Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 05:24 am GMT

PDB ID	:	6RWE
EMDB ID	:	EMD-10038
Title	:	RNA Polymerase I Open Complex conformation 2
Authors	:	Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on	:	2019-06-04
Resolution	:	3.00 Å(reported)

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

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

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

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

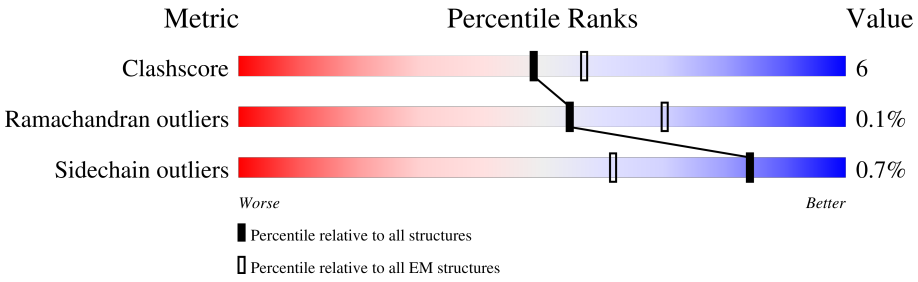
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	T	70	34% 51% 20% 29%
2	U	70	27% 43% 21% 36%
3	M	415	82% 81% 14% 6%
4	A	1664	26% 76% 12% 12%
5	B	1203	33% 85% 13%
6	C	335	21% 81% 10% 9%
7	D	137	13% 45% 6% 49%
8	E	215	30% 88% 11%

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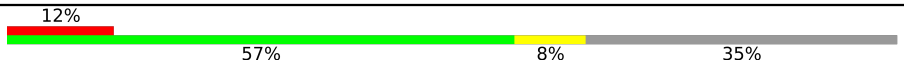
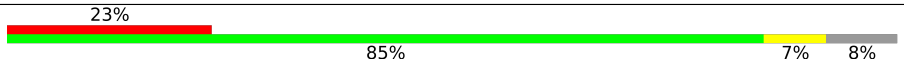
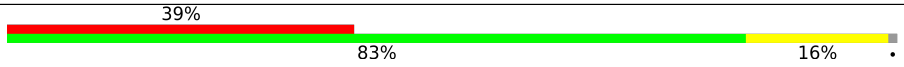
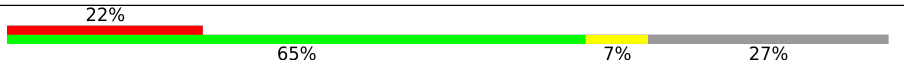
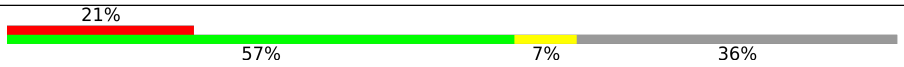
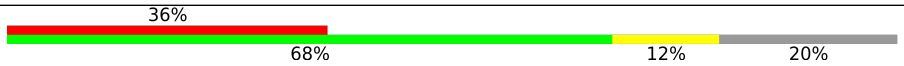
Mol	Chain	Length	Quality of chain
9	F	155	
10	G	326	
11	H	146	
12	I	125	
13	J	70	
14	K	142	
15	L	70	
16	N	233	
17	O	627	
18	Q	514	
19	S	894	
20	R	507	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 53719 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 DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	T	50	1000	481	164	305	50	0	0

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	U	45	944	447	192	261	44	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	392	3100	1978	525	593	4	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1464	11558	7303	2011	2183	61	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1180	9371	5923	1644	1754	50	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	304	2418	1536	414	460	8	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	70	Total	C	N	O	S	0	0
			551	340	100	109	2		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	199	Total	C	N	O	S	0	0
			1576	1012	273	286	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	134	Total	C	N	O	S	0	0
			1072	676	181	211	4		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	124	Total	C	N	O	S	0	0
			942	584	160	189	9		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			810	506	132	167	5		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	499	Total	C	N	O	S	0	0
			4086	2636	661	767	22		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	477	Total	C	N	O	S	0	0
			3936	2529	675	712	20		

- Molecule 19 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	610	Total	C	N	O	S	0	0
			4963	3160	842	950	11		

- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	330	Total	C	N	O	S	0	0
			2771	1791	489	480	11		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

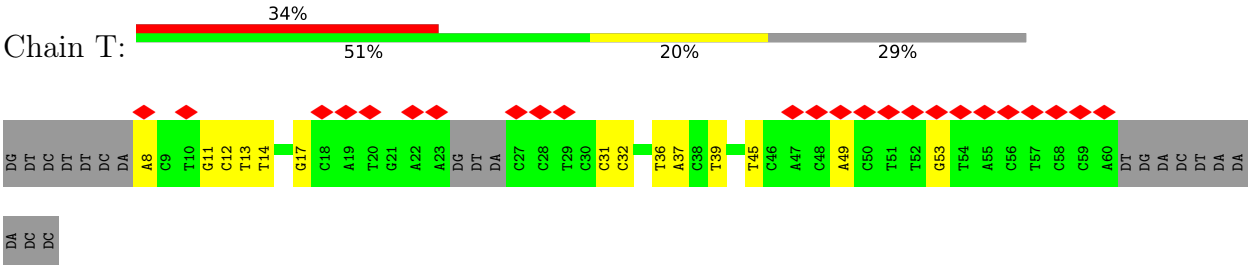
Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0
21	Q	1	Total Zn 1 1	0

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.

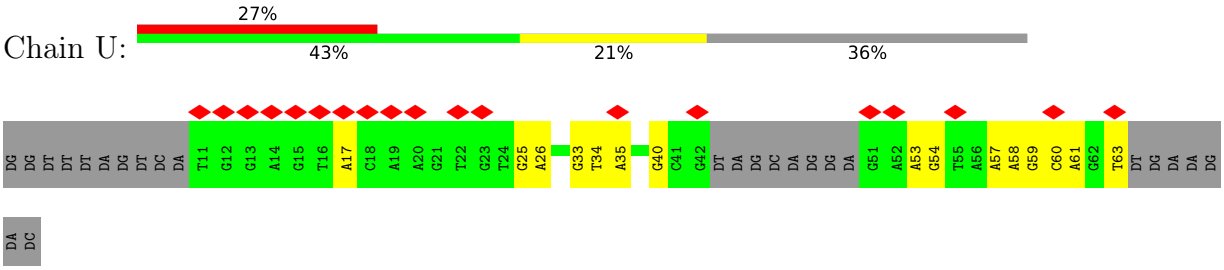
• Molecule 1: Template strand

Chain T:



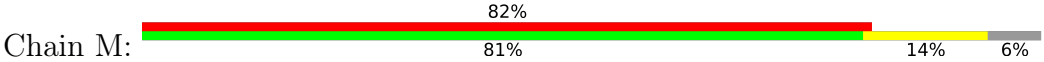
• Molecule 2: Nontemplate strand

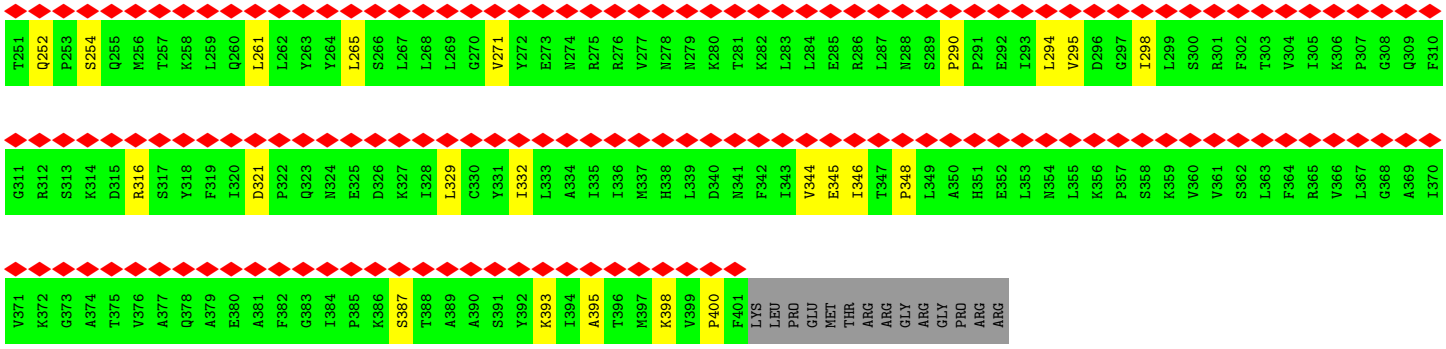
Chain U:



• Molecule 3: DNA-directed RNA polymerase I subunit RPA49

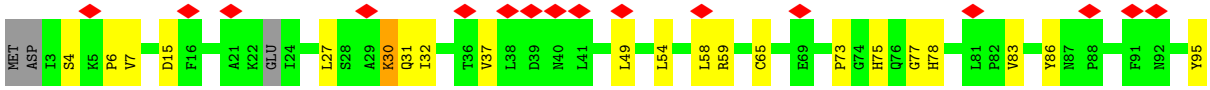
Chain M:

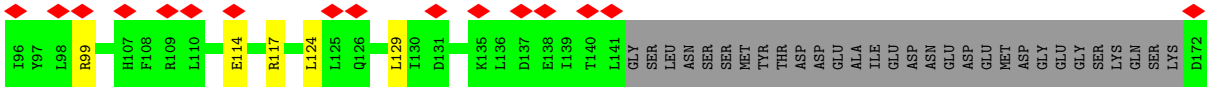


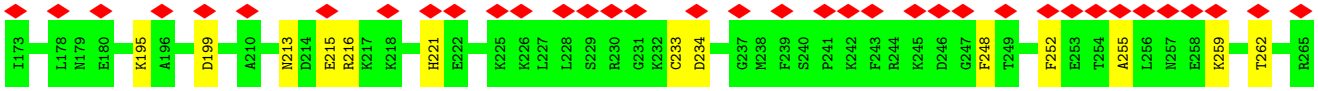


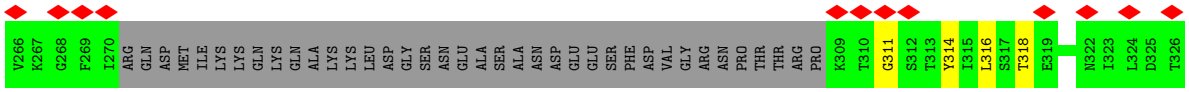
• Molecule 4: DNA-directed RNA polymerase I subunit RPA190

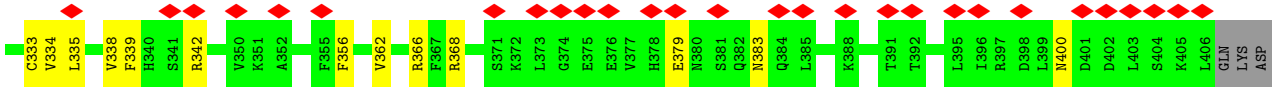
Chain A:

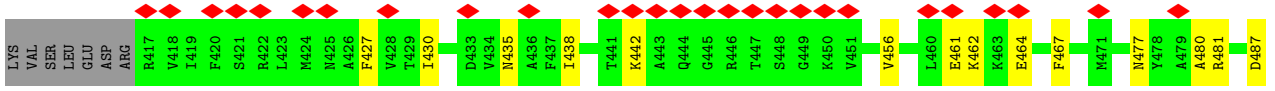


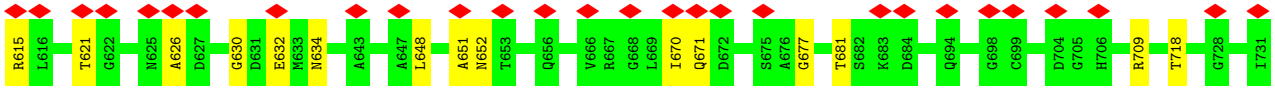


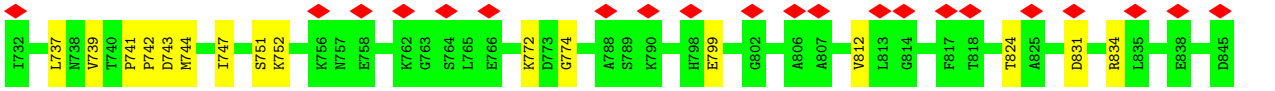


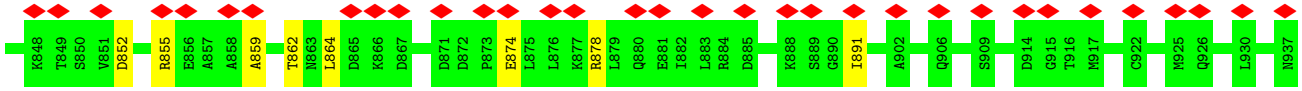


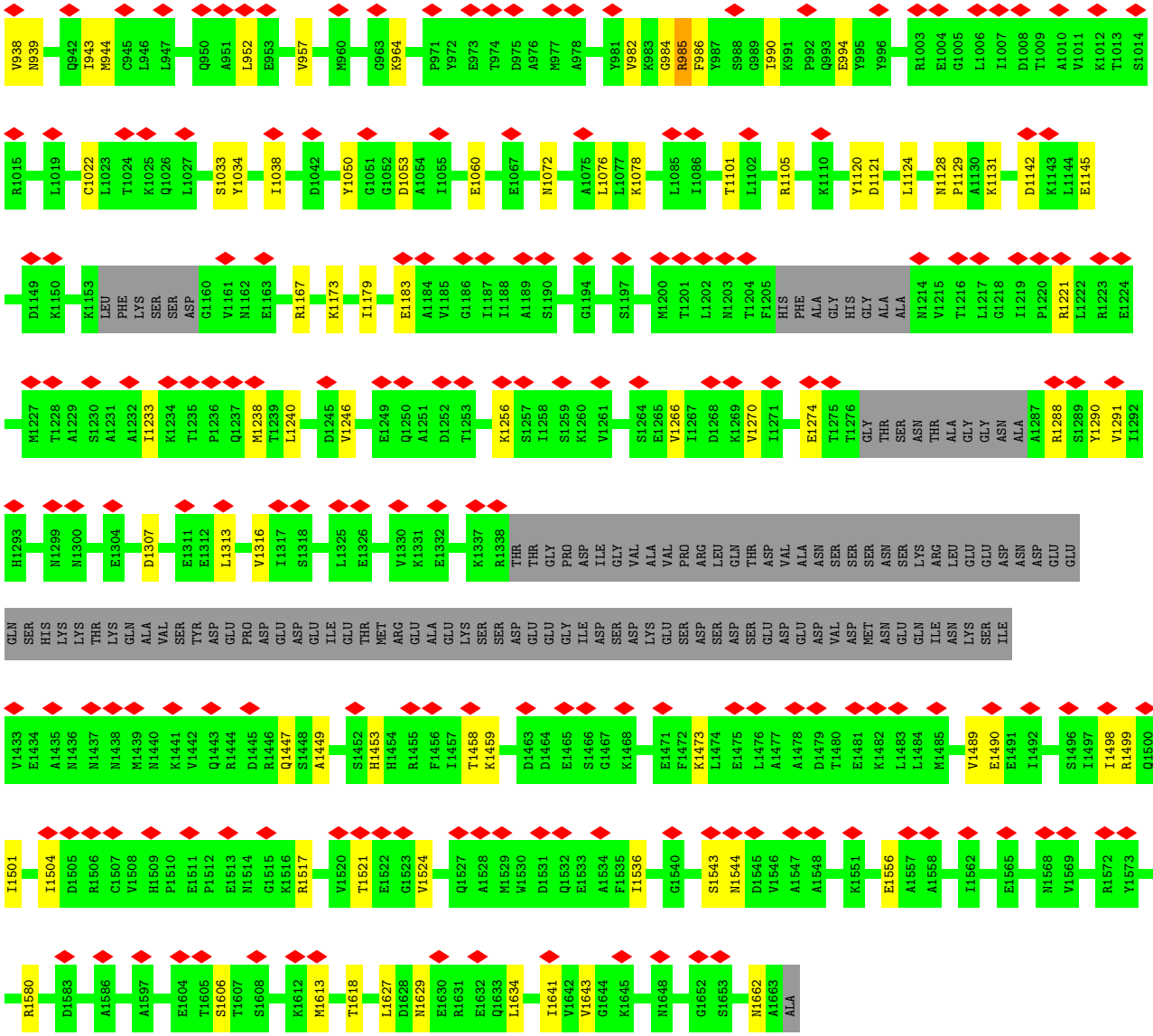






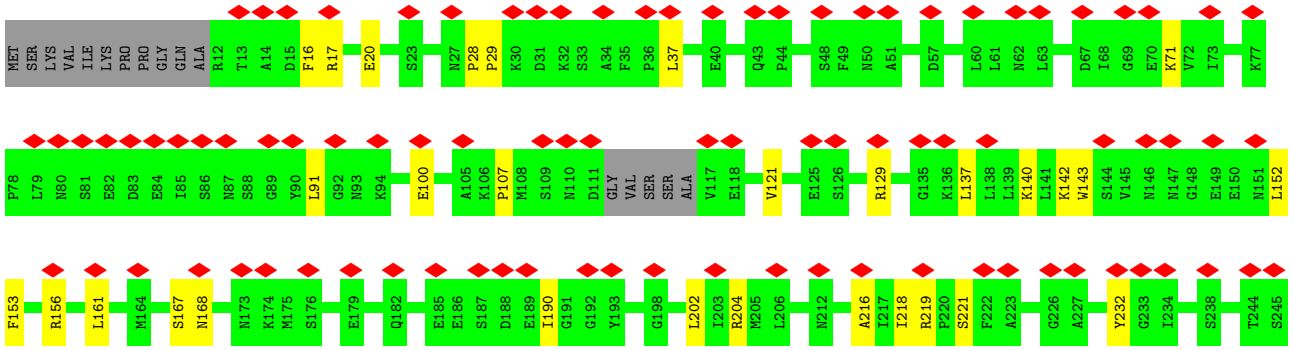


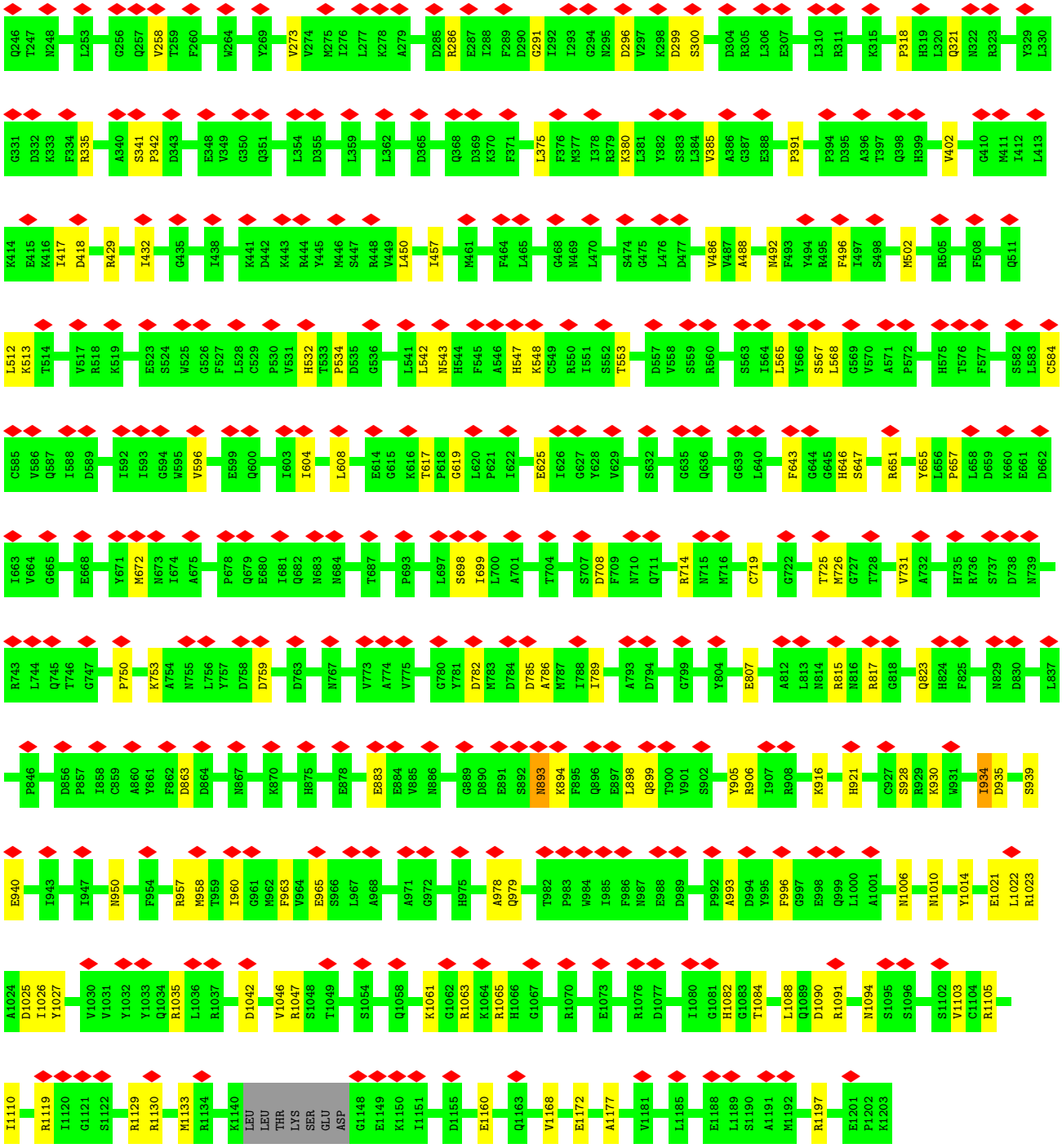




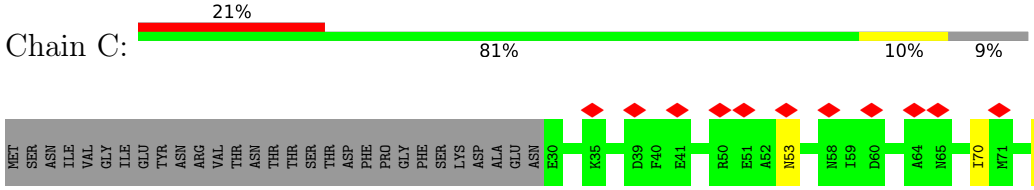
• Molecule 5: DNA-directed RNA polymerase I subunit RPA135

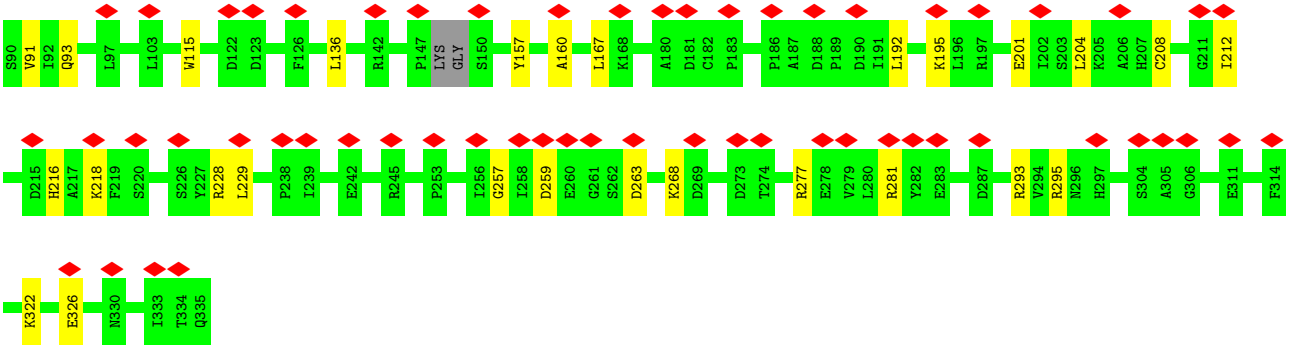
Chain B:



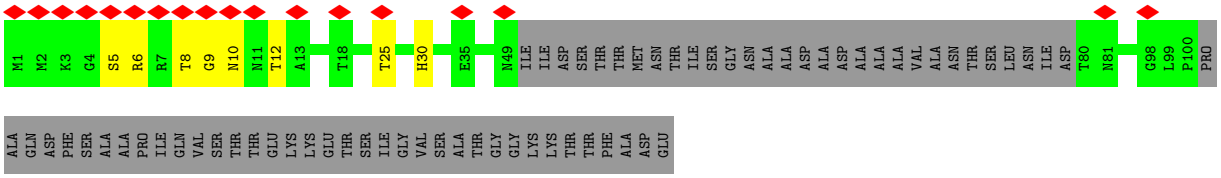


• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

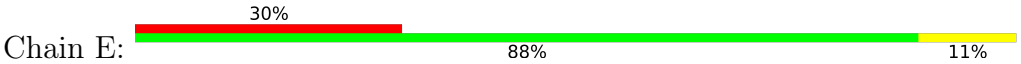


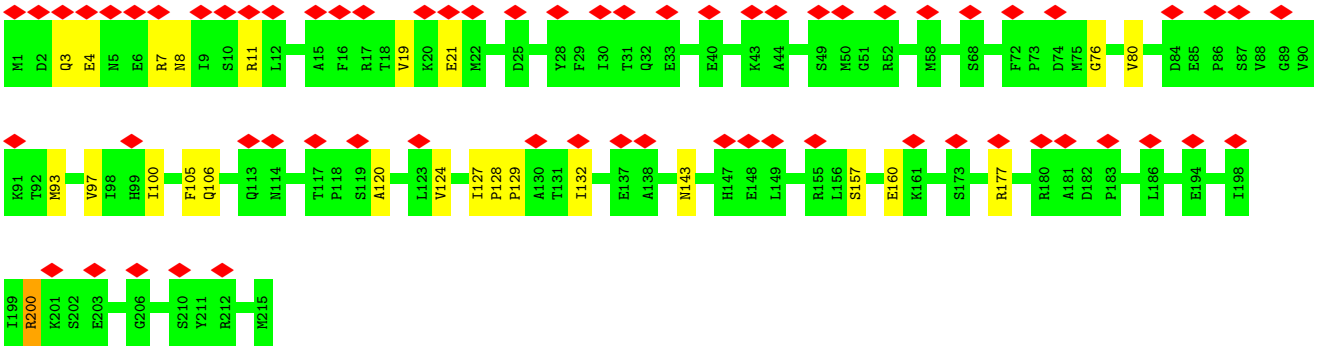


• Molecule 7: DNA-directed RNA polymerase I subunit RPA14

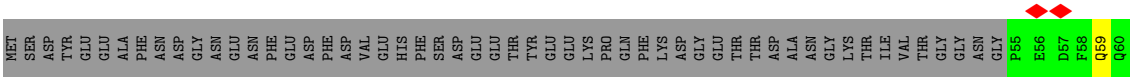


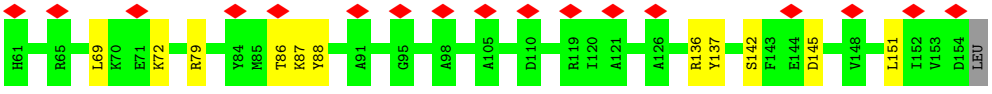
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



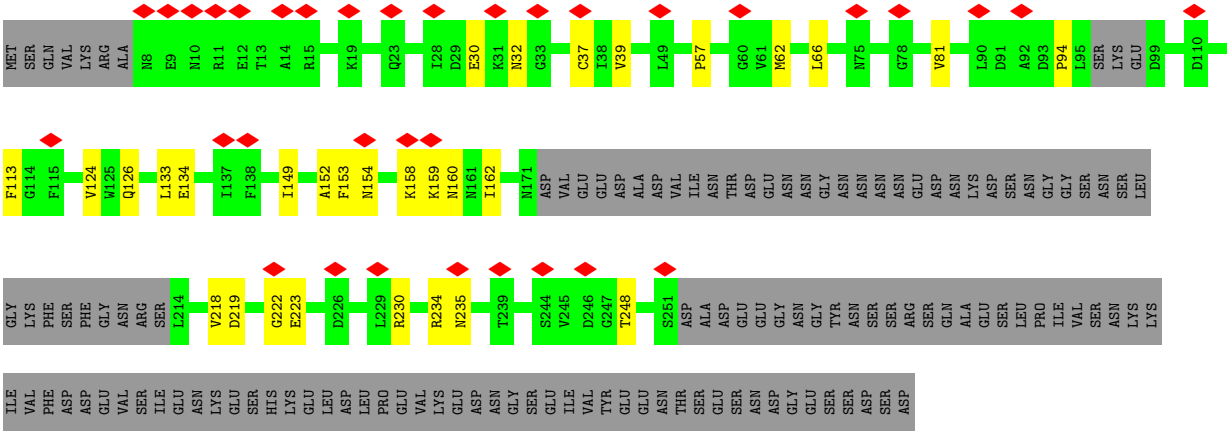


• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



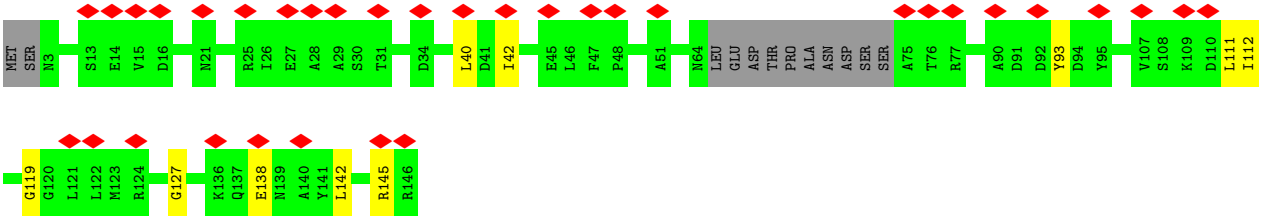


• Molecule 10: DNA-directed RNA polymerase I subunit RPA43



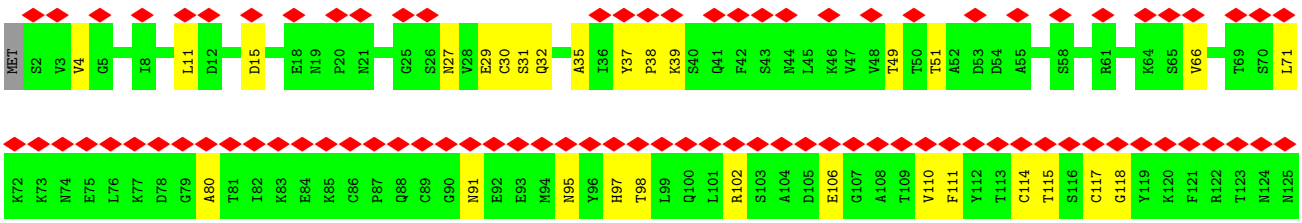
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



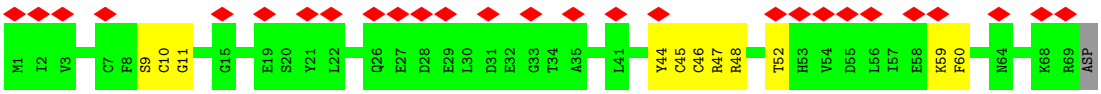
• Molecule 12: DNA-directed RNA polymerase I subunit RPA12

Chain I:



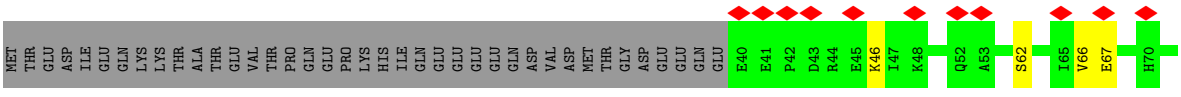
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

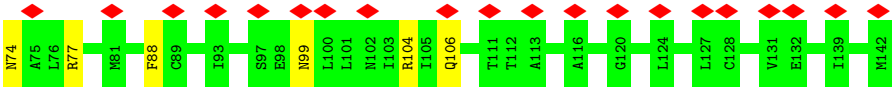
Chain J:



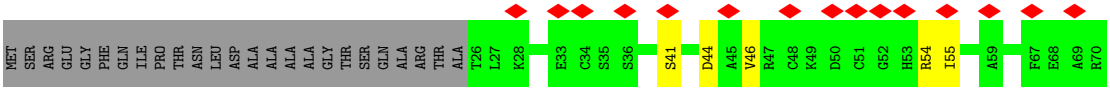
• Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:

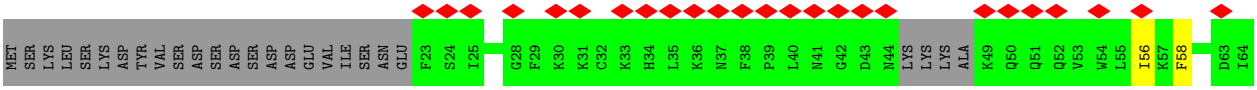


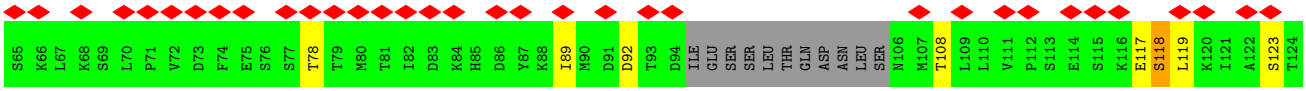


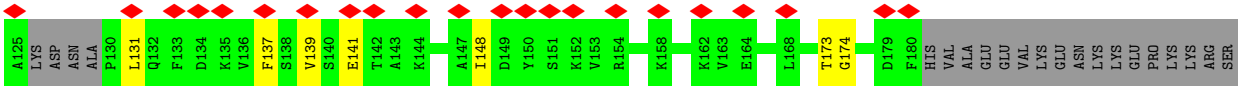
• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4



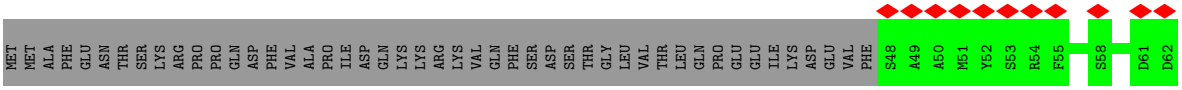
• Molecule 16: DNA-directed RNA polymerase I subunit RPA34

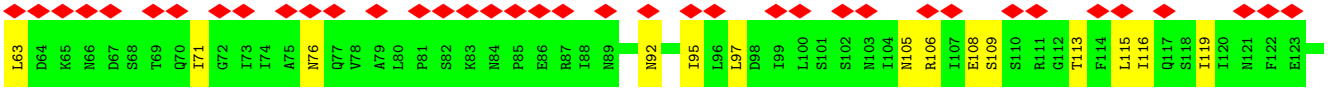


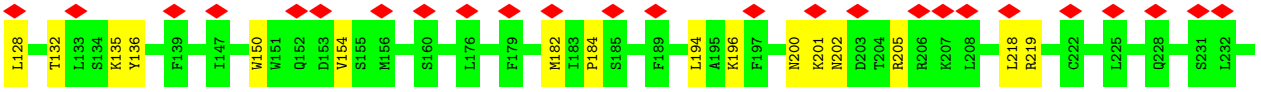


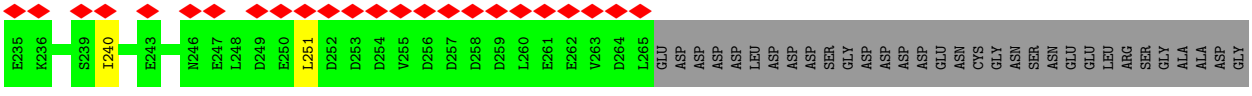


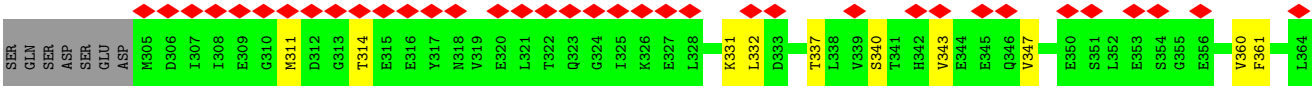
• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN3

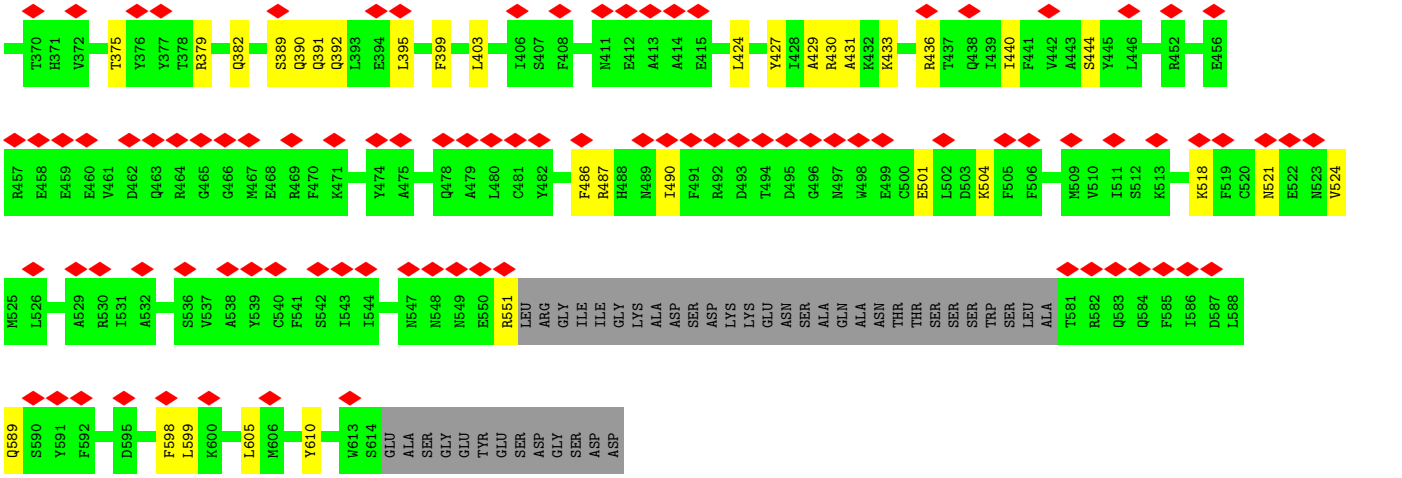






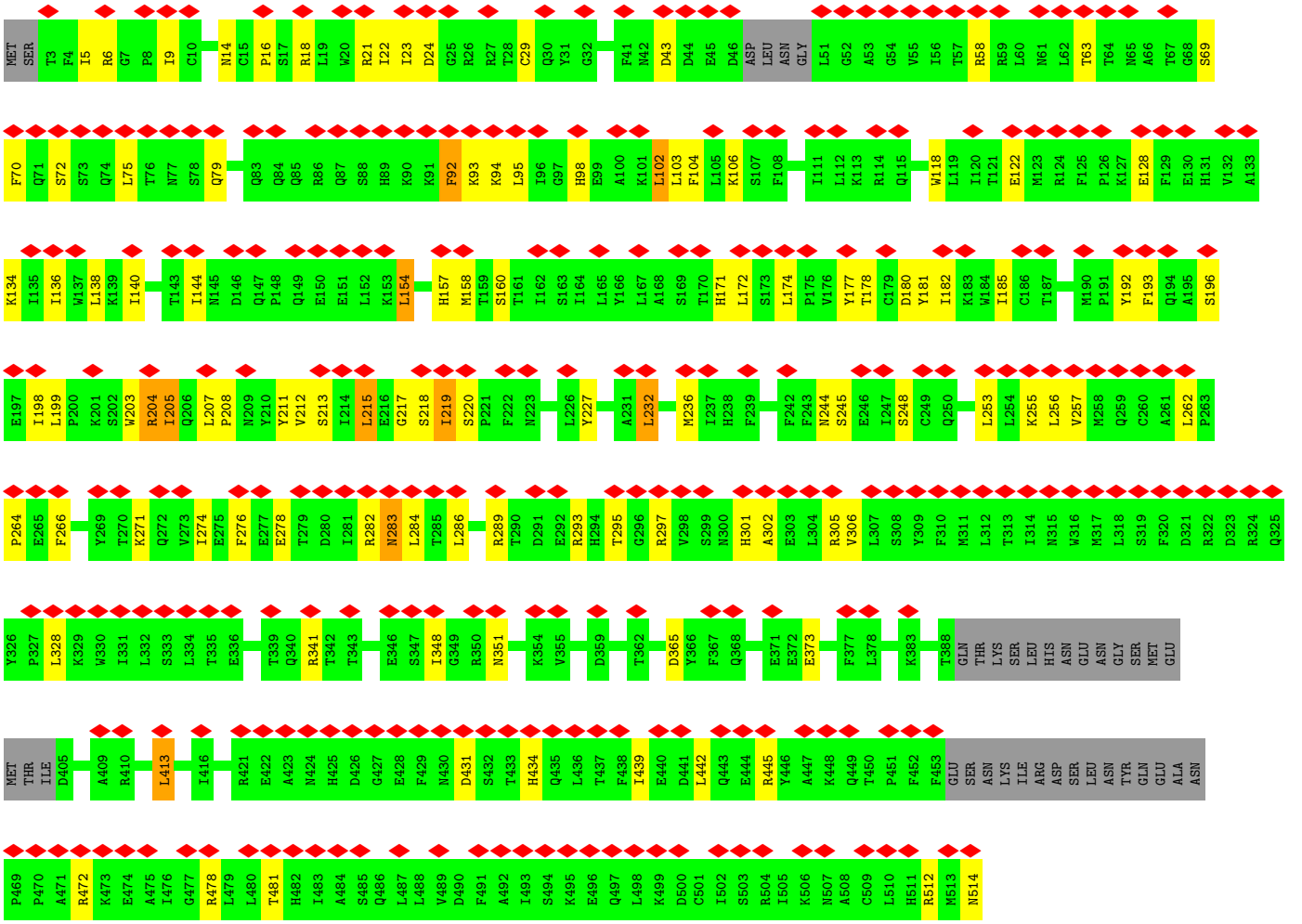






• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN7

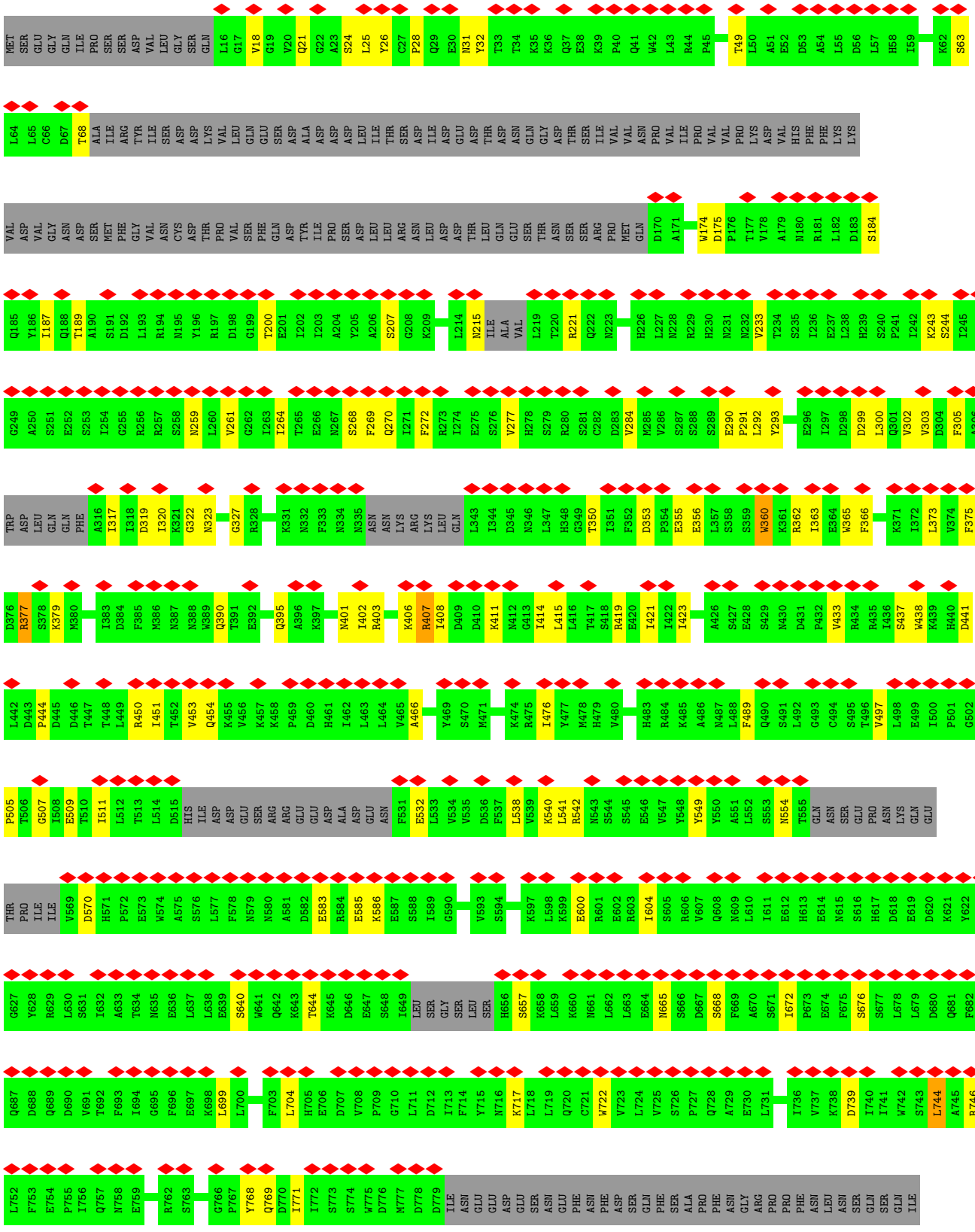
Chain Q:

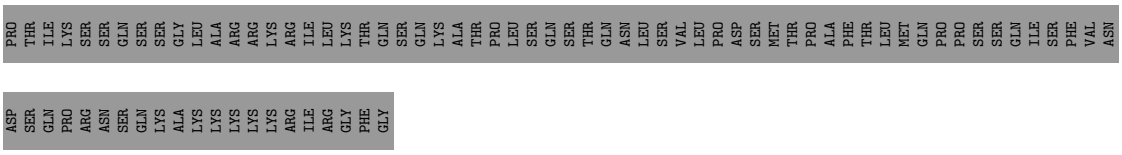


• Molecule 19: RNA polymerase I-specific transcription initiation factor RRN6

Chain S:

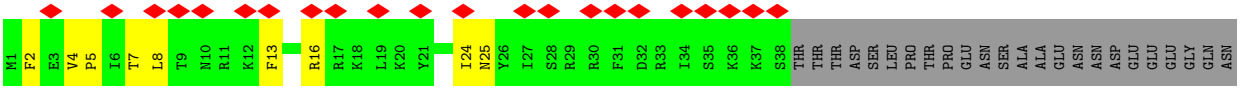

48%
54%
14%
32%

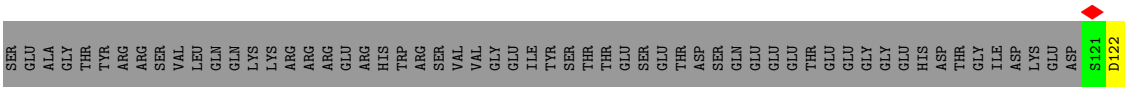

MET SER GLU GLY GLN ILE PRO SER SER ASP VAL LEU GLY SER GLN L16 G17 V18 G19 V20 Q21 G22 A23 S24 L25 Y26 C27 P28 Q29 E30 N31 Y32 T33 T34 K35 K36 Q37 E38 K39 P40 Q41 W42 L43 R44 P45 T49 L50 A51 E52 D53 A54 L55 D56 L57 H58 I59 K62 S63
L64 L65 C66 D67 T68 ALA ILE ARG TYR ILE SER ASP ASP LYS VAL LEU GLN GLU SER ASP ALA ASP ASP ASP LEU ILE THR SER ASP ILE ASP GLU ASP THR ASP ASN GLN GLY ASP THR SER ILE VAL VAL ASN PRO VAL ILE PRO VAL VAL PRO LYS ASP VAL HIS PHE PHE LYS LYS
VAL ASP VAL GLY ASN ASP SER MET PHE GLY VAL ASN CYS ASP THR PRO VAL SER PHE GLN ASP TYR ILE PRO SER ASP LEU LEU ARG ASN LEU ASP ASP THR LEU GLN GLU SER THR ASN SER SER ARG PRO MET GLN D170 A171 W174 D175 P176 T177 V178 A179 N180 R181 L182 D183 S184
Q185 Y186 I187 Q188 T189 A190 S191 D192 L193 R194 N195 Y196 R197 D198 G199 T200 E201 I202 I203 A204 Y205 A206 S207 G208 K209 L214 N215 ILE ALA VAL L219 T220 R221 Q222 N223 H226 L227 N228 R229 H230 N231 N232 V233 T234 S235 I236 E237 L238 H239 S240 P241 I242 K243 S244 I245 K246 I247 P248
G249 A250 S251 E252 S253 I254 G255 R256 R257 S258 N259 L260 V261 G262 I263 I264 T265 E266 N267 S268 F269 Q270 I271 F272 R273 I274 E275 S276 V277 H278 S279 R280 S281 C282 D283 V284 M285 V286 S287 S288 S289 E290 P291 L292 Y293 E296 I297 D298 D299 L300 Q301 V302 V303 D304 F305 A306 PHE ASN PRO
TRP ASP LEU GLN GLN PHE A316 I317 I318 D319 I320 K321 G322 N323 G327 R328 K331 N332 F333 N334 N335 ASN ASN LYS ARG LYS LEU GLN L343 I344 D345 N346 L347 H348 G349 T350 I351 F352 D353 P354 E355 E356 L357 S358 S359 W360 K361 R362 I363 E364 W365 F366 K371 I372 L373 V374 F375
D376 R377 S378 K379 M380 I383 D384 F385 M386 N387 N388 W389 Q390 T391 E392 Q395 A396 K397 N401 I402 R403 K406 R407 I408 D409 D410 K411 N412 G413 I414 L415 L416 T417 S418 R419 E420 I421 I422 I423 A426 S427 E428 S429 N430 D431 P432 V433 R434 R435 I436 S437 W438 K439 H440 D441
L442 D443 P444 D445 D446 T447 T448 L449 R450 I451 T452 V453 Q454 K455 V456 K457 K458 P459 D460 H461 I462 L463 L464 V465 A466 Y469 S470 M471 K474 R475 I476 Y477 M478 H479 V480 H483 R484 K485 A486 N487 L488 F489 Q490 S491 L492 G493 C494 S495 T496 V497 L498 E499 I500 P501 G502 G503 T504
P505 T506 G507 I508 E509 T510 I511 L512 T513 L514 D515 HIS ILE ASP ASP GLU SER ARG ARG GLU GLU ASP ALA ASP GLU ASN F531 E532 L533 V534 V535 D536 F537 L538 V539 K540 L541 R542 N543 S544 S545 E546 V547 Y548 Y549 Y550 A551 L552 S553 N554 T555 GLN ASN SER GLU PRO ASN LYS GLN GLU
THR PRO ILE ILE V569 D570 H571 P572 E573 W574 A575 S576 L577 F578 N579 N580 A581 D582 E583 R584 E585 K586 E587 S588 I589 G590 V593 S594 K597 L598 K599 E600 R601 E602 R603 I604 S605 R606 V607 Q608 N609 L610 I611 E612 H613 E614 N615 S616 H617 D618 E619 D620 K621 Y622 L623 Q624 D625 L626
G627 Y628 R629 L630 S631 I632 A633 T634 N635 E636 L637 L638 E639 S640 W641 Q642 K643 T644 K645 D646 E647 S648 I649 LEU SER GLY SER LEU SER H656 S657 K658 L659 K660 N661 L662 L663 E664 N665 S666 D667 S668 F669 A670 S671 I672 P673 E674 F675 S676 S677 L678 L679 D680 Q681 F682 F683 Q684 Y685 Y686
Q687 D688 Q689 D690 V691 T692 F693 I694 G695 F696 E697 K698 L699 L700 F703 L704 H705 E706 D707 V708 P709 G710 L711 D712 I713 F714 Y715 N716 K717 L718 L719 Q720 C721 W722 V723 L724 V725 S726 P727 Q728 A729 E730 L731 T736 V737 K738 D739 I740 I741 W742 S743 L744 A745 R746 L747 E748 K749
L752 F753 E754 P755 I756 Q757 N758 E759 R762 S763 G766 P767 Y768 Q769 D770 I771 I772 S773 S774 W775 D776 M777 D778 D779 ILE ASN GLU GLU ASP GLU SER ASN GLU PHE ASN PHE ASP SER GLN PHE SER ALA PRO PHE ASN GLY ARG PRO PRO PHE ASN LEU ASN SER GLN SER GLN ILE

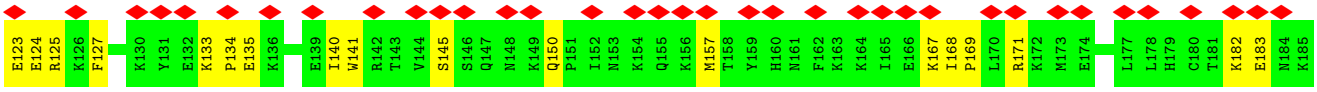


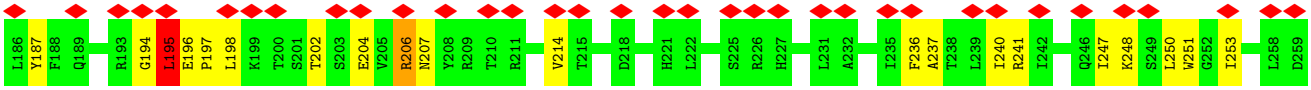
• Molecule 20: RNA polymerase I-specific transcription initiation factor RRN11

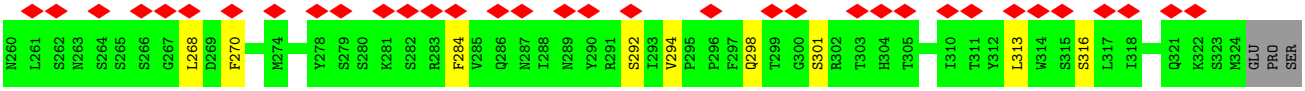
Chain R:

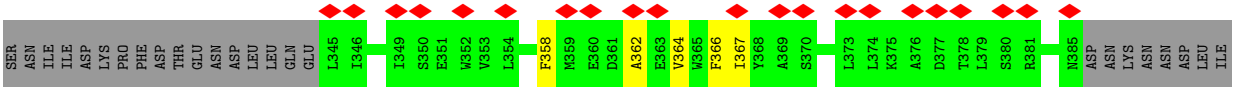


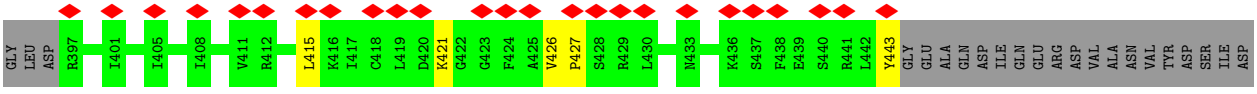












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59963	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 ($e^-/Å^2$)	1.57175	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	T	0.55	0/1113	0.91	1/1707 (0.1%)
2	U	0.44	0/1065	0.80	0/1645
3	M	0.30	0/3152	0.55	0/4252
4	A	0.49	1/11769 (0.0%)	0.59	0/15896
5	B	0.54	0/9578	0.63	0/12948
6	C	0.51	0/2469	0.59	0/3347
7	D	0.37	0/557	0.54	0/750
8	E	0.42	0/1795	0.52	0/2416
9	F	0.51	1/838 (0.1%)	0.57	0/1129
10	G	0.40	0/1613	0.57	0/2193
11	H	0.49	0/1090	0.60	0/1476
12	I	0.34	0/955	0.56	0/1288
13	J	0.59	0/578	0.68	0/775
14	K	0.48	0/821	0.58	0/1108
15	L	0.48	0/361	0.70	0/478
16	N	0.35	0/1124	0.56	0/1512
17	O	0.34	0/4173	0.55	0/5645
18	Q	0.36	0/4028	0.61	0/5441
19	S	0.34	0/5065	0.61	0/6859
20	R	0.42	0/2836	0.60	0/3817
All	All	0.45	2/54980 (0.0%)	0.61	1/74682 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1022	CYS	CB-SG	-5.05	1.73	1.81
9	F	137	TYR	C-N	-5.01	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	49	DA	O3'-P-O5'	6.08	115.55	104.00

There are no chirality outliers.

There are no planarity outliers.

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	T	1000	0	568	22	0
2	U	944	0	507	31	0
3	M	3100	0	3207	34	0
4	A	11558	0	11648	133	0
5	B	9371	0	9238	109	0
6	C	2418	0	2401	21	0
7	D	551	0	558	6	0
8	E	1759	0	1788	15	0
9	F	823	0	841	6	0
10	G	1576	0	1581	22	0
11	H	1072	0	1042	6	0
12	I	942	0	931	19	0
13	J	569	0	586	6	0
14	K	810	0	801	5	0
15	L	359	0	381	4	0
16	N	1103	0	1106	13	0
17	O	4086	0	4024	44	0
18	Q	3936	0	3918	110	0
19	S	4963	0	4890	103	0
20	R	2771	0	2844	50	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
21	Q	1	0	0	0	0
All	All	53719	0	52860	646	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 6.

All (646) 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)
19:S:31:ASN:OD1	19:S:32:TYR:N	1.97	0.96
18:Q:92:PHE:CD1	18:Q:205:ILE:HG21	2.02	0.95
18:Q:218:SER:HB3	20:R:207:ASN:OD1	1.70	0.92
18:Q:92:PHE:CD1	18:Q:205:ILE:CG2	2.57	0.88
19:S:450:ARG:HH11	19:S:450:ARG:HG2	1.40	0.87
18:Q:193:PHE:HD1	18:Q:217:GLY:O	1.59	0.85
18:Q:104:PHE:CD1	18:Q:211:TYR:CD1	2.65	0.85
20:R:122:ASP:CB	20:R:125:ARG:HD3	2.09	0.83
18:Q:193:PHE:CD1	18:Q:217:GLY:O	2.33	0.80
18:Q:104:PHE:CD1	18:Q:211:TYR:HD1	2.00	0.80
18:Q:144:ILE:HD12	18:Q:154:LEU:HB2	1.64	0.79
20:R:204:GLU:N	20:R:204:GLU:OE1	2.16	0.79
19:S:292:LEU:HD12	19:S:292:LEU:O	1.84	0.78
1:T:17:DG:H1	2:U:53:DA:H2	1.33	0.76
19:S:31:ASN:CG	19:S:32:TYR:H	1.88	0.76
7:D:9:GLY:HA2	7:D:12:THR:HG23	1.70	0.74
18:Q:196:SER:OG	18:Q:215:LEU:HB3	1.86	0.74
20:R:122:ASP:HB3	20:R:125:ARG:HD3	1.68	0.74
18:Q:219:ILE:HG12	18:Q:219:ILE:O	1.87	0.73
19:S:377:ARG:HG3	19:S:402:ILE:O	1.90	0.72
20:R:125:ARG:NH1	20:R:125:ARG:HG2	2.04	0.71
18:Q:196:SER:O	18:Q:204:ARG:HD2	1.89	0.71
20:R:125:ARG:HG2	20:R:125:ARG:HH11	1.55	0.71
18:Q:289:ARG:NH1	18:Q:295:THR:HA	2.04	0.71
4:A:15:ASP:HB2	5:B:1197:ARG:HB3	1.73	0.70
4:A:670:ILE:HG12	4:A:671:GLN:HG3	1.74	0.70
19:S:268:SER:HB3	19:S:293:TYR:CE1	2.26	0.70
20:R:122:ASP:HB2	20:R:125:ARG:HD3	1.72	0.70
18:Q:92:PHE:HB3	18:Q:205:ILE:HD12	1.74	0.70
4:A:477:ASN:OD1	5:B:1047:ARG:NH1	2.25	0.69
19:S:360:TRP:CD2	19:S:377:ARG:NH2	2.60	0.69
18:Q:282:ARG:HG3	18:Q:283:ASN:N	2.09	0.67
3:M:66:THR:HB	3:M:71:GLN:HG3	1.77	0.67
19:S:360:TRP:CG	19:S:377:ARG:NH2	2.63	0.66
18:Q:136:ILE:O	18:Q:140:ILE:HG12	1.95	0.66
20:R:167:LYS:HG2	20:R:171:ARG:HE	1.60	0.66
18:Q:22:ILE:HG23	18:Q:23:ILE:HG13	1.78	0.66
18:Q:92:PHE:CB	18:Q:205:ILE:HD12	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:59:DG:OP1	4:A:221:HIS:HE1	1.79	0.65
18:Q:232:LEU:CD2	18:Q:289:ARG:HH21	2.08	0.65
18:Q:282:ARG:HG3	18:Q:283:ASN:H	1.61	0.65
18:Q:232:LEU:HD23	18:Q:289:ARG:HH21	1.61	0.64
18:Q:278:GLU:HA	18:Q:278:GLU:OE1	1.96	0.64
19:S:360:TRP:CB	19:S:377:ARG:HH21	2.10	0.64
6:C:70:ILE:HG23	6:C:74:GLU:HB2	1.81	0.64
18:Q:193:PHE:HZ	18:Q:220:SER:HB3	1.63	0.63
4:A:1101:THR:HG22	4:A:1120:TYR:HB3	1.80	0.63
4:A:964:LYS:NZ	5:B:672:MET:O	2.25	0.63
4:A:233:CYS:SG	4:A:234:ASP:N	2.72	0.63
4:A:65:CYS:SG	4:A:75:HIS:NE2	2.64	0.62
19:S:270:GLN:CG	19:S:291:PRO:HB3	2.29	0.62
17:O:430:ARG:NH1	17:O:610:TYR:OH	2.32	0.62
3:M:38:PHE:HB2	16:N:119:LEU:HB2	1.80	0.62
20:R:124:GLU:O	20:R:127:PHE:HB3	2.00	0.62
19:S:317:ILE:HG13	19:S:327:GLY:H	1.64	0.62
4:A:27:LEU:HB3	5:B:1130:ARG:HB3	1.81	0.61
18:Q:93:LYS:HB3	18:Q:95:LEU:HD22	1.82	0.61
18:Q:481:THR:HG21	19:S:570:ASP:HA	1.82	0.61
4:A:982:VAL:HG22	4:A:994:GLU:HB2	1.81	0.61
8:E:97:VAL:HG13	8:E:127:ILE:HD11	1.82	0.61
19:S:451:ILE:HD11	19:S:466:ALA:HB1	1.81	0.61
12:I:27:ASN:HA	12:I:38:PRO:HA	1.81	0.61
5:B:726:MET:SD	5:B:1035:ARG:NH1	2.74	0.61
20:R:122:ASP:O	20:R:123:GLU:HB2	2.01	0.61
18:Q:154:LEU:HD23	18:Q:154:LEU:O	2.01	0.61
19:S:63:SER:HB3	19:S:549:TYR:HB3	1.83	0.61
20:R:206:ARG:HG3	20:R:206:ARG:O	2.01	0.61
12:I:30:CYS:SG	12:I:31:SER:N	2.74	0.60
5:B:143:TRP:HB3	5:B:152:LEU:HB2	1.83	0.60
18:Q:293:ARG:O	18:Q:293:ARG:HG3	2.01	0.60
4:A:709:ARG:NH1	4:A:737:LEU:O	2.33	0.60
19:S:395:GLN:HB3	20:R:140:ILE:HG23	1.82	0.60
3:M:344:VAL:HB	3:M:395:ALA:HB3	1.84	0.60
18:Q:276:PHE:O	18:Q:512:ARG:NH1	2.34	0.60
18:Q:103:LEU:HD12	18:Q:103:LEU:O	2.02	0.59
10:G:159:LYS:HA	10:G:162:ILE:HD12	1.85	0.59
18:Q:14:ASN:ND2	18:Q:29:CYS:SG	2.76	0.59
18:Q:274:ILE:O	18:Q:278:GLU:HB2	2.03	0.59
4:A:1145:GLU:OE2	4:A:1167:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:97:HIS:HB3	12:I:111:PHE:HB2	1.85	0.59
20:R:194:GLY:O	20:R:195:LEU:O	2.20	0.59
3:M:127:ALA:HA	3:M:131:ALA:HB3	1.84	0.59
6:C:229:LEU:HB2	6:C:293:ARG:HH11	1.68	0.59
18:Q:102:LEU:HD21	19:S:769:GLN:OE1	2.03	0.58
18:Q:104:PHE:HD1	18:Q:211:TYR:CD1	2.19	0.58
4:A:824:THR:HG23	5:B:1023:ARG:HB2	1.84	0.58
17:O:501:GLU:HB3	17:O:504:LYS:HB3	1.85	0.58
3:M:53:LEU:HB2	3:M:96:LEU:HD13	1.85	0.58
5:B:565:LEU:HD21	5:B:608:LEU:HD11	1.85	0.58
19:S:401:ASN:H	19:S:419:ARG:HG2	1.66	0.58
4:A:86:TYR:HA	4:A:356:PHE:HA	1.86	0.57
17:O:431:ALA:O	17:O:487:ARG:NH2	2.36	0.57
2:U:54:DG:H1'	5:B:513:LYS:NZ	2.19	0.57
3:M:234:PHE:O	3:M:237:GLN:NE2	2.37	0.57
9:F:136:ARG:HH12	9:F:151:LEU:HD21	1.70	0.57
3:M:13:GLU:HB2	3:M:89:GLN:HB3	1.87	0.57
4:A:114:GLU:OE2	4:A:117:ARG:NH2	2.38	0.57
18:Q:278:GLU:OE2	18:Q:284:LEU:CD2	2.52	0.57
3:M:398:LYS:HG2	3:M:400:PRO:HD2	1.87	0.57
6:C:53:ASN:HD22	16:N:174:GLY:HA3	1.70	0.57
19:S:270:GLN:HG2	19:S:291:PRO:HB3	1.86	0.57
18:Q:271:LYS:NZ	19:S:739:ASP:OD2	2.36	0.57
4:A:592:GLN:OE1	4:A:634:ASN:ND2	2.38	0.56
6:C:192:LEU:HD21	6:C:195:LYS:HE3	1.87	0.56
2:U:54:DG:H8	2:U:54:DG:H5"	1.69	0.56
4:A:1459:LYS:HD2	4:A:1473:LYS:HD3	1.87	0.56
4:A:32:ILE:HD11	4:A:54:LEU:HD11	1.88	0.56
17:O:518:LYS:HD2	17:O:551:ARG:HB2	1.87	0.56
19:S:25:LEU:HD23	19:S:437:SER:HA	1.88	0.56
2:U:25:DG:N2	18:Q:293:ARG:NH2	2.53	0.56
19:S:433:VAL:HG21	20:R:145:SER:HB3	1.88	0.56
19:S:454:GLN:NE2	19:S:511:ILE:O	2.39	0.56
18:Q:103:LEU:HD11	18:Q:203:TRP:HB3	1.88	0.56
18:Q:118:TRP:NE1	18:Q:122:GLU:OE1	2.38	0.56
5:B:71:LYS:NZ	5:B:418:ASP:OD1	2.37	0.55
20:R:237:ALA:O	20:R:241:ARG:NH2	2.39	0.55
17:O:92:ASN:HA	17:O:95:ILE:HD12	1.87	0.55
19:S:31:ASN:OD1	19:S:32:TYR:O	2.24	0.55
4:A:1288:ARG:NH2	4:A:1290:TYR:OH	2.40	0.55
4:A:462:LYS:HD2	4:A:464:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1053:ASP:OD2	4:A:1580:ARG:NH2	2.38	0.55
20:R:294:VAL:H	20:R:298:GLN:HE21	1.54	0.55
5:B:1014:TYR:OH	6:C:293:ARG:NH1	2.36	0.55
2:U:26:DA:H8	3:M:387:SER:HG	1.47	0.55
19:S:290:GLU:OE2	19:S:290:GLU:HA	2.07	0.55
19:S:362:ARG:HB3	19:S:375:PHE:HB2	1.87	0.55
18:Q:92:PHE:CD1	18:Q:205:ILE:HG23	2.41	0.54
6:C:257:GLY:HA3	6:C:268:LYS:HE2	1.89	0.54
18:Q:204:ARG:NH1	18:Q:212:VAL:HG21	2.23	0.54
16:N:56:ILE:HG22	16:N:137:PHE:HB2	1.90	0.54
19:S:407:ARG:HH11	19:S:411:LYS:HG2	1.71	0.54
4:A:1449:ALA:O	4:A:1453:HIS:ND1	2.37	0.54
18:Q:182:ILE:HD12	18:Q:185:ILE:HD11	1.89	0.54
19:S:215:ASN:HB2	19:S:233:VAL:HB	1.90	0.54
2:U:26:DA:C8	3:M:387:SER:OG	2.61	0.54
4:A:438:ILE:HA	4:A:456:VAL:HG22	1.90	0.54
17:O:337:THR:HG23	17:O:605:LEU:HD11	1.89	0.54
19:S:423:ILE:HD13	20:R:141:TRP:HZ2	1.72	0.54
19:S:450:ARG:HH11	19:S:450:ARG:CG	2.12	0.54
19:S:174:TRP:CD1	20:R:198:LEU:HD13	2.43	0.54
4:A:1179:ILE:HD11	4:A:1183:GLU:HG2	1.90	0.53
5:B:894:LYS:HG2	15:L:54:ARG:HH22	1.72	0.53
4:A:874:GLU:OE2	4:A:878:ARG:NH2	2.41	0.53
5:B:167:SER:OG	5:B:168:ASN:N	2.41	0.53
19:S:300:LEU:HA	19:S:320:ILE:HA	1.90	0.53
4:A:747:ILE:HG22	4:A:774:GLY:HA2	1.90	0.53
18:Q:302:ALA:HA	18:Q:305:ARG:HE	1.72	0.53
4:A:435:ASN:ND2	4:A:442:LYS:O	2.42	0.53
10:G:158:LYS:NZ	17:O:108:GLU:OE1	2.40	0.53
20:R:8:LEU:HD21	20:R:202:THR:HG22	1.90	0.53
5:B:37:LEU:HD12	5:B:759:ASP:HB3	1.91	0.53
18:Q:351:ASN:ND2	18:Q:373:GLU:OE2	2.41	0.53
17:O:109:SER:O	17:O:113:THR:OG1	2.27	0.53
20:R:4:VAL:HG11	20:R:214:VAL:HG22	1.89	0.53
5:B:429:ARG:HA	5:B:432:ILE:HG12	1.91	0.53
6:C:87:ASN:ND2	6:C:201:GLU:OE2	2.40	0.53
1:T:8:DA:O5'	1:T:8:DA:H8	1.92	0.52
4:A:4:SER:OG	4:A:576:LYS:NZ	2.39	0.52
4:A:1274:GLU:OE2	4:A:1288:ARG:NH2	2.42	0.52
5:B:1014:TYR:HE2	6:C:228:ARG:HA	1.75	0.52
18:Q:177:TYR:OH	18:Q:248:SER:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:11:DG:H2"	1:T:12:DC:H5'	1.91	0.52
18:Q:21:ARG:NH1	18:Q:24:ASP:OD1	2.41	0.52
20:R:313:LEU:HB3	20:R:367:ILE:HD13	1.90	0.52
1:T:37:DA:C2	2:U:35:DA:C2	2.98	0.52
5:B:534:PRO:HG3	5:B:542:LEU:HD23	1.92	0.52
17:O:71:ILE:HG23	17:O:115:LEU:HD23	1.91	0.52
12:I:80:ALA:O	12:I:95:ASN:ND2	2.40	0.52
4:A:1124:LEU:HD22	4:A:1129:PRO:HG3	1.92	0.52
4:A:1291:VAL:HG22	4:A:1473:LYS:HG2	1.91	0.52
8:E:4:GLU:O	8:E:8:ASN:ND2	2.41	0.52
5:B:91:LEU:HD21	5:B:342:PRO:HB2	1.90	0.52
5:B:142:LYS:HG3	5:B:153:PHE:HE1	1.74	0.52
10:G:149:ILE:HB	10:G:153:PHE:HB2	1.92	0.52
18:Q:103:LEU:HD13	18:Q:106:LYS:HE3	1.91	0.52
19:S:243:LYS:NZ	19:S:299:ASP:OD2	2.43	0.52
19:S:269:PHE:HB3	19:S:292:LEU:HG	1.92	0.52
4:A:248:PHE:HD2	4:A:442:LYS:HG3	1.74	0.52
4:A:536:ILE:HG12	4:A:557:LEU:HD21	1.91	0.52
14:K:74:ASN:OD1	14:K:77:ARG:NH2	2.43	0.52
4:A:7:VAL:HG21	5:B:1177:ALA:HB2	1.91	0.52
4:A:772:LYS:NZ	11:H:138:GLU:OE2	2.43	0.52
6:C:157:TYR:HB2	6:C:160:ALA:HB2	1.92	0.52
4:A:1662:ASN:HB3	10:G:57:PRO:HD2	1.92	0.52
13:J:45:CYS:SG	13:J:46:CYS:N	2.83	0.52
18:Q:295:THR:O	18:Q:295:THR:OG1	2.27	0.52
19:S:355:GLU:HB2	20:R:24:ILE:HG23	1.91	0.52
19:S:476:ILE:HG22	19:S:497:VAL:H	1.74	0.52
5:B:1105:ARG:NH2	5:B:1172:GLU:OE1	2.43	0.52
20:R:5:PRO:HB3	20:R:248:LYS:HB2	1.92	0.52
3:M:212:GLU:HA	3:M:215:PHE:HD2	1.75	0.51
5:B:1090:ASP:HA	5:B:1094:ASN:HB2	1.91	0.51
4:A:878:ARG:NH1	12:I:66:VAL:O	2.44	0.51
4:A:259:LYS:O	4:A:262:THR:OG1	2.27	0.51
18:Q:94:LYS:NZ	18:Q:207:LEU:O	2.33	0.51
3:M:345:GLU:HG2	3:M:348:PRO:HD2	1.92	0.51
19:S:175:ASP:OD1	20:R:195:LEU:CD2	2.58	0.51
4:A:944:MET:O	4:A:985:ARG:NH1	2.44	0.51
5:B:100:GLU:OE2	5:B:140:LYS:NZ	2.44	0.51
14:K:67:GLU:HA	14:K:99:ASN:HB3	1.92	0.51
18:Q:198:ILE:HG13	18:Q:199:LEU:HG	1.91	0.51
18:Q:9:ILE:HG22	18:Q:16:PRO:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:292:LEU:HD12	19:S:292:LEU:C	2.31	0.51
3:M:88:ILE:HD12	3:M:90:LEU:HD21	1.91	0.51
5:B:202:LEU:HD23	5:B:488:ALA:HB2	1.92	0.51
13:J:10:CYS:SG	13:J:11:GLY:N	2.83	0.51
18:Q:514:ASN:ND2	19:S:585:GLU:OE2	2.44	0.51
19:S:184:SER:N	19:S:509:GLU:OE2	2.43	0.51
1:T:17:DG:N2	2:U:54:DG:N2	2.59	0.51
2:U:60:DC:H2"	2:U:61:DA:C8	2.46	0.51
4:A:1221:ARG:HH12	4:A:1233:ILE:HG12	1.75	0.51
17:O:205:ARG:HG2	17:O:331:LYS:HG2	1.91	0.51
17:O:390:GLN:HE21	17:O:433:LYS:H	1.59	0.51
14:K:62:SER:OG	14:K:104:ARG:NH1	2.40	0.50
17:O:200:ASN:ND2	17:O:202:ASN:OD1	2.44	0.50
5:B:785:ASP:OD1	5:B:957:ARG:NH2	2.43	0.50
18:Q:154:LEU:HD23	18:Q:154:LEU:N	2.26	0.50
19:S:269:PHE:HZ	19:S:303:VAL:HG21	1.76	0.50
5:B:1021:GLU:OE2	6:C:295:ARG:NH2	2.44	0.50
6:C:80:ALA:HA	6:C:208:CYS:HA	1.94	0.50
1:T:39:DT:N3	2:U:33:DG:N2	2.60	0.50
4:A:1105:ARG:NH2	4:A:1142:ASP:OD1	2.45	0.50
10:G:62:MET:HA	10:G:66:LEU:HB2	1.94	0.50
19:S:244:SER:HB3	19:S:264:ILE:HB	1.93	0.50
19:S:504:THR:O	19:S:542:ARG:N	2.42	0.50
5:B:300:SER:HB3	12:I:49:THR:HG22	1.93	0.50
5:B:417:ILE:HG22	5:B:457:ILE:HD13	1.92	0.50
12:I:15:ASP:OD2	12:I:32:GLN:NE2	2.44	0.50
1:T:39:DT:C2	2:U:33:DG:N2	2.79	0.50
18:Q:171:HIS:ND1	18:Q:244:ASN:OD1	2.44	0.50
4:A:648:LEU:O	4:A:652:ASN:ND2	2.44	0.50
17:O:201:LYS:HG3	17:O:240:ILE:HG13	1.93	0.50
9:F:72:LYS:HB3	9:F:142:SER:HA	1.94	0.50
17:O:200:ASN:ND2	18:Q:14:ASN:O	2.45	0.50
17:O:392:GLN:HB2	17:O:395:LEU:HD13	1.93	0.50
18:Q:178:THR:HA	18:Q:181:TYR:HB2	1.94	0.50
4:A:30:LYS:NZ	5:B:1129:ARG:CZ	2.74	0.50
5:B:898:LEU:HB3	15:L:46:VAL:HG21	1.94	0.50
8:E:100:ILE:HG23	8:E:105:PHE:HB2	1.93	0.50
17:O:379:ARG:HA	17:O:382:GLN:HE22	1.76	0.50
19:S:189:THR:HA	19:S:259:ASN:HD22	1.76	0.50
19:S:323:ASN:HA	19:S:350:THR:HA	1.92	0.50
2:U:57:DA:H2'	2:U:58:DA:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:58:LEU:HD22	18:Q:70:PHE:HD1	1.75	0.49
18:Q:92:PHE:CE1	18:Q:205:ILE:HG21	2.45	0.49
19:S:407:ARG:HA	19:S:414:ILE:HG23	1.94	0.49
4:A:799:GLU:OE2	4:A:1173:LYS:NZ	2.35	0.49
4:A:1246:VAL:O	4:A:1517:ARG:NH2	2.41	0.49
5:B:335:ARG:NH2	5:B:341:SER:O	2.45	0.49
5:B:402:VAL:O	5:B:647:SER:OG	2.25	0.49
4:A:952:LEU:HD12	4:A:957:VAL:HA	1.93	0.49
19:S:438:TRP:CD1	19:S:489:PHE:HB2	2.46	0.49
18:Q:439:ILE:HG22	19:S:704:LEU:HD22	1.93	0.49
6:C:53:ASN:ND2	16:N:173:THR:O	2.45	0.49
18:Q:262:LEU:HD13	18:Q:266:PHE:HB2	1.94	0.49
19:S:421:ILE:HA	19:S:441:ASP:HA	1.93	0.49
4:A:938:VAL:HG11	12:I:98:THR:HG21	1.95	0.49
19:S:31:ASN:O	19:S:32:TYR:CG	2.66	0.49
4:A:1447:GLN:HE21	4:A:1459:LYS:HA	1.77	0.49
5:B:129:ARG:HB2	15:L:55:ILE:HD11	1.95	0.49
5:B:568:LEU:HD23	5:B:604:ILE:HG12	1.94	0.49
18:Q:203:TRP:CD1	18:Q:203:TRP:N	2.77	0.49
19:S:26:TYR:HB3	19:S:28:PRO:HD3	1.94	0.49
4:A:83:VAL:HG11	4:A:427:PHE:HE1	1.77	0.49
4:A:1038:ILE:HD11	4:A:1050:TYR:HB2	1.95	0.49
18:Q:104:PHE:CE1	18:Q:211:TYR:HD1	2.29	0.49
5:B:204:ARG:HH21	5:B:486:VAL:HG11	1.78	0.48
12:I:98:THR:HG22	12:I:110:VAL:HG22	1.95	0.48
17:O:440:ILE:O	17:O:444:SER:N	2.41	0.48
2:U:26:DA:H8	3:M:387:SER:OG	1.95	0.48
3:M:192:ASN:HB3	3:M:201:ILE:HA	1.94	0.48
4:A:480:ALA:HB2	5:B:1046:VAL:HG23	1.94	0.48
5:B:1025:ASP:OD2	6:C:277:ARG:NH1	2.46	0.48
18:Q:75:LEU:HD22	18:Q:79:GLN:HG3	1.95	0.48
19:S:746:ARG:HH22	19:S:749:LYS:HD2	1.77	0.48
3:M:271:VAL:HG21	3:M:298:ILE:HG21	1.95	0.48
4:A:1307:ASP:HB3	4:A:1499:ARG:HH12	1.78	0.48
5:B:807:GLU:OE1	5:B:905:TYR:OH	2.26	0.48
19:S:444:PRO:HA	20:R:2:PHE:HA	1.94	0.48
1:T:37:DA:C2	2:U:34:DT:N3	2.81	0.48
4:A:602:GLY:N	4:A:651:ALA:O	2.46	0.48
4:A:739:VAL:HG11	4:A:812:VAL:HG21	1.95	0.48
4:A:1053:ASP:OD1	4:A:1053:ASP:N	2.45	0.48
11:H:93:TYR:HE1	11:H:145:ARG:HH11	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:13:PHE:HA	20:R:16:ARG:HG2	1.96	0.48
4:A:621:THR:OG1	4:A:626:ALA:O	2.31	0.48
5:B:698:SER:OG	5:B:699:ILE:N	2.46	0.48
4:A:1033:SER:OG	4:A:1034:TYR:N	2.45	0.48
17:O:63:LEU:HD22	17:O:106:ARG:HA	1.96	0.48
18:Q:264:PRO:HD3	19:S:722:TRP:CD1	2.49	0.48
4:A:718:THR:HG21	11:H:119:GLY:HA3	1.96	0.48
4:A:891:ILE:HD12	12:I:71:LEU:HG	1.96	0.48
5:B:219:ARG:HG2	5:B:221:SER:H	1.79	0.48
5:B:883:GLU:OE1	5:B:906:ARG:NH1	2.37	0.48
19:S:450:ARG:CG	19:S:450:ARG:NH1	2.73	0.48
20:R:187:TYR:HE1	20:R:197:PRO:HB3	1.79	0.48
3:M:216:ILE:HD11	3:M:294:LEU:HD11	1.95	0.48
4:A:30:LYS:NZ	5:B:1129:ARG:NH2	2.60	0.48
5:B:258:VAL:HG12	5:B:273:VAL:HG21	1.95	0.48
4:A:339:PHE:HE1	4:A:1627:LEU:HD22	1.79	0.48
4:A:342:ARG:NH1	4:A:1629:ASN:O	2.47	0.48
5:B:786:ALA:HB1	5:B:928:SER:HB2	1.96	0.48
7:D:25:THR:OG1	9:F:59:GLN:OE1	2.32	0.48
5:B:1061:LYS:O	5:B:1065:ARG:NH1	2.47	0.48
10:G:152:ALA:HA	17:O:184:PRO:HG2	1.96	0.48
19:S:21:GLN:OE1	19:S:24:SER:OG	2.28	0.48
5:B:963:PHE:O	5:B:1027:TYR:OH	2.31	0.47
5:B:1006:ASN:HD22	5:B:1010:ASN:HB2	1.79	0.47
17:O:219:ARG:HH22	17:O:360:VAL:HG22	1.78	0.47
19:S:505:PRO:HA	19:S:541:LEU:HA	1.94	0.47
4:A:943:ILE:HG12	5:B:960:ILE:HD11	1.95	0.47
5:B:291:GLY:HA3	5:B:375:LEU:HD13	1.95	0.47
5:B:750:PRO:HG2	5:B:753:LYS:HB3	1.96	0.47
5:B:1065:ARG:NH2	18:Q:43:ASP:O	2.47	0.47
18:Q:193:PHE:CZ	18:Q:220:SER:HB3	2.48	0.47
20:R:122:ASP:CB	20:R:125:ARG:CD	2.87	0.47
20:R:247:ILE:HA	20:R:250:LEU:HD12	1.96	0.47
16:N:117:GLU:HG2	16:N:118:SER:H	1.79	0.47
18:Q:232:LEU:CD2	18:Q:232:LEU:N	2.76	0.47
4:A:195:LYS:NZ	4:A:199:ASP:OD2	2.47	0.47
6:C:136:LEU:HB3	6:C:204:LEU:HG	1.97	0.47
7:D:6:ARG:O	7:D:10:ASN:N	2.47	0.47
3:M:203:PRO:HG2	3:M:206:SER:HB3	1.97	0.47
4:A:1270:VAL:HG11	4:A:1489:VAL:HG11	1.97	0.47
5:B:296:ASP:HB3	5:B:299:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:403:LEU:HD22	17:O:424:LEU:HD13	1.97	0.47
18:Q:144:ILE:HD12	18:Q:154:LEU:CB	2.41	0.47
18:Q:154:LEU:N	18:Q:154:LEU:CD2	2.78	0.47
18:Q:284:LEU:HD13	18:Q:306:VAL:HG22	1.97	0.47
19:S:360:TRP:CE3	19:S:377:ARG:NH2	2.80	0.47
19:S:511:ILE:HD11	19:S:538:LEU:HD23	1.95	0.47
5:B:815:ARG:NH2	5:B:899:GLN:OE1	2.47	0.47
5:B:1091:ARG:HA	5:B:1091:ARG:HD3	1.61	0.47
5:B:934:ILE:H	5:B:934:ILE:HG13	1.54	0.46
12:I:91:ASN:ND2	12:I:115:THR:OG1	2.48	0.46
3:M:290:PRO:HB2	3:M:295:VAL:HG21	1.96	0.46
3:M:116:LYS:HE3	3:M:118:ASP:HB3	1.97	0.46
4:A:834:ARG:HH21	5:B:993:ALA:HB1	1.80	0.46
5:B:921:HIS:NE2	5:B:965:GLU:OE1	2.38	0.46
19:S:360:TRP:CD1	19:S:360:TRP:C	2.88	0.46
19:S:450:ARG:HG2	19:S:450:ARG:NH1	2.17	0.46
19:S:406:LYS:HD3	19:S:453:VAL:H	1.80	0.46
4:A:551:VAL:HG12	4:A:554:ARG:HH21	1.80	0.46
17:O:314:THR:HG22	18:Q:5:ILE:HG22	1.96	0.46
5:B:492:ASN:ND2	5:B:725:THR:OG1	2.49	0.46
13:J:9:SER:HB2	13:J:45:CYS:HB2	1.97	0.46
4:A:316:LEU:HD23	4:A:318:THR:H	1.81	0.46
5:B:286:ARG:HH12	12:I:4:VAL:HG21	1.80	0.46
17:O:97:LEU:HD22	17:O:135:LYS:HG2	1.96	0.46
18:Q:439:ILE:HD12	19:S:717:LYS:HE2	1.97	0.46
19:S:270:GLN:HG3	19:S:291:PRO:HB3	1.98	0.46
4:A:73:PRO:O	4:A:366:ARG:NH2	2.49	0.46
4:A:1634:LEU:HD13	4:A:1643:VAL:HG11	1.98	0.46
8:E:3:GLN:HB2	8:E:7:ARG:HH12	1.80	0.46
19:S:18:VAL:HG21	20:R:366:PHE:CZ	2.51	0.46
19:S:507:GLY:O	19:S:540:LYS:N	2.48	0.46
19:S:583:GLU:HA	19:S:586:LYS:HB2	1.97	0.46
12:I:37:TYR:HD1	12:I:39:LYS:HE2	1.80	0.46
18:Q:92:PHE:HB3	18:Q:205:ILE:HG23	1.97	0.46
19:S:532:GLU:HA	19:S:554:ASN:HB3	1.97	0.46
1:T:17:DG:N1	2:U:53:DA:H2	2.09	0.46
5:B:190:ILE:HD13	5:B:496:PHE:HE2	1.80	0.46
6:C:216:HIS:HD2	6:C:218:LYS:H	1.64	0.46
10:G:133:LEU:HD13	10:G:149:ILE:HD13	1.98	0.46
4:A:481:ARG:HH21	4:A:632:GLU:HB2	1.81	0.45
4:A:1238:MET:HE3	4:A:1524:VAL:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:93:MET:HG3	8:E:120:ALA:HB1	1.98	0.45
3:M:31:ARG:HG3	12:I:11:LEU:HB3	1.98	0.45
3:M:261:LEU:O	3:M:265:LEU:N	2.48	0.45
4:A:216:ARG:NH2	4:A:338:VAL:O	2.49	0.45
5:B:906:ARG:HD2	6:C:93:GLN:HG2	1.98	0.45
4:A:124:LEU:HD22	4:A:129:LEU:HD11	1.99	0.45
4:A:215:GLU:OE2	8:E:177:ARG:NH2	2.40	0.45
4:A:1641:ILE:HD11	5:B:1088:LEU:HD21	1.97	0.45
10:G:134:GLU:OE2	10:G:230:ARG:NE	2.46	0.45
18:Q:245:SER:HB2	18:Q:286:LEU:HB3	1.98	0.45
20:R:415:LEU:HD11	20:R:426:VAL:HG21	1.98	0.45
3:M:221:ILE:HG23	3:M:230:LYS:HG3	1.99	0.45
4:A:77:GLY:O	4:A:362:VAL:N	2.40	0.45
5:B:1103:VAL:HG22	5:B:1110:ILE:HG12	1.98	0.45
10:G:234:ARG:HB2	10:G:248:THR:HG23	1.98	0.45
19:S:360:TRP:CD1	19:S:360:TRP:O	2.70	0.45
2:U:61:DA:O5'	2:U:61:DA:H8	1.99	0.45
4:A:982:VAL:HG12	4:A:984:GLY:H	1.81	0.45
4:A:1556:GLU:OE1	8:E:200:ARG:NH1	2.50	0.45
5:B:532:HIS:ND1	5:B:719:CYS:HB3	2.31	0.45
6:C:136:LEU:HB2	6:C:167:LEU:HD23	1.99	0.45
18:Q:98:HIS:O	18:Q:98:HIS:CG	2.70	0.45
2:U:59:DG:OP1	4:A:221:HIS:CE1	2.66	0.45
6:C:115:TRP:HH2	6:C:212:ILE:HG23	1.82	0.45
4:A:1121:ASP:OD1	4:A:1121:ASP:N	2.49	0.45
5:B:1119:ARG:NH2	5:B:1160:GLU:OE2	2.49	0.45
7:D:30:HIS:HA	10:G:39:VAL:HG23	1.99	0.45
12:I:29:GLU:HA	12:I:35:ALA:HB3	1.99	0.45
17:O:97:LEU:HD11	17:O:136:TYR:HA	1.97	0.45
17:O:429:ALA:HB1	17:O:486:PHE:HD2	1.81	0.45
19:S:353:ASP:OD2	19:S:356:GLU:N	2.49	0.45
19:S:600:GLU:O	19:S:604:ILE:N	2.45	0.45
3:M:51:PHE:CD2	3:M:94:PRO:HG3	2.52	0.45
4:A:555:LYS:O	4:A:559:ASN:ND2	2.49	0.45
18:Q:442:LEU:HD23	18:Q:445:ARG:HD2	1.98	0.45
19:S:360:TRP:CB	19:S:377:ARG:NH2	2.79	0.45
1:T:12:DC:H2"	1:T:13:DT:H5"	1.99	0.45
4:A:1240:LEU:HB3	4:A:1536:ILE:HD12	1.98	0.45
5:B:584:CYS:HB3	5:B:596:VAL:HG23	1.99	0.45
5:B:647:SER:OG	5:B:647:SER:O	2.34	0.45
5:B:731:VAL:HG21	13:J:59:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:78:THR:OG1	16:N:89:ILE:O	2.31	0.45
20:R:358:PHE:HB2	20:R:364:VAL:HG21	1.99	0.45
20:R:5:PRO:HA	20:R:248:LYS:HD2	1.98	0.45
20:R:7:THR:HG23	20:R:292:SER:HB3	1.98	0.45
20:R:135:GLU:OE2	20:R:301:SER:OG	2.34	0.45
1:T:11:DG:OP2	1:T:11:DG:C8	2.70	0.44
4:A:461:GLU:HG2	4:A:1618:THR:HB	2.00	0.44
5:B:216:ALA:HB2	5:B:380:LYS:HD3	1.99	0.44
10:G:134:GLU:HG2	10:G:230:ARG:HA	1.99	0.44
16:N:89:ILE:HG13	16:N:139:VAL:HG22	1.98	0.44
4:A:255:ALA:HB2	4:A:311:GLY:HA2	2.00	0.44
19:S:768:TYR:HA	19:S:771:ILE:HG12	1.98	0.44
20:R:251:TRP:HA	20:R:270:PHE:HE2	1.81	0.44
4:A:852:ASP:OD1	4:A:855:ARG:NH2	2.51	0.44
4:A:1128:ASN:HB3	4:A:1131:LYS:HB3	1.99	0.44
8:E:21:GLU:OE1	8:E:143:ASN:ND2	2.43	0.44
10:G:219:ASP:OD1	10:G:223:GLU:N	2.43	0.44
18:Q:158:MET:HB3	18:Q:192:TYR:CE1	2.52	0.44
18:Q:282:ARG:HA	18:Q:282:ARG:NE	2.32	0.44
12:I:114:CYS:SG	12:I:115:THR:N	2.90	0.44
4:A:527:PRO:HB3	4:A:534:THR:HA	1.98	0.44
5:B:935:ASP:OD1	5:B:935:ASP:N	2.41	0.44
9:F:69:LEU:HD23	10:G:94:PRO:HG3	1.98	0.44
16:N:92:ASP:OD1	16:N:92:ASP:N	2.51	0.44
19:S:261:VAL:HG13	19:S:272:PHE:HB2	1.98	0.44
3:M:75:GLN:HG3	16:N:58:PHE:HB2	2.00	0.44
4:A:1238:MET:HB3	4:A:1521:THR:HB	2.00	0.44
17:O:311:MET:HB3	18:Q:6:ARG:HG2	1.99	0.44
17:O:361:PHE:HZ	17:O:399:PHE:HB2	1.82	0.44
19:S:68:THR:HG23	19:S:207:SER:HB3	1.98	0.44
10:G:218:VAL:HG13	10:G:222:GLY:HA2	1.98	0.44
17:O:194:LEU:HD21	17:O:218:LEU:HD23	2.00	0.44
4:A:550:SER:OG	4:A:551:VAL:N	2.51	0.44
4:A:1490:GLU:OE2	12:I:51:THR:OG1	2.33	0.44
5:B:204:ARG:NH1	5:B:502:MET:SD	2.91	0.44
18:Q:219:ILE:HG22	20:R:206:ARG:O	2.18	0.44
3:M:252:GLN:HG3	3:M:254:SER:H	1.83	0.44
3:M:346:ILE:HD13	3:M:393:LYS:HB2	2.00	0.44
4:A:37:VAL:HG12	4:A:49:LEU:HB2	2.00	0.44
5:B:107:PRO:HB2	5:B:121:VAL:HG13	1.99	0.44
5:B:543:ASN:OD1	5:B:543:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:893:ASN:N	5:B:893:ASN:HD22	2.15	0.44
11:H:40:LEU:HG	11:H:42:ILE:HG23	2.00	0.44
19:S:264:ILE:HG23	19:S:300:LEU:HD21	2.00	0.44
19:S:319:ASP:HB2	19:S:363:ILE:HG12	1.99	0.44
19:S:699:LEU:HD22	19:S:744:LEU:HD21	1.98	0.44
4:A:30:LYS:HZ1	5:B:1129:ARG:CZ	2.31	0.43
10:G:234:ARG:HG2	10:G:235:ASN:H	1.82	0.43
18:Q:278:GLU:OE2	18:Q:284:LEU:HD23	2.18	0.43
19:S:390:GLN:N	20:R:150:GLN:O	2.51	0.43
3:M:24:GLY:N	16:N:108:THR:O	2.51	0.43
3:M:321:ASP:OD1	3:M:321:ASP:N	2.50	0.43
4:A:32:ILE:HD12	4:A:362:VAL:HG21	1.99	0.43
4:A:335:LEU:HD23	4:A:335:LEU:HA	1.87	0.43
4:A:741:PRO:HA	4:A:742:PRO:HD3	1.86	0.43
4:A:831:ASP:N	4:A:831:ASP:OD1	2.50	0.43
4:A:1256:LYS:O	4:A:1499:ARG:NH2	2.51	0.43
18:Q:208:PRO:HD2	18:Q:211:TYR:HB2	2.00	0.43
19:S:248:PRO:HB3	19:S:305:PHE:HB2	1.99	0.43
19:S:657:SER:HA	19:S:748:GLU:HB2	2.00	0.43
2:U:54:DG:H1'	5:B:513:LYS:HZ2	1.84	0.43
4:A:213:ASN:ND2	4:A:1606:SER:O	2.52	0.43
6:C:259:ASP:HB3	6:C:263:ASP:HB3	2.00	0.43
7:D:6:ARG:HD2	17:O:196:LYS:HE3	2.00	0.43
18:Q:180:ASP:OD1	18:Q:255:LYS:NZ	2.51	0.43
19:S:421:ILE:HG13	19:S:441:ASP:HA	1.99	0.43
1:T:36:DT:H3	2:U:35:DA:N6	2.17	0.43
4:A:526:GLY:HA3	4:A:554:ARG:NH1	2.33	0.43
5:B:28:PRO:HA	5:B:29:PRO:HD3	1.93	0.43
5:B:547:HIS:CE1	5:B:548:LYS:HE3	2.53	0.43
10:G:149:ILE:N	10:G:153:PHE:O	2.49	0.43
4:A:487:ASP:HB2	4:A:615:ARG:HG2	2.00	0.43
5:B:714:ARG:HD3	5:B:714:ARG:HA	1.77	0.43
17:O:119:ILE:O	17:O:136:TYR:OH	2.30	0.43
1:T:45:DT:O4	2:U:26:DA:N1	2.50	0.43
2:U:59:DG:H2'	2:U:59:DG:O5'	2.18	0.43
4:A:368:ARG:HH11	4:A:383:ASN:HD21	1.66	0.43
4:A:563:THR:HG22	17:O:375:THR:HG22	2.00	0.43
8:E:76:GLY:N	8:E:106:GLN:OE1	2.51	0.43
18:Q:103:LEU:HG	18:Q:207:LEU:HD13	2.00	0.43
18:Q:207:LEU:HD12	18:Q:207:LEU:HA	1.81	0.43
18:Q:413:LEU:HD21	20:R:240:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:36:DT:C2	2:U:35:DA:N1	2.86	0.43
4:A:743:ASP:OD1	4:A:743:ASP:N	2.52	0.43
5:B:823:GLN:HA	5:B:863:ASP:HA	2.01	0.43
18:Q:154:LEU:CD2	18:Q:154:LEU:H	2.32	0.43
19:S:362:ARG:NH1	19:S:363:ILE:O	2.52	0.43
4:A:677:GLY:O	4:A:681:THR:OG1	2.25	0.43
4:A:855:ARG:O	4:A:859:ALA:N	2.45	0.43
4:A:1613:MET:HB3	4:A:1618:THR:HG23	2.00	0.43
5:B:17:ARG:HB3	5:B:20:GLU:HB3	2.00	0.43
5:B:218:ILE:HG23	5:B:391:PRO:HB3	2.01	0.43
8:E:8:ASN:OD1	8:E:11:ARG:NH2	2.51	0.43
12:I:102:ARG:HB2	12:I:106:GLU:HB3	1.99	0.43
14:K:46:LYS:HA	14:K:66:VAL:HG22	1.99	0.43
17:O:113:THR:HA	17:O:116:ILE:HD12	1.99	0.43
18:Q:192:TYR:CD2	18:Q:192:TYR:C	2.92	0.43
18:Q:193:PHE:HZ	18:Q:220:SER:CB	2.30	0.43
19:S:665:ASN:ND2	19:S:668:SER:OG	2.50	0.43
20:R:135:GLU:HG3	20:R:284:PHE:CD2	2.54	0.43
5:B:232:TYR:CD2	5:B:385:VAL:HG12	2.53	0.43
17:O:340:SER:HA	17:O:343:VAL:HG12	2.01	0.43
19:S:322:GLY:O	19:S:350:THR:OG1	2.26	0.43
4:A:58:LEU:HD23	18:Q:69:SER:HA	2.01	0.43
4:A:1543:SER:OG	4:A:1544:ASN:N	2.51	0.43
18:Q:282:ARG:HG3	18:Q:283:ASN:OD1	2.19	0.43
18:Q:282:ARG:HA	18:Q:282:ARG:HE	1.83	0.43
18:Q:431:ASP:OD2	18:Q:434:HIS:ND1	2.52	0.43
19:S:31:ASN:O	19:S:32:TYR:CD1	2.72	0.43
19:S:221:ARG:NH2	19:S:549:TYR:OH	2.52	0.43
20:R:362:ALA:HB2	20:R:421:LYS:HB2	2.01	0.43
5:B:657:PRO:HD3	16:N:148:ILE:HG12	2.00	0.42
10:G:37:CYS:O	10:G:126:GLN:N	2.44	0.42
3:M:198:VAL:HA	3:M:201:ILE:HG12	2.01	0.42
17:O:436:ARG:HG2	17:O:490:ILE:HG23	2.01	0.42
17:O:521:ASN:HB2	17:O:589:GLN:HB3	2.01	0.42
18:Q:253:LEU:O	18:Q:257:VAL:N	2.49	0.42
2:U:53:DA:H5'	5:B:512:LEU:HD22	2.02	0.42
6:C:91:VAL:HG11	13:J:60:PHE:HB3	2.00	0.42
7:D:5:SER:O	7:D:8:THR:OG1	2.32	0.42
15:L:41:SER:OG	15:L:44:ASP:OD2	2.30	0.42
18:Q:172:LEU:HD23	18:Q:174:LEU:HD11	2.01	0.42
18:Q:205:ILE:HD13	18:Q:205:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:59:ARG:HG3	18:Q:69:SER:HB3	2.01	0.42
12:I:117:CYS:SG	12:I:118:GLY:N	2.92	0.42
14:K:88:PHE:HB3	14:K:106:GLN:HB2	2.02	0.42
19:S:264:ILE:HG12	19:S:300:LEU:HD11	2.02	0.42
19:S:408:ILE:HD11	19:S:415:LEU:HB2	2.00	0.42
20:R:125:ARG:HH11	20:R:125:ARG:CG	2.23	0.42
20:R:268:LEU:HD11	20:R:316:SER:HB3	2.01	0.42
9:F:86:THR:O	9:F:88:TYR:N	2.48	0.42
10:G:160:ASN:H	17:O:105:ASN:HD21	1.68	0.42
20:R:122:ASP:HB2	20:R:125:ARG:CD	2.45	0.42
6:C:322:LYS:NZ	6:C:326:GLU:OE2	2.53	0.42
13:J:44:TYR:HA	13:J:47:ARG:HB3	2.02	0.42
17:O:389:SER:O	17:O:427:TYR:OH	2.37	0.42
18:Q:244:ASN:OD1	18:Q:244:ASN:N	2.52	0.42
3:M:166:ARG:NH2	4:A:400:ASN:O	2.52	0.42
5:B:979:GLN:HG2	5:B:996:PHE:HE1	1.85	0.42
5:B:1042:ASP:HA	5:B:1063:ARG:HH12	1.83	0.42
11:H:111:LEU:HD23	11:H:111:LEU:HA	1.92	0.42
17:O:150:TRP:O	17:O:154:VAL:N	2.49	0.42
18:Q:253:LEU:HA	18:Q:256:LEU:HB2	2.02	0.42
1:T:53:DG:N2	2:U:17:DA:N1	2.68	0.42
4:A:333:CYS:SG	4:A:334:VAL:N	2.93	0.42
4:A:427:PHE:HA	4:A:430:ILE:HG22	2.01	0.42
11:H:112:ILE:N	11:H:127:GLY:O	2.53	0.42
4:A:751:SER:OG	4:A:752:LYS:N	2.52	0.42
5:B:553:THR:O	5:B:646:HIS:ND1	2.35	0.42
5:B:655:TYR:CE2	5:B:657:PRO:HG2	2.55	0.42
8:E:19:VAL:HG11	8:E:80:VAL:HG11	2.01	0.42
8:E:124:VAL:HG13	8:E:132:ILE:HB	2.02	0.42
10:G:30:GLU:HG2	10:G:32:ASN:HB2	2.02	0.42
19:S:302:VAL:HG11	19:S:362:ARG:HD2	2.01	0.42
1:T:14:DT:H6	1:T:14:DT:H2'	1.72	0.41
16:N:123:SER:HA	16:N:131:LEU:HB2	2.02	0.41
18:Q:227:TYR:HB3	18:Q:301:HIS:CD2	2.54	0.41
19:S:187:ILE:HD11	19:S:259:ASN:HA	2.02	0.41
20:R:168:ILE:HG23	20:R:169:PRO:HD3	2.02	0.41
18:Q:157:HIS:O	18:Q:160:SER:N	2.36	0.41
19:S:31:ASN:CG	19:S:32:TYR:N	2.58	0.41
20:R:25:ASN:ND2	20:R:123:GLU:OE1	2.53	0.41
1:T:31:DC:H42	2:U:40:DG:H1	1.67	0.41
4:A:630:GLY:HA3	5:B:916:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1501:ILE:HG23	4:A:1504:ILE:HB	2.01	0.41
5:B:137:LEU:HD22	5:B:161:LEU:HD23	2.02	0.41
5:B:617:THR:HG22	5:B:619:GLY:H	1.84	0.41
19:S:187:ILE:O	19:S:200:THR:OG1	2.35	0.41
1:T:32:DC:O2	5:B:817:ARG:NH1	2.53	0.41
3:M:45:LYS:NZ	3:M:48:LYS:O	2.53	0.41
4:A:6:PRO:HG3	10:G:113:PHE:CD2	2.55	0.41
4:A:1266:VAL:HG21	4:A:1313:LEU:HD21	2.02	0.41
5:B:318:PRO:O	5:B:321:GLN:NE2	2.53	0.41
17:O:332:LEU:HD23	17:O:599:LEU:HD11	2.01	0.41
19:S:269:PHE:CZ	19:S:303:VAL:HG21	2.55	0.41
4:A:1072:ASN:O	4:A:1076:LEU:HB2	2.21	0.41
5:B:567:SER:OG	16:N:141:GLU:OE1	2.37	0.41
5:B:708:ASP:OD1	5:B:708:ASP:N	2.54	0.41
5:B:789:ILE:HG22	5:B:930:LYS:HA	2.02	0.41
4:A:1291:VAL:HG22	4:A:1473:LYS:HE3	2.01	0.41
5:B:939:SER:OG	5:B:940:GLU:N	2.53	0.41
17:O:251:LEU:HA	17:O:598:PHE:HE1	1.85	0.41
18:Q:128:GLU:HB3	19:S:749:LYS:HE3	2.01	0.41
18:Q:134:LYS:O	18:Q:138:LEU:N	2.48	0.41
19:S:269:PHE:HD2	19:S:292:LEU:HD21	1.85	0.41
19:S:403:ARG:HE	19:S:419:ARG:HB3	1.86	0.41
20:R:236:PHE:CD1	20:R:253:ILE:HD11	2.56	0.41
1:T:8:DA:H2	2:U:63:DT:H3	1.69	0.41
1:T:36:DT:H3	2:U:35:DA:H61	1.69	0.41
3:M:329:LEU:HD23	3:M:332:ILE:HD12	2.02	0.41
4:A:31:GLN:HG2	4:A:78:HIS:CE1	2.56	0.41
5:B:1022:LEU:HD23	5:B:1026:ILE:HD11	2.03	0.41
18:Q:215:LEU:HD12	18:Q:215:LEU:HA	1.76	0.41
18:Q:341:ARG:NH1	18:Q:365:ASP:OD2	2.54	0.41
19:S:18:VAL:HG23	20:R:427:PRO:HD2	2.03	0.41
2:U:58:DA:H8	2:U:58:DA:O5'	2.04	0.41
4:A:95:TYR:CZ	4:A:99:ARG:HD2	2.56	0.41
4:A:862:THR:HG23	4:A:864:LEU:H	1.86	0.41
5:B:16:PHE:CD1	5:B:978:ALA:HB2	2.56	0.41
10:G:81:VAL:HA	10:G:124:VAL:HG12	2.02	0.41
10:G:154:ASN:ND2	17:O:182:MET:O	2.47	0.41
17:O:128:LEU:HD13	17:O:132:THR:HG22	2.03	0.41
20:R:124:GLU:O	20:R:127:PHE:N	2.53	0.41
5:B:547:HIS:ND1	5:B:548:LYS:HG2	2.36	0.41
5:B:979:GLN:HG2	5:B:996:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:547:ILE:HB	18:Q:22:ILE:HD11	2.03	0.40
4:A:939:ASN:HD22	5:B:958:MET:HE2	1.86	0.40
5:B:782:ASP:O	5:B:950:ASN:ND2	2.54	0.40
17:O:347:VAL:HG11	17:O:391:GLN:HG3	2.03	0.40
19:S:277:VAL:HG12	19:S:284:VAL:HA	2.02	0.40
1:T:17:DG:O6	2:U:53:DA:N1	2.54	0.40
4:A:744:MET:HG2	4:A:1078:LYS:HD2	2.03	0.40
4:A:1060:GLU:OE2	4:A:1580:ARG:NH1	2.54	0.40
5:B:625:GLU:HG2	5:B:643:PHE:HB2	2.03	0.40
8:E:128:PRO:HG2	8:E:129:PRO:HD3	2.03	0.40
8:E:157:SER:OG	8:E:160:GLU:OE1	2.38	0.40
18:Q:328:LEU:HD13	18:Q:472:ARG:HA	2.02	0.40
3:M:62:TYR:HB3	3:M:100:VAL:HA	2.02	0.40
4:A:252:PHE:HE1	4:A:314:TYR:HD1	1.69	0.40
4:A:379:GLU:OE1	18:Q:58:ARG:NE	2.52	0.40
5:B:156:ARG:CZ	5:B:450:LEU:HD22	2.52	0.40
5:B:1082:HIS:HB2	5:B:1084:THR:HG22	2.03	0.40
5:B:1133:MET:O	5:B:1168:VAL:N	2.39	0.40
18:Q:63:THR:HG21	18:Q:72:SER:HB3	2.03	0.40
19:S:366:PHE:HB2	19:S:373:LEU:HG	2.03	0.40
1:T:17:DG:C2	2:U:54:DG:N2	2.90	0.40
9:F:79:ARG:NH1	9:F:145:ASP:O	2.54	0.40
18:Q:348:ILE:HA	18:Q:351:ASN:HD22	1.86	0.40
18:Q:478:ARG:HD3	19:S:570:ASP:HB2	2.04	0.40
19:S:317:ILE:HG21	19:S:365:TRP:HE1	1.87	0.40
19:S:640:SER:O	19:S:644:THR:OG1	2.34	0.40
20:R:133:LYS:HA	20:R:134:PRO:HD3	1.90	0.40
4:A:986:PHE:HB3	5:B:960:ILE:HD12	2.02	0.40
4:A:990:ILE:HB	4:A:994:GLU:HG3	2.04	0.40
4:A:1316:VAL:HG21	4:A:1498:ILE:HG23	2.04	0.40
8:E:100:ILE:HA	8:E:105:PHE:HD2	1.85	0.40
17:O:521:ASN:HB3	17:O:524:VAL:HG12	2.03	0.40
18:Q:102:LEU:HA	18:Q:102:LEU:HD12	1.89	0.40
19:S:672:ILE:O	19:S:676:SER:N	2.53	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	
3	M	388/415 (94%)	356 (92%)	32 (8%)	0	100	100
4	A	1448/1664 (87%)	1368 (94%)	79 (6%)	1 (0%)	51	85
5	B	1174/1203 (98%)	1103 (94%)	71 (6%)	0	100	100
6	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
7	D	66/137 (48%)	62 (94%)	4 (6%)	0	100	100
8	E	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
9	F	98/155 (63%)	93 (95%)	4 (4%)	1 (1%)	15	53
10	G	193/326 (59%)	182 (94%)	11 (6%)	0	100	100
11	H	130/146 (89%)	117 (90%)	13 (10%)	0	100	100
12	I	122/125 (98%)	108 (88%)	14 (12%)	0	100	100
13	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
14	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
15	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
16	N	131/233 (56%)	114 (87%)	16 (12%)	1 (1%)	19	57
17	O	493/627 (79%)	453 (92%)	40 (8%)	0	100	100
18	Q	469/514 (91%)	415 (88%)	53 (11%)	1 (0%)	47	82
19	S	594/894 (66%)	517 (87%)	77 (13%)	0	100	100
20	R	322/507 (64%)	289 (90%)	32 (10%)	1 (0%)	41	76
All	All	6352/7778 (82%)	5874 (92%)	473 (7%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	R	195	LEU
18	Q	283	ASN
4	A	1458	THR
9	F	87	LYS

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Mol	Chain	Res	Type
16	N	118	SER

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
3	M	350/371 (94%)	349 (100%)	1 (0%)	92 97
4	A	1292/1465 (88%)	1287 (100%)	5 (0%)	91 97
5	B	1030/1053 (98%)	1027 (100%)	3 (0%)	92 97
6	C	269/296 (91%)	267 (99%)	2 (1%)	84 94
7	D	65/116 (56%)	65 (100%)	0	100 100
8	E	197/197 (100%)	196 (100%)	1 (0%)	88 96
9	F	90/137 (66%)	90 (100%)	0	100 100
10	G	177/291 (61%)	177 (100%)	0	100 100
11	H	116/128 (91%)	115 (99%)	1 (1%)	78 92
12	I	109/110 (99%)	109 (100%)	0	100 100
13	J	64/65 (98%)	62 (97%)	2 (3%)	40 75
14	K	93/130 (72%)	93 (100%)	0	100 100
15	L	40/57 (70%)	40 (100%)	0	100 100
16	N	128/220 (58%)	128 (100%)	0	100 100
17	O	457/576 (79%)	456 (100%)	1 (0%)	93 98
18	Q	436/476 (92%)	423 (97%)	13 (3%)	41 75
19	S	563/828 (68%)	557 (99%)	6 (1%)	73 90
20	R	313/474 (66%)	306 (98%)	7 (2%)	52 81
All	All	5789/6990 (83%)	5747 (99%)	42 (1%)	84 94

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	316	ARG

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Mol	Chain	Res	Type
4	A	30	LYS
4	A	467	PHE
4	A	590	ASN
4	A	606	ARG
4	A	985	ARG
5	B	651	ARG
5	B	893	ASN
5	B	934	ILE
6	C	89	THR
6	C	281	ARG
8	E	200	ARG
11	H	142	LEU
13	J	48	ARG
13	J	52	THR
17	O	76	ASN
18	Q	18	ARG
18	Q	92	PHE
18	Q	102	LEU
18	Q	154	LEU
18	Q	204	ARG
18	Q	205	ILE
18	Q	213	SER
18	Q	215	LEU
18	Q	219	ILE
18	Q	232	LEU
18	Q	236	MET
18	Q	297	ARG
18	Q	413	LEU
19	S	49	THR
19	S	360	TRP
19	S	377	ARG
19	S	379	LYS
19	S	407	ARG
19	S	744	LEU
20	R	157	MET
20	R	182	LYS
20	R	183	GLU
20	R	195	LEU
20	R	196	GLU
20	R	206	ARG
20	R	443	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
4	A	78	HIS
4	A	221	HIS
4	A	1447	GLN
5	B	893	ASN
7	D	88	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

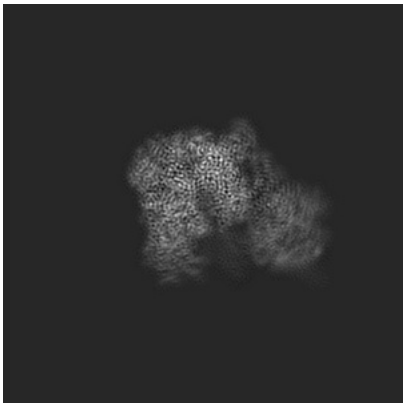
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10038. These allow visual inspection of the internal detail of the map and identification of artifacts.

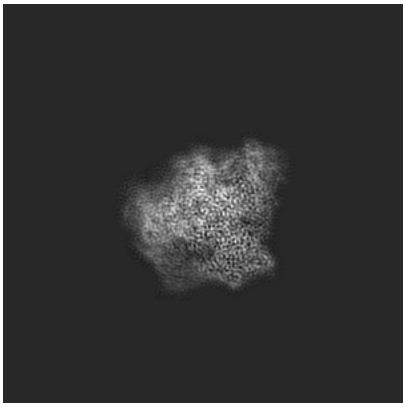
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

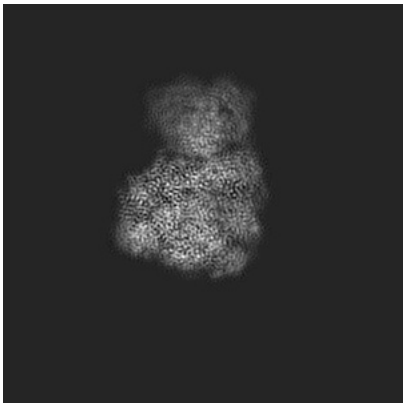
6.1.1 Primary map



X



Y

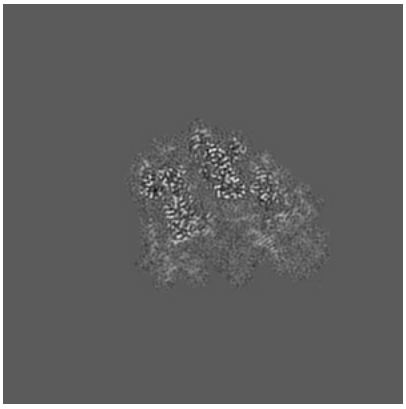


Z

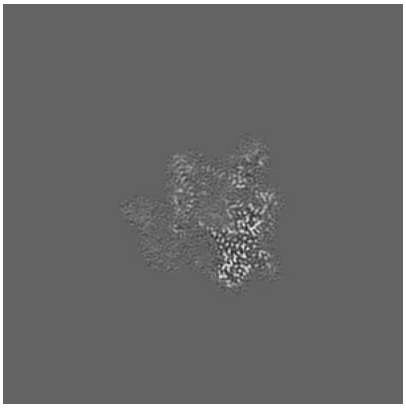
The images above show the map projected in three orthogonal directions.

6.2 Central slices

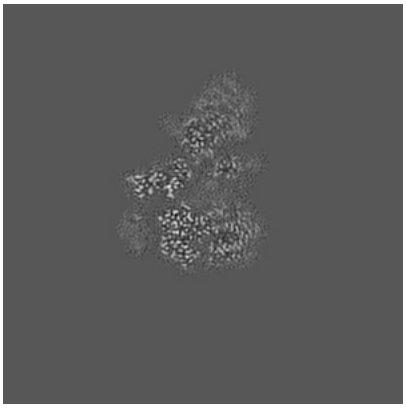
6.2.1 Primary map



X Index: 144



Y Index: 144

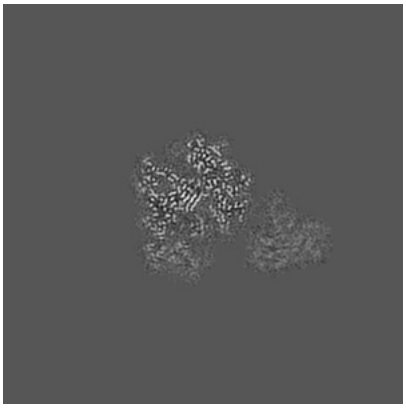


Z Index: 144

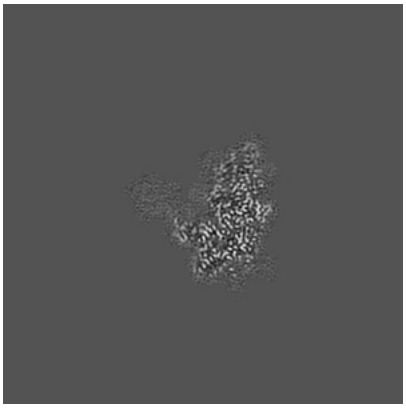
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

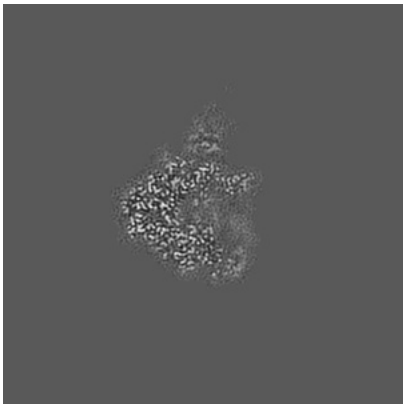
6.3.1 Primary map



X Index: 125



Y Index: 156



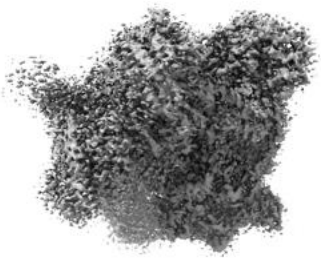
Z Index: 161

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.

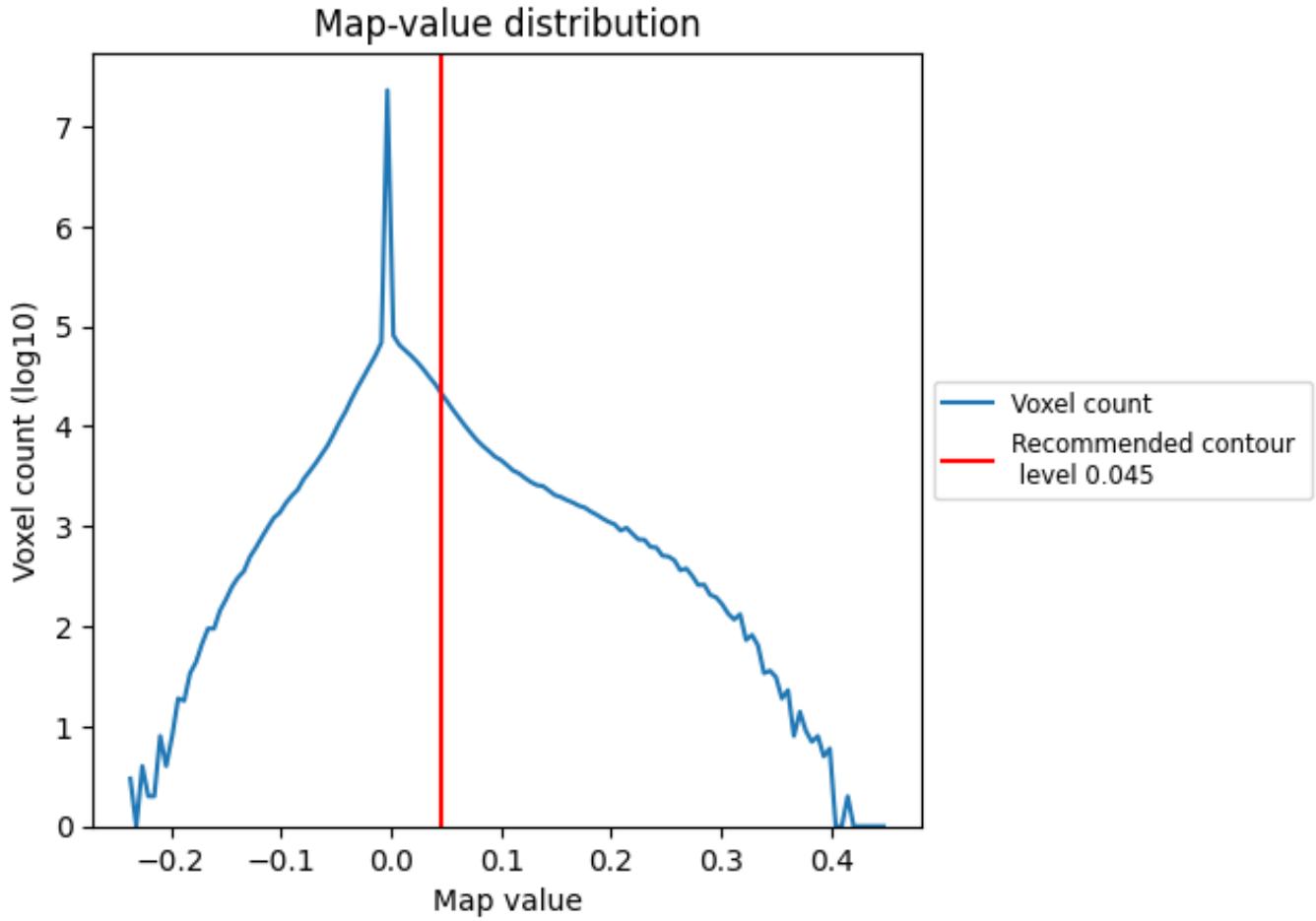
6.5 Mask visualisation (i)

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

7 Map analysis

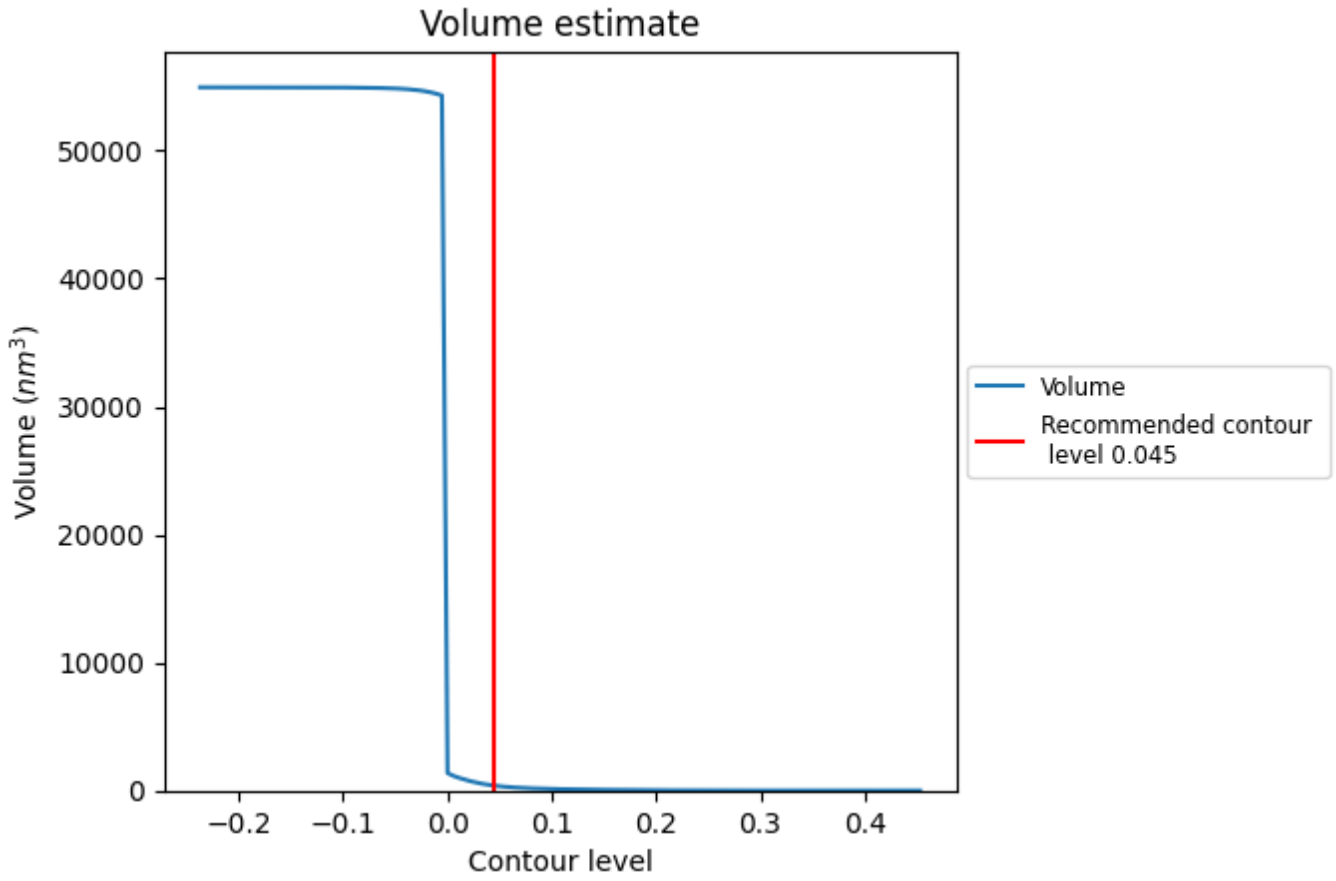
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

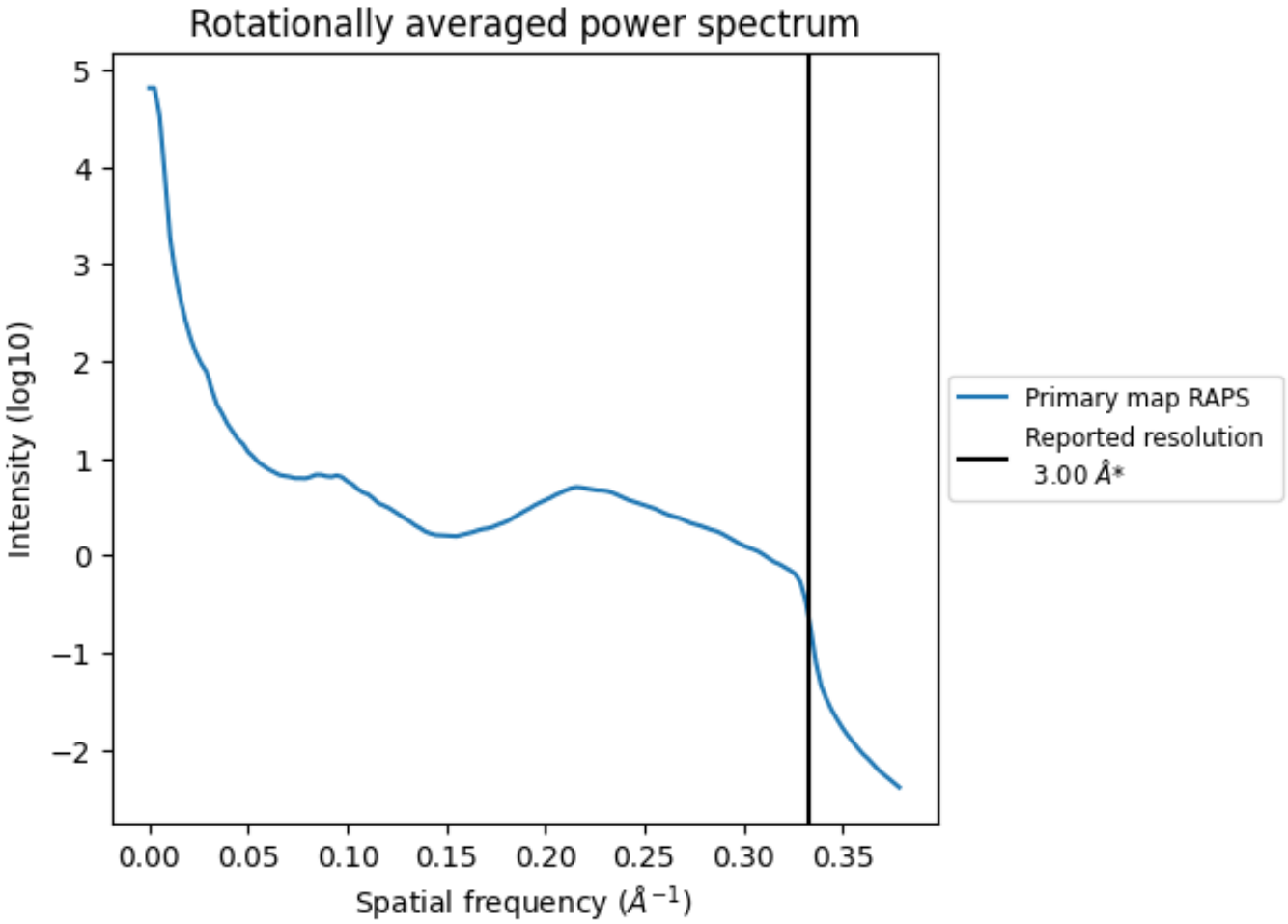
7.2 Volume estimate



The volume at the recommended contour level is 385 nm^3; this corresponds to an approximate mass of 348 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 0.333 Å^{-1}

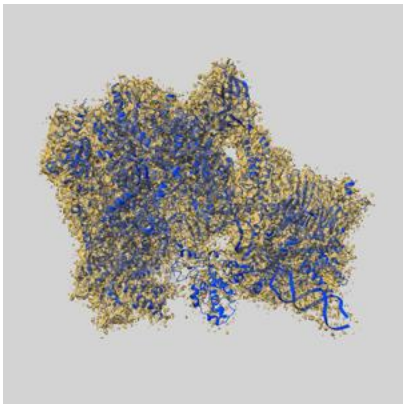
8 Fourier-Shell correlation (i)

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

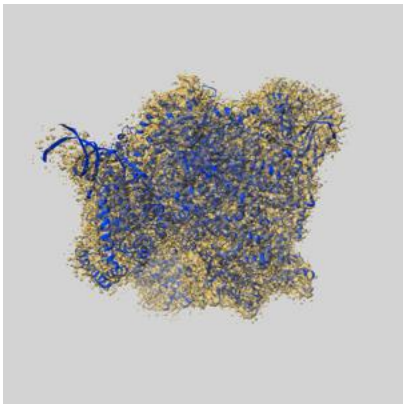
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10038 and PDB model 6RWE. Per-residue inclusion information can be found in section 3 on page 8.

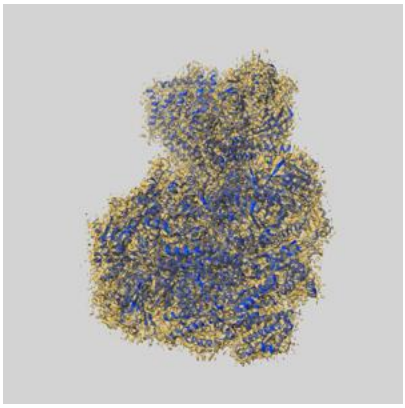
9.1 Map-model overlay



X



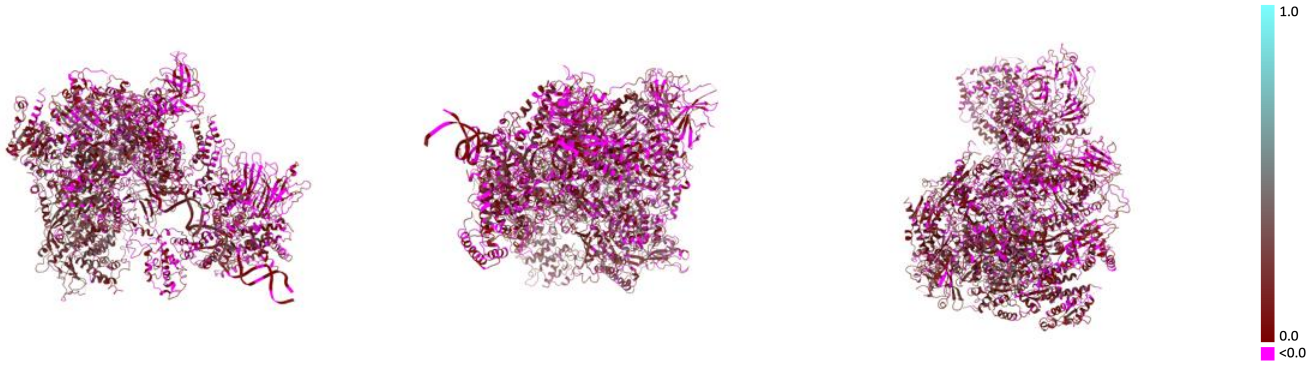
Y



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.

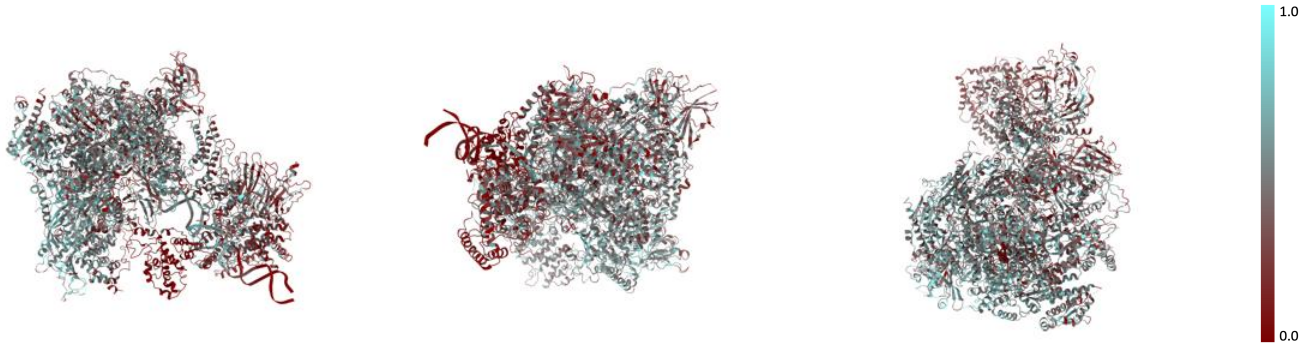
9.2 Q-score mapped to coordinate model (i)



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.

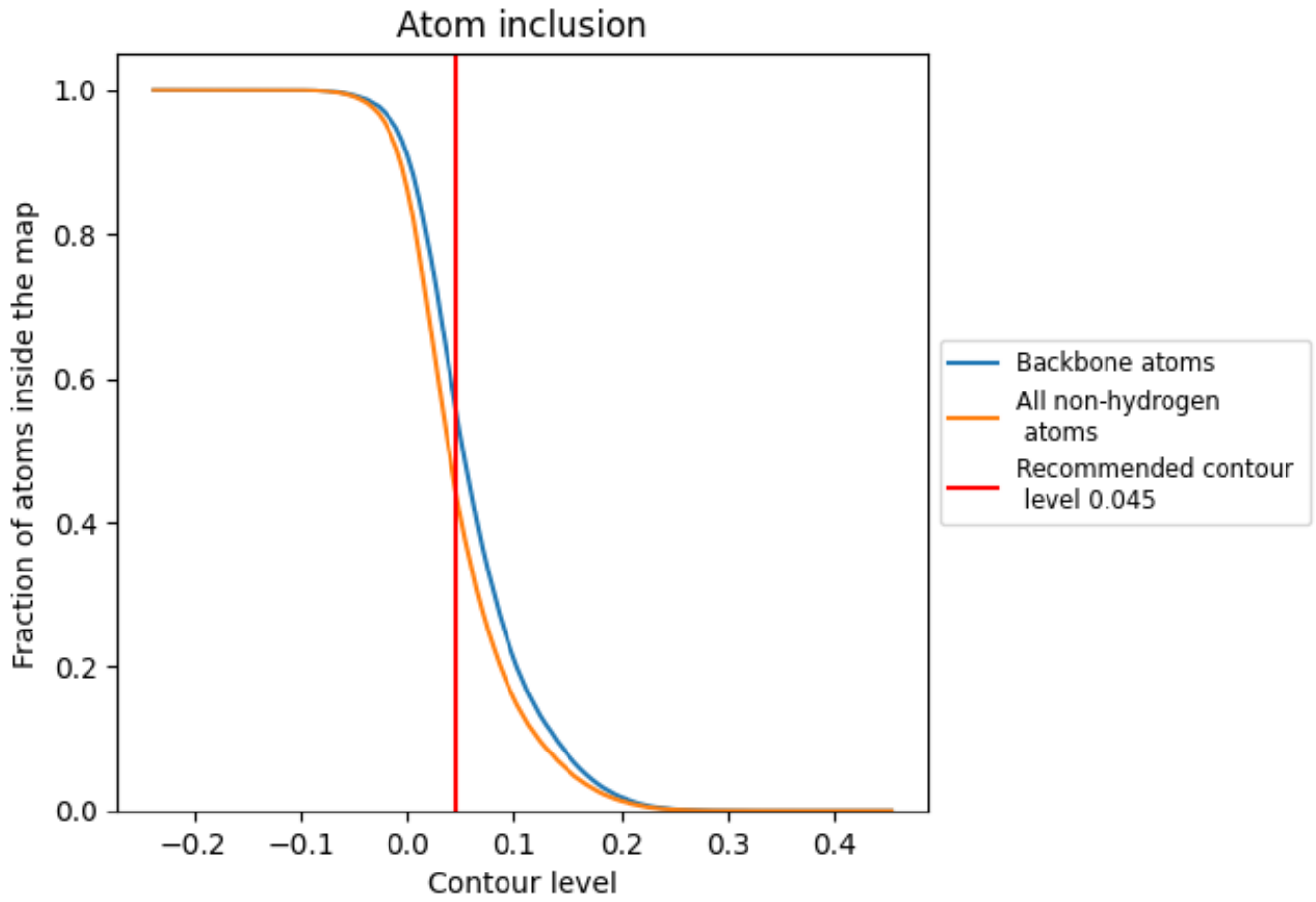
9.3 Atom inclusion mapped to coordinate model (i)



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, 56% of all backbone atoms, 45% 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	0.4462	0.1120
A	0.5291	0.1360
B	0.4995	0.1040
C	0.5527	0.1420
D	0.5414	0.2240
E	0.5216	0.1210
F	0.6155	0.2060
G	0.5837	0.2200
H	0.5670	0.1660
I	0.2730	0.0640
J	0.4746	0.0500
K	0.5468	0.1750
L	0.5274	0.1010
M	0.1443	0.0350
N	0.3516	0.0390
O	0.4411	0.1800
Q	0.3403	0.0880
R	0.4280	0.0650
S	0.3017	0.0370
T	0.3920	0.1090
U	0.4015	0.1240