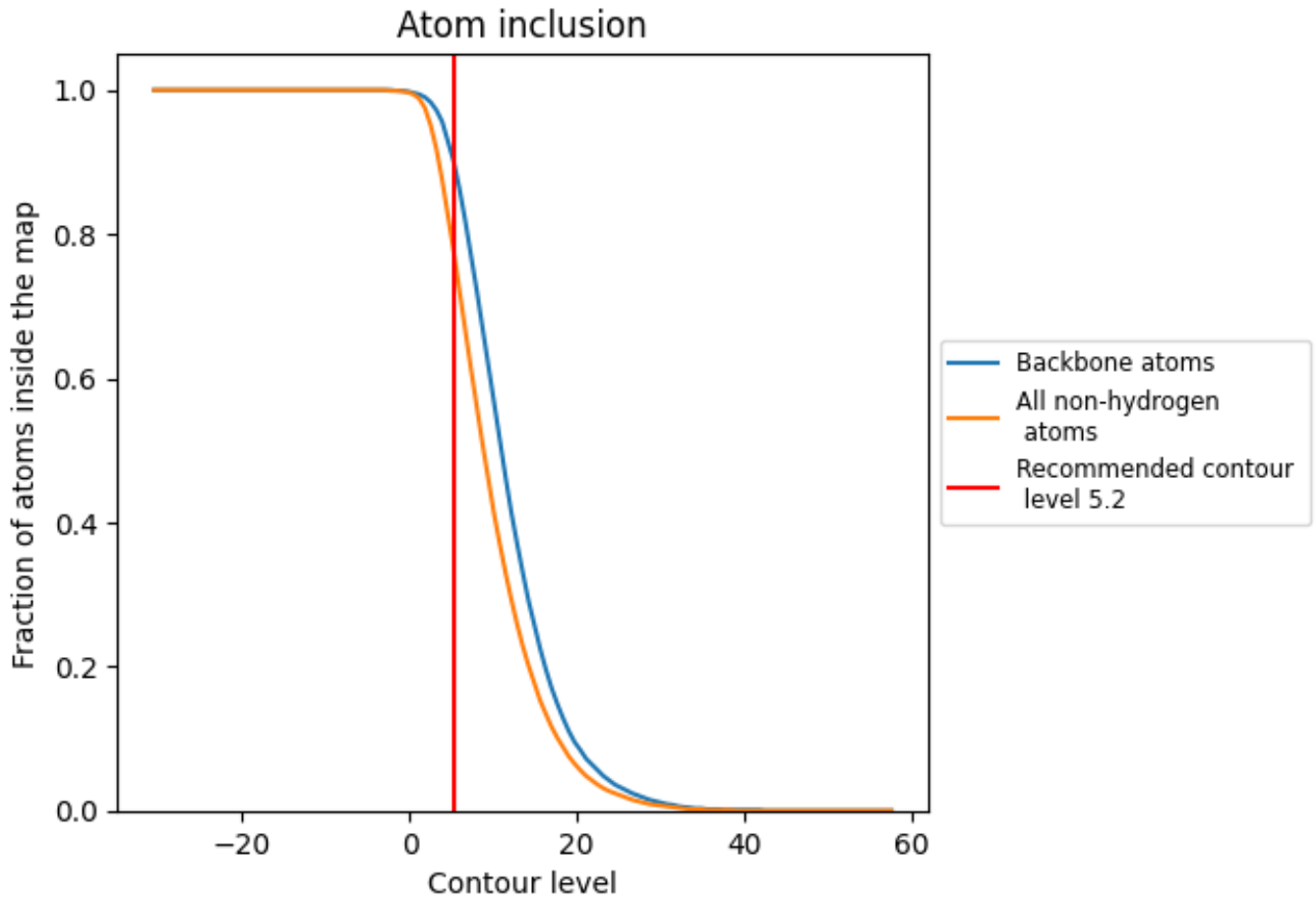
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.2).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.4280
A	0.7570	0.4190
D	0.8340	0.4110
E	0.8580	0.4590
F	0.8440	0.4610
X	0.8110	0.4230
Y	0.8090	0.4170