Full wwPDB EM Validation Report ⓘ

Oct 24, 2022 – 07:19 am BST

PDB ID	:	8A43
EMDB ID	:	EMD-15135
Title	:	Human RNA polymerase I
Authors	:	Daiss, J.L.; Pilsl, M.; Straub, K.; Bleckmann, A.; Hoecherl, M.; Heiss, F.B.; Abascal-Palacios, G.; Ramsay, E.; Tluckova, K.; Mars, J.C.; Fuertges, T.; Bruckmann, A.; Rudack, T.; Bernecky, C.; Lamour, V.; Panov, K.; Vannini, A.; Moss, T.; Engel, C.
Deposited on	:	2022-06-10
Resolution	:	4.09 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:

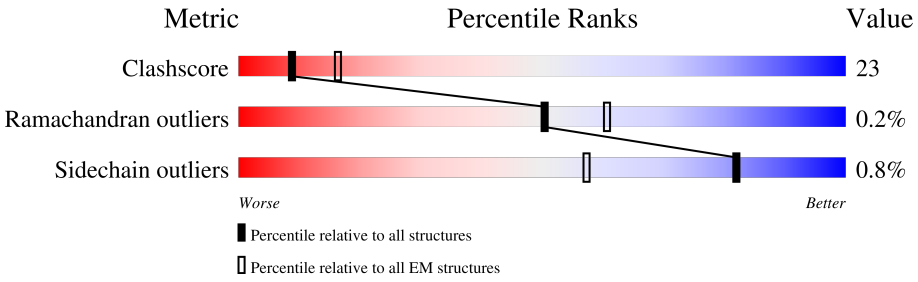
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.09 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1720	35% 49% 41% 10%
2	B	1135	13% 56% 42%
3	C	346	55% 32% 12%
4	E	210	49% 51%
5	F	127	33% 28% 39%
6	H	150	60% 39%
7	I	126	11% 24% 63%
8	J	67	67% 31%

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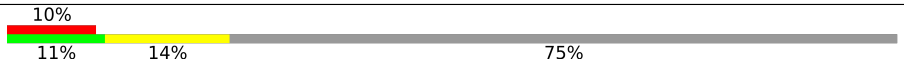
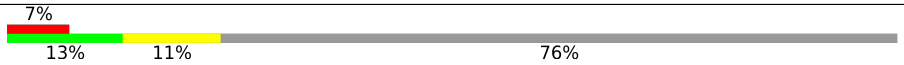
Mol	Chain	Length	Quality of chain
9	K	133	
10	L	58	
11	N	419	
12	M	510	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31109 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-directed RNA polymerase I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1549	12315	7818	2159	2255	83	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	8973	5748	1529	1624	72	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	306	2450	1548	437	455	10	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	209	1715	1083	300	324	8	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	78	627	402	106	114	5	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	148	1186	750	194	237	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	47	Total	C	N	O	S	0	0
			355	223	60	68	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	105	Total	C	N	O	S	0	0
			832	518	154	154	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

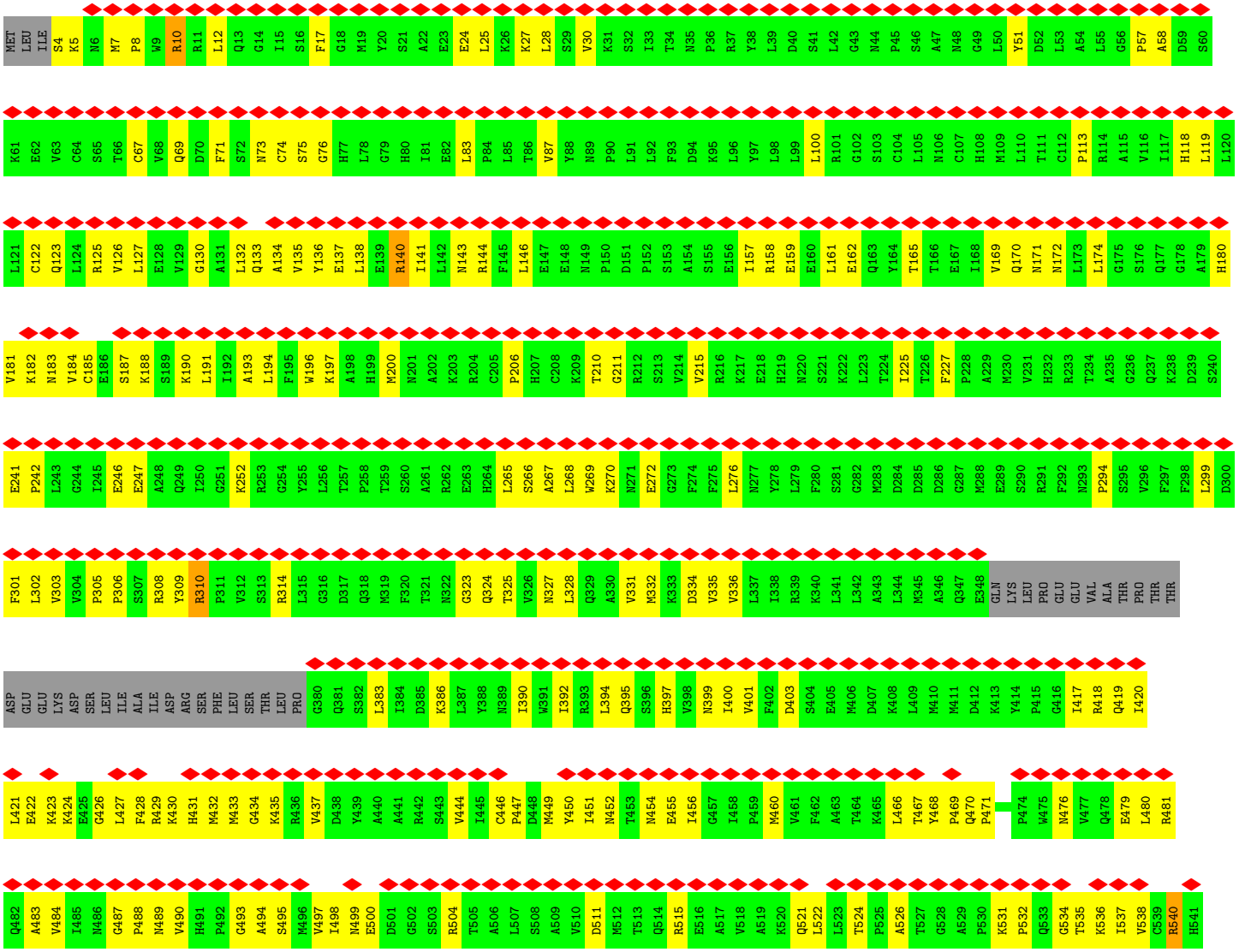
Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	122	Total	C	N	O	S	0	0
			888	559	157	169	3		

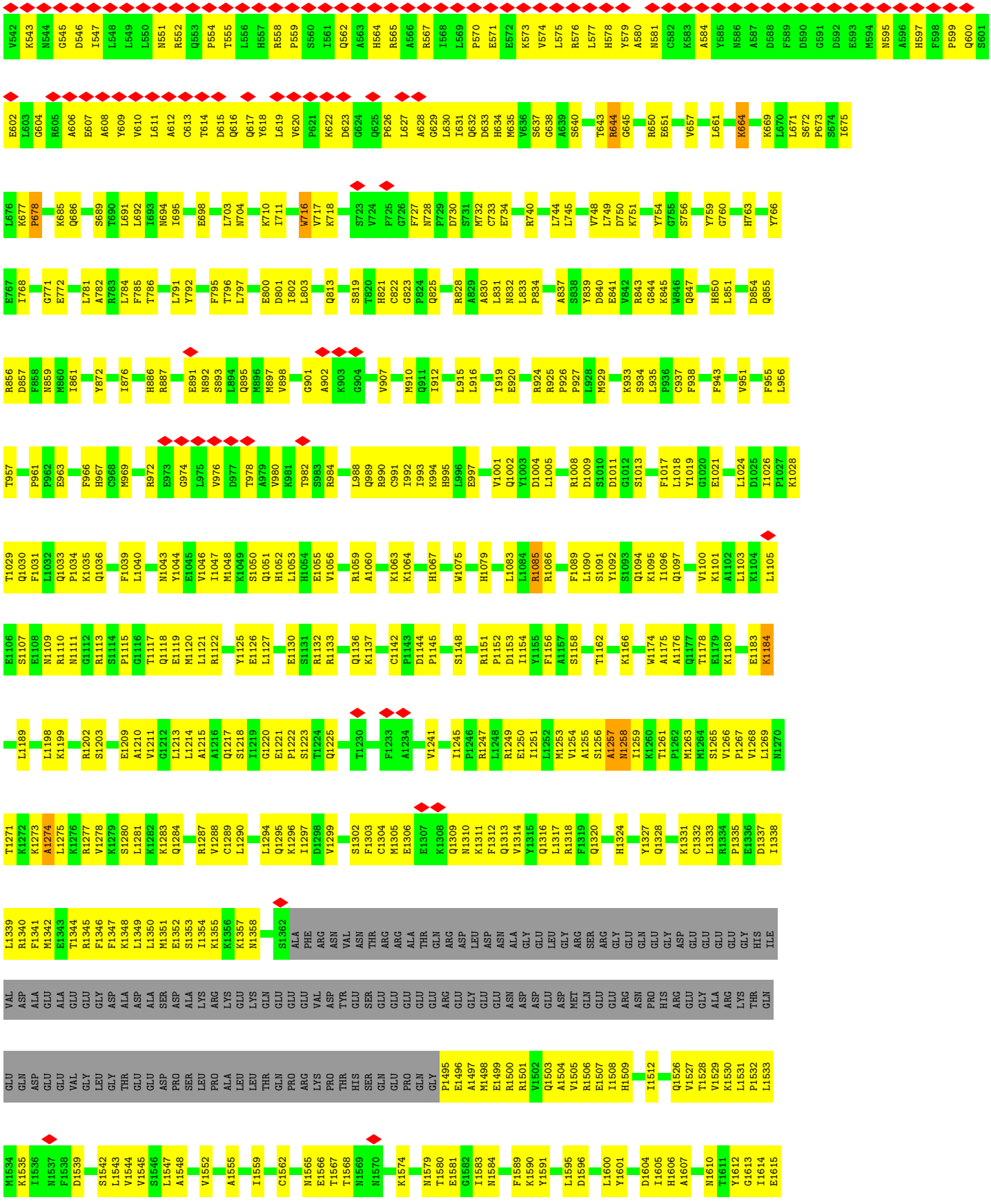
3 Residue-property plots (i)

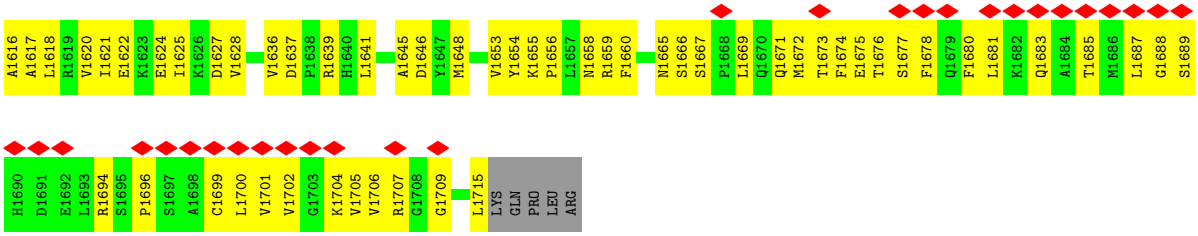
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-directed RNA polymerase I subunit RPA1

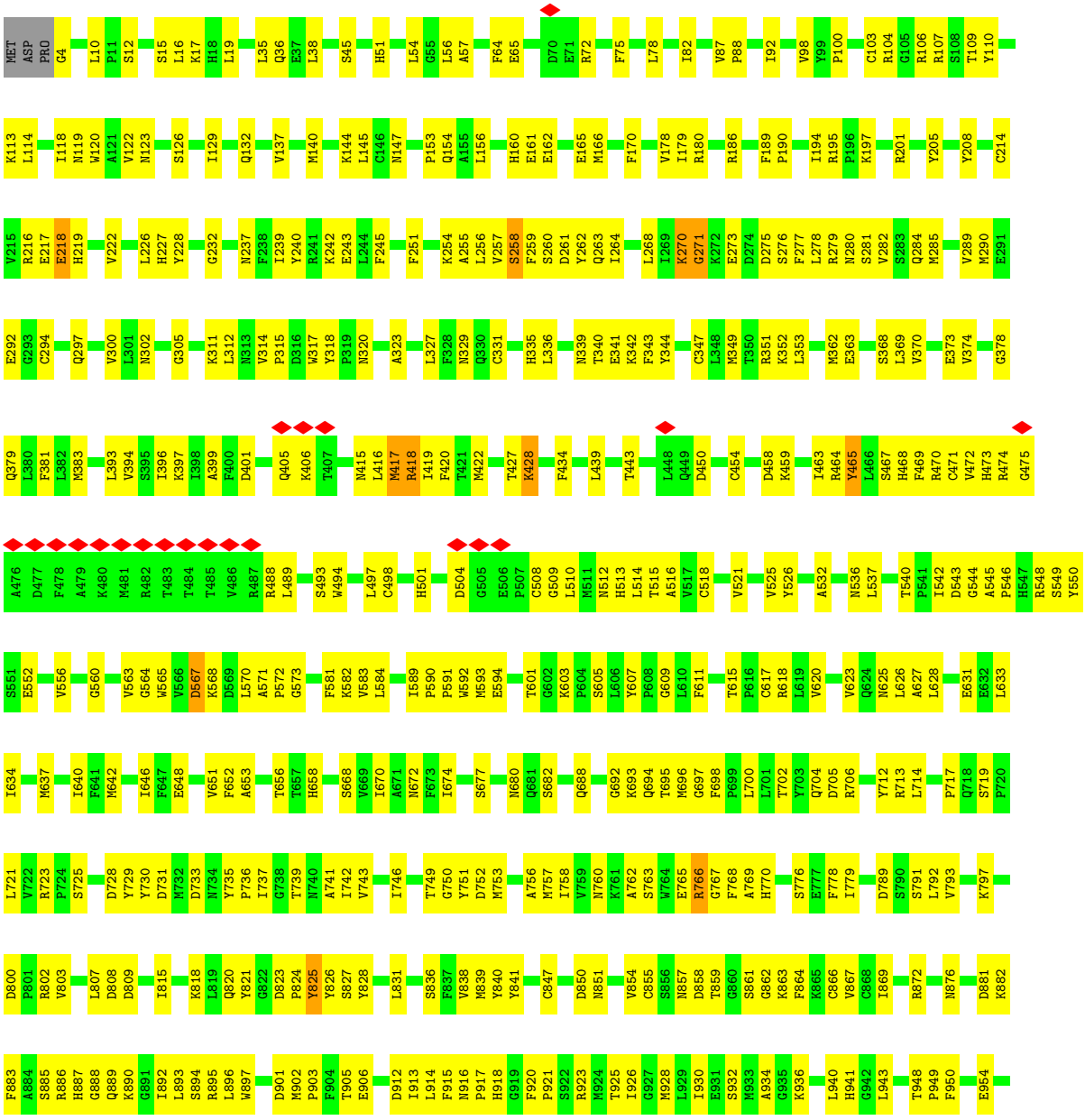
Chain A:

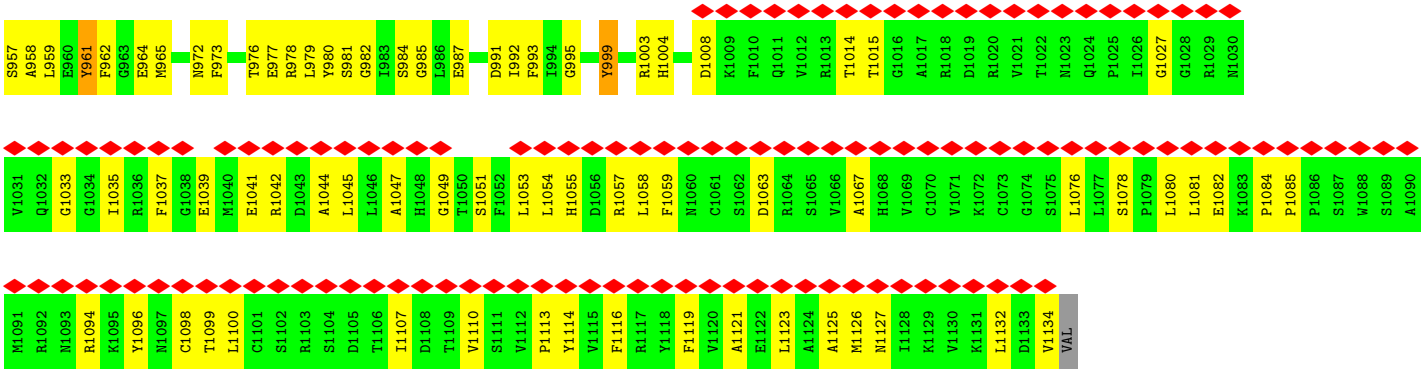



V542 K543 N544 G545 D546 I547 L548 L549 L550 N551 R552 Q553 P554 T555 L556 H557 R558 P559 S560 I561 Q562 A563 H564 R565 A566 R567 I568 L569 P570 E571 E572 K573 V574 L575 R576 L577 H578 Y579 A580 N581 C582 K583 A584 Y585 N586 A587 D588 F589 D590 G591 D592 E593 M594 N595 A596 H597 F598 P599 Q600 S601
E602 K603 G604 R605 A606 E607 A608 Y609 V610 L611 A612 C613 T614 D615 Q616 Q617 Y618 L619 V620 P621 K622 D623 G624 Q625 P626 L627 A628 G629 L630 I631 Q632 D633 H634 M635 V636 S637 G638 A639 S640 T643 R644 G645 R650 E651 V657 L661 K664 K669 L670 L671 S672 P673 S674 I675
L676 K677 P678 K685 Q686 S689 T690 L691 L692 I693 N694 I695 E698 L703 N704 K710 I711 W716 V717 K718 S723 V724 P725 G726 F727 N728 P729 D730 S731 M732 C733 E734 R740 L744 L745 V748 L749 D750 K751 Y754 G755 S756 Y759 G760 H763 Y766
E767 I768 G771 E772 L781 A782 R783 L784 F785 T786 L791 Y792 F795 T796 L797 E800 D801 I802 L803 Q813 S819 T820 H821 C822 G823 P824 Q825 R828 A829 A830 L831 N832 L833 P834 A837 S838 Y839 D840 E841 V842 R843 G844 K845 W846 Q847 H850 L851 D854 Q855
R856 D857 F858 N859 M860 I861 Y872 I876 H886 R887 E891 N892 S893 L894 Q895 M896 M897 V898 G901 A902 K903 G904 V907 M910 Q911 I912 L915 L916 I919 E920 R924 R925 P926 P927 L928 M929 K933 S934 L935 P936 C937 F938 F943 V951 F955 L956
T957 P961 P962 E963 F966 H967 G968 M969 R972 E973 G974 L975 V976 D977 T978 A979 V980 K981 T982 S983 R984 L988 Q989 R990 C991 I992 I993 K994 H995 L996 E997 V1001 Q1002 Y1003 D1004 L1005 R1008 D1009 S1010 D1011 G1012 S1013 F1017 L1018 Y1019 G1020 E1021 L1024 D1025 I1026 P1027 K1028
T1029 Q1030 F1031 L1032 Q1033 P1034 K1035 Q1036 F1039 L1040 N1043 Y1044 E1045 V1046 I1047 M1048 K1049 S1050 Q1051 H1052 L1053 H1054 E1055 V1056 R1059 A1060 K1063 K1064 H1067 W1075 H1079 L1083 L1084 R1085 R1086 F1089 L1090 S1091 Y1092 S1093 Q1094 K1095 I1096 Q1097 V1100 K1101 A1102 L1103 K1104 L1105
E1106 S1107 E1108 N1109 R1110 N1111 G1112 R1113 S1114 P1115 G1116 T1117 Q1118 E1119 M1120 L1121 R1122 Y1125 E1126 L1127 E1130 S1131 R1132 R1133 Q1136 K1137 C1142 P1143 D1144 P1145 S1148 R1151 P1152 D1153 I1154 Y1155 F1156 A1157 S1158 T1162 K1166 W1174 A1175 A1176 Q1177 T1178 E1179 K1180 E1183 K1184
L1189 L1198 K1199 R1202 S1203 E1209 A1210 V1211 G1212 L1213 L1214 A1215 A1216 Q1217 S1218 I1219 G1220 E1221 P1222 S1223 T1224 Q1225 T1230 F1233 A1234 V1241 I1245 P1246 R1247 L1248 R1249 E1250 I1251 L1252 M1253 V1254 A1255 S1256 A1257 N1258 I1259 K1260 T1261 P1262 M1263 M1264 S1265 V1266 P1267 V1268 L1269 N1270
T1271 K1272 K1273 A1274 L1275 K1276 R1277 V1278 K1279 S1280 L1281 K1282 K1283 Q1284 R1287 V1288 C1289 L1290 L1294 Q1295 K1296 I1297 D1298 V1299 S1302 F1303 C1304 M1305 E1306 E1307 K1308 Q1309 N1310 K1311 F1312 Q1313 V1314 Y1315 Q1316 L1317 R1318 F1319 Q1320 H1324 Y1327 Q1328 K1331 C1332 L1333 R1334 P1335 E1336 D1337 I1338
L1339 R1340 F1341 M1342 E1343 T1344 R1345 F1346 F1347 K1348 L1349 L1350 M1351 E1352 S1353 I1354 K1355 K1356 K1357 N1358 S1362 ALA PHE ARG ASN VAL ASN THR ARG ARG ALA THR GLN ARG ASP LEU ASP ASN ALA GLY GLU LEU GLY ARG SER ARG GLY GLU GLN GLU GLY HIS ARG GLU GLY ALA ARG LYS THR GLN
VAL ASP ALA GLU ALA GLU GLU GLY ASP ALA ASP ALA SER ASP ALA LYS ARG LYS GLU LYS GLN GLU GLU GLU VAL ASP TYR GLU SER GLU GLU GLU GLU GLU ARG GLU GLY GLU GLU ASP GLU ASP GLU ASN ASP ASP GLU ASP MET GLN GLU GLU ARG ASN PRO HIS ARG GLU GLY GLU GLU ALA ARG LYS THR GLN
GLU GLN ASP GLU GLU VAL GLY LEU GLY THR GLU GLU ASP PRO SER LEU PRO ALA LEU LEU THR GLN PRO ARG LYS PRO THR HIS SER GLN GLU PRO GLN GLY P1495 E1496 A1497 M1498 E1499 R1500 R1501 V1502 Q1503 A1504 V1505 R1506 E1507 I1508 H1509 I1512 Q1526 V1527 T1528 V1529 K1530 L1531 P1532 L1533
M1534 K1535 I1536 N1537 F1538 D1539 S1542 L1543 V1544 V1545 S1546 L1547 A1548 V1552 A1555 I1559 C1562 N1565 E1566 T1567 T1568 N1569 N1570 K1574 N1579 T1580 E1581 G1582 I1583 N1584 F1589 K1590 Y1591 L1595 D1596 L1600 Y1601 D1604 I1605 H1606 A1607 N1610 T1611 Y1612 G1613 I1614 E1615



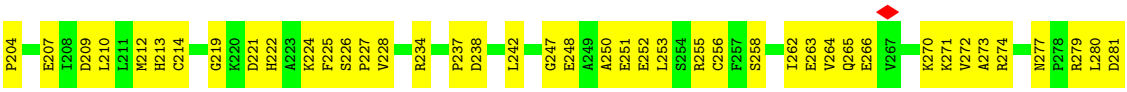
• Molecule 2: DNA-directed RNA polymerase I subunit RPA2

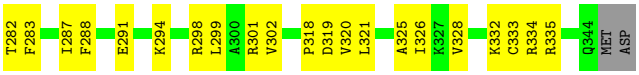




• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

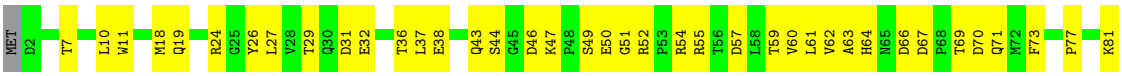
Chain C:

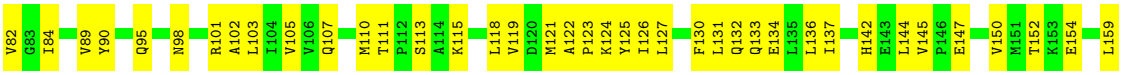


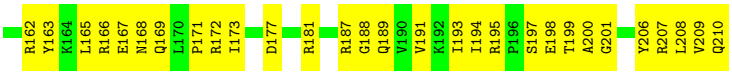


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

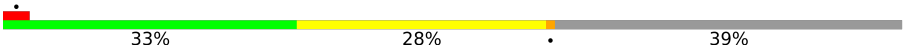


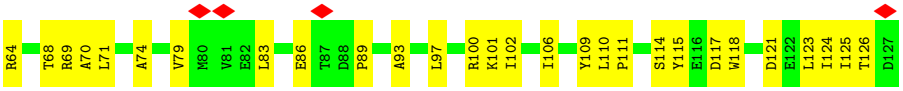




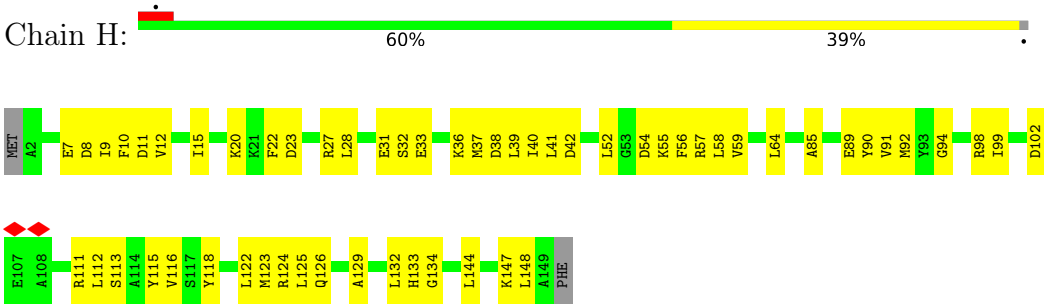
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

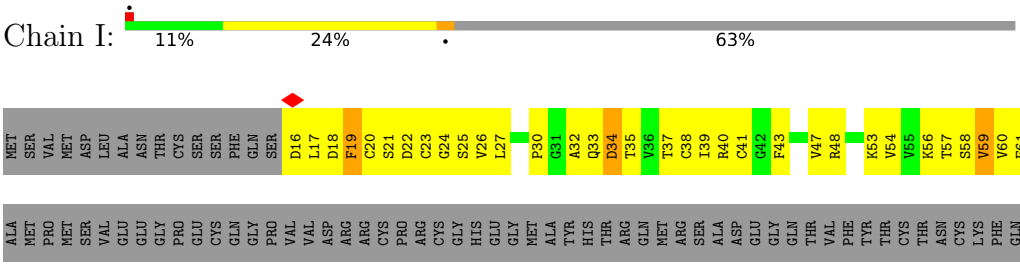




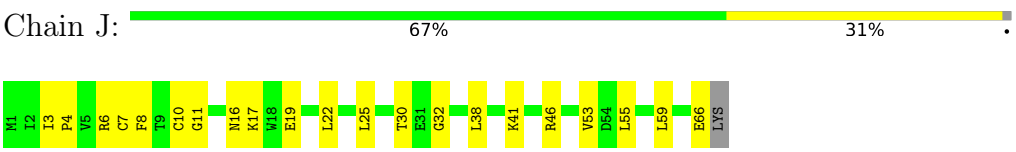
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



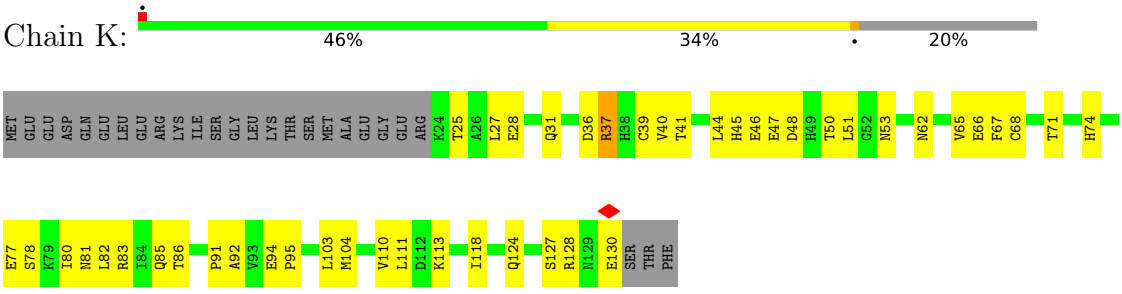
• Molecule 7: DNA-directed RNA polymerase I subunit RPA12



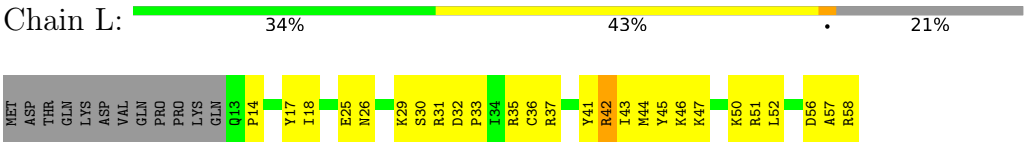
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

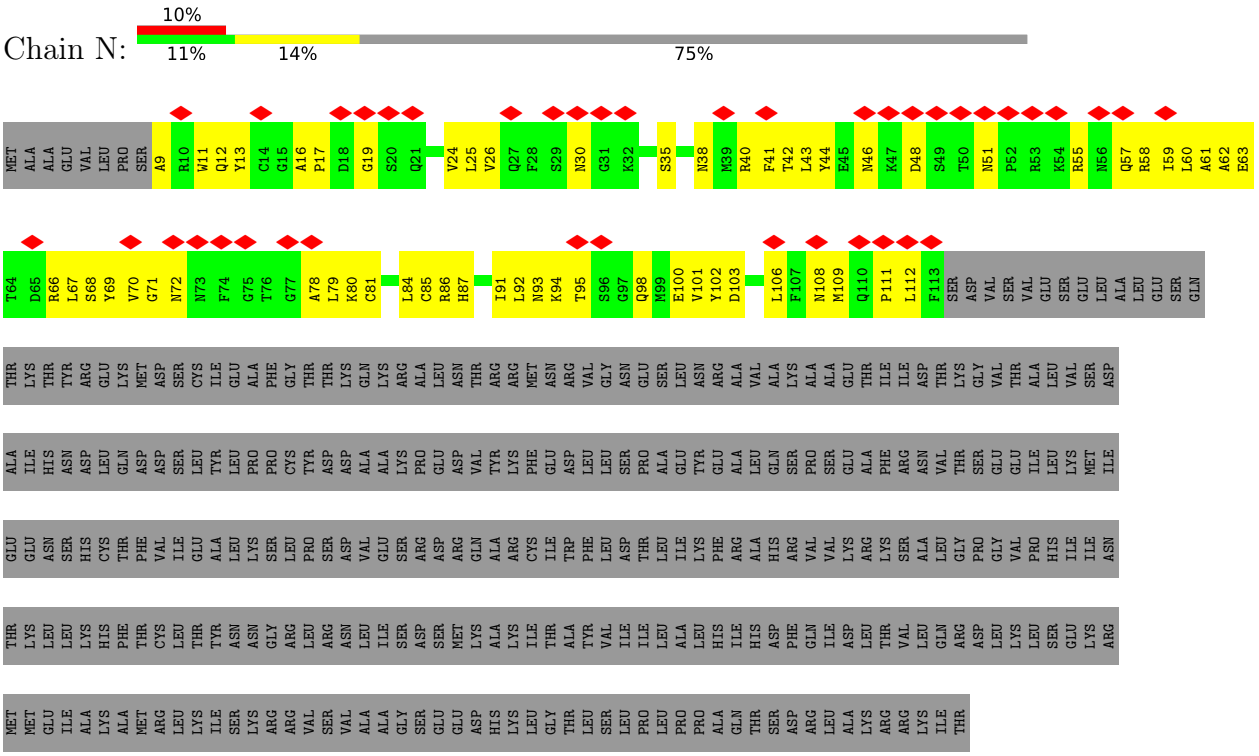


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



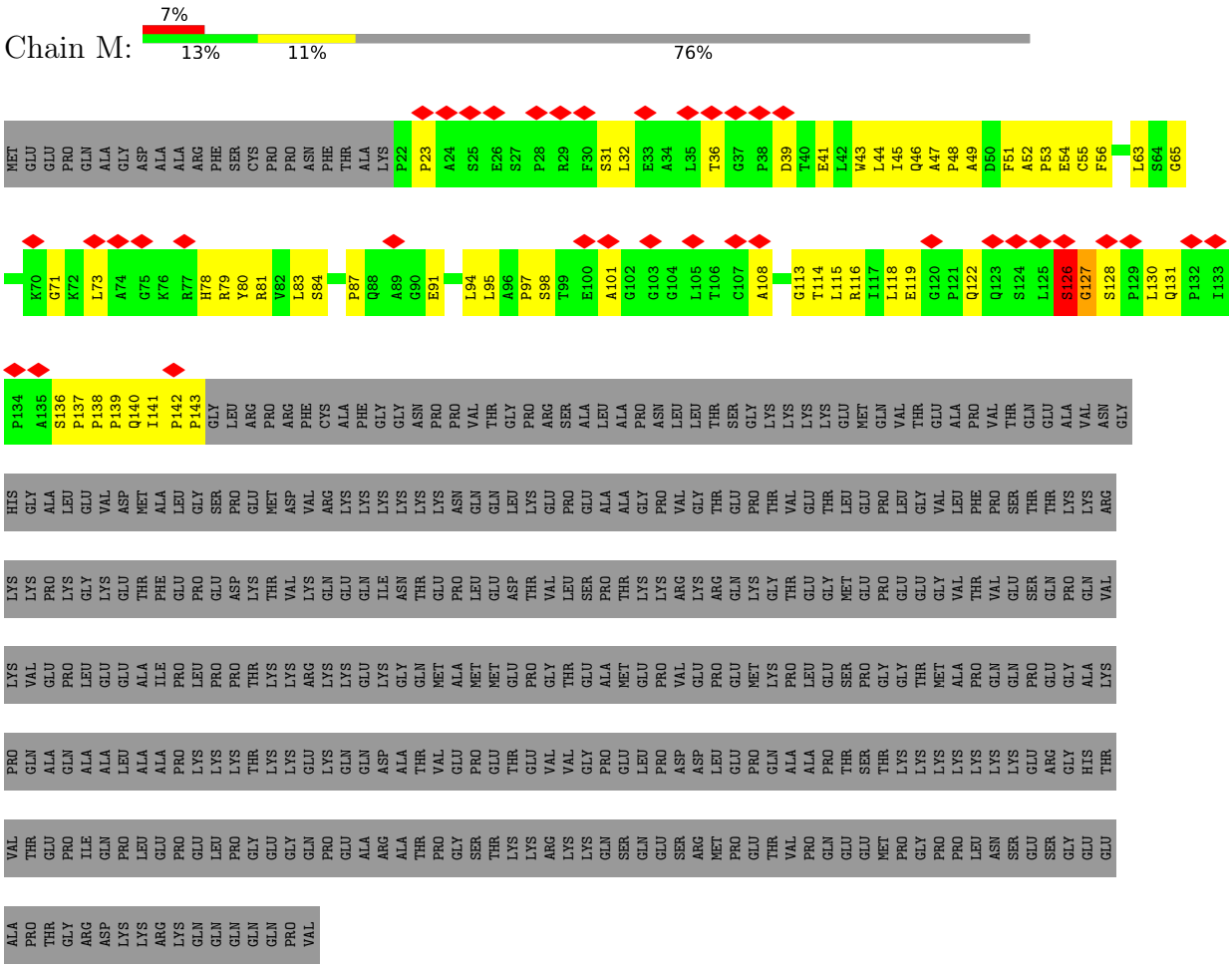
• Molecule 11: DNA-directed RNA polymerase I subunit RPA49

Chain N:



• Molecule 12: DNA-directed RNA polymerase I subunit RPA34

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0154	Depositor
Map size (Å)	286.60742, 286.60742, 286.60742	wwPDB
Map dimensions	190, 190, 190	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5084602, 1.5084602, 1.5084602	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.37	0/12574	0.53	0/16983
2	B	0.53	0/9193	0.58	0/12442
3	C	0.48	0/2498	0.55	0/3386
4	E	0.37	0/1745	0.53	0/2358
5	F	0.31	0/637	0.53	0/861
6	H	0.43	0/1207	0.55	0/1628
7	I	0.35	0/361	0.62	0/489
8	J	0.63	0/533	0.59	0/719
9	K	0.46	0/871	0.52	0/1174
10	L	0.51	0/394	0.58	0/524
11	N	0.34	0/848	0.51	0/1142
12	M	0.31	0/914	0.51	0/1251
All	All	0.44	0/31775	0.55	0/42957

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
3	C	0	1
7	I	0	2
9	K	0	1
12	M	0	2
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1184	LYS	Peptide
1	A	1257	ALA	Peptide
1	A	310	ARG	Peptide
1	A	664	LYS	Peptide
2	B	218	GLU	Peptide
2	B	258	SER	Peptide
2	B	270	LYS	Peptide
3	C	137	THR	Peptide
7	I	19	PHE	Peptide
7	I	57	THR	Peptide
9	K	37	ARG	Peptide
12	M	126	SER	Peptide
12	M	136	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12315	0	12425	660	0
2	B	8973	0	8954	436	0
3	C	2450	0	2452	101	0
4	E	1715	0	1733	113	0
5	F	627	0	659	37	0
6	H	1186	0	1147	44	0
7	I	355	0	345	42	0
8	J	524	0	544	20	0
9	K	856	0	840	41	0
10	L	388	0	395	24	0
11	N	832	0	812	80	0
12	M	888	0	889	57	0
All	All	31109	0	31195	1462	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 23.

All (1462) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASN:H	1:A:1043:ASN:HD21	1.06	1.01
1:A:1700:LEU:HD22	2:B:1054:LEU:HD13	1.45	0.96
11:N:91:ILE:HB	11:N:100:GLU:HB3	1.52	0.90
2:B:180:ARG:NH2	2:B:471:CYS:SG	2.47	0.88
1:A:933:LYS:NZ	2:B:642:MET:O	2.08	0.87
1:A:1539:ASP:O	1:A:1543:LEU:N	2.08	0.85
2:B:347:CYS:SG	2:B:351:ARG:NH1	2.49	0.85
1:A:704:ASN:HD21	1:A:740:ARG:HG3	1.40	0.85
5:F:97:LEU:HA	5:F:102:ILE:HD11	1.59	0.84
5:F:110:LEU:HB3	5:F:111:PRO:HD2	1.57	0.84
3:C:109:ARG:NH2	8:J:3:ILE:O	2.10	0.84
2:B:940:LEU:O	8:J:46:ARG:NH2	2.10	0.83
2:B:179:ILE:HD13	2:B:454:CYS:HB3	1.58	0.83
1:A:1125:TYR:O	1:A:1132:ARG:NH2	2.11	0.83
1:A:446:CYS:SG	1:A:576:ARG:NH1	2.52	0.82
6:H:33:GLU:O	6:H:36:LYS:NZ	2.13	0.81
1:A:797:LEU:HD13	2:B:917:PRO:HB2	1.60	0.81
1:A:1028:LYS:O	1:A:1031:PHE:N	2.14	0.81
2:B:802:ARG:HH12	2:B:824:PRO:HD3	1.46	0.80
2:B:217:GLU:O	2:B:219:HIS:ND1	2.15	0.80
11:N:11:TRP:HH2	12:M:53:PRO:HB2	1.46	0.80
7:I:22:ASP:H	11:N:66:ARG:HE	1.31	0.79
2:B:802:ARG:NH1	2:B:824:PRO:HD3	1.98	0.79
1:A:1119:GLU:OE1	1:A:1122:ARG:NH2	2.16	0.79
9:K:47:GLU:HG3	9:K:48:ASP:H	1.47	0.79
1:A:1055:GLU:O	1:A:1059:ARG:NH2	2.16	0.78
7:I:35:THR:HA	7:I:47:VAL:HB	1.65	0.78
1:A:651:GLU:N	1:A:651:GLU:OE1	2.14	0.78
2:B:515:THR:HG22	2:B:516:ALA:H	1.48	0.78
1:A:140:ARG:NH2	4:E:119:VAL:O	2.16	0.78
1:A:972:ARG:HH21	2:B:509:GLY:HA2	1.49	0.78
1:A:967:HIS:HD2	2:B:682:SER:OG	1.67	0.78
7:I:35:THR:HG22	7:I:47:VAL:H	1.49	0.77
1:A:1297:ILE:HG21	1:A:1544:VAL:HG11	1.66	0.77
1:A:75:SER:H	2:B:1080:LEU:HD22	1.49	0.77
2:B:625:ASN:HD21	2:B:627:ALA:HB3	1.48	0.77
1:A:1107:SER:OG	1:A:1118:GLN:NE2	2.17	0.77
3:C:96:ASN:ND2	3:C:207:GLU:OE2	2.17	0.77
11:N:86:ARG:HH12	12:M:53:PRO:HD3	1.48	0.76
2:B:719:SER:OG	2:B:723:ARG:NH1	2.18	0.76
4:E:167:GLU:O	4:E:172:ARG:NH2	2.19	0.76
2:B:92:ILE:O	10:L:35:ARG:NH2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:LEU:HA	12:M:131:GLN:HE22	1.51	0.75
3:C:116:HIS:HB2	3:C:193:VAL:HG22	1.68	0.75
1:A:73:ASN:HB3	2:B:1081:LEU:HB3	1.68	0.75
3:C:221:ASP:OD2	10:L:58:ARG:NH2	2.17	0.75
2:B:162:GLU:OE1	2:B:735:TYR:OH	2.03	0.75
1:A:1154:ILE:HD11	5:F:52:ILE:HA	1.66	0.75
1:A:133:GLN:HB3	4:E:210:GLN:HE21	1.49	0.75
2:B:54:LEU:HA	2:B:57:ALA:HB3	1.68	0.75
2:B:186:ARG:HH22	2:B:637:MET:HB2	1.51	0.75
1:A:1295:GLN:HE21	1:A:1296:LYS:HG2	1.52	0.75
2:B:930:ILE:HD13	2:B:959:LEU:HD12	1.69	0.75
3:C:149:ASN:ND2	3:C:161:GLU:O	2.20	0.75
1:A:828:ARG:HH22	1:A:844:GLY:HA3	1.51	0.74
2:B:567:ASP:OD1	2:B:567:ASP:N	2.19	0.74
1:A:435:LYS:HG2	2:B:1058:LEU:HD23	1.68	0.74
2:B:194:ILE:HG13	2:B:363:GLU:HG3	1.68	0.74
2:B:232:GLY:O	2:B:281:SER:OG	2.04	0.74
9:K:37:ARG:HB3	9:K:91:PRO:HB3	1.69	0.74
2:B:1096:TYR:HB2	2:B:1107:ILE:HG13	1.70	0.74
6:H:56:PHE:HB3	6:H:147:LYS:HA	1.69	0.74
2:B:178:VAL:HG21	2:B:469:PHE:HE1	1.53	0.73
9:K:36:ASP:OD2	9:K:37:ARG:NH1	2.20	0.73
3:C:96:ASN:HB2	10:L:50:LYS:HG2	1.70	0.73
11:N:24:VAL:HG23	12:M:95:LEU:HB2	1.68	0.73
1:A:418:ARG:O	1:A:422:GLU:HB2	1.87	0.73
1:A:1324:HIS:CE1	1:A:1335:PRO:HD3	2.23	0.73
7:I:22:ASP:N	11:N:66:ARG:HE	1.87	0.73
2:B:260:SER:HB2	11:N:111:PRO:HG2	1.70	0.73
1:A:1113:ARG:HD2	1:A:1118:GLN:HB3	1.70	0.73
1:A:76:GLY:HA3	1:A:306:PRO:HB3	1.70	0.72
1:A:925:ARG:HG2	1:A:926:PRO:HD2	1.70	0.72
1:A:1342:MET:HG2	1:A:1346:PHE:CD2	2.24	0.72
2:B:934:ALA:HA	2:B:962:PHE:HE2	1.52	0.72
2:B:257:VAL:HG22	2:B:259:PHE:HB2	1.69	0.72
1:A:181:VAL:HG12	1:A:182:LYS:H	1.54	0.72
1:A:1699:CYS:HB3	1:A:1706:VAL:HG13	1.69	0.72
4:E:29:THR:N	4:E:32:GLU:OE1	2.21	0.72
1:A:1127:LEU:O	1:A:1132:ARG:NH2	2.21	0.72
2:B:302:ASN:OD1	2:B:320:ASN:ND2	2.23	0.72
1:A:916:LEU:HD22	1:A:951:VAL:HG11	1.69	0.72
4:E:172:ARG:NE	4:E:210:GLN:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:15:ILE:HD11	6:H:52:LEU:HA	1.72	0.71
11:N:92:LEU:HB2	12:M:41:GLU:HB2	1.72	0.71
1:A:452:ASN:HB2	1:A:455:GLU:HB3	1.71	0.71
2:B:642:MET:SD	2:B:658:HIS:NE2	2.63	0.71
2:B:885:SER:OG	2:B:886:ARG:N	2.21	0.71
1:A:796:THR:HG21	2:B:992:ILE:HA	1.72	0.71
1:A:1503:GLN:HA	1:A:1506:ARG:HD2	1.72	0.71
2:B:261:ASP:OD1	2:B:262:TYR:N	2.24	0.71
2:B:263:GLN:HG2	11:N:30:ASN:HD21	1.55	0.71
2:B:694:GLN:HE22	2:B:1003:ARG:HE	1.39	0.71
1:A:399:ASN:O	1:A:403:ASP:N	2.23	0.70
1:A:631:ILE:HD12	1:A:632:GLN:H	1.56	0.70
2:B:498:CYS:SG	2:B:668:SER:N	2.61	0.70
2:B:312:LEU:HD13	2:B:327:LEU:HD12	1.72	0.70
11:N:46:ASN:ND2	11:N:57:GLN:OE1	2.24	0.70
1:A:1498:MET:HG2	1:A:1501:ARG:HE	1.55	0.70
2:B:697:GLY:HA3	2:B:737:ILE:HD12	1.73	0.70
12:M:80:TYR:HA	12:M:119:GLU:HA	1.72	0.70
1:A:801:ASP:O	1:A:892:ASN:ND2	2.24	0.70
1:A:1305:MET:HA	1:A:1310:ASN:HA	1.71	0.70
2:B:1054:LEU:HG	2:B:1058:LEU:HD13	1.74	0.70
2:B:339:ASN:OD1	2:B:340:THR:N	2.24	0.70
3:C:263:GLU:OE2	3:C:274:ARG:NH1	2.24	0.70
1:A:127:LEU:HD11	1:A:191:LEU:HD12	1.73	0.70
1:A:957:THR:HB	2:B:954:GLU:HA	1.74	0.70
1:A:1253:MET:O	1:A:1658:ASN:ND2	2.25	0.70
1:A:266:SER:HA	1:A:294:PRO:HG2	1.74	0.70
5:F:56:TYR:H	5:F:123:LEU:HD22	1.56	0.70
12:M:83:LEU:HD22	12:M:116:ARG:HG3	1.74	0.69
10:L:56:ASP:OD2	10:L:57:ALA:N	2.25	0.69
1:A:429:ARG:NH1	1:A:1675:GLU:O	2.25	0.69
1:A:855:GLN:O	1:A:859:ASN:ND2	2.20	0.69
1:A:1052:HIS:HB3	1:A:1055:GLU:HB3	1.75	0.69
1:A:887:ARG:HD3	1:A:891:GLU:HB3	1.74	0.69
2:B:770:HIS:ND1	2:B:876:ASN:OD1	2.26	0.69
11:N:81:CYS:O	11:N:85:CYS:N	2.20	0.69
11:N:94:LYS:N	12:M:39:ASP:O	2.20	0.69
1:A:1566:GLU:OE2	1:A:1574:LYS:NZ	2.25	0.69
2:B:179:ILE:HD11	2:B:434:PHE:HE1	1.58	0.68
7:I:34:ASP:OD1	7:I:34:ASP:N	2.24	0.68
1:A:675:ILE:HG12	6:H:92:MET:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:THR:HG1	2:B:605:SER:HG	1.39	0.68
11:N:48:ASP:OD2	11:N:51:ASN:ND2	2.26	0.68
1:A:935:LEU:O	1:A:937:CYS:N	2.25	0.68
2:B:439:LEU:HB3	2:B:450:ASP:HB2	1.74	0.68
3:C:270:LYS:NZ	3:C:271:LYS:O	2.17	0.68
4:E:173:ILE:O	4:E:210:GLN:N	2.26	0.68
1:A:479:GLU:OE1	1:A:543:LYS:NZ	2.25	0.68
9:K:41:THR:OG1	9:K:83:ARG:NE	2.26	0.68
2:B:255:ALA:O	2:B:297:GLN:NE2	2.27	0.68
1:A:4:SER:OG	1:A:5:LYS:N	2.28	0.67
1:A:1327:TYR:HB2	1:A:1331:LYS:HD2	1.75	0.67
2:B:470:ARG:NH2	2:B:515:THR:O	2.25	0.67
2:B:700:LEU:HD11	2:B:706:ARG:HD2	1.76	0.67
1:A:310:ARG:HH21	1:A:325:THR:HA	1.58	0.67
3:C:96:ASN:HD22	10:L:50:LYS:HE2	1.60	0.67
1:A:171:ASN:OD1	1:A:172:ASN:ND2	2.27	0.67
1:A:51:TYR:HE1	1:A:310:ARG:HD3	1.59	0.67
1:A:1075:TRP:CD2	1:A:1142:CYS:HB3	2.30	0.67
2:B:261:ASP:O	2:B:264:ILE:N	2.27	0.67
6:H:102:ASP:OD1	6:H:106:THR:OG1	2.11	0.67
1:A:620:VAL:HG22	1:A:627:LEU:HD12	1.77	0.67
3:C:97:ASN:HD22	3:C:103:ASP:HB3	1.59	0.67
2:B:905:THR:HG22	2:B:906:GLU:H	1.60	0.67
3:C:156:SER:HA	3:C:162:LEU:HD11	1.76	0.67
7:I:23:CYS:O	11:N:66:ARG:HG3	1.94	0.67
1:A:1004:ASP:OD2	1:A:1008:ARG:NH2	2.28	0.66
1:A:1046:VAL:O	1:A:1050:SER:OG	2.13	0.66
1:A:749:LEU:HB3	1:A:754:TYR:HE1	1.58	0.66
2:B:757:MET:N	2:B:894:SER:OG	2.29	0.66
2:B:934:ALA:HA	2:B:962:PHE:CE2	2.29	0.66
6:H:64:LEU:HD11	6:H:144:LEU:HD21	1.77	0.66
2:B:766:ARG:NH2	8:J:10:CYS:O	2.24	0.66
1:A:447:PRO:HB2	1:A:579:TYR:CE1	2.31	0.66
1:A:1665:ASN:ND2	1:A:1667:SER:O	2.27	0.66
1:A:1306:GLU:OE1	7:I:48:ARG:NH2	2.29	0.66
1:A:606:ALA:HA	1:A:609:TYR:HD2	1.60	0.66
2:B:854:VAL:HG13	10:L:44:MET:HB2	1.78	0.66
7:I:38:CYS:SG	7:I:39:ILE:N	2.69	0.66
1:A:310:ARG:HG3	1:A:324:GLN:HE21	1.61	0.66
1:A:1352:GLU:HA	1:A:1355:LYS:HE3	1.76	0.66
1:A:1002:GLN:NE2	5:F:111:PRO:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:27:ARG:NE	6:H:42:ASP:OD1	2.25	0.66
11:N:86:ARG:NH1	12:M:51:PHE:O	2.29	0.65
2:B:195:ARG:HD3	2:B:197:LYS:HB3	1.77	0.65
1:A:182:LYS:NZ	1:A:1009:ASP:OD2	2.28	0.65
2:B:823:ASP:O	2:B:841:TYR:N	2.28	0.65
2:B:140:MET:HB2	2:B:170:PHE:HE2	1.61	0.65
3:C:142:LEU:HD23	3:C:210:LEU:HD23	1.79	0.65
1:A:113:PRO:HG3	1:A:206:PRO:HG2	1.78	0.65
1:A:551:ASN:HB3	1:A:595:ASN:HD21	1.62	0.65
1:A:821:HIS:O	1:A:825:GLN:NE2	2.30	0.65
2:B:548:ARG:HG3	2:B:550:TYR:CZ	2.32	0.65
1:A:1257:ALA:O	1:A:1259:ILE:N	2.30	0.65
2:B:88:PRO:HB2	2:B:859:THR:HG21	1.78	0.65
6:H:64:LEU:HD21	6:H:85:ALA:HB2	1.78	0.65
1:A:677:LYS:HB2	6:H:91:VAL:H	1.61	0.65
1:A:1221:GLU:HB2	1:A:1222:PRO:HD3	1.79	0.65
12:M:140:GLN:NE2	12:M:141:ILE:O	2.30	0.65
1:A:797:LEU:HD21	2:B:921:PRO:HD3	1.78	0.64
2:B:227:HIS:CE1	2:B:237:ASN:HD22	2.15	0.64
12:M:31:SER:HA	12:M:97:PRO:HG2	1.78	0.64
1:A:428:PHE:CD1	1:A:432:MET:HG3	2.32	0.64
1:A:633:ASP:OD2	2:B:753:MET:HG2	1.98	0.64
1:A:1305:MET:HB3	1:A:1310:ASN:HD22	1.60	0.64
2:B:793:VAL:H	2:B:828:TYR:HA	1.63	0.64
3:C:163:TYR:CE1	3:C:204:PRO:HD3	2.33	0.64
1:A:428:PHE:O	2:B:1042:ARG:NH2	2.31	0.64
1:A:978:THR:O	1:A:982:THR:HG23	1.95	0.64
2:B:594:GLU:OE2	2:B:618:ARG:NE	2.30	0.64
11:N:61:ALA:HA	11:N:70:VAL:HA	1.77	0.64
11:N:84:LEU:HA	12:M:49:ALA:HB2	1.78	0.64
1:A:637:SER:HG	1:A:785:PHE:HD1	1.44	0.64
2:B:1003:ARG:NH1	2:B:1004:HIS:O	2.30	0.64
11:N:60:LEU:O	11:N:71:GLY:N	2.26	0.64
1:A:573:LYS:NZ	2:B:1008:ASP:OD2	2.21	0.64
2:B:292:GLU:N	2:B:292:GLU:OE2	2.31	0.64
2:B:626:LEU:HA	12:M:131:GLN:NE2	2.11	0.64
1:A:132:LEU:HD13	4:E:172:ARG:NH2	2.13	0.64
2:B:762:ALA:O	2:B:765:GLU:N	2.28	0.64
1:A:1324:HIS:O	1:A:1328:GLN:CB	2.46	0.63
12:M:45:ILE:HG23	12:M:115:LEU:HB2	1.79	0.63
1:A:847:GLN:HA	1:A:850:HIS:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:80:LYS:O	11:N:84:LEU:N	2.30	0.63
2:B:779:ILE:HG13	2:B:867:VAL:HB	1.80	0.63
4:E:31:ASP:OD1	4:E:31:ASP:N	2.30	0.63
4:E:52:ARG:NH2	4:E:107:GLN:OE1	2.32	0.63
1:A:1699:CYS:HA	1:A:1702:VAL:HG22	1.81	0.63
1:A:1337:ASP:OD1	1:A:1337:ASP:N	2.31	0.63
2:B:344:TYR:OH	2:B:543:ASP:OD1	2.11	0.63
1:A:1130:GLU:OE2	1:A:1130:GLU:N	2.31	0.63
1:A:1340:ARG:O	1:A:1344:THR:OG1	2.11	0.63
2:B:857:ASN:HB2	2:B:862:GLY:HA3	1.81	0.63
1:A:1110:ARG:HH21	1:A:1111:ASN:HD22	1.46	0.63
2:B:791:SER:OG	2:B:864:PHE:O	2.16	0.63
10:L:26:ASN:ND2	10:L:36:CYS:SG	2.71	0.63
1:A:1052:HIS:ND1	5:F:126:THR:OG1	2.29	0.62
1:A:1316:GLN:OE1	1:A:1317:LEU:N	2.32	0.62
4:E:27:LEU:HG	4:E:64:HIS:CG	2.33	0.62
1:A:955:PHE:O	1:A:956:LEU:HD23	1.99	0.62
5:F:69:ARG:NH2	5:F:101:LYS:O	2.32	0.62
1:A:137:GLU:HG3	4:E:187:ARG:HG2	1.81	0.62
1:A:584:ALA:HB2	1:A:627:LEU:HD21	1.81	0.62
1:A:1051:GLN:OE1	1:A:1051:GLN:N	2.32	0.62
11:N:92:LEU:O	12:M:41:GLU:N	2.33	0.62
1:A:83:LEU:HD22	1:A:302:LEU:HD11	1.81	0.62
7:I:25:SER:OG	7:I:26:VAL:N	2.30	0.62
1:A:1144:ASP:N	1:A:1144:ASP:OD1	2.33	0.62
2:B:949:PRO:HB2	2:B:950:PHE:CD2	2.35	0.62
6:H:133:HIS:CD2	6:H:134:GLY:H	2.17	0.62
11:N:11:TRP:CH2	12:M:53:PRO:HB2	2.33	0.62
2:B:696:MET:HG3	2:B:712:TYR:HB3	1.81	0.62
9:K:39:CYS:HA	9:K:85:GLN:HG2	1.80	0.62
4:E:62:VAL:HG22	4:E:71:GLN:HB2	1.80	0.61
12:M:81:ARG:N	12:M:118:LEU:O	2.29	0.61
2:B:981:SER:OG	2:B:982:GLY:N	2.30	0.61
3:C:112:LEU:HB3	8:J:6:ARG:HD2	1.81	0.61
3:C:242:LEU:HD21	3:C:298:ARG:HD3	1.82	0.61
1:A:1287:ARG:HG3	1:A:1555:ALA:HB2	1.82	0.61
1:A:1612:TYR:HE1	4:E:142:HIS:CD2	2.18	0.61
3:C:334:ARG:NE	9:K:104:MET:SD	2.74	0.61
1:A:452:ASN:OD1	1:A:567:ARG:NH2	2.33	0.61
10:L:25:GLU:N	10:L:25:GLU:OE1	2.31	0.61
1:A:616:GLN:HA	1:A:766:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:ASP:OD1	2:B:277:PHE:N	2.33	0.61
1:A:619:LEU:HA	1:A:626:PRO:HA	1.81	0.61
2:B:825:TYR:N	2:B:839:MET:O	2.34	0.61
1:A:1083:LEU:HD23	1:A:1083:LEU:H	1.66	0.61
1:A:1175:ALA:HB2	1:A:1189:LEU:HD21	1.82	0.61
2:B:583:VAL:HG13	2:B:584:LEU:HD12	1.81	0.61
2:B:980:TYR:OH	3:C:301:ARG:NH1	2.34	0.61
6:H:38:ASP:N	6:H:38:ASP:OD1	2.30	0.61
2:B:903:PRO:HB2	2:B:979:LEU:HD11	1.83	0.61
10:L:30:SER:O	10:L:31:ARG:NH1	2.34	0.61
1:A:1050:SER:O	5:F:126:THR:OG1	2.20	0.60
1:A:1089:PHE:CD1	4:E:27:LEU:HD22	2.36	0.60
2:B:540:THR:HG21	2:B:546:PRO:HB3	1.81	0.60
2:B:825:TYR:HB3	2:B:826:TYR:CD1	2.35	0.60
6:H:11:ASP:HB2	6:H:55:LYS:HG3	1.83	0.60
12:M:65:GLY:O	12:M:84:SER:OG	2.19	0.60
1:A:1145:PRO:O	1:A:1148:SER:OG	2.16	0.60
1:A:1614:ILE:O	1:A:1617:ALA:N	2.34	0.60
1:A:1273:LYS:O	1:A:1275:LEU:N	2.34	0.60
2:B:752:ASP:HB2	2:B:916:ASN:HB2	1.82	0.60
1:A:833:LEU:HD12	1:A:834:PRO:HD2	1.84	0.60
1:A:1274:ALA:O	1:A:1278:VAL:HB	2.01	0.60
1:A:1312:PHE:HB3	1:A:1532:PRO:HA	1.83	0.60
1:A:1604:ASP:OD1	1:A:1605:ILE:N	2.34	0.60
2:B:623:VAL:HG21	2:B:658:HIS:HD2	1.67	0.60
4:E:47:LYS:NZ	4:E:52:ARG:HD2	2.16	0.60
2:B:514:LEU:HD23	2:B:518:CYS:SG	2.41	0.60
2:B:704:GLN:OE1	2:B:851:ASN:ND2	2.32	0.60
1:A:132:LEU:HD13	4:E:172:ARG:HH21	1.66	0.60
1:A:1559:ILE:HD11	1:A:1584:ASN:HB3	1.84	0.60
1:A:1673:THR:HG23	2:B:1042:ARG:HH22	1.67	0.60
2:B:525:VAL:HG11	2:B:590:PRO:HG3	1.84	0.60
2:B:739:THR:HG21	2:B:769:ALA:HB2	1.83	0.60
8:J:17:LYS:HB3	8:J:38:LEU:HD13	1.83	0.60
2:B:932:SER:OG	2:B:995:GLY:HA3	2.02	0.60
1:A:1053:LEU:HD12	1:A:1198:LEU:HD12	1.84	0.60
1:A:1616:ALA:HA	4:E:144:LEU:HD13	1.83	0.59
2:B:275:ASP:OD1	2:B:278:LEU:N	2.32	0.59
1:A:140:ARG:HH21	4:E:123:PRO:HD3	1.66	0.59
1:A:813:GLN:NE2	2:B:954:GLU:OE2	2.35	0.59
1:A:1706:VAL:HG23	2:B:1051:SER:OG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:14:PRO:HB2	10:L:29:LYS:HE3	1.84	0.59
1:A:1355:LYS:HA	1:A:1358:ASN:HD21	1.67	0.59
11:N:11:TRP:CZ3	11:N:13:TYR:HB2	2.37	0.59
1:A:1034:PRO:HB2	1:A:1035:LYS:HZ2	1.66	0.59
1:A:1622:GLU:HG3	1:A:1641:LEU:HB3	1.85	0.59
2:B:615:THR:O	2:B:618:ARG:NH1	2.35	0.59
1:A:577:LEU:HD12	1:A:578:HIS:H	1.67	0.59
1:A:1031:PHE:HE2	1:A:1040:LEU:HD11	1.67	0.59
1:A:470:GLN:HB3	1:A:480:LEU:HD21	1.85	0.59
1:A:751:LYS:HG3	1:A:901:GLY:HA3	1.85	0.59
1:A:887:ARG:O	1:A:892:ASN:HB2	2.02	0.59
1:A:1005:LEU:HD13	1:A:1151:ARG:HH21	1.67	0.59
4:E:133:GLN:HA	4:E:136:LEU:HG	1.84	0.59
12:M:71:GLY:N	12:M:78:HIS:O	2.34	0.59
1:A:677:LYS:HB3	1:A:678:PRO:HD3	1.85	0.59
1:A:1304:CYS:HB2	1:A:1314:VAL:HG13	1.85	0.59
2:B:417:MET:SD	2:B:417:MET:N	2.75	0.59
1:A:460:MET:HG3	1:A:570:PRO:HA	1.84	0.59
1:A:1110:ARG:NH2	1:A:1111:ASN:HD22	2.01	0.59
2:B:916:ASN:HD21	2:B:918:HIS:HB2	1.68	0.59
2:B:941:HIS:CE1	12:M:143:PRO:HD2	2.38	0.59
4:E:26:TYR:HA	4:E:64:HIS:CE1	2.37	0.59
4:E:36:THR:HG22	4:E:38:GLU:H	1.67	0.59
7:I:38:CYS:SG	7:I:40:ARG:N	2.72	0.59
1:A:1034:PRO:HB2	1:A:1035:LYS:NZ	2.17	0.59
2:B:201:ARG:HB2	2:B:205:TYR:HE2	1.66	0.59
2:B:544:GLY:O	2:B:546:PRO:HD3	2.03	0.59
4:E:163:TYR:HB2	4:E:165:LEU:HD22	1.84	0.59
11:N:42:THR:OG1	11:N:61:ALA:O	2.15	0.59
12:M:32:LEU:O	12:M:36:THR:HG23	2.03	0.59
2:B:64:PHE:CE1	2:B:397:LYS:HB2	2.37	0.58
4:E:63:ALA:N	4:E:70:ASP:O	2.34	0.58
1:A:633:ASP:HA	2:B:918:HIS:CE1	2.37	0.58
2:B:521:VAL:HG22	2:B:592:TRP:HD1	1.68	0.58
3:C:253:LEU:HB3	3:C:262:ILE:HD13	1.85	0.58
1:A:1011:ASP:HA	1:A:1694:ARG:NH2	2.18	0.58
1:A:1341:PHE:CZ	1:A:1345:ARG:HG3	2.38	0.58
3:C:103:ASP:OD1	3:C:104:GLU:N	2.37	0.58
1:A:1100:VAL:HG11	1:A:1120:MET:HG2	1.85	0.58
3:C:138:LEU:HB2	3:C:214:CYS:HB2	1.85	0.58
2:B:625:ASN:OD1	2:B:626:LEU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:ALA:HB2	2:B:422:MET:SD	2.44	0.58
2:B:700:LEU:HA	2:B:735:TYR:HE2	1.69	0.58
2:B:741:ALA:HB2	2:B:768:PHE:HZ	1.69	0.58
3:C:116:HIS:ND1	3:C:116:HIS:O	2.37	0.58
1:A:802:ILE:HD11	1:A:912:ILE:HG21	1.86	0.58
1:A:1053:LEU:O	1:A:1056:VAL:C	2.41	0.58
1:A:602:GLU:HG3	5:F:71:LEU:HA	1.86	0.58
2:B:824:PRO:HA	2:B:840:TYR:HA	1.85	0.58
2:B:728:ASP:O	2:B:731:ASP:N	2.28	0.57
1:A:643:THR:O	1:A:645:GLY:N	2.35	0.57
1:A:974:GLY:O	1:A:978:THR:HG23	2.05	0.57
3:C:170:THR:OG1	3:C:195:ASP:HA	2.04	0.57
4:E:77:PRO:HD2	4:E:105:VAL:O	2.05	0.57
1:A:691:LEU:O	1:A:695:ILE:HB	2.04	0.57
1:A:1296:LYS:HB2	1:A:1320:GLN:HB2	1.86	0.57
1:A:703:LEU:HD13	1:A:768:ILE:HD11	1.86	0.57
1:A:897:MET:HA	1:A:902:ALA:HB3	1.86	0.57
3:C:64:ASP:OD2	3:C:279:ARG:NH2	2.37	0.57
1:A:1050:SER:OG	1:A:1051:GLN:OE1	2.15	0.57
2:B:362:MET:N	2:B:605:SER:O	2.32	0.57
3:C:262:ILE:HG13	3:C:262:ILE:O	2.03	0.57
1:A:545:GLY:O	1:A:609:TYR:OH	2.08	0.57
1:A:686:GLN:O	1:A:689:SER:OG	2.22	0.57
1:A:704:ASN:N	1:A:1043:ASN:HD21	1.89	0.57
2:B:368:SER:OG	2:B:369:LEU:N	2.37	0.57
2:B:458:ASP:OD2	2:B:464:ARG:NH1	2.37	0.57
2:B:1067:ALA:HB1	2:B:1076:LEU:HD11	1.87	0.57
4:E:26:TYR:HA	4:E:64:HIS:HE1	1.69	0.57
1:A:1295:GLN:HG3	1:A:1296:LYS:HG3	1.87	0.57
1:A:579:TYR:HB2	1:A:631:ILE:HG12	1.86	0.57
2:B:87:VAL:HG22	2:B:88:PRO:O	2.04	0.57
1:A:847:GLN:HA	1:A:850:HIS:HD2	1.69	0.56
1:A:1354:ILE:O	1:A:1358:ASN:ND2	2.38	0.56
3:C:159:PRO:HA	3:C:162:LEU:HB2	1.86	0.56
3:C:258:SER:OG	3:C:281:ASP:OD1	2.23	0.56
11:N:86:ARG:NH1	12:M:53:PRO:HD3	2.20	0.56
2:B:201:ARG:HB2	2:B:205:TYR:CE2	2.40	0.56
1:A:134:ALA:O	1:A:138:LEU:HG	2.04	0.56
1:A:535:THR:HG22	1:A:536:LYS:H	1.70	0.56
1:A:571:GLU:OE2	2:B:895:ARG:NH1	2.37	0.56
1:A:669:LYS:H	1:A:694:ASN:HD21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLU:N	1:A:698:GLU:OE1	2.38	0.56
1:A:1044:TYR:OH	1:A:1048:MET:SD	2.52	0.56
2:B:104:ARG:NH2	2:B:161:GLU:OE2	2.38	0.56
2:B:290:MET:SD	7:I:25:SER:OG	2.60	0.56
2:B:336:LEU:HD13	2:B:341:GLU:HB3	1.87	0.56
2:B:546:PRO:HG2	2:B:549:SER:OG	2.04	0.56
2:B:591:PRO:HD2	2:B:592:TRP:CZ3	2.41	0.56
3:C:90:GLU:HG2	3:C:224:LYS:NZ	2.20	0.56
6:H:113:SER:HA	6:H:126:GLN:HA	1.87	0.56
11:N:57:GLN:O	11:N:58:ARG:NH1	2.36	0.56
11:N:93:ASN:OD1	11:N:95:THR:OG1	2.19	0.56
1:A:146:LEU:HA	1:A:158:ARG:HD3	1.86	0.56
2:B:542:ILE:HA	2:B:564:GLY:HA2	1.87	0.56
5:F:121:ASP:N	5:F:121:ASP:OD1	2.36	0.56
1:A:1700:LEU:HG	1:A:1706:VAL:HG21	1.88	0.56
4:E:95:GLN:OE1	4:E:125:TYR:OH	2.12	0.56
4:E:132:GLN:HE22	4:E:136:LEU:HD21	1.71	0.56
12:M:87:PRO:HD3	12:M:113:GLY:HA2	1.88	0.56
1:A:433:MET:HB2	2:B:1042:ARG:NE	2.21	0.56
1:A:637:SER:O	1:A:640:SER:OG	2.13	0.56
2:B:601:THR:OG1	2:B:605:SER:OG	2.17	0.56
2:B:702:THR:O	2:B:702:THR:OG1	2.20	0.56
4:E:82:VAL:O	4:E:111:THR:OG1	2.22	0.56
5:F:89:PRO:O	5:F:93:ALA:HB2	2.05	0.56
9:K:44:LEU:HD12	9:K:80:ILE:HD11	1.87	0.56
10:L:42:ARG:HG2	10:L:42:ARG:O	2.05	0.56
1:A:1290:LEU:O	1:A:1294:LEU:HG	2.06	0.56
1:A:1085:ARG:HH12	4:E:19:GLN:HB3	1.71	0.56
1:A:1265:SER:OG	1:A:1601:TYR:O	2.23	0.56
1:A:1604:ASP:CG	1:A:1606:HIS:H	2.08	0.56
2:B:883:PHE:HD2	2:B:999:TYR:HD1	1.53	0.56
3:C:137:THR:OG1	3:C:138:LEU:O	2.24	0.56
3:C:247:GLY:O	3:C:270:LYS:HE2	2.06	0.56
2:B:263:GLN:HG2	11:N:30:ASN:ND2	2.21	0.55
5:F:97:LEU:HD21	5:F:125:ILE:HG21	1.89	0.55
1:A:1338:ILE:HG13	1:A:1339:LEU:N	2.21	0.55
2:B:72:ARG:HG2	2:B:123:ASN:HB2	1.87	0.55
2:B:881:ASP:OD2	2:B:882:LYS:N	2.32	0.55
1:A:1118:GLN:HA	1:A:1121:LEU:HD12	1.89	0.55
1:A:1324:HIS:O	1:A:1328:GLN:HB2	2.05	0.55
1:A:1497:ALA:O	1:A:1500:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1671:GLN:HB3	1:A:1680:PHE:CG	2.41	0.55
1:A:1604:ASP:OD1	1:A:1606:HIS:N	2.37	0.55
1:A:580:ALA:N	1:A:631:ILE:HD13	2.21	0.55
1:A:872:TYR:O	1:A:876:ILE:HG12	2.06	0.55
1:A:1153:ASP:OD1	1:A:1154:ILE:N	2.38	0.55
2:B:56:LEU:O	2:B:218:GLU:HB3	2.06	0.55
2:B:218:GLU:OE1	2:B:218:GLU:N	2.28	0.55
4:E:134:GLU:OE2	4:E:181:ARG:NH2	2.39	0.55
1:A:1567:THR:HG23	1:A:1574:LYS:HD3	1.88	0.55
1:A:1324:HIS:O	1:A:1328:GLN:HB3	2.07	0.55
1:A:140:ARG:NH2	4:E:123:PRO:HD3	2.21	0.55
1:A:165:THR:O	1:A:169:VAL:HG23	2.07	0.55
1:A:692:LEU:HA	1:A:695:ILE:HG22	1.88	0.55
1:A:1567:THR:OG1	1:A:1568:THR:N	2.37	0.55
7:I:37:THR:OG1	7:I:38:CYS:N	2.40	0.55
1:A:69:GLN:HG2	2:B:1082:GLU:HA	1.89	0.55
1:A:854:ASP:OD1	1:A:855:GLN:N	2.31	0.55
1:A:1026:ILE:HG23	1:A:1029:THR:HB	1.89	0.55
1:A:1250:GLU:HA	1:A:1254:VAL:HB	1.88	0.55
1:A:1089:PHE:HD2	1:A:1092:TYR:HD2	1.54	0.55
1:A:1681:LEU:O	1:A:1685:THR:HG23	2.07	0.55
1:A:562:GLN:HE21	1:A:564:HIS:CE1	2.24	0.54
7:I:18:ASP:HB2	7:I:27:LEU:HD22	1.89	0.54
8:J:22:LEU:HD23	8:J:25:LEU:HD12	1.87	0.54
1:A:140:ARG:HH21	4:E:122:ALA:HB3	1.72	0.54
1:A:732:MET:HB3	6:H:122:LEU:HD11	1.90	0.54
2:B:889:GLN:HE21	2:B:925:THR:HG21	1.72	0.54
2:B:912:ASP:OD1	2:B:912:ASP:N	2.38	0.54
2:B:943:LEU:H	2:B:943:LEU:HD23	1.71	0.54
6:H:8:ASP:OD1	6:H:9:ILE:N	2.39	0.54
1:A:24:GLU:HA	1:A:27:LYS:HE3	1.90	0.54
1:A:1092:TYR:O	1:A:1096:ILE:HG12	2.08	0.54
1:A:1342:MET:HG2	1:A:1346:PHE:CE2	2.43	0.54
4:E:82:VAL:HB	4:E:110:MET:HG3	1.90	0.54
1:A:531:LYS:HE3	1:A:534:GLY:HA3	1.90	0.54
2:B:1055:HIS:O	2:B:1059:PHE:HB3	2.07	0.54
11:N:80:LYS:O	11:N:84:LEU:HG	2.06	0.54
1:A:1290:LEU:HD21	1:A:1346:PHE:CZ	2.42	0.54
1:A:1314:VAL:HG12	1:A:1530:LYS:HB2	1.90	0.54
2:B:78:LEU:HD11	2:B:119:ASN:HB3	1.88	0.54
2:B:756:ALA:HA	2:B:892:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:ARG:HG2	2:B:896:LEU:N	2.23	0.54
11:N:67:LEU:HB3	11:N:111:PRO:HB3	1.90	0.54
1:A:327:ASN:HB3	1:A:401:VAL:HG22	1.89	0.54
1:A:456:ILE:HG12	1:A:564:HIS:CB	2.37	0.54
1:A:1299:VAL:HB	7:I:56:LYS:HG3	1.90	0.54
2:B:800:ASP:O	2:B:802:ARG:N	2.32	0.54
1:A:613:CYS:O	1:A:617:GLN:HB2	2.07	0.54
2:B:214:CYS:SG	2:B:335:HIS:ND1	2.70	0.54
1:A:227:PHE:HB2	1:A:252:LYS:HB3	1.90	0.53
1:A:1342:MET:O	1:A:1346:PHE:HB2	2.08	0.53
2:B:393:LEU:O	2:B:396:ILE:HG22	2.08	0.53
5:F:100:ARG:HD2	5:F:100:ARG:N	2.23	0.53
11:N:40:ARG:NE	11:N:63:GLU:OE2	2.41	0.53
1:A:30:VAL:HG11	2:B:1099:THR:HG22	1.89	0.53
1:A:455:GLU:HG2	1:A:565:ARG:O	2.08	0.53
1:A:487:GLY:HA2	1:A:494:ALA:H	1.73	0.53
1:A:710:LYS:HB3	1:A:750:ASP:OD2	2.08	0.53
2:B:467:SER:O	2:B:470:ARG:N	2.36	0.53
2:B:609:GLY:HA3	2:B:611:PHE:HE2	1.73	0.53
7:I:19:PHE:O	11:N:66:ARG:NH1	2.42	0.53
9:K:62:ASN:HD22	9:K:95:PRO:HB3	1.73	0.53
1:A:619:LEU:HD21	1:A:763:HIS:CD2	2.43	0.53
1:A:73:ASN:HD22	2:B:1081:LEU:HB3	1.74	0.53
2:B:258:SER:OG	2:B:259:PHE:N	2.41	0.53
2:B:648:GLU:O	2:B:651:VAL:HG12	2.09	0.53
2:B:800:ASP:OD1	2:B:800:ASP:N	2.38	0.53
6:H:37:MET:HE1	6:H:132:LEU:HD11	1.89	0.53
1:A:187:SER:O	1:A:191:LEU:HG	2.08	0.53
1:A:630:LEU:HD21	1:A:634:HIS:HB2	1.91	0.53
5:F:110:LEU:HB2	5:F:114:SER:O	2.09	0.53
11:N:84:LEU:O	12:M:49:ALA:N	2.41	0.53
1:A:632:GLN:HA	1:A:635:MET:SD	2.49	0.53
1:A:1498:MET:HA	1:A:1501:ARG:HE	1.73	0.53
3:C:189:THR:OG1	3:C:190:ILE:N	2.41	0.53
12:M:98:SER:HB2	12:M:101:ALA:HB3	1.91	0.53
1:A:599:PRO:HB3	2:B:1057:ARG:NH2	2.23	0.53
1:A:1527:VAL:HG22	1:A:1528:THR:H	1.74	0.53
2:B:228:TYR:HB2	2:B:353:LEU:HD21	1.91	0.53
2:B:312:LEU:HD22	2:B:327:LEU:HB2	1.89	0.53
2:B:601:THR:OG1	2:B:603:LYS:O	2.27	0.53
4:E:44:SER:HB3	4:E:50:GLU:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:40:ILE:HB	6:H:124:ARG:HB3	1.90	0.53
1:A:136:TYR:HB3	4:E:187:ARG:NH1	2.24	0.53
3:C:248:GLU:O	3:C:251:GLU:HG2	2.08	0.53
4:E:46:ASP:OD1	4:E:47:LYS:N	2.38	0.53
1:A:607:GLU:HB3	5:F:64:ARG:HH11	1.73	0.53
3:C:318:PRO:HA	3:C:321:LEU:HD12	1.91	0.53
4:E:110:MET:HB3	4:E:115:LYS:NZ	2.24	0.53
5:F:57:MET:HE2	5:F:62:ARG:HB2	1.90	0.53
1:A:1288:VAL:HG11	1:A:1331:LYS:HD3	1.90	0.53
2:B:680:ASN:HD21	2:B:887:HIS:HB3	1.74	0.53
2:B:694:GLN:NE2	2:B:1003:ARG:HE	2.03	0.53
4:E:131:LEU:H	4:E:131:LEU:HD12	1.73	0.53
4:E:172:ARG:HA	4:E:208:LEU:O	2.09	0.53
1:A:447:PRO:O	1:A:579:TYR:OH	2.25	0.52
1:A:1092:TYR:CZ	1:A:1096:ILE:HG13	2.44	0.52
2:B:532:ALA:O	2:B:536:ASN:ND2	2.43	0.52
2:B:751:TYR:CE2	2:B:895:ARG:HD2	2.44	0.52
7:I:23:CYS:H	11:N:66:ARG:NE	2.06	0.52
8:J:10:CYS:SG	8:J:11:GLY:N	2.82	0.52
1:A:608:ALA:HA	1:A:612:ALA:HB3	1.90	0.52
5:F:55:PRO:HG3	5:F:118:TRP:HH2	1.74	0.52
10:L:30:SER:OG	10:L:31:ARG:N	2.42	0.52
11:N:60:LEU:N	11:N:71:GLY:O	2.36	0.52
12:M:137:PRO:HG2	12:M:138:PRO:HD3	1.92	0.52
1:A:819:SER:O	1:A:819:SER:OG	2.23	0.52
1:A:994:LYS:HB3	1:A:1674:PHE:CD1	2.43	0.52
1:A:1011:ASP:HB3	1:A:1666:SER:HB2	1.92	0.52
1:A:1656:PRO:HG2	1:A:1660:PHE:CD1	2.44	0.52
1:A:397:HIS:O	1:A:401:VAL:HG23	2.10	0.52
1:A:717:VAL:O	1:A:718:LYS:NZ	2.31	0.52
11:N:43:LEU:HD21	12:M:23:PRO:HA	1.92	0.52
1:A:57:PRO:HD2	1:A:74:CYS:SG	2.49	0.52
1:A:332:MET:O	1:A:336:VAL:HG23	2.09	0.52
1:A:972:ARG:O	1:A:976:VAL:HG23	2.09	0.52
1:A:1249:ARG:HG2	1:A:1253:MET:SD	2.49	0.52
2:B:38:LEU:HD12	2:B:730:TYR:HE1	1.74	0.52
2:B:261:ASP:OD2	7:I:26:VAL:HG23	2.09	0.52
1:A:401:VAL:HG12	2:B:1126:MET:HG3	1.90	0.52
1:A:417:ILE:N	2:B:1126:MET:HE3	2.25	0.52
2:B:263:GLN:HE21	11:N:111:PRO:CD	2.22	0.52
2:B:753:MET:HA	2:B:916:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:86:ARG:N	12:M:47:ALA:O	2.43	0.52
1:A:618:TYR:CE2	1:A:626:PRO:HB3	2.45	0.52
1:A:1533:LEU:H	1:A:1533:LEU:HD23	1.74	0.52
3:C:159:PRO:HB3	3:C:163:TYR:HD2	1.75	0.52
6:H:94:GLY:HA2	6:H:118:TYR:HD1	1.74	0.52
1:A:119:LEU:HD22	1:A:143:ASN:HB2	1.91	0.52
1:A:130:GLY:HA2	1:A:184:VAL:HG21	1.92	0.52
1:A:421:LEU:O	1:A:1677:SER:OG	2.12	0.52
3:C:319:ASP:OD1	3:C:320:VAL:N	2.41	0.52
4:E:84:ILE:HD11	4:E:113:SER:OG	2.10	0.52
7:I:21:SER:C	11:N:66:ARG:HB2	2.30	0.52
1:A:597:HIS:HE2	2:B:1057:ARG:HD2	1.75	0.52
1:A:1153:ASP:HB2	5:F:54:THR:HB	1.91	0.52
2:B:1003:ARG:HG2	2:B:1004:HIS:N	2.25	0.52
3:C:159:PRO:O	3:C:163:TYR:N	2.43	0.52
6:H:20:LYS:NZ	6:H:22:PHE:O	2.27	0.52
7:I:18:ASP:CG	7:I:27:LEU:HB2	2.30	0.52
1:A:822:CYS:SG	1:A:823:GLY:N	2.83	0.52
1:A:1211:VAL:HA	1:A:1214:LEU:HD22	1.93	0.52
2:B:214:CYS:HB3	2:B:222:VAL:HG12	1.91	0.52
7:I:33:GLN:N	7:I:33:GLN:OE1	2.44	0.52
11:N:26:VAL:HG21	11:N:41:PHE:CE1	2.45	0.52
1:A:716:TRP:O	1:A:718:LYS:NZ	2.43	0.51
2:B:219:HIS:O	2:B:383:MET:HB3	2.11	0.51
1:A:181:VAL:HG22	4:E:166:ARG:HH21	1.75	0.51
1:A:1624:GLU:HA	1:A:1627:ASP:OD2	2.10	0.51
2:B:370:VAL:HG21	2:B:640:ILE:HD11	1.91	0.51
2:B:548:ARG:HH21	2:B:567:ASP:HB2	1.75	0.51
2:B:653:ALA:HA	12:M:130:LEU:HD11	1.91	0.51
3:C:156:SER:HA	3:C:162:LEU:HD21	1.92	0.51
3:C:237:PRO:HB3	3:C:283:PHE:CE1	2.45	0.51
3:C:252:GLU:O	3:C:256:CYS:N	2.43	0.51
6:H:54:ASP:OD1	6:H:147:LYS:HG2	2.11	0.51
1:A:75:SER:H	2:B:1080:LEU:CD2	2.22	0.51
1:A:843:ARG:O	1:A:847:GLN:HG2	2.09	0.51
1:A:934:SER:O	1:A:935:LEU:HD12	2.11	0.51
1:A:1220:GLY:O	1:A:1223:SER:OG	2.20	0.51
1:A:1249:ARG:O	1:A:1253:MET:N	2.41	0.51
3:C:288:PHE:HA	3:C:294:LYS:HG2	1.92	0.51
1:A:685:LYS:HG2	1:A:744:LEU:HD22	1.91	0.51
1:A:1095:LYS:HE3	1:A:1096:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:VAL:HG12	1:A:1600:LEU:HD11	1.91	0.51
1:A:1283:LYS:HB3	1:A:1332:CYS:HB2	1.93	0.51
1:A:1583:ILE:HD12	1:A:1607:ALA:HB2	1.92	0.51
2:B:776:SER:O	2:B:776:SER:OG	2.22	0.51
1:A:1504:ALA:O	1:A:1508:ILE:HG12	2.11	0.51
11:N:87:HIS:CG	11:N:106:LEU:HD13	2.46	0.51
1:A:831:LEU:HD22	1:A:847:GLN:HG3	1.93	0.51
4:E:168:ASN:HA	4:E:172:ARG:NH2	2.26	0.51
11:N:78:ALA:C	11:N:108:ASN:HD21	2.14	0.51
1:A:1290:LEU:HG	1:A:1294:LEU:HD11	1.93	0.51
4:E:11:TRP:CE2	4:E:37:LEU:HB2	2.45	0.51
1:A:749:LEU:HB3	1:A:754:TYR:CE1	2.43	0.51
1:A:1089:PHE:CE1	4:E:27:LEU:HD22	2.46	0.51
1:A:1283:LYS:HD3	1:A:1332:CYS:HB2	1.92	0.51
1:A:1344:THR:O	1:A:1348:LYS:NZ	2.29	0.51
2:B:510:LEU:O	2:B:512:ASN:N	2.43	0.51
3:C:291:GLU:HA	3:C:294:LYS:HE2	1.92	0.51
6:H:7:GLU:OE2	6:H:57:ARG:NH1	2.42	0.51
7:I:23:CYS:HA	7:I:41:CYS:SG	2.50	0.51
10:L:32:ASP:N	10:L:32:ASP:OD1	2.44	0.51
11:N:26:VAL:HG23	12:M:95:LEU:HD11	1.93	0.51
1:A:454:ASN:O	1:A:565:ARG:HG3	2.10	0.51
1:A:469:PRO:HG3	1:A:600:GLN:HE21	1.76	0.51
2:B:314:VAL:HG21	2:B:323:ALA:HB2	1.93	0.51
3:C:222:HIS:ND1	3:C:224:LYS:HG2	2.25	0.51
1:A:631:ILE:O	1:A:635:MET:HG3	2.11	0.50
1:A:1113:ARG:NE	1:A:1118:GLN:OE1	2.45	0.50
2:B:36:GLN:NE2	2:B:165:GLU:O	2.35	0.50
2:B:467:SER:OG	2:B:468:HIS:N	2.44	0.50
2:B:815:ILE:HD11	10:L:46:LYS:HB3	1.94	0.50
1:A:616:GLN:O	1:A:766:TYR:OH	2.28	0.50
1:A:733:CYS:SG	1:A:734:GLU:N	2.83	0.50
2:B:275:ASP:OD1	2:B:276:SER:N	2.44	0.50
2:B:280:ASN:ND2	2:B:284:GLN:OE1	2.43	0.50
2:B:263:GLN:HE21	11:N:111:PRO:HD2	1.76	0.50
3:C:114:PRO:O	3:C:193:VAL:HG23	2.12	0.50
4:E:107:GLN:HG3	4:E:132:GLN:HG2	1.93	0.50
1:A:241:GLU:HG3	1:A:242:PRO:HD2	1.93	0.50
1:A:1060:ALA:HB1	1:A:1156:PHE:HB2	1.93	0.50
1:A:1117:THR:O	1:A:1121:LEU:HG	2.12	0.50
2:B:984:SER:OG	2:B:985:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:92:ALA:O	9:K:95:PRO:HD2	2.12	0.50
1:A:332:MET:HA	1:A:335:VAL:HG22	1.94	0.50
1:A:626:PRO:HD3	1:A:763:HIS:CD2	2.46	0.50
2:B:545:ALA:HB1	12:M:91:GLU:OE2	2.11	0.50
2:B:957:SER:OG	2:B:958:ALA:N	2.45	0.50
1:A:433:MET:HB3	2:B:1042:ARG:HB2	1.94	0.50
1:A:484:VAL:O	1:A:515:ARG:NH2	2.42	0.50
1:A:980:VAL:O	1:A:984:ARG:HG2	2.12	0.50
1:A:1497:ALA:O	1:A:1501:ARG:HG3	2.11	0.50
2:B:239:ILE:HG13	2:B:243:GLU:C	2.32	0.50
2:B:582:LYS:NZ	2:B:593:MET:O	2.31	0.50
2:B:847:CYS:HB2	2:B:872:ARG:O	2.11	0.50
2:B:926:ILE:O	2:B:930:ILE:HG22	2.12	0.50
7:I:22:ASP:HB2	7:I:43:PHE:CD2	2.46	0.50
1:A:499:ASN:HA	1:A:536:LYS:HG2	1.92	0.50
1:A:782:ALA:O	1:A:786:THR:HG23	2.12	0.50
1:A:966:PHE:HA	1:A:969:MET:SD	2.52	0.50
1:A:1342:MET:HG2	1:A:1346:PHE:HD2	1.76	0.50
2:B:256:LEU:HD22	2:B:343:PHE:HB2	1.94	0.50
12:M:83:LEU:O	12:M:115:LEU:HA	2.12	0.50
1:A:1019:TYR:O	1:A:1021:GLU:N	2.45	0.50
1:A:1026:ILE:HA	1:A:1029:THR:OG1	2.11	0.50
1:A:1353:SER:HB2	1:A:1543:LEU:HD21	1.94	0.50
8:J:22:LEU:O	8:J:25:LEU:HB2	2.12	0.50
10:L:32:ASP:HB2	10:L:33:PRO:HD2	1.93	0.50
11:N:81:CYS:HB2	11:N:85:CYS:HB2	1.93	0.50
1:A:638:GLY:HA2	1:A:785:PHE:CE1	2.47	0.49
1:A:1709:GLY:HA3	2:B:1049:GLY:O	2.12	0.49
3:C:146:CYS:SG	3:C:147:THR:N	2.84	0.49
8:J:7:CYS:SG	8:J:8:PHE:N	2.85	0.49
1:A:1213:LEU:HG	2:B:1047:ALA:HA	1.94	0.49
1:A:1615:GLU:N	1:A:1615:GLU:OE1	2.45	0.49
2:B:239:ILE:HG13	2:B:243:GLU:O	2.11	0.49
2:B:991:ASP:N	2:B:991:ASP:OD1	2.44	0.49
1:A:184:VAL:HG22	1:A:188:LYS:NZ	2.28	0.49
1:A:929:MET:HG2	1:A:933:LYS:O	2.12	0.49
1:A:1539:ASP:HB2	1:A:1542:SER:HB3	1.94	0.49
1:A:1618:LEU:HD22	1:A:1645:ALA:HB1	1.94	0.49
2:B:65:GLU:HB2	2:B:75:PHE:CE1	2.46	0.49
1:A:629:GLY:HA3	1:A:756:SER:HB3	1.94	0.49
1:A:1051:GLN:HG3	1:A:1202:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ALA:HA	1:A:1218:SER:OG	2.12	0.49
1:A:1256:SER:OG	1:A:1258:ASN:HB2	2.12	0.49
6:H:55:LYS:O	6:H:148:LEU:N	2.42	0.49
1:A:392:ILE:HA	1:A:395:GLN:HE21	1.78	0.49
1:A:669:LYS:H	1:A:694:ASN:ND2	2.10	0.49
1:A:781:LEU:HG	1:A:785:PHE:CE2	2.47	0.49
1:A:1604:ASP:OD2	1:A:1607:ALA:N	2.44	0.49
2:B:767:GLY:HA2	2:B:770:HIS:CD2	2.47	0.49
3:C:175:TRP:NE1	3:C:176:ILE:O	2.44	0.49
3:C:242:LEU:HG	3:C:298:ARG:HB2	1.94	0.49
4:E:57:ASP:HB3	4:E:59:THR:HG23	1.93	0.49
6:H:98:ARG:HD3	6:H:115:TYR:HD2	1.78	0.49
1:A:183:ASN:HB2	4:E:168:ASN:OD1	2.13	0.49
2:B:329:ASN:HD22	2:B:342:LYS:HZ2	1.61	0.49
2:B:379:GLN:O	2:B:383:MET:HG2	2.12	0.49
2:B:627:ALA:O	12:M:128:SER:OG	2.28	0.49
4:E:47:LYS:HZ2	4:E:52:ARG:HD2	1.78	0.49
4:E:81:LYS:HB3	4:E:111:THR:HG23	1.95	0.49
1:A:1495:PRO:HB2	1:A:1498:MET:HB2	1.94	0.49
2:B:427:THR:OG1	2:B:428:LYS:N	2.45	0.49
2:B:752:ASP:CB	2:B:916:ASN:HB2	2.41	0.49
1:A:551:ASN:N	1:A:595:ASN:OD1	2.40	0.49
1:A:988:LEU:HD13	1:A:1245:ILE:HG23	1.94	0.49
1:A:1034:PRO:O	1:A:1036:GLN:HG2	2.13	0.49
2:B:72:ARG:NH1	2:B:123:ASN:HB2	2.27	0.49
2:B:540:THR:HG22	2:B:565:TRP:O	2.12	0.49
2:B:753:MET:SD	2:B:916:ASN:ND2	2.86	0.49
3:C:84:VAL:HB	3:C:227:PRO:HG3	1.94	0.49
3:C:90:GLU:HG2	3:C:224:LYS:HZ1	1.78	0.49
3:C:160:ASN:HD22	3:C:166:HIS:CE1	2.30	0.49
4:E:60:VAL:HG13	4:E:71:GLN:OE1	2.13	0.49
9:K:27:LEU:HD12	9:K:28:GLU:H	1.78	0.49
1:A:119:LEU:HD13	1:A:143:ASN:HD22	1.78	0.49
1:A:487:GLY:CA	1:A:515:ARG:HH22	2.26	0.49
1:A:1347:PHE:O	1:A:1351:MET:HG2	2.12	0.49
1:A:1501:ARG:O	1:A:1505:VAL:HG23	2.12	0.49
1:A:1672:MET:SD	1:A:1681:LEU:HD21	2.53	0.49
2:B:178:VAL:HG21	2:B:469:PHE:CE1	2.41	0.49
2:B:552:GLU:HB2	2:B:568:LYS:HE3	1.95	0.49
4:E:60:VAL:HG22	4:E:71:GLN:NE2	2.28	0.49
4:E:67:ASP:O	4:E:69:THR:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:187:ARG:HD3	4:E:210:GLN:HA	1.95	0.49
11:N:44:TYR:HB2	11:N:59:ILE:HB	1.95	0.49
11:N:59:ILE:HA	11:N:72:ASN:OD1	2.12	0.49
12:M:54:GLU:H	12:M:54:GLU:CD	2.16	0.49
1:A:497:VAL:HG13	1:A:538:VAL:HA	1.93	0.49
1:A:1021:GLU:HB2	4:E:199:THR:OG1	2.12	0.49
2:B:120:TRP:CG	2:B:416:LEU:HD21	2.48	0.49
2:B:405:GLN:OE1	2:B:406:LYS:HG3	2.13	0.49
2:B:546:PRO:HG2	2:B:549:SER:CB	2.43	0.49
2:B:1039:GLU:O	2:B:1042:ARG:HG2	2.12	0.49
11:N:17:PRO:HD3	11:N:102:TYR:CD1	2.48	0.49
1:A:455:GLU:OE2	1:A:567:ARG:HB2	2.12	0.48
1:A:1621:ILE:O	1:A:1625:ILE:HG13	2.12	0.48
2:B:501:HIS:O	2:B:501:HIS:CD2	2.66	0.48
6:H:133:HIS:CG	6:H:134:GLY:H	2.31	0.48
10:L:41:TYR:HE2	10:L:43:ILE:HG22	1.77	0.48
11:N:80:LYS:C	11:N:84:LEU:HG	2.33	0.48
1:A:630:LEU:HD13	1:A:754:TYR:HB2	1.96	0.48
1:A:727:PHE:HA	6:H:124:ARG:HH12	1.78	0.48
3:C:326:ILE:HG21	9:K:111:LEU:HB2	1.95	0.48
9:K:45:HIS:HB3	9:K:46:GLU:HG2	1.95	0.48
11:N:13:TYR:OH	11:N:103:ASP:OD1	2.24	0.48
12:M:79:ARG:HG3	12:M:122:GLN:HE21	1.76	0.48
1:A:619:LEU:HG	1:A:626:PRO:HA	1.96	0.48
1:A:1100:VAL:HG21	1:A:1120:MET:SD	2.54	0.48
1:A:1289:CYS:HB3	1:A:1552:VAL:HG12	1.95	0.48
2:B:179:ILE:HD11	2:B:434:PHE:CE1	2.44	0.48
2:B:733:ASP:O	2:B:736:PRO:HD3	2.14	0.48
3:C:175:TRP:CD1	3:C:190:ILE:HG21	2.49	0.48
7:I:22:ASP:N	11:N:66:ARG:HB2	2.28	0.48
9:K:47:GLU:N	9:K:78:SER:O	2.35	0.48
10:L:52:LEU:HD23	10:L:52:LEU:H	1.78	0.48
1:A:446:CYS:N	1:A:575:LEU:O	2.44	0.48
1:A:498:ILE:HD12	1:A:504:ARG:HG2	1.94	0.48
1:A:664:LYS:HA	1:A:664:LYS:HE2	1.95	0.48
1:A:1498:MET:HG2	1:A:1501:ARG:NE	2.27	0.48
1:A:133:GLN:OE1	4:E:188:GLY:HA2	2.14	0.48
1:A:449:MET:HG3	2:B:750:GLY:O	2.14	0.48
1:A:449:MET:HG3	2:B:750:GLY:C	2.34	0.48
1:A:555:THR:HB	2:B:1044:ALA:HB2	1.95	0.48
1:A:961:PRO:HA	2:B:950:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:7:THR:HA	4:E:10:LEU:HD12	1.94	0.48
1:A:546:ASP:HA	1:A:609:TYR:OH	2.14	0.48
1:A:1267:PRO:HG2	1:A:1596:ASP:HB3	1.95	0.48
2:B:122:VAL:HB	2:B:126:SER:HB2	1.95	0.48
2:B:473:HIS:CD2	2:B:475:GLY:H	2.32	0.48
1:A:169:VAL:HG22	1:A:174:LEU:HB3	1.95	0.48
1:A:1063:LYS:HB2	1:A:1064:LYS:HZ2	1.78	0.48
1:A:1294:LEU:HD12	1:A:1548:ALA:HB1	1.96	0.48
1:A:1503:GLN:O	1:A:1507:GLU:HG2	2.14	0.48
2:B:279:ARG:HE	7:I:16:ASP:N	2.12	0.48
2:B:1119:PHE:O	2:B:1123:LEU:HD23	2.13	0.48
9:K:71:THR:HG22	9:K:81:ASN:HB2	1.95	0.48
1:A:87:VAL:O	1:A:299:LEU:N	2.46	0.48
1:A:1178:THR:O	1:A:1183:GLU:HB2	2.13	0.48
1:A:1255:ALA:HB1	1:A:1654:TYR:CE2	2.49	0.48
7:I:20:CYS:HA	11:N:66:ARG:HD2	1.94	0.48
1:A:606:ALA:HA	1:A:609:TYR:CD2	2.46	0.48
1:A:677:LYS:HD2	1:A:678:PRO:N	2.27	0.48
3:C:234:ARG:NH2	3:C:279:ARG:O	2.47	0.48
4:E:66:ASP:OD1	4:E:66:ASP:N	2.45	0.48
11:N:46:ASN:CG	11:N:57:GLN:HB3	2.34	0.48
1:A:997:GLU:HG2	1:A:1213:LEU:HD11	1.94	0.48
1:A:1033:GLN:OE1	1:A:1166:LYS:HE3	2.14	0.48
4:E:134:GLU:CD	4:E:181:ARG:HH22	2.16	0.48
1:A:427:LEU:HA	1:A:430:LYS:HB2	1.95	0.47
1:A:1050:SER:O	1:A:1052:HIS:ND1	2.46	0.47
2:B:107:ARG:HD2	2:B:778:PHE:CD1	2.48	0.47
2:B:889:GLN:HE22	2:B:923:ARG:HG3	1.78	0.47
3:C:265:GLN:O	3:C:272:VAL:N	2.38	0.47
4:E:121:MET:O	4:E:125:TYR:HB2	2.14	0.47
4:E:132:GLN:NE2	4:E:136:LEU:HD21	2.28	0.47
7:I:23:CYS:C	11:N:66:ARG:HG3	2.34	0.47
1:A:269:TRP:CZ3	1:A:276:LEU:HB3	2.49	0.47
1:A:1601:TYR:HD2	1:A:1620:VAL:HG13	1.79	0.47
2:B:625:ASN:O	12:M:131:GLN:NE2	2.43	0.47
2:B:674:ILE:HD11	2:B:688:GLN:HG3	1.95	0.47
3:C:251:GLU:HG3	3:C:252:GLU:N	2.30	0.47
7:I:21:SER:H	11:N:66:ARG:NE	2.13	0.47
12:M:126:SER:OG	12:M:127:GLY:N	2.47	0.47
3:C:95:TYR:HD1	10:L:51:ARG:O	1.97	0.47
1:A:650:ARG:NH2	9:K:66:GLU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASP:HB3	1:A:1013:SER:OG	2.14	0.47
2:B:270:LYS:HG3	2:B:271:GLY:H	1.79	0.47
2:B:271:GLY:HA2	2:B:273:GLU:OE2	2.14	0.47
2:B:537:LEU:HA	12:M:118:LEU:HD22	1.97	0.47
3:C:251:GLU:HB2	3:C:255:ARG:HH12	1.79	0.47
4:E:84:ILE:HD12	4:E:84:ILE:H	1.79	0.47
1:A:497:VAL:HG22	1:A:538:VAL:HG13	1.95	0.47
1:A:500:GLU:OE2	1:A:536:LYS:HG3	2.14	0.47
1:A:1002:GLN:HE21	1:A:1707:ARG:NH2	2.12	0.47
1:A:1496:GLU:HA	1:A:1499:GLU:HB3	1.97	0.47
2:B:64:PHE:HE1	2:B:397:LYS:HB2	1.77	0.47
2:B:821:TYR:HA	2:B:841:TYR:HB3	1.96	0.47
2:B:854:VAL:HA	2:B:866:CYS:O	2.15	0.47
6:H:31:GLU:HG2	6:H:32:SER:O	2.15	0.47
12:M:94:LEU:HB3	12:M:108:ALA:HB3	1.95	0.47
1:A:69:GLN:OE1	2:B:1080:LEU:HB2	2.15	0.47
1:A:580:ALA:HB2	1:A:631:ILE:HA	1.96	0.47
1:A:915:LEU:HG	1:A:916:LEU:H	1.79	0.47
1:A:1253:MET:HG2	1:A:1658:ASN:HB3	1.97	0.47
1:A:1273:LYS:HD2	1:A:1274:ALA:N	2.30	0.47
1:A:1281:LEU:HG	1:A:1591:TYR:CZ	2.49	0.47
2:B:12:SER:O	2:B:12:SER:OG	2.29	0.47
2:B:263:GLN:HA	11:N:30:ASN:OD1	2.14	0.47
2:B:857:ASN:ND2	2:B:861:SER:O	2.30	0.47
2:B:958:ALA:O	2:B:962:PHE:HB2	2.14	0.47
2:B:978:ARG:NH2	2:B:987:GLU:OE2	2.48	0.47
3:C:197:ILE:HD13	8:J:16:ASN:HB3	1.95	0.47
3:C:237:PRO:HB3	3:C:283:PHE:HE1	1.80	0.47
3:C:277:ASN:OD1	3:C:279:ARG:HB3	2.15	0.47
10:L:46:LYS:HG2	10:L:47:LYS:H	1.79	0.47
1:A:711:ILE:HD11	1:A:748:VAL:HG21	1.97	0.47
1:A:1051:GLN:HG3	1:A:1202:ARG:CZ	2.45	0.47
1:A:1199:LYS:HD2	1:A:1199:LYS:HA	1.80	0.47
1:A:1269:LEU:HD22	1:A:1595:LEU:N	2.30	0.47
1:A:1349:LEU:HB3	1:A:1547:LEU:HD21	1.96	0.47
2:B:268:LEU:HD23	2:B:268:LEU:O	2.15	0.47
2:B:417:MET:HG2	2:B:418:ARG:HD3	1.96	0.47
2:B:965:MET:HA	12:M:142:PRO:HG3	1.97	0.47
9:K:37:ARG:O	9:K:91:PRO:HA	2.15	0.47
1:A:828:ARG:HE	1:A:837:ALA:HB2	1.80	0.47
1:A:1273:LYS:HE3	1:A:1273:LYS:HB3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1625:ILE:O	1:A:1628:VAL:HG12	2.15	0.47
2:B:394:VAL:O	2:B:397:LYS:HB3	2.15	0.47
2:B:620:VAL:HG23	2:B:634:ILE:O	2.14	0.47
3:C:95:TYR:O	3:C:209:ASP:HB2	2.15	0.47
6:H:27:ARG:NH2	6:H:42:ASP:OD2	2.47	0.47
9:K:48:ASP:OD2	9:K:50:THR:OG1	2.29	0.47
9:K:94:GLU:HB2	9:K:95:PRO:HD3	1.96	0.47
1:A:456:ILE:HG23	1:A:576:ARG:O	2.14	0.47
1:A:925:ARG:CG	1:A:926:PRO:HD2	2.41	0.47
1:A:1705:VAL:HG13	2:B:1051:SER:HB3	1.95	0.47
2:B:118:ILE:O	2:B:129:ILE:HA	2.15	0.47
2:B:808:ASP:OD1	2:B:809:ASP:N	2.46	0.47
3:C:118:ASP:OD1	3:C:121:LEU:HG	2.15	0.47
1:A:511:ASP:O	1:A:515:ARG:HG2	2.15	0.46
1:A:1277:ARG:HH12	1:A:1591:TYR:HD2	1.63	0.46
1:A:1324:HIS:CE1	1:A:1328:GLN:HB2	2.50	0.46
1:A:1616:ALA:HA	4:E:144:LEU:CD1	2.44	0.46
1:A:1674:PHE:CE2	1:A:1675:GLU:HB2	2.50	0.46
2:B:571:ALA:HB3	2:B:572:PRO:HD3	1.96	0.46
2:B:756:ALA:HB1	2:B:894:SER:OG	2.15	0.46
2:B:792:LEU:H	2:B:792:LEU:HD23	1.80	0.46
2:B:1053:LEU:O	2:B:1057:ARG:HG2	2.15	0.46
3:C:167:LYS:NZ	8:J:19:GLU:OE2	2.45	0.46
3:C:256:CYS:SG	3:C:287:ILE:HD12	2.54	0.46
8:J:30:THR:O	8:J:32:GLY:N	2.48	0.46
8:J:59:LEU:O	8:J:59:LEU:HD23	2.15	0.46
9:K:25:THR:HG21	9:K:28:GLU:HB2	1.96	0.46
10:L:17:TYR:HD1	10:L:45:TYR:O	1.98	0.46
11:N:87:HIS:NE2	11:N:106:LEU:HD22	2.29	0.46
1:A:766:TYR:HD1	1:A:771:GLY:HA2	1.80	0.46
1:A:1174:TRP:NE1	1:A:1178:THR:HB	2.30	0.46
1:A:1269:LEU:HD22	1:A:1595:LEU:O	2.15	0.46
2:B:521:VAL:CG2	2:B:592:TRP:HD1	2.28	0.46
2:B:544:GLY:HA2	11:N:79:LEU:HD11	1.96	0.46
9:K:67:PHE:HB3	9:K:85:GLN:HB2	1.96	0.46
1:A:118:HIS:CE1	1:A:158:ARG:HE	2.33	0.46
1:A:1269:LEU:O	1:A:1271:THR:N	2.48	0.46
2:B:19:LEU:HD22	8:J:53:VAL:HG23	1.97	0.46
2:B:282:VAL:HA	2:B:285:MET:HE2	1.97	0.46
2:B:570:LEU:O	2:B:573:GLY:N	2.48	0.46
4:E:49:SER:OG	4:E:50:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TYR:HB3	2:B:1121:ALA:HB2	1.98	0.46
1:A:992:ILE:O	1:A:995:HIS:HB2	2.15	0.46
1:A:1011:ASP:OD1	1:A:1011:ASP:N	2.43	0.46
1:A:1303:PHE:CG	1:A:1303:PHE:O	2.68	0.46
2:B:153:PRO:O	2:B:156:LEU:HB2	2.15	0.46
2:B:515:THR:HG22	2:B:516:ALA:N	2.23	0.46
2:B:867:VAL:HG12	2:B:869:ILE:HG13	1.97	0.46
11:N:68:SER:HB2	11:N:112:LEU:O	2.16	0.46
1:A:5:LYS:HE2	1:A:531:LYS:HE3	1.97	0.46
1:A:122:CYS:O	1:A:126:VAL:HG23	2.16	0.46
1:A:710:LYS:HE3	1:A:751:LYS:HD2	1.98	0.46
1:A:994:LYS:HB3	1:A:1674:PHE:HD1	1.80	0.46
1:A:1162:THR:CG2	4:E:200:ALA:HA	2.45	0.46
1:A:1613:GLY:HA2	4:E:177:ASP:OD1	2.16	0.46
1:A:876:ILE:HG21	1:A:915:LEU:HD13	1.98	0.46
1:A:1706:VAL:HG12	1:A:1707:ARG:H	1.80	0.46
3:C:266:GLU:HG3	3:C:271:LYS:HA	1.98	0.46
1:A:144:ARG:O	1:A:158:ARG:HD2	2.16	0.46
1:A:306:PRO:O	1:A:310:ARG:HB2	2.16	0.46
1:A:841:GLU:HG3	1:A:844:GLY:H	1.80	0.46
1:A:934:SER:OG	1:A:938:PHE:HD2	1.98	0.46
1:A:972:ARG:NH1	2:B:489:LEU:HD21	2.31	0.46
1:A:1706:VAL:H	2:B:1051:SER:CB	2.28	0.46
2:B:329:ASN:HD22	2:B:342:LYS:NZ	2.14	0.46
2:B:474:ARG:HH11	2:B:510:LEU:HA	1.81	0.46
2:B:698:PHE:HE1	2:B:713:ARG:HH21	1.61	0.46
2:B:797:LYS:HE2	2:B:836:SER:H	1.80	0.46
2:B:888:GLY:O	2:B:890:LYS:N	2.48	0.46
2:B:901:ASP:O	2:B:982:GLY:HA3	2.16	0.46
3:C:148:ARG:NH2	8:J:66:GLU:O	2.38	0.46
9:K:62:ASN:ND2	9:K:95:PRO:HB3	2.30	0.46
1:A:67:CYS:HG	2:B:1099:THR:HG1	1.62	0.46
1:A:303:VAL:HG12	2:B:1127:ASN:HA	1.97	0.46
1:A:471:PRO:HG3	1:A:537:ILE:HG22	1.98	0.46
1:A:555:THR:CB	2:B:1044:ALA:HB2	2.45	0.46
1:A:579:TYR:CE1	2:B:753:MET:HB3	2.51	0.46
1:A:704:ASN:ND2	1:A:740:ARG:HG3	2.20	0.46
1:A:1091:SER:HA	1:A:1094:GLN:CD	2.36	0.46
1:A:1268:VAL:HA	1:A:1595:LEU:HA	1.97	0.46
1:A:1508:ILE:HG13	1:A:1509:HIS:ND1	2.31	0.46
2:B:467:SER:O	2:B:469:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:LYS:H	2:B:863:LYS:HD2	1.80	0.46
1:A:1075:TRP:CE3	1:A:1142:CYS:HB3	2.51	0.46
1:A:422:GLU:HG2	1:A:1677:SER:OG	2.16	0.46
1:A:452:ASN:HB2	1:A:455:GLU:CB	2.44	0.46
1:A:1017:PHE:O	1:A:1018:LEU:HD23	2.16	0.46
2:B:240:TYR:HB2	2:B:331:CYS:SG	2.56	0.46
7:I:23:CYS:HB2	7:I:38:CYS:HB2	1.98	0.46
9:K:74:HIS:HD2	9:K:77:GLU:HG3	1.81	0.46
11:N:63:GLU:HG3	11:N:63:GLU:O	2.16	0.46
1:A:967:HIS:CD2	2:B:682:SER:OG	2.58	0.45
1:A:976:VAL:O	1:A:980:VAL:HG22	2.16	0.45
1:A:1280:SER:O	1:A:1284:GLN:HG3	2.16	0.45
1:A:1567:THR:CG2	1:A:1574:LYS:HD3	2.46	0.45
4:E:122:ALA:O	4:E:125:TYR:N	2.49	0.45
5:F:57:MET:HA	5:F:123:LEU:HD13	1.99	0.45
12:M:127:GLY:O	12:M:128:SER:OG	2.34	0.45
1:A:1257:ALA:O	1:A:1259:ILE:HG23	2.16	0.45
2:B:4:GLY:HA3	2:B:631:GLU:HG2	1.99	0.45
2:B:923:ARG:HB3	2:B:925:THR:HG23	1.98	0.45
4:E:162:ARG:HH11	4:E:163:TYR:HE2	1.63	0.45
9:K:51:LEU:O	9:K:53:ASN:N	2.49	0.45
11:N:70:VAL:O	11:N:109:MET:HA	2.15	0.45
12:M:55:CYS:HB3	12:M:73:LEU:HG	1.99	0.45
1:A:469:PRO:CG	1:A:600:GLN:HE21	2.29	0.45
1:A:500:GLU:CD	1:A:536:LYS:HG3	2.36	0.45
1:A:791:LEU:HB3	1:A:792:TYR:CD2	2.51	0.45
2:B:254:LYS:NZ	2:B:261:ASP:HB3	2.31	0.45
3:C:127:GLN:OE1	3:C:128:GLY:N	2.49	0.45
3:C:283:PHE:HE2	3:C:299:LEU:HB3	1.81	0.45
4:E:95:GLN:O	4:E:98:ASN:ND2	2.50	0.45
9:K:80:ILE:O	9:K:81:ASN:ND2	2.49	0.45
9:K:124:GLN:OE1	9:K:127:SER:OG	2.34	0.45
1:A:17:PHE:HB2	1:A:1688:GLY:HA2	1.98	0.45
1:A:487:GLY:HA3	1:A:515:ARG:HH22	1.81	0.45
1:A:555:THR:HG21	2:B:1041:GLU:HA	1.99	0.45
1:A:1318:ARG:NH2	1:A:1526:GLN:OE1	2.49	0.45
2:B:742:ILE:O	2:B:913:ILE:HG22	2.16	0.45
2:B:758:ILE:HD13	2:B:894:SER:HB2	1.98	0.45
3:C:198:LEU:HD11	3:C:200:ALA:O	2.17	0.45
4:E:60:VAL:O	4:E:61:LEU:HD22	2.16	0.45
1:A:132:LEU:HD22	4:E:172:ARG:NE	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PRO:HD3	2:B:1125:ALA:HA	1.97	0.45
1:A:310:ARG:HH22	1:A:328:LEU:HD22	1.82	0.45
1:A:1133:ARG:HA	1:A:1136:GLN:HG3	1.99	0.45
1:A:1176:ALA:O	1:A:1180:LYS:HE2	2.16	0.45
1:A:1658:ASN:HB2	1:A:1659:ARG:HH11	1.82	0.45
2:B:625:ASN:ND2	2:B:628:LEU:H	2.14	0.45
2:B:972:ASN:OD1	2:B:973:PHE:N	2.49	0.45
4:E:124:LYS:O	4:E:126:ILE:HD12	2.17	0.45
5:F:109:TYR:CD1	5:F:115:TYR:HB3	2.52	0.45
9:K:124:GLN:OE1	9:K:128:ARG:NE	2.50	0.45
12:M:31:SER:CA	12:M:97:PRO:HG2	2.45	0.45
1:A:435:LYS:O	2:B:1037:PHE:HB2	2.16	0.45
1:A:456:ILE:HG12	1:A:564:HIS:HB2	1.98	0.45
1:A:1615:GLU:OE2	4:E:207:ARG:NH2	2.47	0.45
2:B:154:GLN:OE1	2:B:154:GLN:N	2.40	0.45
2:B:472:VAL:HG13	2:B:514:LEU:HD11	1.98	0.45
3:C:234:ARG:NH1	3:C:281:ASP:O	2.50	0.45
11:N:85:CYS:SG	12:M:48:PRO:HA	2.56	0.45
1:A:616:GLN:HA	1:A:766:TYR:HE1	1.82	0.45
1:A:759:TYR:H	1:A:763:HIS:CE1	2.35	0.45
2:B:35:LEU:HD11	2:B:166:MET:CE	2.47	0.45
2:B:51:HIS:CD2	2:B:144:LYS:HD2	2.52	0.45
2:B:815:ILE:HD12	2:B:815:ILE:H	1.82	0.45
6:H:54:ASP:OD2	6:H:147:LYS:HE3	2.17	0.45
1:A:428:PHE:CE1	1:A:432:MET:HG3	2.51	0.45
1:A:630:LEU:CD2	1:A:634:HIS:HB2	2.47	0.45
2:B:459:LYS:NZ	2:B:465:TYR:OH	2.48	0.45
2:B:760:ASN:OD1	2:B:762:ALA:N	2.50	0.45
2:B:807:LEU:HD21	2:B:824:PRO:HG2	1.99	0.45
3:C:238:ASP:OD1	3:C:238:ASP:N	2.41	0.45
3:C:252:GLU:H	3:C:252:GLU:HG2	1.47	0.45
4:E:150:VAL:HA	4:E:191:VAL:HG22	1.99	0.45
6:H:39:LEU:HD13	6:H:125:LEU:HB2	1.99	0.45
1:A:140:ARG:HD3	1:A:141:ILE:HD13	1.99	0.45
1:A:631:ILE:HD12	1:A:632:GLN:N	2.29	0.45
1:A:1115:PRO:HA	1:A:1118:GLN:NE2	2.32	0.45
7:I:18:ASP:OD2	7:I:27:LEU:HB2	2.16	0.45
1:A:331:VAL:HG22	1:A:397:HIS:HB3	1.98	0.45
1:A:499:ASN:OD1	1:A:500:GLU:N	2.48	0.45
1:A:800:GLU:OE2	1:A:887:ARG:NH2	2.50	0.45
1:A:919:ILE:HG22	1:A:920:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:THR:HG22	4:E:200:ALA:HA	1.98	0.45
1:A:1357:LYS:HA	1:A:1357:LYS:HD3	1.79	0.45
2:B:893:LEU:HD12	2:B:893:LEU:HA	1.74	0.45
12:M:43:TRP:CZ3	12:M:113:GLY:HA3	2.52	0.45
1:A:123:GLN:HE22	1:A:135:VAL:HG13	1.82	0.44
1:A:193:ALA:O	1:A:197:LYS:HD2	2.17	0.44
1:A:711:ILE:HG23	1:A:750:ASP:OD2	2.17	0.44
1:A:907:VAL:HA	1:A:910:MET:SD	2.57	0.44
1:A:1052:HIS:CG	5:F:126:THR:HG1	2.33	0.44
2:B:467:SER:HB3	2:B:670:ILE:HD11	1.99	0.44
3:C:92:VAL:HG21	3:C:110:LEU:HD12	1.99	0.44
3:C:95:TYR:HB2	3:C:209:ASP:HB3	1.99	0.44
1:A:75:SER:HA	1:A:308:ARG:HB3	1.99	0.44
1:A:309:TYR:HB3	2:B:1121:ALA:CB	2.47	0.44
1:A:429:ARG:HH22	1:A:1676:THR:HA	1.81	0.44
1:A:429:ARG:NH2	1:A:1676:THR:HA	2.32	0.44
1:A:488:PRO:HB3	1:A:495:SER:HB3	1.99	0.44
1:A:991:CYS:HB3	1:A:1253:MET:CE	2.48	0.44
1:A:1247:ARG:O	1:A:1251:ILE:HG12	2.17	0.44
2:B:100:PRO:O	2:B:103:CYS:N	2.49	0.44
2:B:260:SER:HB2	11:N:111:PRO:CG	2.44	0.44
2:B:763:SER:O	2:B:768:PHE:HB2	2.18	0.44
4:E:102:ALA:O	4:E:103:LEU:HD23	2.17	0.44
4:E:147:GLU:O	4:E:194:ILE:HG22	2.17	0.44
9:K:127:SER:HA	9:K:130:GLU:OE2	2.17	0.44
1:A:12:LEU:HB3	1:A:1704:LYS:HE2	2.00	0.44
1:A:1086:ARG:HA	1:A:1086:ARG:HD3	1.74	0.44
1:A:1109:ASN:HD21	4:E:43:GLN:HB2	1.82	0.44
1:A:1351:MET:HE1	1:A:1512:ILE:HD11	1.99	0.44
2:B:725:SER:H	2:B:948:THR:CG2	2.30	0.44
2:B:746:ILE:CG2	2:B:992:ILE:HD12	2.47	0.44
4:E:122:ALA:HA	4:E:125:TYR:O	2.17	0.44
7:I:21:SER:H	11:N:66:ARG:CZ	2.30	0.44
11:N:81:CYS:HA	11:N:84:LEU:HD12	1.98	0.44
1:A:685:LYS:HE2	1:A:685:LYS:HB2	1.75	0.44
1:A:1335:PRO:HA	1:A:1338:ILE:HG12	1.99	0.44
1:A:1346:PHE:HA	1:A:1349:LEU:HD12	1.98	0.44
1:A:1715:LEU:HD11	5:F:68:THR:HG21	1.99	0.44
2:B:504:ASP:HA	2:B:508:CYS:SG	2.58	0.44
2:B:961:TYR:CE1	12:M:139:PRO:HG2	2.53	0.44
2:B:976:THR:HG22	2:B:993:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:280:LEU:HD23	3:C:280:LEU:HA	1.80	0.44
1:A:552:ARG:NH1	1:A:554:PRO:HD2	2.32	0.44
1:A:781:LEU:HA	1:A:781:LEU:HD12	1.66	0.44
1:A:1266:VAL:HA	1:A:1600:LEU:CD1	2.47	0.44
2:B:305:GLY:HA3	2:B:320:ASN:O	2.17	0.44
2:B:746:ILE:HG21	2:B:992:ILE:HD12	2.00	0.44
2:B:936:LYS:HB2	2:B:936:LYS:HE3	1.69	0.44
4:E:90:TYR:HD1	4:E:90:TYR:HA	1.59	0.44
4:E:105:VAL:HA	4:E:130:PHE:O	2.16	0.44
4:E:187:ARG:HD3	4:E:209:VAL:O	2.17	0.44
6:H:116:VAL:O	6:H:123:MET:N	2.49	0.44
7:I:23:CYS:H	11:N:66:ARG:HE	1.65	0.44
9:K:66:GLU:N	9:K:85:GLN:O	2.41	0.44
1:A:935:LEU:HD13	1:A:966:PHE:CE1	2.53	0.44
1:A:1089:PHE:HD2	1:A:1092:TYR:CD2	2.34	0.44
1:A:1089:PHE:CZ	4:E:29:THR:HG22	2.53	0.44
1:A:1222:PRO:HA	1:A:1225:GLN:HB2	1.98	0.44
1:A:1340:ARG:HA	1:A:1340:ARG:HD3	1.60	0.44
1:A:1669:LEU:CD1	1:A:1701:VAL:HG21	2.48	0.44
1:A:1696:PRO:HA	1:A:1706:VAL:HG11	2.00	0.44
2:B:336:LEU:HD21	2:B:560:GLY:O	2.18	0.44
2:B:652:PHE:O	2:B:656:THR:HG22	2.18	0.44
2:B:746:ILE:CG2	2:B:992:ILE:HG23	2.48	0.44
4:E:54:ARG:NH2	4:E:90:TYR:HE2	2.16	0.44
4:E:199:THR:OG1	4:E:200:ALA:N	2.50	0.44
5:F:83:LEU:H	5:F:83:LEU:HD23	1.83	0.44
7:I:20:CYS:CA	11:N:66:ARG:HD2	2.47	0.44
1:A:100:LEU:HD12	1:A:265:LEU:HD21	2.00	0.44
1:A:246:GLU:HG3	1:A:247:GLU:N	2.33	0.44
1:A:677:LYS:HG3	6:H:89:GLU:O	2.17	0.44
1:A:1031:PHE:HZ	1:A:1039:PHE:CD2	2.35	0.44
1:A:1040:LEU:HD23	1:A:1047:ILE:HG21	1.98	0.44
1:A:1063:LYS:HB2	1:A:1064:LYS:NZ	2.32	0.44
1:A:1209:GLU:OE1	1:A:1214:LEU:HD21	2.17	0.44
1:A:1309:GLN:HB3	1:A:1311:LYS:HG2	2.00	0.44
1:A:1565:ASN:CG	1:A:1579:ASN:HD21	2.21	0.44
1:A:1672:MET:HE3	1:A:1681:LEU:HD11	1.99	0.44
2:B:396:ILE:HD12	2:B:396:ILE:HA	1.93	0.44
2:B:627:ALA:HB1	12:M:127:GLY:HA3	2.00	0.44
2:B:714:LEU:O	2:B:717:PRO:HD3	2.18	0.44
4:E:115:LYS:HA	4:E:118:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:110:LEU:HB3	5:F:111:PRO:CD	2.37	0.44
7:I:20:CYS:HA	11:N:66:ARG:CD	2.47	0.44
1:A:1053:LEU:O	1:A:1056:VAL:O	2.36	0.44
1:A:1669:LEU:O	1:A:1672:MET:HB3	2.18	0.44
2:B:189:PHE:HE1	2:B:611:PHE:CD1	2.35	0.44
2:B:751:TYR:HE2	2:B:895:ARG:HD2	1.82	0.44
3:C:283:PHE:CE2	3:C:299:LEU:HB3	2.53	0.44
1:A:123:GLN:NE2	1:A:135:VAL:HG13	2.32	0.44
1:A:803:LEU:O	1:A:886:HIS:HB2	2.18	0.44
1:A:1184:LYS:HD2	1:A:1184:LYS:HA	1.85	0.44
1:A:1583:ILE:HG13	1:A:1583:ILE:O	2.18	0.44
2:B:15:SER:OG	2:B:17:LYS:HG2	2.18	0.44
2:B:106:ARG:HG3	2:B:855:CYS:HB2	1.99	0.44
2:B:758:ILE:HB	2:B:914:LEU:HD12	2.00	0.44
4:E:152:THR:OG1	4:E:154:GLU:OE1	2.36	0.44
1:A:422:GLU:OE2	1:A:1678:PHE:N	2.32	0.43
1:A:547:ILE:HG13	1:A:564:HIS:O	2.17	0.43
1:A:1052:HIS:HB3	1:A:1055:GLU:CB	2.45	0.43
1:A:1589:PHE:HB2	1:A:1590:LYS:NZ	2.33	0.43
2:B:1063:ASP:HB3	2:B:1114:TYR:H	1.83	0.43
6:H:58:LEU:HD23	6:H:59:VAL:N	2.33	0.43
1:A:185:CYS:HA	1:A:188:LYS:HG2	2.00	0.43
1:A:604:GLY:O	1:A:607:GLU:HG3	2.18	0.43
1:A:1021:GLU:OE1	4:E:200:ALA:HB3	2.17	0.43
1:A:1151:ARG:HH12	5:F:52:ILE:HD12	1.83	0.43
2:B:251:PHE:CD2	2:B:289:VAL:HG23	2.53	0.43
2:B:581:PHE:HB3	2:B:589:ILE:HD12	2.00	0.43
2:B:882:LYS:HG2	2:B:890:LYS:HE3	1.99	0.43
3:C:325:ALA:O	3:C:328:VAL:HG12	2.17	0.43
4:E:197:SER:HB3	4:E:201:GLY:HA2	1.98	0.43
1:A:210:THR:OG1	1:A:211:GLY:N	2.51	0.43
1:A:1210:ALA:O	1:A:1214:LEU:HD13	2.18	0.43
1:A:1312:PHE:HB3	1:A:1531:LEU:O	2.19	0.43
1:A:1358:ASN:HB2	1:A:1535:LYS:NZ	2.33	0.43
2:B:98:VAL:O	2:B:147:ASN:ND2	2.51	0.43
2:B:132:GLN:NE2	2:B:420:PHE:HB3	2.32	0.43
2:B:208:TYR:N	2:B:208:TYR:CD2	2.86	0.43
2:B:276:SER:HB3	7:I:54:VAL:HG13	2.00	0.43
2:B:467:SER:HB3	2:B:670:ILE:CD1	2.48	0.43
2:B:850:ASP:OD2	2:B:872:ARG:HB3	2.19	0.43
4:E:187:ARG:N	4:E:189:GLN:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:90:TYR:HE2	6:H:92:MET:HG3	1.83	0.43
8:J:25:LEU:HD23	8:J:25:LEU:HA	1.75	0.43
1:A:267:ALA:HA	1:A:270:LYS:HG2	2.00	0.43
1:A:444:VAL:HG13	1:A:574:VAL:HG23	1.99	0.43
1:A:711:ILE:N	1:A:750:ASP:OD2	2.50	0.43
1:A:895:GLN:HA	1:A:898:VAL:HG22	2.00	0.43
1:A:990:ARG:O	1:A:993:ILE:HG22	2.18	0.43
2:B:51:HIS:NE2	2:B:144:LYS:HD2	2.34	0.43
2:B:64:PHE:CZ	2:B:397:LYS:HB2	2.53	0.43
2:B:160:HIS:HD2	2:B:705:ASP:OD1	2.01	0.43
2:B:625:ASN:CG	2:B:627:ALA:H	2.21	0.43
2:B:897:TRP:HB3	2:B:902:MET:CE	2.48	0.43
2:B:1084:PRO:HA	2:B:1085:PRO:HD3	1.88	0.43
4:E:29:THR:O	4:E:32:GLU:HB2	2.18	0.43
4:E:197:SER:OG	4:E:198:GLU:N	2.52	0.43
4:E:209:VAL:O	4:E:210:GLN:HG3	2.18	0.43
5:F:97:LEU:HD21	5:F:125:ILE:HD13	2.00	0.43
6:H:111:ARG:O	6:H:112:LEU:HD12	2.18	0.43
1:A:25:LEU:HD23	1:A:301:PHE:HB2	2.00	0.43
1:A:1189:LEU:HD23	1:A:1189:LEU:HA	1.86	0.43
2:B:863:LYS:HD2	2:B:863:LYS:N	2.33	0.43
6:H:112:LEU:HD13	6:H:129:ALA:HB2	1.99	0.43
1:A:28:LEU:HD12	2:B:1100:LEU:HG	2.01	0.43
1:A:137:GLU:OE2	4:E:187:ARG:HB3	2.18	0.43
1:A:268:LEU:O	1:A:272:GLU:HG2	2.18	0.43
1:A:704:ASN:ND2	1:A:740:ARG:HA	2.33	0.43
1:A:1097:GLN:HG2	1:A:1101:LYS:HZ2	1.82	0.43
1:A:1529:VAL:HG12	1:A:1530:LYS:N	2.33	0.43
2:B:15:SER:C	2:B:16:LEU:HD12	2.38	0.43
2:B:281:SER:HA	2:B:284:GLN:NE2	2.34	0.43
4:E:51:GLY:H	4:E:55:ARG:HG3	1.83	0.43
6:H:98:ARG:O	6:H:115:TYR:HB2	2.19	0.43
10:L:18:ILE:HD11	10:L:47:LYS:HG3	2.00	0.43
1:A:83:LEU:HD11	1:A:394:LEU:HD11	1.99	0.43
1:A:635:MET:HE3	1:A:754:TYR:HE2	1.84	0.43
1:A:797:LEU:HD21	2:B:921:PRO:CD	2.49	0.43
1:A:972:ARG:NH2	2:B:509:GLY:HA2	2.26	0.43
2:B:189:PHE:CD1	2:B:190:PRO:HD2	2.54	0.43
8:J:41:LYS:HA	8:J:41:LYS:HD3	1.69	0.43
10:L:41:TYR:CE2	10:L:43:ILE:HG22	2.52	0.43
1:A:433:MET:CB	2:B:1042:ARG:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLN:CD	1:A:476:ASN:HD22	2.21	0.43
1:A:607:GLU:O	1:A:611:LEU:HB2	2.18	0.43
2:B:493:SER:OG	2:B:497:LEU:HB2	2.19	0.43
2:B:494:TRP:HZ2	2:B:646:ILE:HD11	1.83	0.43
2:B:620:VAL:HG22	2:B:633:LEU:HD12	2.00	0.43
2:B:915:PHE:CE2	2:B:920:PHE:HZ	2.36	0.43
2:B:1027:GLY:HA2	2:B:1033:GLY:HA3	2.01	0.43
2:B:1132:LEU:HD22	2:B:1134:VAL:HG13	2.00	0.43
9:K:27:LEU:HD12	9:K:28:GLU:N	2.33	0.43
11:N:44:TYR:HD2	11:N:59:ILE:HB	1.84	0.43
1:A:190:LYS:O	1:A:194:LEU:HG	2.19	0.43
1:A:606:ALA:O	1:A:610:VAL:HG22	2.18	0.43
1:A:615:ASP:OD2	1:A:772:GLU:HA	2.18	0.43
1:A:1316:GLN:CD	1:A:1526:GLN:HE21	2.22	0.43
1:A:1350:LEU:O	1:A:1354:ILE:HG12	2.19	0.43
2:B:72:ARG:HB3	2:B:317:TRP:HH2	1.84	0.43
2:B:397:LYS:NZ	2:B:401:ASP:HB2	2.34	0.43
2:B:749:THR:HG21	2:B:751:TYR:CD2	2.54	0.43
2:B:1014:THR:HG22	2:B:1015:THR:HG23	2.01	0.43
1:A:579:TYR:HB2	1:A:631:ILE:CD1	2.49	0.43
1:A:599:PRO:HB3	2:B:1057:ARG:HH22	1.82	0.43
1:A:623:ASP:HA	1:A:1026:ILE:HG21	2.01	0.43
1:A:989:GLN:O	1:A:992:ILE:HG22	2.19	0.43
1:A:1050:SER:C	1:A:1052:HIS:HD1	2.23	0.43
1:A:1302:SER:O	1:A:1303:PHE:HB3	2.19	0.43
1:A:1324:HIS:HE1	1:A:1333:LEU:O	2.02	0.43
2:B:374:VAL:O	2:B:617:CYS:HB3	2.19	0.43
2:B:719:SER:HG	2:B:723:ARG:NH1	2.15	0.43
2:B:800:ASP:O	2:B:803:VAL:HG12	2.18	0.43
2:B:827:SER:OG	2:B:838:VAL:HG12	2.18	0.43
2:B:902:MET:SD	2:B:914:LEU:HD11	2.59	0.43
4:E:193:ILE:HG22	4:E:195:ARG:H	1.84	0.43
5:F:86:GLU:CD	5:F:86:GLU:H	2.22	0.43
6:H:41:LEU:HD13	6:H:123:MET:HG3	2.01	0.43
12:M:44:LEU:O	12:M:114:THR:HA	2.19	0.43
1:A:961:PRO:HA	2:B:950:PHE:CE1	2.54	0.42
1:A:1137:LYS:HE2	1:A:1137:LYS:HB3	1.74	0.42
1:A:1324:HIS:HA	1:A:1327:TYR:CE2	2.54	0.42
2:B:474:ARG:NH1	2:B:510:LEU:HA	2.34	0.42
2:B:694:GLN:HE22	2:B:1003:ARG:NE	2.13	0.42
3:C:332:LYS:HD2	3:C:335:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:78:ALA:HA	11:N:108:ASN:HD21	1.83	0.42
1:A:623:ASP:O	1:A:1030:GLN:HB2	2.19	0.42
1:A:1309:GLN:HB3	1:A:1311:LYS:CG	2.49	0.42
1:A:1677:SER:O	1:A:1681:LEU:HG	2.19	0.42
2:B:857:ASN:HB2	2:B:862:GLY:CA	2.48	0.42
2:B:964:GLU:HG3	12:M:142:PRO:CD	2.48	0.42
3:C:238:ASP:HB3	3:C:302:VAL:HG23	2.00	0.42
4:E:110:MET:HB3	4:E:115:LYS:HZ3	1.84	0.42
7:I:25:SER:HB2	7:I:40:ARG:NH2	2.35	0.42
1:A:927:PRO:HG3	2:B:488:ARG:NH2	2.34	0.42
1:A:1026:ILE:HD11	1:A:1639:ARG:HD2	2.00	0.42
1:A:1589:PHE:HE1	4:E:137:ILE:HG22	1.83	0.42
2:B:109:THR:HG22	2:B:110:TYR:H	1.84	0.42
3:C:334:ARG:HH21	9:K:104:MET:HB3	1.84	0.42
8:J:38:LEU:HD23	8:J:38:LEU:HA	1.76	0.42
1:A:451:ILE:HD11	1:A:577:LEU:HA	2.00	0.42
1:A:521:GLN:O	1:A:524:THR:OG1	2.33	0.42
12:M:83:LEU:HB3	12:M:116:ARG:HB2	2.01	0.42
1:A:188:LYS:HD2	1:A:1687:LEU:HD11	2.01	0.42
1:A:383:LEU:O	1:A:386:LYS:HG2	2.19	0.42
1:A:643:THR:C	1:A:645:GLY:H	2.21	0.42
1:A:830:ALA:HB1	1:A:861:ILE:HG12	2.00	0.42
1:A:1090:LEU:O	1:A:1094:GLN:HG3	2.19	0.42
2:B:336:LEU:HD23	2:B:336:LEU:HA	1.70	0.42
2:B:474:ARG:CZ	2:B:512:ASN:HD21	2.32	0.42
2:B:548:ARG:HG3	2:B:550:TYR:OH	2.19	0.42
2:B:590:PRO:HB3	2:B:592:TRP:HE3	1.84	0.42
2:B:702:THR:OG1	2:B:706:ARG:NH1	2.53	0.42
3:C:49:PHE:CZ	9:K:110:VAL:HG22	2.54	0.42
5:F:50:LYS:C	5:F:51:ARG:HD3	2.40	0.42
5:F:101:LYS:HA	5:F:101:LYS:HD3	1.75	0.42
9:K:118:ILE:HD13	9:K:118:ILE:HA	1.89	0.42
1:A:386:LYS:O	1:A:390:ILE:HG23	2.20	0.42
1:A:483:ALA:O	1:A:494:ALA:N	2.52	0.42
1:A:760:GLY:H	1:A:763:HIS:HB3	1.84	0.42
1:A:851:LEU:HD22	1:A:857:ASP:OD2	2.19	0.42
1:A:1562:CYS:HA	1:A:1580:THR:HA	2.02	0.42
1:A:1706:VAL:HG12	1:A:1707:ARG:N	2.34	0.42
2:B:818:LYS:NZ	2:B:820:GLN:HE21	2.18	0.42
3:C:201:GLN:O	3:C:202:LEU:HD23	2.19	0.42
1:A:718:LYS:HD3	1:A:718:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:LEU:HD13	1:A:1105:LEU:HG	2.01	0.42
1:A:1303:PHE:O	1:A:1305:MET:N	2.53	0.42
1:A:1545:VAL:HG13	7:I:61:PHE:CZ	2.54	0.42
2:B:858:ASP:OD1	2:B:858:ASP:N	2.52	0.42
2:B:905:THR:HG21	2:B:977:GLU:OE1	2.20	0.42
3:C:272:VAL:HG12	3:C:273:ALA:H	1.85	0.42
1:A:419:GLN:O	1:A:423:LYS:N	2.53	0.42
1:A:581:ASN:HD21	1:A:628:ALA:HB2	1.84	0.42
1:A:1659:ARG:HG3	1:A:1674:PHE:CZ	2.54	0.42
2:B:315:PRO:HG2	2:B:318:TYR:CZ	2.55	0.42
2:B:463:ILE:HG22	2:B:693:LYS:HG2	2.02	0.42
2:B:556:VAL:O	2:B:563:VAL:HG12	2.19	0.42
2:B:1039:GLU:HA	2:B:1042:ARG:HD3	2.01	0.42
3:C:159:PRO:HB3	3:C:163:TYR:CD2	2.55	0.42
3:C:219:GLY:HA2	3:C:225:PHE:HB2	2.02	0.42
3:C:281:ASP:OD1	3:C:282:THR:N	2.53	0.42
4:E:159:LEU:HD22	4:E:206:TYR:CD1	2.55	0.42
1:A:795:PHE:CZ	1:A:893:SER:HB3	2.55	0.42
1:A:1559:ILE:HD12	1:A:1559:ILE:H	1.85	0.42
2:B:107:ARG:HD2	2:B:778:PHE:CE1	2.55	0.42
2:B:855:CYS:H	2:B:866:CYS:HB3	1.84	0.42
7:I:30:PRO:O	7:I:32:ALA:N	2.53	0.42
11:N:48:ASP:O	11:N:55:ARG:HA	2.20	0.42
1:A:429:ARG:HA	2:B:1042:ARG:CZ	2.49	0.42
1:A:483:ALA:HA	1:A:493:GLY:HA2	2.01	0.42
1:A:562:GLN:NE2	1:A:614:THR:HB	2.35	0.42
1:A:622:LYS:NZ	1:A:1636:VAL:HG12	2.34	0.42
1:A:672:SER:OG	1:A:673:PRO:HD2	2.20	0.42
1:A:728:ASN:C	1:A:730:ASP:H	2.22	0.42
1:A:1275:LEU:HA	1:A:1278:VAL:HG12	2.00	0.42
1:A:1637:ASP:O	1:A:1639:ARG:N	2.50	0.42
2:B:82:ILE:HG23	2:B:113:LYS:O	2.20	0.42
2:B:294:CYS:SG	2:B:300:VAL:HG12	2.60	0.42
2:B:700:LEU:HA	2:B:735:TYR:CE2	2.51	0.42
3:C:207:GLU:OE1	3:C:207:GLU:N	2.53	0.42
3:C:319:ASP:OD1	3:C:319:ASP:N	2.50	0.42
9:K:39:CYS:CA	9:K:85:GLN:HG2	2.49	0.42
11:N:12:GLN:OE1	11:N:98:GLN:NE2	2.52	0.42
12:M:52:ALA:HB3	12:M:73:LEU:HD13	2.01	0.42
1:A:323:GLY:O	1:A:327:ASN:ND2	2.50	0.41
1:A:644:ARG:HB2	1:A:734:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HD11	1:A:784:LEU:HD22	2.02	0.41
1:A:1152:PRO:HB3	1:A:1158:SER:HB2	2.02	0.41
1:A:1303:PHE:HB3	7:I:53:LYS:NZ	2.35	0.41
2:B:694:GLN:OE1	2:B:1003:ARG:NH2	2.53	0.41
2:B:1113:PRO:HD2	2:B:1116:PHE:CD2	2.55	0.41
4:E:18:MET:SD	4:E:32:GLU:HB3	2.60	0.41
9:K:128:ARG:HD3	9:K:128:ARG:HA	1.84	0.41
1:A:157:ILE:HB	1:A:159:GLU:OE1	2.20	0.41
1:A:466:LEU:HD23	1:A:467:THR:N	2.34	0.41
1:A:1122:ARG:HA	1:A:1125:TYR:HD2	1.85	0.41
2:B:214:CYS:HB3	2:B:222:VAL:CG1	2.50	0.41
2:B:415:ASN:O	2:B:419:ILE:HG23	2.20	0.41
2:B:760:ASN:OD1	2:B:760:ASN:C	2.59	0.41
3:C:333:CYS:SG	9:K:103:LEU:HD23	2.60	0.41
4:E:142:HIS:O	4:E:145:VAL:HG12	2.20	0.41
1:A:184:VAL:HG22	1:A:188:LYS:HZ2	1.85	0.41
1:A:558:ARG:HB3	1:A:559:PRO:HD3	2.01	0.41
1:A:1671:GLN:NE2	1:A:1683:GLN:HE22	2.18	0.41
2:B:137:VAL:HG21	2:B:381:PHE:HZ	1.85	0.41
2:B:590:PRO:HB3	2:B:592:TRP:CE3	2.55	0.41
2:B:1045:LEU:HD21	2:B:1054:LEU:HD12	2.03	0.41
4:E:11:TRP:CD2	4:E:37:LEU:HB2	2.54	0.41
4:E:115:LYS:O	4:E:118:LEU:HB2	2.20	0.41
4:E:162:ARG:HE	4:E:163:TYR:HE2	1.66	0.41
7:I:58:SER:O	7:I:60:VAL:HG22	2.21	0.41
9:K:40:VAL:HG22	9:K:41:THR:H	1.85	0.41
9:K:68:CYS:HA	9:K:83:ARG:O	2.19	0.41
9:K:82:LEU:HD12	9:K:82:LEU:HA	1.78	0.41
12:M:114:THR:O	12:M:115:LEU:HD23	2.20	0.41
1:A:481:ARG:O	1:A:484:VAL:HG12	2.20	0.41
1:A:1263:MET:HA	1:A:1581:GLU:HA	2.03	0.41
1:A:1269:LEU:HG	1:A:1271:THR:HG23	2.02	0.41
1:A:1604:ASP:CG	1:A:1607:ALA:H	2.23	0.41
1:A:1621:ILE:HD13	1:A:1648:MET:CE	2.50	0.41
1:A:1646:ASP:OD1	4:E:195:ARG:NH2	2.41	0.41
2:B:275:ASP:CG	2:B:278:LEU:HB2	2.40	0.41
2:B:312:LEU:CD2	2:B:327:LEU:HB2	2.51	0.41
2:B:546:PRO:HG2	2:B:549:SER:HB2	2.03	0.41
2:B:698:PHE:CE2	8:J:55:LEU:HD23	2.55	0.41
3:C:187:GLU:OE1	3:C:187:GLU:N	2.48	0.41
5:F:106:ILE:O	5:F:117:ASP:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:16:ALA:HB3	11:N:19:GLY:HA2	2.01	0.41
11:N:35:SER:OG	11:N:38:ASN:ND2	2.53	0.41
1:A:215:VAL:HG12	1:A:225:ILE:HD13	2.01	0.41
1:A:397:HIS:O	1:A:400:ILE:HG22	2.20	0.41
1:A:451:ILE:HD12	1:A:456:ILE:HA	2.01	0.41
1:A:626:PRO:HG2	1:A:756:SER:C	2.41	0.41
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.90	0.41
1:A:935:LEU:HD23	2:B:494:TRP:CE3	2.55	0.41
1:A:1031:PHE:CE2	1:A:1040:LEU:HD11	2.52	0.41
1:A:1198:LEU:HA	1:A:1198:LEU:HD23	1.82	0.41
1:A:1653:VAL:CG2	1:A:1655:LYS:HE3	2.51	0.41
2:B:889:GLN:HG3	2:B:928:MET:SD	2.60	0.41
3:C:154:LYS:HD2	3:C:155:ASP:HA	2.02	0.41
6:H:28:LEU:HB2	6:H:41:LEU:O	2.21	0.41
10:L:46:LYS:HG2	10:L:47:LYS:N	2.36	0.41
11:N:62:ALA:N	11:N:69:TYR:O	2.49	0.41
1:A:161:LEU:HB3	1:A:162:GLU:OE2	2.21	0.41
1:A:489:ASN:OD1	1:A:490:VAL:N	2.54	0.41
1:A:657:VAL:O	1:A:661:LEU:HD12	2.21	0.41
1:A:951:VAL:HA	1:A:963:GLU:OE2	2.21	0.41
1:A:1067:HIS:N	1:A:1067:HIS:CD2	2.87	0.41
1:A:1217:GLN:O	1:A:1221:GLU:HG3	2.21	0.41
2:B:10:LEU:HD23	2:B:729:TYR:CD1	2.56	0.41
2:B:144:LYS:C	2:B:145:LEU:HD22	2.40	0.41
2:B:243:GLU:HG3	2:B:245:PHE:CE1	2.56	0.41
2:B:721:LEU:HD23	2:B:721:LEU:HA	1.76	0.41
2:B:743:VAL:HG12	2:B:913:ILE:CG2	2.50	0.41
2:B:1094:ARG:O	2:B:1094:ARG:HG3	2.20	0.41
11:N:24:VAL:O	11:N:25:LEU:HD23	2.20	0.41
11:N:42:THR:OG1	11:N:42:THR:O	2.38	0.41
12:M:94:LEU:O	12:M:108:ALA:N	2.51	0.41
1:A:7:MET:CE	1:A:8:PRO:HD2	2.51	0.41
1:A:581:ASN:HD21	1:A:628:ALA:CB	2.33	0.41
1:A:607:GLU:CB	5:F:64:ARG:HH11	2.34	0.41
1:A:791:LEU:HB3	1:A:792:TYR:CE2	2.56	0.41
1:A:1153:ASP:OD1	1:A:1154:ILE:HG13	2.21	0.41
1:A:1202:ARG:HG2	5:F:56:TYR:OH	2.20	0.41
2:B:471:CYS:CB	2:B:513:HIS:HD2	2.34	0.41
2:B:692:GLY:O	2:B:695:THR:HG23	2.21	0.41
2:B:991:ASP:O	2:B:992:ILE:HD13	2.20	0.41
3:C:250:ALA:HB1	3:C:264:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:171:PRO:HB2	4:E:207:ARG:NH1	2.36	0.41
5:F:57:MET:SD	5:F:125:ILE:HG12	2.61	0.41
1:A:423:LYS:N	1:A:426:GLY:HA2	2.36	0.41
1:A:578:HIS:NE2	1:A:631:ILE:HB	2.36	0.41
1:A:1241:VAL:HG12	1:A:1261:THR:HB	2.03	0.41
2:B:702:THR:H	2:B:702:THR:HG23	1.66	0.41
2:B:760:ASN:HB3	2:B:912:ASP:HA	2.02	0.41
2:B:792:LEU:HA	2:B:828:TYR:HA	2.03	0.41
3:C:212:MET:O	3:C:213:HIS:CD2	2.74	0.41
12:M:55:CYS:HG	12:M:56:PHE:HD1	1.66	0.41
1:A:252:LYS:O	1:A:252:LYS:HG2	2.21	0.41
1:A:420:ILE:HG22	1:A:427:LEU:HD12	2.02	0.41
1:A:431:HIS:HA	1:A:434:GLY:O	2.21	0.41
1:A:484:VAL:C	1:A:515:ARG:HH21	2.23	0.41
1:A:526:ALA:HB2	1:A:532:PRO:HA	2.03	0.41
1:A:551:ASN:OD1	1:A:552:ARG:N	2.48	0.41
1:A:839:TYR:CE1	1:A:943:PHE:HB2	2.56	0.41
1:A:1001:VAL:HG12	1:A:1209:GLU:O	2.21	0.41
1:A:1024:LEU:HD13	1:A:1203:SER:O	2.20	0.41
1:A:1096:ILE:O	1:A:1100:VAL:HG22	2.21	0.41
1:A:1672:MET:HG3	1:A:1677:SER:CB	2.51	0.41
2:B:45:SER:OG	2:B:378:GLY:HA3	2.21	0.41
2:B:57:ALA:HA	2:B:218:GLU:HB3	2.02	0.41
2:B:186:ARG:NE	2:B:373:GLU:OE1	2.50	0.41
2:B:242:LYS:NZ	2:B:443:THR:HA	2.35	0.41
3:C:137:THR:O	3:C:138:LEU:HD23	2.21	0.41
4:E:73:PHE:O	4:E:103:LEU:N	2.54	0.41
5:F:70:ALA:O	5:F:74:ALA:HB2	2.21	0.41
6:H:38:ASP:O	6:H:125:LEU:HA	2.21	0.41
6:H:98:ARG:O	6:H:99:ILE:HD13	2.20	0.41
7:I:17:LEU:HD23	7:I:18:ASP:O	2.21	0.41
9:K:65:VAL:HG12	9:K:86:THR:HG22	2.02	0.41
11:N:12:GLN:O	11:N:101:VAL:HB	2.20	0.41
11:N:87:HIS:CD2	12:M:46:GLN:HG2	2.56	0.41
12:M:87:PRO:HB3	12:M:114:THR:CG2	2.51	0.41
1:A:609:TYR:O	1:A:613:CYS:HB3	2.21	0.41
1:A:1075:TRP:O	1:A:1079:HIS:HD2	2.04	0.41
2:B:226:LEU:HD11	2:B:349:MET:SD	2.60	0.41
2:B:352:LYS:HG3	2:B:607:TYR:CD1	2.55	0.41
2:B:789:ASP:H	2:B:831:LEU:HB2	1.86	0.41
3:C:95:TYR:HB2	3:C:209:ASP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLN:HG3	3:C:105:ILE:HG12	2.03	0.41
3:C:163:TYR:HE1	3:C:204:PRO:HD3	1.84	0.41
3:C:226:SER:OG	3:C:228:VAL:O	2.38	0.41
4:E:166:ARG:H	4:E:169:GLN:NE2	2.18	0.41
6:H:11:ASP:OD2	6:H:12:VAL:N	2.54	0.41
9:K:113:LYS:HD2	9:K:113:LYS:HA	1.83	0.41
11:N:78:ALA:CA	11:N:108:ASN:HD21	2.34	0.41
1:A:10:ARG:HG3	2:B:1110:VAL:HG12	2.03	0.40
1:A:170:GLN:OE1	1:A:171:ASN:HB2	2.21	0.40
1:A:450:TYR:CG	2:B:751:TYR:HE1	2.39	0.40
1:A:840:ASP:HB3	1:A:845:LYS:HZ2	1.85	0.40
1:A:1304:CYS:HB3	1:A:1313:GLN:HA	2.03	0.40
1:A:1612:TYR:CE1	4:E:142:HIS:CD2	3.05	0.40
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.84	0.40
2:B:311:LYS:HD3	2:B:311:LYS:HA	1.79	0.40
3:C:251:GLU:HG3	3:C:252:GLU:H	1.86	0.40
4:E:89:VAL:HG12	4:E:90:TYR:CD1	2.57	0.40
6:H:9:ILE:HA	6:H:57:ARG:HA	2.02	0.40
8:J:3:ILE:HG13	8:J:4:PRO:HD2	2.03	0.40
11:N:9:ALA:HB2	12:M:63:LEU:HD21	2.03	0.40
1:A:196:TRP:O	1:A:200:MET:HG2	2.21	0.40
1:A:468:TYR:HB3	1:A:540:ARG:NH1	2.36	0.40
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.94	0.40
1:A:1295:GLN:HG3	1:A:1296:LYS:CG	2.49	0.40
2:B:216:ARG:NE	2:B:218:GLU:OE2	2.54	0.40
2:B:525:VAL:HG12	2:B:526:TYR:N	2.37	0.40
3:C:272:VAL:HG12	3:C:273:ALA:N	2.35	0.40
4:E:24:ARG:HD2	4:E:24:ARG:HA	1.75	0.40
5:F:79:VAL:HG11	5:F:83:LEU:HD22	2.04	0.40
6:H:22:PHE:HB3	6:H:23:ASP:H	1.79	0.40
1:A:180:HIS:CE1	1:A:1689:SER:HG	2.38	0.40
1:A:424:LYS:HB2	1:A:424:LYS:HE2	1.89	0.40
1:A:437:VAL:O	2:B:1035:ILE:HG22	2.21	0.40
1:A:483:ALA:HB1	1:A:540:ARG:HB2	2.03	0.40
1:A:1059:ARG:HE	5:F:124:ILE:HD11	1.86	0.40
1:A:1126:GLU:OE1	1:A:1126:GLU:N	2.33	0.40
2:B:668:SER:O	2:B:672:ASN:HB2	2.22	0.40
2:B:1078:SER:HB2	2:B:1098:CYS:HB2	2.04	0.40
3:C:118:ASP:OD1	3:C:120:ARG:N	2.53	0.40
3:C:155:ASP:OD1	3:C:155:ASP:N	2.54	0.40
5:F:56:TYR:N	5:F:123:LEU:HD22	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:23:CYS:SG	7:I:24:GLY:N	2.95	0.40
1:A:58:ALA:HA	1:A:71:PHE:CD2	2.56	0.40
1:A:269:TRP:HB2	1:A:294:PRO:HG3	2.04	0.40
1:A:334:ASP:HB2	1:A:397:HIS:CE1	2.56	0.40
1:A:828:ARG:NH2	1:A:844:GLY:HA3	2.27	0.40
1:A:1296:LYS:HG2	7:I:59:VAL:HA	2.02	0.40
1:A:1341:PHE:CE2	1:A:1345:ARG:HG3	2.57	0.40
1:A:1627:ASP:OD1	1:A:1628:VAL:N	2.55	0.40
2:B:464:ARG:O	2:B:468:HIS:HB2	2.22	0.40
2:B:592:TRP:O	2:B:618:ARG:NH2	2.55	0.40
2:B:674:ILE:HG22	2:B:677:SER:HB2	2.04	0.40
2:B:883:PHE:CD2	2:B:999:TYR:HD1	2.38	0.40
2:B:1081:LEU:HD23	2:B:1082:GLU:N	2.37	0.40
6:H:8:ASP:HB3	6:H:10:PHE:CE2	2.56	0.40
9:K:31:GLN:HA	9:K:40:VAL:HG23	2.03	0.40
1:A:535:THR:HG22	1:A:536:LYS:N	2.36	0.40
1:A:744:LEU:HD23	1:A:745:LEU:N	2.36	0.40
1:A:1100:VAL:HA	1:A:1103:LEU:HG	2.04	0.40
2:B:227:HIS:CD2	2:B:227:HIS:N	2.88	0.40
2:B:1003:ARG:HG2	2:B:1004:HIS:O	2.21	0.40
2:B:1037:PHE:CD2	2:B:1041:GLU:HB3	2.56	0.40
3:C:265:GLN:NE2	3:C:274:ARG:HB3	2.35	0.40
4:E:73:PHE:N	4:E:101:ARG:O	2.55	0.40
4:E:102:ALA:O	4:E:127:LEU:HA	2.21	0.40
4:E:110:MET:HB3	4:E:115:LYS:HE2	2.03	0.40
10:L:47:LYS:HE3	10:L:47:LYS:HB3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1543/1720 (90%)	1328 (86%)	211 (14%)	4 (0%)	41 75
2	B	1129/1135 (100%)	944 (84%)	184 (16%)	1 (0%)	51 84
3	C	304/346 (88%)	241 (79%)	63 (21%)	0	100 100
4	E	207/210 (99%)	184 (89%)	23 (11%)	0	100 100
5	F	76/127 (60%)	62 (82%)	14 (18%)	0	100 100
6	H	146/150 (97%)	119 (82%)	27 (18%)	0	100 100
7	I	45/126 (36%)	29 (64%)	15 (33%)	1 (2%)	6 37
8	J	64/67 (96%)	51 (80%)	13 (20%)	0	100 100
9	K	105/133 (79%)	92 (88%)	13 (12%)	0	100 100
10	L	44/58 (76%)	34 (77%)	10 (23%)	0	100 100
11	N	103/419 (25%)	98 (95%)	5 (5%)	0	100 100
12	M	120/510 (24%)	107 (89%)	11 (9%)	2 (2%)	9 42
All	All	3886/5001 (78%)	3289 (85%)	589 (15%)	8 (0%)	50 80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1258	ASN
1	A	1274	ALA
2	B	271	GLY
1	A	644	ARG
1	A	678	PRO
7	I	59	VAL
12	M	126	SER
12	M	127	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1356/1504 (90%)	1345 (99%)	11 (1%)	81 88
2	B	988/992 (100%)	979 (99%)	9 (1%)	78 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	269/302 (89%)	267 (99%)	2 (1%)	84 90
4	E	191/192 (100%)	191 (100%)	0	100 100
5	F	68/111 (61%)	67 (98%)	1 (2%)	65 79
6	H	129/131 (98%)	129 (100%)	0	100 100
7	I	42/111 (38%)	41 (98%)	1 (2%)	49 69
8	J	55/56 (98%)	55 (100%)	0	100 100
9	K	96/119 (81%)	96 (100%)	0	100 100
10	L	43/55 (78%)	41 (95%)	2 (5%)	26 53
11	N	89/366 (24%)	89 (100%)	0	100 100
12	M	97/427 (23%)	97 (100%)	0	100 100
All	All	3423/4366 (78%)	3397 (99%)	26 (1%)	82 88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	125	ARG
1	A	140	ARG
1	A	314	ARG
1	A	540	ARG
1	A	716	TRP
1	A	832	ASN
1	A	856	ARG
1	A	924	ARG
1	A	1085	ARG
1	A	1610	ASN
2	B	417	MET
2	B	418	ARG
2	B	428	LYS
2	B	465	TYR
2	B	567	ASP
2	B	766	ARG
2	B	825	TYR
2	B	961	TYR
2	B	999	TYR
3	C	120	ARG
3	C	154	LYS
5	F	51	ARG

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Mol	Chain	Res	Type
7	I	34	ASP
10	L	37	ARG
10	L	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	73	ASN
1	A	143	ASN
1	A	177	GLN
1	A	324	GLN
1	A	562	GLN
1	A	600	GLN
1	A	694	ASN
1	A	704	ASN
1	A	850	HIS
1	A	967	HIS
1	A	1002	GLN
1	A	1030	GLN
1	A	1043	ASN
1	A	1067	HIS
1	A	1079	HIS
1	A	1081	ASN
1	A	1111	ASN
1	A	1240	ASN
1	A	1295	GLN
1	A	1310	ASN
1	A	1329	GLN
1	A	1358	ASN
1	A	1359	ASN
1	A	1579	ASN
1	A	1683	GLN
2	B	18	HIS
2	B	59	GLN
2	B	97	ASN
2	B	160	HIS
2	B	227	HIS
2	B	237	ASN
2	B	263	GLN
2	B	329	ASN
2	B	473	HIS

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Mol	Chain	Res	Type
2	B	512	ASN
2	B	536	ASN
2	B	672	ASN
2	B	688	GLN
2	B	734	ASN
2	B	820	GLN
2	B	846	ASN
2	B	889	GLN
2	B	918	HIS
2	B	941	HIS
2	B	1030	ASN
2	B	1048	HIS
3	C	59	ASN
3	C	160	ASN
3	C	213	HIS
3	C	305	HIS
4	E	64	HIS
4	E	98	ASN
4	E	132	GLN
4	E	133	GLN
4	E	169	GLN
6	H	133	HIS
9	K	38	HIS
9	K	45	HIS
9	K	81	ASN
9	K	85	GLN
9	K	101	ASN
10	L	13	GLN
11	N	38	ASN
12	M	131	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

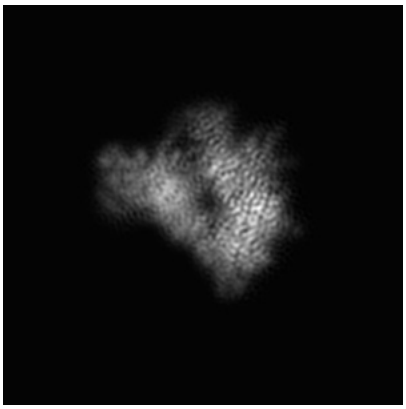
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15135. These allow visual inspection of the internal detail of the map and identification of artifacts.

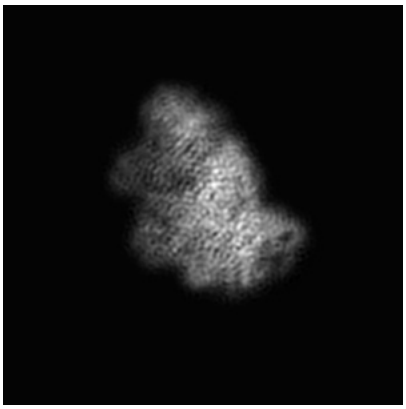
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

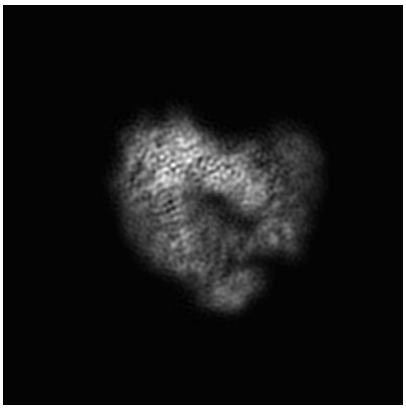
6.1.1 Primary map



X

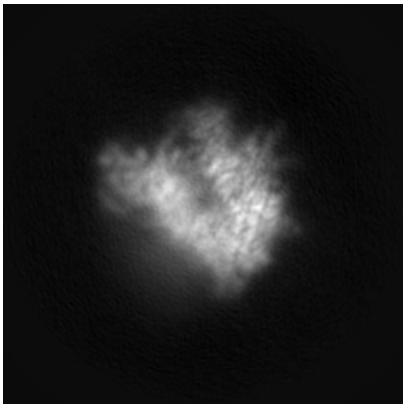


Y

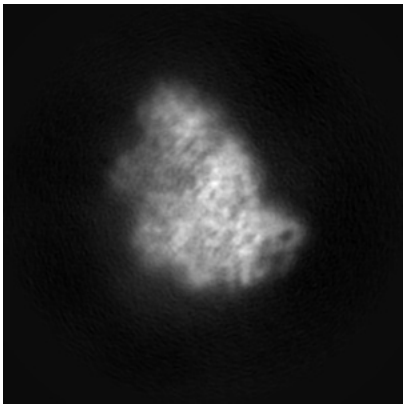


Z

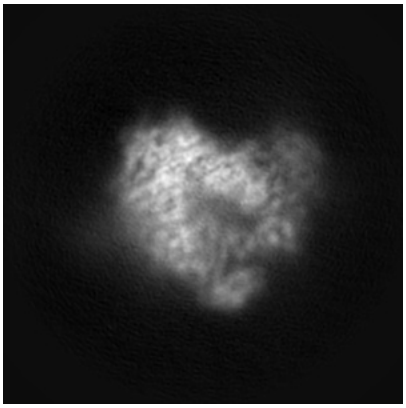
6.1.2 Raw map



X



Y

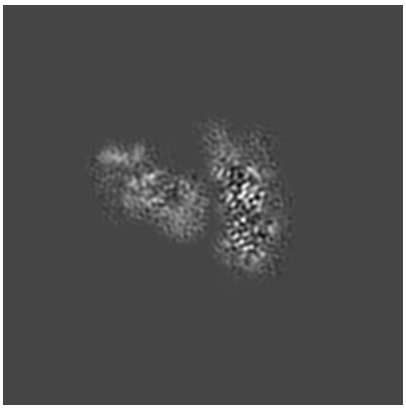


Z

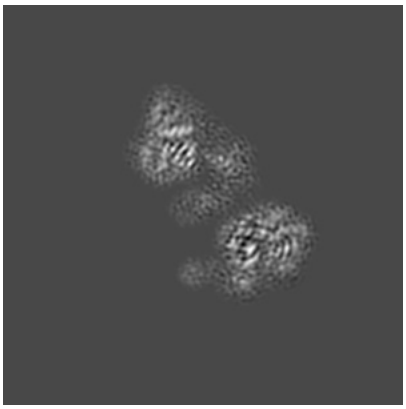
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

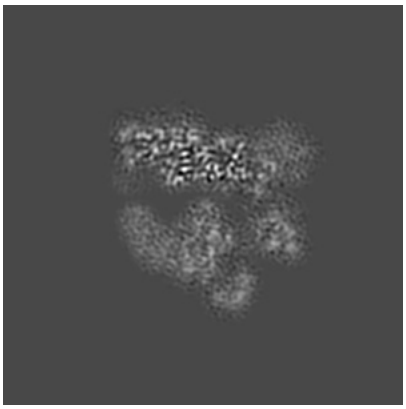
6.2.1 Primary map



X Index: 95

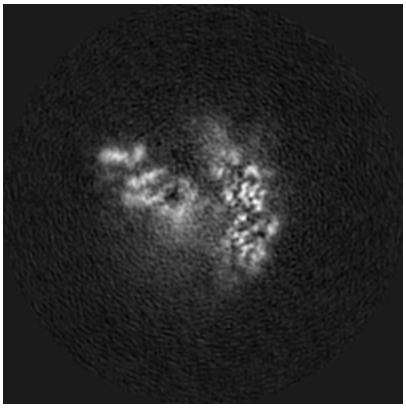


Y Index: 95

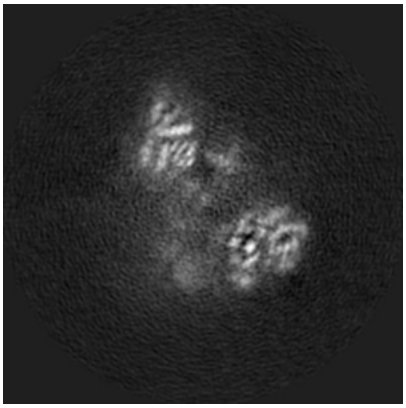


Z Index: 95

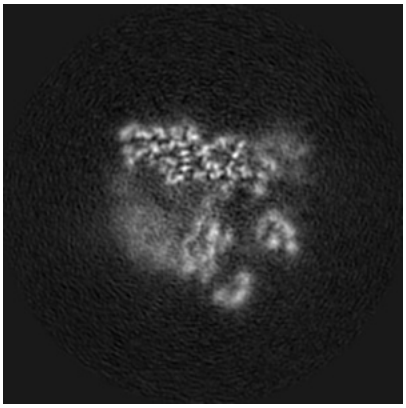
6.2.2 Raw map



X Index: 95



Y Index: 95

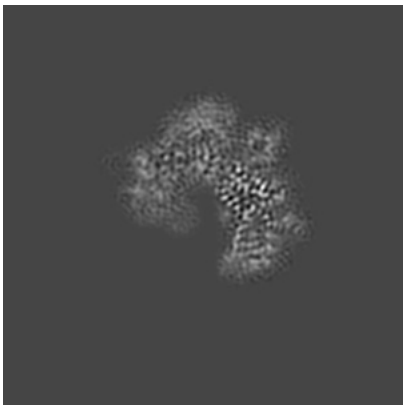


Z Index: 95

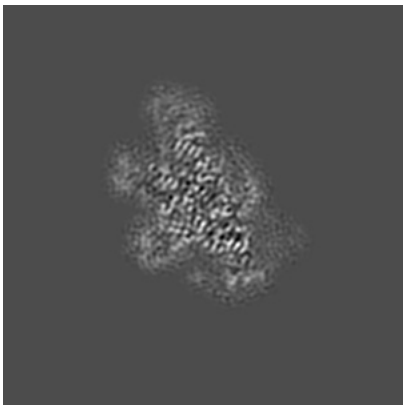
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

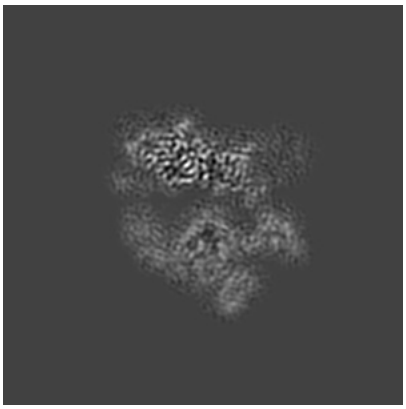
6.3.1 Primary map



X Index: 83

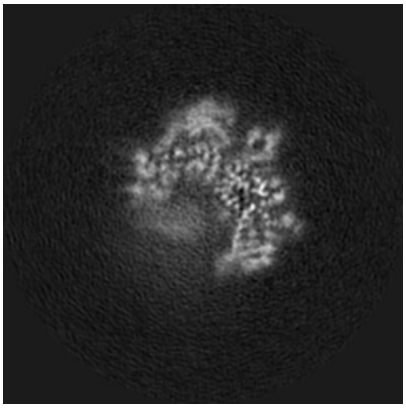


Y Index: 111

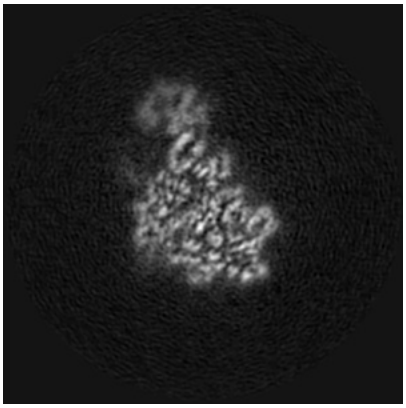


Z Index: 99

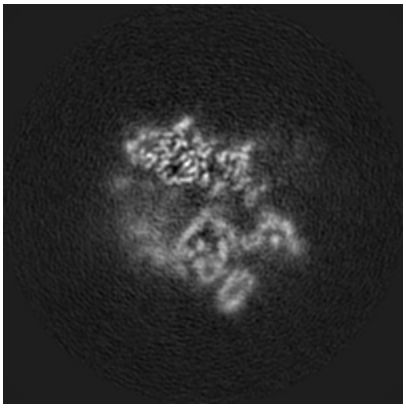
6.3.2 Raw map



X Index: 83



Y Index: 118



Z Index: 99

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

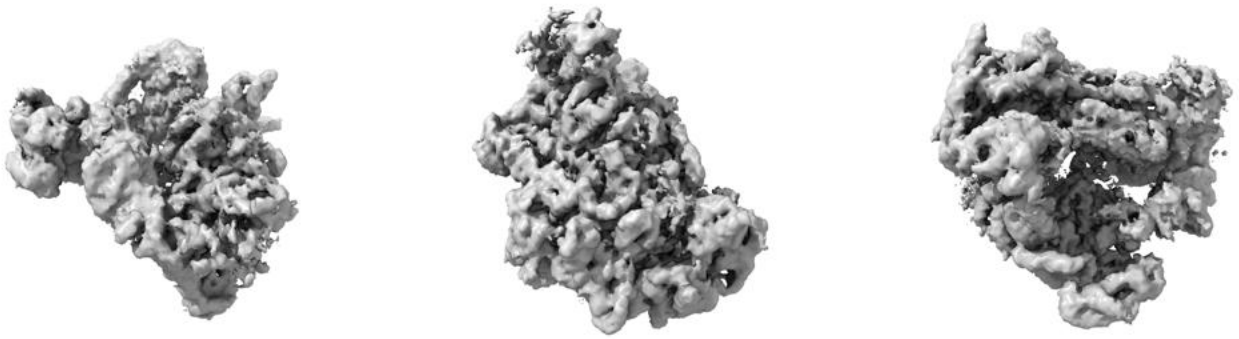
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

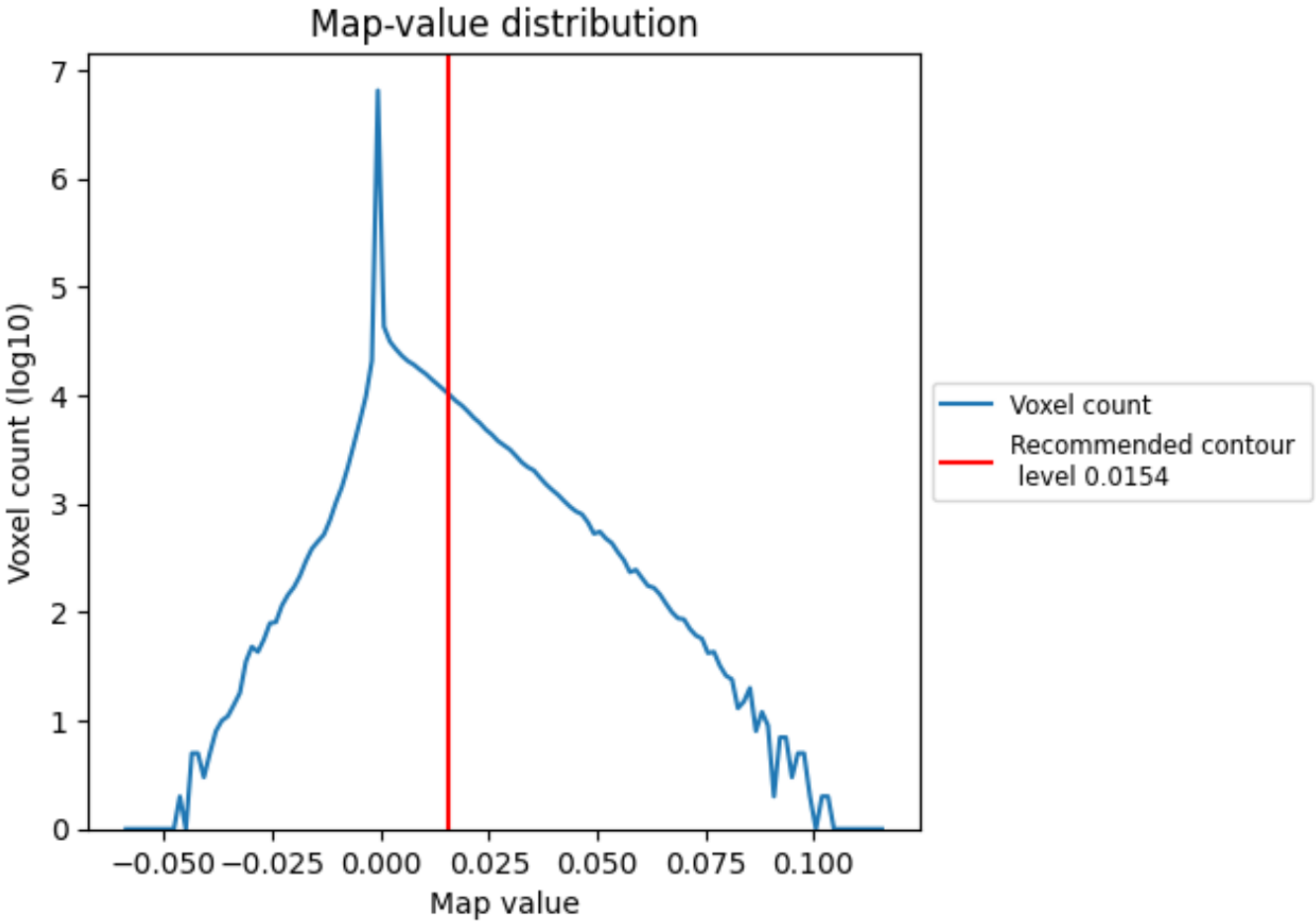
6.5 Mask visualisation (i)

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

7 Map analysis

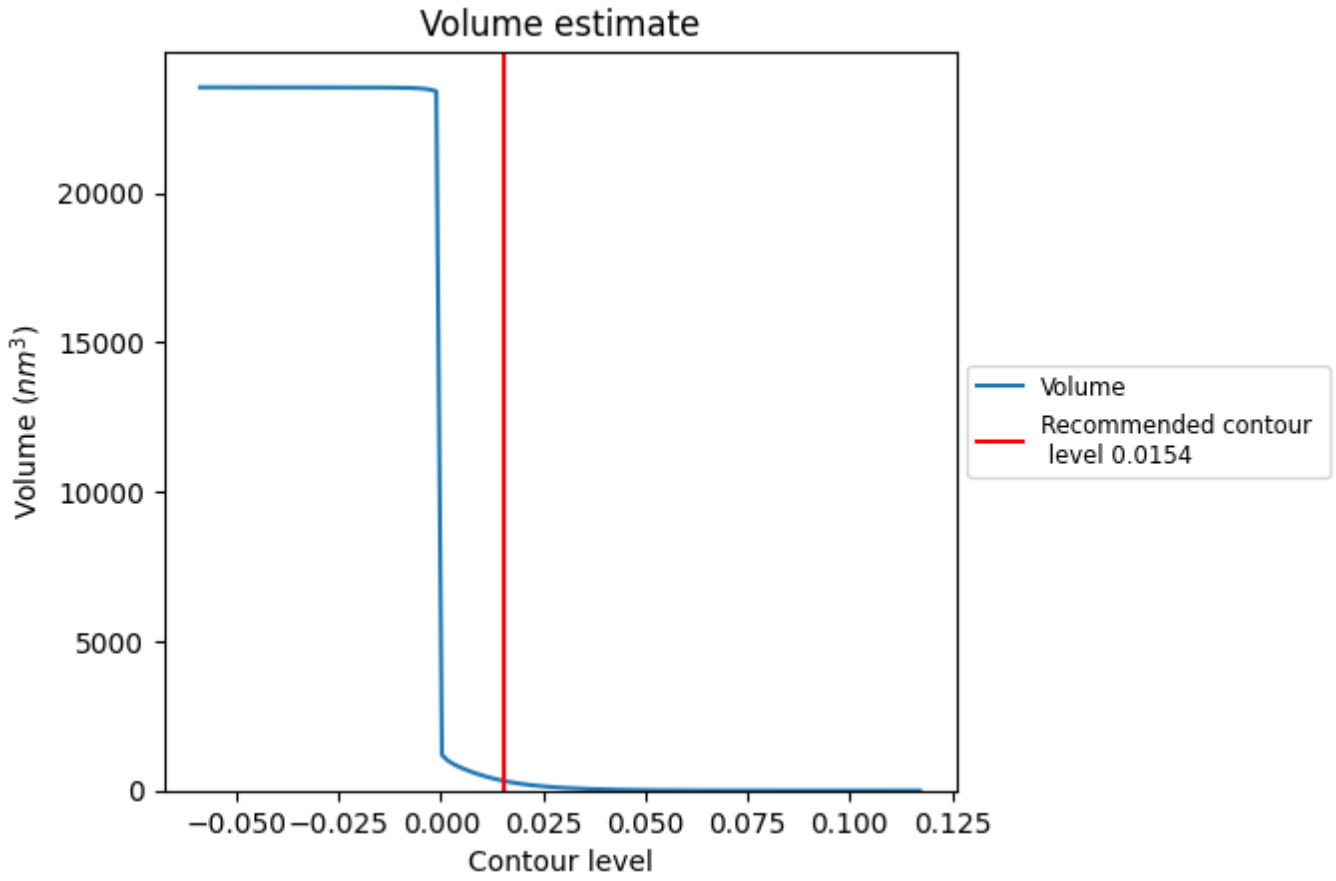
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

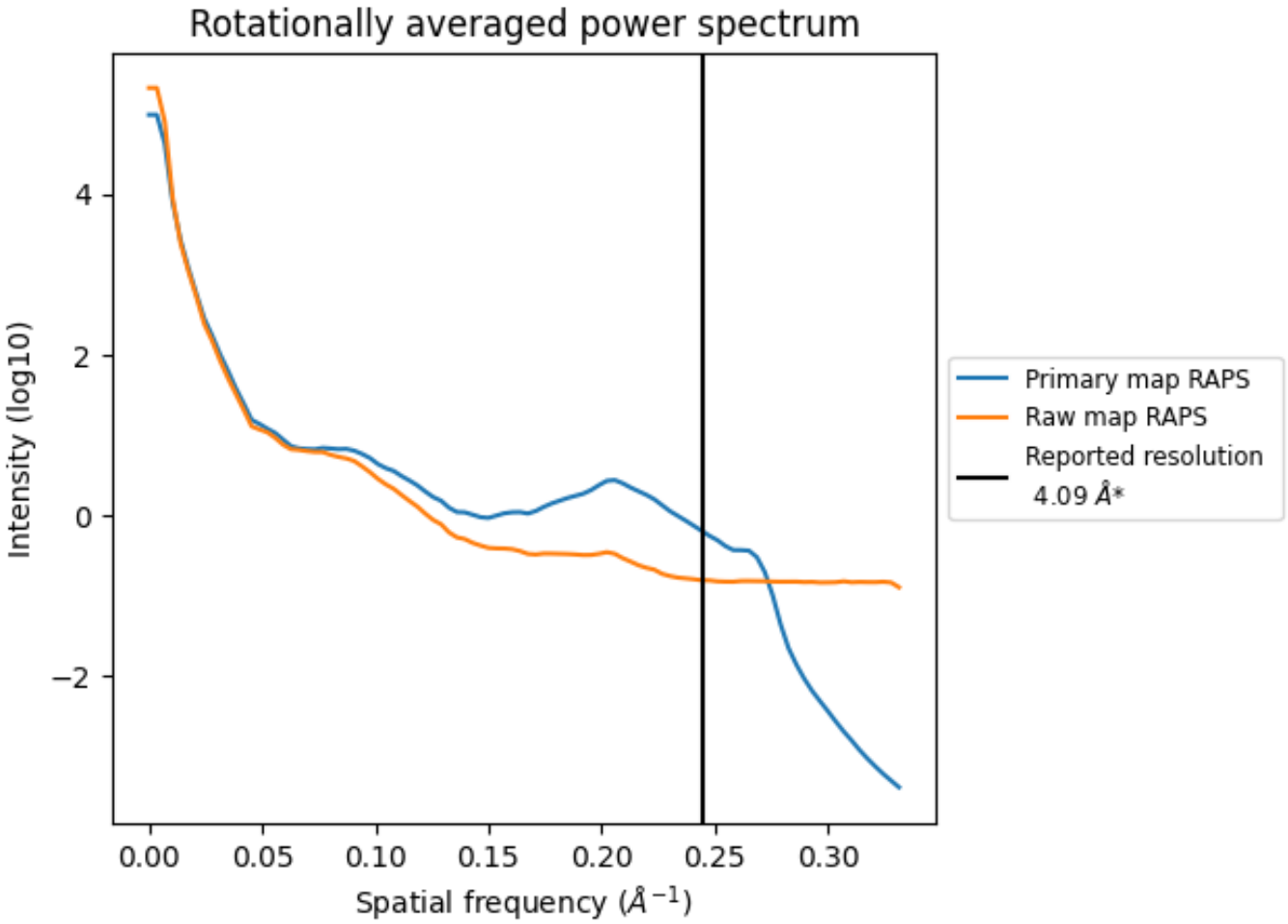
7.2 Volume estimate



The volume at the recommended contour level is 324 nm^3; this corresponds to an approximate mass of 293 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)

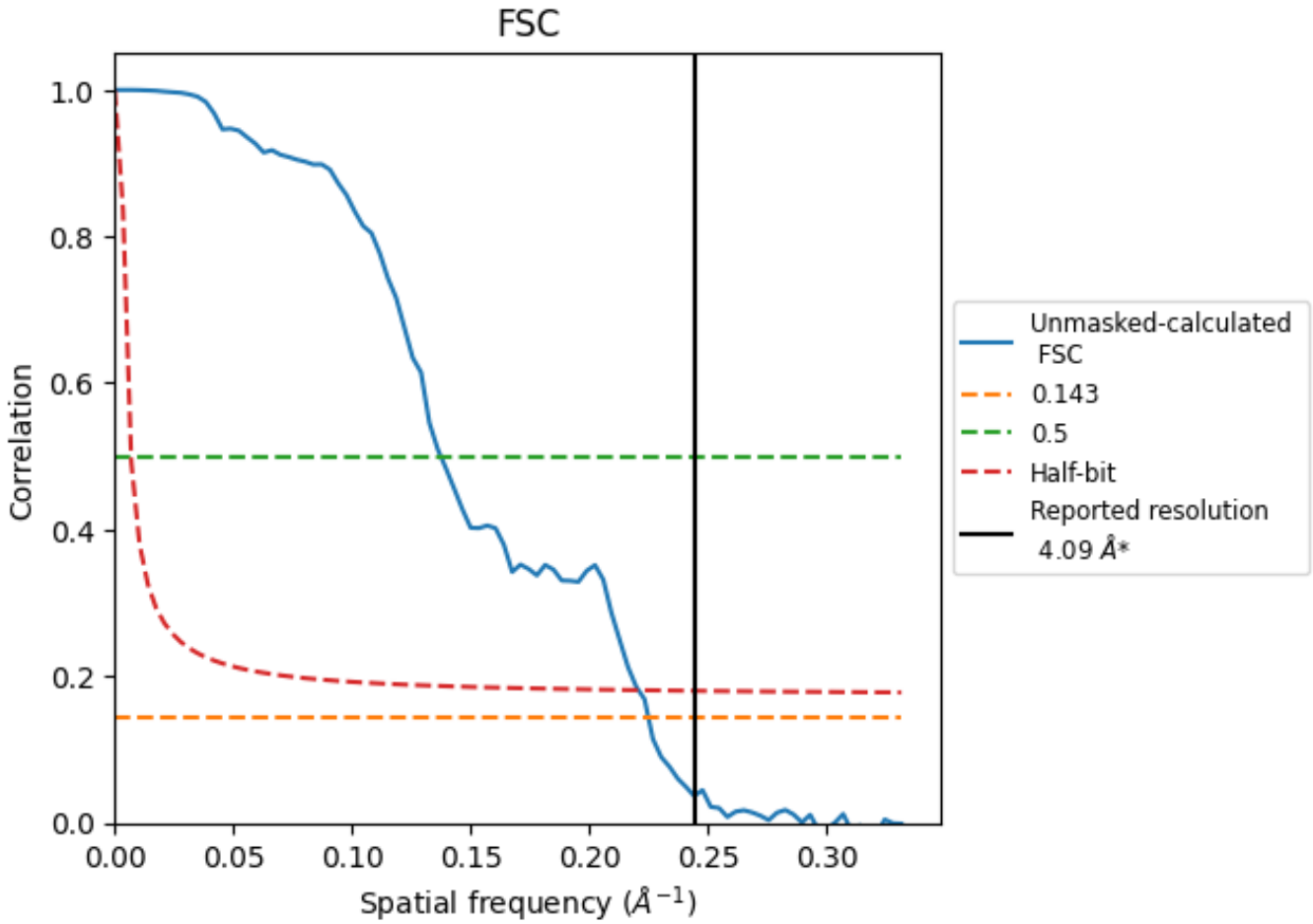


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

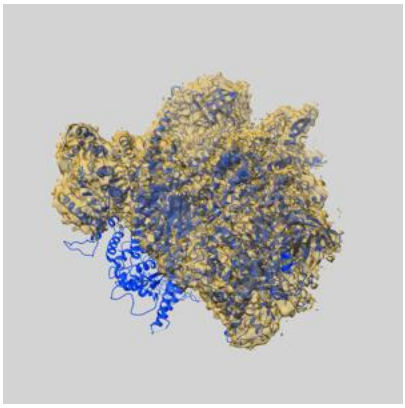
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.45	7.28	4.53

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

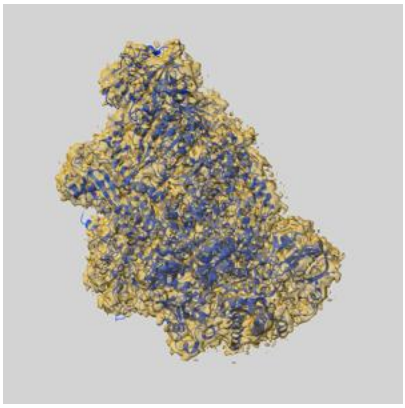
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15135 and PDB model 8A43. Per-residue inclusion information can be found in section 3 on page 6.

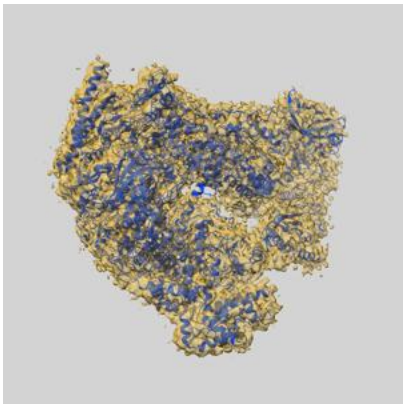
9.1 Map-model overlay



X



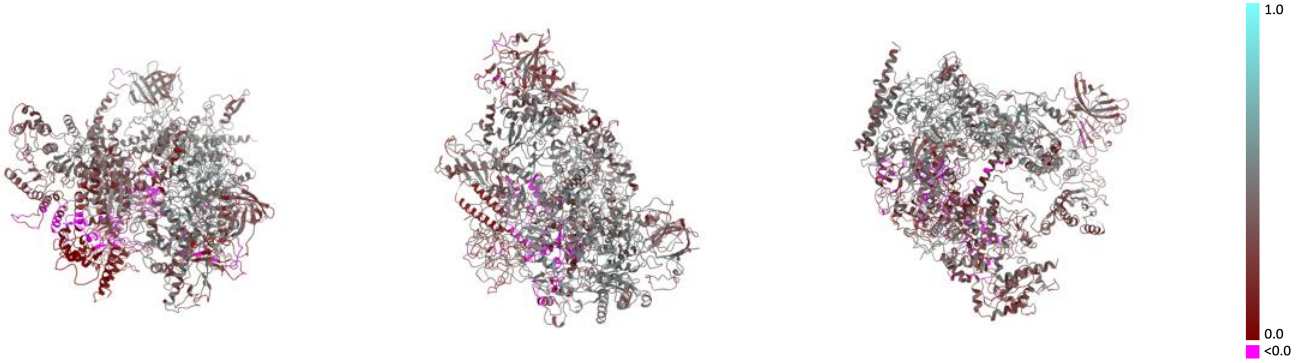
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0154 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.

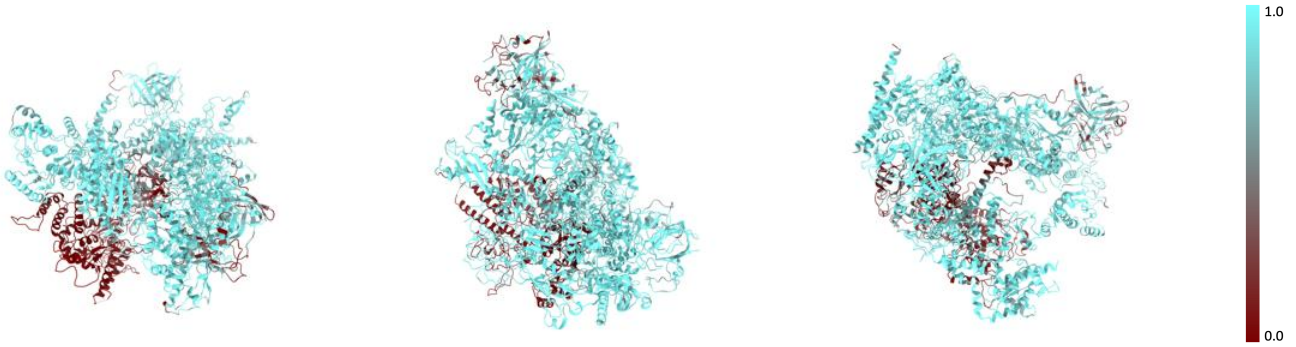
9.2 Q-score mapped to coordinate model (i)



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.

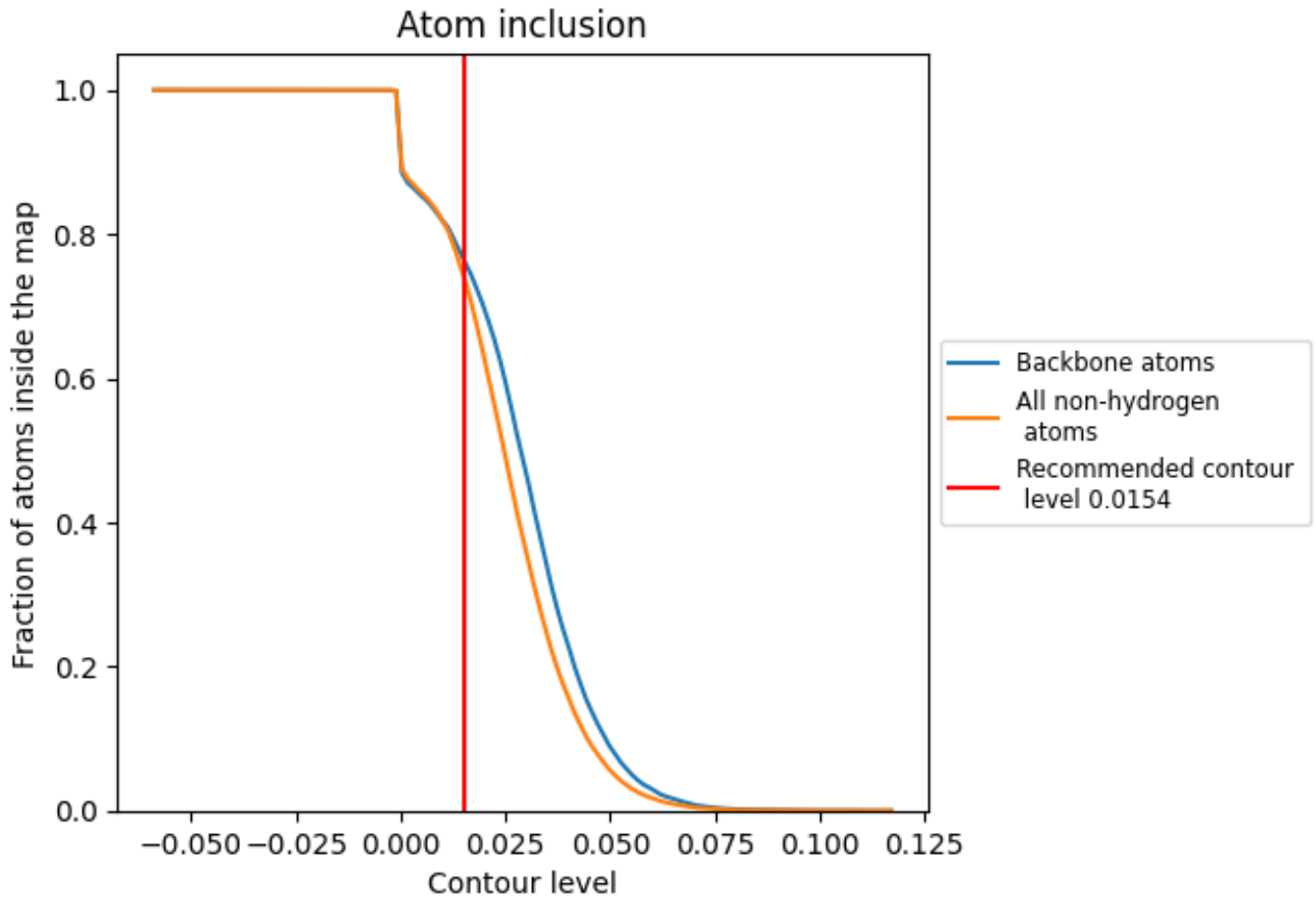
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0154).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7346	0.3370
A	0.5680	0.2480
B	0.8326	0.4060
C	0.9440	0.4530
E	0.9313	0.3660
F	0.8207	0.3330
H	0.8913	0.3880
I	0.8860	0.3530
J	0.9569	0.4890
K	0.9227	0.4300
L	0.9380	0.4330
M	0.5549	0.2790
N	0.5376	0.2490