Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:02 am GMT

PDB ID	:	5M3F
EMDB ID	:	EMD-4147
Title	:	Yeast RNA polymerase I elongation complex at 3.8A
Authors	:	Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.; Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on	:	2016-10-14
Resolution	:	3.80 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:

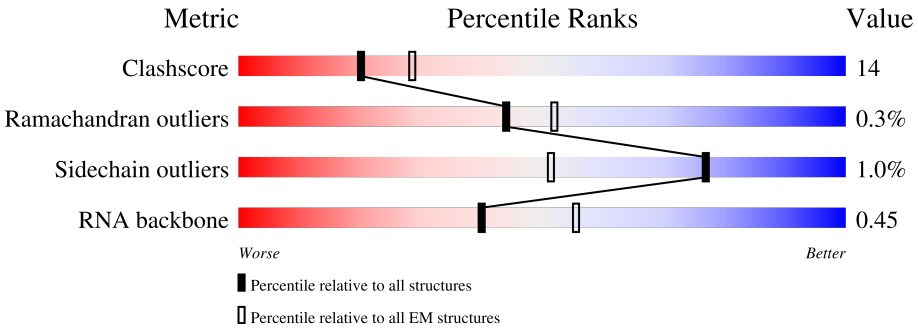
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.80 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
RNA backbone	4643	859

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	1664	38% 65% 22% 12%
2	B	1203	32% 71% 27% ·
3	C	335	35% 72% 19% 9%
4	E	215	67% 81% 17% ·
5	F	155	30% 49% 15% 35%
6	H	146	36% 71% 19% 10%
7	I	125	50% 30% 20% 50%

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Mol	Chain	Length	Quality of chain
8	J	70	17% 76% 23%
9	K	142	22% 57% 14% 29%
10	L	70	23% 51% 11% 37%
11	T	39	51% 26% 38% 36%
12	U	39	36% 13% 23% 64%
13	R	20	25% 15% 20% 5% 60%
14	M	415	26% 17% 8% 74%
15	N	233	62% 42% 19% 38%
16	D	137	39% 28% 10% 61%
17	G	326	59% 45% 13% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	SO4	B	1301	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 34032 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 RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1459	11526	7281	2004	2180	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1177	9350	5913	1639	1747	51	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	305	2423	1539	416	460	8	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	212	1735	1102	306	316	11	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	100	823	522	144	154	3	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	131	1052	664	176	208	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	63	Total	C	N	O	S	0	0
			466	292	77	93	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	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	25	Total	C	N	O	P	0	0
			509	244	95	146	24		

- Molecule 12 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	14	Total	C	N	O	P	0	0
			285	138	51	83	13		

- Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	8	Total	C	N	O	P	0	0
			173	77	34	54	8		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	108	Total 856	C 543	N 142	O 171	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	145	Total 1151	C 735	N 188	O 224	S 4	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	D	54	Total 431	C 270	N 73	O 88	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	193	Total 1526	C 985	N 262	O 274	S 5	0	0

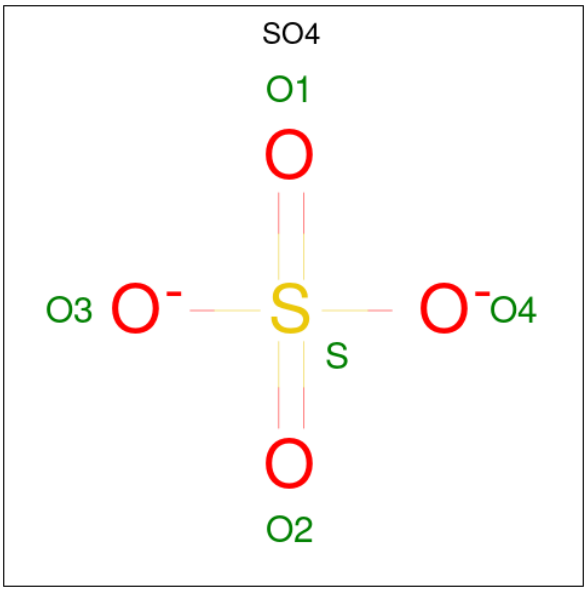
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total 2	Zn 2	0
18	B	1	Total 1	Zn 1	0
18	I	1	Total 1	Zn 1	0
18	J	1	Total 1	Zn 1	0
18	L	1	Total 1	Zn 1	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total 1	Mg 1	0

- Molecule 20 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



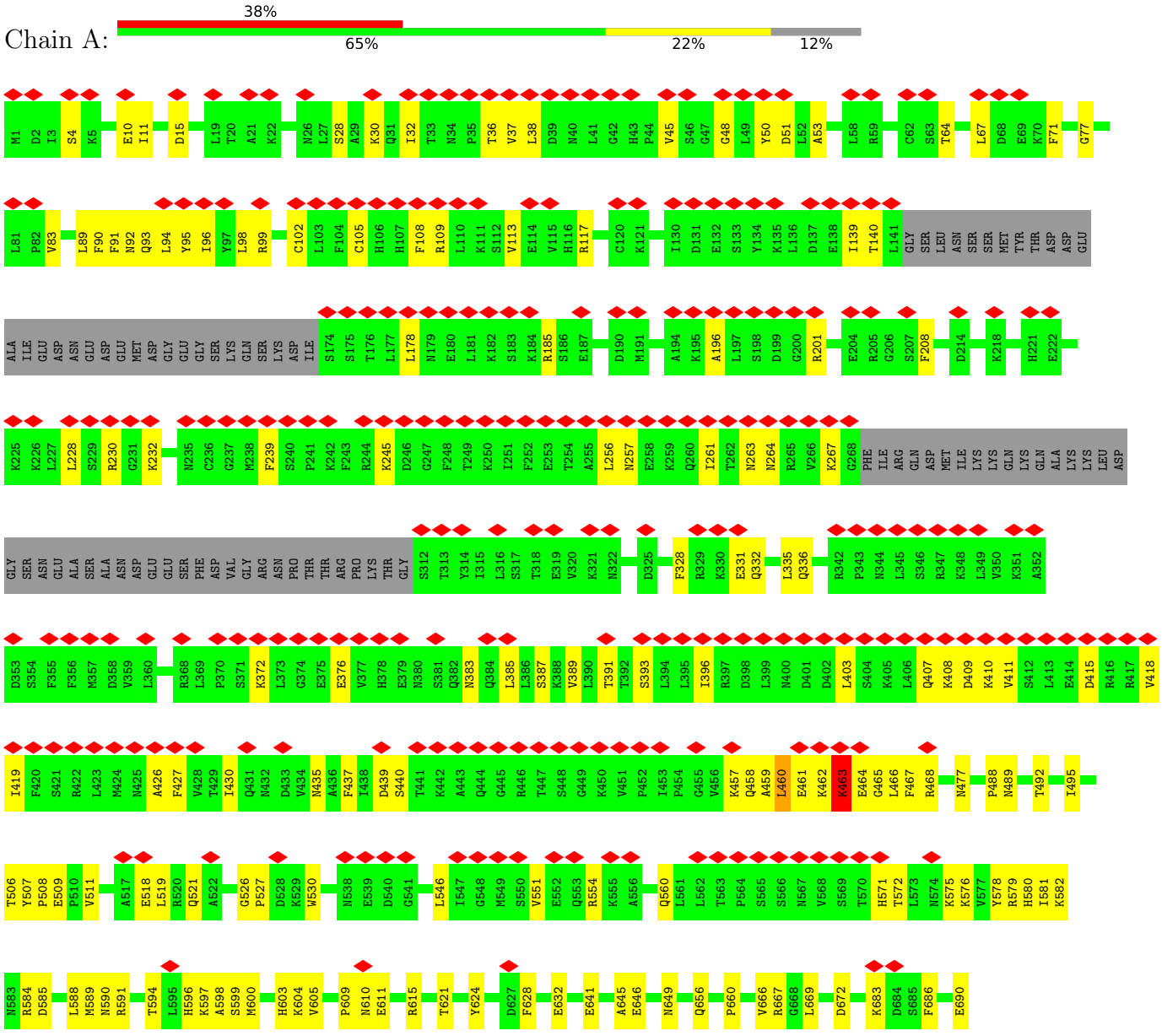
Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
20	B	1	5	4	1	0

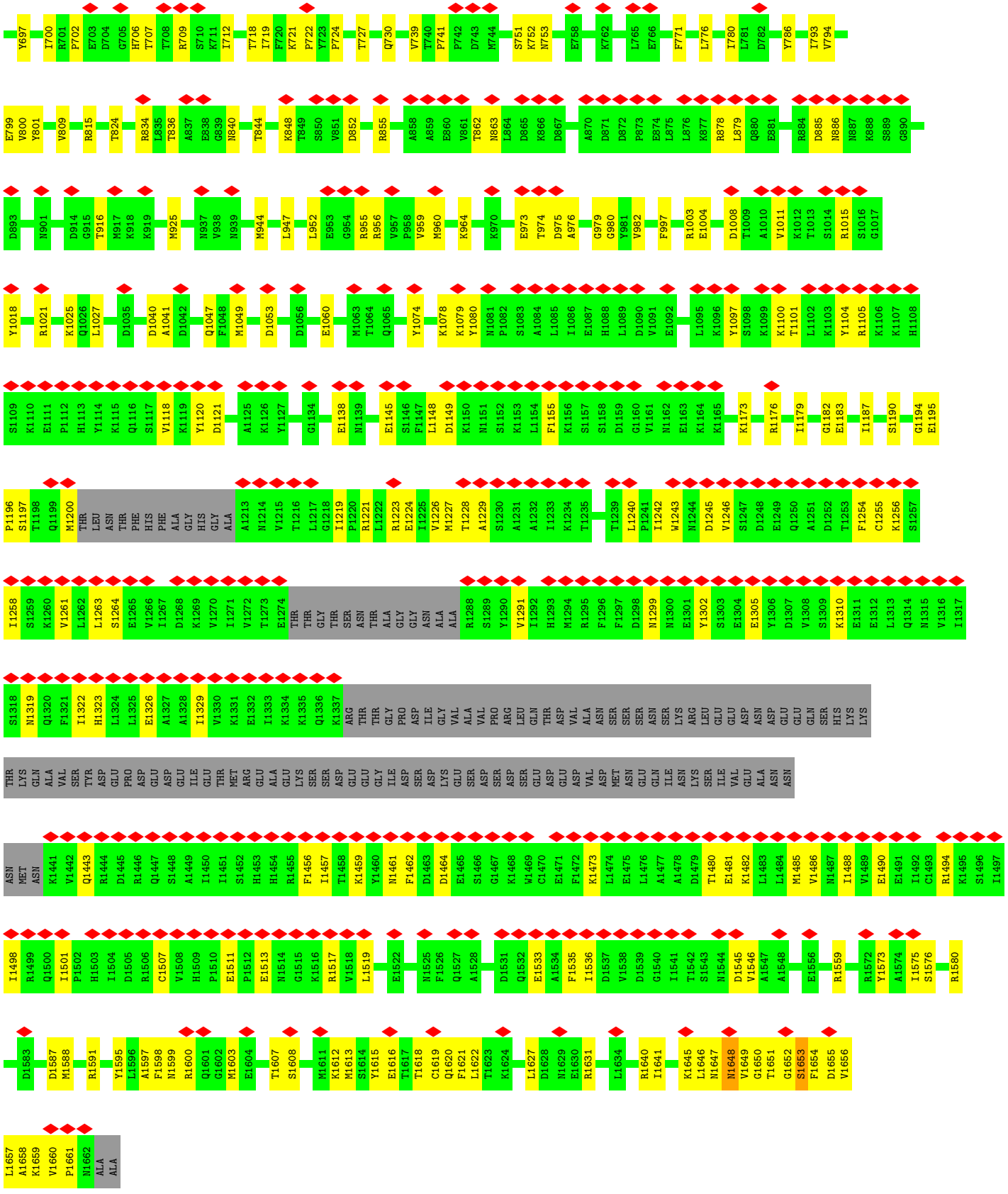
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase I subunit RPA190

Chain A:

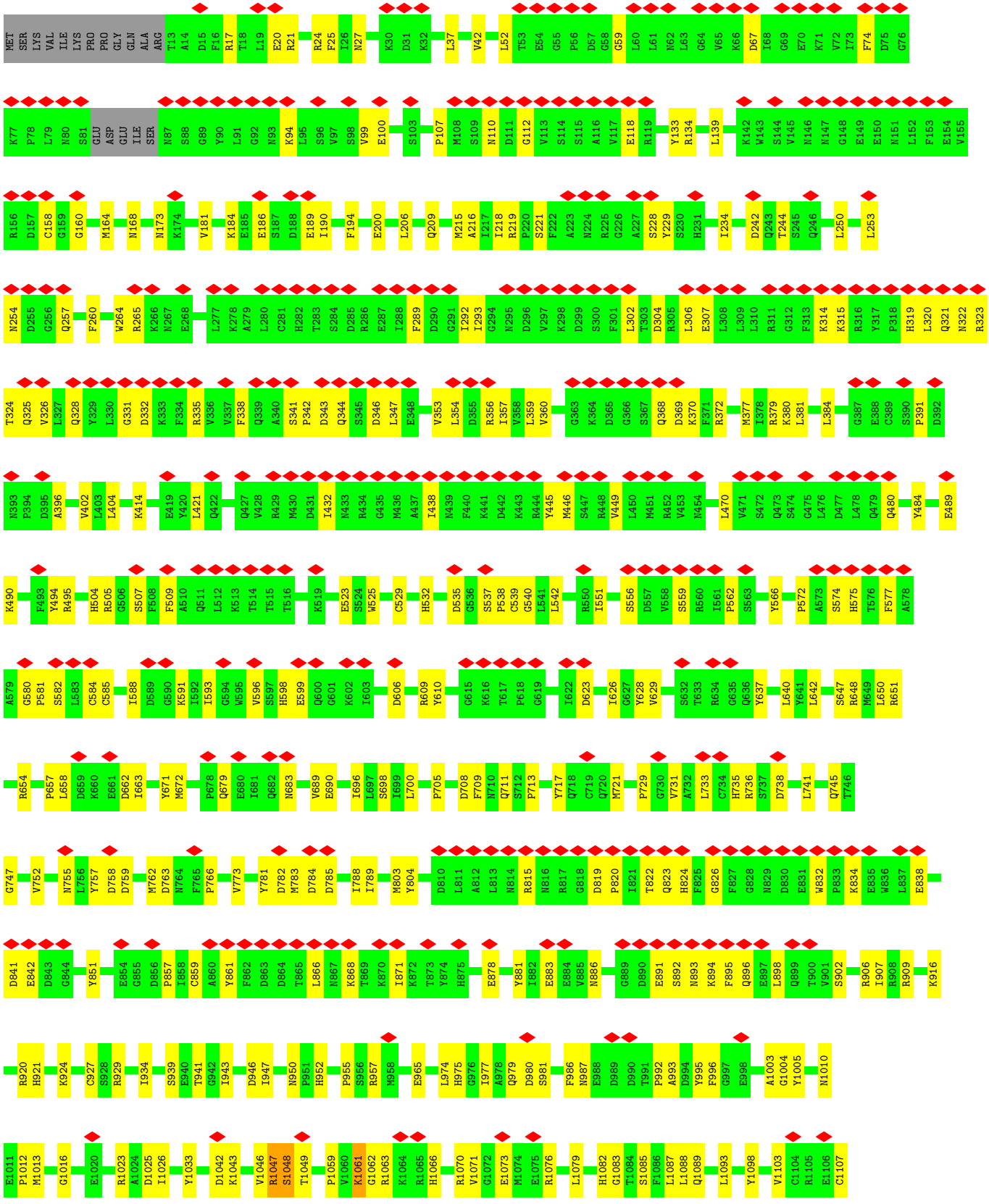


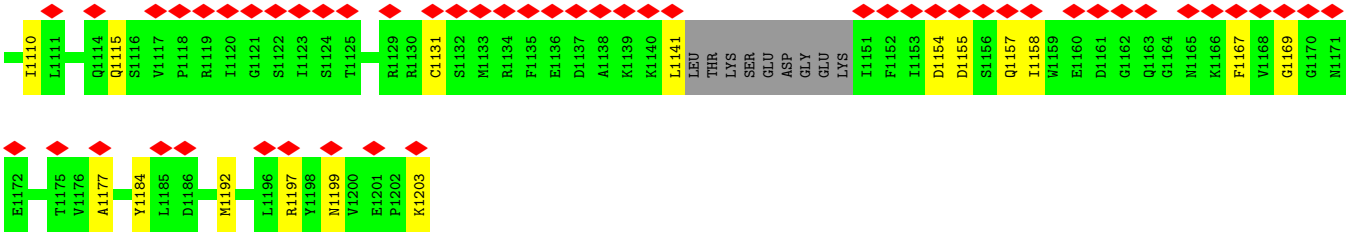


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

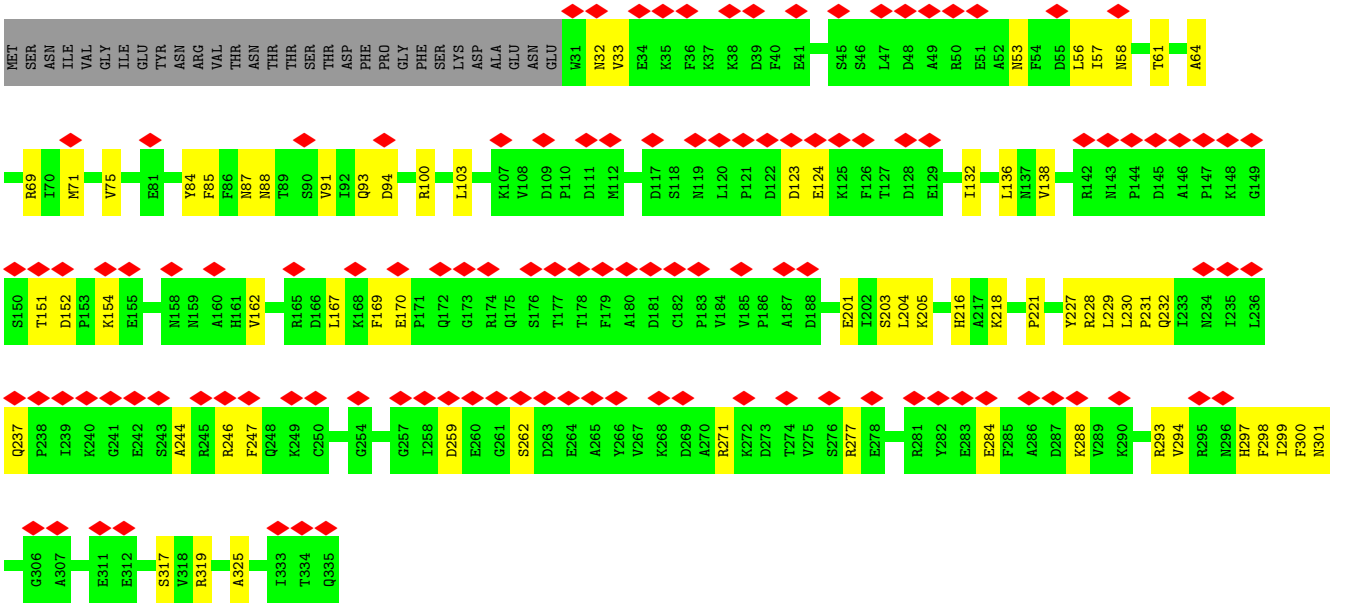
Chain B:


32%
71%
27%

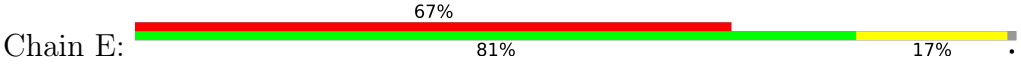

MET SER LYS VAL ILE LYS PRO PRO GLY GLN ALA ARG T13 A14 D15 F16 R17 T18 L19 E20 R21 R24 P25 I26 N27 K30 D31 K32 L37 V42 L52 T53 E54 G55 P56 D57 G58 G59 L60 L61 N62 L63 G64 V65 K66 D67 I68 G69 E70 K71 V72 I73 F74 D75 G76
K77 P78 L79 N80 S81 GLU ASP GLU ILE SER N87 S88 G89 Y90 L91 G92 N93 K94 L95 S96 V97 S98 V99 E100 S103 P107 M108 S109 N110 D111 G112 V113 S114 S115 A116 V117 E118 R119 Y133 R134 L139 K142 W143 S144 V145 N146 N147 G148 E149 E150 N151 L152 F153 E154 V155
R156 D157 C158 G159 G160 M164 N168 N173 K174 V181 K184 E185 E186 S187 D188 E189 I190 F194 E200 L206 Q209 M215 A216 I217 I218 R219 P220 S221 F222 A223 N224 R225 G226 A227 S228 Y229 S230 H231 I234 D242 Q243 T244 S245 Q246 L250 L253
N254 D255 G256 Q257 F260 W264 R265 K266 N267 E268 L277 K278 A279 L280 C281 H282 T283 S284 D285 R286 E287 I288 F289 D290 G291 I292 I293 G294 N295 D296 V297 K298 D299 S300 F301 L302 T303 D304 R305 L306 E307 L308 L309 L310 R311 G312 F313 K314 K315 R316 Y317 P318 H319 L320 Q321 N322 R323
T324 Q325 V326 L327 Q328 Y329 L330 G331 D332 K333 F334 R335 V336 V337 F338 Q339 A340 S341 P342 D343 Q344 S345 D346 L347 E348 V353 L354 D355 R356 I357 V358 L359 V360 G363 K364 D365 G366 S367 Q368 D369 K370 F371 R372 M377 I378 R379 K380 L381 L384 G387 E388 C389 S390 P391 D392
N393 P394 D395 A396 V402 L403 L404 K414 E419 Y420 L421 Q422 Q427 V428 R429 M430 D431 I432 N433 R434 G435 M436 A437 I438 N439 F440 K441 D442 K443 R444 Y445 M446 S447 R448 V449 L450 M451 R452 V453 N454 L470 V471 S472 Q473 S474 G475 L476 D477 L478 Q479 Q480 Y484 E489
K490 F493 Y494 R495 H504 R505 G506 S507 F508 F509 A510 Q511 L512 K513 T514 T515 T516 K519 E523 S524 W525 C529 H532 D535 G536 S537 P538 C539 G540 L541 L542 R550 I551 S556 D557 V558 S559 R560 I561 P562 S563 Y566 P572 A573 S574 H575 T576 F577 A578
A579 G580 P581 S582 L583 C584 C585 I588 D589 G590 K591 I592 I593 G594 W595 V596 S597 H598 E599 Q600 G601 K602 I603 D606 R609 Y610 G615 K616 T617 P618 G619 I622 D623 I626 G627 Y628 V629 S632 T633 R634 G635 Q636 Y637 L640 Y641 L642 S647 R648 M649 L650 R651
R654 P657 L658 D659 K660 E661 D662 I663 Y671 M672 P678 Q679 E680 I681 Q682 N683 V689 E690 I696 L697 S698 I699 L700 P705 D708 F709 W710 Q711 S712 P713 Y717 Q718 C719 Q720 M721 P729 G730 V731 A732 L733 C734 H735 R736 S737 D738 L741 Q745 T746
G747 V752 N755 L756 Y757 D758 D759 M762 D763 N764 F765 P766 V773 Y781 D782 M783 D784 D785 I788 I789 M803 Y804 D810 L811 A812 L813 N814 R815 N816 R817 G818 D819 P820 I821 T822 Q823 H824 F825 G826 F827 G828 N829 D830 E831 W832 P833 K834 E835 W836 L837 E838
D841 E842 D843 G844 Y851 E854 G855 D856 P857 I858 C859 A860 Y861 F862 D863 D864 T865 L866 N867 K868 T869 K870 I871 K872 T873 Y874 H875 E878 Y881 I882 E883 E884 V885 N886 G889 D890 E891 S892 N893 K894 F895 Q896 E897 L898 Q899 T900 V901 S902 R906 I907 R908 R909 K916
R920 H921 K924 C927 S928 R929 I934 S939 E940 T941 G942 I943 D946 I947 N950 P951 H952 P955 S956 R957 M958 E965 L974 H975 G976 I977 A978 Q979 D980 S981 F986 N987 E988 D989 D990 T991 P992 A993 D994 Y995 F996 G997 E998 A1003 G1004 Y1005 N1010
E1011 P1012 M1013 G1016 E1020 R1023 A1024 D1025 I1026 Y1033 D1042 K1043 V1046 R1047 S1048 T1049 P1059 V1060 K1061 G1062 R1063 K1064 R1065 H1066 R1070 V1071 G1072 E1073 M1074 E1075 R1076 L1079 H1082 G1083 T1084 S1085 F1086 L1087 L1088 Q1089 L1093 Y1098 V1103 C1104 R1105 E1106 C1107

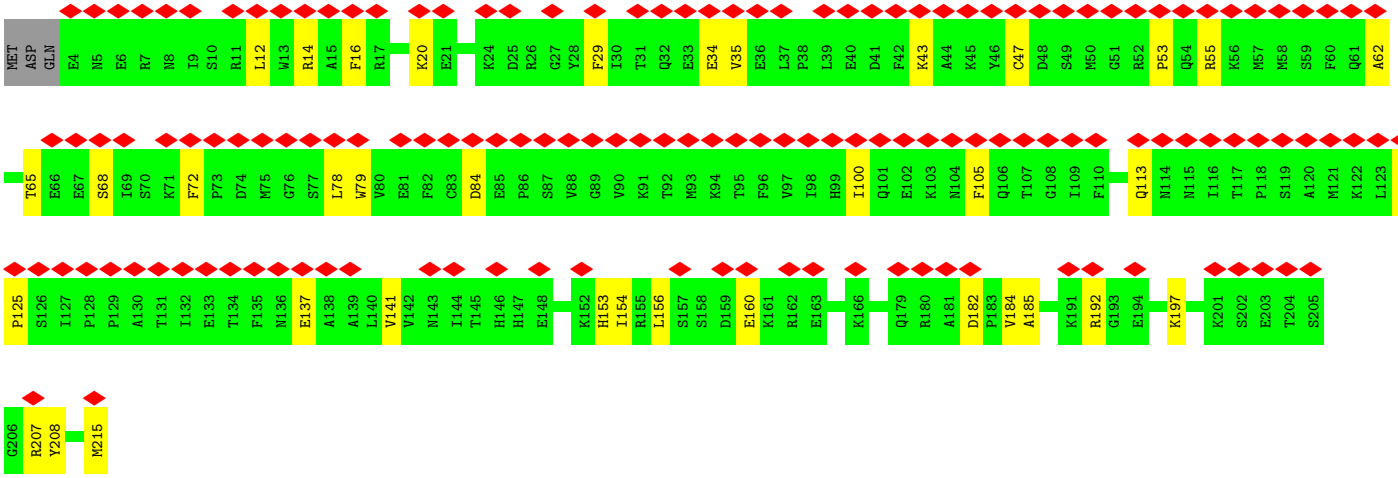


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



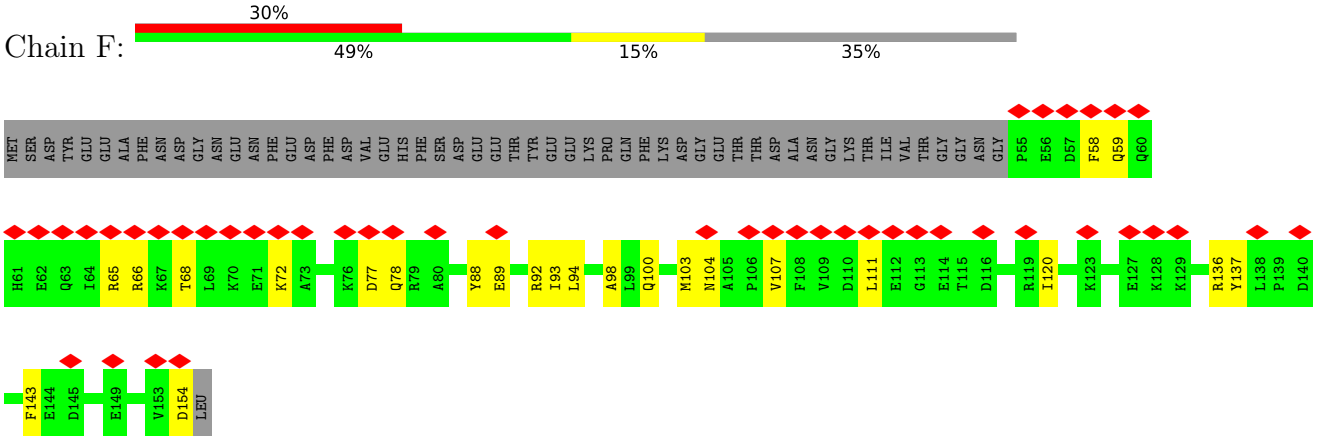
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1





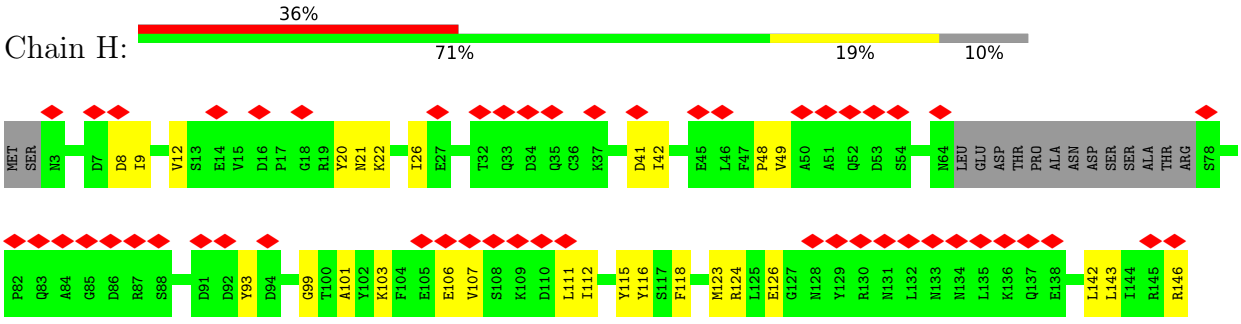
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



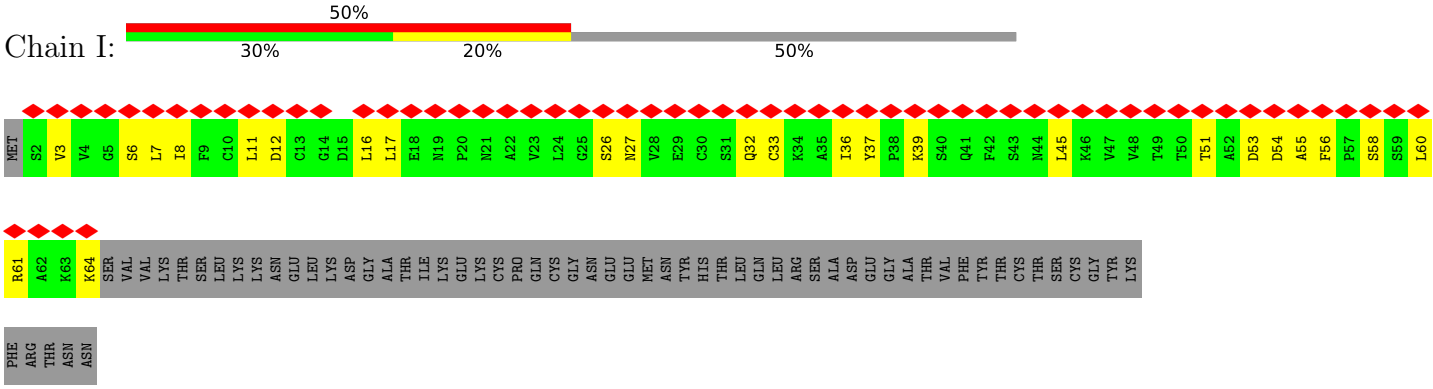
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



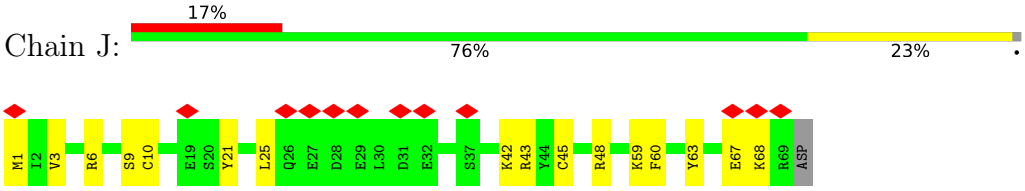
• Molecule 7: DNA-directed RNA polymerase I subunit RPA12

Chain I:



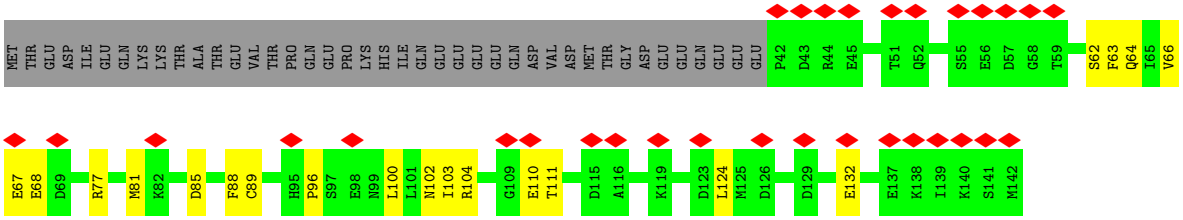
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



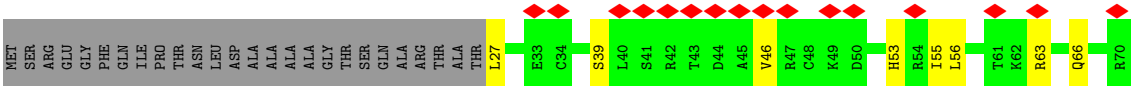
• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



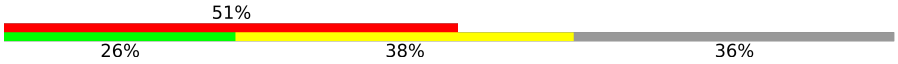
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

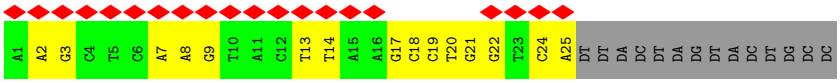
Chain L:



• Molecule 11: template DNA

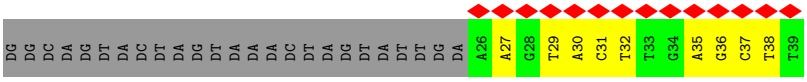
Chain T:





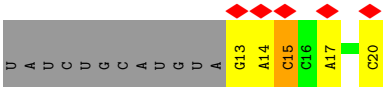
• Molecule 12: non-template DNA

Chain U:



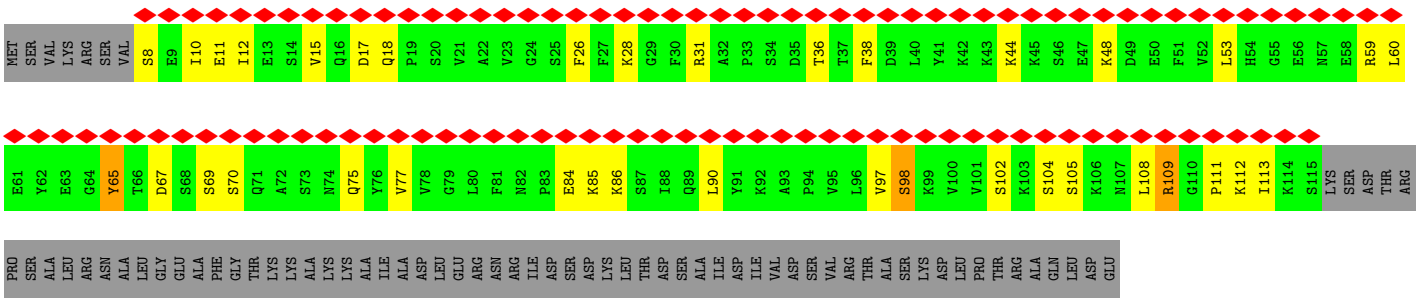
• Molecule 13: RNA

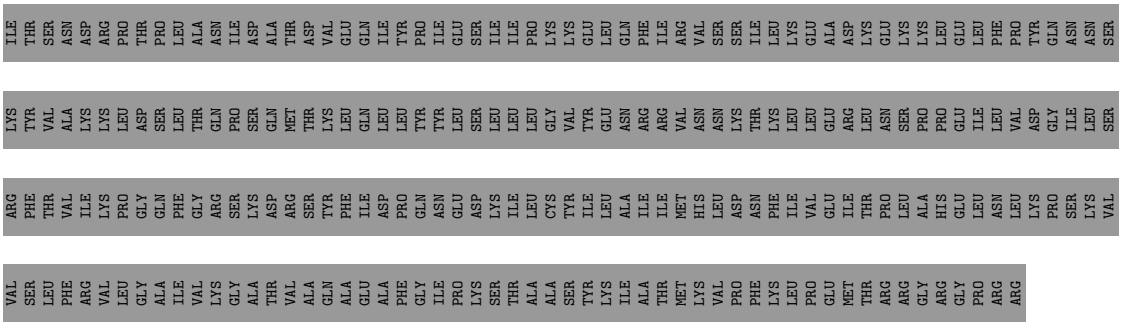
Chain R:



• Molecule 14: DNA-directed RNA polymerase I subunit RPA49

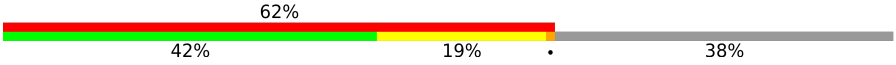
Chain M:

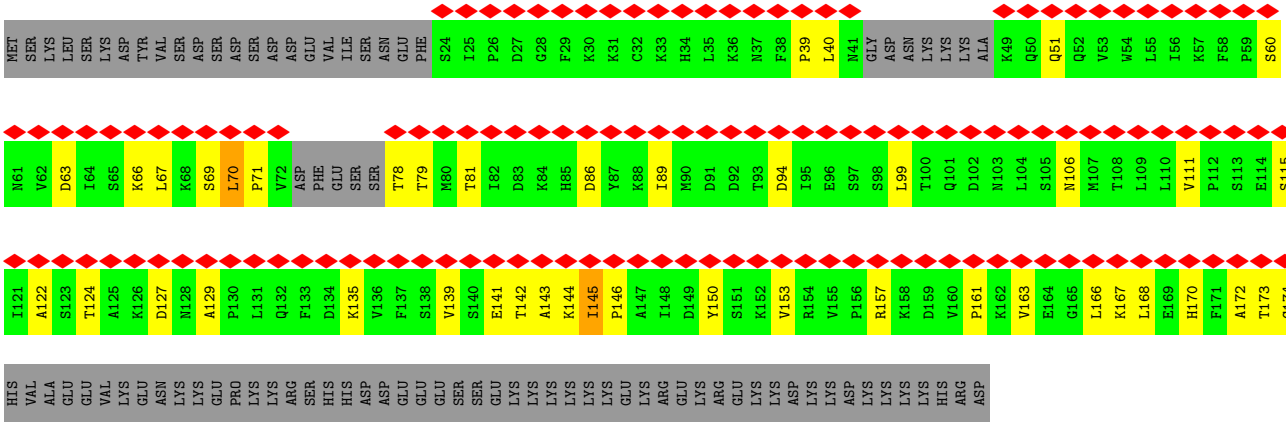




• Molecule 15: DNA-directed RNA polymerase I subunit RPA34

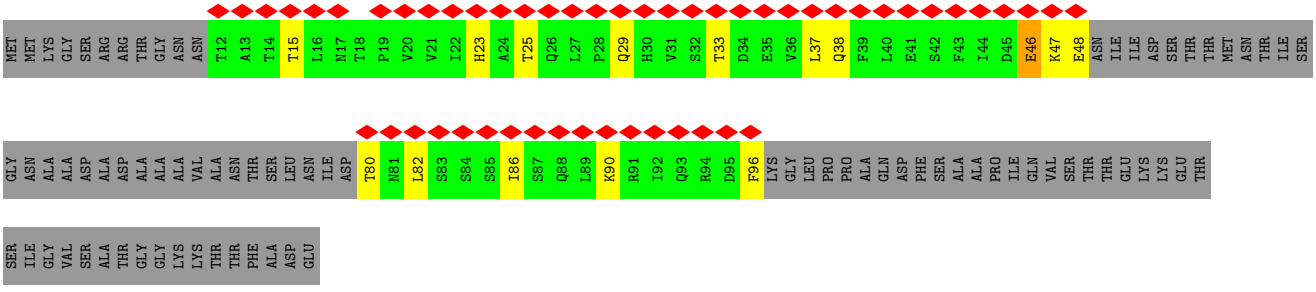
Chain N:





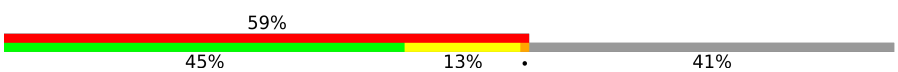
• Molecule 16: DNA-directed RNA polymerase I subunit RPA14

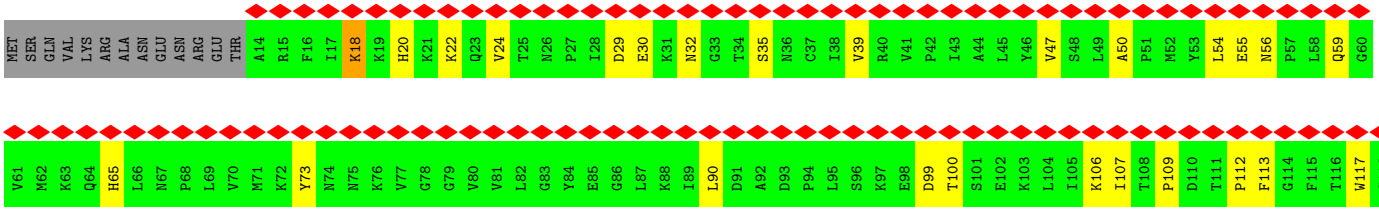
Chain D:

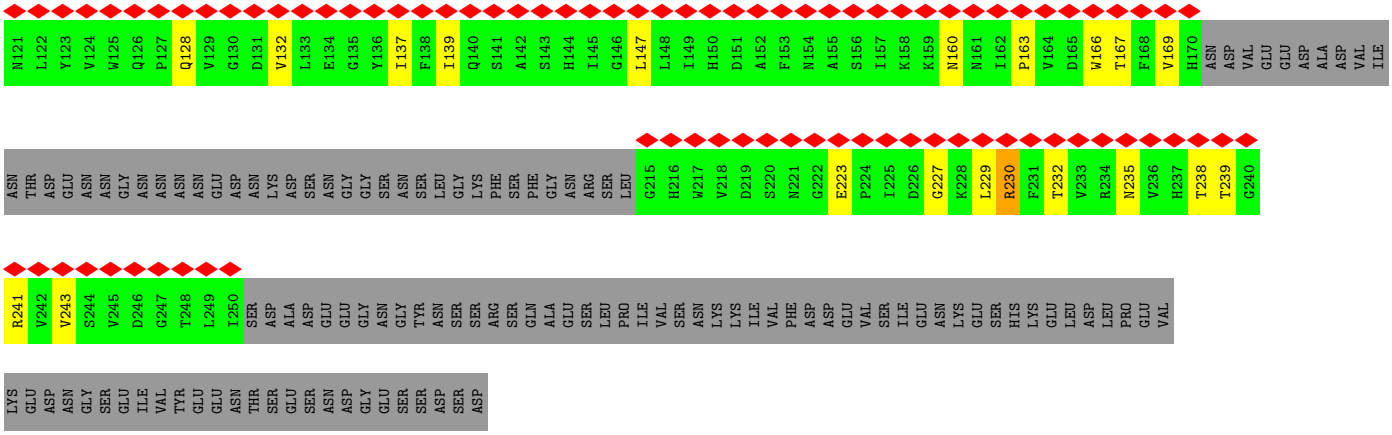


• Molecule 17: DNA-directed RNA polymerase I subunit RPA43

Chain G:






N121 L122 Y123 V124 W125 Q126 P127 Q128 V129 G130 D131 V132 L133 E134 G135 Y136 I137 F138 I139 Q140 S141 A142 S143 H144 I145 G146 L147 L148 I149 H150 D151 A152 F153 N154 A155 S156 I157 K158 K159 N160 N161 I162 P163 V164 D165 W166 T167 F168 V169 H170 ASN ASP VAL GLU GLU ASP ALA ASP VAL ILE
ASN THR ASP GLU ASN ASN GLY ASN ASN ASN ASN GLU ASP ASN LYS ASP SER ASN GLY GLY SER ASN SER LEU GLY LYS PHE SER PHE GLY ASN ARG SER LEU G215 H216 W217 V218 D219 S220 N221 G222 E223 P224 T225 D226 G227 K228 L229 R230 F231 T232 V233 R234 N235 V236 H237 T238 T239 G240
R241 V242 V243 S244 V245 D246 G247 T248 L249 I250 SER ASP ALA ASP GLU GLU GLY ASN GLY TYR ASN SER SER ARG SER GLN ALA GLU SER LEU PRO ILE VAL SER ASN LYS LYS ILE VAL PHE ASP ASP GLU VAL SER ILE GLU ASN LYS GLU SER HIS LYS GLU LEU ASP LEU PRO GLU VAL
LYS GLU ASP ASN GLY SER GLU ILE VAL TYR GLU GLU ASN THR SER GLU SER ASN ASP GLY GLU SER SER ASP SER ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, MG

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	0.35	0/11738	0.50	0/15851
2	B	0.37	0/9557	0.52	0/12918
3	C	0.35	0/2475	0.49	0/3354
4	E	0.31	0/1771	0.46	0/2383
5	F	0.32	0/838	0.46	0/1129
6	H	0.34	0/1070	0.49	0/1449
7	I	0.26	0/472	0.48	0/639
8	J	0.37	0/578	0.47	0/775
9	K	0.35	0/804	0.51	0/1083
10	L	0.33	0/354	0.50	0/468
11	T	0.60	0/571	0.87	0/879
12	U	0.58	0/319	0.97	0/491
13	R	0.48	0/193	1.08	0/299
14	M	0.41	0/872	0.55	0/1170
15	N	0.42	0/1172	0.57	1/1580 (0.1%)
16	D	0.38	0/436	0.51	0/591
17	G	0.37	0/1564	0.66	3/2127 (0.1%)
All	All	0.37	0/34784	0.54	4/47186 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	241	ARG	NE-CZ-NH1	11.89	126.25	120.30
17	G	241	ARG	NE-CZ-NH2	-11.70	114.45	120.30
17	G	241	ARG	CD-NE-CZ	6.04	132.05	123.60
15	N	145	ILE	C-N-CD	5.04	138.99	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1048	SER	Peptide
2	B	1061	LYS	Peptide
2	B	319	HIS	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	11526	0	11614	326	0
2	B	9350	0	9240	362	0
3	C	2423	0	2412	68	0
4	E	1735	0	1764	25	0
5	F	823	0	840	46	0
6	H	1052	0	1021	20	0
7	I	466	0	466	29	0
8	J	569	0	585	21	0
9	K	793	0	790	17	0
10	L	352	0	376	7	0
11	T	509	0	283	16	0
12	U	285	0	161	9	0
13	R	173	0	89	6	0
14	M	856	0	852	97	0
15	N	1151	0	1169	99	0
16	D	431	0	428	11	0
17	G	1526	0	1540	90	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1	0	0	0	0
19	A	1	0	0	0	0
20	B	5	0	0	2	0
All	All	34032	0	33630	918	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 14.

All (918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLN:NE2	14:M:112:LYS:HA	1.22	1.49
1:A:1661:PRO:CD	17:G:55:GLU:CA	1.86	1.44
2:B:987:ASN:ND2	15:N:157:ARG:CD	1.85	1.39
2:B:328:GLN:CD	14:M:112:LYS:HA	1.39	1.39
3:C:301:ASN:ND2	15:N:173:THR:HB	1.37	1.37
1:A:1661:PRO:CD	17:G:55:GLU:HA	1.11	1.36
2:B:977:ILE:CD1	15:N:163:VAL:HG21	1.59	1.29
1:A:1182:GLY:O	1:A:1649:VAL:CB	1.81	1.29
2:B:575:HIS:HB3	14:M:97:VAL:CG2	1.63	1.27
1:A:460:LEU:HD23	1:A:466:LEU:CB	1.65	1.25
1:A:1661:PRO:HD3	17:G:55:GLU:CA	1.52	1.25
2:B:977:ILE:CD1	15:N:163:VAL:CG2	2.14	1.24
5:F:100:GLN:HE21	17:G:112:PRO:CB	1.48	1.24
1:A:1660:VAL:CA	17:G:54:LEU:O	1.86	1.24
2:B:987:ASN:ND2	15:N:157:ARG:NE	1.86	1.23
2:B:321:GLN:OE1	14:M:108:LEU:HD13	1.33	1.22
2:B:577:PHE:CZ	15:N:106:ASN:OD1	1.91	1.22
2:B:328:GLN:OE1	14:M:111:PRO:O	1.57	1.21
1:A:460:LEU:CD2	1:A:466:LEU:HB3	1.71	1.20
2:B:987:ASN:HD21	15:N:157:ARG:NE	1.37	1.20
1:A:1656:VAL:O	17:G:107:ILE:HB	1.38	1.19
3:C:271:ARG:NH1	15:N:175:TYR:OH	1.75	1.19
1:A:1658:ALA:N	17:G:107:ILE:HG12	1.56	1.19
2:B:572:PRO:HG3	14:M:70:SER:CB	1.73	1.19
1:A:1658:ALA:N	17:G:107:ILE:CG1	2.06	1.18
1:A:1659:LYS:O	17:G:54:LEU:HD22	1.45	1.17
2:B:346:ASP:OD2	14:M:113:ILE:HD13	1.45	1.17
3:C:301:ASN:HD22	15:N:173:THR:CB	1.56	1.16
2:B:346:ASP:OD2	14:M:113:ILE:CD1	1.93	1.16
2:B:977:ILE:HD13	15:N:163:VAL:CG2	1.70	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:VAL:HA	17:G:54:LEU:O	0.97	1.14
2:B:584:CYS:HB3	2:B:596:VAL:O	1.43	1.14
5:F:100:GLN:NE2	17:G:112:PRO:HB2	1.59	1.14
5:F:58:PHE:CZ	16:D:23:HIS:HB2	1.78	1.14
2:B:987:ASN:ND2	15:N:157:ARG:HD3	1.56	1.13
1:A:1657:LEU:HG	17:G:106:LYS:HA	1.15	1.12
5:F:58:PHE:CE2	16:D:23:HIS:HB2	1.84	1.12
2:B:346:ASP:CG	14:M:113:ILE:CD1	2.17	1.12
2:B:328:GLN:NE2	14:M:112:LYS:CA	2.13	1.09
3:C:53:ASN:ND2	15:N:174:GLY:HA3	1.66	1.09
1:A:1658:ALA:HB3	17:G:107:ILE:HD11	1.33	1.08
1:A:1660:VAL:HG12	17:G:54:LEU:HA	1.35	1.08
1:A:457:LYS:NZ	1:A:461:GLU:OE2	1.85	1.08
2:B:572:PRO:CG	14:M:70:SER:CB	2.32	1.08
2:B:577:PHE:CE2	14:M:28:LYS:HE2	1.88	1.08
3:C:53:ASN:HD22	15:N:174:GLY:HA3	1.05	1.07
2:B:575:HIS:CB	14:M:97:VAL:HG22	1.85	1.07
2:B:346:ASP:OD2	14:M:113:ILE:CG1	2.02	1.07
2:B:572:PRO:CG	14:M:70:SER:HB2	1.83	1.07
1:A:460:LEU:HD21	1:A:466:LEU:HD23	1.30	1.07
2:B:328:GLN:CD	14:M:112:LYS:CA	2.25	1.04
2:B:975:HIS:CG	15:N:166:LEU:HD22	1.92	1.02
2:B:987:ASN:HD22	15:N:157:ARG:CD	1.53	1.02
5:F:58:PHE:CE2	16:D:23:HIS:CB	2.42	1.02
1:A:1651:THR:O	5:F:92:ARG:NH1	1.91	1.01
2:B:21:ARG:HH12	2:B:763:ASP:HB3	1.25	1.01
1:A:460:LEU:HD23	1:A:466:LEU:HB3	1.01	1.00
1:A:1651:THR:OG1	2:B:1085:SER:HB2	1.62	1.00
3:C:301:ASN:HD22	15:N:173:THR:HB	0.86	1.00
1:A:1658:ALA:H	17:G:107:ILE:CG1	1.68	1.00
1:A:1661:PRO:HD2	17:G:55:GLU:CA	1.89	1.00
2:B:572:PRO:HB3	14:M:70:SER:HB3	1.44	0.99
2:B:1003:ALA:C	15:N:168:LEU:HD23	1.83	0.98
7:I:32:GLN:O	14:M:104:SER:OG	1.80	0.98
7:I:12:ASP:HB3	14:M:60:LEU:HD21	1.45	0.97
1:A:1658:ALA:H	17:G:107:ILE:HG12	1.15	0.97
2:B:346:ASP:CB	14:M:113:ILE:HG12	1.94	0.97
2:B:572:PRO:HG3	14:M:70:SER:HB2	0.99	0.97
2:B:566:TYR:CE2	14:M:69:SER:O	2.18	0.96
2:B:346:ASP:HB2	14:M:113:ILE:HG12	1.43	0.96
2:B:575:HIS:HB3	14:M:97:VAL:HG22	0.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLN:OE1	14:M:111:PRO:C	2.03	0.95
2:B:987:ASN:HD22	15:N:157:ARG:HD3	1.15	0.95
5:F:100:GLN:HE21	17:G:112:PRO:HB2	0.77	0.94
5:F:100:GLN:NE2	17:G:112:PRO:CB	2.21	0.93
1:A:466:LEU:HD21	2:B:1184:TYR:HE2	1.31	0.92
2:B:577:PHE:HE2	14:M:28:LYS:HE2	1.20	0.92
2:B:346:ASP:OD2	14:M:113:ILE:HG12	1.68	0.92
2:B:683:ASN:ND2	15:N:150:TYR:CE2	2.38	0.92
2:B:1107:CYS:HB3	2:B:1131:CYS:SG	2.09	0.91
1:A:466:LEU:HD21	2:B:1184:TYR:CE2	2.06	0.90
2:B:977:ILE:CD1	15:N:163:VAL:HG22	1.98	0.90
3:C:301:ASN:CG	15:N:173:THR:HB	1.91	0.90
3:C:301:ASN:ND2	15:N:173:THR:CB	2.22	0.90
2:B:328:GLN:HB3	14:M:112:LYS:O	1.72	0.89
2:B:683:ASN:ND2	15:N:150:TYR:CZ	2.40	0.89
3:C:271:ARG:CZ	15:N:175:TYR:OH	2.20	0.88
3:C:228:ARG:NH1	15:N:172:ALA:HB1	1.88	0.88
2:B:328:GLN:NE2	14:M:112:LYS:CG	2.37	0.88
3:C:53:ASN:HD22	15:N:174:GLY:CA	1.87	0.88
1:A:1657:LEU:HA	17:G:107:ILE:HG12	1.55	0.87
2:B:321:GLN:OE1	14:M:108:LEU:CD1	2.20	0.87
2:B:346:ASP:CG	14:M:113:ILE:HG12	1.93	0.87
15:N:143:ALA:C	15:N:144:LYS:HD2	1.94	0.87
3:C:228:ARG:NH1	15:N:172:ALA:CB	2.38	0.87
1:A:1658:ALA:HB3	17:G:107:ILE:CD1	2.05	0.86
1:A:1657:LEU:CG	17:G:106:LYS:HA	2.03	0.85
2:B:346:ASP:CG	14:M:113:ILE:CG1	2.44	0.85
2:B:977:ILE:HD12	15:N:163:VAL:CG1	2.06	0.84
1:A:1658:ALA:CB	17:G:107:ILE:HD11	2.07	0.84
2:B:941:THR:OG1	15:N:170:HIS:NE2	2.09	0.84
2:B:346:ASP:CG	14:M:113:ILE:HD11	1.95	0.84
1:A:1657:LEU:CA	17:G:107:ILE:HG12	2.07	0.84
2:B:1047:ARG:HH21	2:B:1049:THR:HG21	1.42	0.83
5:F:66:ARG:NH1	17:G:90:LEU:HB3	1.93	0.83
1:A:1661:PRO:CD	17:G:54:LEU:O	2.26	0.83
3:C:301:ASN:CB	15:N:173:THR:HB	2.09	0.82
2:B:574:SER:OG	14:M:67:ASP:CG	2.17	0.82
2:B:368:GLN:HG3	2:B:372:ARG:HH12	1.44	0.82
2:B:134:ARG:HD3	2:B:160:GLY:HA3	1.62	0.82
1:A:1657:LEU:C	17:G:107:ILE:HG12	1.99	0.82
7:I:12:ASP:OD1	14:M:60:LEU:HD11	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:26:SER:HA	7:I:39:LYS:HE2	1.62	0.82
1:A:1658:ALA:N	17:G:107:ILE:HG13	1.95	0.81
2:B:977:ILE:HD13	15:N:163:VAL:HG21	0.85	0.81
7:I:33:CYS:HA	14:M:104:SER:HB3	1.61	0.81
2:B:572:PRO:CB	14:M:70:SER:HB3	2.09	0.81
1:A:466:LEU:CD2	2:B:1184:TYR:HE2	1.94	0.81
1:A:372:LYS:HA	1:A:376:GLU:O	1.81	0.80
1:A:1256:LYS:NZ	1:A:1305:GLU:O	2.15	0.80
1:A:1661:PRO:HD2	17:G:54:LEU:O	1.82	0.80
2:B:975:HIS:CE1	15:N:166:LEU:HB3	2.17	0.80
1:A:440:SER:H	1:A:458:GLN:HE22	1.28	0.79
5:F:92:ARG:NH2	17:G:109:PRO:HA	1.98	0.79
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	1.65	0.79
1:A:1659:LYS:O	17:G:54:LEU:CD2	2.28	0.78
17:G:22:LYS:HD3	17:G:128:GLN:HG2	1.65	0.78
1:A:460:LEU:CD2	1:A:466:LEU:CB	2.45	0.78
2:B:977:ILE:HD12	15:N:163:VAL:CG2	2.11	0.78
2:B:1003:ALA:O	15:N:168:LEU:HD23	1.83	0.77
2:B:328:GLN:HE22	14:M:112:LYS:HA	1.43	0.77
2:B:566:TYR:HE2	14:M:69:SER:O	1.66	0.77
1:A:1660:VAL:HG12	17:G:54:LEU:CA	2.15	0.76
1:A:460:LEU:CD2	1:A:466:LEU:HD23	2.13	0.75
5:F:100:GLN:CG	17:G:112:PRO:HB3	2.17	0.75
2:B:322:ASN:HB2	14:M:108:LEU:O	1.87	0.75
7:I:12:ASP:OD2	14:M:59:ARG:NH1	2.18	0.75
1:A:1652:GLY:C	1:A:1654:PHE:H	1.90	0.74
1:A:509:GLU:OE2	1:A:584:ARG:NH2	2.20	0.74
1:A:489:ASN:ND2	2:B:781:TYR:OH	2.19	0.74
2:B:328:GLN:NE2	14:M:109:ARG:HH21	1.85	0.74
7:I:6:SER:H	7:I:45:LEU:HD21	1.51	0.74
2:B:987:ASN:HD22	15:N:157:ARG:HD2	1.50	0.74
2:B:1155:ASP:HB2	17:G:235:ASN:HD21	1.52	0.74
1:A:30:LYS:NZ	1:A:51:ASP:OD2	2.21	0.74
1:A:1652:GLY:O	1:A:1654:PHE:N	2.20	0.74
1:A:1657:LEU:HG	17:G:106:LYS:CA	2.07	0.74
2:B:328:GLN:NE2	14:M:109:ARG:NH2	2.36	0.74
1:A:666:VAL:HG23	1:A:667:ARG:HG3	1.69	0.73
2:B:346:ASP:OD2	14:M:113:ILE:CG2	2.36	0.73
1:A:95:TYR:OH	1:A:99:ARG:NH1	2.22	0.73
2:B:346:ASP:HB2	14:M:113:ILE:CG1	2.19	0.73
1:A:707:THR:HG22	1:A:709:ARG:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:ASP:CG	14:M:113:ILE:HD13	1.99	0.73
1:A:460:LEU:HD21	1:A:466:LEU:CD2	2.15	0.73
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.70	0.72
1:A:886:ASN:OD1	1:A:955:ARG:NH1	2.16	0.72
5:F:58:PHE:CE2	16:D:23:HIS:HB3	2.25	0.72
2:B:838:GLU:O	10:L:63:ARG:NH2	2.23	0.72
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.70	0.72
1:A:1647:ASN:ND2	2:B:1085:SER:OG	2.22	0.72
2:B:328:GLN:NE2	14:M:112:LYS:HG2	2.04	0.72
1:A:700:ILE:O	1:A:706:HIS:ND1	2.23	0.71
2:B:1012:PRO:HG3	3:C:277:ARG:HH12	1.55	0.71
1:A:1658:ALA:H	17:G:107:ILE:CD1	2.02	0.71
2:B:857:PRO:HB3	2:B:871:ILE:HD11	1.72	0.71
8:J:42:LYS:NZ	15:N:176:ASP:HB3	2.04	0.71
2:B:338:PHE:HE2	2:B:353:VAL:HG22	1.55	0.71
1:A:690:GLU:HB3	9:K:77:ARG:HH22	1.56	0.71
15:N:144:LYS:HD2	15:N:144:LYS:N	2.06	0.71
2:B:328:GLN:CB	14:M:112:LYS:O	2.38	0.71
2:B:987:ASN:ND2	15:N:157:ARG:CZ	2.53	0.70
3:C:271:ARG:NH1	15:N:175:TYR:CZ	2.59	0.70
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.73	0.70
1:A:645:ALA:O	1:A:649:ASN:ND2	2.21	0.70
1:A:753:ASN:ND2	1:A:780:ILE:O	2.25	0.69
2:B:328:GLN:HE21	14:M:112:LYS:HG2	1.56	0.69
2:B:815:ARG:NH2	2:B:819:ASP:O	2.25	0.69
5:F:58:PHE:CD2	16:D:23:HIS:HB3	2.27	0.69
13:R:13:G:H2'	13:R:14:A:C8	2.27	0.69
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.21	0.69
2:B:582:SER:O	2:B:598:HIS:NE2	2.25	0.69
3:C:301:ASN:HD22	15:N:173:THR:CG2	2.06	0.69
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.26	0.69
9:K:85:ASP:OD2	9:K:111:THR:OG1	2.11	0.69
2:B:293:ILE:HD12	2:B:302:LEU:HB3	1.73	0.69
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.75	0.69
2:B:228:SER:O	2:B:254:ASN:ND2	2.25	0.68
14:M:38:PHE:HB3	14:M:53:LEU:HD11	1.73	0.68
5:F:66:ARG:HH12	17:G:90:LEU:HB3	1.58	0.68
1:A:594:THR:HG23	1:A:599:SER:HB2	1.75	0.68
1:A:956:ARG:HE	1:A:979:GLY:HA3	1.57	0.68
2:B:320:LEU:HD13	2:B:326:VAL:HG22	1.76	0.68
1:A:90:PHE:O	1:A:92:ASN:N	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:7:DA:H2'	11:T:8:DA:C8	2.28	0.68
1:A:1658:ALA:CB	17:G:107:ILE:CD1	2.68	0.68
2:B:574:SER:HG	14:M:67:ASP:CG	1.96	0.67
2:B:1004:GLY:HA3	15:N:168:LEU:CD2	2.24	0.67
1:A:99:ARG:HH21	1:A:228:LEU:HD13	1.57	0.67
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.59	0.67
5:F:100:GLN:CG	17:G:112:PRO:CB	2.72	0.67
2:B:941:THR:HG1	15:N:170:HIS:HE2	1.25	0.67
3:C:271:ARG:HG2	15:N:175:TYR:OH	1.94	0.67
2:B:773:VAL:HG21	2:B:1033:TYR:HE2	1.59	0.67
1:A:656:GLN:HE22	2:B:1082:HIS:CE1	2.14	0.66
2:B:572:PRO:CG	14:M:70:SER:HB3	2.21	0.66
2:B:939:SER:HA	2:B:1013:MET:HG2	1.77	0.66
2:B:783:MET:HA	2:B:950:ASN:HD22	1.60	0.66
1:A:1224:GLU:O	1:A:1228:THR:OG1	2.12	0.66
1:A:89:LEU:HD11	2:B:1192:MET:HB3	1.78	0.65
6:H:106:GLU:HG2	6:H:112:ILE:HG12	1.77	0.65
11:T:22:DG:H1	13:R:15:C:H42	1.43	0.65
1:A:109:ARG:NH1	1:A:230:ARG:O	2.26	0.65
2:B:324:THR:HG21	14:M:109:ARG:NE	2.10	0.65
2:B:785:ASP:OD1	2:B:957:ARG:NH2	2.29	0.65
5:F:100:GLN:HG3	17:G:112:PRO:HB3	1.78	0.65
2:B:322:ASN:CB	14:M:108:LEU:O	2.45	0.65
7:I:27:ASN:HA	7:I:37:TYR:O	1.96	0.65
1:A:672:ASP:OD2	2:B:950:ASN:ND2	2.29	0.65
2:B:184:LYS:HD2	2:B:735:HIS:CD2	2.32	0.65
1:A:683:LYS:NZ	6:H:41:ASP:OD2	2.26	0.65
1:A:1145:GLU:O	1:A:1149:ASP:HB2	1.96	0.65
1:A:1661:PRO:HD2	17:G:54:LEU:C	2.16	0.65
2:B:328:GLN:CG	14:M:112:LYS:O	2.45	0.65
5:F:92:ARG:NH2	17:G:109:PRO:CA	2.60	0.65
2:B:975:HIS:ND1	15:N:166:LEU:HD22	2.12	0.65
2:B:209:GLN:NE2	2:B:215:MET:SD	2.70	0.65
2:B:328:GLN:HE22	14:M:112:LYS:HG3	1.62	0.65
1:A:460:LEU:HD23	1:A:466:LEU:HB2	1.70	0.64
2:B:112:GLY:HA3	2:B:893:ASN:HB3	1.79	0.64
2:B:328:GLN:OE1	14:M:112:LYS:HA	1.92	0.64
1:A:706:HIS:CE1	1:A:815:ARG:HH22	2.14	0.64
2:B:891:GLU:HG2	2:B:892:SER:H	1.62	0.64
2:B:977:ILE:HD12	15:N:163:VAL:HG11	1.78	0.64
3:C:228:ARG:CZ	15:N:172:ALA:HB1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:3:DG:N2	12:U:38:DT:O2	2.32	0.63
3:C:32:ASN:OD1	3:C:33:VAL:N	2.32	0.63
3:C:229:LEU:HB2	3:C:293:ARG:HD2	1.79	0.63
5:F:92:ARG:HH22	17:G:109:PRO:HB3	1.64	0.63
3:C:103:LEU:HD22	8:J:6:ARG:HD2	1.80	0.63
2:B:328:GLN:OE1	14:M:112:LYS:CA	2.47	0.63
2:B:480:GLN:OE1	2:B:507:SER:N	2.28	0.63
2:B:987:ASN:HD21	15:N:157:ARG:HE	1.40	0.63
2:B:332:ASP:HB2	14:M:113:ILE:HG23	1.81	0.63
7:I:12:ASP:CG	14:M:60:LEU:HD11	2.19	0.63
13:R:13:G:H2'	13:R:14:A:H8	1.64	0.63
1:A:1600:ARG:NH2	1:A:1620:GLN:OE1	2.31	0.63
2:B:74:PHE:HE1	2:B:94:LYS:HG3	1.62	0.63
1:A:462:LYS:O	1:A:463:LYS:C	2.38	0.62
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.63	0.62
2:B:17:ARG:NH1	2:B:758:ASP:OD2	2.31	0.62
2:B:977:ILE:HD11	15:N:163:VAL:HG22	1.80	0.62
7:I:3:VAL:HG22	7:I:8:ILE:HG12	1.80	0.62
2:B:218:ILE:HD12	2:B:391:PRO:HG3	1.81	0.62
2:B:577:PHE:HE2	14:M:28:LYS:CE	2.04	0.62
2:B:328:GLN:HE22	14:M:109:ARG:NH2	1.97	0.62
2:B:379:ARG:HH21	2:B:581:PRO:HD2	1.63	0.62
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.32	0.62
1:A:1104:TYR:HB3	1:A:1120:TYR:OH	2.00	0.62
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.81	0.62
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.65	0.62
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.81	0.62
2:B:577:PHE:HZ	15:N:106:ASN:OD1	1.70	0.62
1:A:551:VAL:HA	1:A:554:ARG:HH21	1.63	0.62
1:A:1008:ASP:HA	1:A:1011:VAL:HG12	1.81	0.62
1:A:1310:LYS:NZ	1:A:1464:ASP:O	2.23	0.62
2:B:577:PHE:CZ	14:M:28:LYS:HE2	2.34	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.82	0.61
1:A:94:LEU:O	1:A:98:LEU:HB2	2.00	0.61
2:B:979:GLN:HE21	2:B:996:PHE:HE1	1.47	0.61
7:I:32:GLN:CA	14:M:105:SER:HB3	2.28	0.61
2:B:1089:GLN:HE21	2:B:1093:LEU:HD23	1.66	0.61
2:B:328:GLN:HE22	14:M:112:LYS:CG	2.11	0.61
1:A:263:ASN:OD1	1:A:267:LYS:NZ	2.25	0.61
2:B:606:ASP:OD2	15:N:145:ILE:HD11	1.99	0.61
2:B:773:VAL:HG21	2:B:1033:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:PHE:CE1	15:N:106:ASN:OD1	2.53	0.61
7:I:32:GLN:HA	14:M:105:SER:HB3	1.83	0.61
7:I:12:ASP:CB	14:M:60:LEU:HD21	2.26	0.61
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.28	0.60
2:B:532:HIS:ND1	20:B:1301:SO4:O4	2.31	0.60
2:B:987:ASN:HD21	15:N:157:ARG:CD	1.76	0.60
4:E:14:ARG:HD2	4:E:141:VAL:HG13	1.83	0.60
1:A:90:PHE:C	1:A:92:ASN:H	2.04	0.60
1:A:1651:THR:HG1	2:B:1085:SER:HB2	1.62	0.60
8:J:42:LYS:HZ3	15:N:176:ASP:HB3	1.67	0.60
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.35	0.60
3:C:228:ARG:HH12	15:N:172:ALA:CB	2.13	0.60
1:A:560:GLN:O	1:A:575:LYS:NZ	2.32	0.60
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.34	0.60
5:F:66:ARG:CZ	17:G:90:LEU:HB3	2.32	0.60
1:A:1655:ASP:OD2	5:F:137:TYR:OH	2.12	0.59
1:A:67:LEU:HD11	2:B:1115:GLN:HG3	1.84	0.59
1:A:526:GLY:HA3	1:A:554:ARG:HH11	1.66	0.59
1:A:546:LEU:HD22	1:A:554:ARG:HG2	1.84	0.59
2:B:99:VAL:HG23	2:B:421:LEU:HD11	1.84	0.59
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.37	0.59
1:A:1631:ARG:HH22	2:B:1199:ASN:HD22	1.50	0.59
2:B:37:LEU:HD12	2:B:759:ASP:HB3	1.85	0.59
2:B:1103:VAL:HG22	2:B:1110:ILE:HG22	1.85	0.59
5:F:66:ARG:NH1	17:G:90:LEU:CB	2.63	0.59
4:E:20:LYS:HB3	4:E:35:VAL:HG22	1.85	0.59
2:B:307:GLU:HB2	7:I:7:LEU:HD11	1.84	0.58
17:G:30:GLU:HA	17:G:32:ASN:N	2.18	0.58
11:T:8:DA:N6	12:U:32:DT:H3	2.01	0.58
1:A:102:CYS:CB	1:A:105:CYS:SG	2.84	0.58
15:N:69:SER:OG	15:N:70:LEU:N	2.37	0.58
15:N:89:ILE:HG12	15:N:139:VAL:HG22	1.85	0.58
1:A:1261:VAL:HG12	1:A:1498:ILE:HD12	1.84	0.58
4:E:68:SER:O	4:E:72:PHE:N	2.24	0.58
7:I:33:CYS:HA	14:M:102:SER:OG	2.03	0.58
9:K:62:SER:HA	9:K:103:ILE:O	2.03	0.58
6:H:48:PRO:O	6:H:146:ARG:NH2	2.28	0.58
4:E:16:PHE:CZ	4:E:20:LYS:HE3	2.39	0.58
1:A:1194:GLY:O	1:A:1197:SER:OG	2.16	0.58
9:K:64:GLN:HE21	9:K:100:LEU:HD13	1.69	0.58
2:B:331:GLY:HA3	2:B:346:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.28	0.57
1:A:1657:LEU:HA	17:G:107:ILE:CG1	2.32	0.57
1:A:1657:LEU:C	17:G:107:ILE:CG1	2.65	0.57
5:F:92:ARG:HH21	17:G:109:PRO:HA	1.66	0.57
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.27	0.57
2:B:651:ARG:NH1	2:B:690:GLU:OE2	2.36	0.57
7:I:8:ILE:HG22	7:I:17:LEU:HD12	1.86	0.57
1:A:117:ARG:HB3	1:A:185:ARG:NH1	2.19	0.57
1:A:879:LEU:HD21	1:A:974:THR:HG22	1.86	0.57
1:A:1229:ALA:HB2	1:A:1597:ALA:HB2	1.87	0.57
2:B:741:LEU:HD22	2:B:804:TYR:HD2	1.70	0.57
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.32	0.57
1:A:1619:CYS:HA	1:A:1622:LEU:HB3	1.86	0.57
2:B:657:PRO:HB3	15:N:146:PRO:HD2	1.86	0.57
1:A:440:SER:OG	1:A:458:GLN:NE2	2.38	0.57
2:B:572:PRO:CB	14:M:70:SER:CB	2.75	0.57
1:A:706:HIS:HE1	1:A:815:ARG:HH12	1.51	0.56
2:B:181:VAL:HG13	8:J:63:TYR:HE1	1.69	0.56
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.39	0.56
2:B:1085:SER:O	2:B:1088:LEU:N	2.38	0.56
1:A:385:LEU:HD23	1:A:437:PHE:HA	1.86	0.56
2:B:584:CYS:CB	2:B:596:VAL:O	2.36	0.56
3:C:227:TYR:HA	3:C:299:ILE:O	2.05	0.56
1:A:53:ALA:O	1:A:64:THR:OG1	2.17	0.56
1:A:1182:GLY:C	1:A:1649:VAL:CB	2.71	0.56
1:A:1660:VAL:CB	17:G:54:LEU:O	2.53	0.56
1:A:1661:PRO:HD3	17:G:55:GLU:HA	0.56	0.56
17:G:56:ASN:HB3	17:G:59:GLN:HB3	1.87	0.56
2:B:322:ASN:OD1	2:B:323:ARG:N	2.38	0.56
2:B:977:ILE:HD12	15:N:163:VAL:HG13	1.86	0.56
14:M:10:ILE:HB	15:N:70:LEU:HB3	1.86	0.56
1:A:1319:ASN:O	1:A:1323:HIS:ND1	2.33	0.56
7:I:32:GLN:O	14:M:104:SER:CB	2.53	0.56
1:A:507:TYR:OH	1:A:641:GLU:OE2	2.24	0.56
1:A:975:ASP:OD1	1:A:976:ALA:N	2.39	0.56
2:B:556:SER:OG	2:B:623:ASP:OD2	2.22	0.56
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.06	0.56
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.41	0.56
2:B:1079:LEU:HB2	2:B:1088:LEU:HD12	1.87	0.56
14:M:15:VAL:HG22	14:M:90:LEU:HB2	1.88	0.56
2:B:784:ASP:OD1	2:B:785:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:LEU:HG	1:A:1155:PHE:HE2	1.71	0.55
2:B:346:ASP:CB	14:M:113:ILE:CG1	2.73	0.55
6:H:8:ASP:OD1	6:H:9:ILE:N	2.36	0.55
1:A:697:TYR:CE1	9:K:104:ARG:HG3	2.41	0.55
2:B:328:GLN:NE2	14:M:112:LYS:CB	2.69	0.55
2:B:335:ARG:HH21	2:B:342:PRO:HA	1.70	0.55
1:A:37:VAL:HG12	1:A:38:LEU:HG	1.89	0.55
1:A:468:ARG:HD3	2:B:1073:GLU:OE2	2.06	0.55
1:A:925:MET:SD	2:B:955:PRO:HB3	2.46	0.55
1:A:1661:PRO:HD2	17:G:55:GLU:N	2.21	0.55
1:A:435:ASN:O	1:A:439:ASP:N	2.40	0.55
1:A:589:MET:HG3	1:A:603:HIS:HD2	1.70	0.55
1:A:964:LYS:NZ	2:B:672:MET:O	2.39	0.55
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.88	0.55
2:B:729:PRO:HG2	2:B:733:LEU:HD21	1.88	0.55
5:F:89:GLU:OE2	5:F:136:ARG:NE	2.40	0.55
1:A:1329:ILE:HG12	1:A:1488:ILE:HD13	1.87	0.55
1:A:462:LYS:O	1:A:465:GLY:N	2.39	0.55
1:A:1227:MET:O	1:A:1599:ASN:ND2	2.39	0.55
7:I:11:LEU:N	7:I:37:TYR:OH	2.37	0.55
9:K:77:ARG:O	9:K:81:MET:HG2	2.08	0.54
1:A:1121:ASP:OD2	4:E:197:LYS:NZ	2.39	0.54
1:A:1661:PRO:CD	17:G:55:GLU:N	2.66	0.54
6:H:21:ASN:OD1	6:H:22:LYS:N	2.40	0.54
1:A:799:GLU:OE2	1:A:1173:LYS:NZ	2.41	0.54
2:B:1089:GLN:O	2:B:1093:LEU:N	2.39	0.54
11:T:17:DG:H2'	11:T:18:DC:O4'	2.08	0.54
3:C:237:GLN:HE21	3:C:288:LYS:HE3	1.72	0.54
15:N:145:ILE:CG2	15:N:146:PRO:CD	2.86	0.54
1:A:1612:LYS:HB3	1:A:1621:PHE:CD2	2.43	0.54
3:C:301:ASN:CB	15:N:173:THR:CB	2.82	0.54
1:A:1588:MET:O	1:A:1591:ARG:NH1	2.39	0.54
2:B:731:VAL:HG21	8:J:59:LYS:HE3	1.88	0.54
17:G:229:LEU:HD12	17:G:230:ARG:H	1.72	0.54
3:C:136:LEU:HB2	3:C:167:LEU:HD23	1.90	0.54
5:F:65:ARG:HH12	17:G:117:TRP:HZ2	1.53	0.54
1:A:597:LYS:HE3	1:A:660:PRO:HG2	1.88	0.54
1:A:1657:LEU:HA	17:G:107:ILE:H	1.73	0.54
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.41	0.54
3:C:84:TYR:HE1	10:L:66:GLN:HG3	1.72	0.53
2:B:494:TYR:HB3	2:B:700:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:12:ILE:HD12	15:N:67:LEU:HB2	1.90	0.53
2:B:314:LYS:HZ1	7:I:16:LEU:H	1.55	0.53
2:B:574:SER:OG	14:M:67:ASP:CB	2.56	0.53
17:G:132:VAL:HG22	17:G:232:THR:HG22	1.90	0.53
1:A:885:ASP:OD1	1:A:886:ASN:N	2.42	0.53
1:A:1179:ILE:HD11	1:A:1183:GLU:OE2	2.07	0.53
2:B:662:ASP:OD1	2:B:663:ILE:N	2.35	0.53
2:B:745:GLN:NE2	8:J:1:MET:SD	2.81	0.53
3:C:75:VAL:HB	3:C:221:PRO:HG3	1.90	0.53
1:A:83:VAL:HG21	1:A:427:PHE:CE1	2.44	0.53
3:C:271:ARG:HG2	15:N:175:TYR:HH	1.73	0.53
4:E:156:LEU:HD22	4:E:160:GLU:HG2	1.89	0.53
5:F:66:ARG:CZ	17:G:90:LEU:HD13	2.39	0.53
5:F:100:GLN:HG2	17:G:112:PRO:CB	2.37	0.53
8:J:9:SER:HB2	8:J:45:CYS:SG	2.48	0.53
1:A:632:GLU:OE2	2:B:1043:LYS:HE2	2.09	0.53
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.90	0.53
3:C:132:ILE:HG23	3:C:169:PHE:HE1	1.73	0.53
1:A:973:GLU:HG3	1:A:975:ASP:H	1.74	0.53
1:A:1240:LEU:HB2	1:A:1519:LEU:HB2	1.91	0.53
1:A:1661:PRO:CD	17:G:54:LEU:C	2.77	0.53
3:C:100:ARG:NH2	8:J:3:VAL:O	2.31	0.53
8:J:10:CYS:SG	8:J:45:CYS:CB	2.90	0.53
1:A:403:LEU:HD13	1:A:419:ILE:HG21	1.91	0.53
5:F:100:GLN:NE2	17:G:112:PRO:HB3	2.20	0.52
14:M:11:GLU:N	14:M:86:LYS:O	2.36	0.52
14:M:75:GLN:HB2	15:N:60:SER:HA	1.91	0.52
17:G:20:HIS:O	17:G:20:HIS:ND1	2.38	0.52
17:G:30:GLU:HA	17:G:32:ASN:H	1.74	0.52
1:A:468:ARG:HH22	1:A:1021:ARG:NH1	2.07	0.52
1:A:1242:ILE:HD11	1:A:1517:ARG:NE	2.24	0.52
7:I:60:LEU:O	7:I:64:LYS:N	2.38	0.52
1:A:1074:TYR:O	1:A:1078:LYS:NZ	2.30	0.52
2:B:752:VAL:HG12	2:B:981:SER:HB3	1.92	0.52
11:T:7:DA:H2'	11:T:8:DA:H8	1.74	0.52
1:A:256:LEU:HD13	1:A:264:ASN:HD21	1.74	0.52
2:B:826:GLY:H	2:B:861:TYR:HA	1.75	0.52
2:B:986:PHE:HA	15:N:157:ARG:HH12	1.74	0.52
2:B:1013:MET:SD	2:B:1026:ILE:HD11	2.50	0.52
1:A:683:LYS:HD2	6:H:20:TYR:CE2	2.44	0.52
1:A:1485:MET:O	1:A:1488:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:ASN:ND2	14:M:108:LEU:O	2.35	0.52
2:B:346:ASP:OD2	14:M:113:ILE:HG21	2.07	0.52
2:B:599:GLU:OE1	2:B:599:GLU:N	2.38	0.52
2:B:832:TRP:CZ3	2:B:834:LYS:HA	2.44	0.52
5:F:66:ARG:HH12	17:G:90:LEU:CB	2.20	0.52
8:J:10:CYS:SG	8:J:45:CYS:HB3	2.49	0.52
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.90	0.52
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.91	0.52
15:N:144:LYS:N	15:N:144:LYS:CD	2.73	0.52
1:A:1613:MET:HE1	1:A:1622:LEU:HD13	1.92	0.52
1:A:863:ASN:O	1:A:878:ARG:NH1	2.42	0.52
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.91	0.52
1:A:1641:ILE:HD13	2:B:1076:ARG:HD2	1.92	0.51
1:A:1660:VAL:HG13	17:G:54:LEU:HD23	1.91	0.51
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.45	0.51
16:D:48:GLU:OE2	16:D:90:LYS:NZ	2.43	0.51
1:A:771:PHE:HE2	1:A:793:ILE:HD13	1.76	0.51
2:B:851:TYR:HD1	2:B:881:TYR:CE1	2.28	0.51
3:C:136:LEU:O	3:C:203:SER:HA	2.10	0.51
1:A:108:PHE:CE2	1:A:331:GLU:HG3	2.45	0.51
6:H:124:ARG:NH1	6:H:126:GLU:OE1	2.43	0.51
1:A:257:ASN:O	1:A:261:ILE:HD12	2.10	0.51
1:A:418:VAL:HG13	1:A:419:ILE:HG13	1.93	0.51
1:A:461:GLU:O	1:A:461:GLU:HG2	2.09	0.51
1:A:495:ILE:HG22	1:A:604:LYS:O	2.10	0.51
3:C:57:ILE:HG22	3:C:58:ASN:ND2	2.25	0.51
1:A:952:LEU:HD22	1:A:1004:GLU:HG3	1.93	0.51
2:B:987:ASN:ND2	15:N:157:ARG:HD2	2.04	0.51
2:B:1154:ASP:OD1	2:B:1155:ASP:N	2.44	0.51
3:C:138:VAL:HG11	3:C:162:VAL:HG22	1.91	0.51
3:C:170:GLU:OE2	3:C:205:LYS:NZ	2.43	0.51
2:B:878:GLU:OE2	2:B:909:ARG:NH1	2.43	0.51
2:B:314:LYS:O	2:B:315:LYS:HG2	2.11	0.51
2:B:574:SER:OG	14:M:67:ASP:HB2	2.11	0.51
3:C:123:ASP:OD1	3:C:124:GLU:N	2.44	0.51
1:A:706:HIS:CE1	1:A:815:ARG:HH12	2.28	0.50
1:A:1559:ARG:HD2	1:A:1587:ASP:OD1	2.11	0.50
1:A:1652:GLY:C	1:A:1654:PHE:N	2.58	0.50
2:B:1157:GLN:NE2	2:B:1169:GLY:HA2	2.25	0.50
11:T:2:DA:H2"	11:T:3:DG:C8	2.45	0.50
1:A:1645:LYS:HG3	1:A:1646:LEU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:LEU:O	2:B:370:LYS:HE2	2.11	0.50
2:B:946:ASP:OD1	8:J:9:SER:OG	2.26	0.50
2:B:1004:GLY:CA	15:N:168:LEU:CD2	2.88	0.50
3:C:71:MET:HG2	3:C:317:SER:OG	2.10	0.50
7:I:27:ASN:HB3	7:I:36:ILE:HG23	1.94	0.50
1:A:94:LEU:O	1:A:98:LEU:CB	2.59	0.50
2:B:346:ASP:OD1	14:M:113:ILE:HD11	2.11	0.50
2:B:584:CYS:SG	2:B:585:CYS:N	2.84	0.50
2:B:705:PRO:HA	2:B:981:SER:HB2	1.93	0.50
2:B:941:THR:CB	15:N:170:HIS:HE2	2.24	0.50
6:H:103:LYS:HD2	6:H:115:TYR:CD2	2.47	0.50
15:N:145:ILE:HG23	15:N:146:PRO:CD	2.41	0.50
1:A:1003:ARG:HH22	2:B:540:GLY:HA2	1.77	0.50
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.94	0.50
2:B:1042:ASP:O	2:B:1063:ARG:NH1	2.44	0.50
7:I:33:CYS:HB3	14:M:102:SER:HB2	1.93	0.50
15:N:63:ASP:OD2	15:N:66:LYS:NZ	2.35	0.50
1:A:672:ASP:OD1	2:B:952:HIS:ND1	2.45	0.50
1:A:771:PHE:CE2	1:A:793:ILE:HD13	2.47	0.49
4:E:53:PRO:HG2	4:E:55:ARG:HH12	1.77	0.49
11:T:8:DA:H61	12:U:32:DT:H3	1.58	0.49
1:A:621:THR:HG21	1:A:628:PHE:HE2	1.77	0.49
2:B:929:ARG:NH1	9:K:96:PRO:HB2	2.27	0.49
3:C:228:ARG:NH1	15:N:172:ALA:HB2	2.24	0.49
1:A:4:SER:HB3	1:A:576:LYS:NZ	2.27	0.49
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.95	0.49
4:E:20:LYS:NZ	4:E:34:GLU:O	2.30	0.49
12:U:31:DC:H1'	12:U:32:DT:H5'	1.95	0.49
1:A:1187:ILE:O	1:A:1190:SER:N	2.44	0.49
1:A:1511:GLU:O	1:A:1513:GLU:N	2.44	0.49
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.78	0.49
2:B:924:LYS:NZ	13:R:20:C:OP1	2.43	0.49
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.76	0.49
17:G:47:VAL:HB	17:G:65:HIS:CD2	2.47	0.49
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.46	0.49
1:A:1101:THR:HA	1:A:1120:TYR:CE1	2.48	0.49
2:B:609:ARG:HH21	2:B:626:ILE:HB	1.76	0.49
4:E:55:ARG:HB2	4:E:84:ASP:HB2	1.93	0.49
1:A:460:LEU:CD2	1:A:466:LEU:CG	2.90	0.49
1:A:800:VAL:O	1:A:1079:LYS:HD2	2.13	0.49
1:A:1018:TYR:HE1	1:A:1021:ARG:HH21	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLN:OE1	14:M:112:LYS:N	2.45	0.49
2:B:803:MET:HE3	2:B:907:ILE:HD13	1.94	0.49
1:A:852:ASP:OD2	1:A:855:ARG:NH2	2.44	0.49
1:A:1658:ALA:HB2	17:G:107:ILE:HG13	1.94	0.49
2:B:941:THR:CG2	15:N:170:HIS:HE2	2.26	0.49
2:B:995:TYR:OH	15:N:161:PRO:O	2.25	0.49
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.95	0.49
5:F:107:VAL:HG11	5:F:111:LEU:HD21	1.95	0.49
12:U:29:DT:H2'	12:U:30:DA:C8	2.47	0.49
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.94	0.49
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.47	0.49
2:B:709:PHE:CZ	2:B:992:PRO:HG2	2.48	0.49
3:C:246:ARG:NH1	3:C:284:GLU:OE1	2.46	0.49
5:F:94:LEU:O	5:F:98:ALA:HB2	2.13	0.49
1:A:1240:LEU:HD22	1:A:1536:ILE:HD12	1.94	0.48
2:B:21:ARG:O	2:B:24:ARG:N	2.45	0.48
2:B:353:VAL:HG13	2:B:357:ILE:HD12	1.95	0.48
6:H:93:TYR:CE1	6:H:143:LEU:HD23	2.48	0.48
1:A:1223:ARG:HG3	1:A:1227:MET:HG3	1.95	0.48
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.95	0.48
1:A:1533:GLU:HA	1:A:1536:ILE:O	2.13	0.48
2:B:733:LEU:HD22	2:B:741:LEU:HD11	1.96	0.48
2:B:1047:ARG:NH2	2:B:1049:THR:HG21	2.21	0.48
2:B:1157:GLN:HE21	2:B:1169:GLY:HA2	1.78	0.48
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.49	0.48
14:M:65:TYR:CE1	14:M:97:VAL:HB	2.48	0.48
1:A:492:THR:HB	1:A:667:ARG:HH21	1.77	0.48
1:A:1660:VAL:CG1	17:G:54:LEU:HA	2.24	0.48
2:B:292:ILE:HG22	2:B:293:ILE:HD13	1.94	0.48
2:B:783:MET:HA	2:B:950:ASN:ND2	2.26	0.48
3:C:91:VAL:HG21	8:J:60:PHE:HB3	1.96	0.48
3:C:259:ASP:OD2	3:C:262:SER:OG	2.25	0.48
15:N:111:VAL:HG13	15:N:122:ALA:HB2	1.95	0.48
1:A:1660:VAL:CG1	17:G:54:LEU:HD23	2.44	0.48
2:B:380:LYS:HE3	2:B:637:TYR:HB3	1.95	0.48
2:B:789:ILE:HD12	2:B:927:CYS:SG	2.53	0.48
2:B:916:LYS:HD3	2:B:924:LYS:HD2	1.96	0.48
15:N:145:ILE:HG22	15:N:146:PRO:N	2.27	0.48
1:A:102:CYS:HB3	1:A:105:CYS:SG	2.51	0.48
1:A:1015:ARG:HG3	1:A:1219:ILE:HG21	1.94	0.48
1:A:1025:LYS:HG2	1:A:1615:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:ILE:HA	2:B:438:ILE:HD11	1.95	0.48
1:A:834:ARG:HH21	2:B:993:ALA:HB1	1.76	0.48
1:A:1118:VAL:HG21	4:E:154:ILE:HD11	1.95	0.48
2:B:648:ARG:HH12	2:B:650:LEU:HD21	1.78	0.48
2:B:1098:TYR:CE1	2:B:1177:ALA:HB1	2.49	0.48
2:B:841:ASP:OD1	2:B:842:GLU:N	2.41	0.48
1:A:460:LEU:CD2	1:A:466:LEU:CD2	2.84	0.48
1:A:508:PRO:HB3	1:A:578:TYR:CE1	2.49	0.48
1:A:656:GLN:NE2	2:B:1082:HIS:CE1	2.80	0.48
1:A:1658:ALA:CB	17:G:107:ILE:HG13	2.44	0.48
2:B:975:HIS:CB	15:N:166:LEU:HD22	2.43	0.48
2:B:1079:LEU:HD13	2:B:1088:LEU:HA	1.94	0.48
5:F:111:LEU:HD22	5:F:120:ILE:HD13	1.96	0.48
10:L:27:LEU:HA	10:L:39:SER:HB2	1.96	0.48
11:T:13:DT:H2"	11:T:14:DT:H5'	1.95	0.48
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.41	0.48
2:B:628:TYR:HB2	2:B:640:LEU:HD13	1.96	0.48
2:B:1003:ALA:O	15:N:168:LEU:CD2	2.58	0.48
5:F:89:GLU:O	5:F:93:ILE:HG12	2.14	0.48
1:A:139:ILE:O	1:A:140:THR:OG1	2.28	0.47
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.49	0.47
3:C:301:ASN:HB3	15:N:173:THR:HB	1.90	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.94	0.47
6:H:26:ILE:HD11	6:H:49:VAL:HG11	1.96	0.47
1:A:113:VAL:HG21	1:A:178:LEU:HD22	1.95	0.47
1:A:208:PHE:CE2	1:A:1607:THR:HG23	2.48	0.47
1:A:332:GLN:O	1:A:336:GLN:HB2	2.14	0.47
1:A:1546:VAL:HG11	1:A:1595:TYR:CE1	2.49	0.47
1:A:96:ILE:HG23	1:A:228:LEU:HD11	1.96	0.47
1:A:1486:VAL:HG11	7:I:51:THR:HG21	1.95	0.47
2:B:651:ARG:HH12	2:B:690:GLU:CD	2.16	0.47
2:B:1063:ARG:HG2	11:T:20:DT:H5"	1.96	0.47
1:A:751:SER:OG	1:A:752:LYS:N	2.48	0.47
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	1.95	0.47
1:A:1482:LYS:HZ3	2:B:304:ASP:HA	1.79	0.47
1:A:1221:ARG:O	1:A:1224:GLU:N	2.47	0.47
2:B:396:ALA:HB1	2:B:523:GLU:OE1	2.13	0.47
17:G:137:ILE:HG13	17:G:227:GLY:O	2.13	0.47
1:A:589:MET:CG	1:A:603:HIS:HD2	2.27	0.47
1:A:739:VAL:HG21	1:A:809:VAL:HG22	1.96	0.47
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:21:DG:H2'	11:T:22:DG:C8	2.49	0.47
1:A:511:VAL:HG22	1:A:519:LEU:HD12	1.97	0.47
1:A:590:ASN:OD1	1:A:591:ARG:N	2.48	0.47
1:A:1080:TYR:OH	1:A:1173:LYS:HG3	2.15	0.47
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.46	0.47
1:A:1658:ALA:H	17:G:107:ILE:HD11	1.78	0.47
2:B:445:TYR:O	2:B:449:VAL:HG23	2.15	0.47
2:B:535:ASP:HA	2:B:539:CYS:HB2	1.95	0.47
2:B:581:PRO:HB3	2:B:637:TYR:CE1	2.50	0.47
2:B:1046:VAL:HG22	2:B:1047:ARG:HG3	1.97	0.47
12:U:29:DT:H2'	12:U:30:DA:H8	1.78	0.47
7:I:53:ASP:HB3	7:I:61:ARG:NH2	2.29	0.47
16:D:46:GLU:OE1	16:D:47:LYS:HE2	2.15	0.47
1:A:793:ILE:HG23	1:A:794:VAL:H	1.80	0.47
2:B:343:ASP:OD1	2:B:344:GLN:N	2.48	0.47
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.79	0.47
1:A:95:TYR:CD1	1:A:245:LYS:HD3	2.50	0.47
2:B:566:TYR:CE2	14:M:69:SER:C	2.86	0.47
2:B:588:ILE:HG12	2:B:642:LEU:HD12	1.97	0.47
11:T:19:DC:H2'	11:T:20:DT:C6	2.50	0.47
2:B:21:ARG:HH22	2:B:763:ASP:CG	2.19	0.46
1:A:1443:GLN:NE2	1:A:1462:PHE:O	2.48	0.46
2:B:654:ARG:HB3	2:B:689:VAL:HG13	1.98	0.46
2:B:832:TRP:HZ3	2:B:834:LYS:HA	1.79	0.46
5:F:137:TYR:HD1	5:F:143:PHE:HB3	1.80	0.46
11:T:13:DT:H3	12:U:27:DA:H61	1.63	0.46
1:A:1631:ARG:HH12	2:B:1199:ASN:HD21	1.64	0.46
15:N:145:ILE:CG2	15:N:146:PRO:HD2	2.45	0.46
16:D:33:THR:HG23	16:D:96:PHE:HD1	1.80	0.46
1:A:1105:ARG:NH2	4:E:207:ARG:HD3	2.31	0.46
1:A:1200:MET:SD	1:A:1219:ILE:HG13	2.55	0.46
1:A:1490:GLU:HB3	1:A:1494:ARG:HH12	1.81	0.46
2:B:577:PHE:CZ	14:M:28:LYS:HG3	2.51	0.46
5:F:103:MET:O	5:F:104:ASN:HB2	2.16	0.46
2:B:200:GLU:OE2	2:B:736:ARG:NH1	2.45	0.46
5:F:92:ARG:HH22	17:G:109:PRO:CB	2.27	0.46
1:A:669:LEU:HD12	1:A:786:TYR:CD2	2.50	0.46
1:A:697:TYR:HB2	9:K:88:PHE:HZ	1.80	0.46
2:B:99:VAL:HG12	2:B:100:GLU:H	1.81	0.46
1:A:1097:TYR:O	1:A:1101:THR:HG23	2.16	0.46
1:A:1658:ALA:N	17:G:107:ILE:CD1	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG13	8:J:63:TYR:CE1	2.51	0.46
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.51	0.46
14:M:65:TYR:HE1	14:M:97:VAL:HB	1.81	0.46
1:A:1545:ASP:OD1	1:A:1546:VAL:N	2.48	0.46
5:F:77:ASP:OD1	5:F:78:GLN:HG3	2.15	0.46
5:F:92:ARG:HH21	17:G:109:PRO:CA	2.27	0.46
1:A:527:PRO:O	1:A:580:HIS:HE1	1.99	0.46
2:B:99:VAL:HG12	2:B:100:GLU:N	2.31	0.46
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.49	0.46
5:F:100:GLN:CD	17:G:112:PRO:CB	2.83	0.46
1:A:686:PHE:CE1	1:A:727:THR:HG22	2.51	0.45
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.97	0.45
1:A:862:THR:O	1:A:878:ARG:NH1	2.48	0.45
1:A:1229:ALA:HA	1:A:1595:TYR:CE2	2.52	0.45
2:B:629:VAL:HG22	2:B:671:TYR:CE2	2.51	0.45
1:A:328:PHE:CE1	1:A:335:LEU:HD13	2.52	0.45
2:B:1061:LYS:HG2	2:B:1062:GLY:H	1.81	0.45
14:M:26:PHE:CE1	14:M:98:SER:HB2	2.51	0.45
1:A:530:TRP:HZ2	1:A:582:LYS:HA	1.81	0.45
1:A:1242:ILE:HD11	1:A:1517:ARG:HE	1.82	0.45
2:B:52:LEU:O	2:B:59:GLY:HA3	2.17	0.45
2:B:747:GLY:HA3	2:B:766:PRO:HB2	1.97	0.45
2:B:941:THR:HG1	15:N:170:HIS:CE1	2.31	0.45
3:C:301:ASN:ND2	15:N:173:THR:CA	2.79	0.45
1:A:1631:ARG:HH22	2:B:1199:ASN:ND2	2.12	0.45
5:F:65:ARG:NH1	17:G:117:TRP:CZ2	2.84	0.45
1:A:1097:TYR:O	1:A:1100:LYS:HB3	2.17	0.45
1:A:1575:ILE:HG22	1:A:1576:SER:N	2.31	0.45
2:B:219:ARG:HG2	2:B:221:SER:H	1.81	0.45
1:A:10:GLU:OE2	1:A:1645:LYS:HD3	2.17	0.45
1:A:1661:PRO:HG3	17:G:55:GLU:HB3	1.99	0.45
3:C:228:ARG:HH12	15:N:172:ALA:HB2	1.80	0.45
6:H:101:ALA:HA	6:H:116:TYR:HA	1.98	0.45
2:B:379:ARG:NH2	2:B:581:PRO:HD2	2.31	0.45
2:B:731:VAL:HG13	8:J:60:PHE:HD1	1.81	0.45
2:B:1048:SER:O	2:B:1048:SER:OG	2.25	0.45
11:T:24:DC:H2"	11:T:25:DA:N7	2.32	0.45
1:A:719:ILE:O	1:A:724:PRO:HA	2.17	0.45
1:A:1658:ALA:CB	17:G:107:ILE:CG1	2.95	0.45
2:B:577:PHE:CE2	14:M:28:LYS:CE	2.79	0.45
1:A:836:THR:O	1:A:840:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:LEU:HD21	1:A:1588:MET:HG2	1.98	0.45
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.82	0.45
2:B:341:SER:OG	2:B:343:ASP:OD1	2.24	0.45
2:B:402:VAL:O	2:B:647:SER:HB3	2.17	0.45
2:B:1004:GLY:N	15:N:168:LEU:HD23	2.29	0.45
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.50	0.45
9:K:85:ASP:OD1	9:K:110:GLU:HB2	2.17	0.45
1:A:32:ILE:HD12	1:A:48:GLY:O	2.18	0.44
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.50	0.44
2:B:229:TYR:HE1	2:B:253:LEU:HD11	1.82	0.44
2:B:368:GLN:HG3	2:B:372:ARG:NH1	2.21	0.44
3:C:84:TYR:CE1	10:L:66:GLN:HG3	2.52	0.44
4:E:100:ILE:HA	4:E:105:PHE:HD2	1.82	0.44
1:A:408:LYS:HA	1:A:411:VAL:HB	1.99	0.44
1:A:609:PRO:HB2	1:A:610:ASN:HD22	1.83	0.44
2:B:369:ASP:OD2	2:B:591:LYS:HE2	2.17	0.44
2:B:610:TYR:HE1	2:B:658:LEU:HD13	1.82	0.44
1:A:427:PHE:HA	1:A:430:ILE:HG22	1.99	0.44
1:A:1101:THR:HG22	1:A:1120:TYR:CE1	2.53	0.44
1:A:1264:SER:HB2	7:I:56:PHE:CD1	2.52	0.44
15:N:142:THR:HG23	15:N:144:LYS:HE2	1.99	0.44
2:B:21:ARG:NH1	2:B:763:ASP:HB3	2.10	0.44
2:B:559:SER:O	2:B:562:PRO:HD2	2.18	0.44
1:A:1200:MET:HG2	1:A:1573:TYR:CE2	2.52	0.44
2:B:354:LEU:O	2:B:370:LYS:NZ	2.51	0.44
2:B:708:ASP:OD1	2:B:708:ASP:N	2.49	0.44
2:B:886:ASN:HB2	2:B:902:SER:OG	2.18	0.44
8:J:45:CYS:O	8:J:48:ARG:HG2	2.17	0.44
2:B:324:THR:HG23	2:B:347:LEU:HD13	1.99	0.44
6:H:107:VAL:HB	6:H:111:LEU:HD11	2.00	0.44
1:A:457:LYS:O	1:A:461:GLU:HB3	2.16	0.44
2:B:588:ILE:HD12	2:B:593:ILE:HG13	2.00	0.44
2:B:859:CYS:O	2:B:871:ILE:HG13	2.17	0.44
11:T:8:DA:H2"	11:T:9:DG:H8	1.83	0.44
11:T:14:DT:H6	11:T:14:DT:H2'	1.67	0.44
17:G:163:PRO:HG2	17:G:166:TRP:CD1	2.52	0.44
1:A:1254:PHE:CD2	1:A:1255:CYS:HB2	2.52	0.44
1:A:1650:GLY:HA2	5:F:88:TYR:HB3	2.00	0.44
2:B:446:MET:O	2:B:449:VAL:N	2.50	0.44
7:I:26:SER:O	7:I:39:LYS:N	2.50	0.44
15:N:78:THR:HB	15:N:79:THR:H	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:37:LEU:HD23	16:D:37:LEU:HA	1.88	0.44
1:A:196:ALA:HA	1:A:201:ARG:HH21	1.82	0.44
2:B:1048:SER:OG	2:B:1059:PRO:HB3	2.18	0.44
3:C:319:ARG:NH2	9:K:132:GLU:OE2	2.51	0.44
1:A:93:GLN:HG3	1:A:1627:LEU:HD13	1.99	0.43
1:A:1040:ASP:CG	1:A:1041:ALA:H	2.21	0.43
1:A:1322:ILE:HG21	1:A:1457:ILE:HD11	1.99	0.43
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.53	0.43
3:C:325:ALA:HB2	9:K:124:LEU:HD23	1.99	0.43
1:A:36:THR:HG22	1:A:45:VAL:HG21	2.01	0.43
2:B:490:LYS:HE2	2:B:736:ARG:CZ	2.48	0.43
2:B:898:LEU:HD13	10:L:46:VAL:HG21	2.00	0.43
1:A:824:THR:HB	2:B:1023:ARG:NH1	2.34	0.43
1:A:959:VAL:HG12	1:A:960:MET:O	2.19	0.43
1:A:1651:THR:CB	2:B:1085:SER:HB2	2.45	0.43
2:B:67:ASP:HB2	2:B:242:ASP:OD2	2.18	0.43
2:B:505:ARG:HB3	2:B:509:PHE:HD2	1.83	0.43
9:K:64:GLN:NE2	9:K:100:LEU:HD13	2.32	0.43
9:K:81:MET:SD	9:K:89:CYS:HB3	2.59	0.43
1:A:947:LEU:HD22	1:A:982:VAL:HG11	2.01	0.43
1:A:1615:TYR:CD2	1:A:1616:GLU:HG3	2.53	0.43
2:B:324:THR:CG2	14:M:109:ARG:NE	2.79	0.43
2:B:585:CYS:O	2:B:640:LEU:N	2.50	0.43
17:G:106:LYS:HE3	17:G:106:LYS:HB2	1.82	0.43
1:A:409:ASP:OD1	1:A:410:LYS:N	2.51	0.43
2:B:698:SER:HB2	20:B:1301:SO4:O3	2.18	0.43
8:J:67:GLU:HG2	8:J:68:LYS:N	2.34	0.43
1:A:588:LEU:HD21	2:B:1087:LEU:HD21	2.01	0.43
2:B:741:LEU:HD22	2:B:804:TYR:CD2	2.52	0.43
6:H:99:GLY:HA3	6:H:118:PHE:CD1	2.54	0.43
9:K:66:VAL:O	9:K:68:GLU:HG2	2.19	0.43
1:A:509:GLU:CD	1:A:579:ARG:HE	2.22	0.43
1:A:834:ARG:NH2	2:B:993:ALA:HB1	2.33	0.43
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.01	0.43
1:A:1263:LEU:HA	1:A:1498:ILE:HD11	2.00	0.43
2:B:1141:LEU:HD13	17:G:18:LYS:NZ	2.34	0.43
3:C:64:ALA:HB3	3:C:298:PHE:CE2	2.54	0.43
3:C:230:LEU:HD12	3:C:231:PRO:HD2	1.99	0.43
5:F:59:GLN:NE2	16:D:25:THR:HB	2.33	0.43
13:R:14:A:H2'	13:R:15:C:C6	2.53	0.43
5:F:92:ARG:HH22	17:G:109:PRO:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:HIS:CD2	1:A:572:THR:HG23	2.54	0.43
1:A:611:GLU:CB	1:A:615:ARG:HH22	2.32	0.43
1:A:1049:MET:HB2	4:E:208:TYR:HE1	1.84	0.43
2:B:216:ALA:HB1	2:B:384:LEU:HD22	2.00	0.43
2:B:1048:SER:CB	2:B:1059:PRO:HB3	2.49	0.43
1:A:526:GLY:HA3	1:A:554:ARG:NH1	2.34	0.42
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.52	0.42
4:E:29:PHE:HB2	4:E:65:THR:HG22	2.00	0.42
4:E:192:ARG:HG2	4:E:215:MET:O	2.19	0.42
15:N:145:ILE:HG23	15:N:146:PRO:HD2	2.01	0.42
1:A:10:GLU:HG3	1:A:11:ILE:H	1.85	0.42
1:A:1480:THR:HG22	1:A:1481:GLU:N	2.34	0.42
1:A:1645:LYS:HG3	1:A:1646:LEU:N	2.33	0.42
1:A:1649:VAL:O	2:B:1083:GLY:O	2.37	0.42
2:B:139:LEU:HD13	2:B:158:CYS:SG	2.59	0.42
2:B:525:TRP:CZ2	2:B:696:ILE:HG21	2.54	0.42
2:B:1199:ASN:HB3	2:B:1203:LYS:NZ	2.34	0.42
6:H:103:LYS:HB3	6:H:115:TYR:HD2	1.84	0.42
1:A:232:LYS:HE2	1:A:239:PHE:CZ	2.55	0.42
1:A:1243:TRP:HD1	1:A:1535:PHE:O	2.03	0.42
2:B:934:ILE:HD12	3:C:69:ARG:HG3	2.01	0.42
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.54	0.42
7:I:58:SER:OG	7:I:61:ARG:HB2	2.18	0.42
1:A:1105:ARG:HH12	1:A:1138:GLU:HG2	1.84	0.42
2:B:346:ASP:OD1	14:M:113:ILE:CD1	2.62	0.42
17:G:29:ASP:OD1	17:G:30:GLU:N	2.52	0.42
17:G:160:ASN:OD1	17:G:160:ASN:N	2.52	0.42
1:A:518:GLU:O	1:A:521:GLN:N	2.52	0.42
1:A:960:MET:SD	2:B:523:GLU:HG2	2.59	0.42
2:B:27:ASN:HD21	3:C:151:THR:HG23	1.83	0.42
2:B:264:TRP:CH2	2:B:356:ARG:HD3	2.54	0.42
2:B:822:THR:HG22	2:B:823:GLN:HG3	2.01	0.42
2:B:891:GLU:O	2:B:892:SER:OG	2.34	0.42
9:K:66:VAL:HG12	9:K:67:GLU:N	2.35	0.42
12:U:37:DC:H2"	12:U:38:DT:C5	2.54	0.42
14:M:8:SER:O	15:N:71:PRO:HA	2.19	0.42
15:N:94:ASP:HB3	15:N:99:LEU:HG	2.00	0.42
1:A:488:PRO:HD2	2:B:781:TYR:CE2	2.55	0.42
1:A:1647:ASN:HB2	1:A:1648:ASN:H	1.70	0.42
2:B:206:LEU:HD11	2:B:484:TYR:CE1	2.54	0.42
3:C:132:ILE:HG23	3:C:169:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:649:ASN:N	2.53	0.42
1:A:1003:ARG:NH2	2:B:540:GLY:HA2	2.35	0.42
1:A:1226:VAL:HG13	1:A:1598:PHE:CD2	2.54	0.42
2:B:470:LEU:HD22	2:B:484:TYR:HE2	1.84	0.42
2:B:894:LYS:C	2:B:896:GLN:H	2.23	0.42
10:L:53:HIS:CD2	10:L:55:ILE:HG22	2.54	0.42
1:A:67:LEU:HD13	1:A:71:PHE:HB3	2.01	0.42
1:A:411:VAL:HG13	1:A:415:ASP:HB2	2.02	0.42
1:A:1255:CYS:HG	1:A:1507:CYS:HB2	1.84	0.42
2:B:25:PHE:CE1	8:J:59:LYS:HD2	2.55	0.42
2:B:943:ILE:HD11	8:J:43:ARG:HB3	2.01	0.42
1:A:90:PHE:C	1:A:92:ASN:N	2.71	0.42
1:A:459:ALA:O	1:A:466:LEU:HB2	2.20	0.42
2:B:705:PRO:HG3	2:B:920:ARG:NH2	2.35	0.42
2:B:731:VAL:HG13	8:J:60:PHE:CD1	2.54	0.42
3:C:56:LEU:O	3:C:297:HIS:HD2	2.02	0.42
3:C:232:GLN:HB2	3:C:294:VAL:HG23	2.01	0.42
1:A:396:ILE:HD11	1:A:426:ALA:HB1	2.02	0.42
2:B:289:PHE:HD1	2:B:306:LEU:HD22	1.85	0.42
2:B:489:GLU:HG3	2:B:495:ARG:HE	1.85	0.42
2:B:755:ASN:ND2	2:B:980:ASP:OD1	2.53	0.42
2:B:368:GLN:O	2:B:372:ARG:NH1	2.53	0.41
2:B:1003:ALA:HA	15:N:168:LEU:HA	2.02	0.41
1:A:1226:VAL:HG13	1:A:1598:PHE:HD2	1.85	0.41
1:A:1575:ILE:HG22	1:A:1576:SER:H	1.86	0.41
2:B:357:ILE:O	2:B:360:VAL:HG13	2.20	0.41
3:C:244:ALA:O	3:C:247:PHE:HB3	2.19	0.41
9:K:63:PHE:O	9:K:102:ASN:HA	2.21	0.41
16:D:82:LEU:O	16:D:86:ILE:HG23	2.20	0.41
1:A:1299:ASN:HA	1:A:1302:TYR:CE1	2.55	0.41
1:A:1326:GLU:OE2	1:A:1456:PHE:HB2	2.21	0.41
2:B:325:GLN:HG3	14:M:109:ARG:HA	1.47	0.41
2:B:781:TYR:OH	2:B:929:ARG:NH2	2.53	0.41
2:B:1063:ARG:O	2:B:1066:HIS:N	2.37	0.41
4:E:43:LYS:O	4:E:47:CYS:HB2	2.20	0.41
7:I:54:ASP:OD1	7:I:55:ALA:N	2.46	0.41
1:A:844:THR:O	1:A:848:LYS:HG3	2.20	0.41
1:A:1245:ASP:OD1	1:A:1246:VAL:N	2.53	0.41
2:B:819:ASP:OD1	2:B:820:PRO:HD2	2.20	0.41
12:U:35:DA:H2"	12:U:36:DG:C8	2.55	0.41
1:A:407:GLN:O	1:A:411:VAL:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LYS:HG3	1:A:722:PRO:HA	2.03	0.41
2:B:20:GLU:OE2	2:B:24:ARG:NH2	2.54	0.41
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.56	0.41
4:E:182:ASP:O	4:E:185:ALA:N	2.46	0.41
1:A:389:VAL:O	1:A:393:SER:HB2	2.20	0.41
1:A:506:THR:HG22	1:A:580:HIS:HD2	1.86	0.41
2:B:324:THR:CG2	14:M:109:ARG:HE	2.34	0.41
2:B:537:SER:N	2:B:538:PRO:HD2	2.36	0.41
2:B:781:TYR:HB2	2:B:788:ILE:HD11	2.03	0.41
2:B:866:LEU:O	2:B:868:LYS:HG3	2.21	0.41
8:J:42:LYS:HZ1	15:N:176:ASP:HB3	1.83	0.41
1:A:477:ASN:OD1	2:B:1048:SER:HB3	2.21	0.41
1:A:1176:ARG:NH2	5:F:154:ASP:HB3	2.35	0.41
1:A:460:LEU:O	1:A:1618:THR:CB	2.69	0.41
1:A:589:MET:O	1:A:600:MET:HA	2.21	0.41
1:A:741:PRO:HD2	1:A:801:TYR:CD1	2.56	0.41
2:B:253:LEU:HB2	2:B:257:GLN:O	2.20	0.41
2:B:328:GLN:CD	14:M:112:LYS:C	2.77	0.41
2:B:332:ASP:CB	14:M:113:ILE:HG23	2.49	0.41
2:B:1070:ARG:HG2	2:B:1071:VAL:O	2.20	0.41
15:N:40:LEU:HD12	15:N:40:LEU:HA	1.84	0.41
15:N:81:THR:HG22	15:N:86:ASP:HB3	2.01	0.41
1:A:387:SER:O	1:A:391:THR:HG23	2.21	0.41
1:A:467:PHE:CZ	1:A:1613:MET:HE2	2.56	0.41
1:A:1482:LYS:NZ	2:B:304:ASP:HA	2.36	0.41
2:B:974:LEU:HD21	2:B:1005:TYR:HE2	1.86	0.41
10:L:46:VAL:HG13	10:L:56:LEU:HD12	2.03	0.41
13:R:13:G:C2	13:R:14:A:C5	3.09	0.41
15:N:141:GLU:HG2	15:N:142:THR:N	2.36	0.41
2:B:404:LEU:HD21	2:B:551:ILE:HG21	2.03	0.41
2:B:1079:LEU:HD22	2:B:1087:LEU:HD23	2.03	0.41
4:E:12:LEU:HD22	4:E:55:ARG:NH1	2.35	0.41
17:G:50:ALA:HA	17:G:113:PHE:CD2	2.56	0.41
1:A:28:SER:OG	1:A:77:GLY:HA2	2.20	0.40
1:A:916:THR:HG22	1:A:944:MET:CE	2.51	0.40
1:A:1654:PHE:CE1	5:F:92:ARG:HD3	2.55	0.40
2:B:335:ARG:HD2	2:B:346:ASP:OD1	2.21	0.40
3:C:61:THR:HA	3:C:298:PHE:HZ	1.86	0.40
5:F:68:THR:O	5:F:72:LYS:HG2	2.21	0.40
6:H:101:ALA:HB2	6:H:116:TYR:CD2	2.57	0.40
2:B:206:LEU:HD11	2:B:484:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:CYS:HB2	2:B:698:SER:HB3	2.04	0.40
3:C:271:ARG:NH1	15:N:175:TYR:CE1	2.89	0.40
5:F:100:GLN:CD	17:G:112:PRO:HB3	2.41	0.40
6:H:123:MET:HE3	6:H:142:LEU:HD22	2.03	0.40
9:K:66:VAL:HG12	9:K:67:GLU:HG2	2.03	0.40
15:N:127:ASP:OD2	15:N:129:ALA:HB2	2.21	0.40
15:N:145:ILE:HG22	15:N:146:PRO:CD	2.50	0.40
1:A:460:LEU:O	1:A:1618:THR:HB	2.21	0.40
2:B:244:THR:HG21	2:B:414:LYS:NZ	2.37	0.40
3:C:216:HIS:ND1	3:C:218:LYS:HG2	2.37	0.40
4:E:47:CYS:SG	4:E:53:PRO:HB3	2.61	0.40
7:I:6:SER:N	7:I:45:LEU:HD21	2.27	0.40
15:N:145:ILE:CG2	15:N:146:PRO:N	2.85	0.40
17:G:73:TYR:CZ	17:G:238:THR:HG21	2.57	0.40
1:A:603:HIS:NE2	1:A:624:TYR:OH	2.48	0.40
1:A:1060:GLU:HG2	1:A:1060:GLU:O	2.22	0.40
2:B:250:LEU:HD23	2:B:260:PHE:HA	2.04	0.40
2:B:359:LEU:HD21	2:B:377:MET:HE1	2.04	0.40
2:B:679:GLN:OE1	2:B:679:GLN:N	2.52	0.40
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.22	0.40
2:B:824:HIS:O	2:B:861:TYR:HB2	2.21	0.40
3:C:152:ASP:OD2	3:C:154:LYS:HB2	2.22	0.40
1:A:1480:THR:HG22	1:A:1481:GLU:H	1.87	0.40
2:B:717:TYR:O	2:B:721:MET:HG2	2.22	0.40
2:B:757:TYR:CE1	2:B:762:MET:HB2	2.57	0.40
2:B:782:ASP:HB3	2:B:788:ILE:HG12	2.03	0.40
4:E:113:GLN:HA	4:E:137:GLU:CD	2.42	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	1447/1664 (87%)	1325 (92%)	119 (8%)	3 (0%)	47 79
2	B	1171/1203 (97%)	1109 (95%)	60 (5%)	2 (0%)	47 79
3	C	303/335 (90%)	286 (94%)	17 (6%)	0	100 100
4	E	210/215 (98%)	200 (95%)	10 (5%)	0	100 100
5	F	98/155 (63%)	96 (98%)	2 (2%)	0	100 100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100 100
7	I	61/125 (49%)	53 (87%)	8 (13%)	0	100 100
8	J	67/70 (96%)	63 (94%)	4 (6%)	0	100 100
9	K	99/142 (70%)	93 (94%)	6 (6%)	0	100 100
10	L	42/70 (60%)	37 (88%)	5 (12%)	0	100 100
14	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	8 42
15	N	139/233 (60%)	122 (88%)	14 (10%)	3 (2%)	6 39
16	D	50/137 (36%)	48 (96%)	2 (4%)	0	100 100
17	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	14 51
All	All	4109/5236 (78%)	3826 (93%)	271 (7%)	12 (0%)	44 74

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	A	1653	SER
1	A	91	PHE
2	B	1047	ARG
14	M	85	LYS
17	G	99	ASP
14	M	36	THR
15	N	115	SER
17	G	100	THR
2	B	895	PHE
15	N	70	LEU
15	N	39	PRO

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	1289/1465 (88%)	1284 (100%)	5 (0%)	91 95
2	B	1030/1053 (98%)	1030 (100%)	0	100 100
3	C	269/296 (91%)	269 (100%)	0	100 100
4	E	194/197 (98%)	194 (100%)	0	100 100
5	F	90/137 (66%)	90 (100%)	0	100 100
6	H	115/128 (90%)	115 (100%)	0	100 100
7	I	55/110 (50%)	55 (100%)	0	100 100
8	J	64/65 (98%)	64 (100%)	0	100 100
9	K	91/130 (70%)	91 (100%)	0	100 100
10	L	39/57 (68%)	39 (100%)	0	100 100
14	M	98/371 (26%)	88 (90%)	10 (10%)	7 31
15	N	135/220 (61%)	129 (96%)	6 (4%)	28 57
16	D	52/116 (45%)	47 (90%)	5 (10%)	8 34
17	G	171/291 (59%)	159 (93%)	12 (7%)	15 46
All	All	3692/4636 (80%)	3654 (99%)	38 (1%)	77 86

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	LEU
1	A	463	LYS
1	A	464	GLU
1	A	1648	ASN
1	A	1653	SER
14	M	17	ASP
14	M	18	GLN
14	M	31	ARG
14	M	44	LYS
14	M	48	LYS
14	M	65	TYR
14	M	77	VAL
14	M	84	GLU
14	M	98	SER
14	M	109	ARG
15	N	51	GLN

Continued on next page...

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Mol	Chain	Res	Type
15	N	124	THR
15	N	135	LYS
15	N	153	VAL
15	N	167	LYS
15	N	178	GLU
16	D	15	THR
16	D	29	GLN
16	D	38	GLN
16	D	46	GLU
16	D	80	THR
17	G	18	LYS
17	G	24	VAL
17	G	35	SER
17	G	39	VAL
17	G	139	ILE
17	G	147	LEU
17	G	167	THR
17	G	169	VAL
17	G	223	GLU
17	G	230	ARG
17	G	239	THR
17	G	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	264	ASN
1	A	383	ASN
1	A	458	GLN
1	A	489	ASN
1	A	580	HIS
1	A	610	ASN
1	A	730	GLN
1	A	1108	HIS
1	A	1314	GLN
1	A	1453	HIS
1	A	1662	ASN
2	B	27	ASN
2	B	328	GLN
2	B	504	HIS
2	B	646	HIS

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Mol	Chain	Res	Type
2	B	715	ASN
2	B	720	GLN
2	B	975	HIS
2	B	987	ASN
2	B	1082	HIS
2	B	1089	GLN
2	B	1157	GLN
2	B	1171	ASN
2	B	1199	ASN
3	C	237	GLN
3	C	297	HIS
3	C	301	ASN
5	F	59	GLN
5	F	100	GLN
7	I	44	ASN
9	K	64	GLN
9	K	106	GLN
10	L	53	HIS
16	D	23	HIS
17	G	235	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/20 (35%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	15	C
13	R	17	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	SO4	B	1301	-	4,4,4	0.16	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1301	SO4	2	0

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.

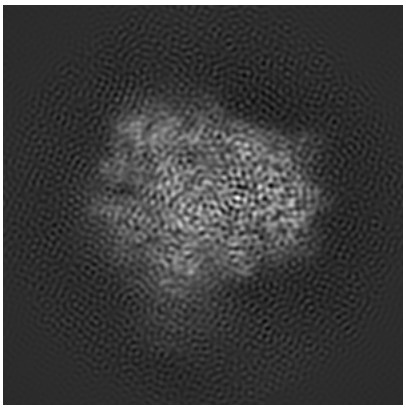
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4147. These allow visual inspection of the internal detail of the map and identification of artifacts.

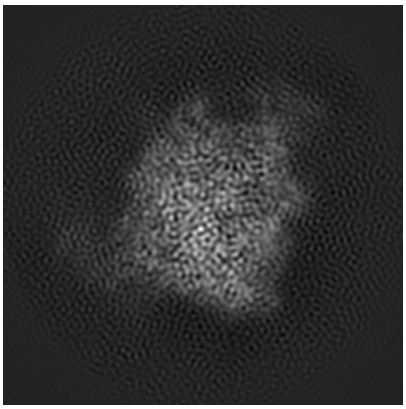
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

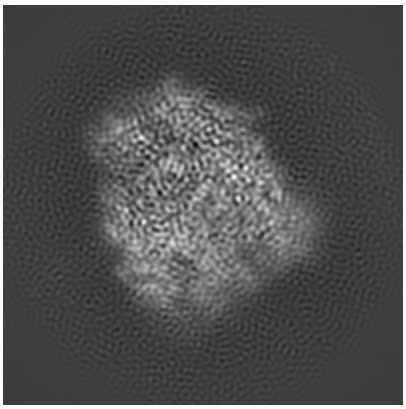
6.1.1 Primary map



X

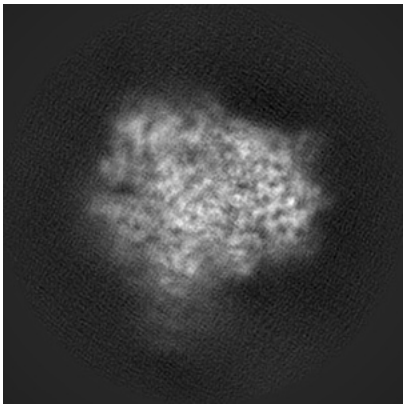


Y

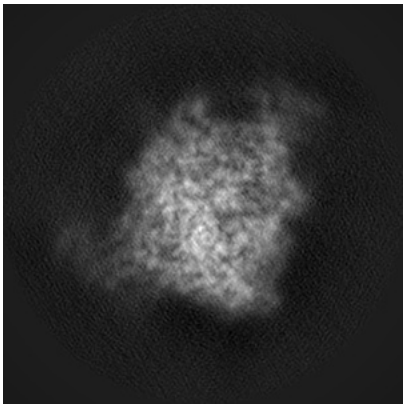


Z

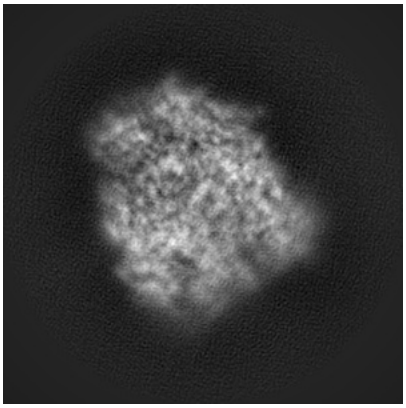
6.1.2 Raw map



X



Y

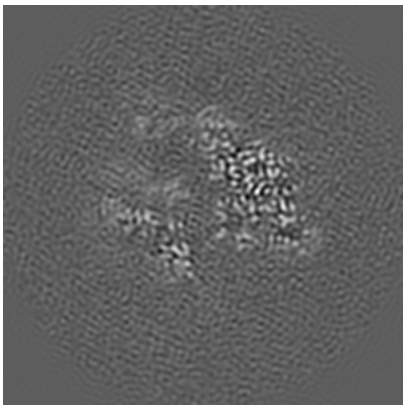


Z

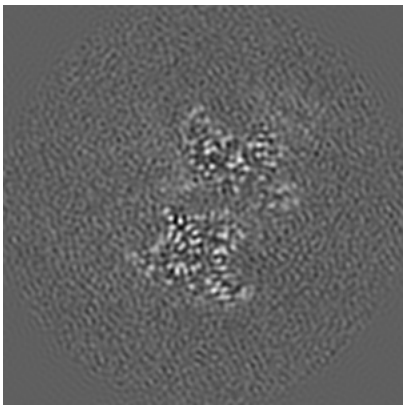
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

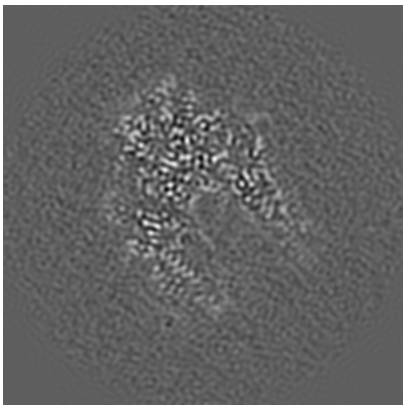
6.2.1 Primary map



X Index: 115

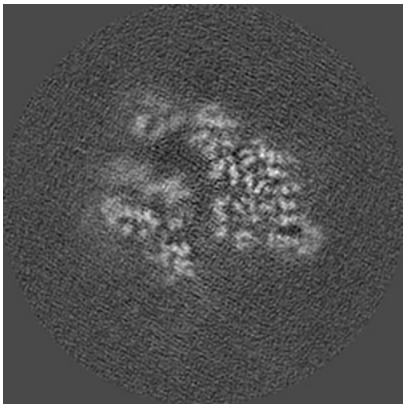


Y Index: 115

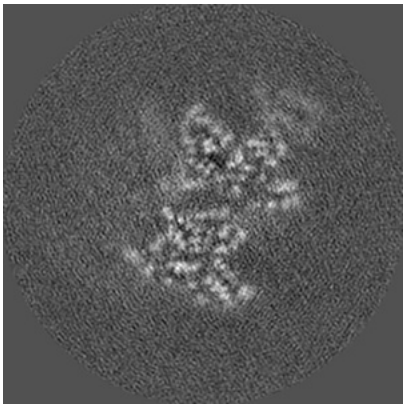


Z Index: 115

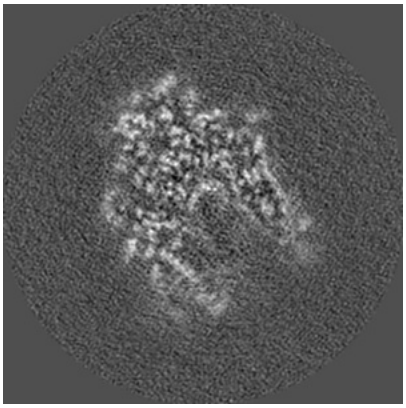
6.2.2 Raw map



X Index: 115



Y Index: 115

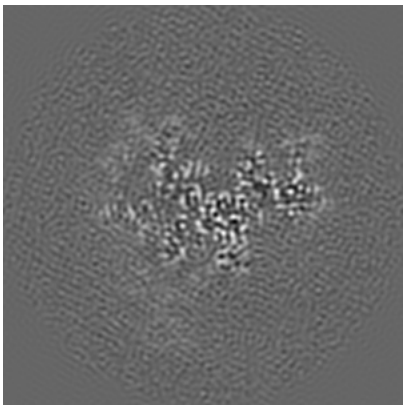


Z Index: 115

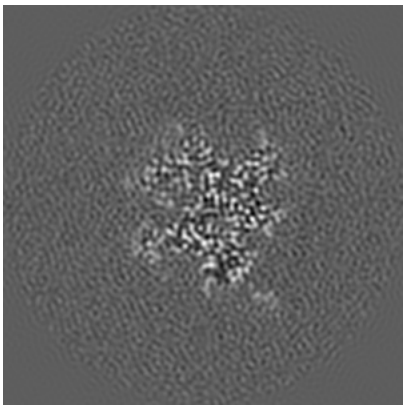
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

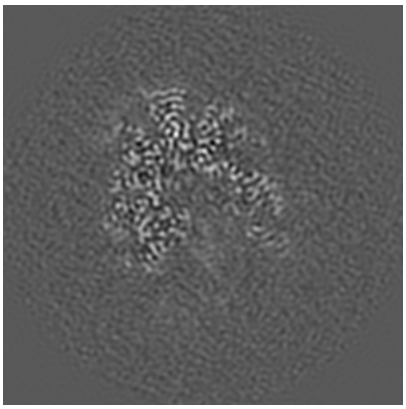
6.3.1 Primary map



X Index: 94

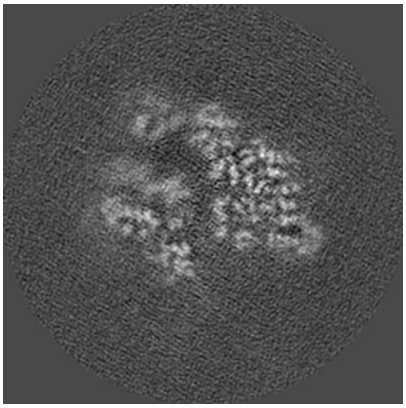


Y Index: 135

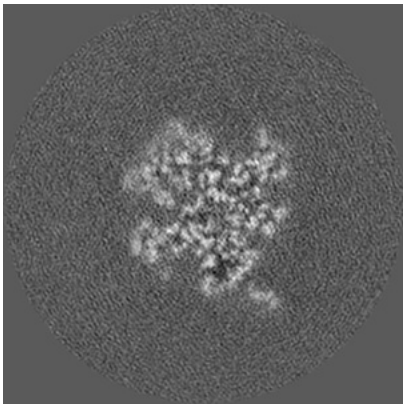


Z Index: 122

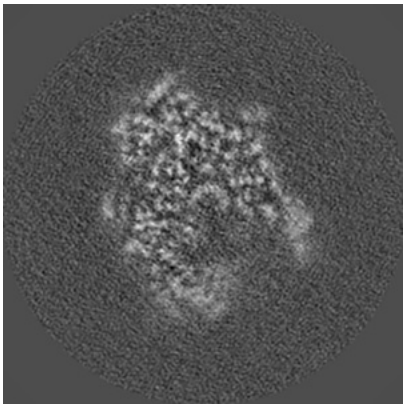
6.3.2 Raw map



X Index: 115



Y Index: 135



Z Index: 113

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 0.045. 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.

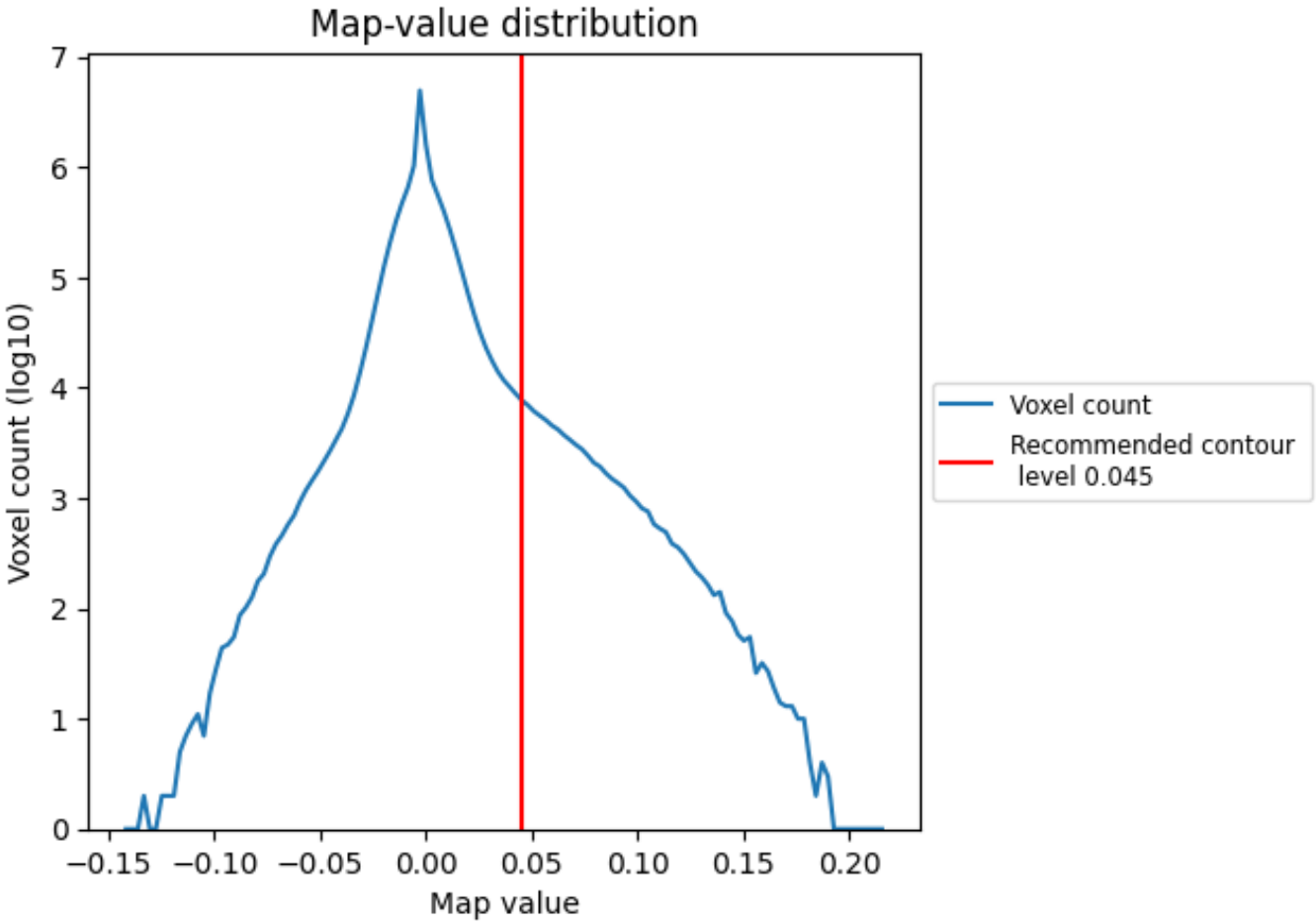
6.5 Mask visualisation (i)

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

7 Map analysis

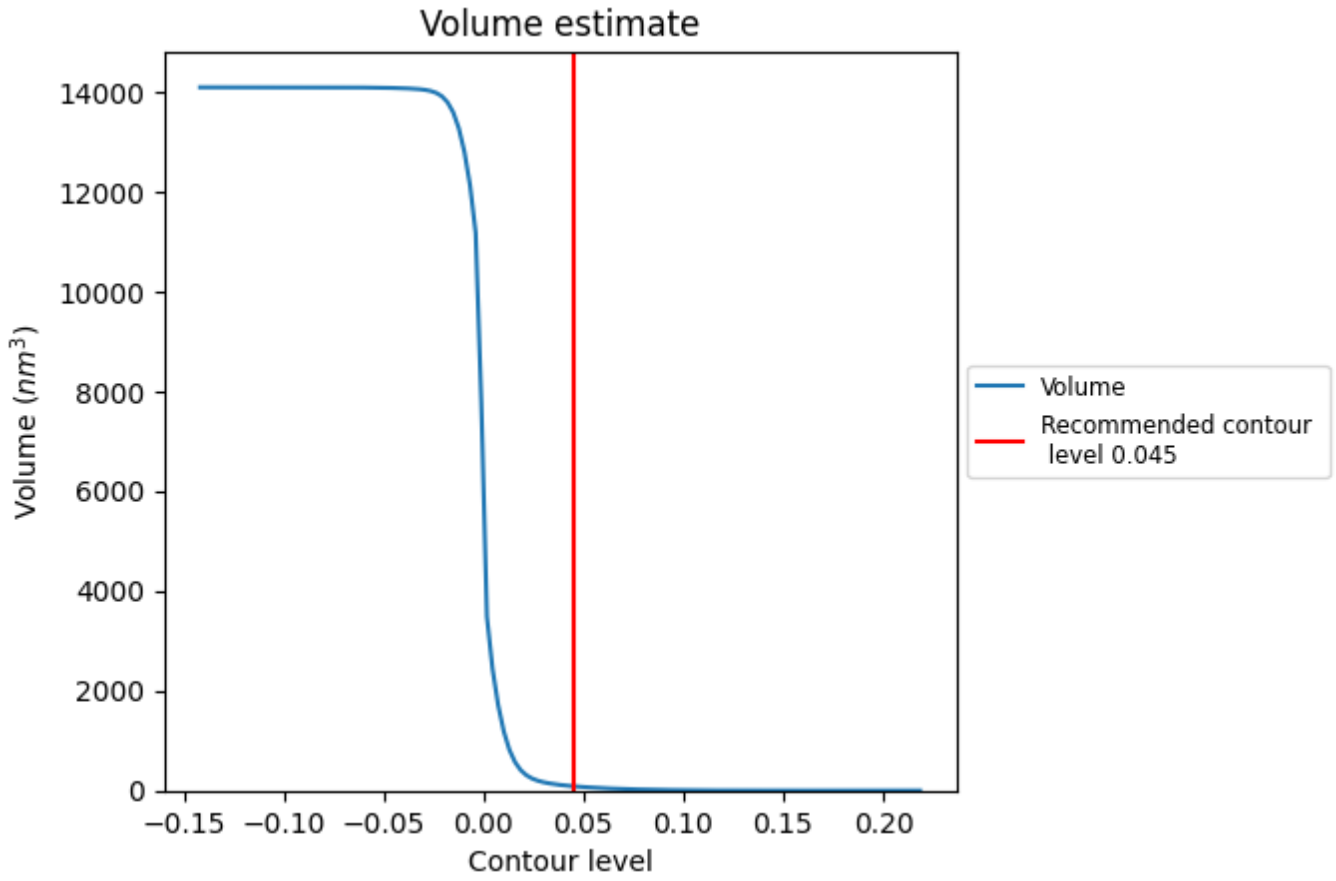
This section contains the results of statistical analysis of the map.

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.

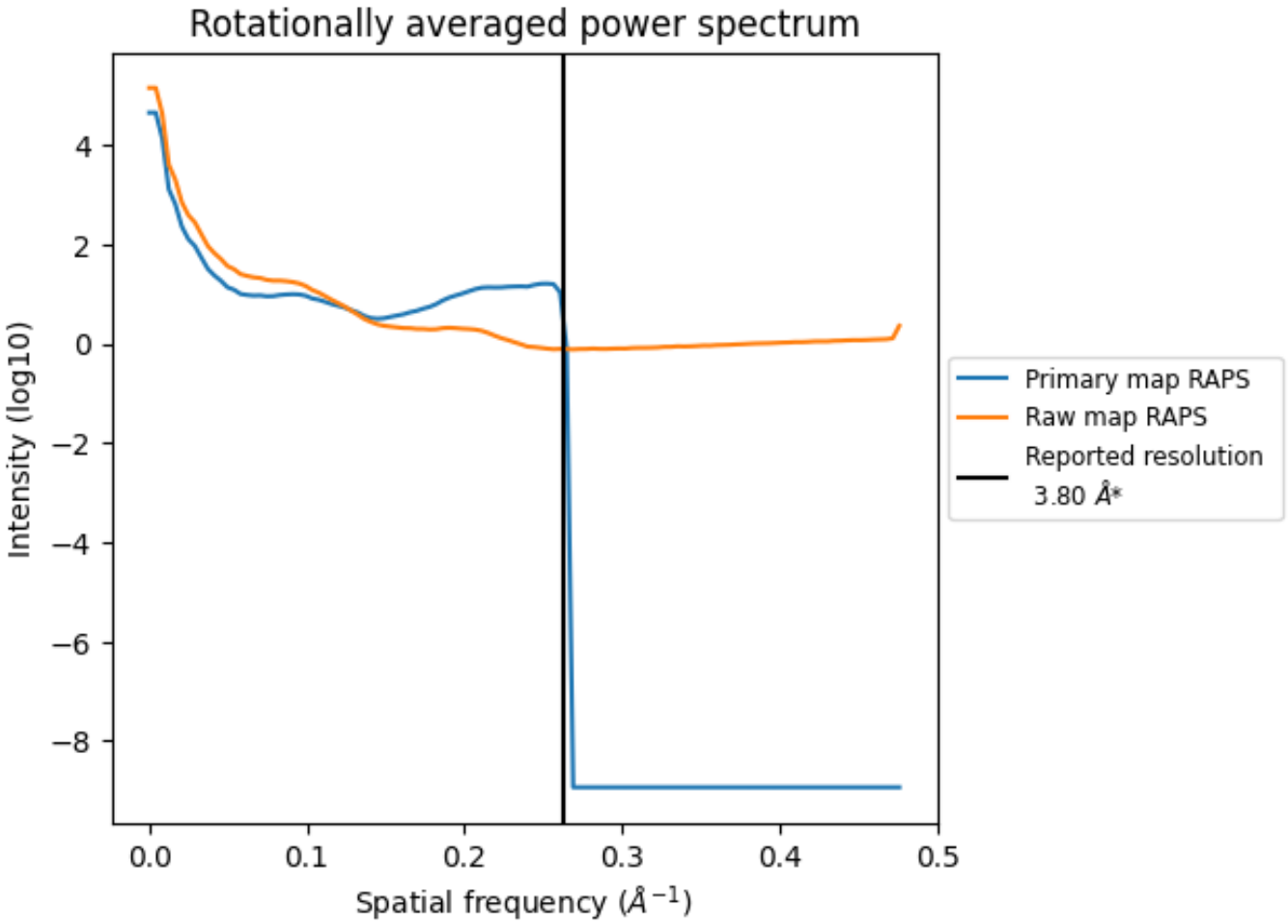
7.2 Volume estimate (i)



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 78 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)

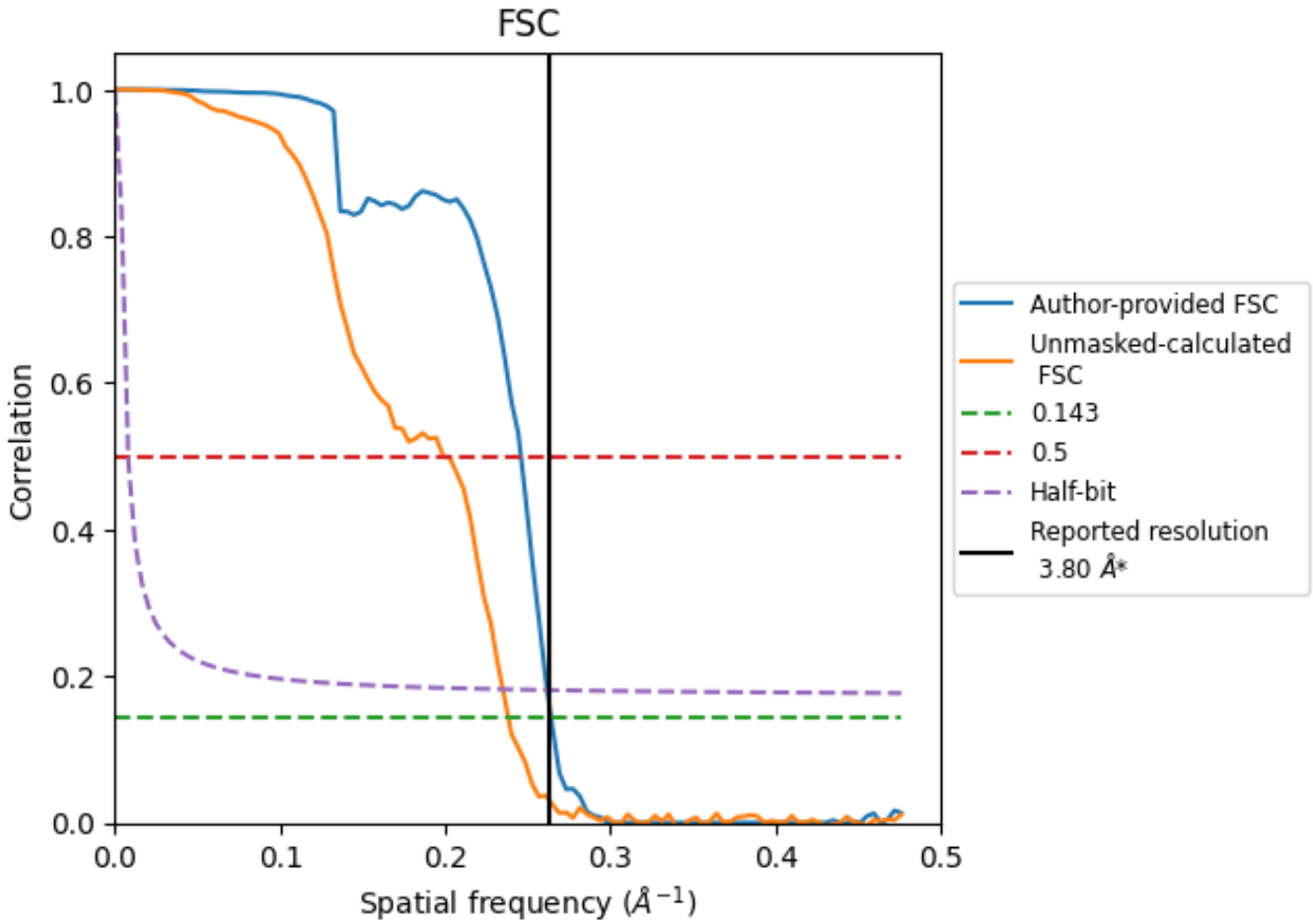


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

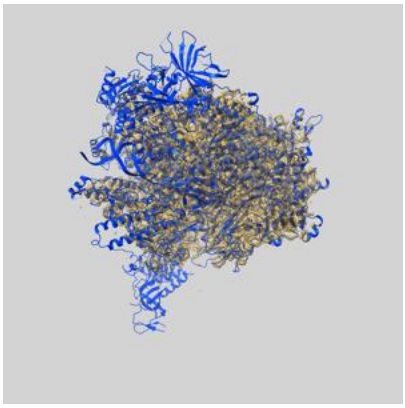
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.07	3.82
Unmasked-calculated*	4.20	5.01	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.8 by more than 10 %

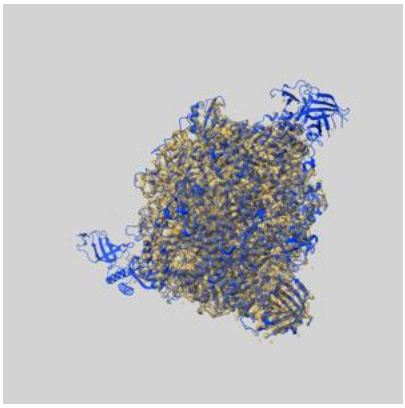
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4147 and PDB model 5M3F. Per-residue inclusion information can be found in section 3 on page 8.

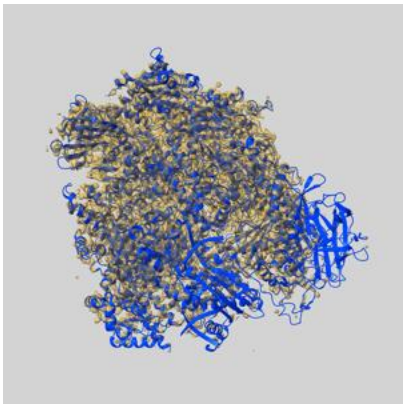
9.1 Map-model overlay



X



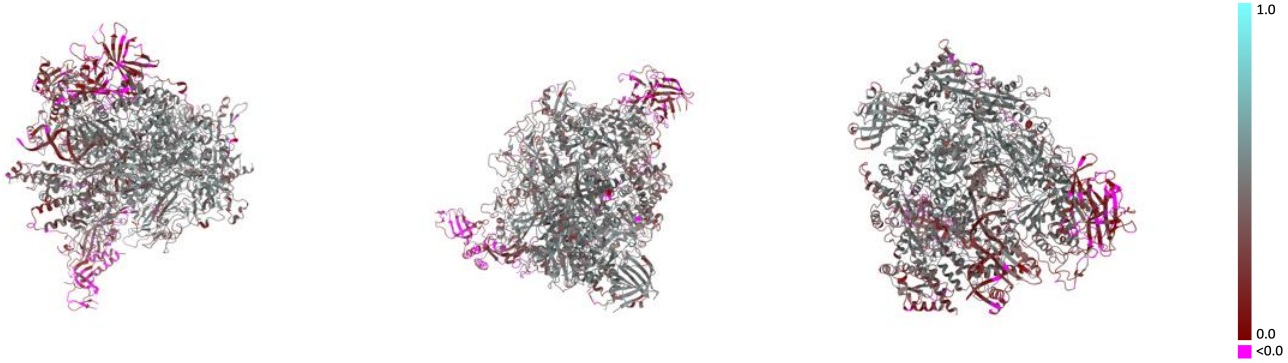
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

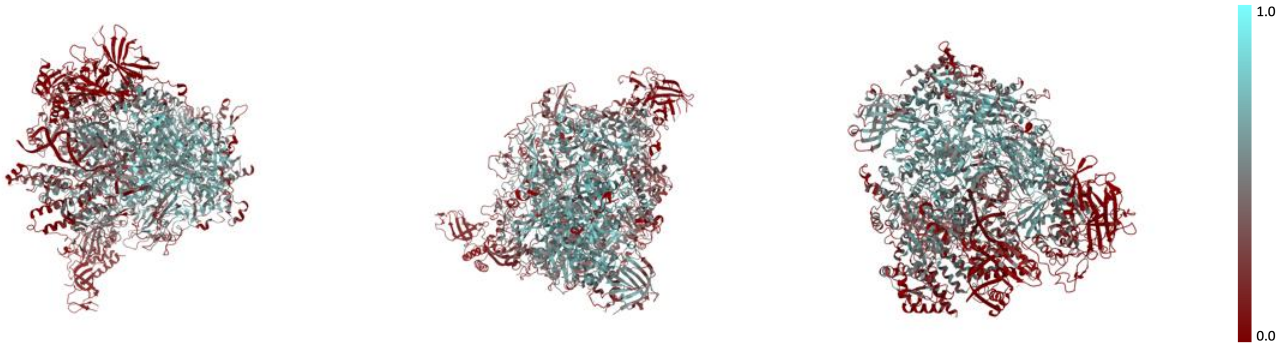
9.2 Q-score mapped to coordinate model (i)



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.

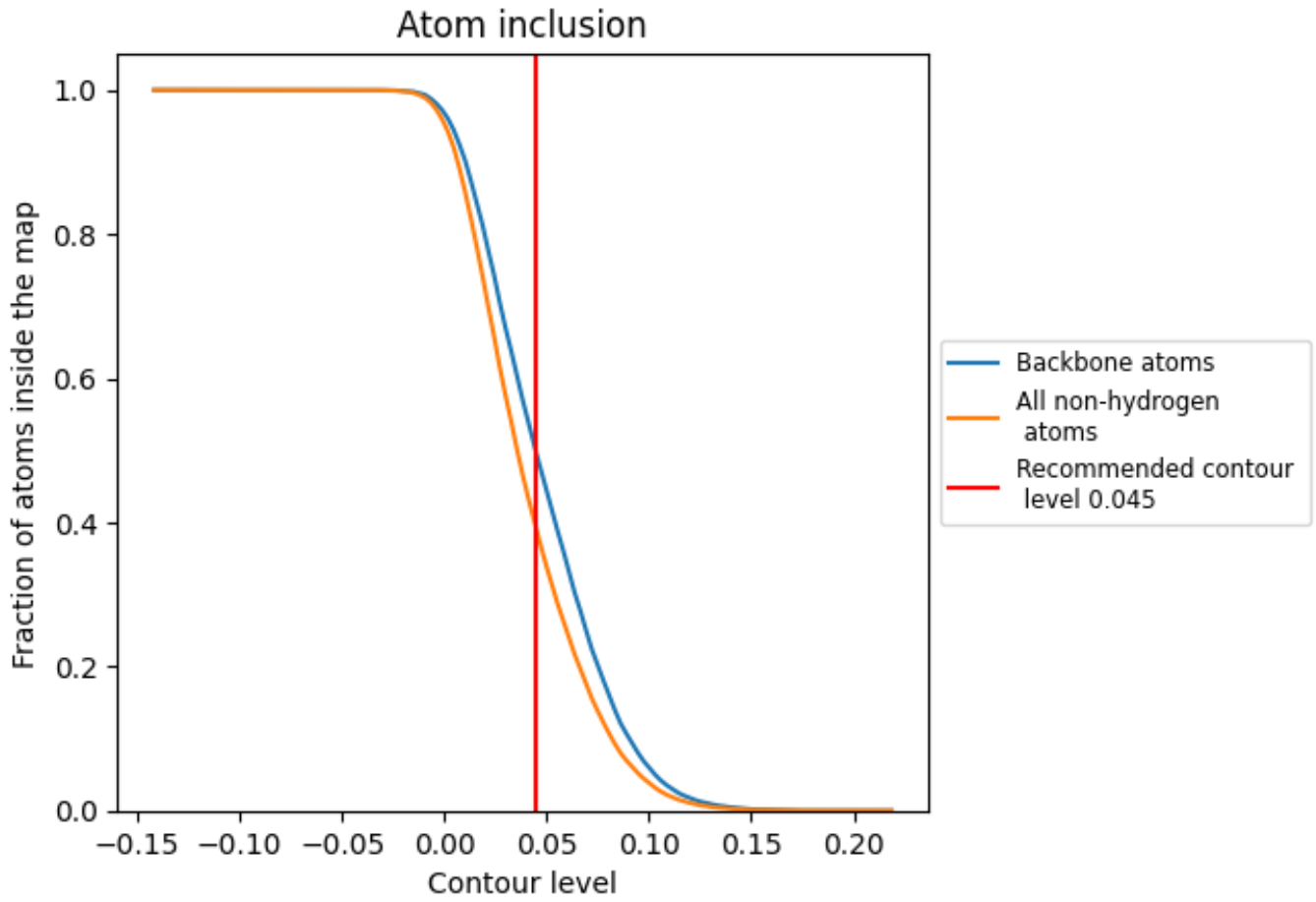
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 39% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3900	0.3830
A	0.4301	0.4240
B	0.5100	0.4500
C	0.4636	0.4480
D	0.0211	0.0430
E	0.2908	0.3670
F	0.4207	0.4200
G	0.0332	0.0420
H	0.4327	0.4430
I	0.0409	0.2560
J	0.6033	0.4880
K	0.4987	0.4600
L	0.4706	0.4510
M	0.0024	0.0870
N	0.0026	0.0760
R	0.2948	0.3370
T	0.1709	0.2880
U	0.0246	0.1580