Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 04:01 PM UTC

PDB ID	:	9GD7 / pdb_00009gd7
EMDB ID	:	EMD-51249
Title	:	DNA-PK Ku80 mediated dimer bound to DNA polymerase Lambda and DNA ligase 4/XRCC4
Authors	:	Chaplin, A.K.; Amin, H.; Zahid, S.; Hardwick, S.W.
Deposited on	:	2024-08-05
Resolution	:	4.25 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

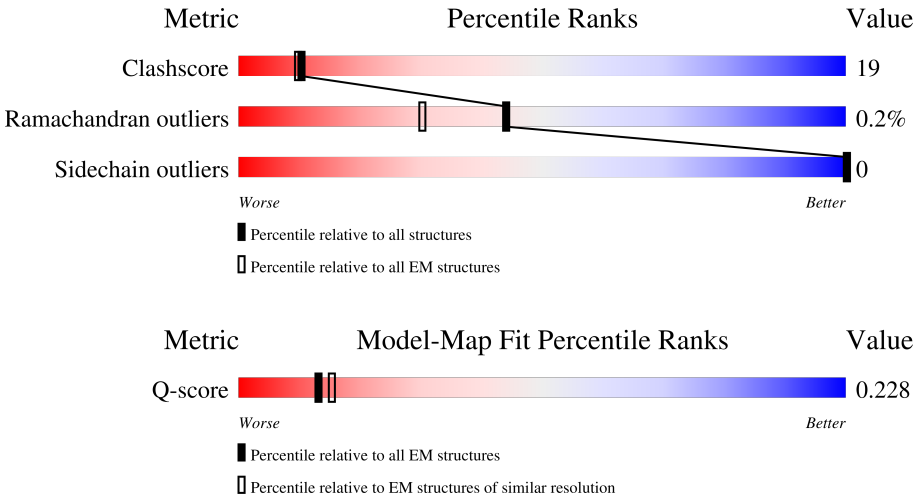
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4654 (3.75 - 4.75)

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	E	911	17% 16% 10% 73%
2	L	732	19% 53% 35% 12%
3	M	204	8% 89%
4	P	336	16% 9% 8% 83%

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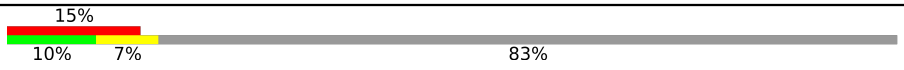
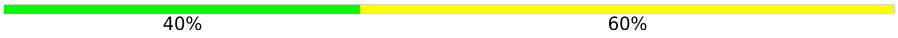
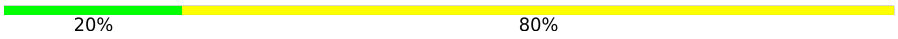
Mol	Chain	Length	Quality of chain
4	Q	336	
5	S	4128	
6	T	609	
7	i	25	
8	j	25	
9	A	575	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41717 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 ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	246	Total	C	N	O	S	0	0
			1956	1240	332	371	13		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	641	Total	C	N	O	S	0	0
			5084	3250	859	950	25		

- Molecule 3 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	23	Total	C	N	O	S	0	0
			160	102	27	30	1		

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	57	Total	C	N	O	S	0	0
			480	303	90	86	1		
4	Q	57	Total	C	N	O	S	0	0
			475	301	89	84	1		

- Molecule 5 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	3535	Total	C	N	O	S	0	0
			27773	17865	4705	5020	183		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	501	Total	C	N	O	S	0	0
			4001	2561	679	743	18		

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	25	Total	C	N	O	P	0	0
			510	247	92	146	25		

- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	25	Total	C	N	O	P	0	0
			514	250	86	154	24		

- Molecule 9 is a protein called DNA polymerase lambda.

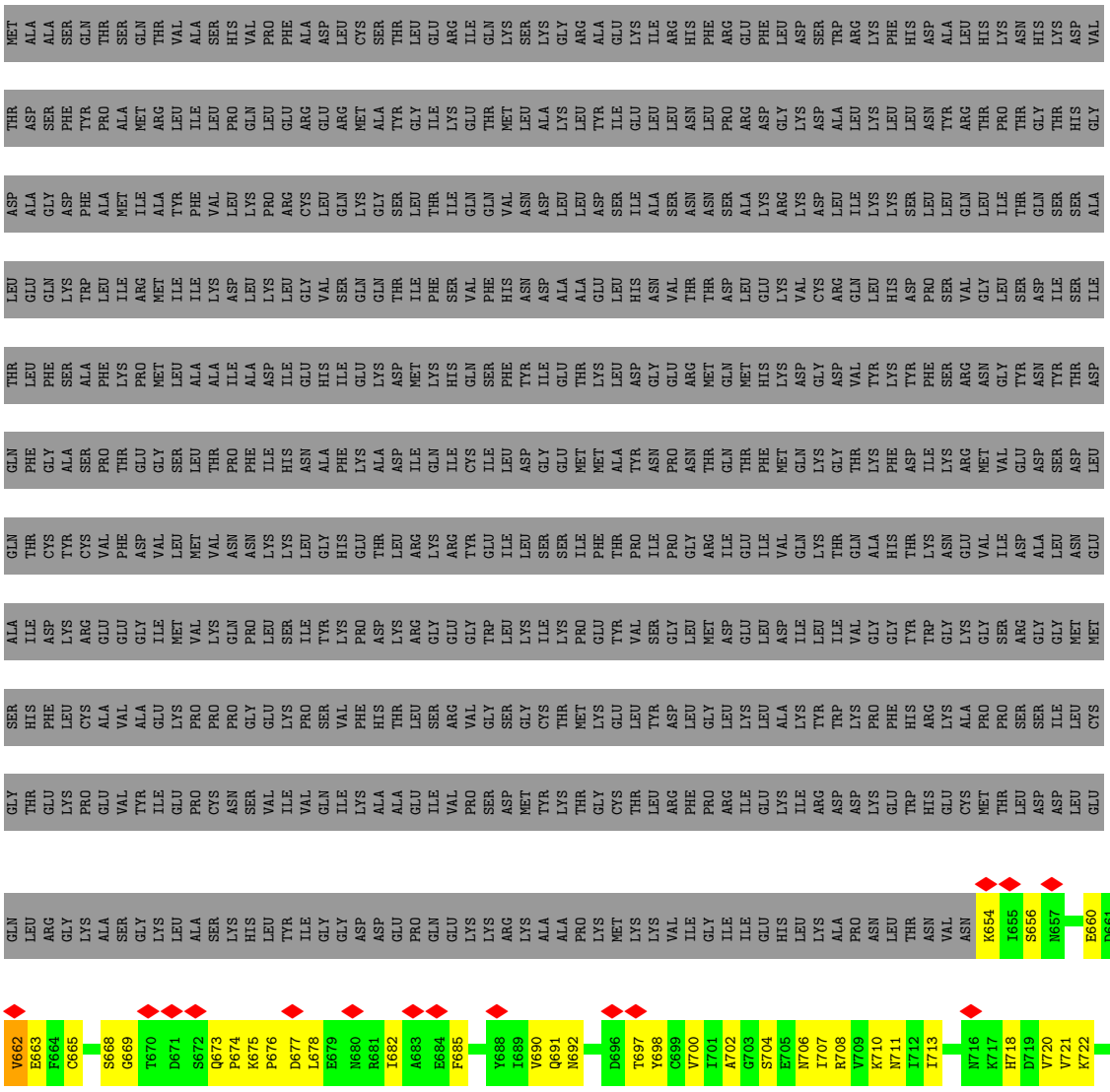
Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	98	Total	C	N	O	S	0	0
			764	487	142	132	3		

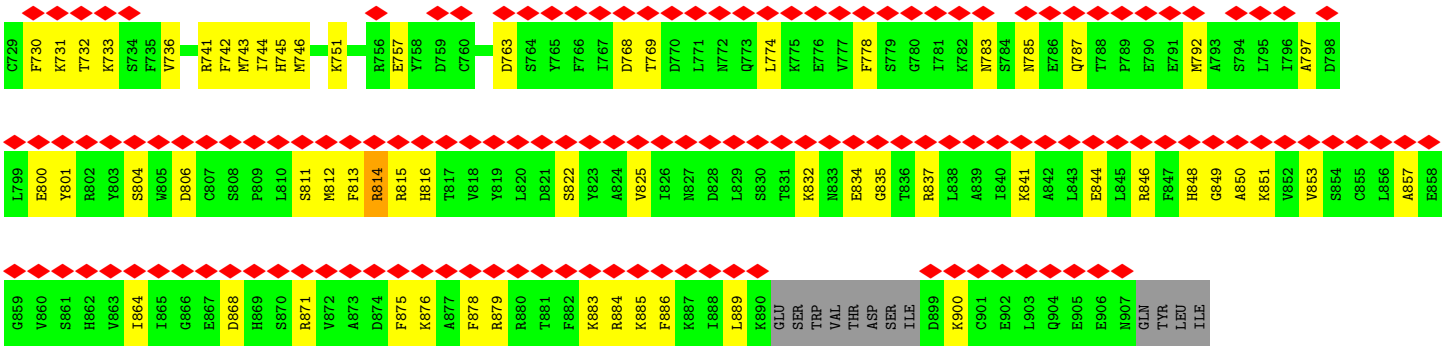
3 Residue-property plots (i)

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 ligase 4

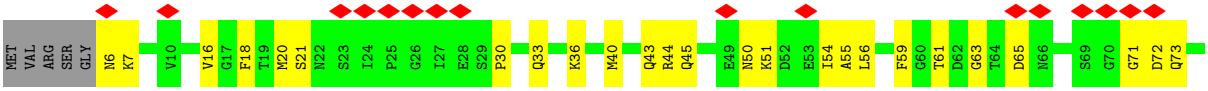
Chain E:

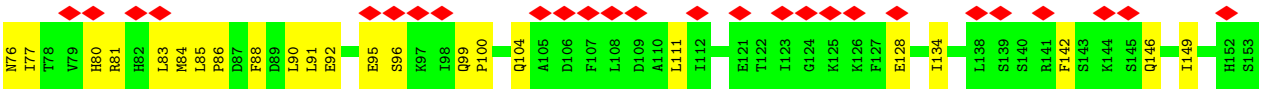


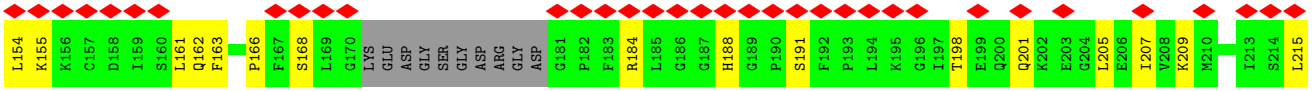


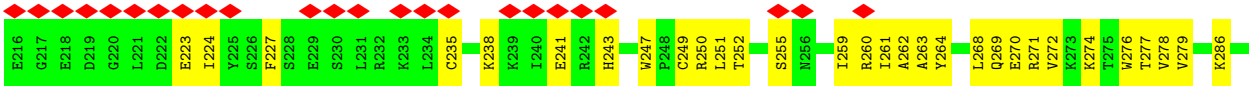
• Molecule 2: X-ray repair cross-complementing protein 5

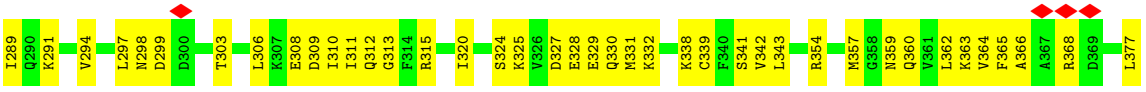
Chain L:

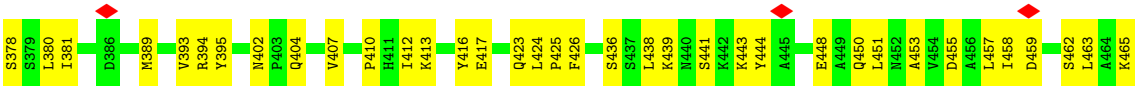


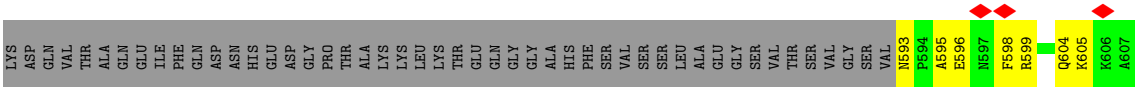


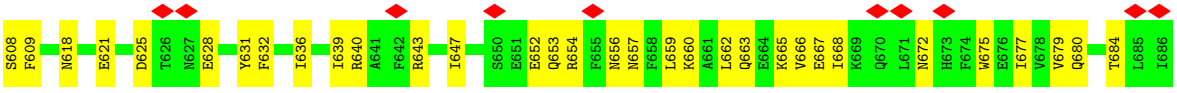


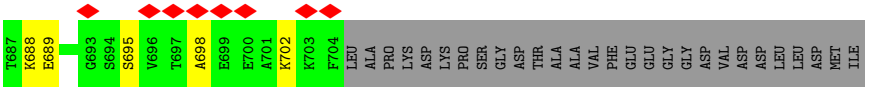






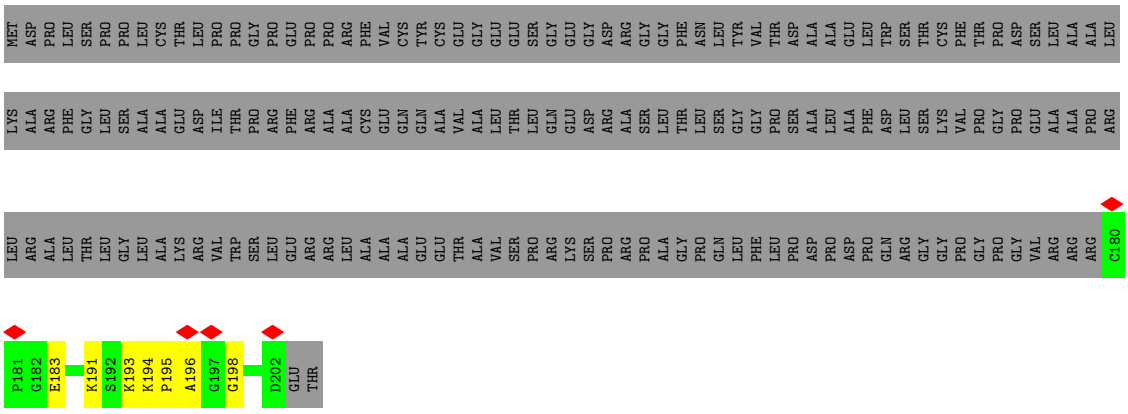






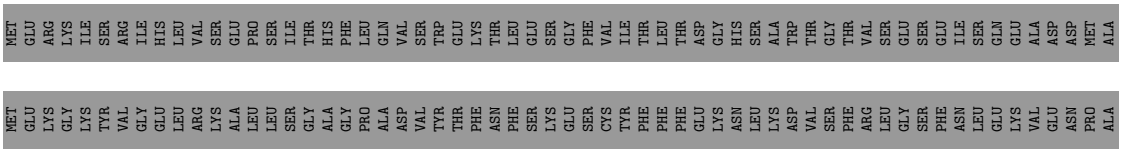
• Molecule 3: Protein PAXX

Chain M:



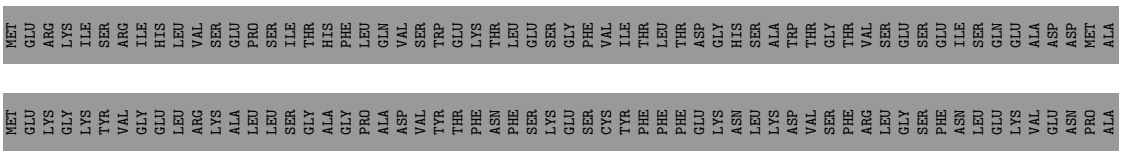
• Molecule 4: DNA repair protein XRCC4

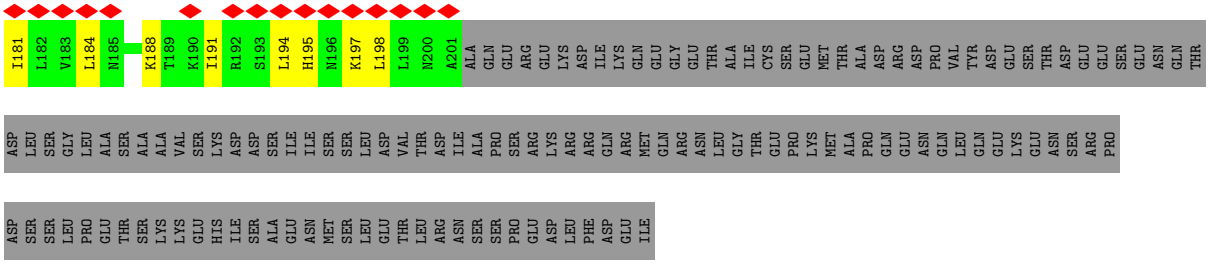
Chain P:



• Molecule 4: DNA repair protein XRCC4

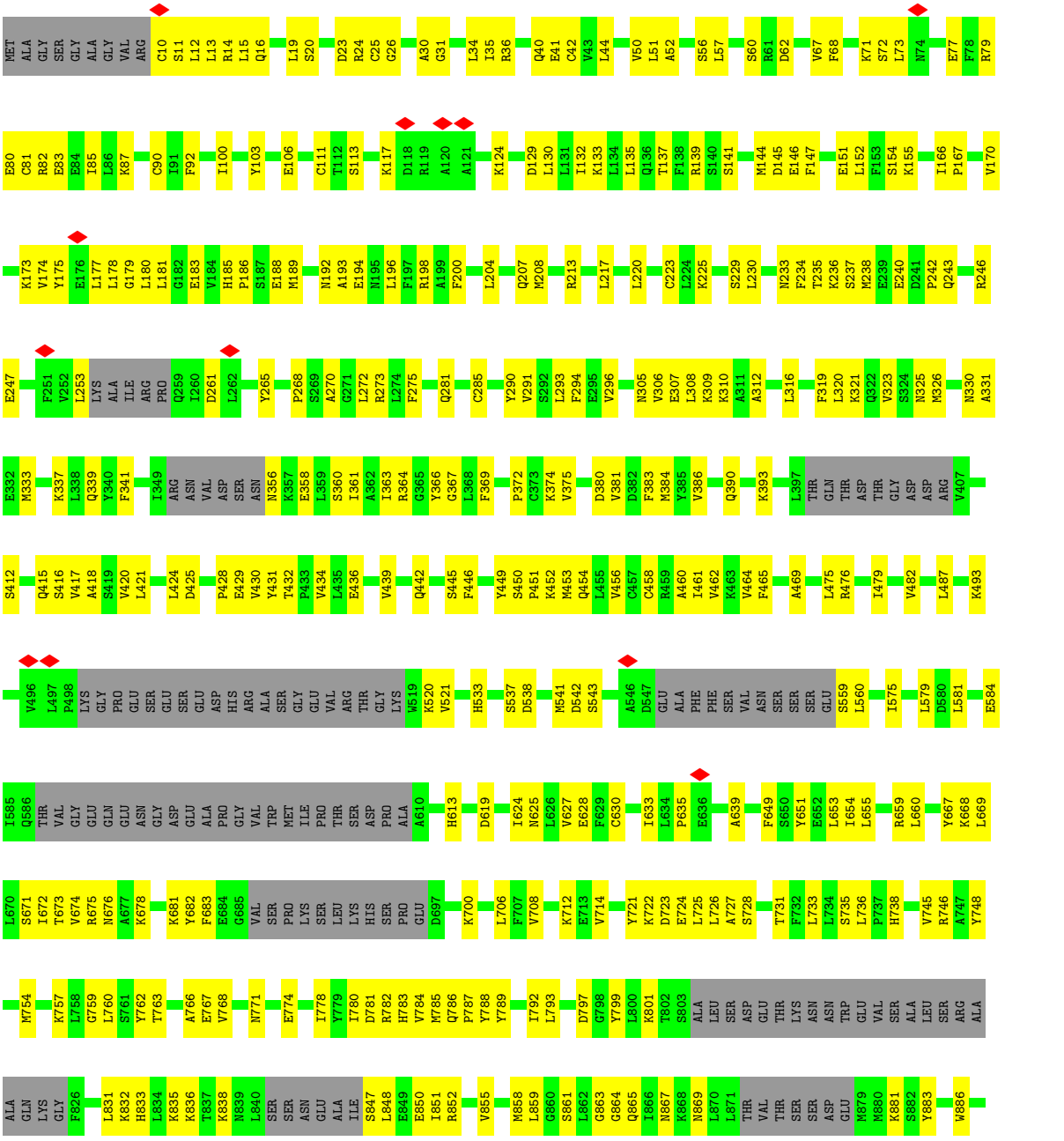
Chain Q:

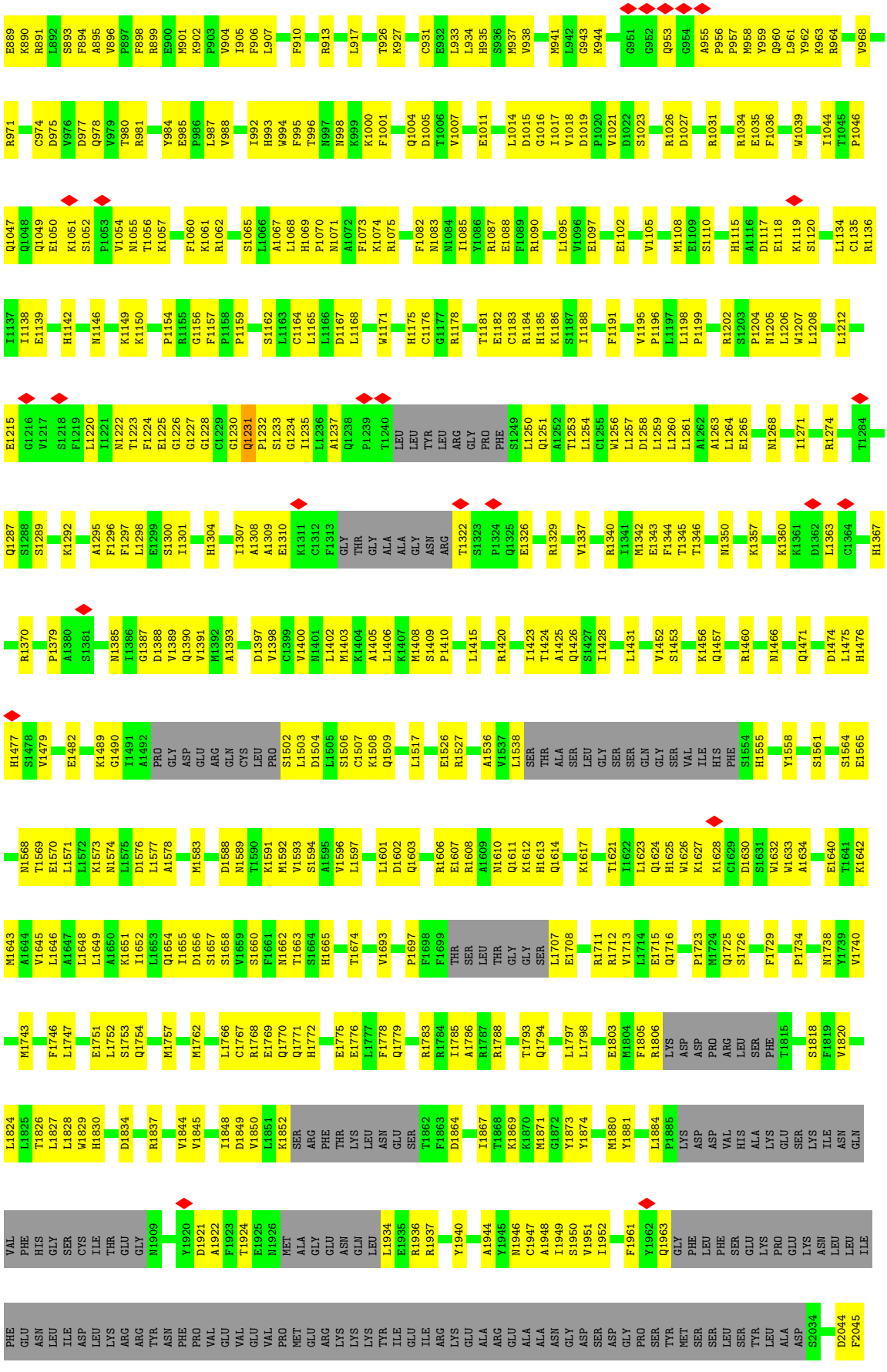




• Molecule 5: DNA-dependent protein kinase catalytic subunit

Chain S:

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R971 C974 D975 V976 D977 Q978 V979 T980 R981 Y984 E985 P986 L987 V988 I992 H993 W994 F995 T996 N997 N998 K999 K1000 F1001 Q1004 D1005 T1006 V1007 E1011 L1014 D1015 G1016 I1017 V1018 D1019 P1020 V1021 D1022 S1023 R1026 D1027 R1031 R1034 E1035 F1036 W1039 I1044 T1045 P1046
Q1047 Q1048 Q1049 E1050 K1051 S1052 P1053 V1054 N1055 T1056 K1057 F1060 K1061 R1062 S1065 L1066 A1067 L1068 H1069 P1070 N1071 A1072 F1073 K1074 R1075 F1082 N1083 N1084 I1085 Y1086 R1087 E1088 F1089 R1090 L1095 V1096 E1097 E1102 V1105 M1108 E1109 S1110 H1115 A1116 D1117 E1118 K1119 S1120 L1134 C1135 R1136
I1137 I1138 E1139 H1142 N1146 K1149 K1150 P1154 R1155 G1156 F1157 P1158 P1159 S1162 L1163 C1164 L1165 L1166 D1167 L1168 W1171 H1175 C1176 G1177 R1178 T1181 E1182 C1183 R1184 H1185 K1186 S1187 I1188 F1191 V1195 P1196 L1197 L1198 P1199 R1202 S1203 P1204 N1205 L1206 W1207 L1208 L1212
E1215 G1216 V1217 S1218 F1219 L1220 I1221 N1222 T1223 F1224 E1225 G1226 G1227 G1228 C1229 G1230 Q1231 P1232 S1233 G1234 I1235 L1236 A1237 Q1238 P1239 T1240 LEU LEU TYR LEU ARG GLY PRO PHE S1249 L1250 Q1251 A1252 T1253 L1254 C1255 W1256 L1257 D1258 L1259 L1260 L1261 A1262 A1263 L1264 E1265 N1268 I1271 R1274 T1284
Q1287 S1288 S1289 K1292 A1295 F1296 F1297 L1298 E1299 S1300 I1301 H1304 I1307 A1308 A1309 E1310 K1311 C1312 F1313 GLY THR GLY ALA ALA GLY ASN ARG T1322 S1323 P1324 Q1325 E1326 R1329 V1337 R1340 I1341 M1342 E1343 F1344 T1345 T1346 N1350 K1357 K1360 K1361 D1362 L1363 C1364 H1367
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H1477 S1478 V1479 E1482 K1489 G1490 I1491 A1492 PRO GLY ASP GLU ARG GLN CYS LEU PRO S1502 L1503 D1504 L1505 S1506 C1507 K1508 Q1509 L1517 E1526 R1527 A1536 V1537 L1538 SER THR ALA SER LEU GLY SER SER GLN GLY SER VAL ILE HIS PHE S1554 H1555 Y1558 S1561 S1564 E1565
N1568 T1569 E1570 L1571 L1572 K1573 N1574 L1575 D1576 L1577 A1578 M1583 D1588 N1589 T1590 K1591 M1592 V1593 S1594 A1595 V1596 L1597 L1601 D1602 Q1603 R1606 E1607 R1608 A1609 N1610 Q1611 K1612 H1613 Q1614 K1617 T1621 I1622 L1623 Q1624 H1625 W1626 K1627 K1628 C1629 D1630 S1631 W1632 W1633 A1634 E1640 T1641 K1642
M1643 A1644 V1645 L1646 A1647 L1648 L1649 A1650 K1651 I1652 L1653 Q1654 I1655 D1656 S1657 S1658 V1659 S1660 F1661 N1662 T1663 S1664 H1665 T1674 V1693 P1697 F1698 F1699 THR SER LEU THR GLY GLY SER L1707 E1708 R1711 R1712 V1713 L1714 E1715 Q1716 P1723 M1724 Q1725 S1726 F1729 P1734 N1738 Y1739 V1740
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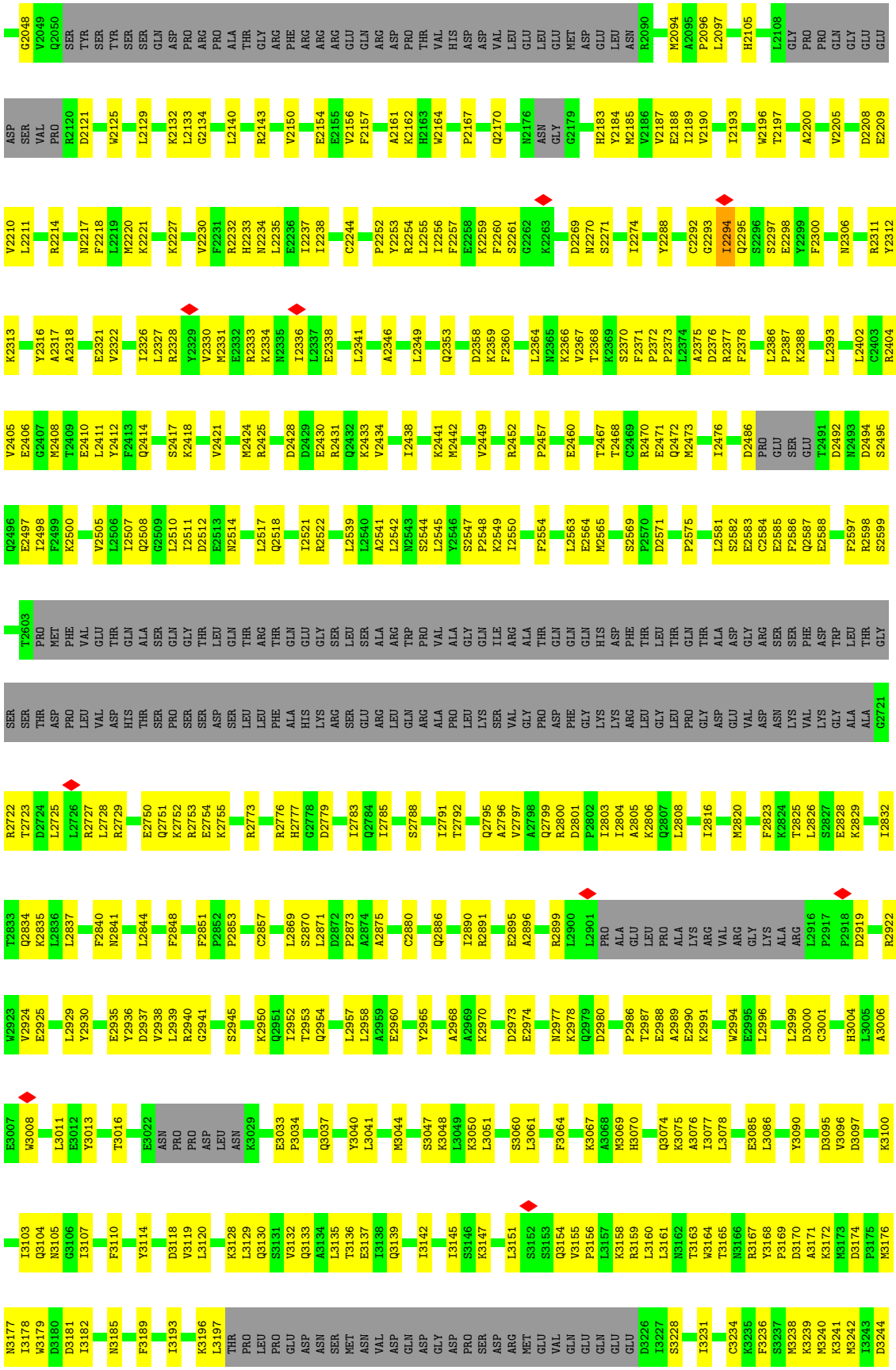
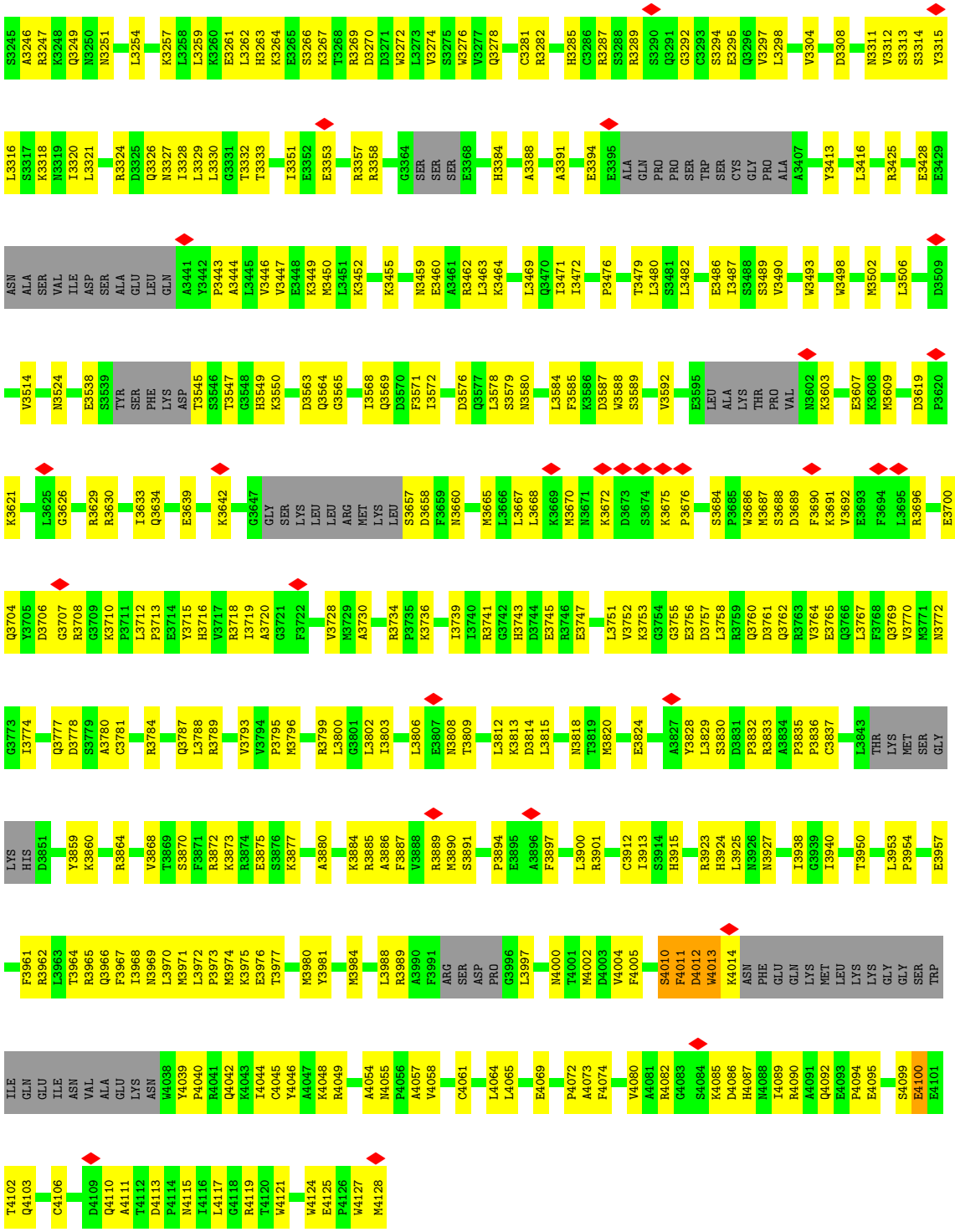
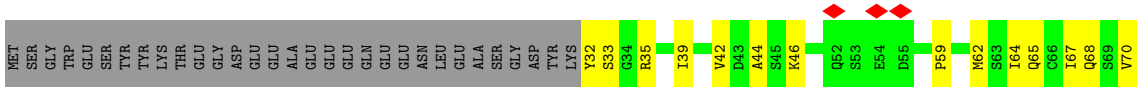
L1824 L1825 T1826 L1827 L1828 W1829 H1830 D1834 R1837 V1844 V1845 I1848 D1849 V1850 L1851 K1852 SER ARG PHE THR LYS LEU ASN GLU SER T1862 F1863 D1864 I1867 T1868 K1869 K1870 M1871 G1872 Y1873 Y1874 M1880 Y1881 L1884 P1885 LYS ASP ASP VAL HIS ALA LYS GLU SER LYS ILE ASN GLN
VAL PHE HIS GLY SER CYS ILE THR GLU GLY N1909 Y1920 D1921 A1922 F1923 T1924 E1925 N1926 MET ALA GLY GLU ASN GLN LEU L1934 E1935 R1936 R1937 Y1940 A1944 Y1945 N1946 C1947 A1948 I1949 S1950 V1951 I1952 F1961 Y1962 Q1963 GLY PHE LEU PHE SER GLU LYS PRO GLU LYS ASN LEU LEU ILE
PHE GLU ASN LEU ILE ASP LEU LYS ARG ARG TYR ASN PHE PRO VAL GLU VAL VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP S2034 D2044 F2045

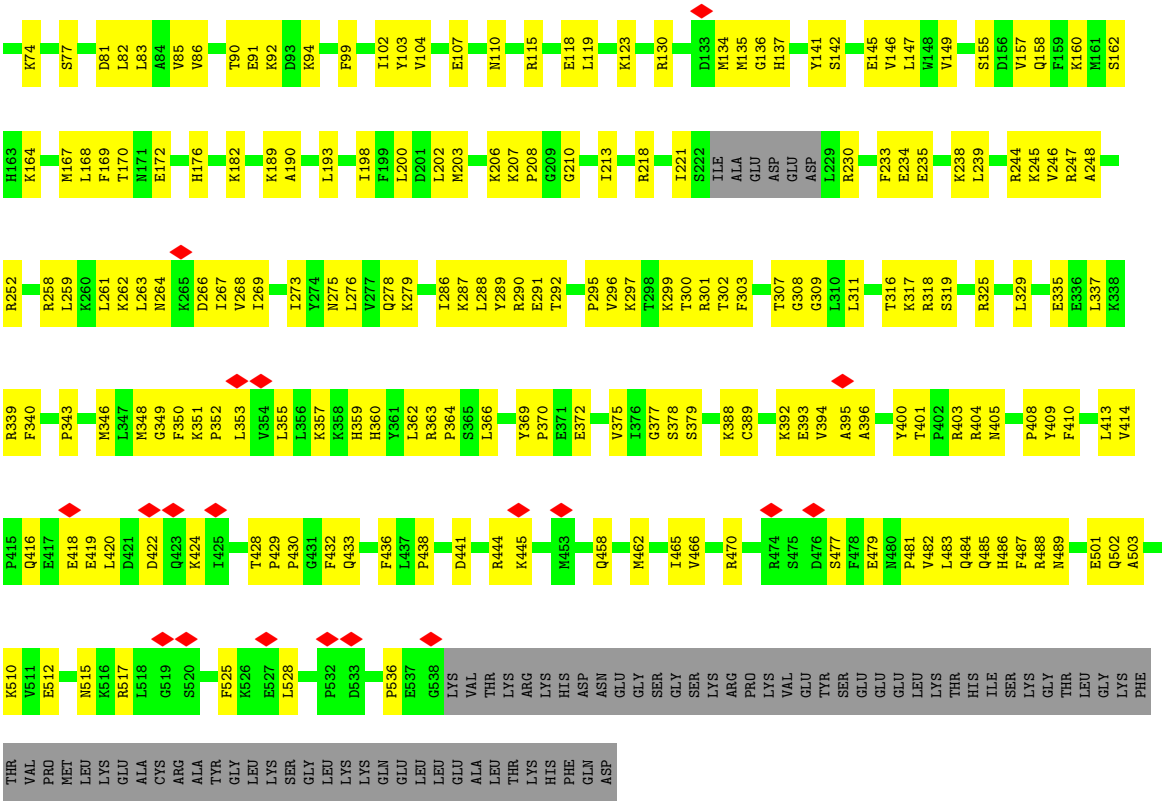




• Molecule 6: X-ray repair cross-complementing protein 6

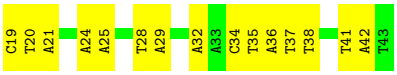
Chain T:





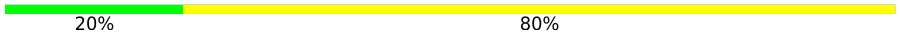
• Molecule 7: DNA

Chain i:



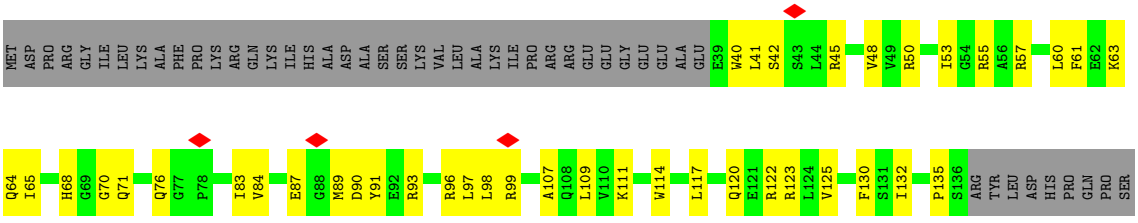
• Molecule 8: DNA

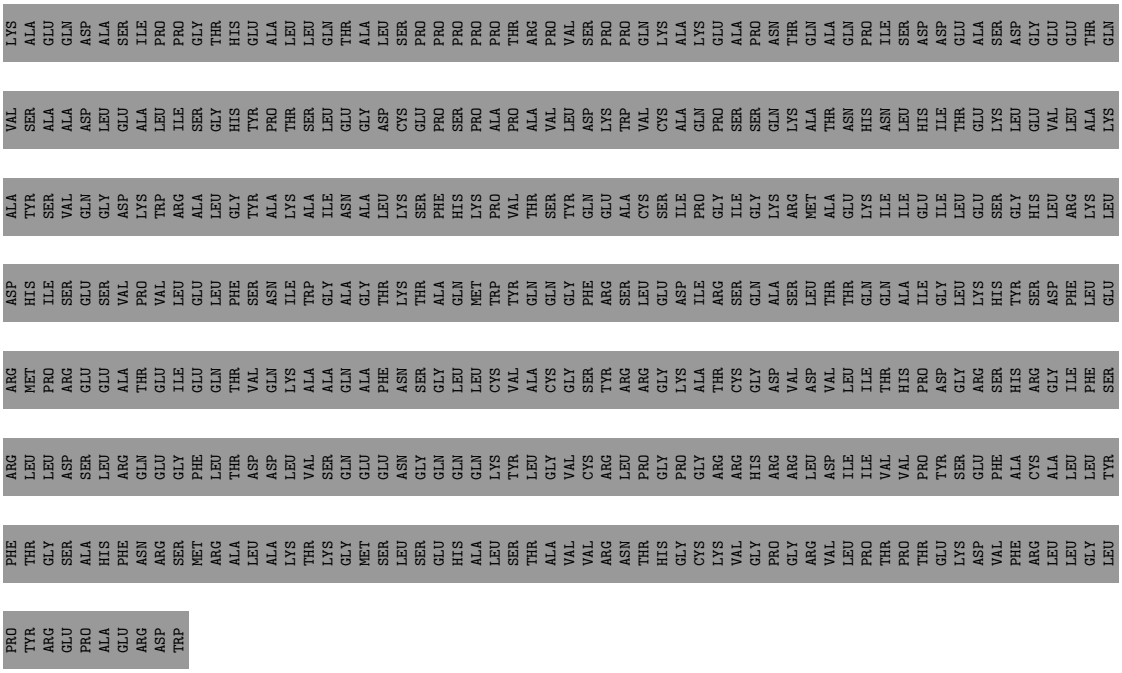
Chain j:



• Molecule 9: DNA polymerase lambda

Chain A:




LYS ALA GLU GLN ASP ALA SER ILE PRO PRO GLY THR HIS GLU ALA LEU LEU GLN THR ALA LEU SER PRO PRO PRO PRO THR ARG PRO VAL SER PRO PRO GLN LYS ALA LYS GLU ALA PRO ASN THR GLN ALA GLN PRO ILE SER ASP ASP GLU ALA SER ASP GLY GLU GLU THR GLN
VAL SER ALA ALA ASP LEU GLU ALA LEU ILE SER GLY HIS TYR PRO THR SER LEU GLU GLY HIS TYR PRO ALA PRO ALA VAL LEU ASP LYS TRP VAL CYS ALA GLN PRO SER SER GLN LYS ALA THR ASN HIS ASN LEU HIS ILE THR GLU LYS LEU GLU VAL LEU ALA LYS
ALA TYR SER VAL GLN GLY ASP LYS TRP ARG ALA LEU GLY TYR ALA LYS ALA ILE ASN ALA LEU LYS SER PHE HIS LYS PRO VAL THR SER TYR GLN GLU ALA CYS SER ILE PRO GLY ILE GLY LYS ARG MET ALA GLU LYS ILE ILE GLU ILE LEU GLU SER GLY HIS LEU ARG LYS LEU
ASP HIS ILE SER GLU SER VAL PRO VAL LEU GLU GLU LEU PHE SER ASN ILE TRP GLY ALA GLY THR LYS THR ALA GLN MET TRP TYR GLN GLN GLY PHE ARG SER LEU GLU ASP ILE ARG SER GLN ALA SER LEU THR THR GLN GLN ALA ILE GLY LEU LYS HIS TYR SER ASP PHE LEU GLU
ARG MET PRO ARG GLU GLU ILE GLU GLN THR VAL GLN LYS ALA ALA GLN ALA PHE ASN SER GLY LEU LEU CYS VAL ALA CYS GLY SER TYR ARG ARG GLY LYS ALA THR CYS GLY ASP VAL ASP VAL LEU ILE THR HIS PRO ASP GLY ARG SER HIS ARG GLY ILE PHE SER
ARG LEU LEU ASP SER LEU ARG GLN GLU GLY PHE LEU THR ASP ASP LEU VAL SER GLN GLU GLU ASN GLY GLN GLN GLN LYS TYR LEU GLY VAL CYS ARG LEU PRO GLY PRO GLY ARG ARG HIS ARG ARG LEU ASP ILE ILE VAL VAL PRO TYR SER GLU PHE ALA CYS ALA LEU LEU TYR
PHE THR GLY SER ALA HIS PHE ASN ARG SER MET ARG ALA LEU ALA LYS THR LYS GLY MET SER LEU SER GLU HIS ALA LEU SER THR ALA VAL VAL ARG ASN THR HIS GLY CYS LYS VAL GLY PRO GLY ARG VAL LEU PRO THR PRO THR GLU LYS ASP VAL PHE ARG LEU LEU GLY LEU
PRO TYR ARG GLU PRO ALA GLU ARG ASP TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14964	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 ($e^-/Å^2$)	51.96	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.211	Depositor
Map size (Å)	417.28, 417.28, 417.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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	E	0.14	0/1997	0.40	0/2695
2	L	0.14	0/5182	0.36	0/6990
3	M	0.17	0/164	0.44	0/220
4	P	0.11	0/485	0.34	0/647
4	Q	0.13	0/480	0.35	0/640
5	S	0.19	0/28315	0.48	0/38300
6	T	0.17	0/4079	0.41	0/5499
7	i	0.28	0/572	0.50	0/879
8	j	0.32	0/575	0.58	0/888
9	A	0.16	0/780	0.44	0/1057
All	All	0.18	0/42629	0.46	0/57815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1956	0	1905	76	0
2	L	5084	0	5080	206	0
3	M	160	0	148	6	0
4	P	480	0	501	27	0
4	Q	475	0	492	25	0
5	S	27773	0	27732	1057	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	4001	0	4050	188	0
7	i	510	0	285	18	0
8	j	514	0	290	20	0
9	A	764	0	785	35	0
All	All	41717	0	41268	1564	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 19.

All (1564) 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)
5:S:2806:LYS:HG3	5:S:2857:CYS:HB3	1.59	0.84
1:E:757:GLU:HB3	1:E:763:ASP:H	1.42	0.83
5:S:835:LYS:HA	5:S:838:LYS:HG2	1.62	0.81
5:S:1300:SER:HA	5:S:1304:HIS:HB2	1.65	0.79
5:S:1820:VAL:HA	5:S:1824:LEU:HD23	1.64	0.79
5:S:3913:ILE:HG21	5:S:3984:MET:HG2	1.64	0.78
5:S:111:CYS:HB2	5:S:130:LEU:HD11	1.64	0.77
5:S:2844:LEU:HD22	5:S:2875:ALA:HB1	1.66	0.77
5:S:3472:ILE:HD13	5:S:3479:THR:HB	1.67	0.76
5:S:3988:LEU:HD23	5:S:4100:GLU:HA	1.68	0.75
5:S:1307:ILE:HG13	5:S:1309:ALA:H	1.50	0.74
5:S:2256:ILE:HA	5:S:2259:LYS:HG2	1.68	0.74
5:S:3974:MET:HE2	5:S:3980:MET:HE1	1.69	0.73
5:S:667:TYR:HB2	5:S:728:SER:HB2	1.69	0.73
2:L:380:LEU:HD23	6:T:462:MET:HG3	1.71	0.73
5:S:931:CYS:HG	5:S:984:TYR:HH	1.35	0.72
2:L:628:GLU:HB2	2:L:631:TYR:HB3	1.72	0.72
5:S:487:LEU:HD11	5:S:575:ILE:HD13	1.71	0.72
6:T:273:ILE:HD11	6:T:366:LEU:HB3	1.71	0.72
5:S:913:ARG:HH11	5:S:2804:ILE:HG23	1.55	0.72
5:S:1536:ALA:O	5:S:1555:HIS:ND1	2.23	0.72
5:S:2217:ASN:HA	5:S:2220:MET:HE2	1.72	0.72
5:S:1235:ILE:HG13	5:S:1292:LYS:HE2	1.73	0.71
9:A:87:GLU:HA	9:A:111:LYS:HG2	1.73	0.71
5:S:2563:LEU:HD23	5:S:2795:GLN:HB3	1.70	0.71
1:E:663:GLU:HB3	1:E:697:THR:HA	1.72	0.70
5:S:2507:ILE:HA	5:S:2510:LEU:HD23	1.73	0.70
5:S:3064:PHE:HA	5:S:3067:LYS:HE3	1.72	0.70
2:L:462:SER:HA	6:T:350:PHE:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:656:ASN:HB3	2:L:688:LYS:HE3	1.72	0.70
5:S:738:HIS:HB2	5:S:780:ILE:HD11	1.73	0.70
5:S:1198:LEU:O	5:S:1202:ARG:NH2	2.24	0.70
5:S:25:CYS:SG	5:S:26:GLY:N	2.64	0.69
7:i:41:DT:H2"	7:i:42:DA:C8	2.27	0.69
5:S:1070:PRO:O	5:S:1075:ARG:NH2	2.26	0.69
5:S:1828:LEU:HD11	5:S:1880:MET:HB3	1.74	0.69
5:S:2965:TYR:HB3	5:S:3001:CYS:HB2	1.75	0.69
5:S:79:ARG:HA	5:S:82:ARG:HD2	1.74	0.69
5:S:1226:GLY:HA2	5:S:1259:LEU:HG	1.74	0.69
5:S:2405:VAL:HA	5:S:2441:LYS:HE3	1.73	0.69
5:S:3160:LEU:O	5:S:3167:ARG:NH2	2.26	0.69
6:T:351:LYS:HD2	6:T:355:LEU:HD13	1.75	0.69
5:S:2753:ARG:NH2	8:j:14:DT:O4	2.26	0.68
3:M:195:PRO:HG3	6:T:244:ARG:HE	1.58	0.68
1:E:813:PHE:H	1:E:848:HIS:HB2	1.58	0.68
6:T:458:GLN:HE21	6:T:528:LEU:HB3	1.59	0.68
5:S:917:LEU:O	5:S:927:LYS:NZ	2.26	0.68
2:L:497:ARG:NH2	2:L:503:GLU:O	2.26	0.67
5:S:3444:ALA:HB1	5:S:3482:LEU:HD12	1.76	0.67
5:S:2795:GLN:O	5:S:2799:GLN:NE2	2.27	0.67
5:S:170:VAL:O	5:S:173:LYS:NZ	2.28	0.67
5:S:2750:GLU:HA	5:S:2753:ARG:HD2	1.77	0.67
5:S:3161:LEU:HA	5:S:3167:ARG:HH12	1.58	0.67
5:S:757:LYS:HA	5:S:760:LEU:HD12	1.75	0.67
5:S:1934:LEU:HD13	5:S:1937:ARG:HH12	1.60	0.67
5:S:3130:GLN:NE2	5:S:3174:ASP:OD1	2.28	0.67
5:S:4039:TYR:HD2	5:S:4042:GLN:HG2	1.60	0.67
5:S:1178:ARG:NH2	5:S:1183:CYS:SG	2.63	0.67
5:S:1097:GLU:HG3	5:S:1149:LYS:HE2	1.77	0.67
5:S:1471:GLN:NE2	5:S:1475:LEU:O	2.28	0.67
5:S:722:LYS:NZ	5:S:1027:ASP:OD2	2.27	0.66
7:i:41:DT:H3	8:j:17:DT:H3	1.43	0.66
5:S:4082:ARG:NH2	5:S:4092:GLN:OE1	2.28	0.66
1:E:846:ARG:HB3	4:Q:166:VAL:HG11	1.78	0.66
6:T:482:VAL:HG12	6:T:486:HIS:HE1	1.61	0.66
1:E:673:GLN:HG3	1:E:678:LEU:HD21	1.78	0.66
1:E:692:ASN:ND2	6:T:290:ARG:O	2.25	0.66
5:S:1156:GLY:HA3	5:S:1171:TRP:HE1	1.59	0.66
2:L:20:MET:HB2	2:L:30:PRO:HB2	1.78	0.66
5:S:412:SER:O	5:S:415:GLN:NE2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:449:TYR:O	5:S:454:GLN:NE2	2.29	0.65
5:S:3274:VAL:HG13	5:S:3278:GLN:HE22	1.60	0.65
5:S:2328:ARG:HH21	5:S:2371:PHE:HA	1.60	0.65
2:L:249:CYS:SG	2:L:250:ARG:N	2.70	0.65
5:S:995:PHE:HD1	5:S:1000:LYS:HZ1	1.43	0.65
6:T:170:THR:HG22	6:T:172:GLU:H	1.61	0.65
5:S:2220:MET:HE1	5:S:2252:PRO:HG3	1.77	0.65
5:S:3885:ARG:HB3	5:S:3889:ARG:HH21	1.60	0.65
2:L:310:ILE:HD11	6:T:287:LYS:HD3	1.78	0.65
5:S:3884:LYS:NZ	5:S:3969:ASN:OD1	2.29	0.65
5:S:3239:LYS:NZ	5:S:3261:GLU:OE2	2.29	0.65
2:L:85:LEU:HD12	2:L:86:PRO:HD2	1.77	0.65
4:Q:166:VAL:HA	4:Q:169:LYS:HD2	1.77	0.65
5:S:1871:MET:HE1	5:S:1940:TYR:HA	1.78	0.65
5:S:992:ILE:HG23	5:S:1036:PHE:HD1	1.62	0.65
5:S:3006:ALA:O	5:S:3050:LYS:NZ	2.30	0.65
6:T:441:ASP:O	6:T:444:ARG:NH2	2.29	0.65
5:S:23:ASP:OD1	5:S:24:ARG:NH1	2.27	0.65
5:S:584:GLU:N	5:S:613:HIS:O	2.29	0.65
5:S:1504:ASP:H	5:S:1507:CYS:HB2	1.61	0.65
5:S:2349:LEU:O	5:S:2353:GLN:HB3	1.97	0.65
5:S:3730:ALA:HA	5:S:3734:ARG:HA	1.78	0.65
5:S:1783:ARG:NH1	5:S:1826:THR:O	2.29	0.64
5:S:2260:PHE:O	5:S:2306:ASN:ND2	2.29	0.64
6:T:485:GLN:O	6:T:489:ASN:ND2	2.30	0.64
5:S:1231:GLN:NE2	5:S:1287:GLN:OE1	2.30	0.64
5:S:1946:ASN:HA	5:S:1949:ILE:HD12	1.79	0.64
1:E:690:VAL:HG23	6:T:291:GLU:HG2	1.78	0.64
5:S:225:LYS:HZ1	5:S:273:ARG:HE	1.45	0.64
9:A:48:VAL:HA	9:A:84:VAL:HB	1.78	0.64
3:M:183:GLU:HA	3:M:191:LYS:HA	1.78	0.64
5:S:1178:ARG:H	5:S:1184:ARG:HD3	1.62	0.64
5:S:2327:LEU:O	5:S:2333:ARG:NH2	2.30	0.64
6:T:91:GLU:H	6:T:136:GLY:HA3	1.62	0.64
5:S:306:VAL:HA	5:S:309:LYS:HE2	1.79	0.64
2:L:466:LYS:NZ	2:L:470:THR:O	2.31	0.64
5:S:4055:ASN:HD22	5:S:4058:VAL:HG23	1.63	0.63
5:S:380:ASP:HB3	5:S:384:MET:HE1	1.78	0.63
5:S:2188:GLU:OE2	5:S:2729:ARG:NH2	2.31	0.63
5:S:913:ARG:NH1	5:S:2804:ILE:HG23	2.13	0.63
5:S:1630:ASP:HB3	5:S:1633:TRP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1171:TRP:O	5:S:1175:HIS:ND1	2.31	0.63
5:S:2449:VAL:HA	5:S:2452:ARG:HE	1.63	0.63
5:S:2837:LEU:O	5:S:2841:ASN:ND2	2.31	0.63
5:S:3657:SER:N	5:S:3660:ASN:OD1	2.31	0.63
5:S:3741:ARG:HH11	5:S:3747:GLU:HB2	1.64	0.63
5:S:253:LEU:HD21	5:S:268:PRO:HA	1.80	0.63
9:A:45:ARG:HH21	9:A:70:GLY:HA2	1.63	0.63
5:S:13:LEU:HD21	5:S:3069:MET:HB3	1.81	0.63
5:S:767:GLU:O	5:S:771:ASN:ND2	2.32	0.63
5:S:3859:TYR:O	5:S:4119:ARG:NH2	2.32	0.63
5:S:3244:ASP:OD1	5:S:3247:ARG:NH2	2.31	0.63
6:T:81:ASP:O	6:T:110:ASN:ND2	2.31	0.63
2:L:465:LYS:H	2:L:474:GLU:HG2	1.63	0.63
6:T:396:ALA:HB3	6:T:413:LEU:HB2	1.81	0.63
2:L:271:ARG:HE	2:L:272:VAL:H	1.46	0.63
5:S:907:LEU:HD13	5:S:937:MET:HG2	1.81	0.63
6:T:287:LYS:NZ	6:T:296:VAL:O	2.30	0.63
5:S:1707:LEU:O	5:S:1711:ARG:NH1	2.32	0.62
5:S:2233:HIS:NE2	5:S:2727:ARG:O	2.30	0.62
5:S:2328:ARG:O	5:S:2333:ARG:NE	2.32	0.62
1:E:654:LYS:N	1:E:660:GLU:OE2	2.33	0.62
5:S:958:MET:O	5:S:962:TYR:N	2.29	0.62
5:S:1227:GLY:O	5:S:1292:LYS:NZ	2.32	0.62
6:T:65:GLN:HB3	6:T:123:LYS:HD3	1.81	0.62
1:E:783:ASN:HA	4:Q:179:ARG:HH21	1.64	0.62
3:M:193:LYS:O	6:T:244:ARG:NH2	2.32	0.62
5:S:3997:LEU:O	5:S:4000:ASN:ND2	2.32	0.62
6:T:164:LYS:HG3	6:T:198:ILE:HA	1.81	0.62
9:A:96:ARG:O	9:A:99:ARG:NH1	2.32	0.62
4:P:176:LEU:HD11	4:Q:173:GLU:HG3	1.80	0.62
9:A:114:TRP:NE1	9:A:125:VAL:O	2.33	0.62
6:T:363:ARG:NH1	8:j:28:DA:OP1	2.33	0.62
5:S:10:CYS:SG	5:S:11:SER:N	2.72	0.62
5:S:1031:ARG:HH22	5:S:1034:ARG:HH11	1.47	0.62
5:S:193:ALA:HA	5:S:196:LEU:HD12	1.81	0.62
5:S:797:ASP:O	5:S:801:LYS:NZ	2.32	0.62
6:T:168:LEU:HD11	6:T:202:LEU:HG	1.81	0.62
2:L:44:ARG:HH12	2:L:488:GLN:HA	1.63	0.62
5:S:2218:PHE:HA	5:S:2221:LYS:HE3	1.82	0.62
5:S:2725:LEU:HD13	5:S:2728:LEU:HD21	1.82	0.62
2:L:146:GLN:HG3	2:L:149:ILE:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3278:GLN:NE2	5:S:3326:GLN:HE21	1.97	0.61
2:L:377:LEU:HD23	2:L:380:LEU:HD12	1.81	0.61
5:S:217:LEU:HA	5:S:220:LEU:HD13	1.82	0.61
5:S:1360:LYS:HZ3	5:S:1363:LEU:HB3	1.64	0.61
5:S:174:VAL:HA	5:S:177:LEU:HB2	1.83	0.61
6:T:94:LYS:H	6:T:103:TYR:HA	1.64	0.61
6:T:167:MET:HE2	6:T:203:MET:HB2	1.82	0.61
5:S:67:VAL:HA	5:S:71:LYS:HD3	1.83	0.61
5:S:799:TYR:O	5:S:852:ARG:NH1	2.32	0.61
5:S:890:LYS:HD2	5:S:906:PHE:HB3	1.82	0.61
5:S:3962:ARG:NH1	5:S:4124:TRP:O	2.33	0.61
1:E:778:PHE:O	4:Q:179:ARG:NH1	2.33	0.61
5:S:2094:MET:HB2	5:S:2097:LEU:HD12	1.83	0.61
5:S:2896:ALA:HB1	5:S:2922:ARG:HH21	1.66	0.61
5:S:3974:MET:HG3	5:S:3976:GLU:H	1.66	0.61
5:S:3880:ALA:O	5:S:3885:ARG:NH2	2.34	0.61
5:S:2473:MET:HA	5:S:2476:ILE:HD12	1.82	0.61
9:A:50:ARG:NH1	9:A:53:ILE:O	2.34	0.61
1:E:697:THR:O	1:E:718:HIS:NE2	2.31	0.60
2:L:184:ARG:NH1	2:L:514:ASN:O	2.34	0.60
5:S:2587:GLN:O	5:S:2777:HIS:N	2.28	0.60
5:S:3728:VAL:HA	5:S:3736:LYS:HG3	1.82	0.60
5:S:4046:TYR:HA	5:S:4049:ARG:HH11	1.65	0.60
5:S:867:ASN:HB2	5:S:3129:LEU:HD21	1.83	0.60
6:T:488:ARG:HE	6:T:501:GLU:HG3	1.66	0.60
2:L:269:GLN:NE2	2:L:359:ASN:O	2.26	0.60
5:S:1326:GLU:O	5:S:1329:ARG:NH1	2.33	0.60
5:S:2588:GLU:HA	5:S:2776:ARG:HA	1.81	0.60
5:S:3154:GLN:O	5:S:3159:ARG:NH2	2.35	0.60
5:S:3789:ARG:HH12	5:S:3938:ILE:HB	1.67	0.60
6:T:482:VAL:O	6:T:486:HIS:ND1	2.35	0.60
5:S:984:TYR:HA	5:S:987:LEU:HD12	1.84	0.60
5:S:2547:SER:H	5:S:2554:PHE:HE2	1.48	0.60
5:S:3686:TRP:HB2	5:S:3696:ARG:HH22	1.67	0.60
5:S:3924:HIS:N	5:S:3927:ASN:OD1	2.35	0.60
2:L:541:GLU:HG3	6:T:375:VAL:HG13	1.84	0.60
5:S:678:LYS:NZ	5:S:735:SER:O	2.35	0.60
5:S:1881:TYR:HB2	5:S:1950:SER:HB2	1.84	0.60
5:S:2511:ILE:HD11	5:S:2550:ILE:HG23	1.84	0.60
5:S:14:ARG:HH12	5:S:3070:HIS:HA	1.66	0.60
5:S:881:LYS:NZ	5:S:883:TYR:O	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1322:THR:O	5:S:1326:GLU:N	2.34	0.60
5:S:1621:THR:O	5:S:1625:HIS:ND1	2.33	0.60
5:S:2358:ASP:OD1	5:S:2359:LYS:N	2.35	0.60
5:S:2467:THR:HG22	5:S:2470:ARG:HH21	1.65	0.60
5:S:4094:PRO:HB3	5:S:4103:GLN:HG2	1.82	0.60
2:L:477:PHE:CZ	2:L:519:PRO:HD2	2.37	0.60
5:S:538:ASP:HA	5:S:541:MET:HG3	1.84	0.60
5:S:3772:ASN:ND2	5:S:3788:LEU:O	2.34	0.60
2:L:510:GLN:HA	2:L:513:TRP:HD1	1.67	0.60
2:L:628:GLU:O	2:L:632:PHE:N	2.30	0.60
5:S:393:LYS:HD2	5:S:434:VAL:HG11	1.83	0.60
5:S:3690:PHE:O	5:S:3696:ARG:NH1	2.35	0.60
5:S:1961:PHE:HB2	5:S:2125:TRP:CZ2	2.36	0.59
5:S:40:GLN:NE2	5:S:2425:ARG:O	2.36	0.59
6:T:213:ILE:HG13	6:T:218:ARG:HH21	1.67	0.59
2:L:659:LEU:HD23	2:L:662:LEU:HD21	1.84	0.59
5:S:895:ALA:HA	5:S:904:VAL:HA	1.85	0.59
5:S:1232:PRO:HA	5:S:1235:ILE:HD12	1.85	0.59
5:S:2134:GLY:HA2	5:S:2167:PRO:HB3	1.83	0.59
4:P:150:ARG:NH1	4:P:154:ASP:OD2	2.35	0.59
5:S:1783:ARG:HH12	5:S:1829:TRP:HB2	1.68	0.59
5:S:2388:LYS:NZ	6:T:157:VAL:O	2.35	0.59
1:E:720:VAL:HB	1:E:745:HIS:H	1.67	0.59
1:E:813:PHE:N	1:E:848:HIS:HB2	2.17	0.59
2:L:198:THR:HG23	2:L:201:GLN:HE21	1.68	0.59
5:S:1611:GLN:NE2	5:S:1614:GLN:OE1	2.36	0.59
5:S:1634:ALA:O	5:S:1642:LYS:NZ	2.34	0.59
5:S:2973:ASP:O	5:S:2977:ASN:ND2	2.34	0.59
1:E:704:SER:O	1:E:708:ARG:NH2	2.36	0.59
2:L:463:LEU:HG	6:T:350:PHE:H	1.67	0.59
6:T:363:ARG:HH22	8:j:27:DT:H5"	1.67	0.59
2:L:359:ASN:OD1	2:L:360:GLN:N	2.35	0.59
7:i:41:DT:H2"	7:i:42:DA:H8	1.68	0.59
1:E:674:PRO:HB2	1:E:676:PRO:HD2	1.85	0.59
6:T:351:LYS:O	6:T:395:ALA:N	2.35	0.59
1:E:721:VAL:HG22	1:E:743:MET:HE1	1.84	0.58
5:S:330:ASN:HB3	5:S:333:MET:HE3	1.85	0.58
5:S:859:LEU:O	5:S:867:ASN:ND2	2.36	0.58
5:S:1222:ASN:OD1	5:S:1223:THR:N	2.34	0.58
5:S:1231:GLN:O	5:S:1292:LYS:NZ	2.33	0.58
5:S:3569:GLN:HA	5:S:3572:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:268:LEU:O	6:T:444:ARG:NH1	2.36	0.58
5:S:1922:ALA:HB2	5:S:1944:ALA:HB3	1.85	0.58
6:T:203:MET:HE1	6:T:238:LYS:H	1.68	0.58
6:T:363:ARG:HB3	6:T:436:PHE:CD2	2.38	0.58
2:L:412:ILE:HA	2:L:417:GLU:HA	1.85	0.58
5:S:651:TYR:HE1	5:S:1388:ASP:HB3	1.69	0.58
5:S:1663:THR:OG1	5:S:1665:HIS:NE2	2.37	0.58
5:S:2507:ILE:HD12	5:S:2545:LEU:HB2	1.84	0.58
8:j:30:DT:H2'	8:j:31:DT:H71	1.86	0.58
2:L:647:ILE:HA	2:L:652:GLU:HB3	1.84	0.58
5:S:2880:CYS:HB3	5:S:2886:GLN:HA	1.85	0.58
5:S:3313:SER:HB3	5:S:3316:LEU:HA	1.85	0.58
6:T:357:LYS:HB2	6:T:360:HIS:CD2	2.38	0.58
1:E:682:ILE:HG13	1:E:730:PHE:HZ	1.68	0.58
1:E:728:GLU:OE1	1:E:741:ARG:NH2	2.37	0.58
5:S:1420:ARG:NH2	5:S:1466:ASN:O	2.36	0.58
5:S:3912:CYS:HA	5:S:3915:HIS:CD2	2.38	0.58
6:T:418:GLU:HB2	6:T:430:PRO:HB3	1.85	0.58
2:L:96:SER:O	2:L:99:GLN:NE2	2.37	0.58
2:L:324:SER:OG	2:L:325:LYS:N	2.36	0.58
5:S:3545:THR:OG1	5:S:3549:HIS:N	2.37	0.58
6:T:141:TYR:O	6:T:182:LYS:NZ	2.37	0.58
2:L:423:GLN:NE2	2:L:424:LEU:O	2.37	0.58
5:S:1117:ASP:OD1	5:S:1118:GLU:N	2.37	0.58
5:S:3870:SER:OG	5:S:4117:LEU:O	2.21	0.58
5:S:4012:ASP:O	5:S:4014:LYS:N	2.36	0.58
1:E:774:LEU:HD22	4:P:181:ILE:HG23	1.85	0.58
5:S:649:PHE:O	5:S:653:LEU:HG	2.04	0.58
5:S:782:ARG:HG2	5:S:786:GLN:HE22	1.68	0.58
5:S:1747:LEU:HD21	5:S:1778:PHE:HD1	1.69	0.58
5:S:1000:LYS:NZ	5:S:1005:ASP:OD1	2.37	0.58
5:S:2161:ALA:HA	5:S:2164:TRP:HB2	1.85	0.58
5:S:2269:ASP:OD1	5:S:2270:ASN:N	2.37	0.58
6:T:46:LYS:NZ	6:T:137:HIS:O	2.37	0.58
2:L:640:ARG:NH2	2:L:684:THR:OG1	2.34	0.57
5:S:891:ARG:NH1	5:S:956:PRO:O	2.36	0.57
5:S:899:ARG:NH1	5:S:2565:MET:O	2.36	0.57
5:S:3155:VAL:HG22	5:S:3158:LYS:HZ1	1.69	0.57
6:T:85:VAL:HG21	6:T:119:LEU:HD11	1.86	0.57
2:L:463:LEU:HD11	6:T:349:GLY:HA3	1.85	0.57
6:T:416:GLN:OE1	6:T:433:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2129:LEU:HD23	5:S:2132:LYS:HZ3	1.69	0.57
5:S:2257:PHE:HA	5:S:2260:PHE:CE2	2.39	0.57
5:S:4082:ARG:HG3	5:S:4089:ILE:HG22	1.85	0.57
2:L:354:ARG:HD3	6:T:433:GLN:HE21	1.70	0.57
2:L:490:LEU:HA	6:T:337:LEU:HD21	1.84	0.57
5:S:2936:TYR:HA	5:S:2939:LEU:HD13	1.86	0.57
9:A:93:ARG:HE	9:A:97:LEU:HG	1.68	0.57
2:L:277:THR:OG1	6:T:319:SER:OG	2.21	0.57
2:L:278:VAL:HG22	6:T:318:ARG:HH21	1.68	0.57
5:S:243:GLN:O	5:S:246:ARG:NH1	2.37	0.57
5:S:321:LYS:NZ	5:S:325:ASN:OD1	2.37	0.57
5:S:1182:GLU:OE2	5:S:1185:HIS:ND1	2.37	0.57
5:S:1389:VAL:HG23	5:S:1391:VAL:HG22	1.86	0.57
5:S:1490:GLY:O	5:S:1502:SER:N	2.37	0.57
5:S:1592:MET:SD	5:S:1592:MET:N	2.77	0.57
5:S:1803:GLU:OE1	5:S:1806:ARG:NH2	2.36	0.57
5:S:682:TYR:O	5:S:700:LYS:NZ	2.32	0.57
5:S:3706:ASP:OD2	5:S:3708:ARG:NH2	2.38	0.57
6:T:176:HIS:HD2	6:T:182:LYS:HD3	1.70	0.57
2:L:497:ARG:HG2	2:L:505:LEU:HD11	1.86	0.57
5:S:1082:PHE:HA	5:S:1085:ILE:HG12	1.87	0.57
5:S:2986:PRO:O	5:S:2991:LYS:NZ	2.38	0.57
6:T:318:ARG:N	6:T:329:LEU:O	2.38	0.57
5:S:2832:ILE:HA	5:S:2835:LYS:HD2	1.85	0.57
1:E:785:ASN:HA	1:E:792:MET:HE1	1.87	0.57
2:L:81:ARG:NH2	2:L:85:LEU:O	2.38	0.57
4:Q:151:LEU:HA	4:Q:154:ASP:HB2	1.87	0.57
5:S:926:THR:HG22	5:S:2800:ARG:HB3	1.87	0.57
5:S:1623:LEU:HD12	5:S:1624:GLN:HG3	1.87	0.57
5:S:3118:ASP:OD1	5:S:3119:VAL:N	2.38	0.57
5:S:3668:LEU:O	5:S:3672:LYS:NZ	2.35	0.57
5:S:3675:LYS:NZ	5:S:3676:PRO:O	2.37	0.57
5:S:579:LEU:HD11	5:S:619:ASP:HB3	1.87	0.57
5:S:1019:ASP:O	5:S:1026:ARG:NH2	2.31	0.57
8:j:29:DG:H2"	8:j:30:DT:H5"	1.87	0.57
2:L:44:ARG:HH22	2:L:488:GLN:HB2	1.71	0.56
5:S:913:ARG:CZ	5:S:2803:ILE:HB	2.35	0.56
6:T:502:GLN:NE2	6:T:503:ALA:O	2.38	0.56
8:j:18:DA:H2"	8:j:19:DA:C8	2.40	0.56
1:E:814:ARG:N	1:E:850:ALA:H	2.04	0.56
2:L:270:GLU:OE1	6:T:444:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1182:GLU:HG3	5:S:1186:LYS:HZ3	1.70	0.56
5:S:1611:GLN:OE1	5:S:1613:HIS:ND1	2.38	0.56
5:S:2510:LEU:HA	5:S:2521:ILE:HD12	1.87	0.56
5:S:2954:GLN:HE21	5:S:2958:LEU:HD23	1.69	0.56
5:S:3965:ARG:O	5:S:3969:ASN:ND2	2.38	0.56
8:j:23:DT:H2'	8:j:24:DT:H71	1.86	0.56
2:L:643:ARG:HH11	2:L:659:LEU:HD12	1.70	0.56
4:Q:191:ILE:O	4:Q:195:HIS:ND1	2.29	0.56
5:S:20:SER:O	5:S:24:ARG:NH1	2.38	0.56
5:S:2470:ARG:NH1	5:S:2512:ASP:OD1	2.39	0.56
5:S:3830:SER:O	5:S:3833:ARG:NH1	2.38	0.56
6:T:203:MET:HE2	6:T:239:LEU:HD23	1.88	0.56
6:T:352:PRO:HA	6:T:394:VAL:HA	1.88	0.56
2:L:81:ARG:HD3	2:L:90:LEU:HD11	1.87	0.56
5:S:998:ASN:HA	5:S:1001:PHE:HB2	1.88	0.56
8:j:16:DA:H2"	8:j:17:DT:C5	2.40	0.56
5:S:229:SER:O	5:S:233:ASN:ND2	2.38	0.56
5:S:1864:ASP:HA	5:S:1867:ILE:HD12	1.87	0.56
5:S:3667:LEU:HD12	5:S:3670:MET:HG2	1.88	0.56
5:S:3707:GLY:HA3	5:S:3712:LEU:HD21	1.86	0.56
5:S:520:LYS:NZ	5:S:521:VAL:O	2.39	0.56
5:S:1251:GLN:HA	5:S:1254:LEU:HD12	1.87	0.56
5:S:2197:THR:HG23	5:S:2244:CYS:HB2	1.86	0.56
5:S:3064:PHE:HD1	5:S:3067:LYS:HZ1	1.54	0.56
5:S:4012:ASP:O	5:S:4013:TRP:C	2.49	0.56
6:T:482:VAL:HG12	6:T:486:HIS:CE1	2.40	0.56
5:S:669:LEU:O	5:S:673:THR:HG23	2.06	0.56
5:S:893:SER:H	5:S:944:LYS:HZ1	1.54	0.56
5:S:2987:THR:HG23	5:S:2990:GLU:H	1.70	0.56
5:S:913:ARG:NH1	5:S:2801:ASP:OD2	2.39	0.56
5:S:2788:SER:HA	5:S:2791:ILE:HG12	1.88	0.56
5:S:2945:SER:HB2	5:S:3975:LYS:HD3	1.87	0.56
5:S:3814:ASP:O	5:S:3818:ASN:ND2	2.39	0.56
5:S:1071:ASN:HD22	5:S:1074:LYS:HG3	1.71	0.56
1:E:871:ARG:O	1:E:875:PHE:N	2.35	0.56
2:L:33:GLN:HA	2:L:36:LYS:HE2	1.88	0.56
5:S:246:ARG:NH2	5:S:281:GLN:O	2.39	0.56
5:S:1379:PRO:HB3	5:S:1385:ASN:HB3	1.88	0.56
5:S:1589:ASN:HB3	5:S:1592:MET:SD	2.46	0.56
5:S:1651:LYS:NZ	5:S:2045:PHE:O	2.39	0.56
2:L:466:LYS:NZ	2:L:467:ASP:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:593:ASN:HB2	5:S:1723:PRO:HG3	1.88	0.55
3:M:196:ALA:HA	6:T:477:SER:HA	1.88	0.55
5:S:2549:LYS:HG3	5:S:2550:ILE:HG13	1.88	0.55
5:S:3261:GLU:HA	5:S:3264:LYS:HB2	1.88	0.55
2:L:484:ASN:HD21	2:L:486:ARG:HB3	1.71	0.55
2:L:595:ALA:HA	2:L:598:PHE:CE1	2.40	0.55
5:S:1611:GLN:HB2	5:S:1613:HIS:HD1	1.70	0.55
5:S:1762:MET:O	5:S:1766:LEU:HB2	2.06	0.55
5:S:1837:ARG:HH22	5:S:1884:LEU:HD22	1.70	0.55
5:S:3033:GLU:OE1	5:S:3033:GLU:N	2.29	0.55
5:S:3578:LEU:HD11	5:S:3752:VAL:HG21	1.88	0.55
5:S:3684:SER:HB3	5:S:3687:MET:HB2	1.88	0.55
2:L:459:ASP:OD1	6:T:392:LYS:NZ	2.40	0.55
5:S:307:GLU:HA	5:S:310:LYS:HG2	1.88	0.55
5:S:668:LYS:NZ	5:S:728:SER:HB3	2.21	0.55
5:S:2467:THR:HA	5:S:2470:ARG:HE	1.71	0.55
2:L:378:SER:HA	2:L:381:ILE:HD12	1.88	0.55
5:S:4125:GLU:HA	5:S:4127:TRP:CZ3	2.41	0.55
1:E:662:VAL:HG13	1:E:698:TYR:HB2	1.88	0.55
2:L:297:LEU:HB2	2:L:303:THR:HB	1.89	0.55
5:S:330:ASN:OD1	5:S:331:ALA:N	2.40	0.55
5:S:453:MET:HA	5:S:456:VAL:HB	1.89	0.55
5:S:1657:SER:O	5:S:1660:SER:OG	2.21	0.55
5:S:1734:PRO:O	5:S:1738:ASN:ND2	2.40	0.55
5:S:2254:ARG:HD3	5:S:2293:GLY:H	1.71	0.55
5:S:3097:ASP:N	5:S:3097:ASP:OD1	2.39	0.55
5:S:3829:LEU:HA	5:S:3833:ARG:HD2	1.89	0.55
5:S:2129:LEU:HA	5:S:2132:LYS:HZ3	1.71	0.55
5:S:3576:ASP:O	5:S:3629:ARG:NH1	2.39	0.55
5:S:3707:GLY:HA2	5:S:3710:LYS:HE2	1.88	0.55
5:S:3793:VAL:HG23	5:S:3803:ILE:HG13	1.89	0.55
5:S:3812:LEU:HB2	5:S:3925:LEU:HB3	1.88	0.55
6:T:64:ILE:HG22	6:T:123:LYS:HE2	1.88	0.55
5:S:316:LEU:HD13	5:S:361:ILE:HG21	1.88	0.55
5:S:3263:HIS:O	5:S:3267:LYS:NZ	2.33	0.55
6:T:35:ARG:N	6:T:160:LYS:O	2.40	0.55
5:S:129:ASP:HA	5:S:132:ILE:HG22	1.88	0.55
5:S:364:ARG:HA	5:S:415:GLN:HE22	1.72	0.55
5:S:417:VAL:HA	5:S:420:VAL:HG12	1.89	0.55
5:S:1346:THR:O	5:S:1350:ASN:ND2	2.39	0.55
5:S:2349:LEU:O	5:S:2353:GLN:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:311:ILE:O	6:T:288:LEU:N	2.35	0.55
4:P:151:LEU:HA	4:P:154:ASP:HB2	1.88	0.55
5:S:3813:LYS:HG3	5:S:3925:LEU:HB2	1.89	0.55
9:A:76:GLN:NE2	9:A:98:LEU:O	2.40	0.55
2:L:513:TRP:HA	2:L:516:LEU:HB3	1.89	0.55
5:S:72:SER:HA	5:S:117:LYS:HE2	1.88	0.55
5:S:1342:MET:HE1	5:S:1398:VAL:HG13	1.87	0.55
5:S:1640:GLU:HA	5:S:1643:MET:HE3	1.89	0.55
5:S:2410:GLU:O	5:S:2414:GLN:NE2	2.40	0.55
5:S:2940:ARG:NH1	5:S:3977:THR:O	2.40	0.55
2:L:247:TRP:HZ2	2:L:338:LYS:HB2	1.72	0.54
5:S:1608:ARG:O	5:S:1608:ARG:NE	2.41	0.54
5:S:1806:ARG:HA	5:S:1869:LYS:HZ1	1.71	0.54
5:S:3130:GLN:HB3	5:S:3178:ILE:HG12	1.89	0.54
6:T:90:THR:OG1	6:T:92:LYS:O	2.25	0.54
6:T:207:LYS:HD2	6:T:208:PRO:HD2	1.89	0.54
6:T:245:LYS:NZ	6:T:246:VAL:O	2.41	0.54
5:S:1798:LEU:HD22	5:S:1827:LEU:HD13	1.89	0.54
7:i:19:DC:O2	7:i:20:DT:N3	2.40	0.54
5:S:1233:SER:O	5:S:1237:ALA:N	2.40	0.54
5:S:1608:ARG:HD2	5:S:1612:LYS:HG3	1.89	0.54
5:S:3044:MET:O	5:S:3047:SER:OG	2.21	0.54
6:T:210:GLY:HA2	6:T:233:PHE:HA	1.88	0.54
2:L:76:ASN:ND2	2:L:104:GLN:O	2.41	0.54
5:S:68:PHE:O	5:S:72:SER:OG	2.25	0.54
5:S:1697:PRO:HG2	5:S:1752:LEU:HD23	1.90	0.54
5:S:2803:ILE:O	5:S:2806:LYS:HB3	2.07	0.54
6:T:316:THR:HB	6:T:318:ARG:HH22	1.72	0.54
2:L:251:LEU:N	2:L:259:ILE:O	2.33	0.54
2:L:531:SER:HA	2:L:534:LYS:HG2	1.89	0.54
5:S:50:VAL:HG13	5:S:51:LEU:HG	1.90	0.54
5:S:998:ASN:HB3	5:S:1044:ILE:HG23	1.89	0.54
5:S:1271:ILE:O	5:S:1274:ARG:NH1	2.38	0.54
5:S:1295:ALA:HA	5:S:1298:LEU:HD12	1.89	0.54
5:S:2919:ASP:N	5:S:2919:ASP:OD1	2.40	0.54
6:T:419:GLU:HB2	6:T:428:THR:HB	1.89	0.54
5:S:1050:GLU:HA	5:S:1055:ASN:HD22	1.73	0.54
5:S:1471:GLN:HE22	5:S:1476:HIS:HA	1.73	0.54
5:S:3177:ASN:OD1	5:S:3178:ILE:HD12	2.07	0.54
5:S:360:SER:HA	5:S:363:ILE:HD12	1.89	0.54
5:S:1952:ILE:HD12	5:S:1961:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3684:SER:O	5:S:3688:SER:OG	2.24	0.54
5:S:3758:LEU:HB2	5:S:3795:PRO:HB3	1.88	0.54
5:S:3780:ALA:HB1	5:S:3784:ARG:HH12	1.73	0.54
6:T:363:ARG:HB3	6:T:436:PHE:HD2	1.72	0.54
9:A:123:ARG:HH12	9:A:125:VAL:HG22	1.72	0.54
2:L:455:ASP:HB2	6:T:388:LYS:HD2	1.90	0.54
5:S:42:CYS:HA	5:S:92:PHE:HZ	1.73	0.54
5:S:2313:LYS:HA	5:S:2316:TYR:CZ	2.42	0.54
5:S:2373:PRO:HA	5:S:2404:ARG:HH22	1.72	0.54
5:S:2408:MET:N	5:S:2408:MET:SD	2.81	0.54
5:S:3158:LYS:HG3	5:S:3159:ARG:HD3	1.89	0.54
5:S:3455:LYS:NZ	5:S:3489:SER:O	2.41	0.54
6:T:230:ARG:NH1	6:T:234:GLU:OE1	2.40	0.54
5:S:1342:MET:HG2	5:S:1402:LEU:HD22	1.90	0.53
5:S:1565:GLU:O	5:S:1569:THR:OG1	2.22	0.53
5:S:1726:SER:HA	5:S:1729:PHE:HD2	1.73	0.53
5:S:3181:ASP:O	5:S:3185:ASN:ND2	2.41	0.53
5:S:3962:ARG:NH2	5:S:4125:GLU:O	2.38	0.53
1:E:691:GLN:NE2	6:T:291:GLU:O	2.40	0.53
2:L:533:ILE:HG23	2:L:537:PHE:HD2	1.73	0.53
5:S:1264:LEU:HD11	5:S:1340:ARG:HB3	1.89	0.53
5:S:2973:ASP:OD1	5:S:2977:ASN:ND2	2.40	0.53
5:S:3136:THR:HA	5:S:3139:GLN:HG3	1.89	0.53
5:S:3179:TRP:HB3	5:S:3242:MET:SD	2.48	0.53
5:S:3587:ASP:OD2	5:S:3799:ARG:NH1	2.41	0.53
5:S:3891:SER:HB2	5:S:3900:LEU:HD21	1.89	0.53
2:L:7:LYS:O	2:L:128:GLU:N	2.33	0.53
5:S:1220:LEU:HD11	5:S:1287:GLN:HB2	1.91	0.53
5:S:1428:ILE:HD12	5:S:1431:LEU:HD12	1.89	0.53
5:S:1656:ASP:OD2	5:S:1660:SER:OG	2.27	0.53
5:S:2940:ARG:HH22	5:S:3981:TYR:HB3	1.74	0.53
5:S:3728:VAL:HG13	5:S:3736:LYS:HD2	1.89	0.53
1:E:868:ASP:HB3	1:E:871:ARG:HG3	1.91	0.53
5:S:894:PHE:N	5:S:905:ILE:O	2.38	0.53
5:S:1070:PRO:HG3	5:S:3715:TYR:HB2	1.90	0.53
5:S:2425:ARG:NH1	5:S:2457:PRO:O	2.42	0.53
5:S:2941:GLY:O	5:S:3975:LYS:NZ	2.38	0.53
1:E:792:MET:HE3	4:Q:178:LYS:HD2	1.90	0.53
5:S:2996:LEU:HA	5:S:2999:LEU:HD12	1.91	0.53
5:S:3090:TYR:O	5:S:3095:ASP:N	2.38	0.53
5:S:3145:ILE:HG23	5:S:3196:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:LEU:HB3	5:S:41:GLU:OE2	2.08	0.53
5:S:3104:GLN:NE2	5:S:3105:ASN:OD1	2.41	0.53
4:Q:158:VAL:HA	4:Q:161:ARG:HB2	1.90	0.53
5:S:865:GLN:HB2	5:S:3168:TYR:HE2	1.74	0.53
5:S:1608:ARG:HB2	5:S:1612:LYS:HE3	1.91	0.53
5:S:1627:LYS:HG3	5:S:1628:LYS:HD3	1.90	0.53
5:S:2346:ALA:HB2	5:S:2377:ARG:HH21	1.74	0.53
2:L:168:SER:HB3	2:L:191:SER:HB3	1.90	0.53
5:S:420:VAL:O	5:S:424:LEU:N	2.37	0.53
5:S:2133:LEU:HG	5:S:2167:PRO:HB2	1.89	0.53
5:S:2970:LYS:NZ	5:S:2974:GLU:OE1	2.41	0.53
5:S:3751:LEU:N	5:S:3803:ILE:O	2.39	0.53
6:T:308:GLY:O	9:A:57:ARG:NH1	2.42	0.53
2:L:142:PHE:HZ	2:L:207:ILE:HG13	1.73	0.53
2:L:308:GLU:O	6:T:290:ARG:NH2	2.42	0.53
5:S:1570:GLU:HG3	5:S:1571:LEU:HD22	1.89	0.53
5:S:3048:LYS:NZ	5:S:3060:SER:OG	2.37	0.53
2:L:451:LEU:HB3	6:T:388:LYS:HE3	1.89	0.52
4:P:181:ILE:O	4:P:185:ASN:ND2	2.42	0.52
5:S:236:LYS:HE3	5:S:243:GLN:HE22	1.72	0.52
5:S:1071:ASN:HD21	5:S:1073:PHE:HB2	1.74	0.52
5:S:3774:ILE:O	5:S:3777:GLN:NE2	2.36	0.52
6:T:362:LEU:HD11	6:T:438:PRO:HA	1.90	0.52
5:S:152:LEU:HA	5:S:155:LYS:HE2	1.91	0.52
5:S:305:ASN:O	5:S:308:LEU:N	2.33	0.52
5:S:913:ARG:HH12	5:S:2801:ASP:CG	2.17	0.52
5:S:1725:GLN:H	5:S:1768:ARG:CZ	2.22	0.52
5:S:1936:ARG:HH21	5:S:1937:ARG:HH22	1.55	0.52
5:S:2331:MET:O	5:S:2334:LYS:NZ	2.36	0.52
2:L:652:GLU:O	2:L:656:ASN:ND2	2.42	0.52
5:S:100:ILE:HG22	5:S:103:TYR:HB2	1.91	0.52
5:S:358:GLU:HA	5:S:361:ILE:HD12	1.90	0.52
5:S:1228:GLY:HA3	5:S:1234:GLY:H	1.74	0.52
5:S:2550:ILE:HB	5:S:2554:PHE:CE1	2.44	0.52
5:S:3603:LYS:NZ	5:S:3607:GLU:OE1	2.39	0.52
2:L:269:GLN:HG3	6:T:362:LEU:HD22	1.92	0.52
5:S:963:LYS:HG2	5:S:1007:VAL:HG11	1.91	0.52
5:S:1633:TRP:CE2	5:S:1674:THR:HG21	2.44	0.52
5:S:1697:PRO:HG3	5:S:1753:SER:HB3	1.91	0.52
5:S:3506:LEU:HD21	5:S:3514:VAL:HG23	1.90	0.52
5:S:3706:ASP:O	5:S:3708:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:MET:H	1:E:849:GLY:H	1.57	0.52
2:L:250:ARG:HH21	6:T:536:PRO:HB2	1.74	0.52
2:L:463:LEU:HD22	2:L:477:PHE:HE2	1.74	0.52
5:S:985:GLU:HA	5:S:988:VAL:HG22	1.90	0.52
5:S:1564:SER:O	5:S:1568:ASN:ND2	2.42	0.52
5:S:1583:MET:HE2	5:S:1628:LYS:HB2	1.91	0.52
5:S:3469:LEU:HD11	5:S:3502:MET:HE1	1.91	0.52
5:S:180:LEU:O	5:S:185:HIS:NE2	2.43	0.52
5:S:272:LEU:HD23	5:S:312:ALA:HA	1.91	0.52
5:S:1457:GLN:HG2	5:S:1460:ARG:HH21	1.75	0.52
5:S:624:ILE:HA	5:S:627:VAL:HG12	1.92	0.52
5:S:1017:ILE:HG13	5:S:1018:VAL:HG23	1.91	0.52
5:S:1225:GLU:O	5:S:1230:GLY:N	2.40	0.52
5:S:2140:LEU:HD23	5:S:2143:ARG:HD2	1.92	0.52
5:S:3156:PRO:HA	5:S:3159:ARG:HE	1.75	0.52
6:T:416:GLN:NE2	6:T:429:PRO:O	2.26	0.52
1:E:668:SER:HB3	1:E:702:ALA:HA	1.92	0.52
2:L:625:ASP:HA	2:L:672:ASN:HD21	1.75	0.52
5:S:320:LEU:HA	5:S:323:VAL:HG22	1.91	0.52
5:S:681:LYS:NZ	5:S:683:PHE:O	2.34	0.52
5:S:958:MET:HB3	5:S:961:LEU:HB2	1.92	0.52
5:S:1115:HIS:HD2	5:S:1119:LYS:HE3	1.73	0.52
5:S:1775:GLU:HA	5:S:1778:PHE:CD2	2.45	0.52
5:S:2582:SER:OG	5:S:2583:GLU:N	2.42	0.52
5:S:3806:LEU:HG	5:S:3808:ASN:H	1.74	0.52
2:L:498:ALA:O	6:T:325:ARG:NH2	2.33	0.52
4:P:189:THR:O	4:P:193:SER:N	2.43	0.52
5:S:1052:SER:OG	5:S:1054:VAL:O	2.28	0.52
5:S:1603:GLN:HG2	5:S:1606:ARG:HH21	1.75	0.52
5:S:2988:GLU:HA	5:S:2991:LYS:HE2	1.92	0.52
1:E:822:SER:HA	1:E:841:LYS:HD2	1.92	0.52
5:S:1601:LEU:HB2	5:S:1655:ILE:HD11	1.91	0.52
6:T:258:ARG:NH1	6:T:259:LEU:O	2.42	0.52
1:E:879:ARG:HB2	1:E:886:PHE:HB2	1.91	0.51
2:L:313:GLY:O	6:T:286:ILE:N	2.34	0.51
4:Q:188:LYS:HA	4:Q:191:ILE:HB	1.91	0.51
5:S:1400:VAL:HA	5:S:1403:MET:HE2	1.92	0.51
5:S:3751:LEU:HB2	5:S:3803:ILE:HB	1.91	0.51
5:S:275:PHE:HE2	5:S:319:PHE:HB2	1.75	0.51
5:S:1805:PHE:O	5:S:1869:LYS:NZ	2.43	0.51
5:S:3753:LYS:HD3	5:S:3756:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:4054:ALA:HA	5:S:4095:GLU:HA	1.91	0.51
2:L:81:ARG:HE	2:L:84:MET:HB2	1.75	0.51
5:S:542:ASP:OD1	5:S:543:SER:N	2.42	0.51
5:S:1164:CYS:SG	5:S:1165:LEU:N	2.83	0.51
5:S:1296:PHE:O	5:S:1300:SER:OG	2.24	0.51
5:S:2234:ASN:HA	5:S:2237:ILE:HD12	1.92	0.51
5:S:2834:GLN:HA	5:S:2837:LEU:HD12	1.92	0.51
5:S:4125:GLU:HB3	5:S:4128:MET:HB2	1.91	0.51
1:E:837:ARG:HG2	4:P:153:ARG:NH2	2.25	0.51
2:L:161:LEU:HD12	2:L:163:PHE:HE1	1.75	0.51
2:L:184:ARG:NH1	2:L:517:ASN:O	2.37	0.51
2:L:272:VAL:HG22	2:L:274:LYS:H	1.76	0.51
2:L:463:LEU:HD22	2:L:477:PHE:CE2	2.44	0.51
5:S:1474:ASP:OD1	5:S:1474:ASP:N	2.44	0.51
6:T:107:GLU:O	6:T:115:ARG:NH2	2.34	0.51
2:L:689:GLU:HA	2:L:695:SER:HB3	1.92	0.51
5:S:146:GLU:HB3	5:S:183:GLU:HG3	1.92	0.51
5:S:186:PRO:HD2	5:S:189:MET:HE1	1.92	0.51
5:S:1502:SER:OG	5:S:1503:LEU:N	2.41	0.51
2:L:88:PHE:HD2	6:T:325:ARG:HD3	1.75	0.51
2:L:608:SER:HB2	2:L:654:ARG:HH12	1.76	0.51
5:S:955:ALA:O	5:S:957:PRO:HD3	2.10	0.51
5:S:2121:ASP:OD1	5:S:2121:ASP:N	2.43	0.51
5:S:3008:TRP:HB2	5:S:3051:LEU:HD23	1.93	0.51
5:S:3176:MET:HA	5:S:3179:TRP:HD1	1.75	0.51
5:S:3923:ARG:HH21	5:S:3924:HIS:HB3	1.76	0.51
5:S:3970:LEU:HD21	5:S:3974:MET:HG2	1.93	0.51
5:S:1786:ALA:HB3	5:S:1830:HIS:HB3	1.92	0.51
5:S:3927:ASN:O	5:S:3940:ILE:N	2.43	0.51
6:T:299:LYS:NZ	6:T:300:THR:O	2.43	0.51
7:i:36:DA:H2"	7:i:37:DT:C5	2.45	0.51
9:A:45:ARG:HE	9:A:71:GLN:H	1.58	0.51
1:E:879:ARG:HD3	1:E:885:LYS:HA	1.92	0.51
2:L:605:LYS:HE3	2:L:609:PHE:HZ	1.76	0.51
5:S:372:PRO:HA	5:S:375:VAL:HB	1.92	0.51
5:S:430:VAL:HG11	5:S:1643:MET:HG3	1.92	0.51
5:S:1602:ASP:HB3	5:S:1606:ARG:HH12	1.75	0.51
5:S:1626:TRP:HH2	5:S:1632:TRP:HB2	1.76	0.51
5:S:3142:ILE:O	5:S:3147:LYS:NZ	2.39	0.51
6:T:414:VAL:O	6:T:433:GLN:N	2.37	0.51
2:L:261:ILE:HA	2:L:366:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1621:THR:O	5:S:1625:HIS:N	2.44	0.51
9:A:90:ASP:HB3	9:A:93:ARG:HB3	1.93	0.51
5:S:35:ILE:HG12	5:S:36:ARG:HH21	1.76	0.51
5:S:493:LYS:O	5:S:625:ASN:ND2	2.44	0.51
5:S:886:TRP:O	5:S:964:ARG:NH1	2.43	0.51
5:S:1538:LEU:HB2	5:S:1555:HIS:CE1	2.46	0.51
5:S:2505:VAL:HA	5:S:2508:GLN:HG2	1.93	0.51
6:T:147:LEU:HD11	6:T:193:LEU:HD23	1.93	0.51
6:T:307:THR:HG22	6:T:309:GLY:H	1.75	0.51
6:T:414:VAL:HB	6:T:433:GLN:HB2	1.92	0.51
2:L:235:CYS:HA	2:L:238:LYS:HB2	1.93	0.50
2:L:458:ILE:O	2:L:462:SER:N	2.44	0.50
5:S:833:HIS:O	5:S:838:LYS:NZ	2.43	0.50
5:S:863:GLY:O	5:S:867:ASN:N	2.40	0.50
5:S:2376:ASP:N	5:S:2376:ASP:OD1	2.43	0.50
5:S:2890:ILE:HD11	5:S:2929:LEU:HB3	1.94	0.50
6:T:413:LEU:HB3	6:T:432:PHE:CD2	2.45	0.50
1:E:816:HIS:HB2	1:E:850:ALA:HA	1.93	0.50
5:S:129:ASP:O	5:S:133:LYS:HG2	2.12	0.50
5:S:1576:ASP:OD1	5:S:1576:ASP:N	2.44	0.50
5:S:3037:GLN:N	5:S:3037:GLN:OE1	2.44	0.50
5:S:3311:ASN:HB3	5:S:3315:TYR:CZ	2.46	0.50
5:S:3657:SER:OG	5:S:3658:ASP:N	2.41	0.50
1:E:746:MET:O	1:E:751:LYS:NZ	2.44	0.50
5:S:3266:SER:HA	5:S:3272:TRP:CD1	2.46	0.50
5:S:2232:ARG:HA	5:S:2235:LEU:HD12	1.93	0.50
5:S:2510:LEU:O	5:S:2518:GLN:NE2	2.31	0.50
5:S:3828:TYR:HD2	5:S:3829:LEU:HD22	1.77	0.50
6:T:389:CYS:O	6:T:393:GLU:N	2.44	0.50
2:L:450:GLN:NE2	2:L:536:LEU:O	2.36	0.50
4:P:161:ARG:HA	4:P:164:LYS:HE2	1.93	0.50
5:S:1479:VAL:O	5:S:1482:GLU:HG2	2.11	0.50
5:S:2255:LEU:HD23	5:S:2255:LEU:H	1.77	0.50
5:S:3321:LEU:O	5:S:3324:ARG:HG2	2.12	0.50
1:E:857:ALA:O	1:E:884:ARG:NH1	2.44	0.50
5:S:668:LYS:HZ2	5:S:728:SER:HB3	1.77	0.50
5:S:1776:GLU:O	5:S:1779:GLN:NE2	2.45	0.50
5:S:3228:SER:HA	5:S:3231:ILE:HG12	1.94	0.50
5:S:3806:LEU:HD23	5:S:3809:THR:HB	1.93	0.50
6:T:261:LEU:HB3	6:T:269:ILE:HB	1.94	0.50
2:L:33:GLN:HB3	2:L:227:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:137:THR:O	5:S:141:SER:OG	2.29	0.50
5:S:931:CYS:O	5:S:935:HIS:ND1	2.45	0.50
5:S:1075:ARG:NH1	5:S:1117:ASP:OD2	2.41	0.50
5:S:2470:ARG:O	5:S:2473:MET:HG2	2.12	0.50
5:S:3132:VAL:HA	5:S:3135:LEU:HD12	1.94	0.50
5:S:3133:GLN:NE2	5:S:3137:GLU:OE2	2.44	0.50
5:S:3796:MET:HB2	5:S:3800:LEU:HB3	1.92	0.50
6:T:343:PRO:HA	6:T:401:THR:HB	1.91	0.50
5:S:630:CYS:HA	5:S:633:ILE:HG12	1.94	0.50
5:S:1057:LYS:HA	5:S:1060:PHE:HD2	1.76	0.50
5:S:1949:ILE:HD13	5:S:2096:PRO:HB2	1.94	0.50
6:T:42:VAL:HG22	6:T:169:PHE:HB2	1.93	0.50
6:T:263:LEU:HD12	6:T:267:ILE:HG21	1.94	0.50
1:E:668:SER:OG	1:E:708:ARG:NH2	2.40	0.49
1:E:707:ILE:HA	1:E:710:LYS:HD3	1.94	0.49
5:S:469:ALA:HA	5:S:475:LEU:HD13	1.93	0.49
5:S:759:GLY:O	5:S:799:TYR:OH	2.28	0.49
5:S:1062:ARG:NH2	5:S:3745:GLU:OE1	2.43	0.49
5:S:189:MET:HA	5:S:192:ASN:HB2	1.94	0.49
5:S:451:PRO:HA	5:S:454:GLN:HB2	1.94	0.49
5:S:1708:GLU:HA	5:S:1711:ARG:HD2	1.94	0.49
5:S:2322:VAL:O	5:S:2326:ILE:HG12	2.12	0.49
5:S:2870:SER:OG	5:S:2899:ARG:NH2	2.43	0.49
5:S:3013:TYR:HA	5:S:3016:THR:HG23	1.94	0.49
6:T:372:GLU:OE1	6:T:377:GLY:N	2.37	0.49
2:L:448:GLU:HA	2:L:451:LEU:HD12	1.93	0.49
2:L:643:ARG:HE	2:L:647:ILE:HG13	1.77	0.49
5:S:425:ASP:OD1	5:S:425:ASP:N	2.43	0.49
5:S:3619:ASP:OD1	5:S:3619:ASP:N	2.45	0.49
6:T:357:LYS:HB3	6:T:359:HIS:CE1	2.47	0.49
2:L:294:VAL:HB	6:T:299:LYS:HB3	1.94	0.49
2:L:298:ASN:OD1	2:L:299:ASP:N	2.46	0.49
5:S:672:ILE:HD12	5:S:675:ARG:HH21	1.78	0.49
5:S:938:VAL:HA	5:S:941:MET:HG3	1.94	0.49
5:S:1118:GLU:OE2	5:S:1120:SER:OG	2.28	0.49
5:S:1250:LEU:O	5:S:1253:THR:OG1	2.25	0.49
5:S:2978:LYS:NZ	5:S:2980:ASP:O	2.37	0.49
5:S:3965:ARG:HA	5:S:3968:ILE:HD12	1.93	0.49
6:T:363:ARG:HH22	8:j:27:DT:H3'	1.77	0.49
7:i:35:DT:O4	7:i:36:DA:N6	2.44	0.49
4:P:187:LYS:O	4:P:191:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1142:HIS:O	5:S:1146:ASN:N	2.44	0.49
5:S:3753:LYS:NZ	5:S:3755:GLY:O	2.32	0.49
6:T:74:LYS:HZ1	6:T:81:ASP:H	1.58	0.49
6:T:147:LEU:HD13	6:T:189:LYS:HB3	1.94	0.49
1:E:853:VAL:HG11	1:E:857:ALA:HB2	1.95	0.49
5:S:52:ALA:O	5:S:56:SER:OG	2.25	0.49
5:S:649:PHE:CE2	5:S:653:LEU:HD11	2.48	0.49
5:S:1181:THR:OG1	5:S:1184:ARG:NH2	2.46	0.49
5:S:1357:LYS:HE3	5:S:1410:PRO:HG2	1.95	0.49
5:S:1571:LEU:HD12	5:S:1578:ALA:HB2	1.94	0.49
5:S:3269:ARG:CZ	5:S:3272:TRP:HB2	2.42	0.49
5:S:3413:TYR:O	5:S:3449:LYS:NZ	2.45	0.49
6:T:301:ARG:HH22	9:A:57:ARG:HE	1.61	0.49
2:L:342:VAL:HG23	2:L:393:VAL:HG22	1.95	0.49
2:L:654:ARG:HA	2:L:657:ASN:HD21	1.77	0.49
5:S:793:LEU:HD22	5:S:869:ASN:HB2	1.94	0.49
5:S:1769:GLU:O	5:S:1772:HIS:ND1	2.33	0.49
5:S:2569:SER:OG	5:S:2571:ASP:OD1	2.29	0.49
5:S:2796:ALA:O	5:S:2800:ARG:HG2	2.11	0.49
5:S:2924:VAL:HG11	5:S:2989:ALA:HB1	1.95	0.49
5:S:3538:GLU:OE1	5:S:3538:GLU:N	2.42	0.49
2:L:473:LEU:HD21	6:T:352:PRO:HG2	1.94	0.49
3:M:198:GLY:H	6:T:477:SER:HB3	1.78	0.49
4:P:194:LEU:HD22	4:Q:194:LEU:HD22	1.95	0.49
5:S:87:LYS:HG3	5:S:831:LEU:HD22	1.95	0.49
5:S:1643:MET:HA	5:S:1646:LEU:HG	1.95	0.49
5:S:2495:SER:HA	5:S:2498:ILE:HD12	1.94	0.49
5:S:2541:ALA:O	5:S:2544:SER:OG	2.26	0.49
5:S:3034:PRO:HD2	5:S:3037:GLN:HB2	1.95	0.49
6:T:266:ASP:N	6:T:266:ASP:OD1	2.44	0.49
6:T:422:ASP:OD1	6:T:422:ASP:N	2.44	0.49
9:A:40:TRP:HE1	9:A:122:ARG:CZ	2.25	0.49
2:L:660:LYS:HZ1	2:L:698:ALA:HB1	1.78	0.49
5:S:3169:PRO:HG3	5:S:3241:LYS:HD2	1.95	0.49
6:T:103:TYR:CG	6:T:135:MET:HE1	2.48	0.49
6:T:142:SER:HB3	6:T:145:GLU:HG2	1.94	0.49
2:L:241:GLU:HG3	6:T:445:LYS:HE2	1.95	0.49
5:S:135:LEU:O	5:S:139:ARG:HG2	2.12	0.49
5:S:672:ILE:HG23	5:S:675:ARG:HH21	1.78	0.49
5:S:3104:GLN:HA	5:S:3107:ILE:HG12	1.94	0.49
9:A:109:LEU:HG	9:A:132:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:402:ASN:O	2:L:404:GLN:NE2	2.46	0.48
2:L:407:VAL:HG12	2:L:424:LEU:HD21	1.94	0.48
5:S:31:GLY:HA2	5:S:34:LEU:HD12	1.95	0.48
5:S:1191:PHE:O	5:S:1195:VAL:HG23	2.13	0.48
5:S:1828:LEU:HD21	5:S:1880:MET:HA	1.95	0.48
5:S:3119:VAL:HG23	5:S:3120:LEU:HD23	1.95	0.48
2:L:329:GLU:HA	2:L:332:LYS:HG2	1.94	0.48
2:L:663:GLN:HA	2:L:666:VAL:HG12	1.95	0.48
2:L:667:GLU:OE2	2:L:702:LYS:NZ	2.46	0.48
5:S:321:LYS:O	5:S:325:ASN:ND2	2.46	0.48
5:S:847:SER:N	5:S:850:GLU:OE2	2.46	0.48
5:S:3037:GLN:O	5:S:3041:LEU:HG	2.13	0.48
5:S:3476:PRO:O	5:S:3480:LEU:HB2	2.13	0.48
7:i:36:DA:H2"	7:i:37:DT:C4	2.48	0.48
5:S:390:GLN:HA	5:S:393:LYS:HE2	1.96	0.48
5:S:768:VAL:HA	5:S:771:ASN:HD22	1.79	0.48
5:S:3193:ILE:HG13	5:S:3196:LYS:HZ3	1.78	0.48
5:S:3780:ALA:HB1	5:S:3784:ARG:NH1	2.28	0.48
5:S:4086:ASP:OD1	5:S:4086:ASP:N	2.45	0.48
6:T:35:ARG:O	6:T:162:SER:N	2.45	0.48
2:L:55:ALA:HB2	2:L:83:LEU:HG	1.95	0.48
5:S:847:SER:OG	5:S:848:LEU:N	2.29	0.48
2:L:277:THR:OG1	6:T:319:SER:O	2.32	0.48
2:L:389:MET:HG2	6:T:466:VAL:HG21	1.96	0.48
4:P:190:LYS:HG3	4:Q:191:ILE:HD13	1.96	0.48
5:S:243:GLN:O	5:S:246:ARG:HD3	2.14	0.48
5:S:1711:ARG:HE	5:S:1757:MET:HE2	1.78	0.48
5:S:2486:ASP:OD1	5:S:2486:ASP:N	2.42	0.48
5:S:2547:SER:HB3	5:S:2554:PHE:HZ	1.79	0.48
2:L:260:ARG:NE	6:T:536:PRO:O	2.37	0.48
4:P:198:LEU:HD12	4:Q:198:LEU:HD13	1.95	0.48
5:S:1150:LYS:HA	5:S:1162:SER:HA	1.96	0.48
5:S:1196:PRO:HA	5:S:1202:ARG:HA	1.95	0.48
5:S:1591:LYS:O	5:S:1594:SER:OG	2.27	0.48
5:S:2406:GLU:N	5:S:2406:GLU:OE1	2.46	0.48
5:S:261:ASP:HB3	5:S:265:TYR:H	1.79	0.48
5:S:625:ASN:O	5:S:628:GLU:HG2	2.13	0.48
5:S:1257:LEU:HA	5:S:1260:LEU:HD12	1.94	0.48
5:S:1867:ILE:O	5:S:1871:MET:HG2	2.14	0.48
5:S:2522:ARG:HH12	5:S:2564:GLU:HG2	1.79	0.48
5:S:3236:PHE:HD2	5:S:3269:ARG:HH12	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3923:ARG:HG2	5:S:4124:TRP:HA	1.96	0.48
5:S:3964:THR:HG23	5:S:3966:GLN:H	1.77	0.48
2:L:457:LEU:HD22	2:L:533:ILE:HD13	1.94	0.48
5:S:476:ARG:HH21	5:S:1561:SER:HG	1.56	0.48
5:S:1649:LEU:HA	5:S:1652:ILE:HD12	1.96	0.48
5:S:2414:GLN:O	5:S:2417:SER:OG	2.28	0.48
5:S:2522:ARG:NH1	5:S:2564:GLU:HG2	2.29	0.48
5:S:3182:ILE:HA	5:S:3185:ASN:HD21	1.79	0.48
5:S:3452:LYS:HA	5:S:3455:LYS:HG2	1.96	0.48
6:T:247:ARG:NH1	6:T:487:PHE:HB2	2.29	0.48
2:L:263:ALA:HA	2:L:364:VAL:HA	1.96	0.48
4:P:188:LYS:O	4:P:192:ARG:N	2.35	0.48
5:S:792:ILE:HG13	5:S:793:LEU:HD12	1.95	0.48
5:S:974:CYS:HA	5:S:981:ARG:HH12	1.79	0.48
5:S:2129:LEU:HA	5:S:2132:LYS:HG2	1.94	0.48
5:S:2318:ALA:HA	5:S:2321:GLU:HG2	1.96	0.48
5:S:2428:ASP:OD1	5:S:2428:ASP:N	2.45	0.48
5:S:2539:LEU:O	5:S:2542:LEU:HG	2.13	0.48
5:S:3240:MET:HE3	5:S:3272:TRP:CH2	2.49	0.48
1:E:731:LYS:HG3	1:E:732:THR:HG23	1.95	0.48
2:L:360:GLN:HE22	2:L:362:LEU:HB2	1.79	0.48
5:S:1083:ASN:O	5:S:1087:ARG:NH1	2.47	0.48
5:S:1184:ARG:NH2	5:S:1265:GLU:OE1	2.47	0.48
5:S:4004:VAL:HG23	5:S:4005:PHE:H	1.78	0.48
6:T:190:ALA:O	6:T:193:LEU:HG	2.14	0.48
7:i:28:DT:H1'	7:i:29:DA:H5'	1.95	0.48
7:i:37:DT:H5"	7:i:37:DT:C6	2.49	0.48
1:E:677:ASP:N	1:E:677:ASP:OD1	2.47	0.47
2:L:311:ILE:HD11	6:T:290:ARG:HD3	1.95	0.47
2:L:312:GLN:NE2	2:L:324:SER:O	2.46	0.47
2:L:541:GLU:HG2	6:T:268:VAL:HB	1.96	0.47
5:S:1115:HIS:NE2	5:S:1182:GLU:HB3	2.28	0.47
5:S:1115:HIS:CD2	5:S:1119:LYS:HE3	2.49	0.47
5:S:2234:ASN:O	5:S:2238:ILE:HD12	2.14	0.47
5:S:3621:LYS:HB2	5:S:3630:ARG:HH12	1.79	0.47
2:L:306:LEU:HG	2:L:308:GLU:H	1.79	0.47
5:S:80:GLU:HA	5:S:83:GLU:OE1	2.13	0.47
5:S:724:GLU:HB2	5:S:2599:SER:HA	1.95	0.47
5:S:1157:PHE:CE1	5:S:1159:PRO:HG2	2.49	0.47
6:T:247:ARG:NH1	6:T:488:ARG:HG3	2.28	0.47
1:E:656:SER:HA	1:E:733:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:343:LEU:HD11	2:L:394:ARG:HB2	1.96	0.47
5:S:1105:VAL:O	5:S:1108:MET:HG3	2.14	0.47
5:S:1740:VAL:HA	5:S:1743:MET:HG2	1.97	0.47
5:S:1793:THR:O	5:S:1797:LEU:HG	2.13	0.47
5:S:672:ILE:O	5:S:676:ASN:ND2	2.48	0.47
5:S:3455:LYS:HZ1	5:S:3489:SER:C	2.22	0.47
5:S:3860:LYS:HG2	5:S:4073:ALA:HB2	1.95	0.47
6:T:39:ILE:O	6:T:167:MET:N	2.44	0.47
5:S:1423:ILE:HD11	5:S:1428:ILE:HB	1.95	0.47
2:L:426:PHE:HB3	6:T:479:GLU:HA	1.97	0.47
5:S:2190:VAL:HA	5:S:2193:ILE:HG22	1.97	0.47
5:S:2205:VAL:HG13	5:S:2208:ASP:H	1.78	0.47
5:S:2826:LEU:HA	5:S:2829:LYS:HE2	1.97	0.47
5:S:3008:TRP:HA	5:S:3011:LEU:HD12	1.97	0.47
5:S:3048:LYS:HA	5:S:3051:LEU:HD12	1.97	0.47
5:S:3312:VAL:O	5:S:3316:LEU:N	2.40	0.47
2:L:18:PHE:HA	2:L:21:SER:HB2	1.96	0.47
2:L:188:HIS:HD1	2:L:519:PRO:HD3	1.80	0.47
5:S:67:VAL:HA	5:S:71:LYS:HB2	1.97	0.47
5:S:364:ARG:HA	5:S:415:GLN:NE2	2.29	0.47
5:S:367:GLY:HA3	5:S:416:SER:HB2	1.97	0.47
5:S:763:THR:O	5:S:766:ALA:N	2.47	0.47
5:S:1342:MET:O	5:S:1345:THR:OG1	2.32	0.47
5:S:2393:LEU:HD12	5:S:2393:LEU:H	1.79	0.47
5:S:3189:PHE:O	5:S:3193:ILE:HD12	2.15	0.47
5:S:3285:HIS:HE2	5:S:3333:THR:HB	1.80	0.47
5:S:3720:ALA:HB3	5:S:3743:HIS:HA	1.95	0.47
5:S:4111:ALA:O	5:S:4115:ASN:ND2	2.41	0.47
6:T:353:LEU:HD23	6:T:395:ALA:HB2	1.96	0.47
5:S:1751:GLU:HA	5:S:1785:ILE:HG22	1.97	0.47
5:S:2825:THR:HG23	5:S:2828:GLU:H	1.80	0.47
1:E:800:GLU:O	1:E:804:SER:N	2.48	0.47
4:P:183:VAL:HA	4:P:186:GLU:HG2	1.96	0.47
5:S:204:LEU:O	5:S:208:MET:HG3	2.15	0.47
5:S:1212:LEU:HD12	5:S:1215:GLU:HB2	1.97	0.47
5:S:2044:ASP:O	5:S:2048:GLY:N	2.47	0.47
5:S:2723:THR:HG23	5:S:2727:ARG:HH21	1.80	0.47
7:i:21:DA:P	8:j:37:DG:H21	2.38	0.47
4:P:191:ILE:HG22	4:P:195:HIS:CE1	2.50	0.47
5:S:1226:GLY:HA3	5:S:1263:ALA:HB2	1.97	0.47
5:S:1452:VAL:HG22	5:S:1517:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1593:VAL:HA	5:S:1596:VAL:HG22	1.96	0.47
5:S:2196:TRP:NE1	5:S:2200:ALA:HB3	2.30	0.47
5:S:3069:MET:HE1	5:S:3078:LEU:HD11	1.96	0.47
5:S:3692:VAL:HG22	5:S:3696:ARG:HD3	1.96	0.47
2:L:496:HIS:CG	2:L:506:PRO:HD3	2.50	0.46
5:S:781:ASP:OD2	5:S:783:HIS:ND1	2.48	0.46
5:S:784:VAL:O	5:S:787:PRO:HD2	2.15	0.46
5:S:1046:PRO:O	5:S:1049:GLN:HG2	2.15	0.46
5:S:2330:VAL:HG12	5:S:2333:ARG:NH2	2.30	0.46
5:S:3758:LEU:O	5:S:3762:GLN:HG2	2.15	0.46
2:L:276:TRP:HB3	6:T:318:ARG:HB3	1.97	0.46
2:L:524:THR:HA	2:L:527:GLN:HG2	1.96	0.46
5:S:723:ASP:C	5:S:725:LEU:H	2.24	0.46
5:S:1406:LEU:HA	5:S:1409:SER:HB3	1.97	0.46
5:S:1824:LEU:HD13	5:S:1827:LEU:HD21	1.97	0.46
5:S:3085:GLU:OE1	5:S:3085:GLU:N	2.41	0.46
5:S:4099:SER:HB3	5:S:4102:THR:OG1	2.15	0.46
6:T:59:PRO:HA	6:T:62:MET:HG2	1.97	0.46
6:T:262:LYS:HA	6:T:267:ILE:O	2.14	0.46
2:L:357:MET:HG3	2:L:425:PRO:HB3	1.96	0.46
5:S:179:GLY:HA3	5:S:230:LEU:HB2	1.98	0.46
5:S:234:PHE:CD2	5:S:235:THR:HG23	2.51	0.46
5:S:782:ARG:HB3	5:S:3164:TRP:CZ2	2.49	0.46
5:S:935:HIS:CE1	5:S:984:TYR:HE1	2.33	0.46
5:S:1268:ASN:ND2	5:S:1343:GLU:OE2	2.49	0.46
5:S:1453:SER:HA	5:S:1456:LYS:HG2	1.97	0.46
5:S:3713:PRO:HB3	5:S:3715:TYR:CZ	2.51	0.46
5:S:4085:LYS:HB3	5:S:4087:HIS:CE1	2.50	0.46
9:A:42:SER:O	9:A:45:ARG:NH2	2.48	0.46
1:E:774:LEU:HD21	4:P:180:PHE:HB2	1.97	0.46
2:L:162:GLN:NE2	2:L:235:CYS:O	2.47	0.46
5:S:12:LEU:HD21	5:S:44:LEU:HD22	1.97	0.46
5:S:16:GLN:NE2	5:S:62:ASP:OD2	2.48	0.46
5:S:429:GLU:O	5:S:432:THR:OG1	2.34	0.46
5:S:1023:SER:HA	5:S:1026:ARG:HG3	1.98	0.46
5:S:2388:LYS:NZ	6:T:155:SER:O	2.39	0.46
5:S:3163:THR:O	5:S:3167:ARG:NH2	2.48	0.46
5:S:3964:THR:HG22	5:S:3967:PHE:HD2	1.80	0.46
8:j:32:DT:H2"	8:j:33:DA:C8	2.50	0.46
2:L:463:LEU:HD13	2:L:477:PHE:CD2	2.51	0.46
2:L:636:ILE:HA	2:L:639:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:176:LEU:HD13	4:Q:176:LEU:HD12	1.98	0.46
5:S:151:GLU:O	5:S:154:SER:OG	2.30	0.46
5:S:1015:ASP:OD1	5:S:1016:GLY:N	2.46	0.46
5:S:1740:VAL:HA	5:S:1743:MET:HE3	1.98	0.46
5:S:1767:CYS:HB3	5:S:1818:SER:OG	2.16	0.46
5:S:2402:LEU:HD13	5:S:2434:VAL:HG23	1.97	0.46
5:S:2414:GLN:OE1	5:S:2414:GLN:N	2.45	0.46
5:S:3133:GLN:O	5:S:3136:THR:HG22	2.14	0.46
5:S:3592:VAL:HB	5:S:3609:MET:HE1	1.98	0.46
5:S:3832:PRO:HB2	5:S:3877:LYS:HG2	1.98	0.46
5:S:4045:CYS:HA	5:S:4048:LYS:HG2	1.98	0.46
9:A:117:LEU:HD12	9:A:120:GLN:HE22	1.81	0.46
2:L:255:SER:OG	6:T:515:ASN:ND2	2.43	0.46
2:L:457:LEU:HD13	2:L:529:PRO:HB2	1.97	0.46
4:P:150:ARG:O	4:P:154:ASP:N	2.41	0.46
5:S:3176:MET:HA	5:S:3179:TRP:CD1	2.50	0.46
5:S:3328:ILE:O	5:S:3332:THR:OG1	2.27	0.46
5:S:4113:ASP:O	5:S:4117:LEU:HG	2.16	0.46
6:T:44:ALA:HB1	6:T:137:HIS:HA	1.98	0.46
9:A:65:ILE:HG13	9:A:70:GLY:HA3	1.98	0.46
1:E:656:SER:HB3	1:E:685:PHE:CD2	2.50	0.46
1:E:832:LYS:HD3	1:E:834:GLU:H	1.80	0.46
5:S:901:MET:SD	5:S:901:MET:N	2.89	0.46
5:S:913:ARG:NH1	5:S:917:LEU:HD11	2.31	0.46
5:S:1261:LEU:HD21	5:S:1337:VAL:HA	1.97	0.46
5:S:3324:ARG:HB3	5:S:3391:ALA:HB3	1.98	0.46
5:S:3493:TRP:CE2	5:S:3524:ASN:HB2	2.50	0.46
6:T:275:ASN:HD21	6:T:278:GLN:HB2	1.81	0.46
1:E:769:THR:HG21	4:P:184:LEU:HD13	1.98	0.46
2:L:252:THR:HB	2:L:341:SER:HA	1.97	0.46
2:L:511:HIS:ND1	2:L:515:MET:HE1	2.31	0.46
4:P:190:LYS:HD3	4:Q:191:ILE:HG21	1.97	0.46
5:S:113:SER:O	5:S:117:LYS:N	2.49	0.46
5:S:1712:ARG:O	5:S:1715:GLU:HG3	2.15	0.46
5:S:3547:THR:HA	5:S:3550:LYS:HZ2	1.80	0.46
5:S:3658:ASP:N	5:S:3658:ASP:OD1	2.48	0.46
5:S:3912:CYS:HB2	5:S:3961:PHE:HB2	1.96	0.46
6:T:102:ILE:HD12	6:T:146:VAL:HG12	1.97	0.46
5:S:31:GLY:HA3	5:S:77:GLU:HB2	1.97	0.46
5:S:996:THR:HG21	5:S:1039:TRP:HB3	1.98	0.46
5:S:2297:SER:OG	5:S:2298:GLU:OE1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3927:ASN:HA	5:S:3940:ILE:HB	1.96	0.46
6:T:372:GLU:OE2	6:T:379:SER:N	2.36	0.46
7:i:37:DT:H5"	7:i:37:DT:H6	1.80	0.46
1:E:725:TRP:NE1	1:E:736:VAL:O	2.43	0.46
5:S:901:MET:SD	5:S:2820:MET:HE1	2.56	0.46
5:S:907:LEU:HA	5:S:910:PHE:CD2	2.51	0.46
5:S:1105:VAL:HA	5:S:1108:MET:HG3	1.98	0.46
5:S:1406:LEU:HD13	5:S:1415:LEU:HD13	1.97	0.46
5:S:1626:TRP:CH2	5:S:1632:TRP:HB2	2.51	0.46
5:S:1770:GLN:NE2	5:S:1775:GLU:OE1	2.49	0.46
5:S:2328:ARG:NE	5:S:2370:SER:O	2.44	0.46
5:S:2375:ALA:O	5:S:2378:PHE:N	2.37	0.46
5:S:2891:ARG:HH22	5:S:3894:PRO:HB2	1.81	0.46
6:T:206:LYS:N	6:T:235:GLU:HB3	2.30	0.46
1:E:711:ASN:OD1	2:L:330:GLN:NE2	2.46	0.45
2:L:21:SER:HB3	2:L:100:PRO:HB3	1.98	0.45
2:L:368:ARG:HD2	2:L:368:ARG:HA	1.86	0.45
2:L:436:SER:O	6:T:369:TYR:OH	2.34	0.45
5:S:166:ILE:N	5:S:167:PRO:HD2	2.31	0.45
5:S:291:VAL:HA	5:S:294:PHE:CD2	2.51	0.45
5:S:861:SER:N	5:S:3136:THR:HG21	2.31	0.45
5:S:891:ARG:HH22	5:S:960:GLN:H	1.65	0.45
5:S:1115:HIS:O	5:S:1119:LYS:NZ	2.36	0.45
5:S:1626:TRP:CZ2	5:S:1630:ASP:HA	2.51	0.45
5:S:2386:LEU:HD12	5:S:2418:LYS:HG3	1.99	0.45
5:S:3247:ARG:NE	5:S:3282:ARG:HE	2.14	0.45
5:S:3837:CYS:SG	5:S:3873:LYS:HB3	2.56	0.45
5:S:3860:LYS:HE3	5:S:4072:PRO:HB2	1.97	0.45
6:T:348:MET:HG3	6:T:410:PHE:CE1	2.50	0.45
1:E:665:CYS:HB3	1:E:700:VAL:HG13	1.98	0.45
1:E:702:ALA:HB3	1:E:720:VAL:HG13	1.98	0.45
1:E:713:ILE:HA	1:E:745:HIS:CE1	2.51	0.45
2:L:65:ASP:N	2:L:77:ILE:O	2.41	0.45
5:S:436:GLU:HA	5:S:439:VAL:HG22	1.98	0.45
5:S:675:ARG:HA	5:S:678:LYS:HG2	1.97	0.45
5:S:1057:LYS:HB3	5:S:1061:LYS:NZ	2.30	0.45
5:S:1651:LYS:O	5:S:1654:GLN:HG2	2.16	0.45
5:S:3177:ASN:OD1	5:S:3178:ILE:N	2.49	0.45
5:S:3689:ASP:N	5:S:3689:ASP:OD1	2.47	0.45
5:S:3767:LEU:HD21	5:S:4002:MET:HA	1.98	0.45
2:L:262:ALA:N	2:L:365:PHE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:81:CYS:O	5:S:85:ILE:HG12	2.17	0.45
5:S:87:LYS:HD3	5:S:831:LEU:HD13	1.98	0.45
5:S:1034:ARG:HH21	5:S:1087:ARG:HB2	1.81	0.45
5:S:1308:ALA:HB3	5:S:1310:GLU:HG2	1.98	0.45
5:S:2227:LYS:HB2	5:S:2230:VAL:HG22	1.98	0.45
5:S:2425:ARG:NH1	5:S:2460:GLU:OE2	2.49	0.45
5:S:3901:ARG:HH21	5:S:3970:LEU:HG	1.81	0.45
5:S:4040:PRO:O	5:S:4044:ILE:HD12	2.17	0.45
2:L:496:HIS:CD2	2:L:505:LEU:HD13	2.52	0.45
2:L:665:LYS:O	2:L:668:ILE:HG12	2.15	0.45
5:S:240:GLU:HB2	5:S:242:PRO:HD2	1.98	0.45
5:S:759:GLY:HA2	5:S:762:TYR:O	2.17	0.45
5:S:771:ASN:O	5:S:774:GLU:HG3	2.14	0.45
5:S:1844:VAL:HG23	5:S:1845:VAL:H	1.80	0.45
5:S:1849:ASP:OD1	5:S:1850:VAL:N	2.49	0.45
5:S:1864:ASP:OD1	5:S:1864:ASP:N	2.46	0.45
5:S:2360:PHE:O	5:S:2364:LEU:HD23	2.17	0.45
5:S:2387:PRO:O	6:T:158:GLN:NE2	2.30	0.45
5:S:2873:PRO:HB2	5:S:2925:GLU:OE1	2.17	0.45
5:S:3000:ASP:O	5:S:3004:HIS:ND1	2.32	0.45
5:S:4055:ASN:HD21	5:S:4057:ALA:HB3	1.80	0.45
1:E:720:VAL:HG23	1:E:745:HIS:HB3	1.98	0.45
2:L:327:ASP:O	2:L:331:MET:HG2	2.16	0.45
5:S:15:LEU:O	5:S:19:LEU:HG	2.16	0.45
5:S:213:ARG:O	6:T:404:ARG:NH2	2.50	0.45
5:S:559:SER:OG	5:S:560:LEU:N	2.38	0.45
5:S:3251:ASN:O	5:S:3254:LEU:HD22	2.16	0.45
6:T:102:ILE:HG21	6:T:149:VAL:HG21	1.98	0.45
9:A:68:HIS:CD2	9:A:122:ARG:HH22	2.35	0.45
1:E:835:GLY:HA2	4:P:150:ARG:HD2	1.98	0.45
2:L:315:ARG:HA	2:L:320:ILE:HA	1.98	0.45
5:S:452:LYS:HE3	5:S:453:MET:HE1	1.98	0.45
5:S:458:CYS:O	5:S:462:VAL:HG23	2.17	0.45
5:S:968:VAL:HA	5:S:971:ARG:HG2	1.98	0.45
5:S:1424:THR:HG23	5:S:1426:GLN:H	1.82	0.45
5:S:1633:TRP:CD2	5:S:1674:THR:HG21	2.51	0.45
5:S:3107:ILE:HG22	5:S:3135:LEU:HD13	1.98	0.45
5:S:3585:PHE:CG	5:S:3667:LEU:HD23	2.52	0.45
6:T:32:TYR:HE2	7:i:34:DC:H4'	1.80	0.45
6:T:200:LEU:HD23	6:T:200:LEU:H	1.82	0.45
6:T:400:TYR:N	6:T:409:TYR:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:THR:OG1	2:L:63:GLY:O	2.33	0.45
2:L:264:TYR:O	2:L:363:LYS:N	2.43	0.45
5:S:144:MET:HE3	5:S:144:MET:HA	1.99	0.45
5:S:476:ARG:NH2	5:S:1558:TYR:O	2.50	0.45
5:S:1397:ASP:OD1	5:S:1398:VAL:N	2.50	0.45
5:S:1952:ILE:HD12	5:S:1961:PHE:HD1	1.79	0.45
5:S:3568:ILE:HA	5:S:3571:PHE:HD2	1.82	0.45
5:S:3589:SER:HA	5:S:3592:VAL:HG12	1.98	0.45
6:T:86:VAL:HG23	6:T:104:VAL:HA	1.99	0.45
9:A:50:ARG:NH1	9:A:50:ARG:O	2.39	0.45
9:A:60:LEU:HA	9:A:63:LYS:HE3	1.98	0.45
9:A:114:TRP:HB2	9:A:130:PHE:CD2	2.51	0.45
4:P:158:VAL:HG22	4:P:161:ARG:HH22	1.81	0.45
5:S:442:GLN:O	5:S:445:SER:OG	2.31	0.45
5:S:978:GLN:OE1	5:S:2598:ARG:N	2.50	0.45
5:S:1297:PHE:HA	5:S:1301:ILE:HG12	1.99	0.45
5:S:1342:MET:O	5:S:1346:THR:HG23	2.17	0.45
6:T:340:PHE:HD2	6:T:408:PRO:HD2	1.82	0.45
8:j:19:DA:H1'	8:j:20:DT:H5'	1.99	0.45
9:A:117:LEU:HD23	9:A:125:VAL:HG21	1.97	0.45
2:L:161:LEU:HD12	2:L:163:PHE:CE1	2.51	0.45
5:S:745:VAL:HA	5:S:748:TYR:CD2	2.51	0.45
5:S:890:LYS:HA	5:S:890:LYS:HD3	1.74	0.45
5:S:994:TRP:CD2	5:S:2581:LEU:HD21	2.52	0.45
5:S:1387:GLY:O	5:S:1389:VAL:HG13	2.17	0.45
5:S:2584:CYS:SG	5:S:2585:GLU:N	2.89	0.45
1:E:825:VAL:HA	1:E:878:PHE:HZ	1.81	0.45
2:L:438:LEU:HD12	2:L:441:SER:HB3	1.99	0.45
5:S:175:TYR:HB2	5:S:223:CYS:HB3	1.98	0.45
5:S:181:LEU:HD23	5:S:181:LEU:HA	1.83	0.45
5:S:1067:ALA:HB1	5:S:1110:SER:HB3	1.98	0.45
5:S:1770:GLN:O	5:S:1771:GLN:HG3	2.16	0.45
5:S:3100:LYS:HA	5:S:3103:ILE:HG22	1.99	0.45
5:S:3311:ASN:HB2	5:S:3314:SER:HA	1.98	0.45
5:S:3326:GLN:HA	5:S:3329:LEU:HD12	1.98	0.45
5:S:2210:VAL:O	5:S:2214:ARG:HG2	2.16	0.44
5:S:2434:VAL:O	5:S:2438:ILE:HG12	2.17	0.44
5:S:3075:LYS:HA	5:S:3078:LEU:HG	1.99	0.44
5:S:3700:GLU:HG3	5:S:3718:ARG:HH11	1.82	0.44
6:T:218:ARG:H	6:T:221:ILE:HG12	1.81	0.44
2:L:45:GLN:NE2	2:L:50:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:LEU:HD12	2:L:80:HIS:HB3	1.98	0.44
2:L:484:ASN:ND2	2:L:486:ARG:HB3	2.32	0.44
2:L:530:LEU:HD13	6:T:264:ASN:HD22	1.82	0.44
5:S:865:GLN:HB2	5:S:3168:TYR:CE2	2.51	0.44
5:S:1227:GLY:HA2	5:S:1260:LEU:HD23	1.97	0.44
5:S:2154:GLU:HA	5:S:2157:PHE:CE1	2.53	0.44
5:S:2254:ARG:CZ	5:S:2292:CYS:HA	2.47	0.44
5:S:2492:ASP:OD2	5:S:2495:SER:N	2.36	0.44
5:S:2832:ILE:N	5:S:2835:LYS:HZ2	2.15	0.44
5:S:3665:MET:HA	5:S:3668:LEU:HG	1.97	0.44
5:S:4085:LYS:O	5:S:4089:ILE:HG12	2.16	0.44
6:T:303:PHE:HA	6:T:311:LEU:H	1.81	0.44
1:E:725:TRP:HA	1:E:741:ARG:HH22	1.82	0.44
5:S:1034:ARG:NH1	5:S:1088:GLU:OE2	2.51	0.44
5:S:2751:GLN:HA	5:S:2754:GLU:CD	2.42	0.44
5:S:3820:MET:HG2	5:S:3824:GLU:HB3	1.99	0.44
5:S:3887:PHE:HA	5:S:3890:MET:HG3	1.99	0.44
5:S:3923:ARG:HD2	5:S:4121:TRP:CD1	2.51	0.44
2:L:71:GLY:O	2:L:73:GLN:N	2.51	0.44
2:L:523:THR:O	2:L:527:GLN:HG2	2.17	0.44
5:S:1071:ASN:ND2	5:S:1074:LYS:HG3	2.33	0.44
5:S:1215:GLU:OE1	5:S:1222:ASN:ND2	2.49	0.44
5:S:1220:LEU:O	5:S:1224:PHE:HB2	2.18	0.44
5:S:1874:TYR:HB3	5:S:1947:CYS:SG	2.57	0.44
5:S:2886:GLN:HB3	5:S:2929:LEU:HD12	1.99	0.44
5:S:3320:ILE:HD11	5:S:3394:GLU:HB2	1.99	0.44
5:S:3327:ASN:HB2	5:S:3388:ALA:HB2	2.00	0.44
5:S:3868:VAL:HG22	5:S:3872:ARG:HH11	1.83	0.44
1:E:702:ALA:N	1:E:721:VAL:O	2.47	0.44
5:S:1597:LEU:HD11	5:S:1648:LEU:HD22	1.99	0.44
5:S:2105:HIS:HB2	5:S:2156:VAL:HG13	2.00	0.44
5:S:2293:GLY:O	5:S:2295:GLN:N	2.50	0.44
5:S:3241:LYS:HE3	5:S:3241:LYS:HB2	1.75	0.44
5:S:3425:ARG:NH2	5:S:3428:GLU:HG2	2.31	0.44
6:T:403:ARG:HD3	6:T:404:ARG:O	2.16	0.44
1:E:668:SER:HG	1:E:708:ARG:HH21	1.63	0.44
5:S:655:LEU:O	5:S:659:ARG:HG2	2.17	0.44
5:S:746:ARG:HH22	5:S:788:TYR:HD2	1.66	0.44
5:S:981:ARG:HA	5:S:984:TYR:HB2	1.99	0.44
5:S:3234:CYS:O	5:S:3238:MET:HG2	2.17	0.44
1:E:864:ILE:HG13	1:E:889:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:653:GLN:O	2:L:657:ASN:ND2	2.51	0.44
5:S:465:PHE:CE1	5:S:479:ILE:HG22	2.53	0.44
5:S:733:LEU:HA	5:S:736:LEU:HD23	2.00	0.44
5:S:953:GLN:H	5:S:956:PRO:HD3	1.82	0.44
5:S:1633:TRP:CD1	5:S:1674:THR:HG21	2.53	0.44
5:S:675:ARG:NH1	5:S:676:ASN:OD1	2.50	0.44
5:S:1207:TRP:HE3	5:S:1208:LEU:HD12	1.82	0.44
5:S:1834:ASP:HA	5:S:1837:ARG:HD2	2.00	0.44
5:S:1850:VAL:HG21	5:S:1873:TYR:CZ	2.53	0.44
5:S:2328:ARG:HH21	5:S:2372:PRO:HD2	1.83	0.44
5:S:2791:ILE:HG13	5:S:2792:THR:N	2.33	0.44
5:S:3877:LYS:HZ2	5:S:4127:TRP:CG	2.36	0.44
5:S:4012:ASP:C	5:S:4014:LYS:N	2.76	0.44
6:T:115:ARG:HA	6:T:118:GLU:HG2	1.99	0.44
7:i:38:DT:N3	8:j:19:DA:N1	2.66	0.44
9:A:114:TRP:HB2	9:A:130:PHE:CG	2.53	0.44
1:E:722:LYS:HB2	1:E:742:PHE:HB2	1.99	0.44
2:L:56:LEU:HG	2:L:81:ARG:HB3	1.99	0.44
2:L:366:ALA:HB2	2:L:377:LEU:HD12	2.00	0.44
2:L:513:TRP:O	2:L:517:ASN:N	2.35	0.44
5:S:188:GLU:HG2	5:S:189:MET:H	1.83	0.44
5:S:374:LYS:HE2	5:S:381:VAL:HG21	2.00	0.44
5:S:1082:PHE:HZ	5:S:1134:LEU:HD21	1.83	0.44
5:S:1136:ARG:O	5:S:1139:GLU:HG2	2.18	0.44
5:S:1146:ASN:ND2	5:S:1199:PRO:HG3	2.33	0.44
5:S:3443:PRO:HA	5:S:3446:VAL:HG22	1.99	0.44
5:S:3447:VAL:HA	5:S:3450:MET:HE2	2.00	0.44
5:S:4064:LEU:HB3	5:S:4074:PHE:HE1	1.83	0.44
6:T:466:VAL:O	6:T:470:ARG:HG3	2.17	0.44
6:T:481:PRO:HA	6:T:484:GLN:HG2	1.99	0.44
6:T:483:LEU:HA	6:T:486:HIS:HD1	1.83	0.44
5:S:12:LEU:HA	5:S:15:LEU:HD12	2.00	0.43
5:S:380:ASP:HA	5:S:383:PHE:HB2	2.00	0.43
5:S:581:LEU:HB3	5:S:660:LEU:HD12	1.99	0.43
5:S:1000:LYS:HB2	5:S:1004:GLN:NE2	2.33	0.43
5:S:1019:ASP:OD1	5:S:1019:ASP:N	2.48	0.43
5:S:1204:PRO:HG2	5:S:1206:LEU:HG	2.00	0.43
5:S:1367:HIS:HB2	5:S:1370:ARG:CZ	2.48	0.43
5:S:1963:GLN:HB2	5:S:2125:TRP:CZ2	2.53	0.43
5:S:2430:GLU:HG2	5:S:2431:ARG:N	2.33	0.43
9:A:64:GLN:O	9:A:68:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:289:ILE:HA	6:T:311:LEU:HD11	2.00	0.43
2:L:402:ASN:N	7:i:25:DA:OP1	2.51	0.43
5:S:754:MET:HE3	5:S:1021:VAL:HG11	2.00	0.43
5:S:1102:GLU:HA	5:S:1154:PRO:HB3	2.00	0.43
5:S:2410:GLU:OE2	5:S:2412:TYR:N	2.51	0.43
1:E:682:ILE:HG13	1:E:730:PHE:CZ	2.50	0.43
2:L:205:LEU:HG	2:L:209:LYS:HD2	1.99	0.43
2:L:413:LYS:N	2:L:416:TYR:O	2.50	0.43
5:S:57:LEU:HB3	5:S:103:TYR:HE2	1.83	0.43
5:S:174:VAL:O	5:S:178:LEU:HG	2.19	0.43
5:S:708:VAL:C	5:S:712:LYS:HZ2	2.26	0.43
5:S:727:ALA:O	5:S:731:THR:OG1	2.30	0.43
5:S:781:ASP:O	5:S:785:MET:HG2	2.18	0.43
5:S:960:GLN:HA	5:S:963:LYS:HZ3	1.84	0.43
5:S:1390:GLN:HA	5:S:1393:ALA:HB3	1.99	0.43
5:S:1794:GLN:O	5:S:1798:LEU:HG	2.18	0.43
5:S:3247:ARG:HE	5:S:3282:ARG:HE	1.65	0.43
5:S:3289:ARG:H	5:S:3292:GLY:HA3	1.83	0.43
5:S:3772:ASN:HD21	5:S:3787:GLN:HE21	1.66	0.43
5:S:196:LEU:HB3	5:S:200:PHE:CE2	2.53	0.43
5:S:896:VAL:O	5:S:902:LYS:HB3	2.17	0.43
5:S:2311:ARG:HG2	5:S:2312:TYR:HD1	1.84	0.43
5:S:2805:ALA:HA	5:S:2808:LEU:HG	2.00	0.43
5:S:3257:LYS:HA	5:S:3257:LYS:HD3	1.71	0.43
5:S:3270:ASP:N	5:S:3270:ASP:OD1	2.50	0.43
5:S:3584:LEU:HD12	5:S:3799:ARG:HH21	1.84	0.43
5:S:3633:ILE:HG13	5:S:3634:GLN:N	2.33	0.43
5:S:3700:GLU:HA	5:S:3718:ARG:HA	2.00	0.43
5:S:3800:LEU:HD12	5:S:3800:LEU:HA	1.93	0.43
5:S:3901:ARG:NH2	5:S:3970:LEU:HG	2.32	0.43
6:T:420:LEU:HB3	6:T:424:LYS:HA	2.00	0.43
5:S:321:LYS:HD2	5:S:321:LYS:HA	1.71	0.43
5:S:417:VAL:O	5:S:421:LEU:HD23	2.18	0.43
5:S:1405:ALA:HA	5:S:1408:MET:HE2	2.00	0.43
5:S:1632:TRP:HD1	5:S:1645:VAL:HB	1.84	0.43
5:S:1948:ALA:O	5:S:1952:ILE:HG12	2.19	0.43
5:S:2254:ARG:HH11	5:S:2294:ILE:HG13	1.83	0.43
5:S:2271:SER:HA	5:S:2274:ILE:HD13	2.01	0.43
5:S:3718:ARG:H	5:S:3743:HIS:HB3	1.84	0.43
6:T:77:SER:HA	6:T:248:ALA:O	2.18	0.43
9:A:89:MET:HE2	9:A:89:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:513:TRP:HB3	2:L:517:ASN:ND2	2.33	0.43
4:Q:194:LEU:HA	4:Q:197:LYS:HE2	2.01	0.43
5:S:207:GLN:C	5:S:217:LEU:HD11	2.44	0.43
5:S:682:TYR:CZ	5:S:700:LYS:HG2	2.54	0.43
5:S:935:HIS:HA	5:S:938:VAL:HG12	2.00	0.43
5:S:1056:THR:HG21	5:S:1095:LEU:HD13	2.00	0.43
5:S:1475:LEU:HB2	5:S:1477:HIS:CE1	2.53	0.43
5:S:3075:LYS:O	5:S:3078:LEU:HG	2.18	0.43
5:S:3287:ARG:HA	5:S:3289:ARG:HH21	1.82	0.43
8:j:27:DT:H2"	8:j:28:DA:C8	2.53	0.43
2:L:662:LEU:HA	2:L:665:LYS:HE2	2.01	0.43
4:Q:161:ARG:HA	4:Q:164:LYS:HE3	2.01	0.43
5:S:290:TYR:OH	5:S:339:GLN:OE1	2.28	0.43
5:S:293:LEU:HA	5:S:296:VAL:HG12	2.01	0.43
5:S:1425:ALA:HA	5:S:1428:ILE:HG22	2.00	0.43
5:S:1504:ASP:O	5:S:1508:LYS:N	2.48	0.43
5:S:2300:PHE:HD2	5:S:2341:LEU:HD13	1.84	0.43
5:S:2467:THR:HB	5:S:2517:LEU:HD11	2.00	0.43
5:S:2497:GLU:HA	5:S:2500:LYS:HD2	2.00	0.43
5:S:2869:LEU:HB2	5:S:2899:ARG:HE	1.83	0.43
5:S:3739:ILE:HG23	5:S:3747:GLU:CD	2.44	0.43
5:S:4080:VAL:HG21	5:S:4119:ARG:HD2	2.01	0.43
1:E:806:ASP:HB3	1:E:816:HIS:CD2	2.53	0.43
2:L:604:GLN:HG3	2:L:605:LYS:HG3	2.01	0.43
4:Q:178:LYS:HA	4:Q:181:ILE:HG22	2.01	0.43
5:S:450:SER:N	5:S:453:MET:SD	2.92	0.43
5:S:864:GLY:N	5:S:3170:ASP:OD1	2.40	0.43
5:S:898:PHE:H	5:S:902:LYS:HE3	1.83	0.43
5:S:1287:GLN:OE1	5:S:1289:SER:N	2.48	0.43
5:S:2431:ARG:HA	5:S:2434:VAL:HG12	2.01	0.43
5:S:2816:ILE:O	5:S:2820:MET:HG2	2.18	0.43
5:S:3078:LEU:HD13	5:S:3086:LEU:HD11	1.99	0.43
5:S:3165:THR:O	5:S:3238:MET:HE1	2.19	0.43
5:S:3828:TYR:OH	5:S:4127:TRP:NE1	2.51	0.43
2:L:6:ASN:HA	2:L:51:LYS:HD2	2.01	0.43
2:L:675:TRP:O	2:L:679:VAL:N	2.48	0.43
4:P:183:VAL:HG11	4:Q:184:LEU:HD13	2.01	0.43
5:S:57:LEU:O	5:S:60:SER:OG	2.33	0.43
5:S:2752:LYS:HD2	5:S:2755:LYS:HZ1	1.84	0.43
5:S:3761:ASP:OD1	5:S:3762:GLN:N	2.51	0.43
5:S:3767:LEU:HA	5:S:3770:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3923:ARG:HH11	5:S:4121:TRP:HE1	1.66	0.43
6:T:99:PHE:CD2	6:T:145:GLU:HB2	2.54	0.43
6:T:357:LYS:HE2	6:T:359:HIS:NE2	2.33	0.43
2:L:154:LEU:HD23	2:L:154:LEU:HA	1.88	0.43
2:L:243:HIS:HD2	2:L:264:TYR:HE2	1.66	0.43
2:L:250:ARG:HA	2:L:260:ARG:HA	2.01	0.43
2:L:291:LYS:HA	6:T:302:THR:HA	2.00	0.43
2:L:463:LEU:C	6:T:351:LYS:HZ3	2.27	0.43
4:P:185:ASN:O	4:P:189:THR:HG23	2.19	0.43
5:S:1011:GLU:HA	5:S:1014:LEU:HG	2.01	0.43
5:S:1304:HIS:CD2	5:S:1307:ILE:HG23	2.54	0.43
5:S:1934:LEU:HA	5:S:1937:ARG:HH12	1.84	0.43
5:S:2150:VAL:HG23	5:S:2157:PHE:CZ	2.54	0.43
5:S:3972:LEU:HB3	5:S:3973:PRO:HD3	2.00	0.43
1:E:787:GLN:HE22	4:Q:178:LYS:NZ	2.17	0.42
1:E:812:MET:HE1	1:E:844:GLU:HB3	2.01	0.42
2:L:88:PHE:HD1	2:L:91:LEU:HD12	1.84	0.42
2:L:163:PHE:HB2	2:L:224:ILE:HG12	2.00	0.42
2:L:311:ILE:HA	2:L:325:LYS:NZ	2.34	0.42
5:S:23:ASP:OD1	5:S:23:ASP:N	2.52	0.42
5:S:247:GLU:OE1	5:S:285:CYS:HB2	2.19	0.42
5:S:851:ILE:O	5:S:855:VAL:HG23	2.19	0.42
5:S:977:ASP:HB3	5:S:980:THR:OG1	2.19	0.42
5:S:2331:MET:HE1	5:S:2338:GLU:OE1	2.18	0.42
5:S:3923:ARG:HD2	5:S:4121:TRP:HD1	1.84	0.42
5:S:3971:MET:SD	5:S:3974:MET:HB2	2.59	0.42
2:L:92:GLU:HA	2:L:95:GLU:HG3	2.01	0.42
5:S:721:TYR:HB2	5:S:726:LEU:HB3	2.00	0.42
5:S:785:MET:HB3	5:S:789:TYR:CZ	2.54	0.42
5:S:933:LEU:HD22	5:S:2797:VAL:HG21	2.00	0.42
5:S:1082:PHE:CZ	5:S:1134:LEU:HD21	2.55	0.42
5:S:2170:GLN:HA	5:S:2211:LEU:HD22	2.01	0.42
5:S:2183:HIS:O	5:S:2187:VAL:HG13	2.18	0.42
5:S:2317:ALA:O	5:S:2366:LYS:HD3	2.20	0.42
5:S:2452:ARG:CZ	5:S:2494:ASP:HB3	2.49	0.42
5:S:3172:LYS:HD2	5:S:3172:LYS:HA	1.77	0.42
5:S:3193:ILE:HA	5:S:3196:LYS:HG2	2.01	0.42
6:T:262:LYS:O	6:T:346:MET:HA	2.19	0.42
1:E:883:LYS:HD3	1:E:883:LYS:HA	1.81	0.42
5:S:1268:ASN:HD21	5:S:1344:PHE:HB2	1.84	0.42
5:S:1569:THR:O	5:S:1573:LYS:NZ	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2421:VAL:HA	5:S:2424:MET:HG3	2.01	0.42
5:S:2548:PRO:HB2	5:S:2848:PHE:CD1	2.55	0.42
5:S:3835:PRO:HB2	5:S:3836:PRO:HD3	2.00	0.42
6:T:301:ARG:NH1	9:A:57:ARG:HH21	2.17	0.42
9:A:41:LEU:HB2	9:A:68:HIS:HB2	2.00	0.42
2:L:61:THR:N	2:L:76:ASN:O	2.52	0.42
2:L:251:LEU:HD23	2:L:259:ILE:HD13	2.02	0.42
5:S:891:ARG:HH12	5:S:959:TYR:H	1.67	0.42
5:S:1256:TRP:CE2	5:S:1260:LEU:HD11	2.54	0.42
5:S:1614:GLN:HA	5:S:1617:LYS:HE2	2.01	0.42
6:T:301:ARG:HH12	9:A:57:ARG:HH21	1.65	0.42
2:L:250:ARG:NH2	6:T:536:PRO:HB2	2.35	0.42
5:S:130:LEU:HD12	5:S:130:LEU:HA	1.79	0.42
5:S:479:ILE:HA	5:S:482:VAL:HG22	2.01	0.42
5:S:858:MET:HE2	5:S:858:MET:HB2	1.94	0.42
5:S:943:GLY:HA3	5:S:2783:ILE:HG21	2.00	0.42
5:S:978:GLN:NE2	5:S:2597:PHE:HA	2.35	0.42
5:S:1017:ILE:HG13	5:S:1018:VAL:N	2.34	0.42
5:S:1658:SER:O	5:S:1662:ASN:HB3	2.19	0.42
5:S:1713:VAL:O	5:S:1716:GLN:HG2	2.20	0.42
5:S:1936:ARG:HH21	5:S:1937:ARG:NH2	2.17	0.42
5:S:2364:LEU:HA	5:S:2367:VAL:HG22	2.02	0.42
5:S:3416:LEU:HB3	5:S:3449:LYS:NZ	2.35	0.42
6:T:465:ILE:HG13	6:T:525:PHE:HE2	1.84	0.42
8:j:32:DT:H2"	8:j:33:DA:N7	2.34	0.42
2:L:298:ASN:HB3	6:T:297:LYS:HG2	2.01	0.42
2:L:327:ASP:OD1	2:L:328:GLU:N	2.51	0.42
2:L:497:ARG:NH2	2:L:500:HIS:O	2.53	0.42
2:L:596:GLU:HA	2:L:599:ARG:HD2	2.01	0.42
4:P:155:TRP:HD1	4:Q:155:TRP:HA	1.85	0.42
5:S:1834:ASP:N	5:S:1834:ASP:OD1	2.51	0.42
5:S:3588:TRP:CZ3	5:S:3609:MET:HG3	2.55	0.42
5:S:3700:GLU:OE2	5:S:3704:GLN:NE2	2.38	0.42
6:T:339:ARG:HA	6:T:405:ASN:HA	2.01	0.42
6:T:363:ARG:HG3	6:T:364:PRO:HD2	2.02	0.42
2:L:223:GLU:OE2	2:L:238:LYS:NZ	2.53	0.42
5:S:993:HIS:O	5:S:996:THR:OG1	2.37	0.42
5:S:1018:VAL:HG22	5:S:1074:LYS:HG2	2.01	0.42
5:S:1031:ARG:NH2	5:S:1034:ARG:HH11	2.14	0.42
5:S:2184:TYR:O	5:S:2187:VAL:HG22	2.19	0.42
5:S:2890:ILE:HD11	5:S:2929:LEU:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2953:THR:OG1	5:S:2994:TRP:NE1	2.52	0.42
6:T:32:TYR:HB2	6:T:252:ARG:HH22	1.83	0.42
6:T:403:ARG:NE	7:i:32:DA:OP1	2.43	0.42
1:E:778:PHE:CG	4:Q:176:LEU:HD22	2.54	0.42
2:L:677:ILE:HA	2:L:680:GLN:HG2	2.01	0.42
5:S:30:ALA:O	5:S:34:LEU:HG	2.20	0.42
5:S:73:LEU:O	5:S:82:ARG:NH2	2.53	0.42
5:S:520:LYS:HA	5:S:520:LYS:HD2	1.90	0.42
5:S:774:GLU:O	5:S:778:ILE:HG12	2.20	0.42
5:S:1258:ASP:HA	5:S:1261:LEU:HD12	2.02	0.42
5:S:2261:SER:O	5:S:2270:ASN:ND2	2.48	0.42
5:S:2584:CYS:HB3	5:S:2586:PHE:CZ	2.55	0.42
5:S:2820:MET:HA	5:S:2823:PHE:HE1	1.85	0.42
5:S:3156:PRO:O	5:S:3160:LEU:N	2.53	0.42
5:S:3741:ARG:HA	5:S:3747:GLU:HA	2.02	0.42
9:A:83:ILE:HG13	9:A:107:ALA:HB1	2.01	0.42
2:L:16:VAL:HG21	2:L:61:THR:HG22	2.02	0.42
2:L:154:LEU:HD13	2:L:215:LEU:HD13	2.02	0.42
2:L:155:LYS:HA	2:L:155:LYS:HD3	1.68	0.42
2:L:453:ALA:O	2:L:533:ILE:HD11	2.20	0.42
5:S:194:GLU:O	5:S:198:ARG:HG2	2.20	0.42
5:S:294:PHE:HE1	5:S:319:PHE:HE2	1.68	0.42
5:S:992:ILE:HG23	5:S:1036:PHE:CD1	2.49	0.42
5:S:2468:THR:HA	5:S:2471:GLU:CD	2.45	0.42
5:S:3295:GLU:O	5:S:3298:LEU:HG	2.20	0.42
5:S:3700:GLU:HG3	5:S:3718:ARG:HD3	2.01	0.42
5:S:3828:TYR:CD2	5:S:3829:LEU:HD22	2.54	0.42
6:T:82:LEU:C	6:T:83:LEU:HD12	2.44	0.42
6:T:488:ARG:CZ	6:T:503:ALA:HA	2.50	0.42
1:E:720:VAL:HG11	1:E:744:ILE:HB	2.02	0.42
1:E:811:SER:O	1:E:900:LYS:HG2	2.18	0.42
5:S:1588:ASP:OD1	5:S:1588:ASP:N	2.52	0.42
5:S:3580:ASN:OD1	5:S:3580:ASN:N	2.53	0.42
5:S:4010:SER:O	5:S:4011:PHE:C	2.62	0.42
6:T:33:SER:HB3	6:T:162:SER:HB2	2.02	0.42
6:T:64:ILE:O	6:T:68:GLN:HG2	2.20	0.42
7:i:20:DT:O2	8:j:38:DG:N1	2.50	0.42
8:j:15:DA:N3	8:j:16:DA:N6	2.67	0.42
1:E:675:LYS:HD2	1:E:675:LYS:HA	1.74	0.41
1:E:815:ARG:O	1:E:816:HIS:ND1	2.53	0.41
2:L:166:PRO:HA	2:L:227:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:366:TYR:HA	5:S:369:PHE:CD1	2.55	0.41
5:S:465:PHE:HE1	5:S:479:ILE:HG22	1.85	0.41
5:S:975:ASP:O	5:S:981:ARG:NH2	2.53	0.41
5:S:1135:CYS:HA	5:S:1138:ILE:HG12	2.01	0.41
5:S:2162:LYS:HZ3	5:S:2200:ALA:HA	1.83	0.41
5:S:2327:LEU:HG	5:S:2371:PHE:CG	2.55	0.41
5:S:2331:MET:O	5:S:2334:LYS:HG2	2.20	0.41
5:S:3110:PHE:HB3	5:S:3128:LYS:HE2	2.02	0.41
5:S:3353:GLU:HG3	5:S:3358:ARG:HH12	1.85	0.41
5:S:3449:LYS:HA	5:S:3452:LYS:HG2	2.02	0.41
5:S:3480:LEU:HD23	5:S:3480:LEU:HA	1.94	0.41
5:S:3765:GLU:OE2	5:S:3769:GLN:NE2	2.53	0.41
5:S:3872:ARG:HA	5:S:3875:GLU:HG2	2.01	0.41
5:S:4106:CYS:SG	5:S:4110:GLN:NE2	2.93	0.41
8:j:24:DT:H1'	8:j:25:DT:H5'	2.02	0.41
2:L:279:VAL:HG23	6:T:317:LYS:HB2	2.02	0.41
4:P:175:ASP:O	4:P:179:ARG:HG2	2.20	0.41
5:S:1607:GLU:OE1	5:S:1610:ASN:ND2	2.52	0.41
5:S:1952:ILE:HG23	5:S:1961:PHE:CE1	2.54	0.41
5:S:2208:ASP:OD1	5:S:2209:GLU:N	2.53	0.41
5:S:3090:TYR:HB3	5:S:3095:ASP:HB2	2.02	0.41
5:S:3171:ALA:HA	5:S:3179:TRP:CZ2	2.56	0.41
5:S:3639:GLU:HA	5:S:3642:LYS:HE2	2.02	0.41
6:T:269:ILE:HG23	6:T:378:SER:HB3	2.02	0.41
6:T:276:LEU:H	6:T:276:LEU:HD23	1.84	0.41
6:T:288:LEU:HA	6:T:295:PRO:HA	2.02	0.41
6:T:418:GLU:HA	6:T:428:THR:O	2.19	0.41
2:L:54:ILE:HG22	2:L:86:PRO:HD3	2.02	0.41
2:L:512:ILE:HA	2:L:515:MET:SD	2.61	0.41
5:S:337:LYS:HA	5:S:341:PHE:CD1	2.55	0.41
5:S:428:PRO:HB2	5:S:431:TYR:CD2	2.55	0.41
5:S:475:LEU:O	5:S:479:ILE:HG12	2.20	0.41
5:S:1506:SER:O	5:S:1509:GLN:NE2	2.53	0.41
5:S:1632:TRP:CD1	5:S:1645:VAL:HB	2.55	0.41
5:S:1713:VAL:HA	5:S:1716:GLN:NE2	2.35	0.41
5:S:1779:GLN:O	5:S:1783:ARG:HG2	2.20	0.41
5:S:3114:TYR:HB2	5:S:3128:LYS:HZ2	1.85	0.41
5:S:3761:ASP:HA	5:S:3764:VAL:HG12	2.02	0.41
5:S:3814:ASP:OD1	5:S:3814:ASP:N	2.54	0.41
5:S:3967:PHE:O	5:S:3970:LEU:HD22	2.20	0.41
2:L:291:LYS:HE2	6:T:300:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:618:ASN:HA	2:L:621:GLU:CD	2.45	0.41
5:S:275:PHE:CE2	5:S:319:PHE:HB2	2.55	0.41
5:S:446:PHE:CE1	5:S:454:GLN:HG2	2.55	0.41
5:S:993:HIS:HE2	5:S:1035:GLU:CD	2.27	0.41
5:S:1693:VAL:HG11	5:S:1746:PHE:CE1	2.55	0.41
5:S:2300:PHE:CD2	5:S:2341:LEU:HD13	2.55	0.41
5:S:2364:LEU:O	5:S:2368:THR:HG22	2.20	0.41
5:S:2514:ASN:HB3	5:S:2517:LEU:HG	2.02	0.41
5:S:2773:ARG:HH21	5:S:2785:ILE:HD13	1.85	0.41
5:S:3778:ASP:HB3	5:S:3781:CYS:HB2	2.02	0.41
5:S:4099:SER:HB3	5:S:4102:THR:HG1	1.86	0.41
6:T:67:ILE:HA	6:T:70:VAL:HG22	2.02	0.41
6:T:510:LYS:NZ	6:T:517:ARG:HH22	2.18	0.41
1:E:706:ASN:HB3	1:E:708:ARG:HH11	1.85	0.41
1:E:815:ARG:HA	1:E:851:LYS:HA	2.03	0.41
2:L:111:LEU:HD21	2:L:134:ILE:HG12	2.03	0.41
2:L:309:ASP:HA	6:T:290:ARG:HE	1.85	0.41
2:L:381:ILE:HG23	2:L:410:PRO:HB2	2.02	0.41
5:S:460:ALA:O	5:S:464:VAL:HG13	2.21	0.41
5:S:1489:LYS:HA	5:S:1489:LYS:HD3	1.82	0.41
5:S:1526:GLU:OE2	5:S:1527:ARG:NE	2.54	0.41
5:S:2840:PHE:HB2	5:S:2871:LEU:HD11	2.03	0.41
5:S:2935:GLU:OE1	5:S:2937:ASP:N	2.53	0.41
5:S:3011:LEU:HB3	5:S:3047:SER:CB	2.50	0.41
5:S:3033:GLU:HG2	5:S:3034:PRO:HD3	2.01	0.41
5:S:3459:ASN:O	5:S:3463:LEU:HG	2.21	0.41
5:S:3460:GLU:O	5:S:3464:LYS:NZ	2.48	0.41
5:S:3498:TRP:O	5:S:3502:MET:HG2	2.20	0.41
5:S:4061:CYS:O	5:S:4065:LEU:HG	2.20	0.41
6:T:512:GLU:H	6:T:512:GLU:CD	2.29	0.41
1:E:797:ALA:HB1	1:E:801:TYR:CZ	2.55	0.41
1:E:876:LYS:HD3	1:E:876:LYS:HA	1.90	0.41
2:L:468:GLU:O	2:L:469:LYS:HG2	2.20	0.41
2:L:529:PRO:HA	2:L:532:LYS:HE2	2.03	0.41
5:S:225:LYS:HD2	5:S:270:ALA:HB1	2.02	0.41
5:S:651:TYR:HD1	5:S:706:LEU:HD11	1.85	0.41
5:S:789:TYR:HA	5:S:792:ILE:HG12	2.02	0.41
5:S:833:HIS:HB2	5:S:835:LYS:NZ	2.36	0.41
5:S:1065:SER:O	5:S:1068:LEU:HG	2.20	0.41
5:S:3330:LEU:HD23	5:S:3384:HIS:CD2	2.56	0.41
5:S:3351:ILE:O	5:S:3357:ARG:NH1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3585:PHE:CD2	5:S:3667:LEU:HD23	2.56	0.41
5:S:3713:PRO:HB2	5:S:3716:HIS:CE1	2.55	0.41
6:T:130:ARG:O	6:T:134:MET:HG3	2.21	0.41
6:T:369:TYR:CG	6:T:370:PRO:HD2	2.56	0.41
2:L:59:PHE:HA	2:L:77:ILE:HA	2.02	0.41
2:L:250:ARG:HG2	2:L:260:ARG:HG2	2.03	0.41
5:S:654:ILE:HD13	5:S:706:LEU:HD22	2.02	0.41
5:S:1205:ASN:OD1	5:S:1206:LEU:N	2.54	0.41
5:S:1753:SER:O	5:S:1754:GLN:HG2	2.20	0.41
5:S:2185:MET:O	5:S:2189:ILE:HG12	2.20	0.41
5:S:2253:TYR:CE1	5:S:2288:TYR:HA	2.55	0.41
5:S:2333:ARG:NH1	5:S:2336:ILE:HD11	2.36	0.41
5:S:3096:VAL:HG12	5:S:3100:LYS:NZ	2.35	0.41
5:S:3246:ALA:HA	5:S:3249:GLN:HB2	2.03	0.41
5:S:3753:LYS:HE3	5:S:3753:LYS:HB3	1.92	0.41
5:S:3780:ALA:HB3	5:S:3989:ARG:HH22	1.86	0.41
5:S:3815:LEU:HA	5:S:3818:ASN:HD21	1.86	0.41
5:S:3894:PRO:O	5:S:3897:PHE:HB3	2.20	0.41
6:T:94:LYS:HD3	6:T:103:TYR:CE1	2.55	0.41
1:E:816:HIS:H	1:E:851:LYS:N	2.19	0.41
4:P:154:ASP:HB3	4:Q:155:TRP:NE1	2.35	0.41
5:S:635:PRO:HA	5:S:675:ARG:HH12	1.86	0.41
5:S:672:ILE:HG23	5:S:675:ARG:NH2	2.36	0.41
5:S:714:VAL:HG13	5:S:733:LEU:HD21	2.03	0.41
5:S:1014:LEU:HA	5:S:1017:ILE:HG12	2.03	0.41
5:S:1047:GLN:C	5:S:1051:LYS:HZ2	2.29	0.41
5:S:1754:GLN:CD	5:S:1788:ARG:HH21	2.29	0.41
5:S:2187:VAL:HA	5:S:2190:VAL:HG22	2.02	0.41
5:S:2825:THR:O	5:S:2829:LYS:HG3	2.20	0.41
5:S:3075:LYS:HG3	5:S:3076:ALA:N	2.36	0.41
5:S:3281:CYS:O	5:S:3285:HIS:ND1	2.54	0.41
5:S:3471:ILE:HD12	5:S:3471:ILE:HA	1.97	0.41
5:S:3487:ILE:HD13	5:S:3487:ILE:HA	1.94	0.41
5:S:3626:GLY:O	5:S:3630:ARG:HD3	2.20	0.41
5:S:4069:GLU:HA	5:S:4074:PHE:CG	2.55	0.41
7:i:24:DA:H1'	7:i:25:DA:O4'	2.21	0.41
9:A:109:LEU:HD23	9:A:132:ILE:HB	2.03	0.41
1:E:768:ASP:OD1	1:E:768:ASP:N	2.54	0.41
2:L:395:TYR:N	2:L:404:GLN:O	2.37	0.41
2:L:528:ILE:O	2:L:531:SER:OG	2.30	0.41
5:S:87:LYS:O	5:S:90:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:135:LEU:HB2	5:S:177:LEU:HD11	2.02	0.41
5:S:418:ALA:HB2	5:S:464:VAL:HG12	2.03	0.41
5:S:832:LYS:NZ	5:S:836:LYS:HG3	2.36	0.41
5:S:931:CYS:O	5:S:934:LEU:HG	2.21	0.41
5:S:993:HIS:ND1	5:S:2779:ASP:HB2	2.36	0.41
5:S:1848:ILE:O	5:S:1852:LYS:NZ	2.43	0.41
5:S:2433:LYS:HG3	5:S:2472:GLN:HE22	1.86	0.41
5:S:2438:ILE:O	5:S:2442:MET:HG3	2.21	0.41
5:S:2575:PRO:HA	5:S:2785:ILE:O	2.20	0.41
5:S:2722:ARG:HA	5:S:2722:ARG:HD3	1.90	0.41
5:S:2869:LEU:HD13	5:S:2895:GLU:HG3	2.02	0.41
5:S:2957:LEU:HA	5:S:2960:GLU:HG3	2.03	0.41
5:S:2960:GLU:HB3	5:S:2968:ALA:HB2	2.03	0.41
5:S:3074:GLN:O	5:S:3077:ILE:HG12	2.20	0.41
5:S:3314:SER:HB3	5:S:3318:LYS:HD2	2.03	0.41
5:S:3563:ASP:O	5:S:3564:GLN:HG3	2.20	0.41
5:S:3686:TRP:CZ3	5:S:3691:LYS:HA	2.56	0.41
5:S:3757:ASP:O	5:S:3760:GLN:NE2	2.49	0.41
5:S:4055:ASN:ND2	5:S:4057:ALA:HB3	2.36	0.41
6:T:335:GLU:O	6:T:339:ARG:N	2.54	0.41
6:T:403:ARG:HE	7:i:32:DA:P	2.42	0.41
8:j:22:DG:H2"	8:j:23:DT:H71	2.03	0.41
9:A:50:ARG:HD3	9:A:55:ARG:NH1	2.36	0.41
2:L:443:LYS:H	2:L:443:LYS:HG2	1.73	0.41
2:L:667:GLU:HG2	2:L:675:TRP:NE1	2.36	0.41
3:M:194:LYS:HD2	3:M:195:PRO:O	2.20	0.41
5:S:326:MET:O	5:S:330:ASN:N	2.54	0.41
5:S:386:VAL:O	5:S:390:GLN:HG2	2.21	0.41
5:S:1176:CYS:HB3	5:S:1188:ILE:HD11	2.03	0.41
5:S:3048:LYS:HZ3	5:S:3061:LEU:HB2	1.85	0.41
5:S:3151:LEU:HA	5:S:3197:LEU:HG	2.03	0.41
5:S:3294:SER:HA	5:S:3297:VAL:HG22	2.02	0.41
5:S:3565:GLY:HA2	5:S:3568:ILE:HD13	2.03	0.41
5:S:3864:ARG:NH2	5:S:4085:LYS:HA	2.36	0.41
9:A:91:TYR:CD2	9:A:135:PRO:HD2	2.56	0.41
2:L:443:LYS:HG3	2:L:444:TYR:CD2	2.56	0.40
5:S:103:TYR:HA	5:S:106:GLU:CD	2.46	0.40
5:S:458:CYS:O	5:S:461:ILE:HG22	2.22	0.40
5:S:1087:ARG:HG3	5:S:1090:ARG:HH21	1.85	0.40
5:S:1164:CYS:N	5:S:1167:ASP:OD2	2.53	0.40
5:S:1947:CYS:O	5:S:1951:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2848:PHE:HD2	5:S:3077:ILE:HG22	1.87	0.40
5:S:3489:SER:OG	5:S:3490:VAL:N	2.53	0.40
6:T:275:ASN:ND2	6:T:278:GLN:HB2	2.37	0.40
6:T:308:GLY:HA3	9:A:61:PHE:HE1	1.87	0.40
2:L:40:MET:HA	2:L:43:GLN:HE21	1.86	0.40
2:L:277:THR:HB	2:L:286:LYS:HD2	2.03	0.40
2:L:466:LYS:HA	2:L:466:LYS:HD2	1.89	0.40
5:S:671:SER:HA	5:S:674:VAL:HG12	2.02	0.40
5:S:1065:SER:O	5:S:1069:HIS:ND1	2.55	0.40
5:S:2233:HIS:O	5:S:2237:ILE:HG13	2.21	0.40
5:S:3462:ARG:HG2	5:S:3498:TRP:HH2	1.85	0.40
6:T:74:LYS:HZ1	6:T:81:ASP:N	2.19	0.40
1:E:669:GLY:H	1:E:675:LYS:HD3	1.85	0.40
2:L:247:TRP:HB3	2:L:263:ALA:HB3	2.03	0.40
4:Q:149:GLU:OE2	4:Q:153:ARG:NH2	2.55	0.40
4:Q:181:ILE:HD12	4:Q:184:LEU:HD23	2.04	0.40
5:S:237:SER:C	5:S:238:MET:HE2	2.47	0.40
5:S:533:HIS:O	5:S:537:SER:HB2	2.21	0.40
5:S:639:ALA:HB2	5:S:676:ASN:HB3	2.03	0.40
5:S:889:GLU:OE2	5:S:891:ARG:HG2	2.21	0.40
5:S:1184:ARG:O	5:S:1188:ILE:HG12	2.21	0.40
5:S:1424:THR:C	5:S:1426:GLN:H	2.30	0.40
5:S:1775:GLU:HA	5:S:1778:PHE:HD2	1.84	0.40
5:S:1921:ASP:O	5:S:1924:THR:OG1	2.32	0.40
5:S:2220:MET:HE3	5:S:2255:LEU:HD21	2.04	0.40
5:S:3037:GLN:HA	5:S:3040:TYR:CD2	2.57	0.40
5:S:3259:LEU:O	5:S:3276:TRP:NE1	2.54	0.40
5:S:3576:ASP:O	5:S:3579:SER:OG	2.36	0.40
6:T:193:LEU:HB2	6:T:198:ILE:HB	2.04	0.40
6:T:278:GLN:OE1	6:T:279:LYS:N	2.55	0.40
9:A:117:LEU:HD12	9:A:120:GLN:NE2	2.36	0.40
2:L:310:ILE:H	6:T:290:ARG:HH21	1.68	0.40
2:L:439:LYS:HB2	2:L:439:LYS:HE2	1.89	0.40
5:S:356:ASN:N	5:S:358:GLU:OE2	2.55	0.40
5:S:1168:LEU:HA	5:S:1171:TRP:HB3	2.02	0.40
5:S:1574:ASN:HD21	5:S:1577:LEU:HB2	1.86	0.40
5:S:2851:PHE:CG	5:S:2853:PRO:HD2	2.57	0.40
5:S:2930:TYR:CE2	5:S:2938:VAL:HG11	2.56	0.40
5:S:3796:MET:HE1	5:S:3802:LEU:HB2	2.03	0.40
5:S:4087:HIS:O	5:S:4090:ARG:HD2	2.22	0.40
2:L:297:LEU:N	2:L:303:THR:O	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:339:CYS:HB2	2:L:394:ARG:HH22	1.85	0.40
5:S:111:CYS:HB2	5:S:130:LEU:CD1	2.44	0.40
5:S:124:LYS:HA	5:S:124:LYS:HD3	1.81	0.40
5:S:145:ASP:HA	5:S:147:PHE:CE2	2.56	0.40
5:S:246:ARG:NH1	5:S:247:GLU:HB2	2.36	0.40
5:S:374:LYS:HD3	5:S:374:LYS:HA	1.89	0.40
5:S:2218:PHE:O	5:S:2221:LYS:HG2	2.21	0.40
5:S:2408:MET:HA	5:S:2411:LEU:HD23	2.04	0.40
5:S:2886:GLN:H	5:S:2886:GLN:CD	2.29	0.40
5:S:2950:LYS:HB3	5:S:2952:ILE:HG22	2.03	0.40
5:S:3262:LEU:O	5:S:3266:SER:CB	2.70	0.40
5:S:3308:ASP:OD1	5:S:3308:ASP:N	2.52	0.40
5:S:3486:GLU:OE2	5:S:3487:ILE:HG12	2.21	0.40
5:S:3701:ILE:HD13	5:S:3719:ILE:HG12	2.02	0.40
5:S:3886:ALA:O	5:S:3889:ARG:HG2	2.20	0.40
5:S:3950:THR:HG23	5:S:3957:GLU:H	1.87	0.40
5:S:3953:LEU:HD13	5:S:3954:PRO:HD2	2.02	0.40
6:T:289:TYR:HD2	6:T:292:THR:H	1.68	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	E	242/911 (27%)	208 (86%)	32 (13%)	2 (1%)	16 52
2	L	635/732 (87%)	598 (94%)	36 (6%)	1 (0%)	43 77
3	M	21/204 (10%)	21 (100%)	0	0	100 100
4	P	55/336 (16%)	55 (100%)	0	0	100 100
4	Q	55/336 (16%)	55 (100%)	0	0	100 100
5	S	3459/4128 (84%)	3188 (92%)	263 (8%)	8 (0%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	497/609 (82%)	461 (93%)	36 (7%)	0	100	100
9	A	96/575 (17%)	96 (100%)	0	0	100	100
All	All	5060/7831 (65%)	4682 (92%)	367 (7%)	11 (0%)	44	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	814	ARG
5	S	4012	ASP
5	S	4013	TRP
5	S	1231	GLN
5	S	4010	SER
5	S	4011	PHE
5	S	4100	GLU
2	L	72	ASP
1	E	662	VAL
5	S	3304	VAL
5	S	2294	ILE

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	E	217/808 (27%)	217 (100%)	0	100	100
2	L	559/649 (86%)	559 (100%)	0	100	100
3	M	16/160 (10%)	16 (100%)	0	100	100
4	P	53/303 (18%)	53 (100%)	0	100	100
4	Q	51/303 (17%)	51 (100%)	0	100	100
5	S	2998/3671 (82%)	2998 (100%)	0	100	100
6	T	444/548 (81%)	444 (100%)	0	100	100
9	A	81/480 (17%)	81 (100%)	0	100	100
All	All	4419/6922 (64%)	4419 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	787	GLN
1	E	904	GLN
2	L	80	HIS
2	L	119	GLN
2	L	201	GLN
2	L	360	GLN
2	L	657	ASN
2	L	672	ASN
3	M	187	ASN
4	P	185	ASN
4	Q	145	GLN
4	Q	148	ASN
5	S	54	GLN
5	S	98	GLN
5	S	771	ASN
5	S	786	GLN
5	S	833	HIS
5	S	1049	GLN
5	S	1055	ASN
5	S	1071	ASN
5	S	1084	ASN
5	S	1125	GLN
5	S	1146	ASN
5	S	1350	ASN
5	S	1426	GLN
5	S	1471	GLN
5	S	1476	HIS
5	S	1509	GLN
5	S	1611	GLN
5	S	1737	ASN
5	S	1830	HIS
5	S	2213	ASN
5	S	2301	GLN
5	S	2306	ASN
5	S	2353	GLN
5	S	2493	ASN
5	S	2508	GLN
5	S	3154	GLN
5	S	3250	ASN

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Mol	Chain	Res	Type
5	S	3278	GLN
5	S	3383	GLN
5	S	3510	GLN
5	S	3549	HIS
5	S	3577	GLN
5	S	3590	ASN
5	S	3787	GLN
5	S	3818	ASN
5	S	4000	ASN
5	S	4042	GLN
5	S	4055	ASN
5	S	4110	GLN
6	T	68	GLN
6	T	152	ASN
6	T	416	GLN
6	T	433	GLN
6	T	484	GLN
6	T	489	ASN
6	T	515	ASN
9	A	82	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

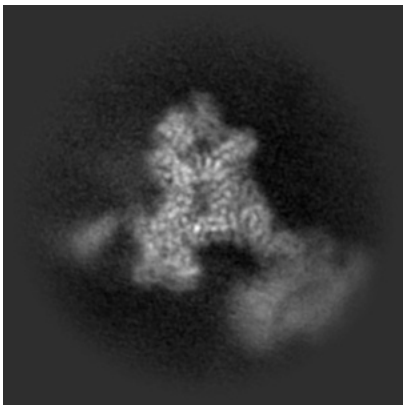
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51249. These allow visual inspection of the internal detail of the map and identification of artifacts.

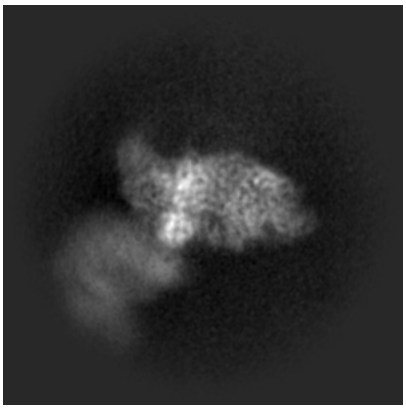
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

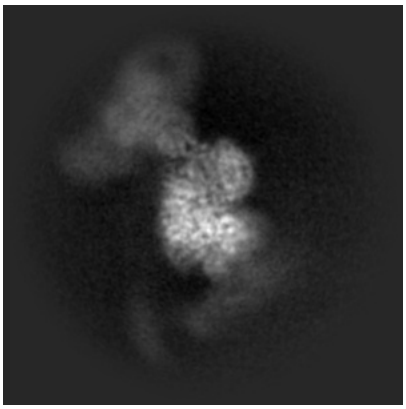
6.1.1 Primary map



X

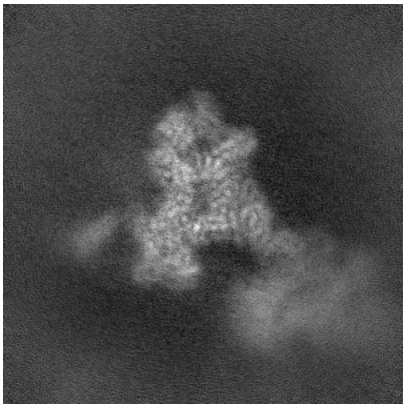


Y

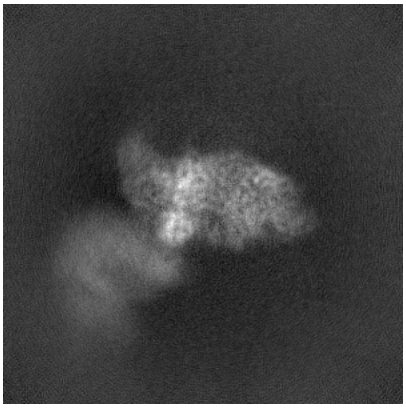


Z

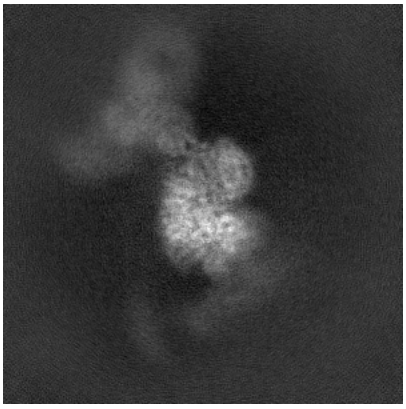
6.1.2 Raw map



X



Y

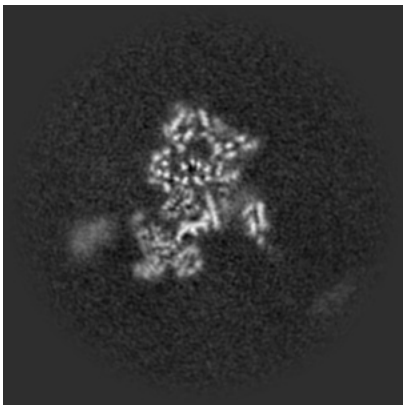


Z

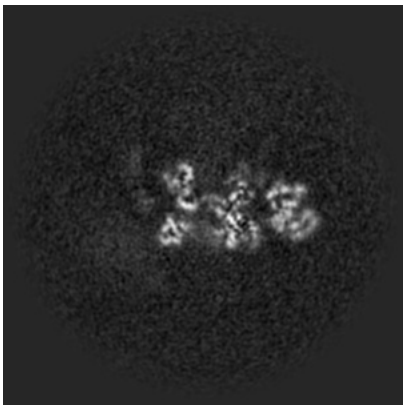
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

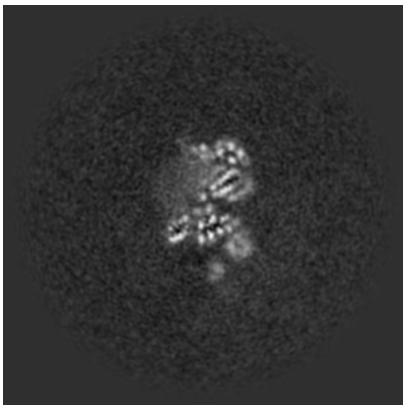
6.2.1 Primary map



X Index: 160

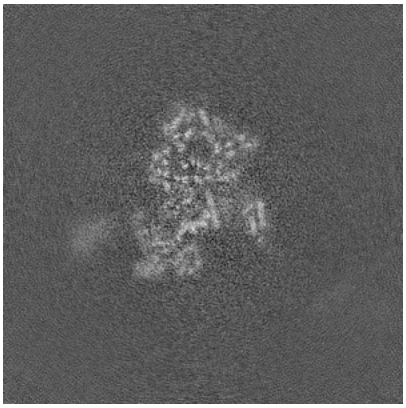


Y Index: 160

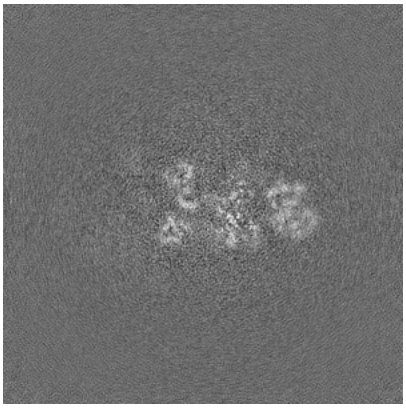


Z Index: 160

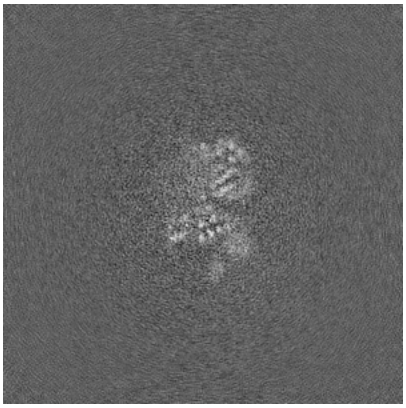
6.2.2 Raw map



X Index: 160



Y Index: 160

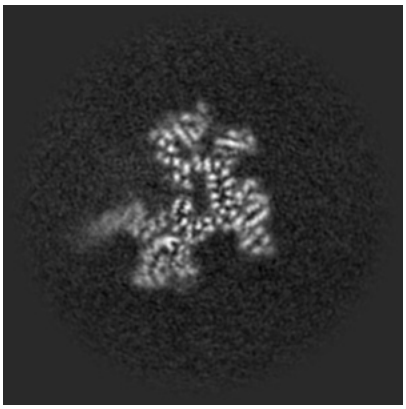


Z Index: 160

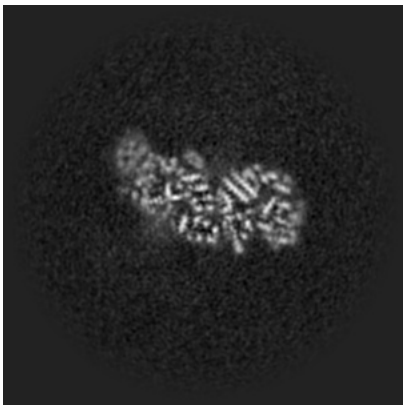
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

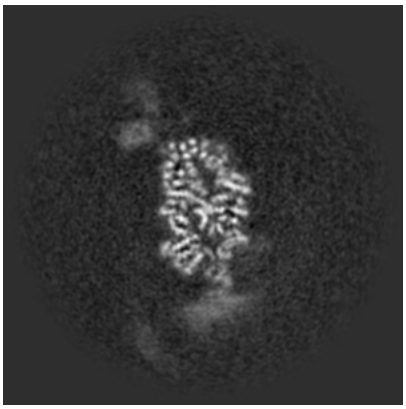
6.3.1 Primary map



X Index: 175

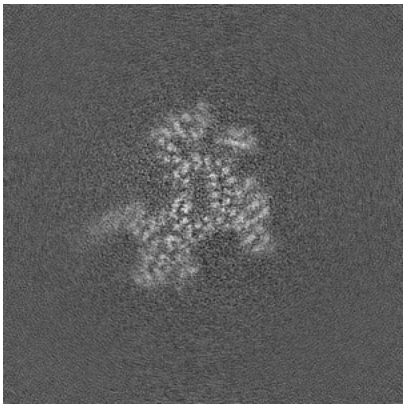


Y Index: 138

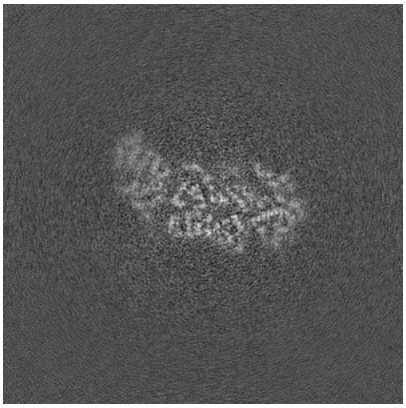


Z Index: 142

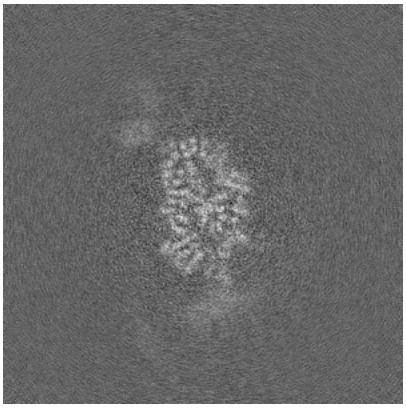
6.3.2 Raw map



X Index: 174



Y Index: 143

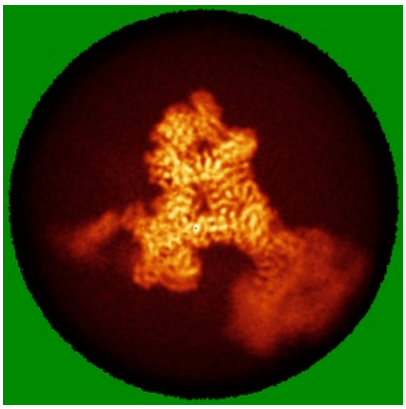


Z Index: 142

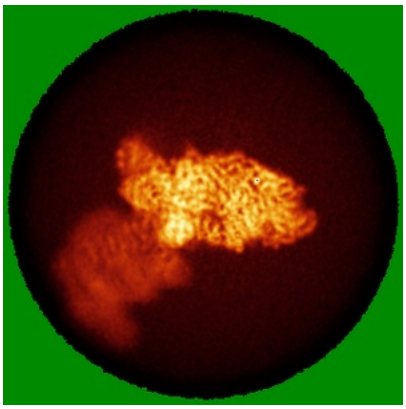
The images above show the largest variance slices of the map in three orthogonal directions.

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

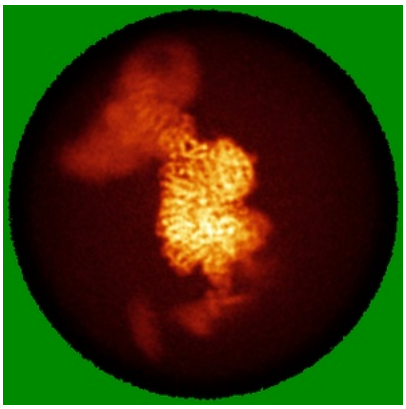
6.4.1 Primary map



X

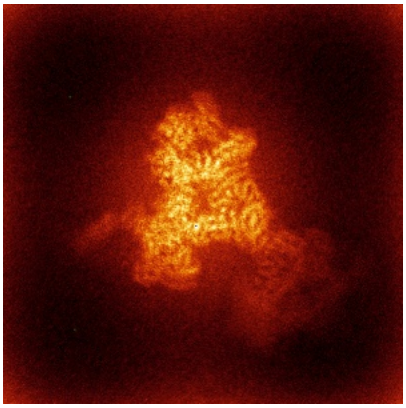


Y

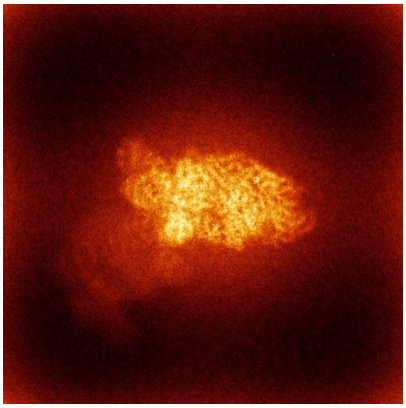


Z

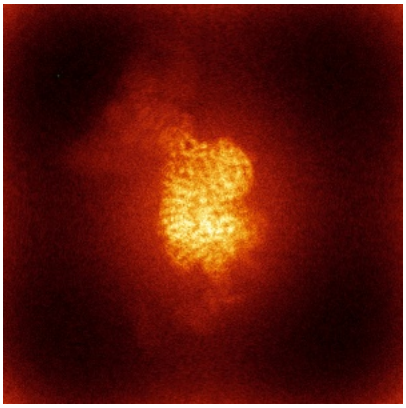
6.4.2 Raw map



X



Y

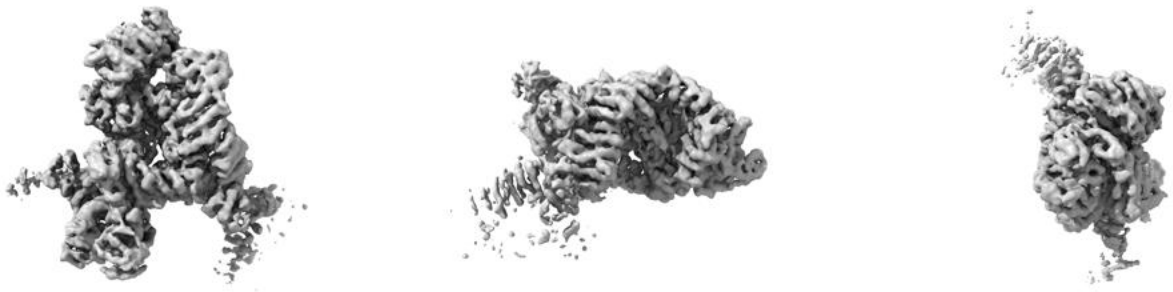


Z

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 0.211. 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.

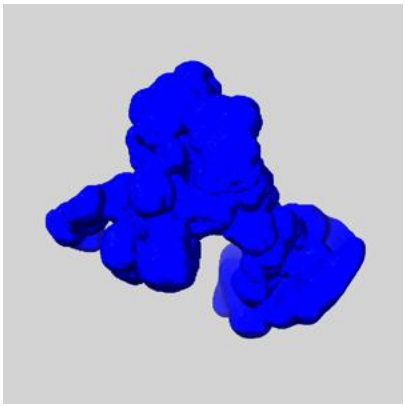
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

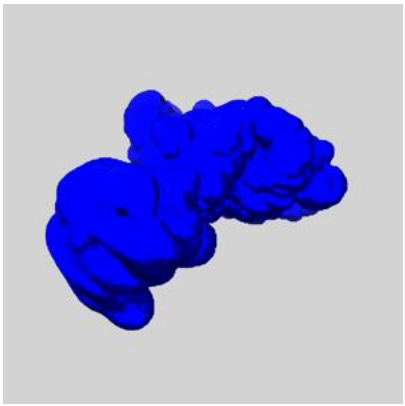
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

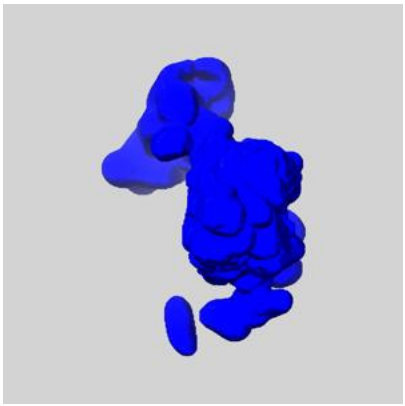
6.6.1 emd_51249_msk_1.map (i)



X



Y

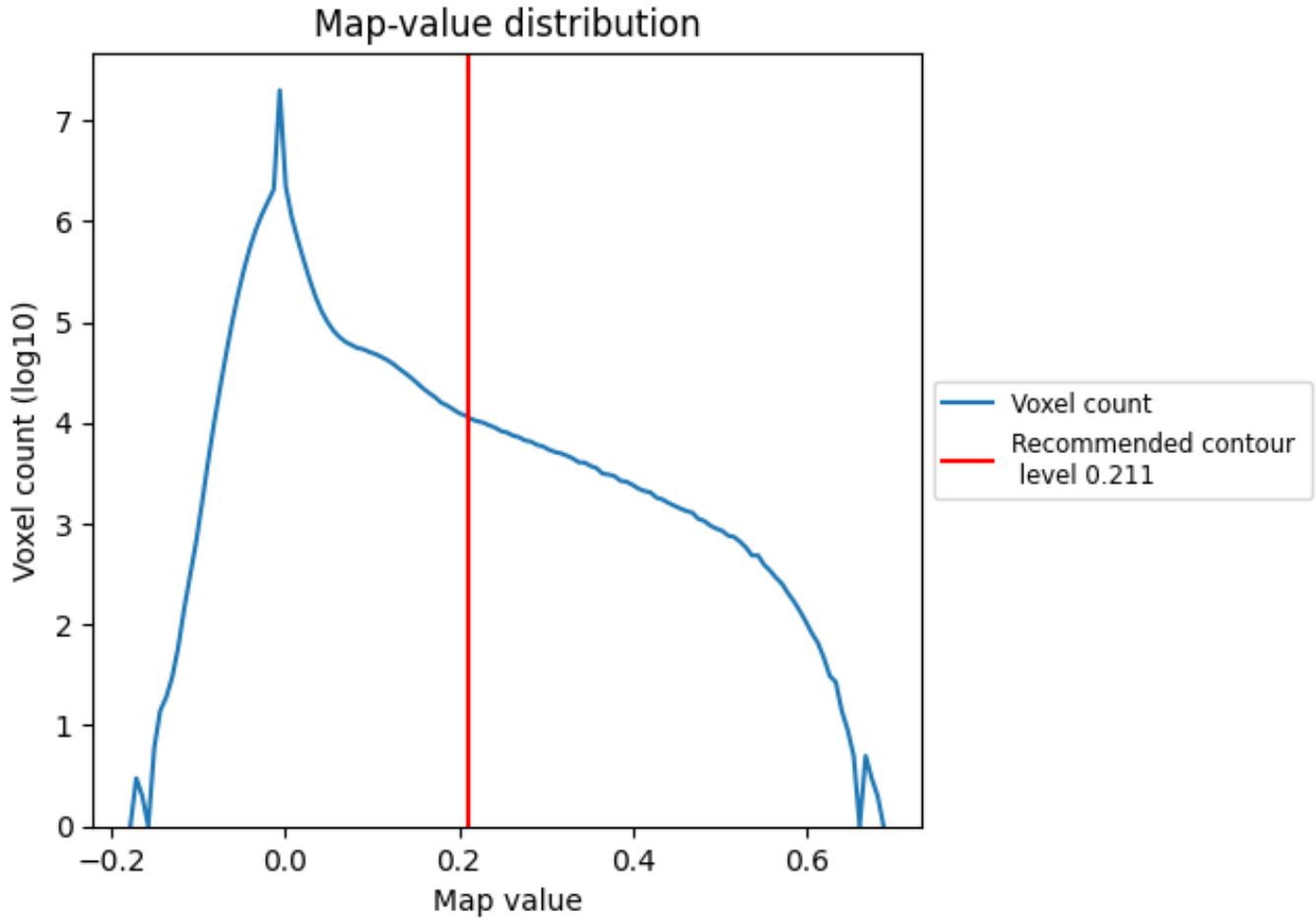


Z

7 Map analysis

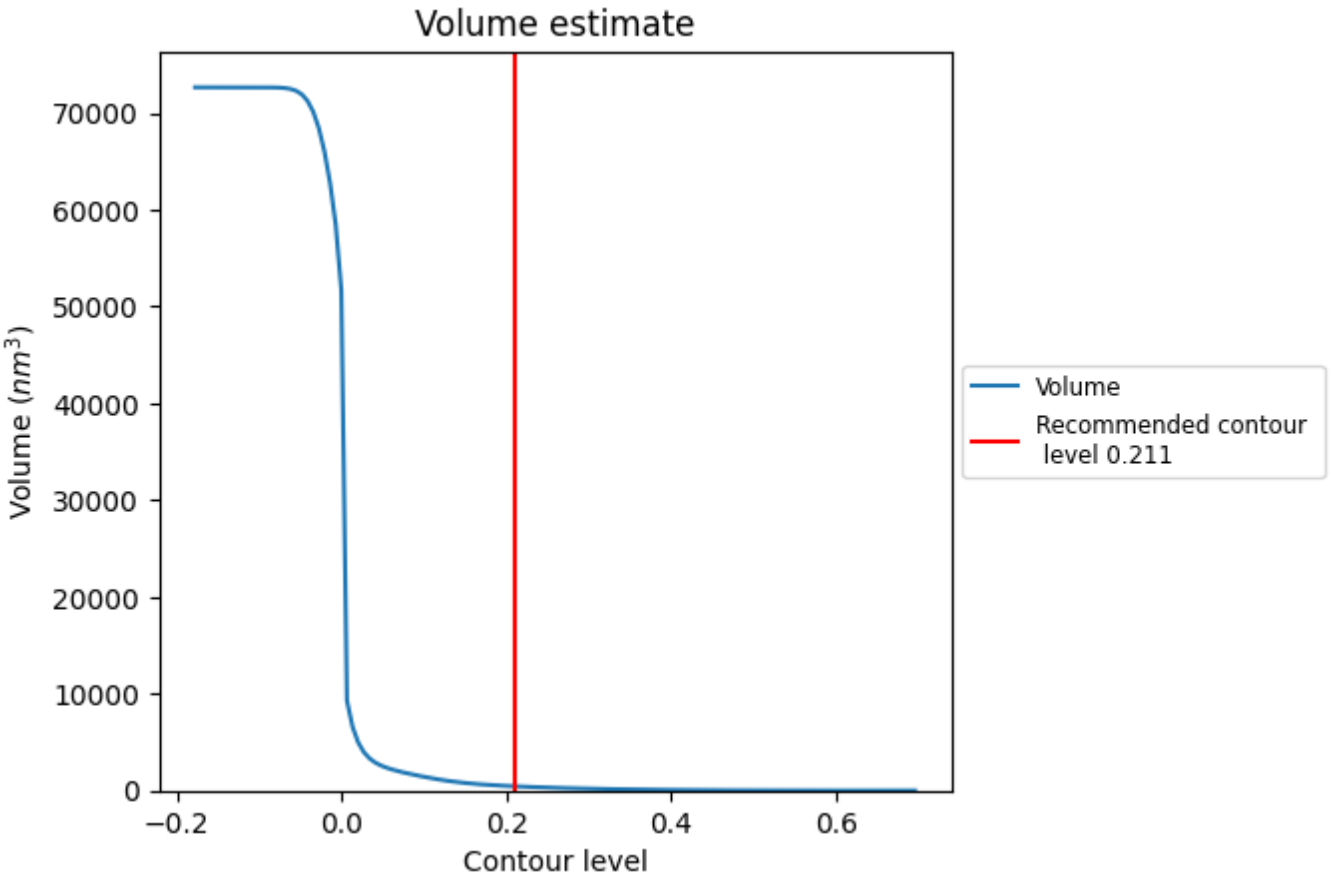
This section contains the results of statistical analysis of the map.

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.

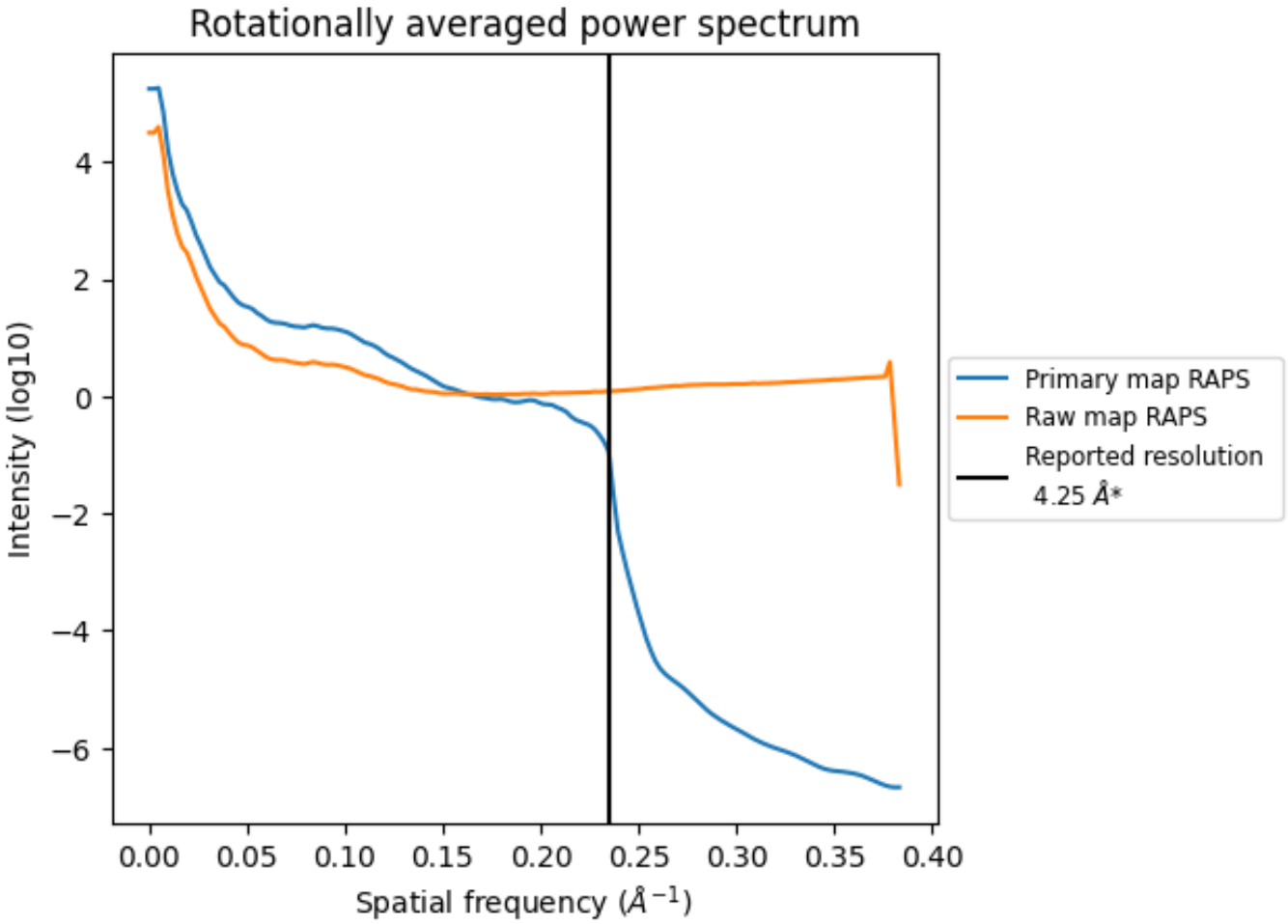
7.2 Volume estimate



The volume at the recommended contour level is 434 nm^3; this corresponds to an approximate mass of 392 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)

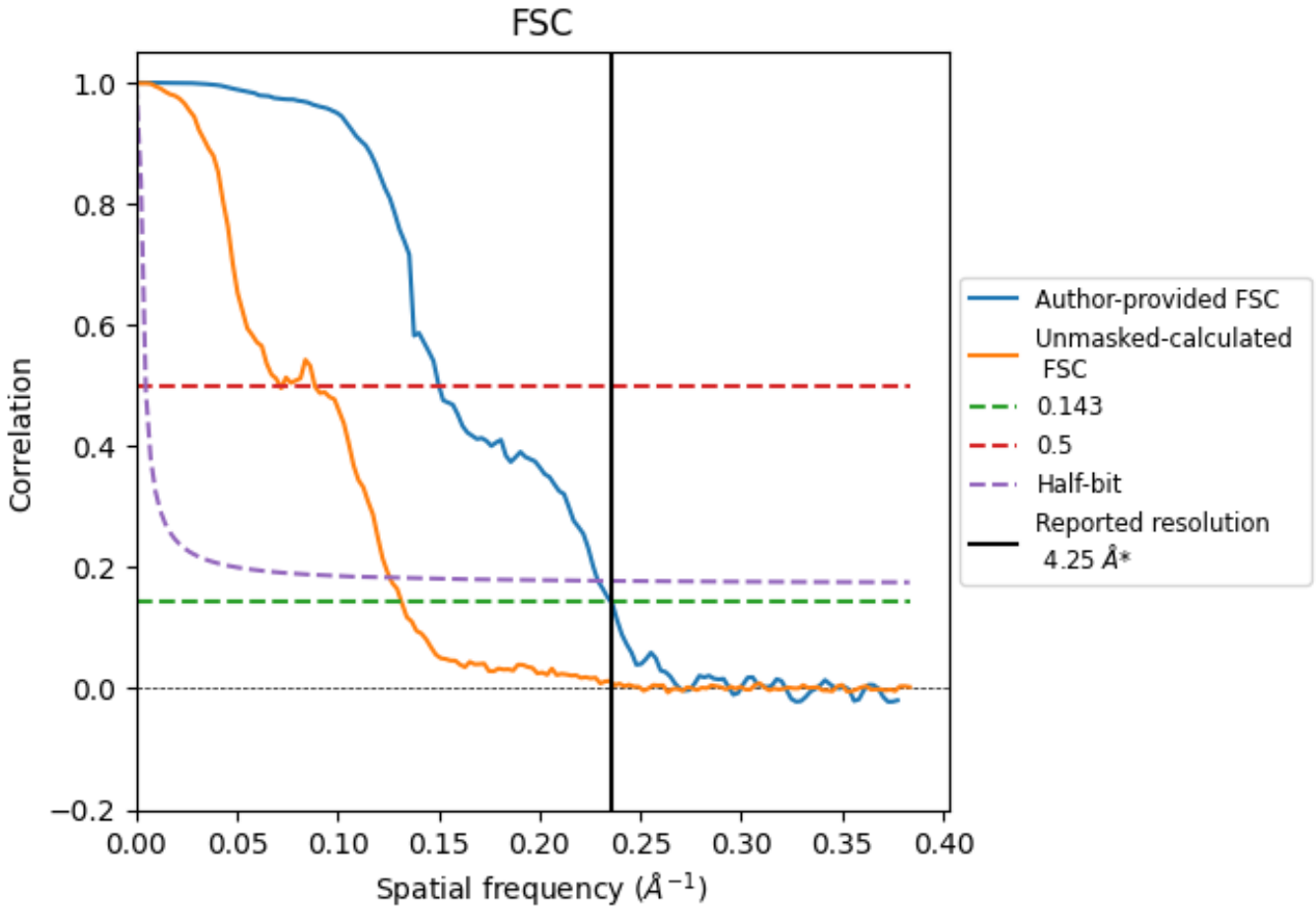


*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

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 0.235 Å^{-1}

8.2 Resolution estimates (i)

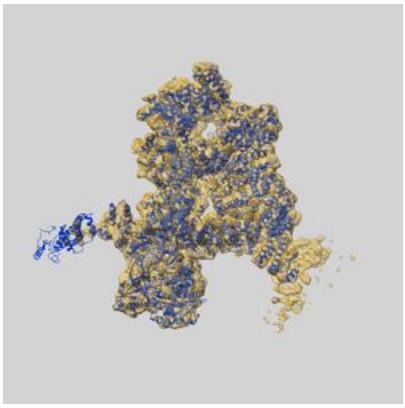
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.25	6.66	4.37
Unmasked-calculated*	7.60	14.04	7.95

*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 7.60 differs from the reported value 4.25 by more than 10 %

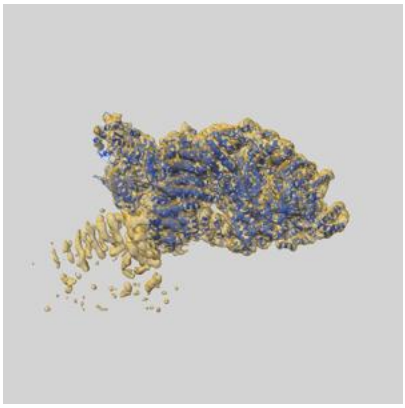
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51249 and PDB model 9GD7. Per-residue inclusion information can be found in section 3 on page 6.

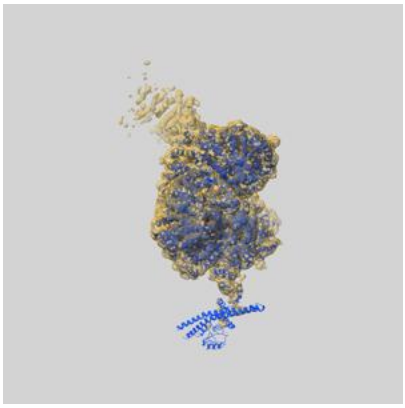
9.1 Map-model overlay



X



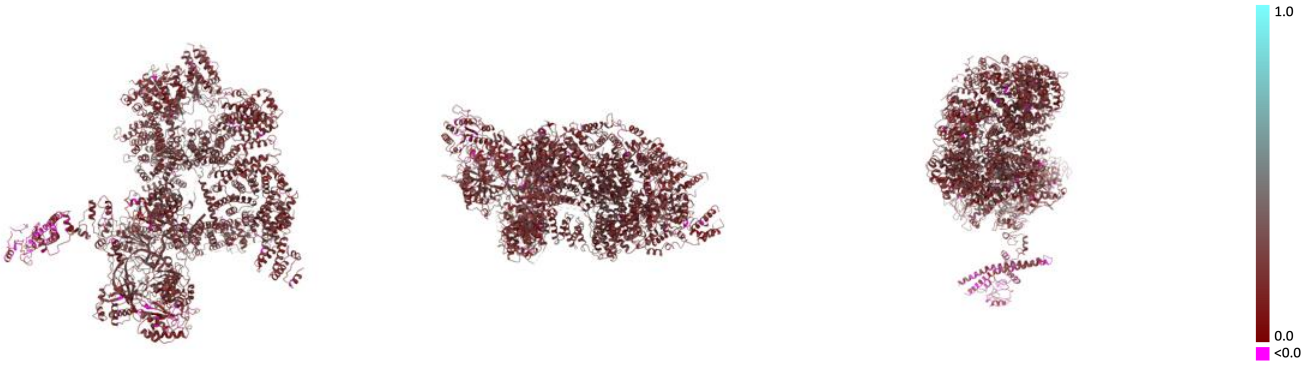
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.211 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.

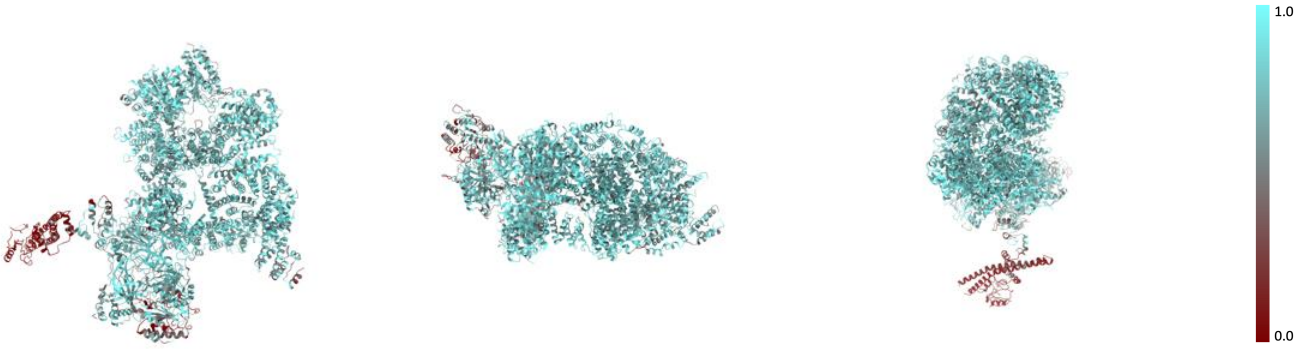
9.2 Q-score mapped to coordinate model (i)



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.

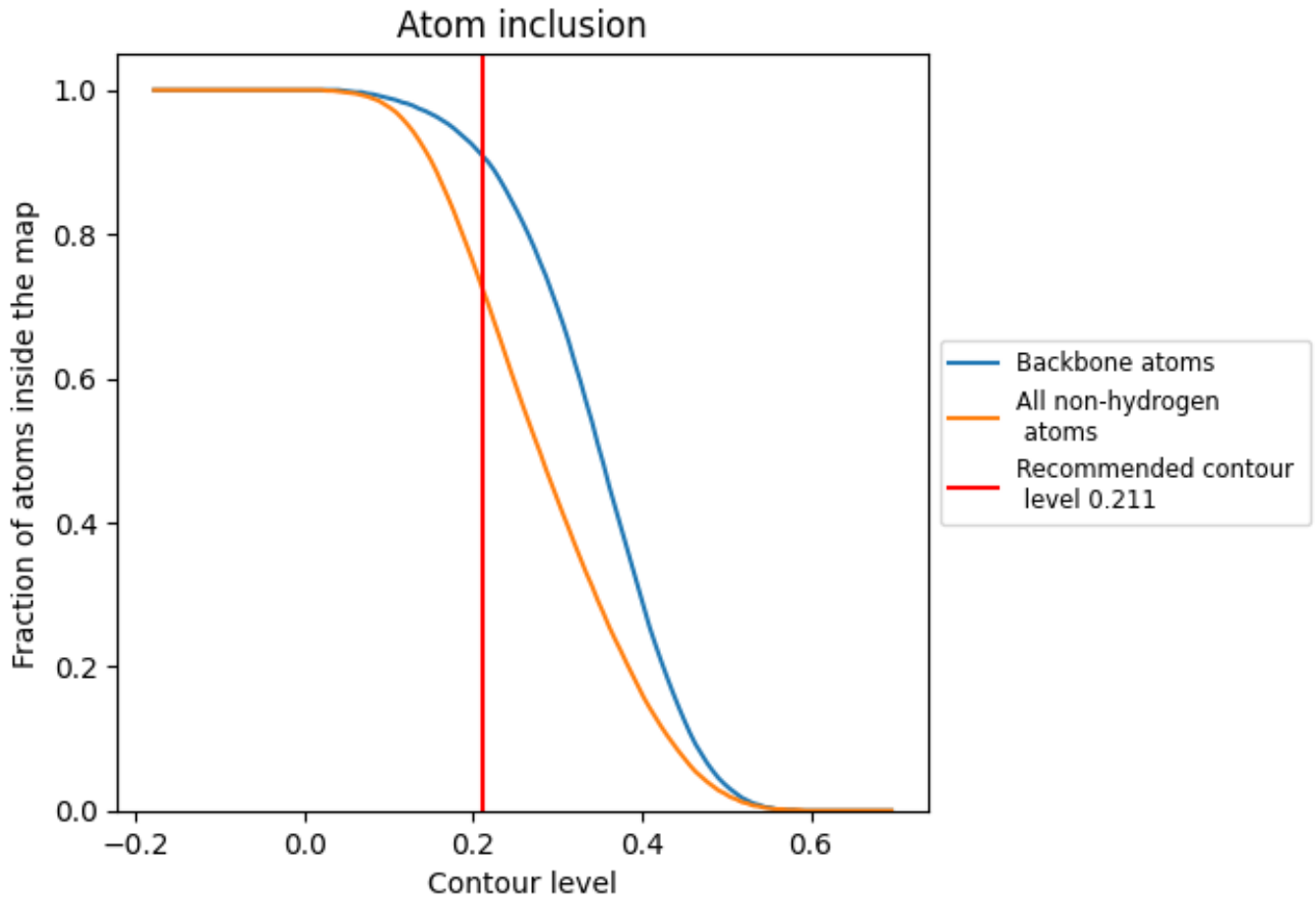
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.211).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.211) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.2280
A	0.7750	0.2160
E	0.2650	0.1390
L	0.6110	0.2070
M	0.6560	0.2950
P	0.0530	0.0970
Q	0.0970	0.0800
S	0.7870	0.2370
T	0.7420	0.2480
i	0.9770	0.3020
j	0.9810	0.2960