Full wwPDB EM Validation Report

Jun 8, 2025 – 04:22 pm BST

PDB ID	:	9G26 / pdb_00009g26
EMDB ID	:	EMD-50965
Title	:	Yeast RNA polymerase I elongation complex stalled by an apurinic site, closed state
Authors	:	Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on	:	2024-07-10
Resolution	:	3.40 Å(reported)
Based on initial model	:	6hko

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 (i) 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 (i)) were used in the production of this report:

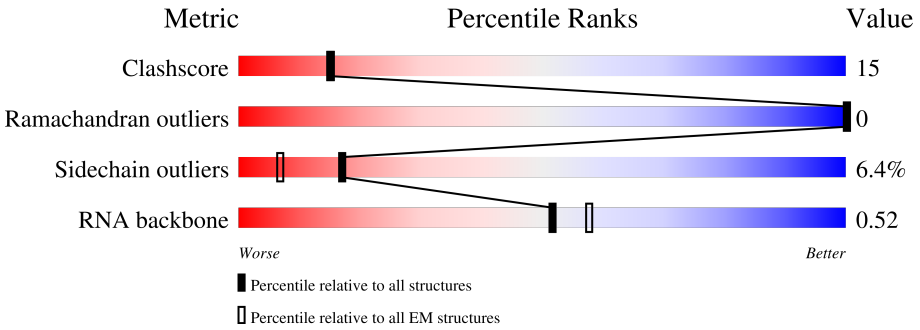
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	17% 54% 31% · 12%
2	B	1203	13% 61% 33% · ·
3	C	335	13% 65% 23% · 9%
4	D	137	36% 27% 15% · 57%
5	E	215	44% 58% 38% ·
6	F	155	14% 39% 24% · 35%
7	G	326	28% 29% 14% · 55%

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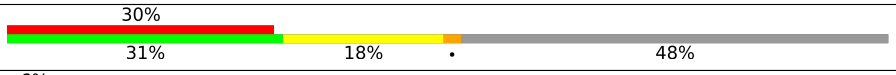
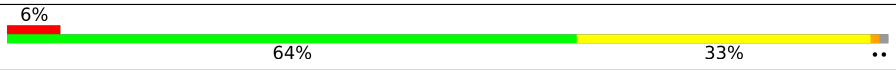
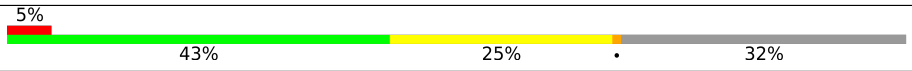
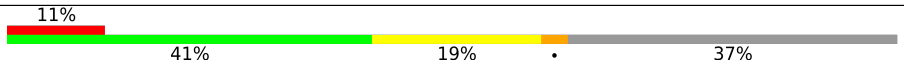
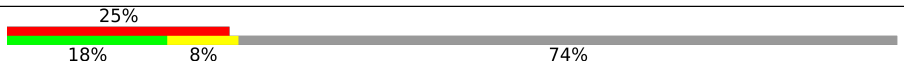
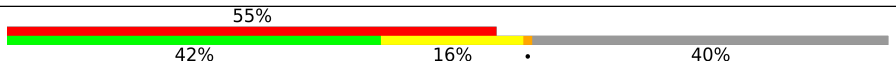
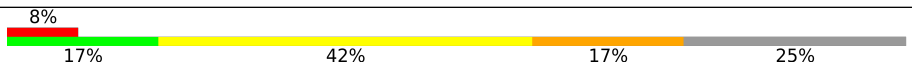
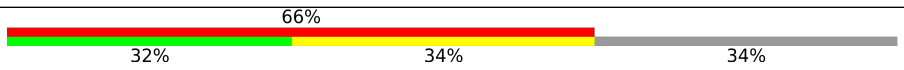
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	12	
16	S	38	
17	T	38	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33973 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	1462	11549	7290	2012	2185	62	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	1164	9254	5852	1626	1725	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	304	2415	1535	414	458	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	0	0

- Molecule 5 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		
5	E	214	1751	1111	309	320	11	0	0

- Molecule 6 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		
6	F	101	827	524	145	155	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	148	Total	C	N	O	S	0	0
			1164	756	196	208	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			758	476	123	155	4		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	139	Total	C	N	O	S	0	0
			1105	705	181	215	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	25	Total	C	N	O	P	0	0
			506	242	85	154	25		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	33	Total	C	N	O	P	0	0
			665	317	117	198	33		

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

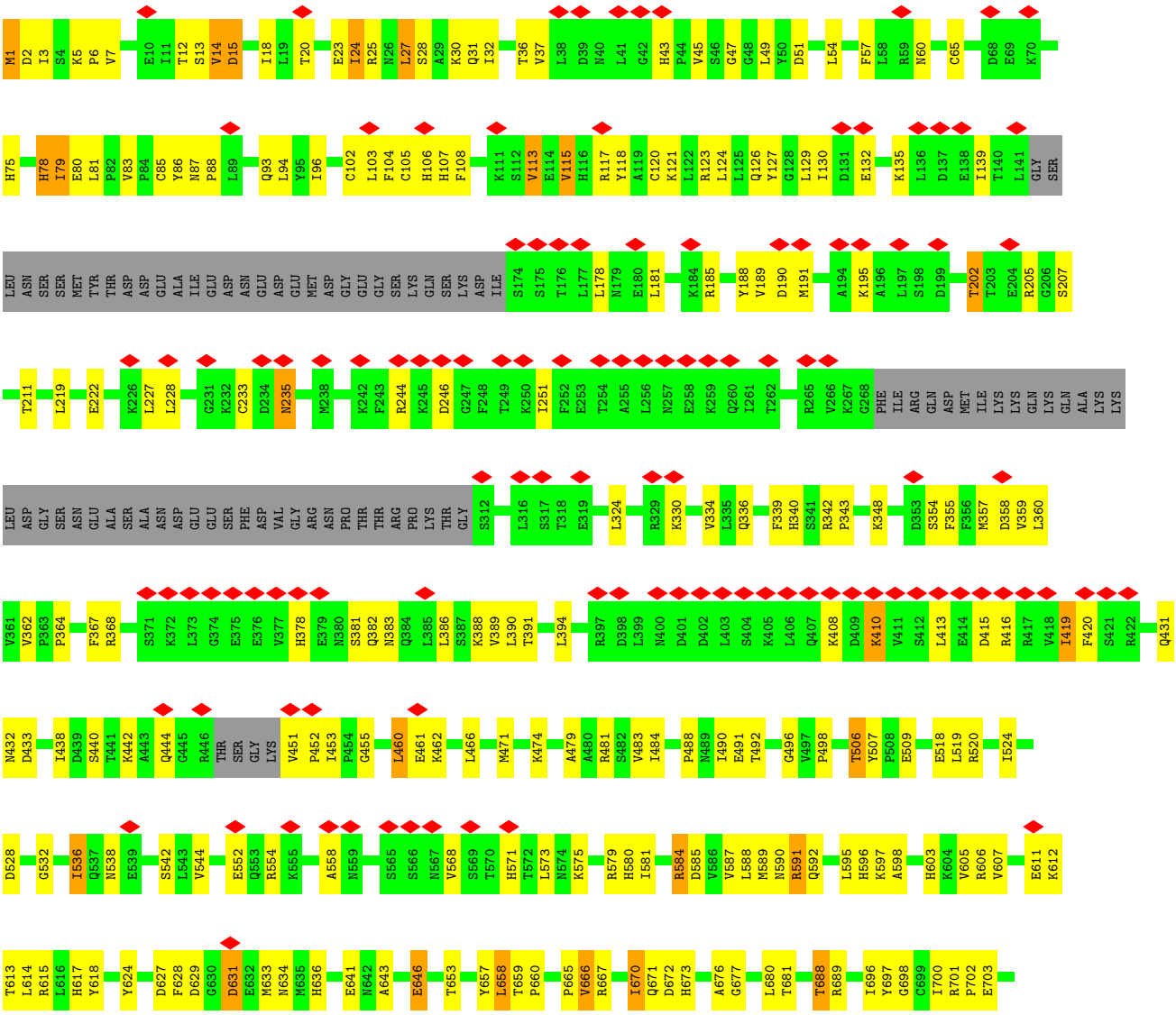
Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	I	1	Total	Zn	0
			1	1	
19	J	1	Total	Zn	0
			1	1	
19	L	1	Total	Zn	0
			1	1	

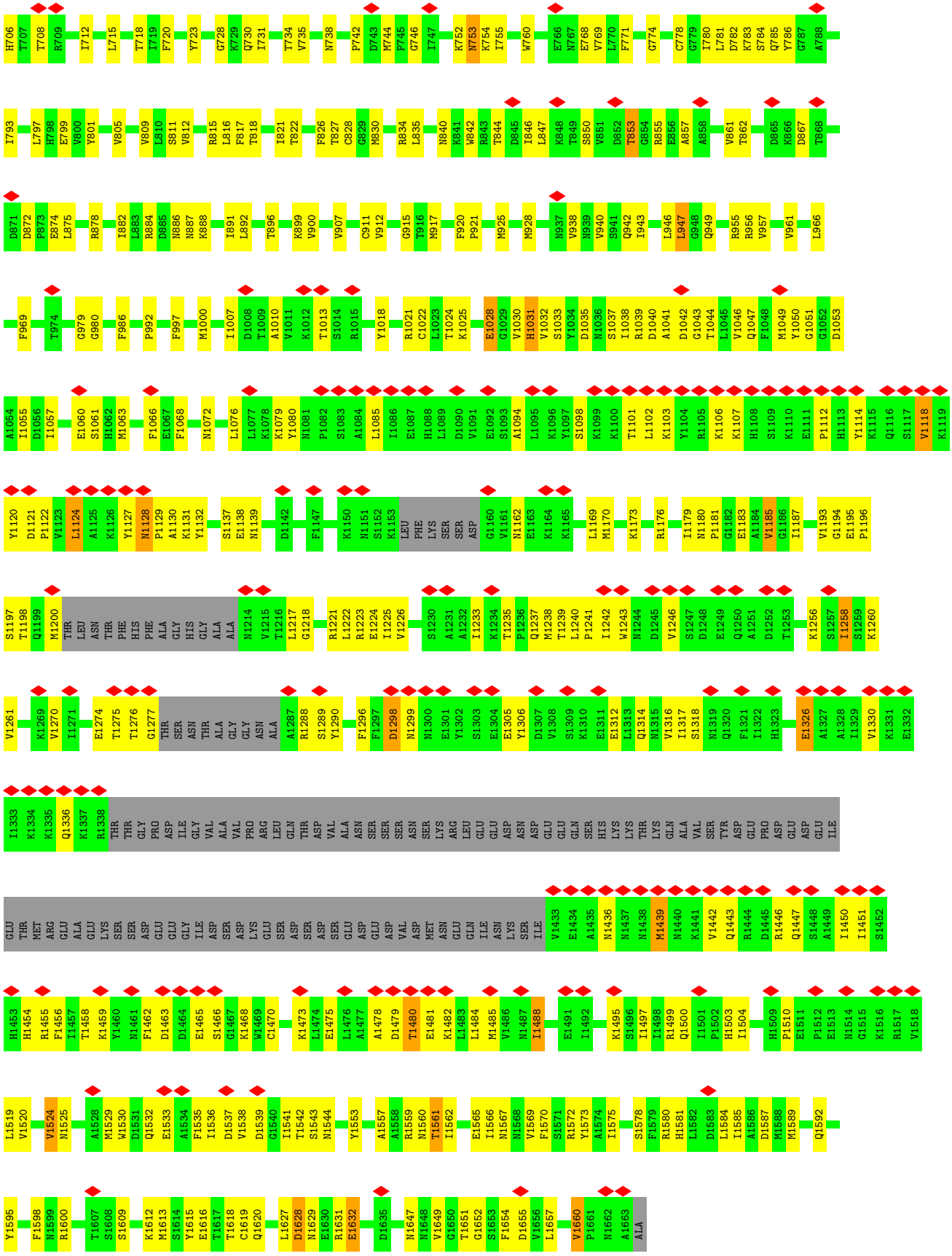
3 Residue-property plots (i)

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:

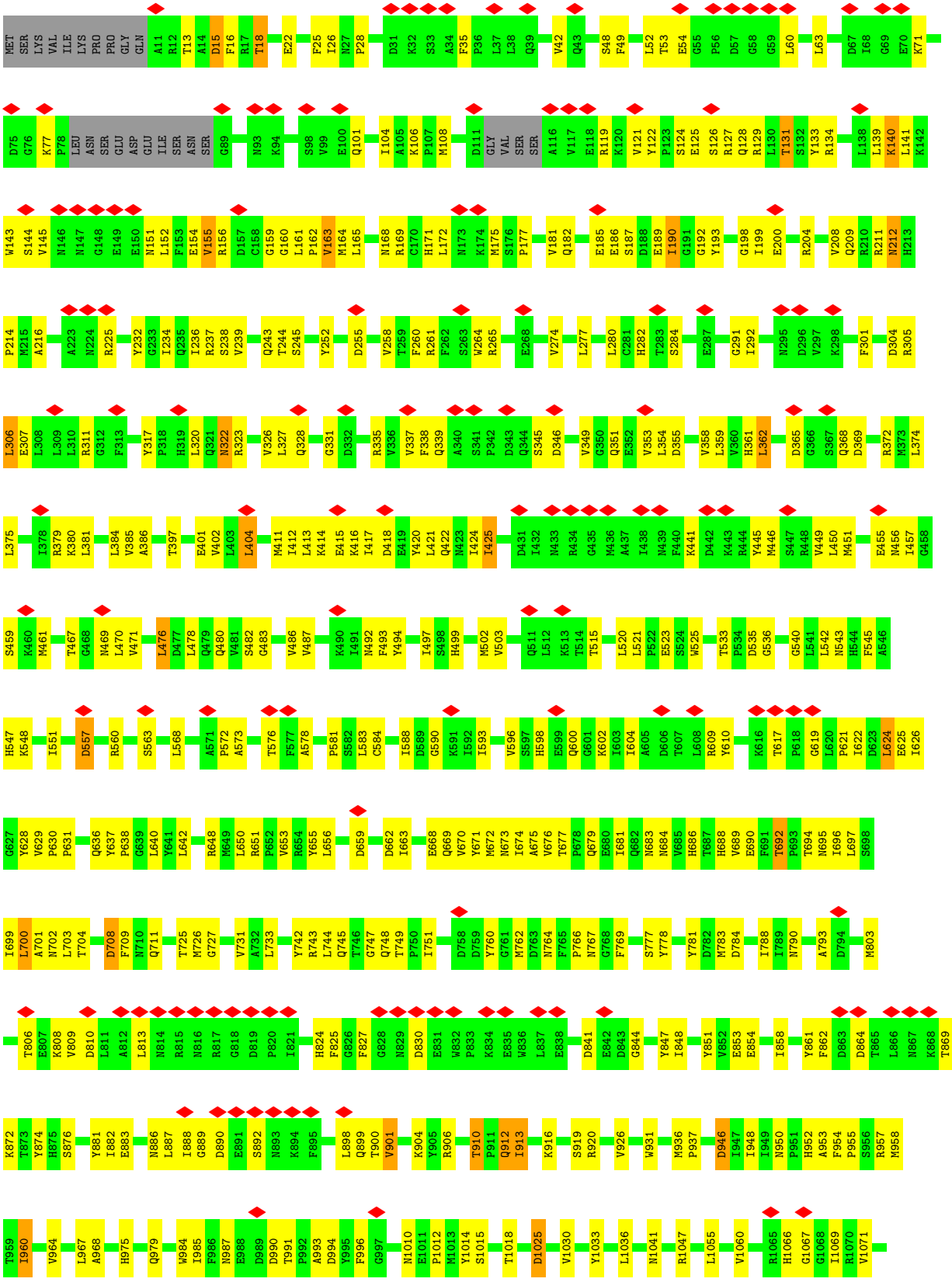


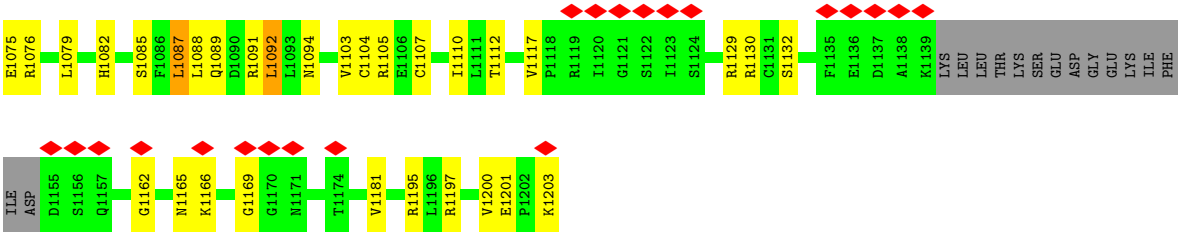


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:

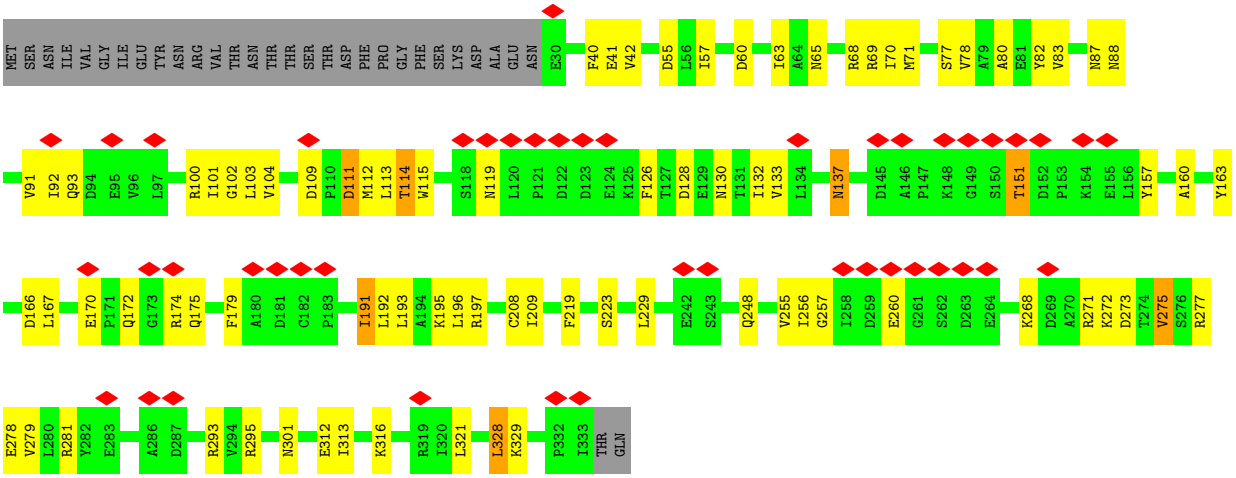

13%
61%
33%


MET SER LYS VAL ILE LYS PRO PRO GLY GLN A11 R12 T13 A14 D15 F16 R17 T18 E22 F25 I26 N27 P28 D31 K32 S33 A34 F35 P36 L37 L38 Q39 V42 Q43 S48 F49 L52 T53 E54 G55 P56 D57 G58 G59 L60 L63 D67 I68 G69 E70 K71
D75 G76 K77 P78 LEU ASN SER GLU ASP GLU ILE SER ASN SER G89 N93 K94 S98 V99 E100 Q101 I104 A105 K106 P107 M108 D111 GLY VAL SER SER A116 V117 E118 R119 K120 V121 Y122 P123 S124 E125 S126 R127 Q128 R129 L130 T131 S132 Y133 R134 L138 L139 K140 L141 K142
W143 S144 V145 N146 N147 G148 E149 E150 N151 L152 F153 E154 V155 R156 D157 C158 G159 G160 L161 P162 V163 M164 L165 N168 R169 C170 H171 L172 N173 K174 M175 S176 P177 V181 Q182 E185 E186 S187 D188 E189 I190 G191 G192 Y193 G198 I199 E200 R204 V208 Q209 R210 R211 N212 H213
P214 M215 A216 A223 N224 R225 Y232 G233 I234 Q235 I236 R237 S238 V239 Q243 T244 S245 Y252 D255 V258 T259 F260 R261 F262 S263 W264 R265 E268 V274 L277 L280 C281 H282 T283 S284 E287 G291 I292 N295 D296 V297 K298 F301 D304 R305
L306 E307 L308 L309 L310 R311 G312 F313 Y317 P318 H319 L320 Q321 N322 R323 V326 L327 Q328 G331 D332 R335 V336 V337 F338 Q339 A340 S341 P342 D343 Q344 S345 D346 V349 G350 Q351 E352 V353 L354 D355 V358 L359 Y360 H361 L362 D365 G366 S367 Q368 D369 R372 M373 L374
L375 I378 R379 K380 L381 L384 V385 A386 T397 E401 V402 L403 L404 M411 I412 L413 K414 E415 K416 I417 D418 E419 Y420 L421 Q422 N423 I424 I425 D431 I432 M433 R434 G435 M436 A437 I438 N439 F440 K441 D442 K443 R444 Y445 M446 S447 R448 V449 L450 M451 E455 N456 I457 G458
S459 K460 M461 T467 G468 N469 L470 V471 L476 D477 L478 Q479 Q480 V481 S482 G483 V486 V487 K490 I491 N492 F493 Y494 I497 S498 H499 M502 V503 Q511 L512 K513 T514 T515 L520 L521 P522 E523 S524 W525 T533 P534 D535 G536 G540 L541 L542 N543 H544 F545 A546
H547 K548 I551 D557 R560 S563 L568 A571 P572 A573 T576 F577 A578 P581 S582 L583 C584 I588 D589 G590 K591 I592 I593 V596 S597 H598 E599 Q600 G601 K602 I603 I604 A605 D606 T607 L608 R609 Y610 K616 T617 P618 G619 L620 P621 I622 D623 L624 E625 I626
G627 Y628 V629 P630 P631 Q636 Y637 P638 G639 L640 Y641 L642 R648 M649 L650 R651 P652 V653 R654 Y655 L656 D659 D662 I663 E668 Q669 V670 Y671 M672 N673 I674 A675 V676 T677 P678 Q679 E680 I681 Q682 N683 N684 V685 H686 T687 H688 V689 E690 F691 T692 P693 T694 N695 I696 L697 S698
I699 L700 A701 N702 L703 T704 D708 F709 N710 Q711 T725 M726 G727 V731 A732 L733 Y742 R743 L744 Q745 T746 G747 Q748 T749 P750 I751 D758 D759 Y760 G761 M762 D763 N764 F765 P766 N767 G768 F769 S777 Y778 Y781 D782 M783 D784 I788 I789 N790 A793 D794 M803
T806 E807 K808 V809 D810 L811 A812 L813 N814 R815 N816 R817 G818 D819 P820 I821 H824 F825 G826 F827 G828 N829 D830 E831 W832 P833 K834 E835 W836 L837 E838 D841 E842 D843 G844 Y847 I848 Y851 V852 E853 E854 I858 Y861 F862 D863 D864 T865 L866 N867 K868 T869 K870 I871
K872 T873 Y874 H875 S876 Y881 I882 E883 N886 L887 I888 G889 D890 E891 S892 N893 K894 F895 L898 Q899 T900 V901 K904 Y905 R906 T910 P911 Q912 I913 K916 S919 R920 V926 W931 M936 P937 D946 I947 I948 I949 N950 P951 H952 A953 F954 P955 S956 R957 M958
T959 I960 V964 L967 A968 H975 Q979 W984 I985 F986 N987 E988 D989 D990 T991 P992 A993 D994 Y995 F996 G997 N1010 E1011 P1012 M1013 Y1014 S1015 T1018 D1025 V1030 Y1033 L1036 N1041 R1047 L1055 V1060 R1065 H1066 G1067 G1068 I1069 R1070 V1071



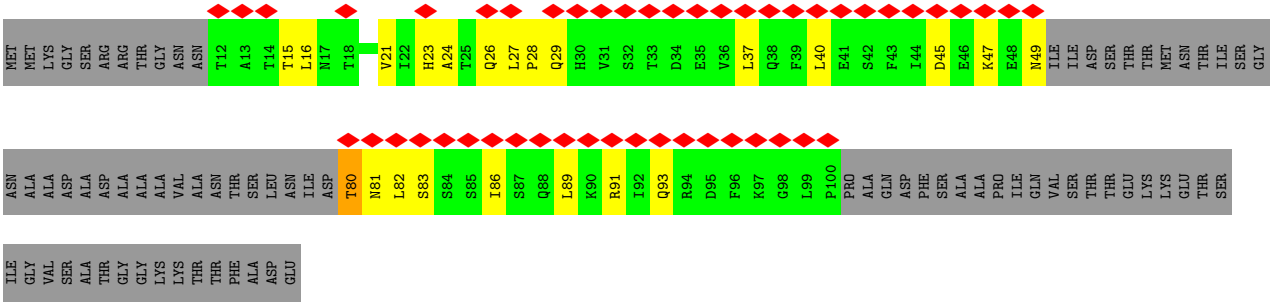
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



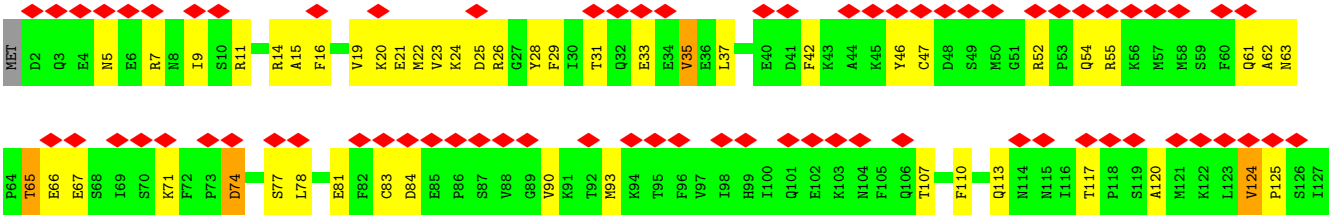
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

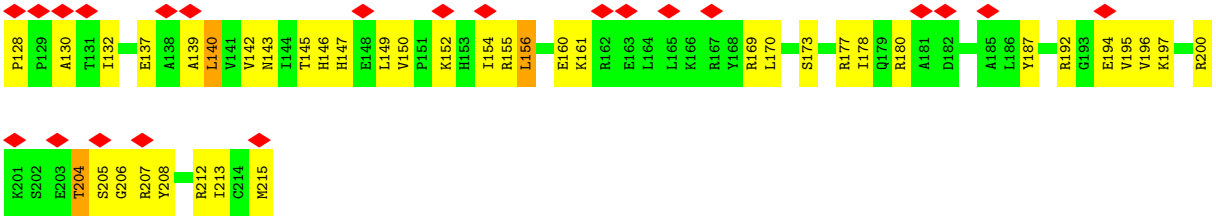
Chain D:



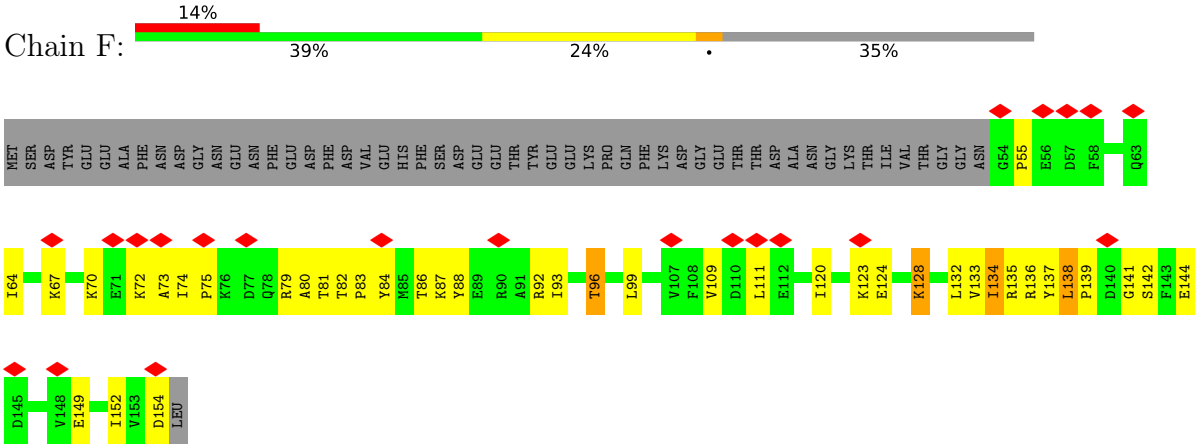
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

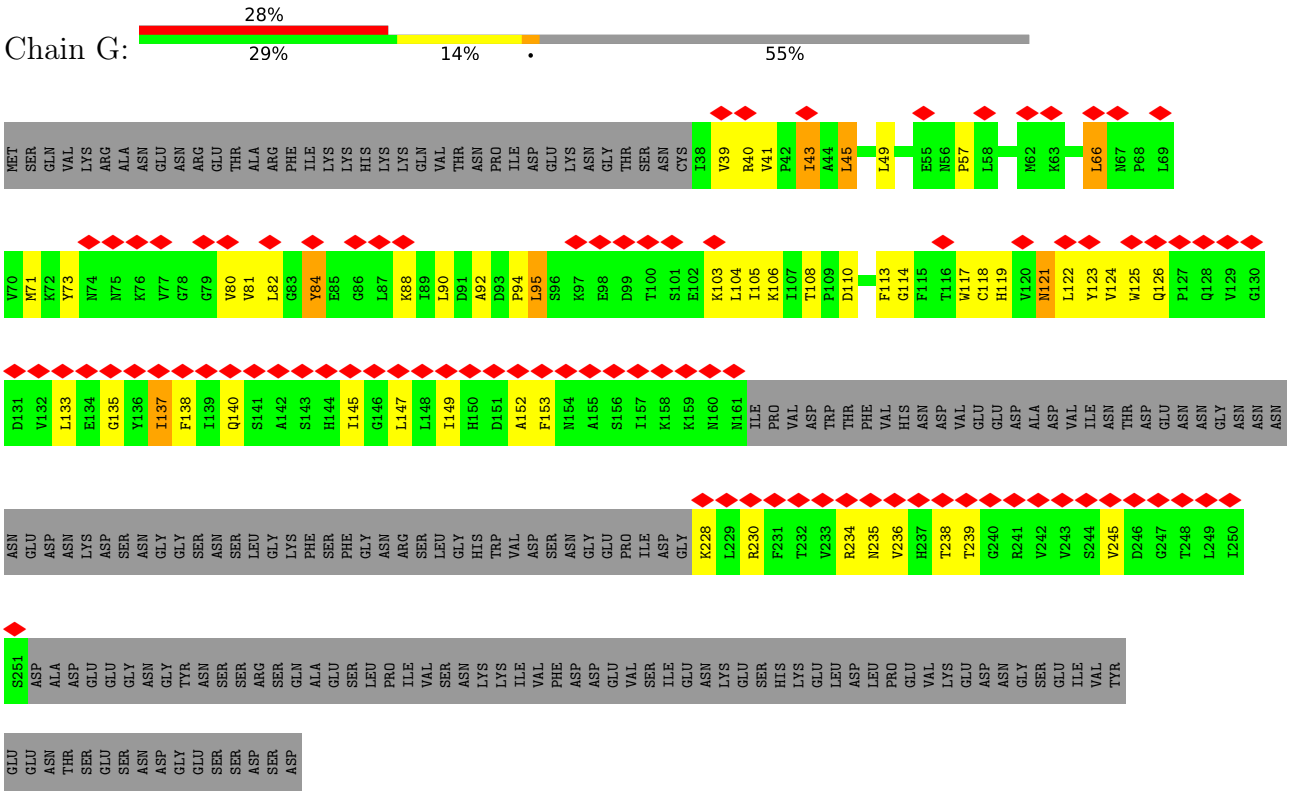




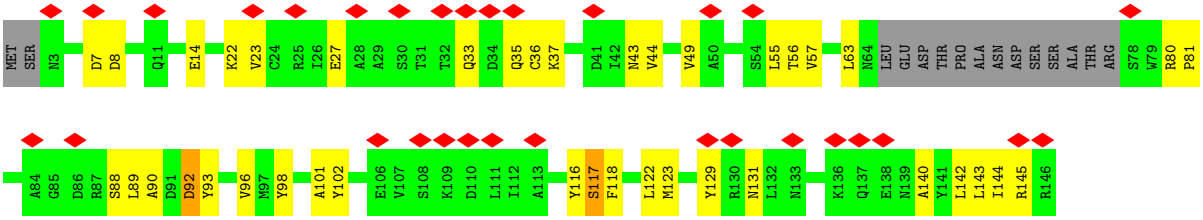
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

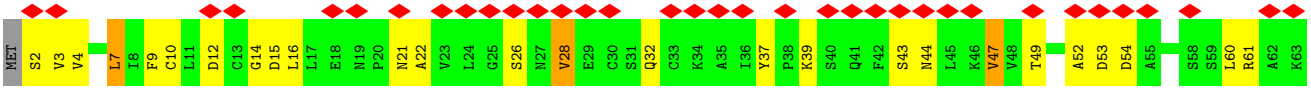


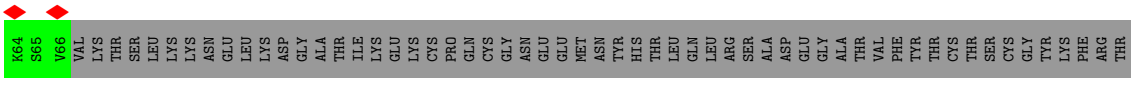
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

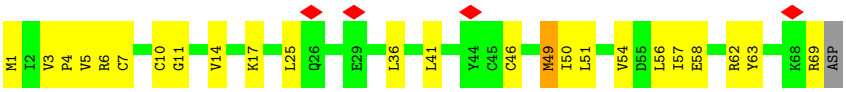
Chain I:





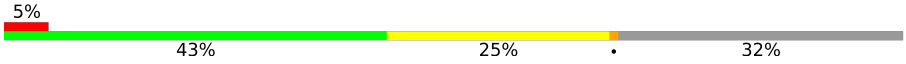
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

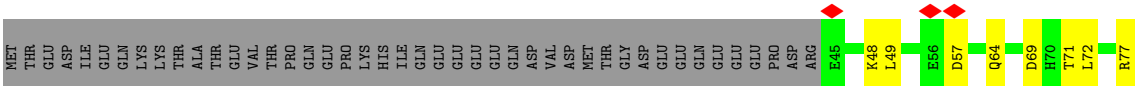
Chain J:

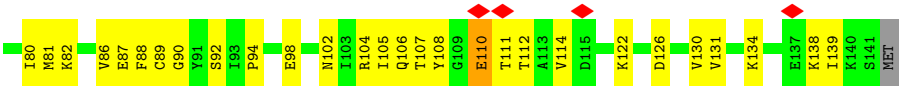


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:

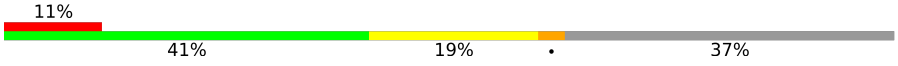


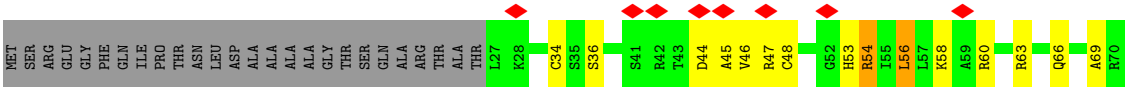




• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

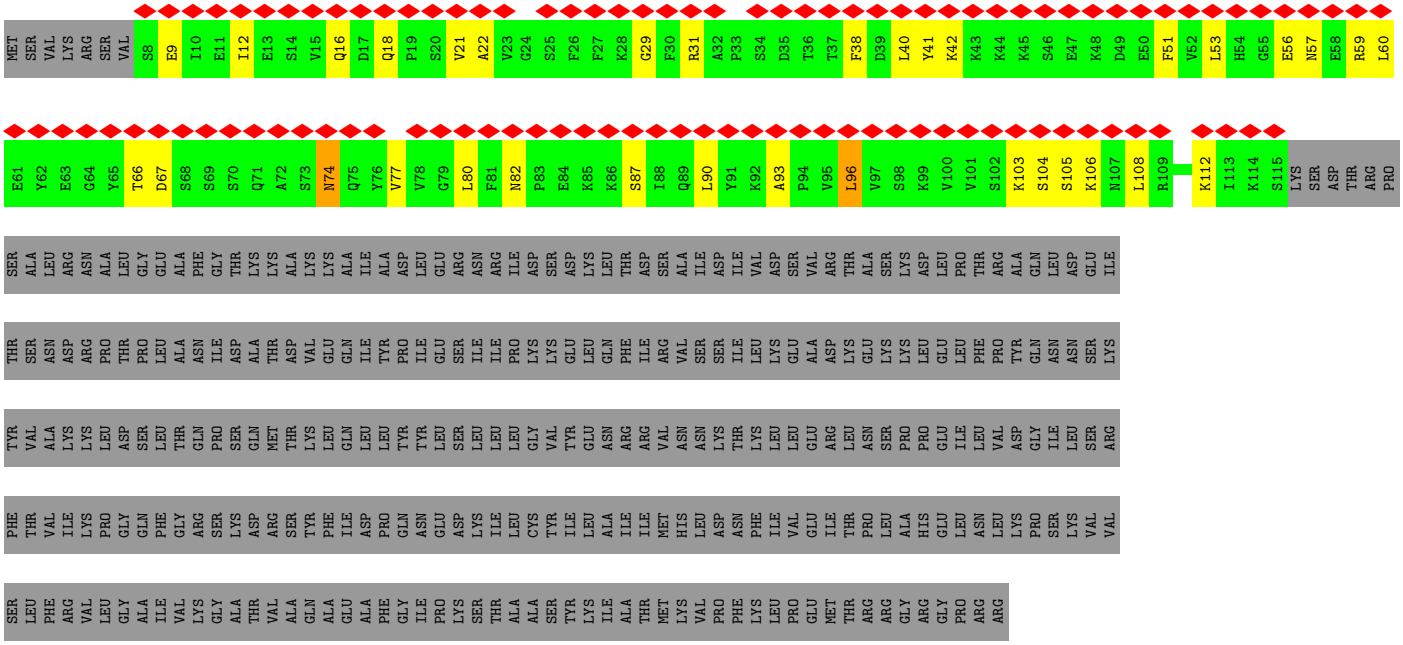
Chain L:





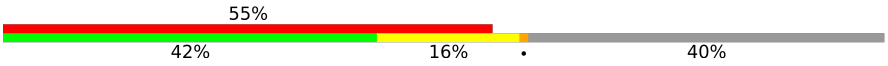
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M:



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain N:

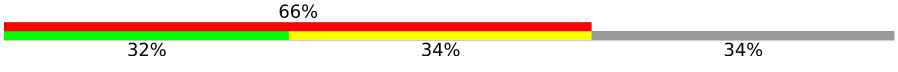


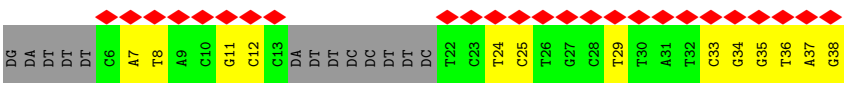
• Molecule 15: RNA

Chain R:

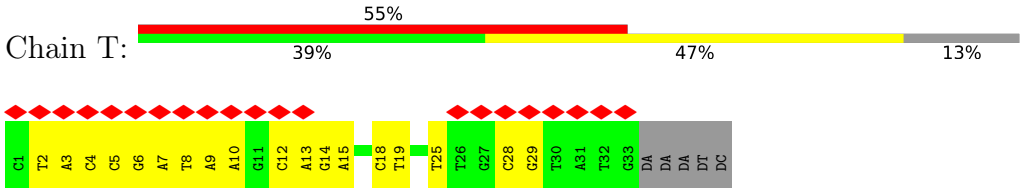
• Molecule 16: Non-template DNA

Chain S:





• Molecule 17: Template DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0237	Depositor
Map size (Å)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, MG, ZN

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	0.21	0/11758	0.33	0/15878
2	B	0.22	0/9459	0.33	0/12785
3	C	0.22	0/2467	0.31	0/3344
4	D	0.11	0/473	0.25	0/641
5	E	0.17	0/1787	0.31	0/2406
6	F	0.20	0/842	0.35	0/1135
7	G	0.15	0/1190	0.32	0/1618
8	H	0.18	0/1070	0.30	0/1449
9	I	0.15	0/485	0.33	0/657
10	J	0.25	0/578	0.34	0/775
11	K	0.23	0/768	0.28	0/1037
12	L	0.17	0/354	0.33	0/468
13	M	0.12	0/872	0.30	0/1170
14	N	0.12	0/1125	0.32	0/1515
15	R	0.22	0/221	0.31	0/343
16	S	0.20	0/563	0.40	0/863
17	T	0.24	0/731	0.41	0/1123
All	All	0.20	0/34743	0.33	0/47207

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11549	0	11632	416	0
2	B	9254	0	9146	321	0
3	C	2415	0	2403	64	0
4	D	467	0	468	14	0
5	E	1751	0	1776	68	0
6	F	827	0	843	33	0
7	G	1164	0	1194	40	0
8	H	1052	0	1021	27	0
9	I	479	0	480	21	0
10	J	569	0	585	19	0
11	K	758	0	756	29	0
12	L	352	0	375	13	0
13	M	856	0	855	25	0
14	N	1105	0	1121	31	0
15	R	197	0	98	9	0
16	S	506	0	285	9	0
17	T	665	0	370	13	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
All	All	33973	0	33408	991	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:SG	1:A:235:ASN:ND2	2.39	0.95
1:A:671:GLN:HB2	2:B:952:HIS:HD2	1.42	0.82
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.62	0.81
1:A:631:ASP:OD2	15:R:12:G:O2'	2.00	0.80
12:L:48:CYS:HB3	12:L:53:HIS:H	1.47	0.79
1:A:942:GLN:HG3	2:B:958:MET:HE1	1.65	0.78
1:A:1226:VAL:HA	1:A:1589:MET:HE1	1.65	0.77
1:A:631:ASP:CG	15:R:12:G:O2'	2.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:PHE:HE1	8:H:98:TYR:HB2	1.51	0.76
1:A:1473:LYS:NZ	1:A:1475:GLU:OE2	2.19	0.75
2:B:1105:ARG:HD3	2:B:1203:LYS:HA	1.68	0.74
2:B:71:LYS:HE2	2:B:422:GLN:HA	1.69	0.74
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.69	0.74
1:A:481:ARG:NH1	1:A:634:ASN:OD1	2.19	0.74
5:E:29:PHE:HB3	5:E:65:THR:HB	1.70	0.74
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.69	0.73
1:A:641:GLU:HB2	6:F:99:LEU:HG	1.68	0.73
3:C:128:ASP:O	3:C:175:GLN:NE2	2.22	0.73
1:A:753:ASN:ND2	1:A:780:ILE:O	2.22	0.73
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.71	0.72
1:A:1124:LEU:HB3	1:A:1129:PRO:HG3	1.72	0.71
2:B:25:PHE:HB3	10:J:58:GLU:HB2	1.72	0.71
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.72	0.71
1:A:1660:VAL:HG22	7:G:103:LYS:H	1.56	0.71
1:A:700:ILE:O	1:A:706:HIS:ND1	2.24	0.71
1:A:1024:THR:O	1:A:1028:GLU:HB3	1.91	0.71
2:B:182:GLN:O	10:J:69:ARG:NH1	2.22	0.71
3:C:100:ARG:NH2	10:J:3:VAL:O	2.16	0.70
5:E:24:LYS:HE3	5:E:35:VAL:HG21	1.72	0.70
1:A:1587:ASP:OD2	5:E:200:ARG:NH1	2.25	0.70
5:E:200:ARG:N	5:E:208:TYR:O	2.20	0.70
1:A:1628:ASP:N	1:A:1628:ASP:OD1	2.23	0.70
1:A:1181:PRO:HD2	6:F:86:THR:HG21	1.72	0.69
1:A:1241:PRO:HB2	1:A:1537:ASP:HB3	1.73	0.69
2:B:129:ARG:NH2	2:B:889:GLY:O	2.25	0.69
15:R:4:A:H2'	15:R:5:A:C8	2.27	0.69
2:B:128:GLN:OE1	2:B:886:ASN:ND2	2.26	0.69
5:E:67:GLU:O	5:E:71:LYS:NZ	2.25	0.69
1:A:105:CYS:SG	1:A:235:ASN:ND2	2.62	0.69
2:B:480:GLN:NE2	2:B:482:SER:O	2.26	0.69
2:B:1079:LEU:HD11	2:B:1087:LEU:HD23	1.74	0.69
1:A:1462:PHE:HD1	1:A:1470:CYS:HB2	1.59	0.68
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.76	0.68
5:E:28:TYR:CZ	5:E:78:LEU:HB2	2.28	0.68
1:A:1559:ARG:NH2	1:A:1560:ASN:OD1	2.27	0.68
1:A:734:THR:O	1:A:738:ASN:ND2	2.26	0.68
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.74	0.68
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.76	0.67
1:A:1439:MET:SD	1:A:1439:MET:N	2.65	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLY:N	1:A:615:ARG:O	2.24	0.67
2:B:53:THR:OG1	2:B:169:ARG:NH1	2.27	0.67
5:E:26:ARG:NE	5:E:187:TYR:O	2.21	0.67
1:A:596:HIS:HD2	1:A:1195:GLU:HG3	1.60	0.67
2:B:568:LEU:HB3	2:B:604:ILE:HD12	1.75	0.67
1:A:389:VAL:HG22	1:A:433:ASP:HB3	1.76	0.67
1:A:1221:ARG:NH1	1:A:1224:GLU:OE2	2.28	0.67
3:C:113:LEU:HB2	3:C:130:ASN:HA	1.76	0.67
2:B:204:ARG:HD2	2:B:486:VAL:HB	1.77	0.66
3:C:103:LEU:HD22	10:J:6:ARG:HD2	1.76	0.66
4:D:47:LYS:NZ	7:G:84:TYR:OH	2.28	0.66
1:A:132:GLU:HG3	1:A:135:LYS:HE2	1.78	0.66
1:A:25:ARG:NH2	1:A:358:ASP:OD2	2.29	0.66
1:A:886:ASN:O	1:A:955:ARG:NH2	2.29	0.66
2:B:320:LEU:HB3	2:B:326:VAL:HG12	1.77	0.66
2:B:809:VAL:HB	2:B:901:VAL:HG23	1.77	0.66
1:A:1063:MET:SD	1:A:1173:LYS:NZ	2.64	0.66
1:A:1053:ASP:HB3	5:E:205:SER:HB3	1.78	0.66
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.78	0.65
5:E:83:CYS:O	5:E:113:GLN:NE2	2.29	0.65
2:B:368:GLN:O	2:B:372:ARG:NH1	2.29	0.65
2:B:733:LEU:O	2:B:904:LYS:NZ	2.29	0.65
1:A:1102:LEU:HG	1:A:1106:LYS:HE2	1.79	0.65
2:B:317:TYR:HB3	2:B:320:LEU:HD13	1.77	0.65
1:A:1094:ALA:O	1:A:1098:SER:OG	2.13	0.65
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.78	0.65
1:A:857:ALA:HB2	1:A:899:LYS:HD2	1.78	0.65
13:M:29:GLY:HA2	14:N:104:LEU:HD11	1.79	0.65
2:B:232:TYR:HD2	2:B:385:VAL:HG22	1.60	0.65
4:D:45:ASP:HA	4:D:49:ASN:HB2	1.78	0.65
1:A:1298:ASP:HA	1:A:1468:LYS:HE3	1.77	0.65
1:A:1299:ASN:H	1:A:1468:LYS:HZ1	1.43	0.65
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.23	0.65
2:B:725:THR:HG21	2:B:767:ASN:HB3	1.79	0.64
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.79	0.64
1:A:23:GLU:OE1	2:B:1130:ARG:NH1	2.31	0.64
1:A:87:ASN:HA	1:A:357:MET:HE2	1.79	0.64
1:A:782:ASP:OD1	1:A:783:LYS:N	2.30	0.64
2:B:209:GLN:HB3	2:B:237:ARG:HD3	1.79	0.64
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.79	0.64
13:M:21:VAL:HG23	13:M:93:ALA:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:SER:OG	3:C:219:PHE:O	2.14	0.64
2:B:626:ILE:HG22	2:B:642:LEU:HD22	1.80	0.64
1:A:671:GLN:HB2	2:B:952:HIS:CD2	2.31	0.64
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.63	0.64
1:A:735:VAL:HG21	1:A:816:LEU:HD22	1.80	0.64
6:F:70:LYS:HA	7:G:94:PRO:HB3	1.80	0.64
1:A:86:TYR:N	1:A:431:GLN:OE1	2.28	0.64
2:B:467:THR:HG22	17:T:25:DT:H4'	1.80	0.64
14:N:108:THR:HG22	14:N:130:PRO:HB3	1.80	0.63
17:T:28:DC:H2'	17:T:29:DG:C8	2.32	0.63
2:B:708:ASP:OD1	2:B:708:ASP:N	2.30	0.63
1:A:57:PHE:O	1:A:60:ASN:ND2	2.23	0.63
1:A:462:LYS:NZ	17:T:15:DA:OP2	2.30	0.63
1:A:536:ILE:HG23	1:A:544:VAL:HB	1.79	0.63
3:C:55:ASP:OD1	3:C:271:ARG:NH1	2.31	0.63
1:A:507:TYR:OH	1:A:641:GLU:OE2	2.16	0.63
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.63	0.63
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.33	0.63
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.81	0.63
4:D:40:LEU:HB3	4:D:93:GLN:HG3	1.80	0.63
2:B:560:ARG:O	2:B:563:SER:OG	2.15	0.63
3:C:170:GLU:OE2	3:C:172:GLN:NE2	2.31	0.63
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.80	0.63
1:A:886:ASN:OD1	1:A:955:ARG:NH2	2.31	0.62
1:A:1587:ASP:OD1	5:E:212:ARG:NH2	2.31	0.62
11:K:80:ILE:HG21	11:K:105:ILE:HD12	1.81	0.62
1:A:1039:ARG:NH1	1:A:1043:GLY:O	2.32	0.62
1:A:1194:GLY:O	1:A:1197:SER:OG	2.10	0.62
1:A:1314:GLN:OE1	1:A:1318:SER:OG	2.17	0.62
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.79	0.62
1:A:573:LEU:HD11	4:D:16:LEU:HD22	1.81	0.62
1:A:413:LEU:HA	1:A:416:ARG:HB3	1.82	0.62
1:A:483:VAL:O	1:A:613:THR:OG1	2.17	0.62
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.64	0.62
1:A:18:ILE:HG21	1:A:354:SER:HB2	1.81	0.62
2:B:557:ASP:OD1	2:B:557:ASP:N	2.33	0.62
2:B:533:THR:HG21	2:B:540:GLY:H	1.65	0.62
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.82	0.62
1:A:874:GLU:OE2	1:A:878:ARG:NH1	2.32	0.61
8:H:92:ASP:N	8:H:92:ASP:OD1	2.33	0.61
1:A:1039:ARG:HH22	5:E:170:LEU:HD11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:THR:OG1	1:A:689:ARG:N	2.31	0.61
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.33	0.61
5:E:21:GLU:OE1	5:E:146:HIS:NE2	2.33	0.61
2:B:327:LEU:HD21	2:B:351:GLN:HB2	1.82	0.61
1:A:20:THR:N	1:A:23:GLU:OE2	2.33	0.61
1:A:1533:GLU:OE1	5:E:14:ARG:NH1	2.34	0.61
2:B:345:SER:HB2	13:M:112:LYS:HE2	1.81	0.61
2:B:244:THR:HA	2:B:411:MET:HE2	1.81	0.61
2:B:760:TYR:HB2	2:B:762:MET:HE2	1.83	0.61
2:B:1104:CYS:HB3	2:B:1107:CYS:HB3	1.83	0.61
1:A:1288:ARG:NH1	1:A:1480:THR:O	2.33	0.61
1:A:126:GLN:NE2	1:A:340:HIS:O	2.33	0.61
1:A:1221:ARG:NH2	1:A:1565:GLU:OE1	2.34	0.60
2:B:26:ILE:O	10:J:62:ARG:NH1	2.34	0.60
3:C:328:LEU:HD12	11:K:72:LEU:HD21	1.82	0.60
1:A:15:ASP:N	1:A:15:ASP:OD1	2.34	0.60
6:F:124:GLU:O	6:F:128:LYS:N	2.33	0.60
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.34	0.60
4:D:26:GLN:NE2	4:D:29:GLN:OE1	2.34	0.60
3:C:102:GLY:HA3	12:L:69:ALA:HB1	1.82	0.60
2:B:154:GLU:OE2	2:B:156:ARG:NH2	2.35	0.60
3:C:42:VAL:O	11:K:138:LYS:NZ	2.35	0.60
16:S:29:DT:H71	17:T:10:DA:H2	1.65	0.60
1:A:1055:ILE:O	1:A:1580:ARG:NH1	2.34	0.60
1:A:1118:VAL:HG21	5:E:154:ILE:HD13	1.82	0.60
3:C:293:ARG:O	3:C:295:ARG:NH1	2.34	0.60
1:A:603:HIS:NE2	1:A:624:TYR:OH	2.30	0.60
2:B:968:ALA:HB1	2:B:979:GLN:HG2	1.84	0.60
1:A:830:MET:HE2	2:B:993:ALA:HB2	1.84	0.59
2:B:890:ASP:OD2	2:B:892:SER:OG	2.20	0.59
3:C:78:VAL:HG21	3:C:113:LEU:HD21	1.84	0.59
1:A:1139:ASN:OD1	5:E:206:GLY:N	2.35	0.59
8:H:23:VAL:HA	8:H:43:ASN:HA	1.84	0.59
1:A:1128:ASN:OD1	1:A:1128:ASN:N	2.35	0.59
2:B:841:ASP:OD2	12:L:58:LYS:NZ	2.30	0.59
2:B:898:LEU:O	2:B:899:GLN:NE2	2.33	0.59
8:H:116:TYR:O	8:H:123:MET:N	2.26	0.59
2:B:683:ASN:OD1	14:N:154:ARG:NH2	2.36	0.59
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.36	0.59
2:B:781:TYR:HB2	2:B:788:ILE:HD11	1.84	0.59
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:ILE:HB	2:B:900:THR:HB	1.84	0.59
1:A:1238:MET:HA	1:A:1543:SER:HA	1.84	0.59
2:B:1088:LEU:HD12	2:B:1092:LEU:HD23	1.84	0.59
2:B:71:LYS:HD3	2:B:421:LEU:HB3	1.85	0.58
2:B:525:TRP:NE1	2:B:690:GLU:OE2	2.32	0.58
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.30	0.58
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.86	0.58
1:A:1124:LEU:HD23	1:A:1129:PRO:HB3	1.84	0.58
1:A:1225:ILE:O	1:A:1595:TYR:OH	2.21	0.58
2:B:1012:PRO:HG2	3:C:275:VAL:HG23	1.85	0.58
1:A:1436:ASN:HD21	1:A:1439:MET:HA	1.68	0.58
7:G:149:ILE:N	7:G:153:PHE:O	2.36	0.58
2:B:351:GLN:NE2	2:B:355:ASP:OD2	2.34	0.58
2:B:745:GLN:NE2	10:J:1:MET:SD	2.73	0.58
2:B:910:THR:O	2:B:912:GLN:NE2	2.37	0.58
1:A:88:PRO:O	1:A:442:LYS:NZ	2.35	0.58
1:A:847:LEU:HD21	1:A:946:LEU:HD22	1.84	0.58
2:B:1103:VAL:HB	2:B:1110:ILE:HD13	1.86	0.58
1:A:491:GLU:OE2	1:A:811:SER:OG	2.16	0.58
1:A:1276:THR:HG23	1:A:1288:ARG:HG2	1.85	0.58
5:E:22:MET:O	5:E:26:ARG:HG2	2.03	0.58
1:A:536:ILE:HD11	1:A:575:LYS:HB3	1.85	0.58
2:B:49:PHE:HZ	2:B:163:VAL:HG12	1.68	0.58
8:H:56:THR:HG21	8:H:145:ARG:HH21	1.68	0.58
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.36	0.58
2:B:1107:CYS:SG	2:B:1130:ARG:NE	2.76	0.58
5:E:61:GLN:O	5:E:63:ASN:ND2	2.36	0.57
1:A:718:THR:OG1	1:A:730:GLN:OE1	2.21	0.57
2:B:369:ASP:OD1	2:B:372:ARG:NH2	2.29	0.57
7:G:140:GLN:HA	7:G:145:ILE:HG23	1.86	0.57
2:B:134:ARG:HA	2:B:162:PRO:HA	1.87	0.57
15:R:4:A:H2'	15:R:5:A:H8	1.68	0.57
1:A:631:ASP:OD1	15:R:12:G:O2'	2.22	0.57
1:A:760:TRP:HZ2	1:A:780:ILE:HD13	1.69	0.57
1:A:1240:LEU:HB3	1:A:1536:ILE:HD12	1.87	0.57
1:A:1447:GLN:HE22	1:A:1459:LYS:HA	1.68	0.57
2:B:412:ILE:HG23	2:B:461:MET:HE1	1.86	0.57
1:A:93:GLN:HG3	1:A:1627:LEU:HD13	1.87	0.57
1:A:106:HIS:O	1:A:107:HIS:ND1	2.38	0.57
1:A:132:GLU:HA	1:A:135:LYS:HG2	1.87	0.57
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10:CYS:SG	10:J:11:GLY:N	2.78	0.57
1:A:1657:LEU:HG	7:G:104:LEU:HD13	1.85	0.57
1:A:1127:TYR:HB3	1:A:1132:TYR:HD2	1.70	0.57
1:A:1447:GLN:O	1:A:1451:ILE:HG12	2.05	0.57
2:B:214:PRO:O	2:B:380:LYS:NZ	2.33	0.57
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.32	0.56
2:B:337:VAL:HG23	2:B:338:PHE:HD1	1.70	0.56
11:K:86:VAL:HA	11:K:107:THR:HA	1.87	0.56
1:A:362:VAL:HG12	1:A:386:LEU:HD13	1.86	0.56
1:A:781:LEU:HB3	1:A:786:TYR:CE1	2.41	0.56
1:A:884:ARG:HH12	1:A:961:VAL:HG23	1.70	0.56
1:A:925:MET:HE1	2:B:955:PRO:HA	1.88	0.56
1:A:1242:ILE:HD12	1:A:1519:LEU:HD11	1.86	0.56
1:A:1463:ASP:OD1	1:A:1466:SER:N	2.30	0.56
1:A:1557:ALA:HB2	5:E:150:VAL:HG22	1.88	0.56
2:B:15:ASP:OD1	2:B:15:ASP:N	2.37	0.56
2:B:280:LEU:HA	2:B:354:LEU:HD21	1.87	0.56
7:G:125:TRP:CD1	7:G:126:GLN:H	2.24	0.56
17:T:7:DA:H2'	17:T:8:DT:H71	1.88	0.56
2:B:129:ARG:HA	2:B:888:ILE:HD12	1.88	0.56
1:A:498:PRO:HB3	1:A:612:LYS:HA	1.88	0.56
1:A:862:THR:HB	1:A:878:ARG:HD3	1.87	0.56
2:B:124:SER:N	2:B:185:GLU:OE2	2.38	0.56
2:B:125:GLU:O	2:B:126:SER:OG	2.23	0.56
2:B:858:ILE:HD11	2:B:874:TYR:HA	1.87	0.56
1:A:771:PHE:HZ	1:A:781:LEU:HD21	1.70	0.56
11:K:104:ARG:NH2	11:K:106:GLN:OE1	2.35	0.56
1:A:65:CYS:HB3	1:A:75:HIS:CE1	2.41	0.56
1:A:811:SER:OG	1:A:815:ARG:NH1	2.32	0.56
2:B:825:PHE:HA	2:B:861:TYR:HB3	1.87	0.56
4:D:83:SER:HA	4:D:86:ILE:HG12	1.87	0.56
1:A:244:ARG:NH1	1:A:246:ASP:OD1	2.39	0.56
1:A:1306:TYR:HE2	9:I:60:LEU:HD22	1.70	0.56
2:B:415:GLU:HG3	2:B:476:LEU:HD21	1.86	0.56
5:E:81:GLU:HB3	5:E:110:PHE:HD1	1.71	0.56
13:M:57:ASN:ND2	13:M:60:LEU:HB2	2.21	0.56
2:B:535:ASP:OD1	2:B:536:GLY:N	2.38	0.56
12:L:48:CYS:N	12:L:53:HIS:O	2.39	0.56
3:C:133:VAL:HG21	3:C:172:GLN:HE21	1.70	0.55
4:D:80:THR:OG1	4:D:81:ASN:N	2.38	0.55
2:B:337:VAL:O	2:B:339:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG23	3:C:130:ASN:HB3	1.88	0.55
5:E:143:ASN:OD1	5:E:145:THR:OG1	2.25	0.55
1:A:628:PHE:HD2	2:B:784:ASP:HB2	1.71	0.55
1:A:1657:LEU:HB2	6:F:133:VAL:HB	1.88	0.55
2:B:335:ARG:NH2	2:B:346:ASP:OD1	2.30	0.55
6:F:109:VAL:HG21	6:F:123:LYS:HG2	1.88	0.55
1:A:1176:ARG:HH21	6:F:154:ASP:HA	1.71	0.55
11:K:110:GLU:HG2	11:K:111:THR:HG23	1.88	0.55
2:B:547:HIS:CE1	2:B:548:LYS:HG2	2.42	0.55
2:B:1015:SER:OG	2:B:1018:THR:OG1	2.21	0.55
1:A:339:PHE:O	1:A:340:HIS:ND1	2.40	0.55
1:A:672:ASP:CG	2:B:950:ASN:HD21	2.15	0.55
7:G:228:LYS:HB3	7:G:230:ARG:HH12	1.71	0.55
9:I:26:SER:H	9:I:39:LYS:HD3	1.71	0.55
1:A:410:LYS:HZ1	1:A:413:LEU:HD12	1.72	0.55
2:B:145:VAL:HG21	2:B:441:LYS:HG2	1.89	0.55
1:A:1530:TRP:HZ3	5:E:139:ALA:HA	1.72	0.55
1:A:1557:ALA:O	1:A:1561:THR:OG1	2.25	0.55
2:B:967:LEU:HD23	2:B:996:PHE:HB2	1.89	0.55
1:A:590:ASN:OD1	1:A:592:GLN:NE2	2.40	0.54
2:B:134:ARG:NE	2:B:160:GLY:O	2.36	0.54
2:B:681:ILE:HD11	2:B:689:VAL:HG21	1.89	0.54
3:C:114:THR:OG1	3:C:115:TRP:N	2.32	0.54
1:A:32:ILE:HG22	1:A:390:LEU:HD22	1.89	0.54
1:A:1654:PHE:HZ	6:F:92:ARG:HB3	1.72	0.54
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.43	0.54
2:B:48:SER:HB3	2:B:404:LEU:HB3	1.89	0.54
2:B:252:TYR:HA	2:B:258:VAL:HG12	1.90	0.54
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.37	0.54
2:B:1010:ASN:HB3	2:B:1025:ASP:HB2	1.88	0.54
1:A:720:PHE:CE1	8:H:98:TYR:HB2	2.37	0.54
2:B:545:PHE:CE2	2:B:551:ILE:HD11	2.42	0.54
13:M:59:ARG:HA	13:M:103:LYS:HB2	1.89	0.54
1:A:627:ASP:OD1	1:A:627:ASP:N	2.41	0.54
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.41	0.54
2:B:129:ARG:HG2	2:B:888:ILE:HG23	1.89	0.54
2:B:547:HIS:HE1	2:B:695:ASN:HA	1.72	0.54
6:F:135:ARG:NH2	7:G:92:ALA:O	2.37	0.54
2:B:808:LYS:HE3	2:B:810:ASP:HB2	1.88	0.54
1:A:1:MET:N	2:B:1094:ASN:O	2.39	0.54
1:A:1478:ALA:HB1	9:I:21:ASN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:ILE:HD11	6:F:134:ILE:HG22	1.89	0.53
2:B:625:GLU:OE1	2:B:648:ARG:NH1	2.41	0.53
2:B:651:ARG:NH2	2:B:669:GLN:OE1	2.41	0.53
3:C:191:ILE:HD11	10:J:5:VAL:HG22	1.90	0.53
12:L:47:ARG:HA	12:L:54:ARG:HA	1.90	0.53
13:M:31:ARG:HE	14:N:129:ALA:HB2	1.74	0.53
1:A:121:LYS:HB3	1:A:219:LEU:HD21	1.90	0.53
1:A:117:ARG:HB2	1:A:185:ARG:NH1	2.24	0.53
14:N:148:ILE:HD12	14:N:148:ILE:H	1.74	0.53
15:R:6:U:H2'	15:R:7:C:C6	2.44	0.53
2:B:307:GLU:OE2	2:B:311:ARG:NE	2.35	0.53
2:B:480:GLN:NE2	2:B:483:GLY:O	2.41	0.53
2:B:672:MET:HE3	2:B:674:ILE:HD11	1.90	0.53
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.25	0.53
11:K:81:MET:HE2	11:K:81:MET:HA	1.91	0.53
1:A:12:THR:HB	2:B:1201:GLU:HG2	1.91	0.53
1:A:850:SER:HA	1:A:853:THR:HB	1.89	0.53
2:B:26:ILE:HG21	3:C:151:THR:HG23	1.90	0.53
13:M:105:SER:HA	13:M:108:LEU:HD23	1.90	0.53
2:B:277:LEU:HD21	2:B:374:LEU:HB3	1.91	0.53
5:E:180:ARG:NH1	5:E:192:ARG:HG3	2.24	0.53
1:A:588:LEU:HD21	2:B:1087:LEU:HD21	1.91	0.53
14:N:113:SER:HB2	14:N:120:LYS:HD3	1.90	0.53
1:A:113:VAL:HG11	1:A:178:LEU:HD22	1.90	0.53
1:A:634:ASN:HB3	2:B:1069:ILE:HD12	1.90	0.53
1:A:1613:MET:HB3	1:A:1618:THR:HG23	1.89	0.53
3:C:248:GLN:NE2	3:C:256:ILE:O	2.42	0.53
15:R:5:A:H2'	15:R:6:U:C6	2.44	0.53
1:A:460:LEU:HA	1:A:466:LEU:H	1.74	0.52
1:A:942:GLN:HB2	1:A:947:LEU:HD23	1.91	0.52
1:A:1218:GLY:H	1:A:1569:VAL:HG23	1.73	0.52
2:B:985:ILE:O	14:N:157:ARG:NH1	2.40	0.52
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.74	0.52
1:A:1237:GLN:H	1:A:1544:ASN:HB3	1.73	0.52
1:A:1589:MET:HB3	1:A:1598:PHE:HE1	1.72	0.52
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.43	0.52
14:N:63:ASP:OD2	14:N:65:SER:OG	2.24	0.52
1:A:611:GLU:HB2	2:B:913:ILE:HG23	1.91	0.52
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.91	0.52
2:B:727:GLY:HA2	2:B:744:LEU:HB2	1.91	0.52
3:C:41:GLU:HA	11:K:134:LYS:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:ILE:O	12:L:60:ARG:NH1	2.42	0.52
9:I:53:ASP:OD1	9:I:61:ARG:NH1	2.42	0.52
1:A:872:ASP:OD2	1:A:875:LEU:N	2.40	0.52
1:A:1330:VAL:HG11	1:A:1455:ARG:HH22	1.74	0.52
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.40	0.52
2:B:854:GLU:OE2	2:B:876:SER:N	2.39	0.52
5:E:161:LYS:HD2	5:E:195:VAL:HG22	1.91	0.52
1:A:124:LEU:HG	1:A:189:VAL:HG13	1.92	0.52
1:A:1183:GLU:OE2	6:F:88:TYR:OH	2.17	0.52
16:S:33:DC:H2"	16:S:34:DG:C8	2.45	0.52
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.74	0.52
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.39	0.52
6:F:111:LEU:HD22	6:F:120:ILE:HD13	1.92	0.52
1:A:1038:ILE:HD11	1:A:1047:GLN:HB2	1.90	0.52
1:A:1600:ARG:NH1	1:A:1616:GLU:OE2	2.41	0.52
2:B:679:GLN:HG2	14:N:157:ARG:HB2	1.92	0.52
1:A:1103:LYS:O	1:A:1107:LYS:HG2	2.10	0.51
1:A:1256:LYS:O	1:A:1499:ARG:NH2	2.43	0.51
2:B:239:VAL:HG22	2:B:245:SER:HB2	1.92	0.51
8:H:80:ARG:HG2	8:H:81:PRO:HD2	1.91	0.51
1:A:518:GLU:OE2	1:A:584:ARG:NH2	2.43	0.51
1:A:595:LEU:HD13	1:A:1198:THR:HG21	1.91	0.51
2:B:936:MET:HE3	2:B:937:PRO:HD2	1.92	0.51
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.91	0.51
2:B:16:PHE:HZ	2:B:751:ILE:HG12	1.75	0.51
10:J:14:VAL:HA	10:J:17:LYS:HD2	1.93	0.51
1:A:1296:PHE:HZ	1:A:1317:ILE:HD11	1.76	0.51
2:B:543:ASN:OD1	2:B:543:ASN:N	2.44	0.51
7:G:121:ASN:OD1	7:G:121:ASN:N	2.42	0.51
1:A:79:ILE:HG23	1:A:360:LEU:HB2	1.91	0.51
1:A:388:LYS:O	1:A:391:THR:OG1	2.24	0.51
2:B:709:PHE:HB3	2:B:960:ILE:HB	1.93	0.51
1:A:1580:ARG:HE	5:E:204:THR:HG21	1.75	0.51
2:B:600:GLN:O	2:B:604:ILE:HG12	2.11	0.51
3:C:312:GLU:HG2	3:C:316:LYS:HZ2	1.74	0.51
3:C:128:ASP:OD1	3:C:174:ARG:NH1	2.44	0.51
17:T:18:DC:H2'	17:T:19:DT:C6	2.45	0.51
1:A:826:PHE:HB3	2:B:777:SER:HB3	1.93	0.51
1:A:1217:LEU:HD13	1:A:1572:ARG:HD2	1.92	0.51
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.93	0.51
2:B:212:ASN:HB3	2:B:590:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:38:PHE:O	14:N:118:SER:OG	2.25	0.51
14:N:111:VAL:HG22	14:N:112:PRO:HD2	1.92	0.51
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.93	0.51
1:A:1243:TRP:NE1	1:A:1533:GLU:O	2.34	0.51
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.91	0.51
6:F:64:ILE:HA	6:F:67:LYS:HE3	1.92	0.51
1:A:1057:ILE:HD11	1:A:1580:ARG:HD2	1.92	0.50
1:A:1130:ALA:HB1	6:F:82:THR:HG23	1.92	0.50
1:A:1221:ARG:HE	1:A:1225:ILE:HD11	1.76	0.50
1:A:1275:THR:O	1:A:1289:SER:N	2.45	0.50
2:B:502:MET:HE3	2:B:542:LEU:HD21	1.93	0.50
2:B:703:LEU:HD11	2:B:762:MET:SD	2.51	0.50
2:B:919:SER:OG	2:B:920:ARG:N	2.44	0.50
5:E:137:GLU:HA	5:E:140:LEU:HB2	1.91	0.50
7:G:135:GLY:HA3	7:G:149:ILE:HG23	1.93	0.50
1:A:708:THR:HB	1:A:742:PRO:HD3	1.94	0.50
1:A:752:LYS:HE2	1:A:768:GLU:HB3	1.94	0.50
1:A:1007:ILE:HG21	2:B:515:THR:HG23	1.91	0.50
2:B:655:TYR:O	2:B:659:ASP:HA	2.10	0.50
1:A:1258:ILE:HD11	1:A:1532:GLN:HE22	1.76	0.50
1:A:1478:ALA:O	9:I:21:ASN:ND2	2.45	0.50
3:C:69:ARG:HB2	11:K:71:THR:HG23	1.94	0.50
17:T:2:DT:H2"	17:T:3:DA:C8	2.46	0.50
1:A:568:VAL:O	1:A:571:HIS:ND1	2.41	0.50
1:A:701:ARG:NH1	11:K:94:PRO:HA	2.27	0.50
2:B:121:VAL:HG12	2:B:133:TYR:CE1	2.46	0.50
2:B:1132:SER:HA	2:B:1169:GLY:HA3	1.92	0.50
6:F:73:ALA:HB2	7:G:94:PRO:HG2	1.92	0.50
1:A:882:ILE:HG12	1:A:888:LYS:HB3	1.94	0.50
1:A:1053:ASP:HB2	1:A:1055:ILE:HG13	1.94	0.50
5:E:154:ILE:HG13	5:E:197:LYS:HB3	1.94	0.50
1:A:135:LYS:HE3	1:A:188:TYR:HE1	1.77	0.50
1:A:697:TYR:HB2	11:K:88:PHE:CZ	2.46	0.50
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.43	0.50
2:B:572:PRO:O	2:B:576:THR:OG1	2.22	0.50
2:B:697:LEU:HD12	2:B:701:ALA:HB1	1.94	0.50
2:B:946:ASP:OD1	2:B:946:ASP:N	2.30	0.50
5:E:155:ARG:NH1	5:E:194:GLU:OE1	2.45	0.50
1:A:368:ARG:HD3	1:A:382:GLN:HG2	1.94	0.50
1:A:1553:TYR:CZ	5:E:147:HIS:HD2	2.29	0.50
2:B:679:GLN:OE1	2:B:679:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:HA	5:E:22:MET:HE2	1.94	0.50
2:B:168:ASN:OD1	2:B:169:ARG:N	2.45	0.49
11:K:89:CYS:SG	11:K:90:GLY:N	2.83	0.49
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.26	0.49
8:H:117:SER:HA	8:H:122:LEU:HA	1.94	0.49
11:K:87:GLU:HB2	11:K:108:TYR:CZ	2.47	0.49
1:A:1032:VAL:HG21	1:A:1179:ILE:HD12	1.94	0.49
2:B:292:ILE:HD12	2:B:306:LEU:HD21	1.94	0.49
2:B:469:ASN:OD1	2:B:470:LEU:N	2.45	0.49
3:C:196:LEU:O	3:C:197:ARG:NH1	2.42	0.49
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.45	0.49
14:N:94:ASP:O	14:N:96:GLU:N	2.42	0.49
2:B:492:ASN:ND2	2:B:494:TYR:HB2	2.26	0.49
2:B:1010:ASN:HB3	2:B:1025:ASP:CB	2.43	0.49
3:C:132:ILE:HD11	3:C:179:PHE:HE2	1.76	0.49
6:F:92:ARG:O	6:F:96:THR:OG1	2.27	0.49
1:A:1589:MET:HE2	1:A:1595:TYR:HE1	1.76	0.49
2:B:525:TRP:HB3	2:B:669:GLN:HE22	1.78	0.49
1:A:27:LEU:HD11	2:B:1112:THR:HG22	1.94	0.49
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.95	0.49
1:A:746:GLY:HA3	1:A:774:GLY:N	2.27	0.49
2:B:887:LEU:HB2	12:L:56:LEU:HB2	1.95	0.49
4:D:89:LEU:HD13	7:G:82:LEU:HD21	1.95	0.49
1:A:992:PRO:HG3	2:B:984:TRP:CD2	2.47	0.49
2:B:862:PHE:HA	2:B:869:THR:HA	1.94	0.49
2:B:140:LYS:HB3	2:B:155:VAL:HG12	1.95	0.49
2:B:670:VAL:HG23	2:B:671:TYR:CD1	2.47	0.49
3:C:70:ILE:HD13	3:C:321:LEU:HB2	1.94	0.49
9:I:10:CYS:HB3	9:I:15:ASP:H	1.78	0.49
2:B:1025:ASP:OD1	2:B:1025:ASP:N	2.45	0.48
16:S:7:DA:H2'	16:S:8:DT:H71	1.94	0.48
2:B:106:LYS:HE2	2:B:171:HIS:HD2	1.78	0.48
2:B:890:ASP:O	12:L:47:ARG:NH2	2.46	0.48
17:T:12:DC:H2"	17:T:13:DA:C8	2.48	0.48
1:A:115:VAL:HG13	1:A:334:VAL:HG21	1.95	0.48
1:A:677:GLY:O	1:A:681:THR:OG1	2.31	0.48
1:A:961:VAL:HG21	2:B:636:GLN:HB2	1.94	0.48
2:B:292:ILE:O	2:B:379:ARG:NH1	2.36	0.48
2:B:1105:ARG:HG3	2:B:1200:VAL:HG21	1.95	0.48
7:G:40:ARG:HG2	7:G:123:TYR:HD1	1.79	0.48
11:K:69:ASP:N	11:K:69:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PRO:HG3	1:A:618:TYR:HE2	1.78	0.48
1:A:657:TYR:CE1	1:A:665:PRO:HB3	2.48	0.48
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.49	0.48
1:A:1122:PRO:HD3	5:E:207:ARG:NH1	2.29	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.14	0.48
2:B:662:ASP:OD1	2:B:663:ILE:N	2.46	0.48
2:B:824:HIS:NE2	2:B:864:ASP:OD2	2.46	0.48
2:B:1010:ASN:ND2	2:B:1025:ASP:O	2.45	0.48
16:S:37:DA:H2"	16:S:38:DG:C8	2.49	0.48
1:A:13:SER:OG	1:A:14:VAL:N	2.47	0.48
1:A:31:GLN:HG2	1:A:78:HIS:CE1	2.48	0.48
1:A:840:ASN:O	1:A:844:THR:OG1	2.28	0.48
2:B:359:LEU:HD21	2:B:374:LEU:HD13	1.95	0.48
2:B:987:ASN:ND2	14:N:157:ARG:HH21	2.10	0.48
2:B:1195:ARG:HH22	2:B:1197:ARG:HH11	1.61	0.48
7:G:138:PHE:HB2	7:G:147:LEU:HA	1.95	0.48
1:A:1533:GLU:HB2	5:E:14:ARG:HH12	1.78	0.48
3:C:80:ALA:HA	3:C:208:CYS:HA	1.95	0.48
6:F:93:ILE:HG13	6:F:132:LEU:HD22	1.95	0.48
1:A:592:GLN:NE2	2:B:1075:GLU:OE2	2.42	0.48
3:C:163:TYR:N	3:C:166:ASP:OD2	2.46	0.48
1:A:103:LEU:HD12	1:A:106:HIS:CD2	2.49	0.48
1:A:506:THR:OG1	1:A:507:TYR:N	2.47	0.48
1:A:1131:LYS:HG2	6:F:83:PRO:HD3	1.95	0.48
2:B:521:LEU:HB3	2:B:523:GLU:OE1	2.14	0.48
2:B:916:LYS:HG2	2:B:926:VAL:HG12	1.94	0.48
1:A:211:THR:OG1	5:E:173:SER:HB2	2.13	0.48
2:B:238:SER:HB3	2:B:361:HIS:H	1.79	0.48
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.95	0.48
5:E:78:LEU:HD12	5:E:107:THR:HB	1.95	0.48
16:S:24:DT:H2"	16:S:25:DC:H5"	1.95	0.48
1:A:1450:ILE:HG23	1:A:1454:HIS:CE1	2.49	0.47
2:B:493:PHE:O	2:B:497:ILE:HG22	2.14	0.47
5:E:31:THR:HG22	5:E:33:GLU:H	1.79	0.47
2:B:881:TYR:O	2:B:906:ARG:N	2.41	0.47
2:B:987:ASN:OD1	2:B:990:ASP:N	2.46	0.47
15:R:6:U:H2'	15:R:7:C:H6	1.79	0.47
1:A:47:GLY:N	1:A:51:ASP:OD2	2.39	0.47
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.22	0.47
2:B:991:THR:HG22	2:B:993:ALA:H	1.78	0.47
1:A:846:ILE:HB	1:A:907:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:ASN:OD1	14:N:150:TYR:OH	2.30	0.47
5:E:20:LYS:HB3	5:E:35:VAL:HG22	1.96	0.47
1:A:730:GLN:O	1:A:734:THR:HG22	2.15	0.47
2:B:673:ASN:HB2	2:B:686:HIS:HA	1.96	0.47
3:C:87:ASN:OD1	3:C:88:ASN:N	2.47	0.47
11:K:112:THR:HG22	11:K:114:VAL:H	1.79	0.47
1:A:102:CYS:SG	1:A:104:PHE:HB2	2.55	0.47
1:A:643:ALA:HB1	2:B:1087:LEU:HD12	1.97	0.47
1:A:32:ILE:HD11	1:A:54:LEU:HD11	1.97	0.47
1:A:410:LYS:NZ	1:A:413:LEU:HD12	2.29	0.47
1:A:589:MET:HE3	1:A:633:MET:HE2	1.96	0.47
1:A:657:TYR:HD1	1:A:658:LEU:HG	1.80	0.47
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.50	0.47
1:A:1000:MET:HG2	2:B:520:LEU:HB3	1.97	0.47
1:A:1305:GLU:HG3	9:I:60:LEU:HD13	1.95	0.47
2:B:851:TYR:CE1	2:B:853:GLU:HG3	2.49	0.47
2:B:861:TYR:HE2	2:B:872:LYS:HE2	1.80	0.47
5:E:25:ASP:OD2	5:E:152:LYS:NZ	2.31	0.47
8:H:93:TYR:HA	8:H:145:ARG:HB2	1.95	0.47
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.95	0.47
1:A:20:THR:O	1:A:23:GLU:HG2	2.14	0.47
1:A:1128:ASN:HD21	6:F:80:ALA:HB1	1.79	0.47
2:B:492:ASN:OD1	2:B:493:PHE:N	2.48	0.47
2:B:630:PRO:HD2	2:B:671:TYR:CE2	2.49	0.47
1:A:1539:ASP:O	5:E:147:HIS:ND1	2.47	0.47
1:A:1542:THR:HG23	5:E:149:LEU:HD22	1.97	0.47
2:B:404:LEU:HD13	2:B:404:LEU:HA	1.79	0.47
1:A:532:GLY:O	1:A:580:HIS:N	2.45	0.47
1:A:697:TYR:HB2	11:K:88:PHE:CE1	2.50	0.47
1:A:1485:MET:H	1:A:1488:ILE:HD11	1.80	0.47
2:B:181:VAL:HG22	2:B:187:SER:HA	1.97	0.47
2:B:747:GLY:HA3	2:B:766:PRO:HB2	1.96	0.47
13:M:74:ASN:OD1	13:M:74:ASN:N	2.48	0.47
1:A:118:TYR:OH	1:A:222:GLU:OE1	2.26	0.46
1:A:591:ARG:HG2	1:A:633:MET:HB3	1.97	0.46
2:B:129:ARG:HG2	2:B:888:ILE:HD12	1.97	0.46
8:H:90:ALA:HA	8:H:143:LEU:HD23	1.98	0.46
2:B:71:LYS:HE3	2:B:71:LYS:HB3	1.72	0.46
4:D:24:ALA:HA	7:G:43:ILE:HG22	1.96	0.46
4:D:91:ARG:HD2	7:G:152:ALA:HB2	1.98	0.46
6:F:72:LYS:HD2	6:F:141:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:THR:O	6:F:136:ARG:NH1	2.38	0.46
12:L:54:ARG:H	12:L:54:ARG:HE	1.61	0.46
1:A:123:ARG:NH1	1:A:190:ASP:OD1	2.47	0.46
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.97	0.46
1:A:986:PHE:HB3	2:B:960:ILE:HG13	1.96	0.46
1:A:1222:LEU:O	1:A:1226:VAL:HG12	2.16	0.46
2:B:703:LEU:HD21	2:B:762:MET:HE1	1.98	0.46
3:C:109:ASP:H	3:C:112:MET:HE2	1.81	0.46
12:L:34:CYS:SG	12:L:36:SER:OG	2.56	0.46
1:A:1657:LEU:HD12	7:G:104:LEU:HB3	1.97	0.46
5:E:15:ALA:O	5:E:19:VAL:HG23	2.15	0.46
1:A:2:ASP:HB3	1:A:5:LYS:HG2	1.98	0.46
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.50	0.46
1:A:1049:MET:N	5:E:208:TYR:OH	2.48	0.46
7:G:41:VAL:HG12	7:G:43:ILE:HG23	1.97	0.46
7:G:73:TYR:CD1	7:G:238:THR:HG21	2.50	0.46
13:M:82:ASN:ND2	13:M:87:SER:O	2.49	0.46
1:A:1289:SER:HA	1:A:1475:GLU:HG3	1.96	0.46
2:B:578:ALA:HB1	2:B:583:LEU:HD12	1.97	0.46
3:C:272:LYS:HD2	14:N:175:TYR:CD2	2.50	0.46
11:K:57:ASP:OD1	11:K:57:ASP:N	2.46	0.46
13:M:22:ALA:HB3	14:N:110:LEU:HD12	1.97	0.46
1:A:31:GLN:HG2	1:A:78:HIS:HE1	1.81	0.46
1:A:96:ILE:HG23	1:A:228:LEU:HD11	1.98	0.46
1:A:191:MET:HE3	1:A:195:LYS:HB2	1.98	0.46
2:B:621:PRO:HG2	2:B:624:LEU:HB2	1.97	0.46
2:B:669:GLN:HA	2:B:672:MET:HE2	1.97	0.46
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.48	0.46
2:B:182:GLN:HA	2:B:182:GLN:HE21	1.81	0.46
6:F:75:PRO:HA	7:G:95:LEU:HD13	1.97	0.46
1:A:135:LYS:HE3	1:A:188:TYR:CE1	2.51	0.46
1:A:202:THR:HG23	1:A:207:SER:HB2	1.97	0.46
1:A:673:HIS:CD2	2:B:783:MET:HE1	2.51	0.46
1:A:938:VAL:O	1:A:942:GLN:HG2	2.16	0.46
1:A:1010:ALA:O	1:A:1013:THR:OG1	2.34	0.46
1:A:1068:PHE:O	1:A:1072:ASN:ND2	2.32	0.46
2:B:301:PHE:CE1	2:B:386:ALA:HB2	2.50	0.46
2:B:1165:ASN:OD1	2:B:1166:LYS:N	2.48	0.46
5:E:16:PHE:CD2	5:E:42:PHE:HE2	2.34	0.46
5:E:52:ARG:O	5:E:55:ARG:HG3	2.15	0.46
7:G:95:LEU:H	7:G:95:LEU:HG	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:111:VAL:HG11	14:N:122:ALA:HB2	1.98	0.46
1:A:440:SER:OG	1:A:455:GLY:N	2.49	0.46
2:B:1047:ARG:HD2	2:B:1067:GLY:O	2.16	0.46
1:A:1101:THR:HG23	1:A:1120:TYR:HB3	1.99	0.45
1:A:1121:ASP:OD1	1:A:1121:ASP:N	2.48	0.45
2:B:18:THR:O	2:B:22:GLU:HG2	2.16	0.45
2:B:260:PHE:CZ	2:B:358:VAL:HG12	2.51	0.45
2:B:629:VAL:HB	2:B:638:PRO:HA	1.98	0.45
2:B:1055:LEU:HD23	2:B:1055:LEU:H	1.81	0.45
3:C:101:ILE:O	3:C:104:VAL:HG22	2.16	0.45
14:N:91:ASP:OD1	14:N:91:ASP:N	2.46	0.45
1:A:94:LEU:HD12	1:A:355:PHE:HB3	1.99	0.45
1:A:415:ASP:O	1:A:419:ILE:HG23	2.16	0.45
1:A:826:PHE:CE2	2:B:952:HIS:HE1	2.34	0.45
1:A:1057:ILE:O	1:A:1060:GLU:HG3	2.15	0.45
1:A:1258:ILE:HD11	1:A:1532:GLN:NE2	2.32	0.45
1:A:1277:GLY:HA3	9:I:43:SER:O	2.16	0.45
2:B:119:ARG:NH1	2:B:125:GLU:OE1	2.46	0.45
2:B:861:TYR:CE1	2:B:870:LYS:HB3	2.51	0.45
3:C:257:GLY:HA3	3:C:268:LYS:HE3	1.98	0.45
9:I:52:ALA:C	9:I:54:ASP:H	2.24	0.45
11:K:104:ARG:O	11:K:105:ILE:HD13	2.16	0.45
12:L:54:ARG:H	12:L:54:ARG:NE	2.13	0.45
1:A:27:LEU:O	2:B:1129:ARG:NH2	2.45	0.45
1:A:1482:LYS:HD2	2:B:307:GLU:HG2	1.99	0.45
1:A:1573:TYR:HB2	1:A:1575:ILE:HG13	1.98	0.45
2:B:692:THR:HB	2:B:694:THR:HG22	1.98	0.45
5:E:66:GLU:CD	5:E:66:GLU:H	2.24	0.45
8:H:116:TYR:CE1	8:H:140:ALA:HB3	2.52	0.45
10:J:7:CYS:HA	10:J:49:MET:SD	2.57	0.45
1:A:88:PRO:HD2	1:A:438:ILE:HD12	1.99	0.45
1:A:378:HIS:O	1:A:378:HIS:ND1	2.49	0.45
1:A:628:PHE:CD2	2:B:784:ASP:HB2	2.49	0.45
1:A:657:TYR:HA	1:A:667:ARG:HD3	1.98	0.45
1:A:703:GLU:OE2	11:K:102:ASN:ND2	2.50	0.45
2:B:420:TYR:O	2:B:424:ILE:HG23	2.16	0.45
3:C:172:GLN:H	3:C:175:GLN:HB2	1.82	0.45
1:A:107:HIS:CE1	1:A:330:LYS:HB3	2.51	0.45
1:A:498:PRO:HG3	1:A:613:THR:O	2.16	0.45
2:B:164:MET:HE3	2:B:192:GLY:HA2	1.97	0.45
5:E:169:ARG:HD2	6:F:138:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:22:LYS:O	8:H:44:VAL:HG22	2.17	0.45
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.98	0.45
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.99	0.45
2:B:172:LEU:HD22	2:B:175:MET:HE2	1.98	0.45
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.97	0.45
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.50	0.45
3:C:329:LYS:HZ1	11:K:122:LYS:N	2.14	0.45
5:E:156:LEU:HG	5:E:160:GLU:HG3	1.99	0.45
14:N:91:ASP:HA	14:N:137:PHE:HA	1.99	0.45
14:N:118:SER:OG	14:N:119:LEU:N	2.50	0.45
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.97	0.45
1:A:1018:TYR:HA	1:A:1021:ARG:HG2	1.99	0.45
1:A:1497:ILE:HD12	1:A:1500:GLN:HB3	1.98	0.45
2:B:143:TRP:CE2	2:B:446:MET:HG2	2.52	0.45
2:B:122:TYR:O	2:B:125:GLU:HB3	2.16	0.45
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.99	0.45
1:A:31:GLN:HA	1:A:78:HIS:O	2.17	0.45
1:A:524:ILE:O	1:A:554:ARG:NH2	2.50	0.45
1:A:1033:SER:OG	1:A:1037:SER:O	2.33	0.45
1:A:1538:VAL:HG11	5:E:142:VAL:HG21	1.98	0.45
1:A:108:PHE:HB3	1:A:227:LEU:HD11	1.98	0.45
1:A:799:GLU:OE1	1:A:1061:SER:OG	2.22	0.45
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.52	0.45
2:B:968:ALA:HB2	2:B:996:PHE:CE2	2.52	0.45
4:D:27:LEU:HD23	6:F:55:PRO:HG2	1.98	0.45
10:J:14:VAL:HB	10:J:50:ILE:HD11	1.97	0.45
13:M:42:LYS:NZ	14:N:32:CYS:HB3	2.32	0.45
1:A:24:ILE:O	1:A:28:SER:N	2.38	0.44
2:B:323:ARG:HA	2:B:326:VAL:HG22	1.99	0.44
3:C:71:MET:HG3	3:C:313:ILE:HG22	1.98	0.44
1:A:358:ASP:OD1	1:A:359:VAL:N	2.50	0.44
1:A:589:MET:HE3	1:A:589:MET:HB3	1.90	0.44
1:A:900:VAL:HG21	1:A:949:GLN:HE21	1.82	0.44
2:B:236:ILE:HG12	2:B:237:ARG:O	2.18	0.44
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.99	0.44
2:B:711:GLN:HG3	2:B:958:MET:HB2	1.99	0.44
2:B:912:GLN:NE2	2:B:1041:ASN:HD21	2.14	0.44
3:C:260:GLU:OE1	3:C:260:GLU:N	2.45	0.44
5:E:62:ALA:HB3	5:E:78:LEU:HB3	2.00	0.44
7:G:228:LYS:HB3	7:G:230:ARG:NH1	2.32	0.44
11:K:48:LYS:HD2	11:K:48:LYS:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:HIS:CE1	2:B:322:ASN:HB2	2.52	0.44
3:C:41:GLU:HG2	3:C:57:ILE:HB	1.99	0.44
7:G:49:LEU:N	7:G:114:GLY:O	2.42	0.44
9:I:12:ASP:HB3	13:M:60:LEU:HD11	1.99	0.44
13:M:9:GLU:OE1	13:M:9:GLU:N	2.51	0.44
13:M:103:LYS:HD2	13:M:106:LYS:HD3	1.99	0.44
1:A:754:LYS:HG3	1:A:784:SER:OG	2.17	0.44
1:A:797:LEU:HD13	1:A:809:VAL:HG21	2.00	0.44
2:B:71:LYS:HE3	2:B:425:ILE:HD12	2.00	0.44
2:B:581:PRO:HG3	2:B:637:TYR:CE1	2.51	0.44
10:J:4:PRO:HG2	10:J:49:MET:HE1	2.00	0.44
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.99	0.44
1:A:127:TYR:HD2	1:A:202:THR:HG21	1.82	0.44
1:A:1038:ILE:HD12	1:A:1584:LEU:HD13	1.99	0.44
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	2.00	0.44
1:A:1314:GLN:NE2	1:A:1462:PHE:HB3	2.33	0.44
2:B:953:ALA:O	2:B:957:ARG:HB2	2.18	0.44
3:C:229:LEU:HB2	3:C:293:ARG:HH11	1.82	0.44
5:E:63:ASN:OD1	5:E:77:SER:OG	2.22	0.44
1:A:496:GLY:O	1:A:614:LEU:HA	2.18	0.44
2:B:106:LYS:O	2:B:108:MET:HG2	2.18	0.44
2:B:1092:LEU:HD13	2:B:1092:LEU:HA	1.77	0.44
3:C:82:TYR:CD2	3:C:126:PHE:HZ	2.36	0.44
9:I:2:SER:HB2	9:I:9:PHE:O	2.18	0.44
15:R:9:A:H2'	15:R:10:G:O4'	2.18	0.44
1:A:597:LYS:HE2	1:A:660:PRO:HG3	1.99	0.44
1:A:1450:ILE:HD12	1:A:1454:HIS:HE1	1.82	0.44
2:B:49:PHE:CZ	2:B:163:VAL:HG12	2.51	0.44
2:B:499:HIS:O	2:B:502:MET:HG2	2.17	0.44
3:C:41:GLU:HG3	3:C:57:ILE:HD13	2.00	0.44
7:G:236:VAL:HG22	7:G:238:THR:HG23	2.00	0.44
1:A:966:LEU:HB2	1:A:969:PHE:CD2	2.53	0.44
1:A:1274:GLU:HB3	9:I:47:VAL:HG13	2.00	0.44
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.74	0.44
2:B:830:ASP:OD2	2:B:869:THR:N	2.48	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.18	0.44
14:N:80:MET:HE2	14:N:80:MET:HB2	1.70	0.44
1:A:911:CYS:O	1:A:915:GLY:N	2.51	0.44
2:B:494:TYR:HB3	2:B:700:LEU:HD11	1.98	0.44
2:B:790:ASN:HB3	2:B:793:ALA:HB3	1.99	0.44
4:D:28:PRO:HB2	7:G:39:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:11:DG:H2"	16:S:12:DC:C4	2.52	0.44
1:A:509:GLU:HB3	1:A:519:LEU:HD11	1.99	0.43
1:A:676:ALA:HB2	1:A:821:ILE:HD13	2.00	0.43
2:B:28:PRO:HG2	2:B:181:VAL:HG21	2.00	0.43
2:B:697:LEU:HB3	2:B:701:ALA:HB3	1.99	0.43
1:A:697:TYR:CE1	1:A:702:PRO:HD2	2.50	0.43
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.75	0.43
5:E:21:GLU:CD	5:E:146:HIS:HE2	2.26	0.43
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.99	0.43
9:I:4:VAL:O	9:I:7:LEU:HD12	2.18	0.43
1:A:14:VAL:HG13	1:A:1632:GLU:HB3	2.01	0.43
1:A:368:ARG:NH1	1:A:383:ASN:OD1	2.47	0.43
2:B:766:PRO:HG2	10:J:54:VAL:HG21	2.00	0.43
9:I:7:LEU:HB2	9:I:16:LEU:HD11	2.00	0.43
1:A:925:MET:HA	1:A:928:MET:HE2	2.00	0.43
1:A:1504:ILE:HD11	1:A:1529:MET:HE1	2.00	0.43
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.92	0.43
3:C:255:VAL:HG11	3:C:273:ASP:HB2	2.00	0.43
13:M:16:GLN:OE1	13:M:18:GLN:N	2.51	0.43
17:T:4:DC:C4	17:T:5:DC:C4	3.06	0.43
1:A:336:GLN:NE2	1:A:348:LYS:O	2.52	0.43
1:A:855:ARG:HH12	1:A:867:ASP:HA	1.84	0.43
1:A:861:VAL:HG11	1:A:892:LEU:HB2	1.99	0.43
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.85	0.43
2:B:144:SER:HA	2:B:151:ASN:HA	2.01	0.43
2:B:1014:TYR:OH	3:C:293:ARG:NH1	2.52	0.43
3:C:167:LEU:HD11	3:C:193:LEU:HD11	2.00	0.43
11:K:82:LYS:HA	11:K:82:LYS:HD3	1.63	0.43
13:M:40:LEU:HD22	13:M:51:PHE:HD2	1.83	0.43
16:S:35:DG:H2"	16:S:36:DT:H5'	1.99	0.43
1:A:677:GLY:HA2	1:A:817:PHE:CE1	2.53	0.43
1:A:1080:TYR:HB2	1:A:1169:LEU:HD11	2.00	0.43
2:B:193:TYR:CD2	2:B:200:GLU:HB3	2.53	0.43
2:B:1079:LEU:HD12	2:B:1079:LEU:HA	1.83	0.43
5:E:200:ARG:HB2	5:E:208:TYR:HB3	2.01	0.43
7:G:88:LYS:HE3	7:G:119:HIS:HB2	2.00	0.43
1:A:129:LEU:HD23	1:A:132:GLU:HG2	2.00	0.43
1:A:1578:SER:HB3	1:A:1581:HIS:CD2	2.54	0.43
1:A:1609:SER:O	1:A:1613:MET:HG3	2.18	0.43
2:B:323:ARG:NH2	2:B:351:GLN:OE1	2.52	0.43
2:B:602:LYS:HE3	2:B:628:TYR:HE2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ASN:OD1	3:C:137:ASN:N	2.51	0.43
7:G:45:LEU:HD12	7:G:118:CYS:HB2	2.01	0.43
8:H:56:THR:HG21	8:H:145:ARG:NH2	2.31	0.43
9:I:10:CYS:N	9:I:15:ASP:O	2.42	0.43
1:A:85:CYS:HB3	1:A:431:GLN:NE2	2.33	0.43
1:A:490:ILE:O	1:A:617:HIS:HD2	2.02	0.43
1:A:942:GLN:HB2	1:A:947:LEU:HA	2.00	0.43
1:A:1197:SER:HA	1:A:1200:MET:HG2	2.01	0.43
2:B:165:LEU:HD22	2:B:193:TYR:CZ	2.54	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.19	0.43
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.88	0.43
7:G:81:VAL:HA	7:G:124:VAL:HG13	2.00	0.43
8:H:92:ASP:O	8:H:145:ARG:HD3	2.18	0.43
8:H:102:TYR:HE2	8:H:117:SER:HB2	1.84	0.43
1:A:368:ARG:HD2	1:A:383:ASN:OD1	2.19	0.43
1:A:1314:GLN:HB2	1:A:1462:PHE:CD2	2.53	0.43
2:B:953:ALA:O	2:B:957:ARG:HD3	2.18	0.43
3:C:119:ASN:OD1	3:C:119:ASN:N	2.52	0.43
14:N:26:PRO:HB2	14:N:29:PHE:CD1	2.54	0.43
17:T:14:DG:H2"	17:T:15:DA:C8	2.54	0.43
1:A:130:ILE:HB	5:E:215:MET:HE2	2.00	0.43
1:A:596:HIS:CE1	1:A:598:ALA:HB3	2.54	0.43
1:A:659:THR:HG23	1:A:666:VAL:HB	2.00	0.43
1:A:24:ILE:H	1:A:24:ILE:HG12	1.60	0.42
1:A:606:ARG:NH2	11:K:98:GLU:OE2	2.52	0.42
1:A:1121:ASP:HA	5:E:207:ARG:HH12	1.83	0.42
1:A:1326:GLU:HG3	1:A:1456:PHE:CZ	2.54	0.42
1:A:1482:LYS:HE2	2:B:304:ASP:HA	2.01	0.42
2:B:49:PHE:O	2:B:52:LEU:HG	2.19	0.42
2:B:125:GLU:C	2:B:127:ARG:H	2.27	0.42
5:E:124:VAL:HG13	5:E:125:PRO:HD3	2.01	0.42
5:E:128:PRO:O	5:E:130:ALA:N	2.52	0.42
8:H:33:GLN:HB2	8:H:36:CYS:HB2	2.01	0.42
1:A:357:MET:HE3	1:A:357:MET:HB2	1.84	0.42
1:A:646:GLU:OE2	1:A:1651:THR:HG21	2.18	0.42
1:A:822:THR:HG22	2:B:778:TYR:O	2.18	0.42
1:A:1180:ASN:HD22	6:F:87:LYS:H	1.67	0.42
1:A:1274:GLU:OE2	1:A:1290:TYR:OH	2.33	0.42
1:A:1495:LYS:HD3	1:A:1495:LYS:HA	1.90	0.42
2:B:131:THR:O	2:B:198:GLY:N	2.51	0.42
1:A:30:LYS:HG3	1:A:31:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HG13	1:A:362:VAL:HG11	2.01	0.42
1:A:769:VAL:HA	1:A:778:CYS:O	2.19	0.42
1:A:842:TRP:O	1:A:846:ILE:HG12	2.20	0.42
1:A:1503:HIS:HB2	1:A:1525:ASN:HB2	2.01	0.42
1:A:1609:SER:HA	1:A:1612:LYS:HE2	2.02	0.42
7:G:105:ILE:HD13	7:G:105:ILE:HA	1.85	0.42
8:H:57:VAL:HG13	8:H:142:LEU:HD11	2.00	0.42
2:B:35:PHE:HE2	2:B:764:ASN:HD21	1.66	0.42
2:B:60:LEU:HA	2:B:63:LEU:HD12	2.00	0.42
2:B:573:ALA:N	2:B:593:ILE:O	2.53	0.42
8:H:98:TYR:C	8:H:118:PHE:HD2	2.28	0.42
1:A:432:ASN:OD1	1:A:444:GLN:HG2	2.19	0.42
1:A:461:GLU:HG3	1:A:462:LYS:HG3	2.02	0.42
1:A:1042:ASP:N	1:A:1042:ASP:OD1	2.49	0.42
1:A:1046:VAL:HG12	1:A:1047:GLN:HG3	2.01	0.42
2:B:727:GLY:O	2:B:743:ARG:HA	2.18	0.42
2:B:847:TYR:CG	12:L:63:ARG:HD2	2.53	0.42
3:C:60:ASP:OD1	3:C:60:ASP:N	2.48	0.42
6:F:137:TYR:HA	6:F:142:SER:O	2.20	0.42
8:H:37:LYS:HE3	8:H:37:LYS:HB3	1.93	0.42
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.54	0.42
12:L:44:ASP:OD1	12:L:45:ALA:N	2.52	0.42
1:A:698:GLY:HA2	11:K:92:SER:HB3	2.01	0.42
1:A:827:THR:OG1	1:A:828:CYS:N	2.52	0.42
1:A:1085:LEU:HD22	6:F:152:ILE:HD12	2.00	0.42
5:E:54:GLN:N	5:E:84:ASP:HB3	2.35	0.42
1:A:1112:PRO:HB2	1:A:1114:TYR:CE1	2.55	0.42
1:A:1238:MET:SD	1:A:1524:VAL:HA	2.59	0.42
2:B:225:ARG:HH12	2:B:261:ARG:CZ	2.33	0.42
2:B:284:SER:HB2	9:I:14:GLY:O	2.20	0.42
2:B:584:CYS:N	2:B:596:VAL:O	2.47	0.42
2:B:861:TYR:CE2	2:B:872:LYS:HE2	2.55	0.42
3:C:69:ARG:HH21	11:K:71:THR:H	1.67	0.42
5:E:74:ASP:OD1	5:E:74:ASP:N	2.52	0.42
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.79	0.42
1:A:589:MET:HE1	1:A:614:LEU:HD13	2.01	0.42
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	2.02	0.42
1:A:1647:ASN:HD22	1:A:1649:VAL:H	1.66	0.42
2:B:177:PRO:O	2:B:181:VAL:HG23	2.20	0.42
3:C:65:ASN:O	3:C:69:ARG:HG3	2.18	0.42
6:F:82:THR:HG22	6:F:84:TYR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:53:VAL:O	14:N:133:PHE:HB3	2.20	0.42
1:A:342:ARG:HH21	1:A:1631:ARG:HB2	1.85	0.42
1:A:381:SER:HB3	1:A:453:ILE:HG23	2.00	0.42
1:A:471:MET:O	1:A:474:LYS:NZ	2.53	0.42
1:A:696:ILE:HD11	1:A:731:ILE:HG23	2.02	0.42
1:A:835:LEU:O	1:A:917:MET:HB3	2.20	0.42
1:A:887:ASN:O	1:A:891:ILE:HG12	2.19	0.42
1:A:1562:ILE:O	1:A:1566:ILE:HG22	2.20	0.42
2:B:354:LEU:O	2:B:358:VAL:HG22	2.20	0.42
2:B:369:ASP:HA	2:B:372:ARG:NH2	2.35	0.42
2:B:413:LEU:HB2	2:B:461:MET:HE2	2.00	0.42
16:S:34:DG:H2"	16:S:35:DG:C8	2.54	0.42
1:A:1050:TYR:OH	1:A:1581:HIS:ND1	2.53	0.42
1:A:1137:SER:OG	1:A:1138:GLU:N	2.53	0.42
2:B:609:ARG:HD2	2:B:655:TYR:CE1	2.55	0.42
2:B:830:ASP:OD1	2:B:830:ASP:N	2.52	0.42
1:A:364:PRO:HD2	1:A:367:PHE:HD2	1.85	0.41
1:A:1076:LEU:O	1:A:1079:LYS:HG2	2.21	0.41
1:A:1260:LYS:HG3	1:A:1500:GLN:HB2	2.02	0.41
1:A:1592:GLN:HB3	5:E:177:ARG:HH21	1.84	0.41
2:B:239:VAL:HA	2:B:245:SER:HA	2.02	0.41
2:B:345:SER:O	2:B:349:VAL:HG12	2.20	0.41
17:T:9:DA:H2"	17:T:10:DA:C8	2.55	0.41
1:A:552:GLU:OE1	1:A:552:GLU:N	2.52	0.41
1:A:589:MET:HB3	1:A:633:MET:HE2	2.02	0.41
2:B:533:THR:CG2	2:B:540:GLY:H	2.30	0.41
2:B:704:THR:HG23	2:B:920:ARG:O	2.20	0.41
8:H:49:VAL:HG11	8:H:55:LEU:HD11	2.02	0.41
9:I:32:GLN:O	13:M:104:SER:OG	2.38	0.41
13:M:53:LEU:HB2	13:M:96:LEU:HD22	2.03	0.41
1:A:896:THR:O	1:A:900:VAL:HG22	2.20	0.41
1:A:1162:ASN:OD1	1:A:1162:ASN:N	2.53	0.41
1:A:1314:GLN:HE22	1:A:1462:PHE:HB3	1.86	0.41
1:A:1317:ILE:HG21	1:A:1470:CYS:SG	2.60	0.41
1:A:1651:THR:OG1	2:B:1085:SER:HB3	2.19	0.41
2:B:412:ILE:HD12	2:B:470:LEU:HD12	2.01	0.41
2:B:547:HIS:CE1	2:B:695:ASN:HA	2.52	0.41
2:B:598:HIS:HB3	2:B:631:PRO:HD3	2.02	0.41
2:B:610:TYR:CG	14:N:145:ILE:HG22	2.55	0.41
2:B:650:LEU:HB3	2:B:663:ILE:HG23	2.02	0.41
6:F:79:ARG:HB3	6:F:144:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:122:LEU:HB3	7:G:124:VAL:HG23	2.02	0.41
17:T:12:DC:H2"	17:T:13:DA:H8	1.85	0.41
1:A:627:ASP:OD2	1:A:629:ASP:CG	2.45	0.41
2:B:414:LYS:O	2:B:417:ILE:HG12	2.21	0.41
2:B:975:HIS:ND1	14:N:166:LEU:HG	2.35	0.41
3:C:111:ASP:N	3:C:111:ASP:OD1	2.50	0.41
5:E:169:ARG:NH1	6:F:74:ILE:HD11	2.35	0.41
9:I:28:VAL:HG13	9:I:37:TYR:HB2	2.01	0.41
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.71	0.41
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.56	0.41
1:A:1042:ASP:OD1	1:A:1044:THR:HG22	2.20	0.41
1:A:1193:VAL:HG21	1:A:1585:ILE:HD12	2.03	0.41
2:B:141:LEU:HD11	2:B:450:LEU:HD11	2.01	0.41
2:B:171:HIS:O	2:B:172:LEU:HD23	2.20	0.41
2:B:186:GLU:OE2	2:B:731:VAL:N	2.51	0.41
13:M:57:ASN:OD1	13:M:60:LEU:N	2.51	0.41
1:A:818:THR:O	1:A:822:THR:HG23	2.20	0.41
1:A:1102:LEU:O	1:A:1106:LYS:HG3	2.21	0.41
2:B:628:TYR:HB2	2:B:640:LEU:HD13	2.03	0.41
2:B:656:LEU:HD23	2:B:656:LEU:HA	1.85	0.41
2:B:675:ALA:HB3	2:B:689:VAL:HG22	2.01	0.41
3:C:40:PHE:CE2	11:K:131:VAL:HA	2.56	0.41
5:E:37:LEU:HD23	5:E:37:LEU:HA	1.86	0.41
7:G:66:LEU:HD13	7:G:66:LEU:HA	1.88	0.41
8:H:93:TYR:HB3	8:H:144:ILE:O	2.20	0.41
1:A:730:GLN:HE21	1:A:730:GLN:HB3	1.58	0.41
1:A:1222:LEU:HD11	1:A:1570:PHE:CE1	2.55	0.41
2:B:52:LEU:O	2:B:60:LEU:N	2.46	0.41
2:B:159:GLY:HA3	2:B:456:ASN:OD1	2.19	0.41
2:B:581:PRO:HG3	2:B:637:TYR:HE1	1.86	0.41
2:B:673:ASN:OD1	2:B:673:ASN:N	2.54	0.41
2:B:912:GLN:CD	2:B:1041:ASN:HD21	2.29	0.41
13:M:12:ILE:HG12	13:M:90:LEU:HD12	2.02	0.41
17:T:5:DC:H2"	17:T:6:DG:C8	2.56	0.41
1:A:498:PRO:HD3	1:A:614:LEU:HD23	2.02	0.41
1:A:1169:LEU:HA	1:A:1169:LEU:HD12	1.88	0.41
1:A:1465:GLU:OE1	1:A:1465:GLU:N	2.50	0.41
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.73	0.41
2:B:122:TYR:O	2:B:125:GLU:N	2.49	0.41
2:B:172:LEU:HA	2:B:175:MET:HG3	2.02	0.41
2:B:282:HIS:HE1	2:B:322:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:GLY:HA3	2:B:349:VAL:HG13	2.02	0.41
2:B:696:ILE:HG13	2:B:697:LEU:HD22	2.03	0.41
2:B:851:TYR:OH	2:B:853:GLU:OE2	2.22	0.41
2:B:916:LYS:HE2	2:B:1036:LEU:HD12	2.03	0.41
2:B:931:TRP:HB3	2:B:936:MET:SD	2.61	0.41
3:C:63:ILE:HD13	3:C:63:ILE:HA	1.94	0.41
3:C:92:ILE:HD11	10:J:57:ILE:HD12	2.03	0.41
8:H:80:ARG:HG3	11:K:108:TYR:CE1	2.56	0.41
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.56	0.41
1:A:6:PRO:HG3	7:G:113:PHE:CG	2.56	0.41
1:A:124:LEU:HD22	1:A:129:LEU:HD22	2.02	0.41
1:A:451:VAL:N	1:A:452:PRO:HD2	2.36	0.41
1:A:538:ASN:N	1:A:542:SER:O	2.38	0.41
1:A:596:HIS:CD2	1:A:1195:GLU:HG3	2.48	0.41
1:A:606:ARG:NH1	1:A:607:VAL:O	2.54	0.41
2:B:523:GLU:OE1	2:B:523:GLU:N	2.49	0.41
2:B:684:ASN:N	14:N:150:TYR:OH	2.53	0.41
2:B:813:LEU:HD23	2:B:813:LEU:H	1.86	0.41
3:C:229:LEU:O	3:C:293:ARG:NH1	2.53	0.41
5:E:7:ARG:O	5:E:11:ARG:HG3	2.20	0.41
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.86	0.41
7:G:108:THR:HG22	7:G:110:ASP:H	1.86	0.41
8:H:14:GLU:HB3	8:H:27:GLU:HB3	2.02	0.41
11:K:126:ASP:O	11:K:130:VAL:HG13	2.20	0.41
14:N:93:THR:O	14:N:93:THR:OG1	2.35	0.41
1:A:80:GLU:HA	1:A:359:VAL:HG22	2.03	0.41
1:A:753:ASN:OD1	1:A:753:ASN:N	2.54	0.41
1:A:1510:PRO:HG3	1:A:1520:VAL:HG12	2.03	0.41
2:B:25:PHE:CE2	10:J:56:LEU:HA	2.56	0.41
2:B:187:SER:N	10:J:63:TYR:OH	2.54	0.41
5:E:178:ILE:N	5:E:213:ILE:O	2.38	0.41
11:K:139:ILE:HD13	11:K:139:ILE:HA	1.87	0.41
1:A:484:ILE:HD11	1:A:631:ASP:HB3	2.03	0.40
2:B:307:GLU:OE1	9:I:7:LEU:HD23	2.21	0.40
2:B:1117:VAL:HG21	2:B:1162:GLY:HA2	2.03	0.40
5:E:47:CYS:HB2	5:E:55:ARG:NH1	2.36	0.40
6:F:82:THR:HG22	6:F:84:TYR:N	2.35	0.40
7:G:137:ILE:HA	7:G:147:LEU:HB2	2.03	0.40
8:H:7:ASP:OD1	8:H:8:ASP:N	2.54	0.40
9:I:21:ASN:OD1	9:I:22:ALA:N	2.53	0.40
1:A:181:LEU:HA	1:A:181:LEU:HD12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:O	1:A:343:PRO:HD2	2.21	0.40
1:A:680:LEU:O	1:A:728:GLY:HA3	2.21	0.40
1:A:1066:PHE:CD1	1:A:1170:MET:HE2	2.57	0.40
1:A:1183:GLU:O	1:A:1185:VAL:N	2.54	0.40
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.47	0.40
2:B:451:MET:HE3	2:B:451:MET:HB3	1.87	0.40
2:B:455:GLU:O	2:B:457:ILE:N	2.52	0.40
2:B:617:THR:HG22	2:B:619:GLY:H	1.85	0.40
3:C:82:TYR:HD2	3:C:126:PHE:HZ	1.69	0.40
4:D:40:LEU:HD22	4:D:93:GLN:HA	2.04	0.40
7:G:234:ARG:HH21	7:G:235:ASN:HB3	1.86	0.40
16:S:35:DG:C5	16:S:36:DT:C4	3.09	0.40
1:A:744:MET:HG2	1:A:801:TYR:CE2	2.56	0.40
1:A:1031:HIS:ND1	1:A:1031:HIS:O	2.55	0.40
1:A:1288:ARG:NH2	1:A:1481:GLU:O	2.47	0.40
1:A:1647:ASN:O	1:A:1652:GLY:HA3	2.21	0.40
2:B:52:LEU:C	2:B:60:LEU:H	2.28	0.40
2:B:445:TYR:O	2:B:449:VAL:HG12	2.21	0.40
2:B:456:ASN:HB3	2:B:459:SER:OG	2.21	0.40
2:B:743:ARG:NH1	3:C:93:GLN:HE22	2.19	0.40
7:G:90:LEU:HD23	7:G:117:TRP:HB2	2.03	0.40
9:I:44:ASN:N	9:I:44:ASN:OD1	2.53	0.40
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.94	0.40
1:A:613:THR:O	1:A:615:ARG:NH2	2.38	0.40
1:A:1458:THR:OG1	1:A:1475:GLU:OE1	2.29	0.40
1:A:1654:PHE:HD2	1:A:1655:ASP:O	2.04	0.40
1:A:1660:VAL:HB	7:G:57:PRO:HG3	2.03	0.40
2:B:101:GLN:HB3	2:B:140:LYS:HG2	2.03	0.40
2:B:208:VAL:N	2:B:401:GLU:O	2.52	0.40
4:D:21:VAL:HG22	4:D:23:HIS:H	1.86	0.40
5:E:5:ASN:O	5:E:9:ILE:HG13	2.22	0.40
7:G:43:ILE:HG12	7:G:122:LEU:HG	2.04	0.40
1:A:460:LEU:HA	1:A:466:LEU:N	2.35	0.40
1:A:1243:TRP:O	1:A:1246:VAL:HG22	2.21	0.40
2:B:418:ASP:O	2:B:422:GLN:HG2	2.22	0.40
2:B:593:ILE:HD13	2:B:593:ILE:HA	1.85	0.40
2:B:827:PHE:HE1	2:B:844:GLY:HA2	1.87	0.40
2:B:936:MET:HE1	2:B:948:ILE:HG13	2.02	0.40
2:B:954:PHE:N	2:B:955:PRO:HD2	2.36	0.40
2:B:960:ILE:O	2:B:964:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1446/1664 (87%)	1364 (94%)	82 (6%)	0	100	100
2	B	1156/1203 (96%)	1064 (92%)	92 (8%)	0	100	100
3	C	302/335 (90%)	284 (94%)	18 (6%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	212/215 (99%)	195 (92%)	17 (8%)	0	100	100
6	F	99/155 (64%)	91 (92%)	8 (8%)	0	100	100
7	G	144/326 (44%)	130 (90%)	14 (10%)	0	100	100
8	H	127/146 (87%)	120 (94%)	7 (6%)	0	100	100
9	I	63/125 (50%)	60 (95%)	3 (5%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
12	L	42/70 (60%)	39 (93%)	3 (7%)	0	100	100
13	M	106/415 (26%)	99 (93%)	7 (7%)	0	100	100
14	N	133/233 (57%)	117 (88%)	16 (12%)	0	100	100
All	All	4047/5236 (77%)	3773 (93%)	274 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	1291/1465 (88%)	1206 (93%)	85 (7%)	14 39
2	B	1017/1053 (97%)	953 (94%)	64 (6%)	15 40
3	C	268/296 (90%)	255 (95%)	13 (5%)	21 48
4	D	56/116 (48%)	52 (93%)	4 (7%)	12 37
5	E	196/197 (100%)	184 (94%)	12 (6%)	15 40
6	F	90/137 (66%)	84 (93%)	6 (7%)	13 38
7	G	131/291 (45%)	119 (91%)	12 (9%)	7 26
8	H	115/128 (90%)	108 (94%)	7 (6%)	15 40
9	I	57/110 (52%)	52 (91%)	5 (9%)	8 28
10	J	64/65 (98%)	62 (97%)	2 (3%)	35 60
11	K	87/130 (67%)	83 (95%)	4 (5%)	23 49
12	L	39/57 (68%)	35 (90%)	4 (10%)	6 22
13	M	98/371 (26%)	91 (93%)	7 (7%)	12 37
14	N	130/220 (59%)	121 (93%)	9 (7%)	13 38
All	All	3639/4636 (78%)	3405 (94%)	234 (6%)	17 39

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	7	VAL
1	A	14	VAL
1	A	15	ASP
1	A	24	ILE
1	A	27	LEU
1	A	36	THR
1	A	43	HIS
1	A	45	VAL
1	A	78	HIS
1	A	79	ILE
1	A	81	LEU
1	A	83	VAL
1	A	113	VAL
1	A	115	VAL
1	A	139	ILE
1	A	202	THR
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	251	ILE
1	A	324	LEU
1	A	408	LYS
1	A	410	LYS
1	A	419	ILE
1	A	420	PHE
1	A	460	LEU
1	A	492	THR
1	A	506	THR
1	A	528	ASP
1	A	536	ILE
1	A	584	ARG
1	A	587	VAL
1	A	591	ARG
1	A	631	ASP
1	A	646	GLU
1	A	658	LEU
1	A	666	VAL
1	A	670	ILE
1	A	688	THR
1	A	715	LEU
1	A	723	TYR
1	A	753	ASN
1	A	805	VAL
1	A	812	VAL
1	A	853	THR
1	A	912	VAL
1	A	940	VAL
1	A	943	ILE
1	A	947	LEU
1	A	957	VAL
1	A	1022	CYS
1	A	1028	GLU
1	A	1030	VAL
1	A	1031	HIS
1	A	1035	ASP
1	A	1118	VAL
1	A	1124	LEU
1	A	1128	ASN
1	A	1185	VAL
1	A	1187	ILE
1	A	1223	ARG

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Mol	Chain	Res	Type
1	A	1233	ILE
1	A	1239	THR
1	A	1258	ILE
1	A	1261	VAL
1	A	1270	VAL
1	A	1298	ASP
1	A	1326	GLU
1	A	1336	GLN
1	A	1439	MET
1	A	1442	VAL
1	A	1443	GLN
1	A	1446	ARG
1	A	1479	ASP
1	A	1480	THR
1	A	1484	LEU
1	A	1488	ILE
1	A	1524	VAL
1	A	1535	PHE
1	A	1561	THR
1	A	1567	ASN
1	A	1628	ASP
1	A	1629	ASN
1	A	1632	GLU
1	A	1660	VAL
2	B	13	THR
2	B	15	ASP
2	B	18	THR
2	B	54	GLU
2	B	104	ILE
2	B	131	THR
2	B	139	LEU
2	B	140	LYS
2	B	155	VAL
2	B	161	LEU
2	B	163	VAL
2	B	189	GLU
2	B	190	ILE
2	B	199	ILE
2	B	212	ASN
2	B	234	ILE
2	B	255	ASP
2	B	274	VAL

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Mol	Chain	Res	Type
2	B	306	LEU
2	B	322	ASN
2	B	328	GLN
2	B	362	LEU
2	B	365	ASP
2	B	397	THR
2	B	402	VAL
2	B	404	LEU
2	B	416	LYS
2	B	425	ILE
2	B	471	VAL
2	B	476	LEU
2	B	478	LEU
2	B	487	VAL
2	B	503	VAL
2	B	557	ASP
2	B	588	ILE
2	B	622	ILE
2	B	624	LEU
2	B	653	VAL
2	B	676	VAL
2	B	677	THR
2	B	692	THR
2	B	699	ILE
2	B	700	LEU
2	B	708	ASP
2	B	749	THR
2	B	803	MET
2	B	806	THR
2	B	882	ILE
2	B	901	VAL
2	B	910	THR
2	B	912	GLN
2	B	913	ILE
2	B	946	ASP
2	B	960	ILE
2	B	1025	ASP
2	B	1030	VAL
2	B	1033	TYR
2	B	1060	VAL
2	B	1071	VAL
2	B	1076	ARG

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Mol	Chain	Res	Type
2	B	1087	LEU
2	B	1089	GLN
2	B	1092	LEU
2	B	1181	VAL
3	C	83	VAL
3	C	91	VAL
3	C	111	ASP
3	C	114	THR
3	C	137	ASN
3	C	151	THR
3	C	191	ILE
3	C	209	ILE
3	C	223	SER
3	C	275	VAL
3	C	279	VAL
3	C	301	ASN
3	C	328	LEU
4	D	15	THR
4	D	37	LEU
4	D	80	THR
4	D	82	LEU
5	E	35	VAL
5	E	46	TYR
5	E	65	THR
5	E	74	ASP
5	E	90	VAL
5	E	117	THR
5	E	124	VAL
5	E	132	ILE
5	E	140	LEU
5	E	156	LEU
5	E	196	VAL
5	E	204	THR
6	F	81	THR
6	F	96	THR
6	F	128	LYS
6	F	134	ILE
6	F	138	LEU
6	F	149	GLU
7	G	43	ILE
7	G	45	LEU
7	G	66	LEU

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Mol	Chain	Res	Type
7	G	71	MET
7	G	80	VAL
7	G	84	TYR
7	G	95	LEU
7	G	121	ASN
7	G	133	LEU
7	G	137	ILE
7	G	239	THR
7	G	245	VAL
8	H	35	GLN
8	H	89	LEU
8	H	92	ASP
8	H	96	VAL
8	H	117	SER
8	H	129	TYR
8	H	131	ASN
9	I	3	VAL
9	I	7	LEU
9	I	28	VAL
9	I	47	VAL
9	I	49	THR
10	J	25	LEU
10	J	49	MET
11	K	49	LEU
11	K	64	GLN
11	K	77	ARG
11	K	110	GLU
12	L	46	VAL
12	L	54	ARG
12	L	56	LEU
12	L	66	GLN
13	M	56	GLU
13	M	66	THR
13	M	67	ASP
13	M	74	ASN
13	M	77	VAL
13	M	80	LEU
13	M	96	LEU
14	N	53	VAL
14	N	56	ILE
14	N	64	ILE
14	N	82	ILE

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Mol	Chain	Res	Type
14	N	111	VAL
14	N	121	ILE
14	N	124	THR
14	N	153	VAL
14	N	155	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	76	GLN
1	A	93	GLN
1	A	384	GLN
1	A	425	ASN
1	A	444	GLN
1	A	596	HIS
1	A	636	HIS
1	A	950	GLN
1	A	1065	GLN
1	A	1081	ASN
1	A	1141	GLN
1	A	1151	ASN
1	A	1180	ASN
1	A	1244	ASN
1	A	1250	GLN
1	A	1300	ASN
1	A	1315	ASN
1	A	1454	HIS
1	A	1503	HIS
1	A	1509	HIS
2	B	128	GLN
2	B	182	GLN
2	B	282	HIS
2	B	427	GLN
2	B	462	GLN
2	B	547	HIS
2	B	739	ASN
2	B	748	GLN
2	B	829	ASN
2	B	886	ASN
2	B	950	ASN
2	B	952	HIS

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Mol	Chain	Res	Type
2	B	1041	ASN
2	B	1157	GLN
3	C	172	GLN
3	C	296	ASN
4	D	30	HIS
5	E	61	GLN
5	E	115	ASN
5	E	179	GLN
7	G	64	GLN
7	G	74	ASN
8	H	3	ASN
8	H	11	GLN
8	H	83	GLN
10	J	23	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	8/12 (66%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	5	A
15	R	10	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\|>2$
17	3DR	T	17	17	8,11,12	0.55	0	9,14,17	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3DR	T	17	17	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	T	17	3DR	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

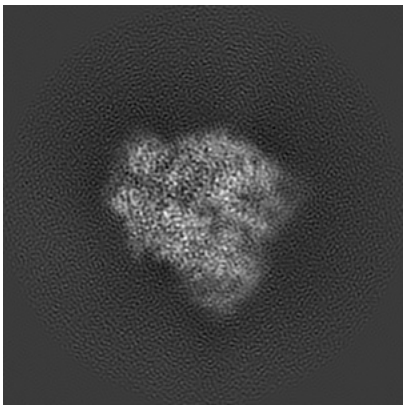
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50965. These allow visual inspection of the internal detail of the map and identification of artifacts.

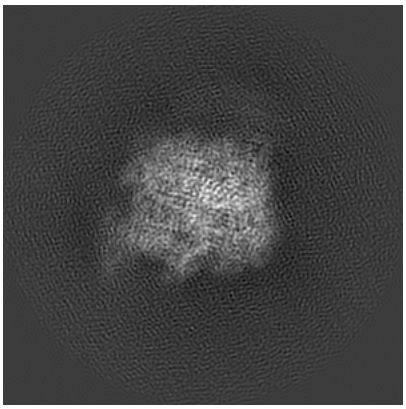
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

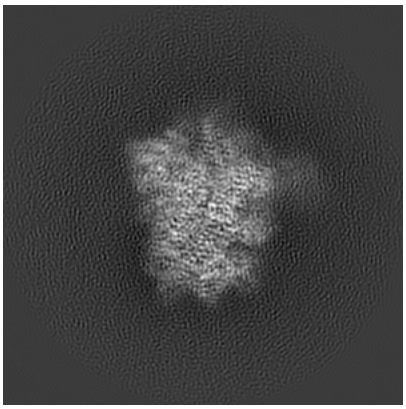
6.1.1 Primary map



X

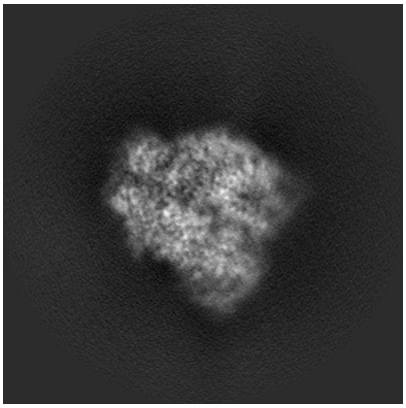


Y

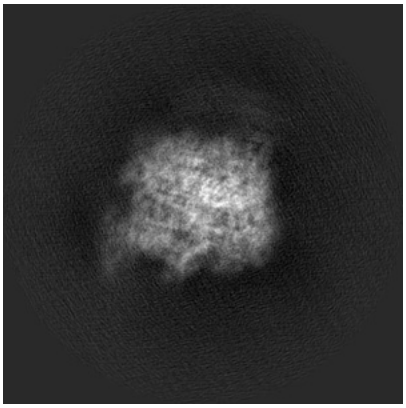


Z

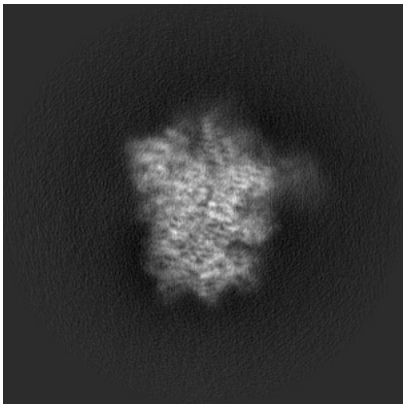
6.1.2 Raw map



X



Y

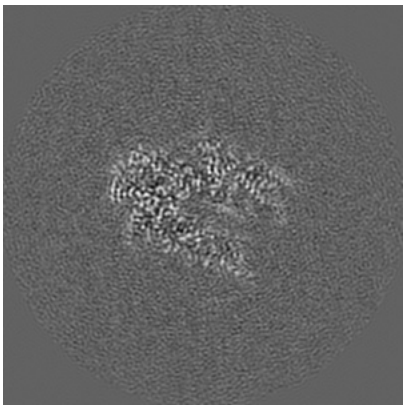


Z

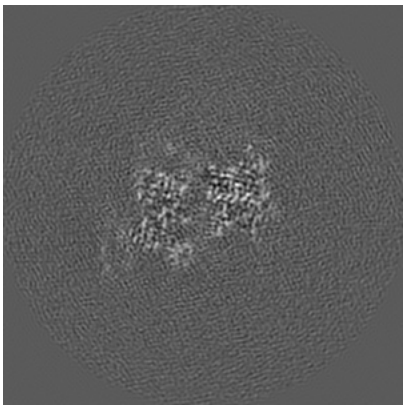
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

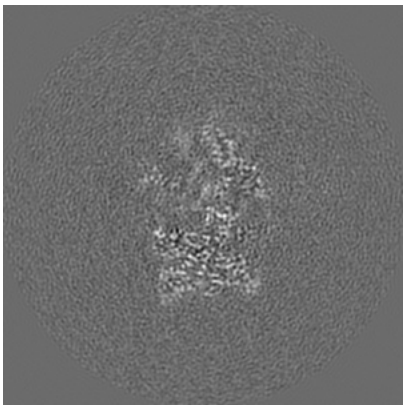
6.2.1 Primary map



X Index: 144

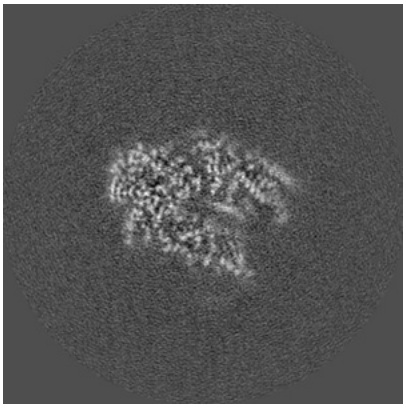


Y Index: 144

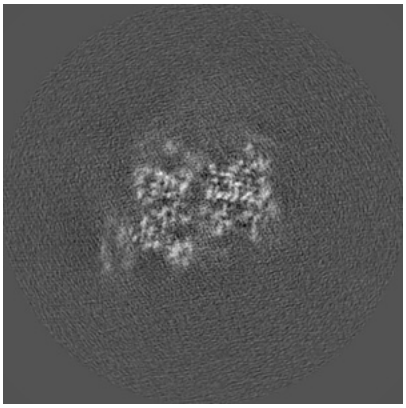


Z Index: 144

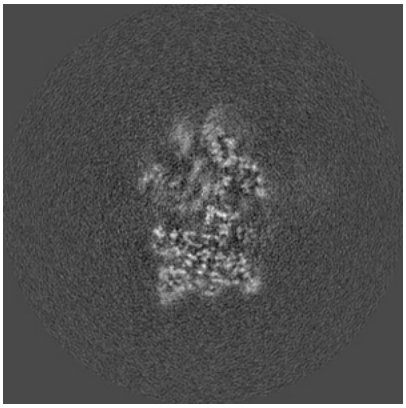
6.2.2 Raw map



X Index: 144



Y Index: 144

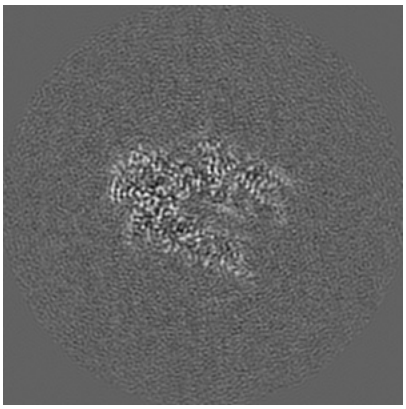


Z Index: 144

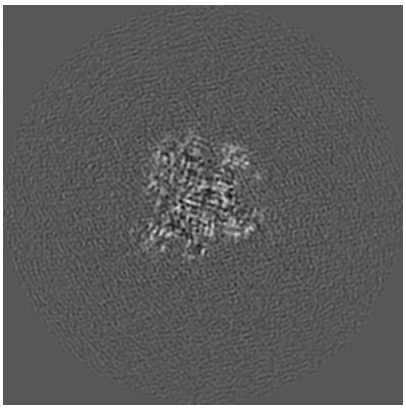
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

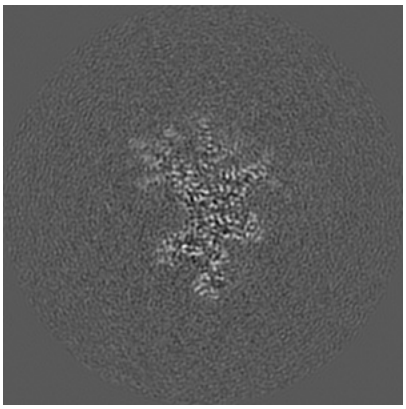
6.3.1 Primary map



X Index: 144

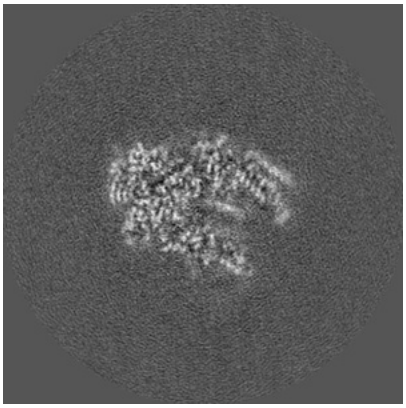


Y Index: 123

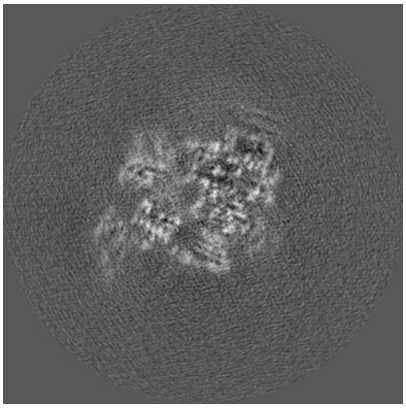


Z Index: 162

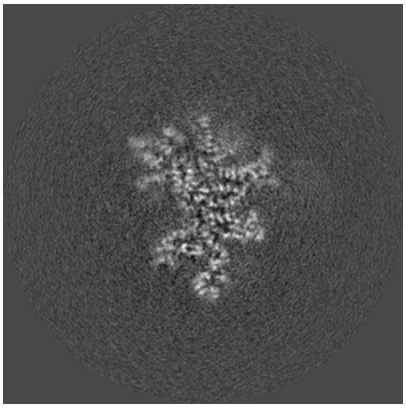
6.3.2 Raw map



X Index: 145



Y Index: 158

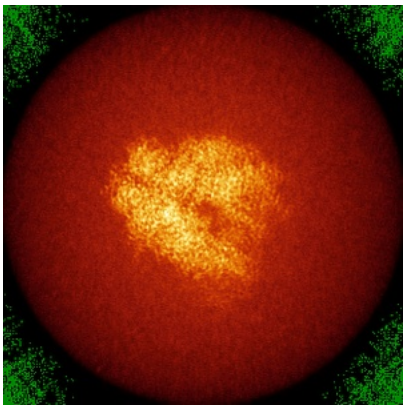


Z Index: 162

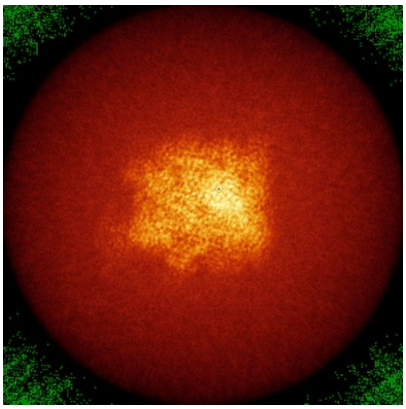
The images above show the largest variance slices of the map in three orthogonal directions.

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

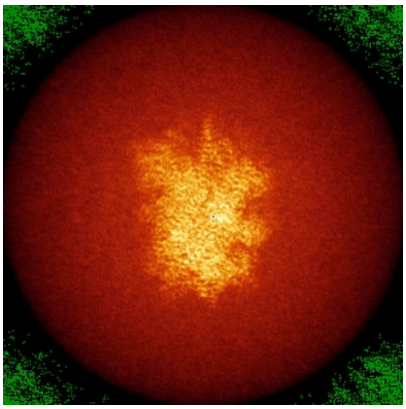
6.4.1 Primary map



X

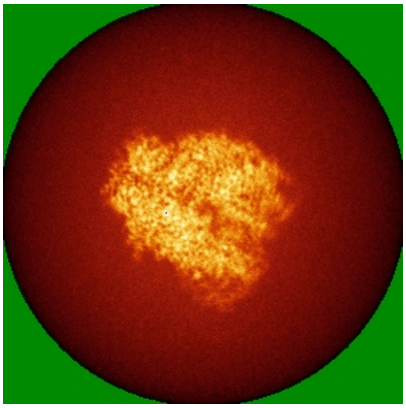


Y

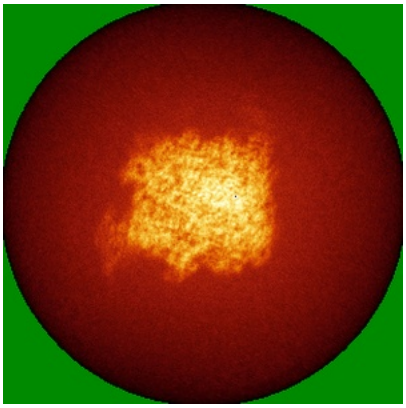


Z

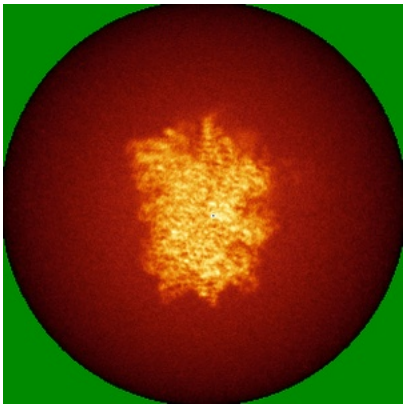
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

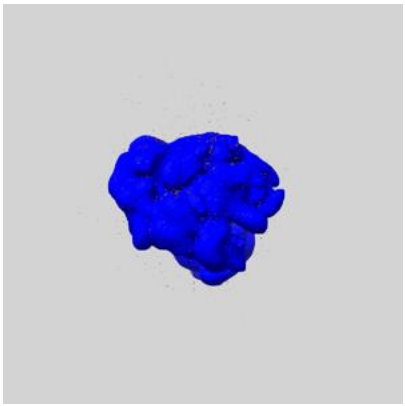
6.6 Mask visualisation (i)

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

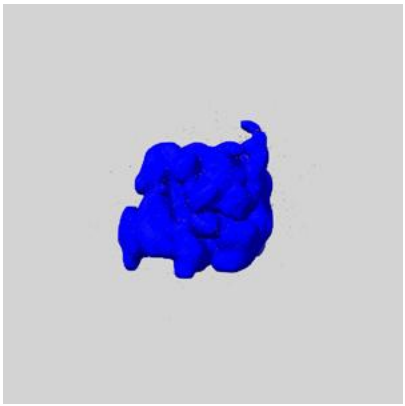
A mask typically either:

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

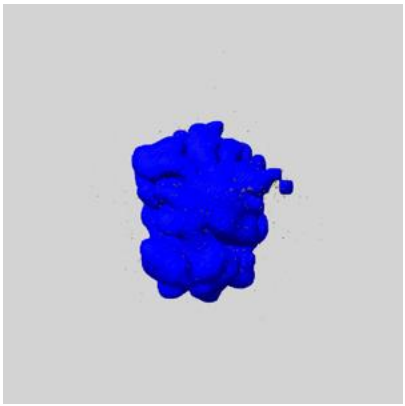
6.6.1 emd_50965_msk_1.map (i)



X



Y

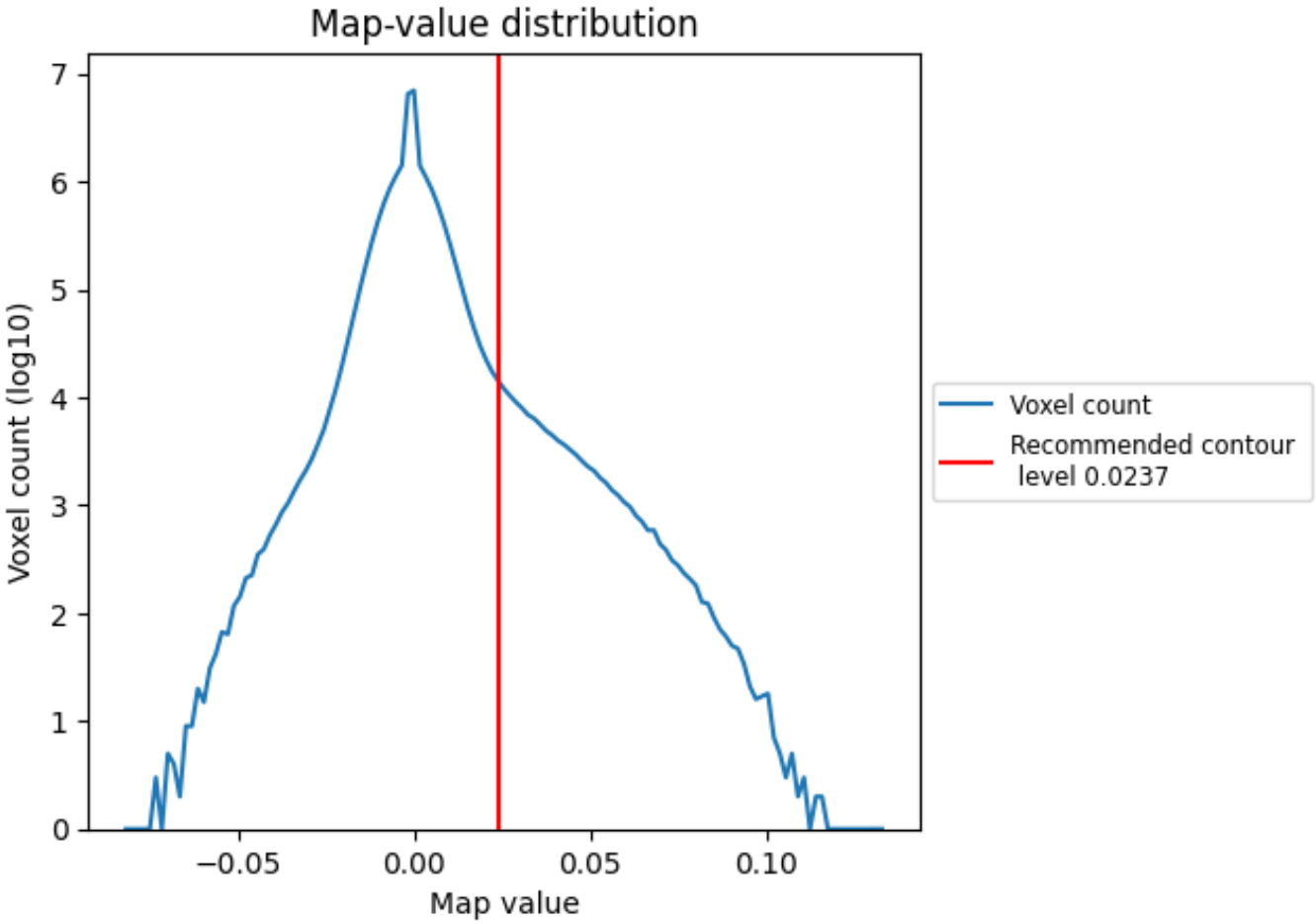


Z

7 Map analysis

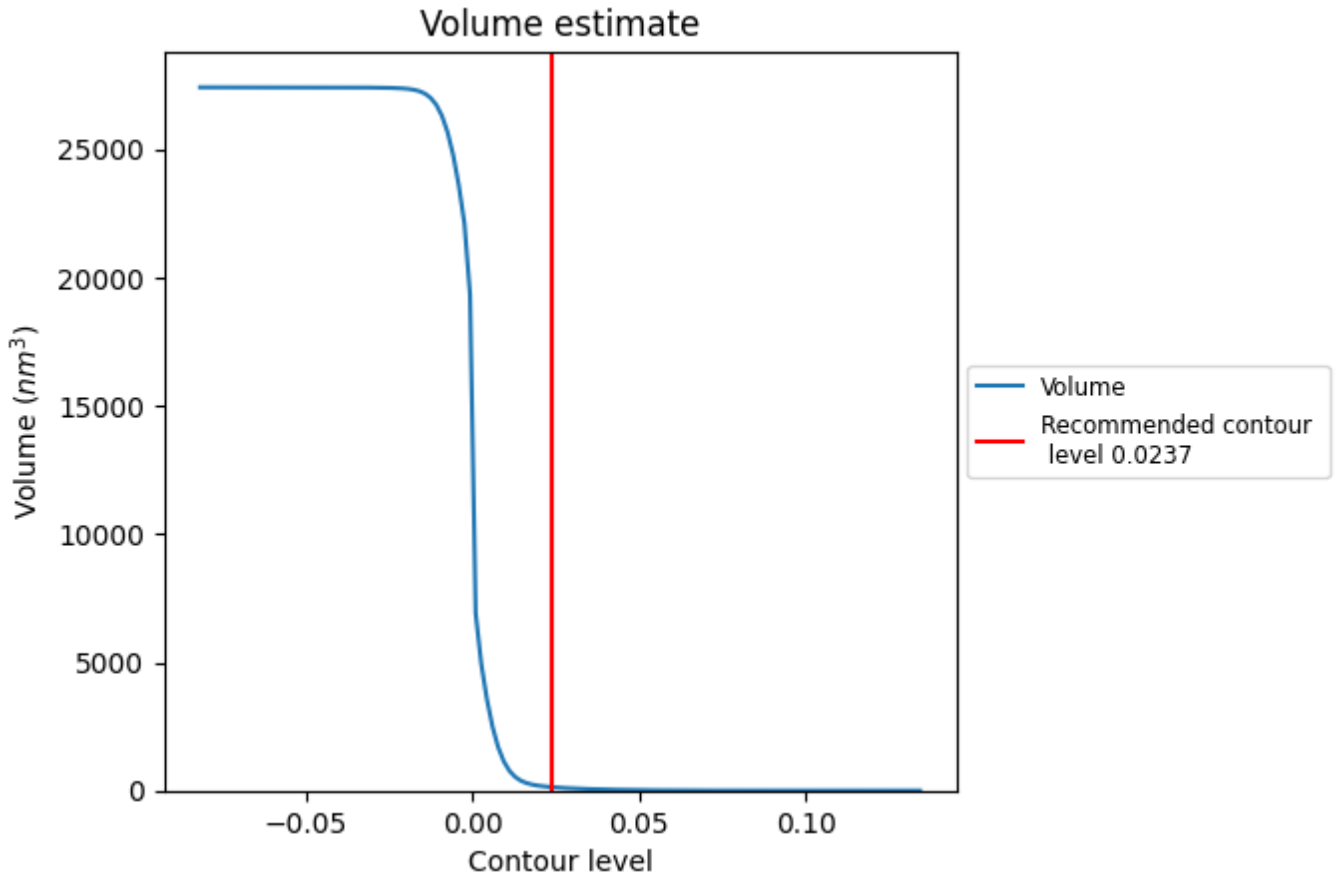
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

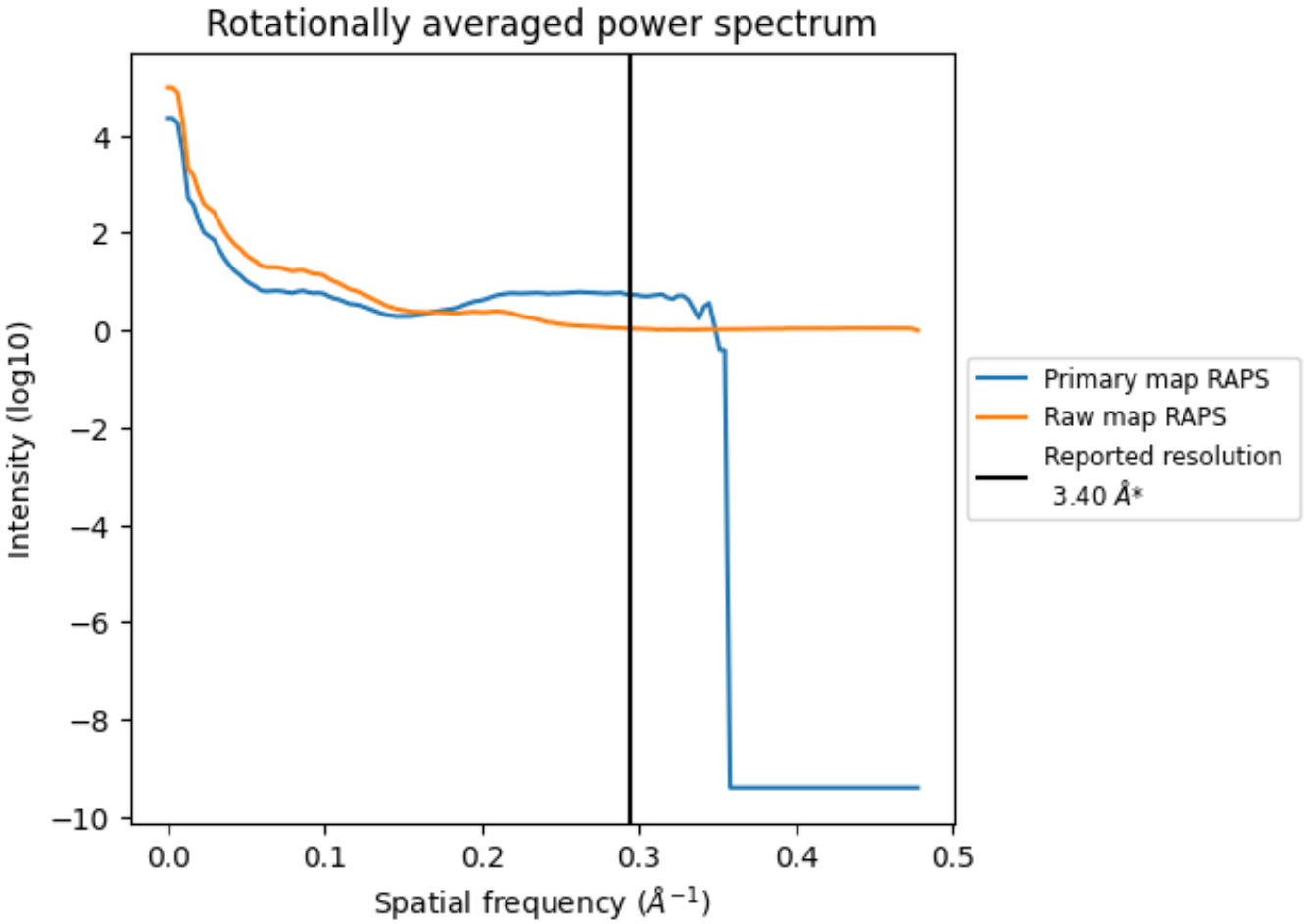
7.2 Volume estimate



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

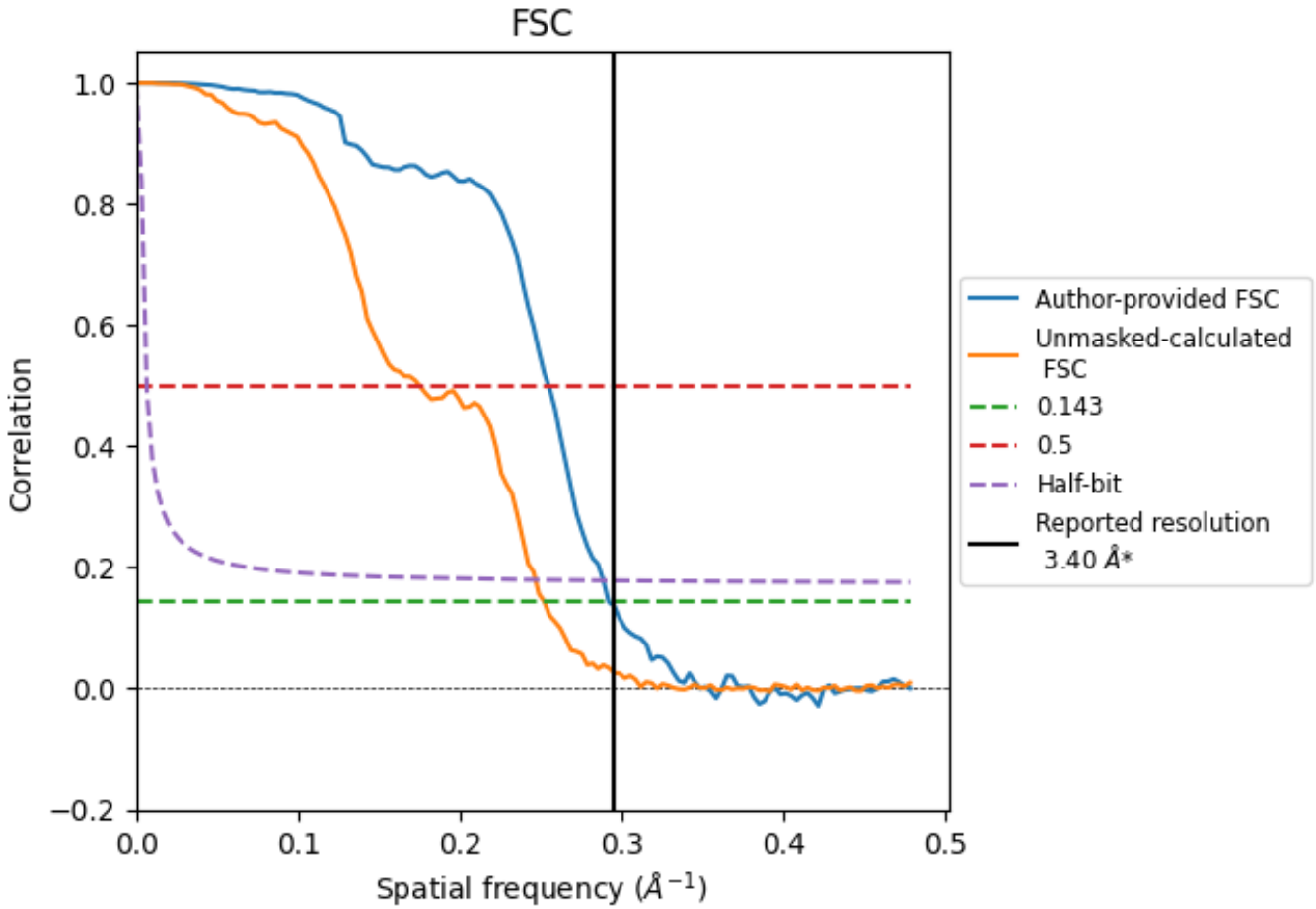


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

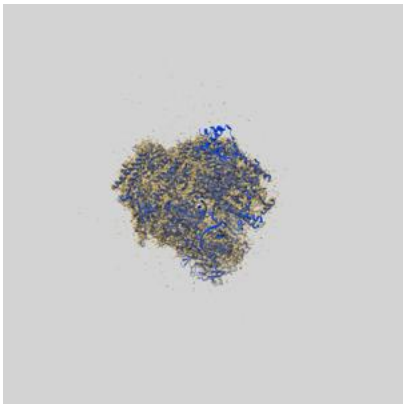
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.93	3.47
Unmasked-calculated*	3.97	5.71	4.06

*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 3.97 differs from the reported value 3.4 by more than 10 %

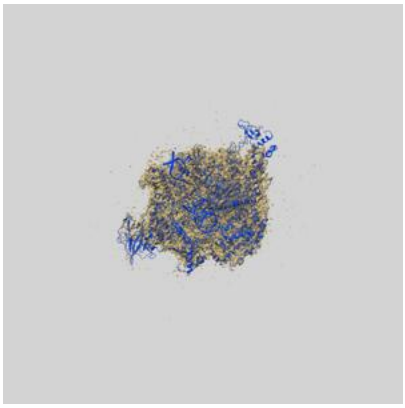
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50965 and PDB model 9G26. Per-residue inclusion information can be found in section 3 on page 7.

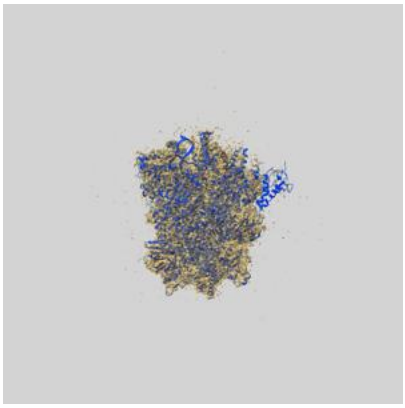
9.1 Map-model overlay



X



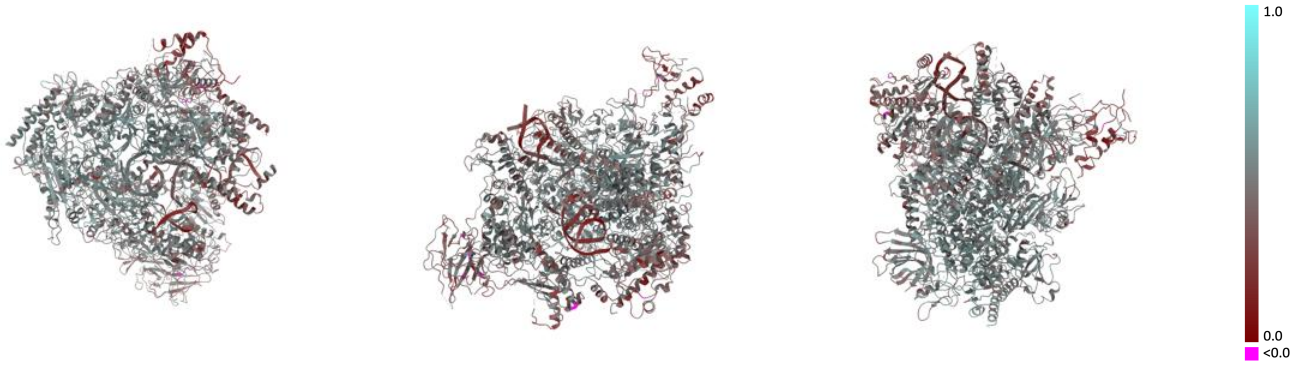
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0237 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.

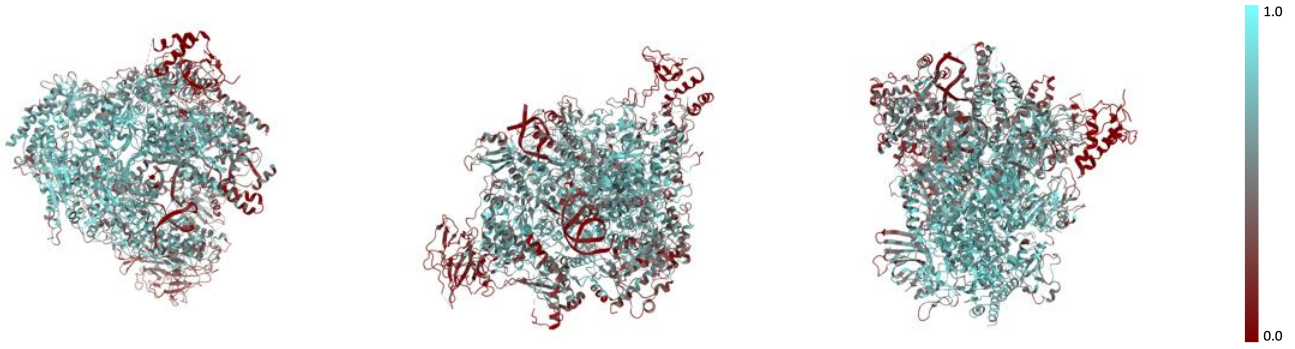
9.2 Q-score mapped to coordinate model (i)



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.

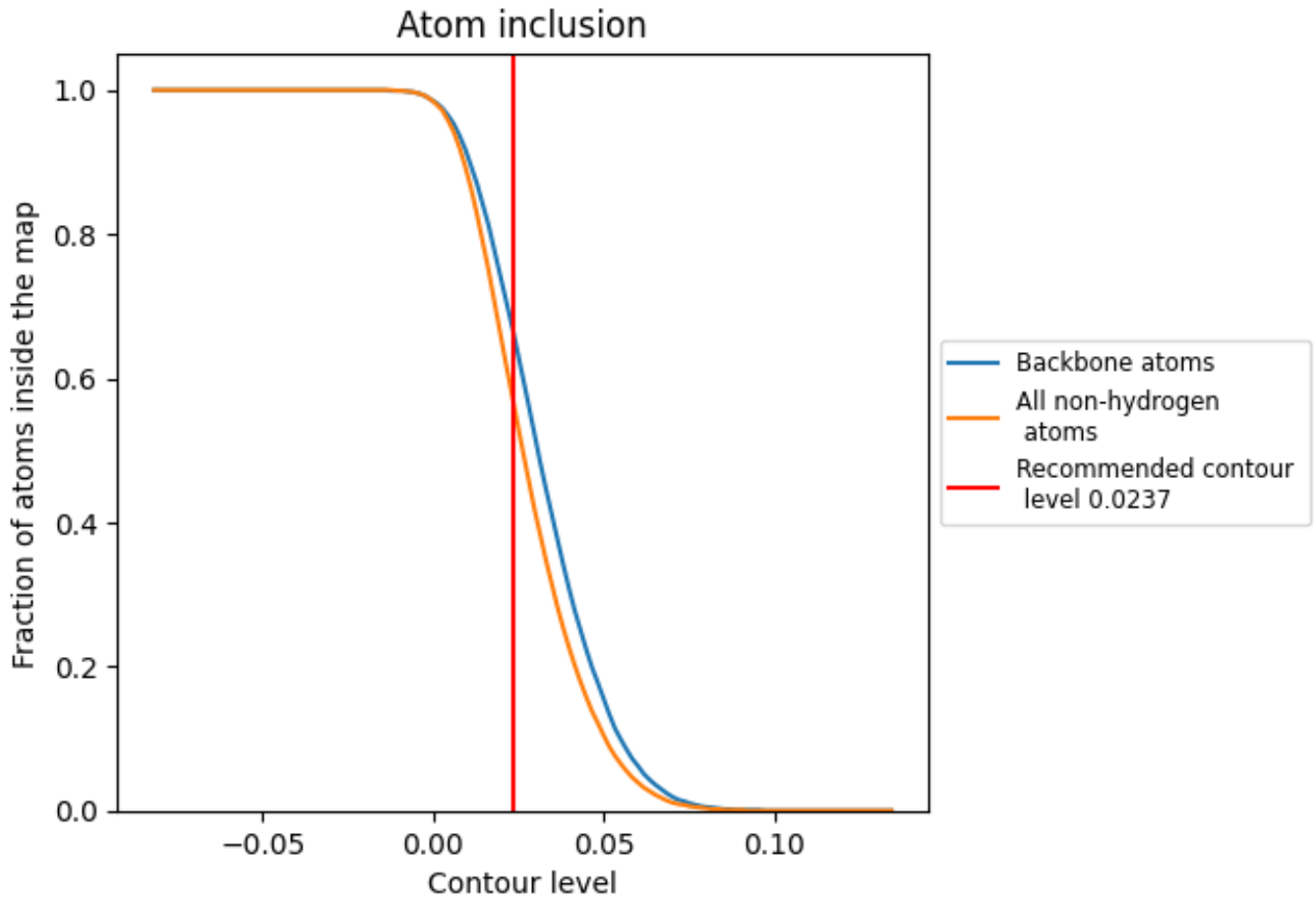
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0237).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 56% 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 (0.0237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5630	0.4650
A	0.6070	0.4800
B	0.6700	0.5010
C	0.6580	0.5070
D	0.1450	0.3180
E	0.4480	0.3900
F	0.6160	0.4770
G	0.3050	0.3880
H	0.5560	0.4750
I	0.3980	0.4190
J	0.7230	0.5230
K	0.7150	0.5050
L	0.6210	0.4900
M	0.1410	0.3670
N	0.1260	0.3710
R	0.7110	0.4660
S	0.1220	0.2320
T	0.3430	0.3190