Full wwPDB EM Validation Report

Aug 27, 2026 – 08:56 am BST

PDB ID	:	7A1G / pdb_00007a1g
EMDB ID	:	EMD-11608
Title	:	Structure of a crosslinked yeast ABCE1-bound 43S pre-initiation complex
Authors	:	Mackens-Kiani, T.; Kratzat, H.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-08-13
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:

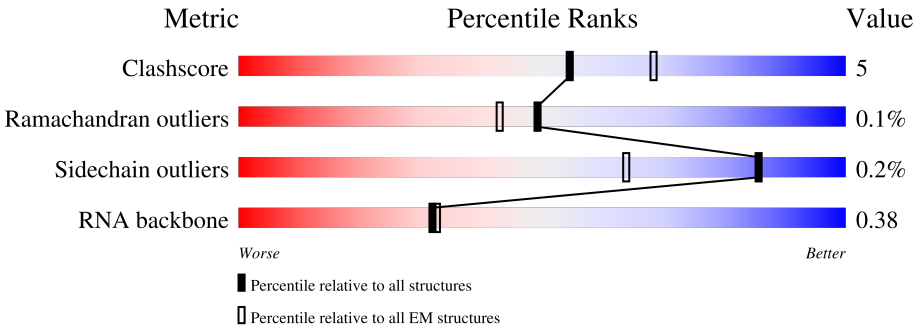
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

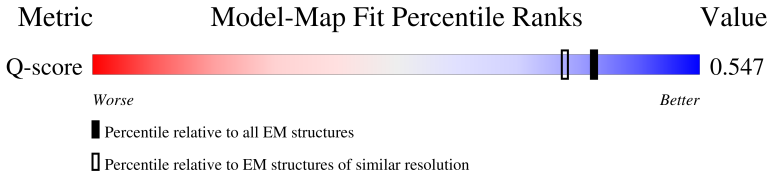
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	2	1771	28% 61% 33% 6%
2	P	206	50% 79% 21%
3	Q	232	68% 77% 20% ·

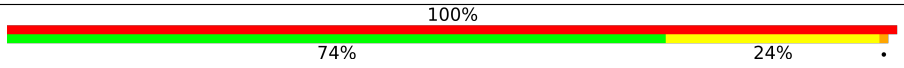
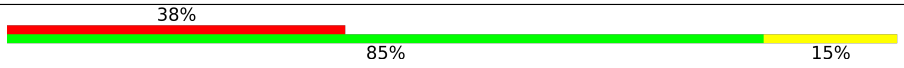
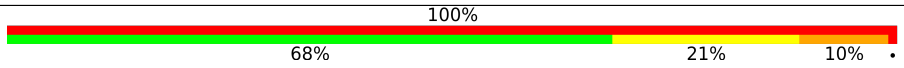
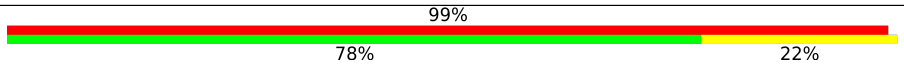
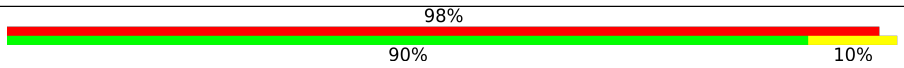
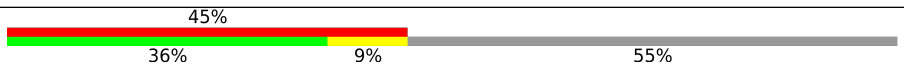
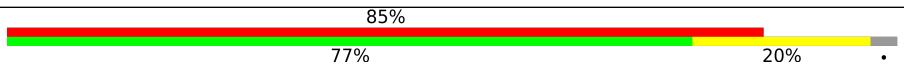
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Mol	Chain	Length	Quality of chain
4	R	216	39% 88% 12%
5	S	258	30% 84% 15%
6	T	228	64% 85% 15%
7	U	184	74% 82% 18%
8	V	200	35% 83% 10% 6%
9	W	184	32% 90% 10%
10	X	142	24% 96%
11	Y	150	41% 94% 5%
12	Z	127	72% 89% 11%
13	a	87	46% 86% 14%
14	b	129	11% 92% 8%
15	c	144	23% 90% 10%
16	d	134	44% 86% 14%
17	e	97	36% 88% 12%
18	f	81	51% 88% 12%
19	g	60	53% 90% 10%
20	E	117	98% 88% 12%
21	A	222	76% 83% 17%
22	B	206	95% 82% 18%
23	C	92	80% 79% 21%
24	D	121	100% 81% 19%
25	F	141	73% 90% 9%
26	H	125	76% 78% 19%
27	I	145	99% 68% 32%
28	J	143	96% 85% 15%

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Mol	Chain	Length	Quality of chain
29	K	100	
30	L	82	
31	M	53	
32	N	73	
33	O	312	
34	h	63	
35	y	265	
35	z	265	
36	x	601	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 81866 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1771	37739	16872	6683	12413	1771	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	206	1603	1030	284	287	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	226	1798	1139	330	325	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	216	1626	1042	287	295	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	258	2056	1308	387	358	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	228	1815	1138	351	323	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	184	Total	C	N	O	0	0
			1473	946	263	264		

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 12 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 17 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 20 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 22 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	92	Total	C	N	O	S	0	0
			754	489	122	141	2		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 26 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 28 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 30 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	L	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	N	73	Total	C	N	O	S	0	0
			560	355	106	95	4		

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 34 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	120	Total 896	C 556	N 172	O 166	S 2	0	0
35	y	79	Total 624	C 389	N 113	O 120	S 2	0	0

- Molecule 36 is a protein called Translation initiation factor RLI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	582	Total 4608	C 2951	N 795	O 839	S 23	0	0

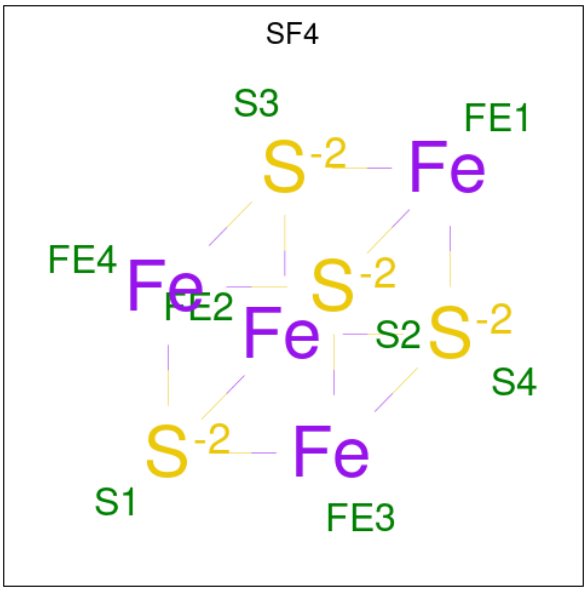
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	76	Total 76	Mg 76	0
37	R	1	Total 1	Mg 1	0
37	S	1	Total 1	Mg 1	0
37	B	1	Total 1	Mg 1	0
37	x	1	Total 1	Mg 1	0

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

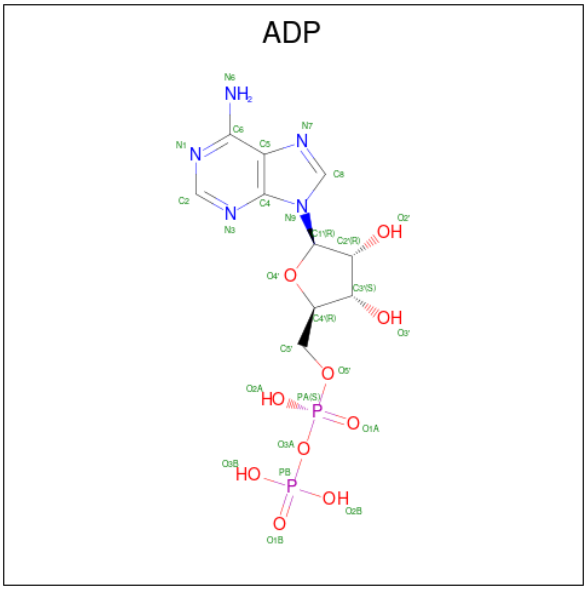
Mol	Chain	Residues	Atoms		AltConf
38	M	1	Total 1	Zn 1	0
38	N	1	Total 1	Zn 1	0

- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
39	x	1	Total	Fe	S	0
			8	4	4	
39	x	1	Total	Fe	S	0
			8	4	4	

- Molecule 40 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
40	x	1	Total	C	N	O	P	0
			27	10	5	10	2	

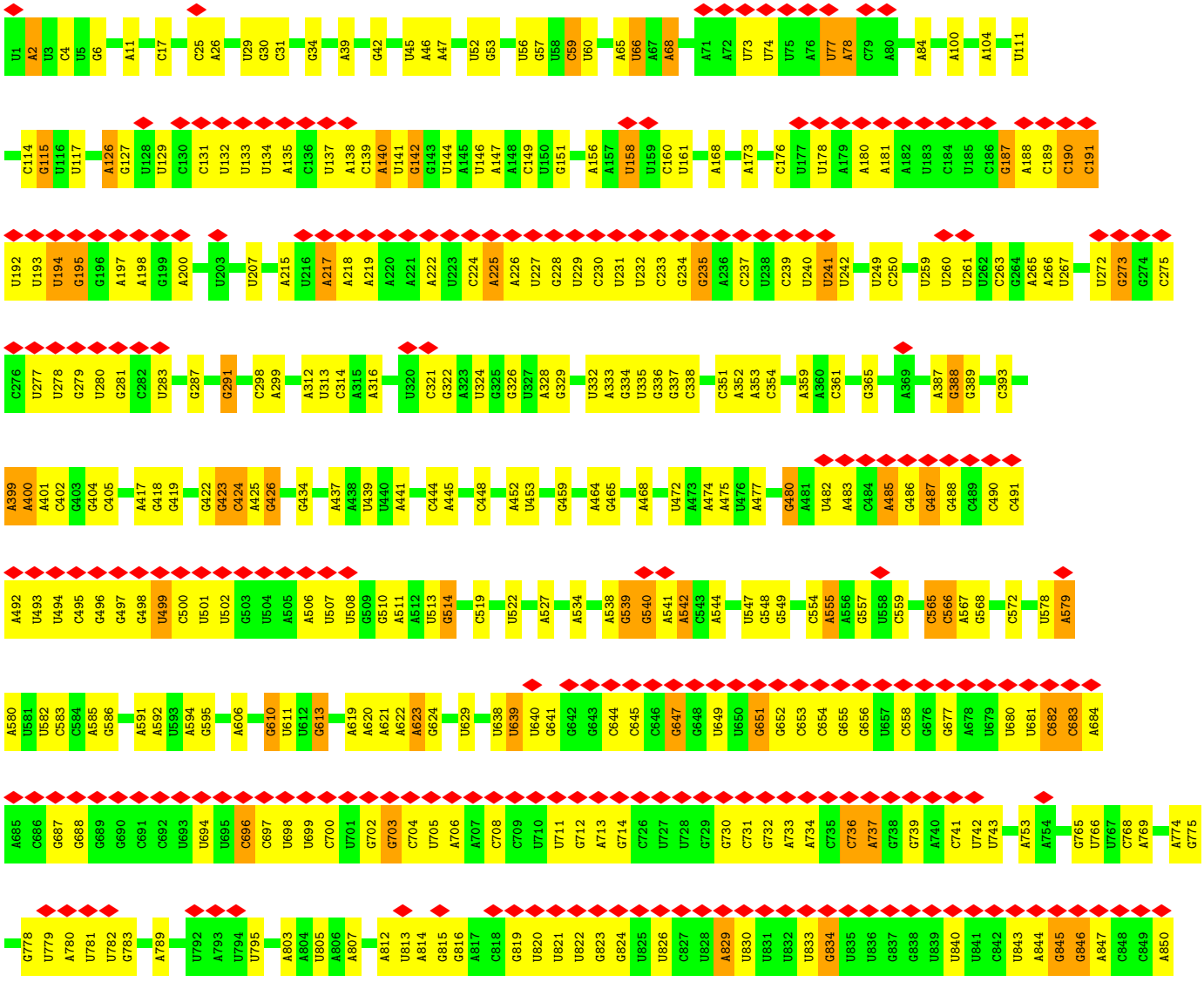
3 Residue-property plots (i)

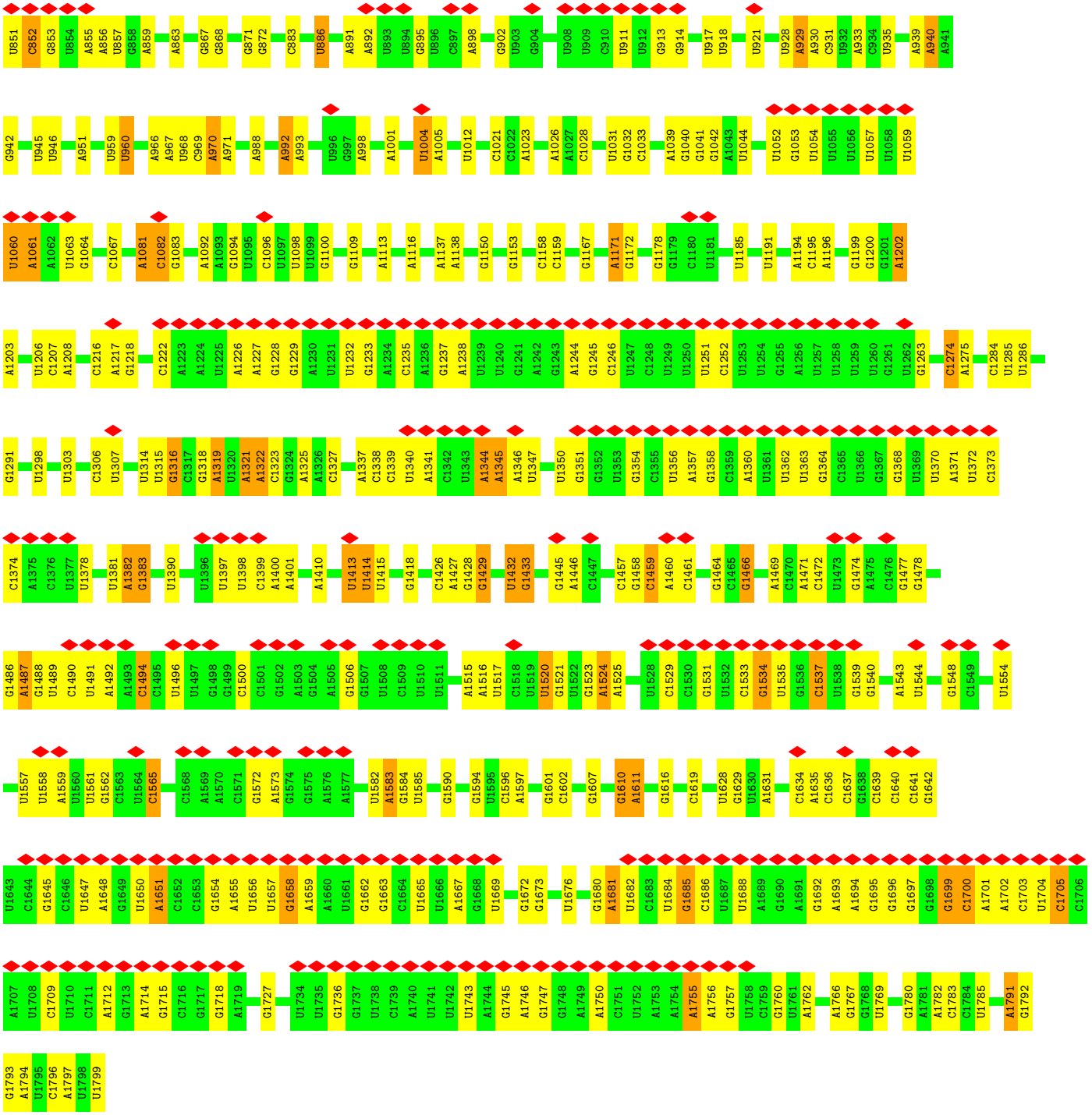
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S ribosomal RNA

Chain 2:

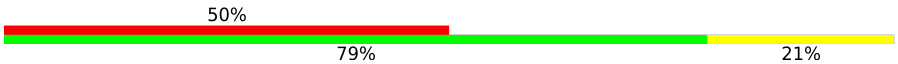


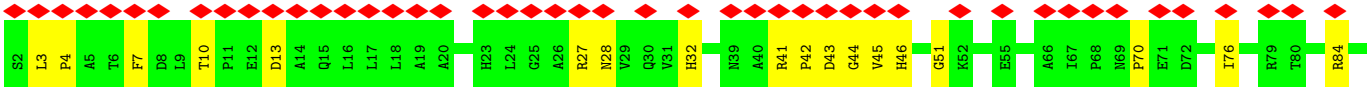


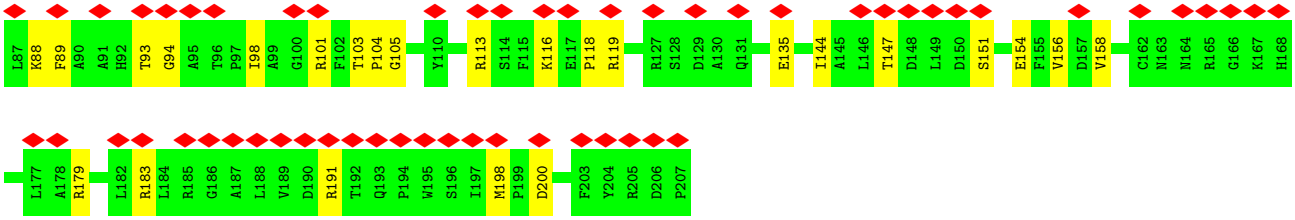


• Molecule 2: 40S ribosomal protein S0-A

Chain P:







• Molecule 3: 40S ribosomal protein S1-A

Chain Q:

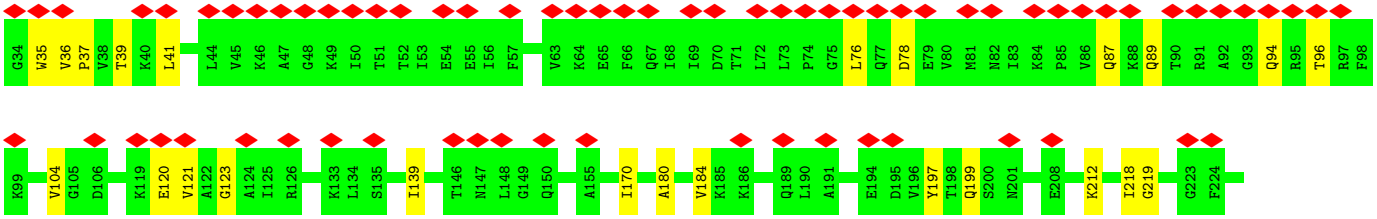


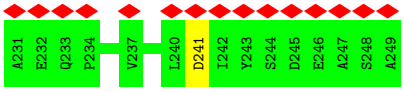


• Molecule 4: 40S ribosomal protein S2

Chain R:



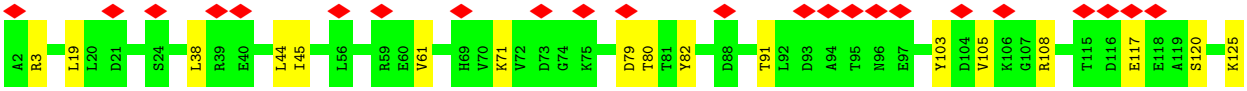


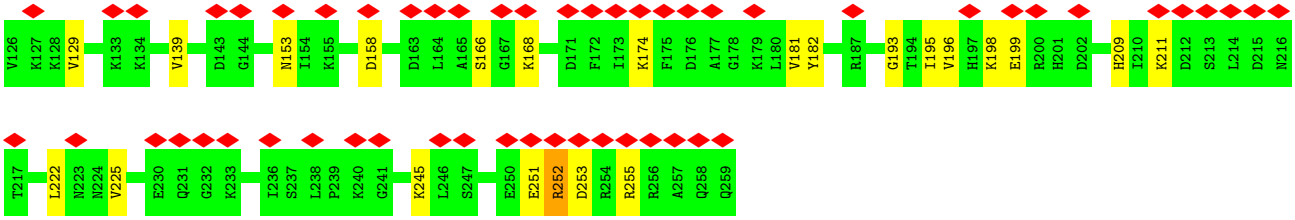


• Molecule 5: 40S ribosomal protein S4-A

Chain S:



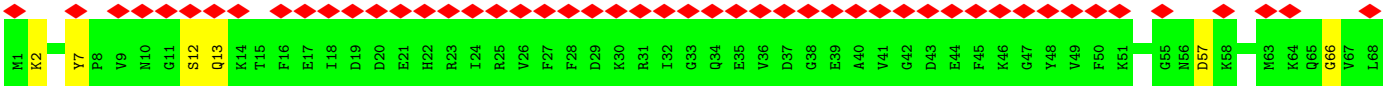




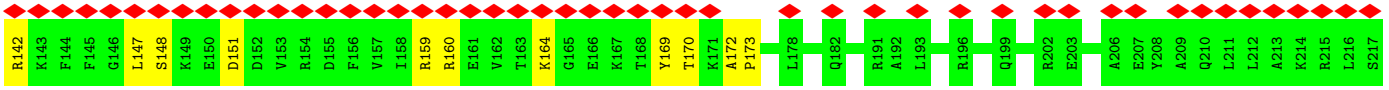
• Molecule 6: 40S ribosomal protein S6-A

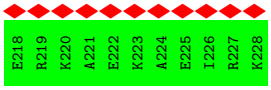
Chain T:







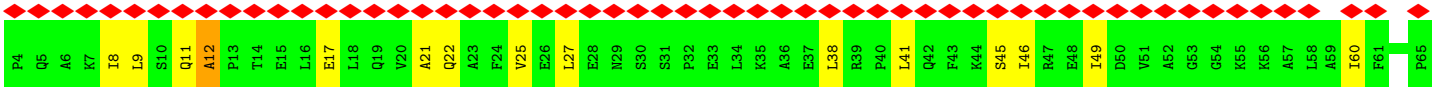


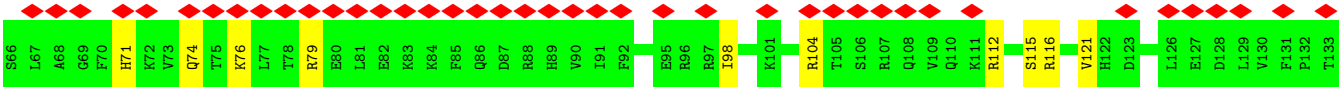


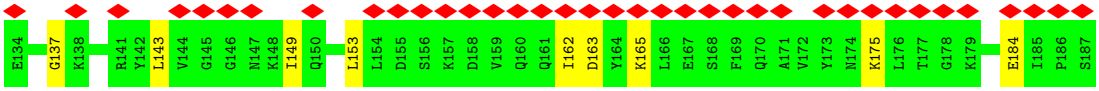
• Molecule 7: 40S ribosomal protein S7-A

Chain U:





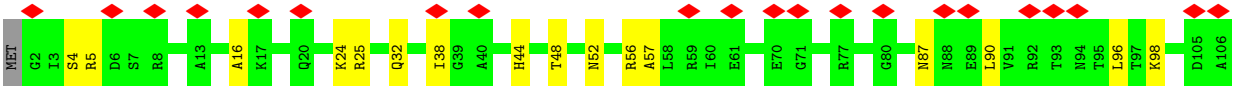




• Molecule 8: 40S ribosomal protein S8-A

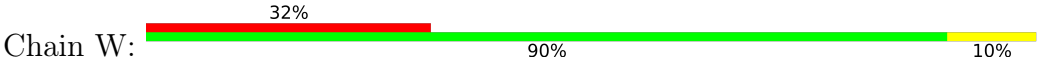
Chain V:

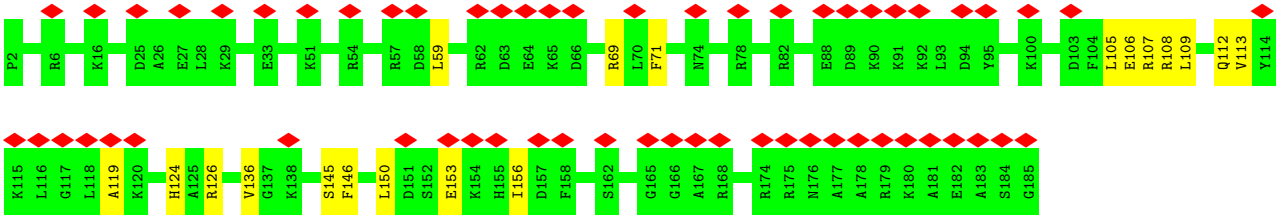






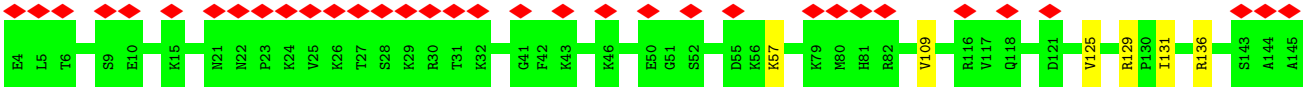
• Molecule 9: 40S ribosomal protein S9-A





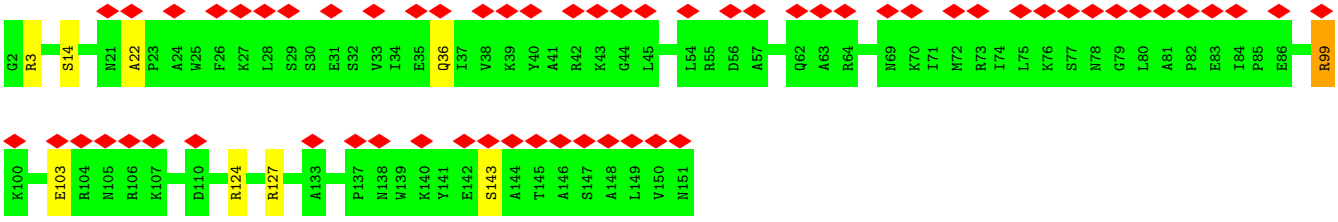
• Molecule 10: 40S ribosomal protein S11-A



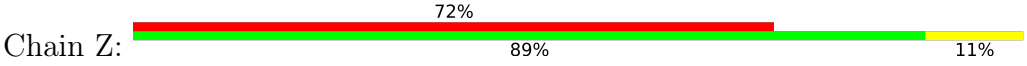


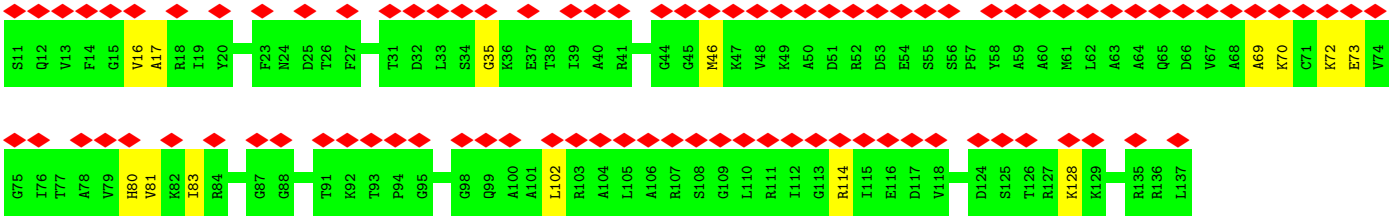
• Molecule 11: 40S ribosomal protein S13





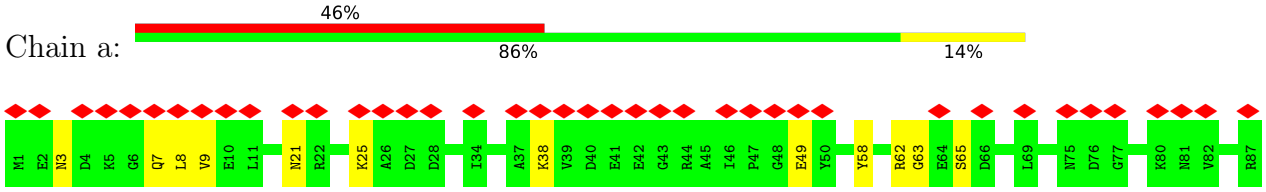
• Molecule 12: 40S ribosomal protein S14-B





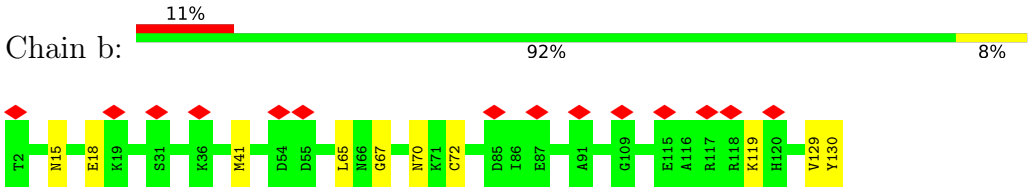
• Molecule 13: 40S ribosomal protein S21-A

Chain a:



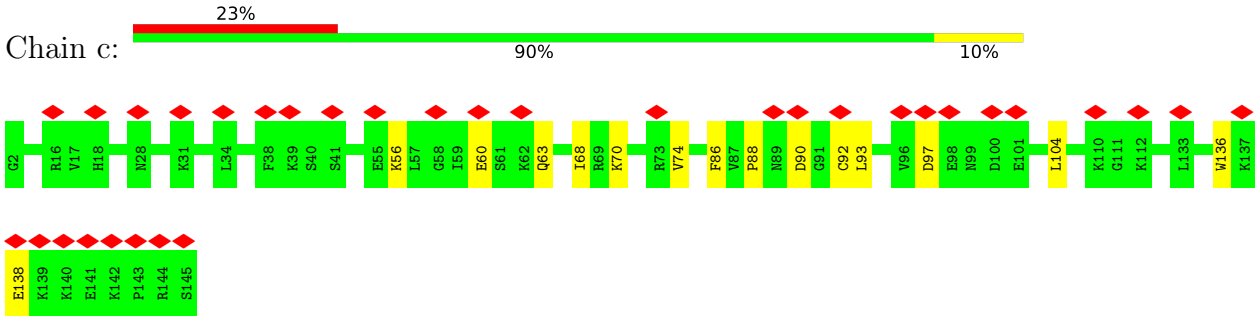
• Molecule 14: 40S ribosomal protein S22-A

Chain b:



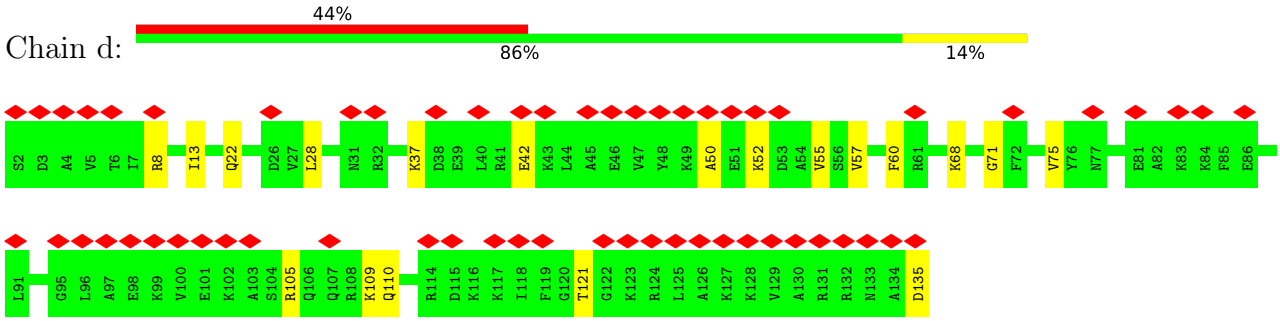
• Molecule 15: 40S ribosomal protein S23-A

Chain c:



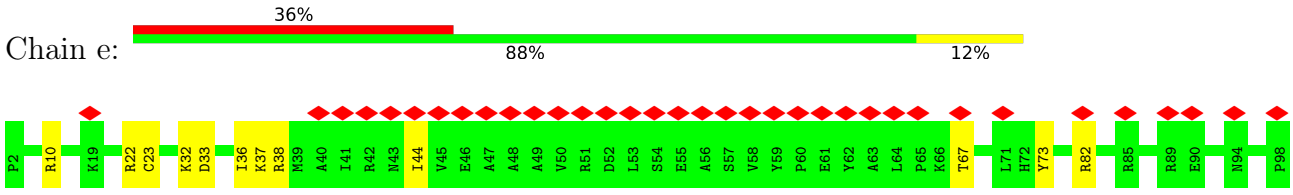
• Molecule 16: 40S ribosomal protein S24-A

Chain d:



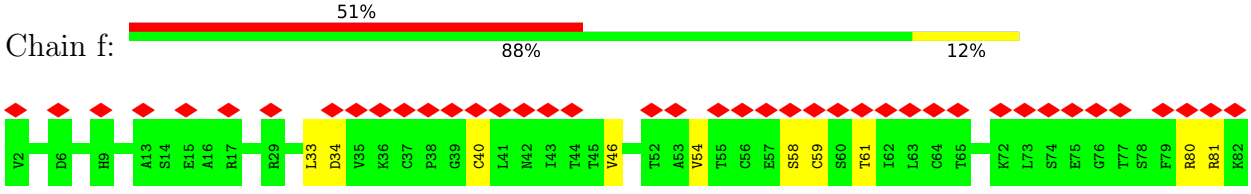
• Molecule 17: 40S ribosomal protein S26-B

Chain e:



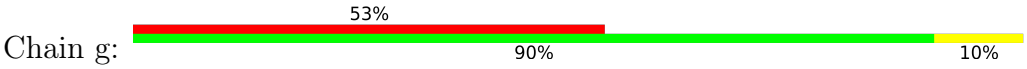
• Molecule 18: 40S ribosomal protein S27-A

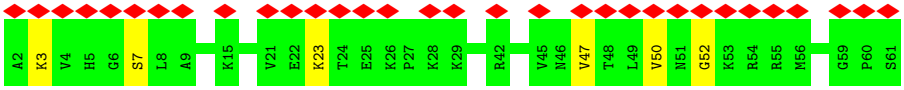
Chain f:



• Molecule 19: 40S ribosomal protein S30-A

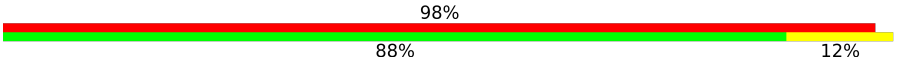
Chain g:

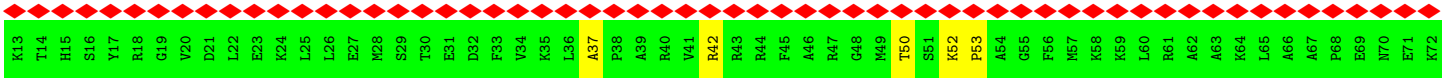


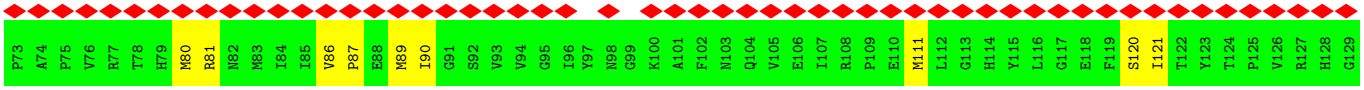


• Molecule 20: 40S ribosomal protein S15

Chain E:



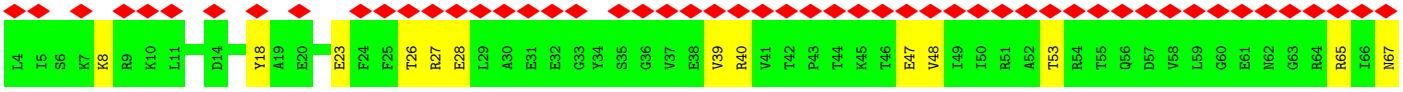


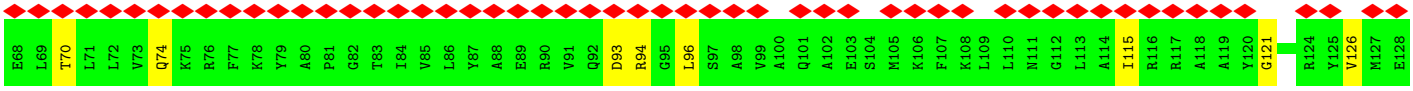


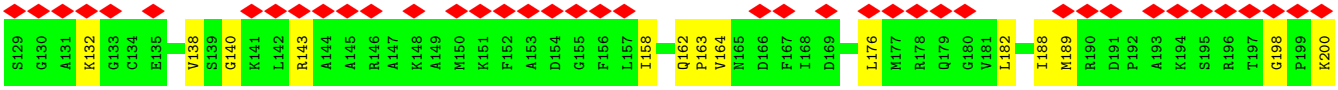
• Molecule 21: 40S ribosomal protein S3

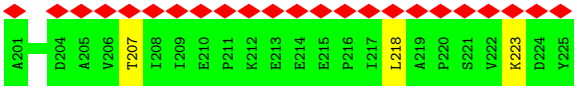
Chain A:





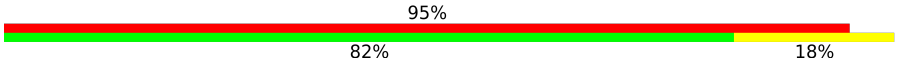


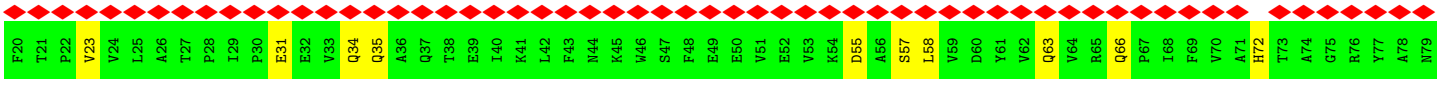


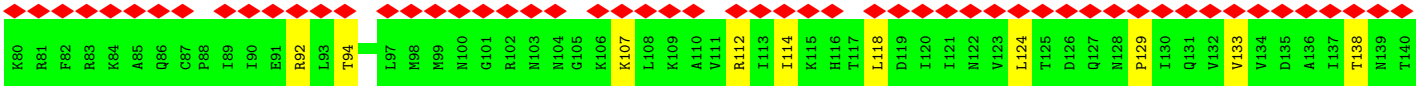


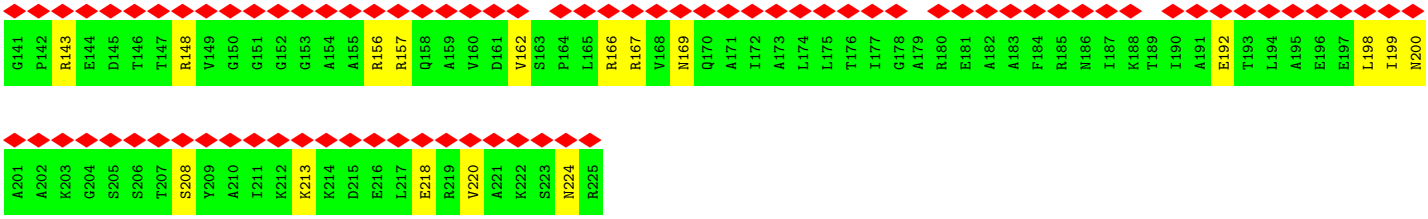
• Molecule 22: 40S ribosomal protein S5

Chain B:

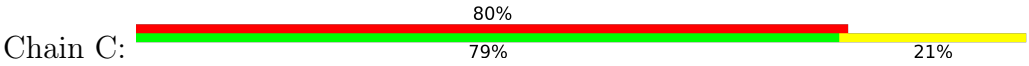


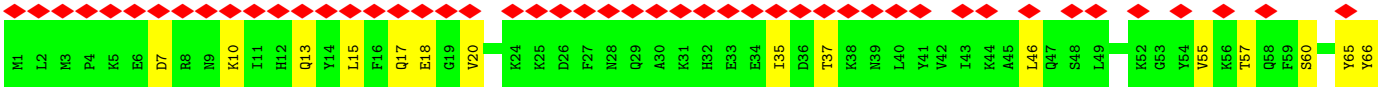


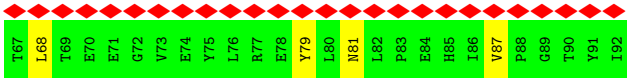




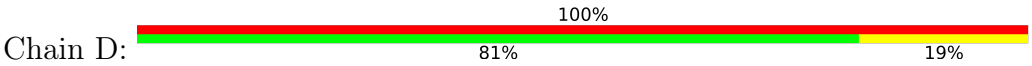
• Molecule 23: 40S ribosomal protein S10-A



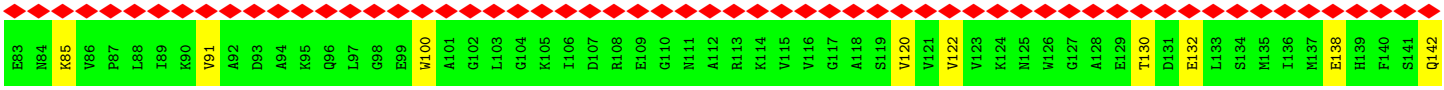




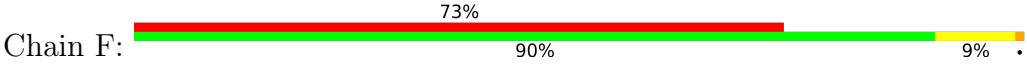
• Molecule 24: 40S ribosomal protein S12

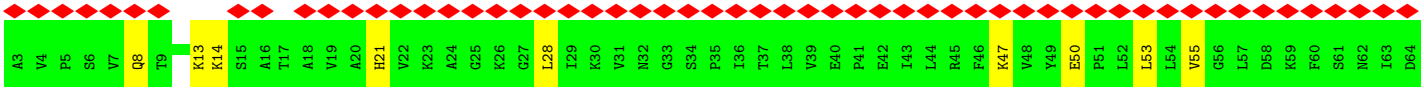


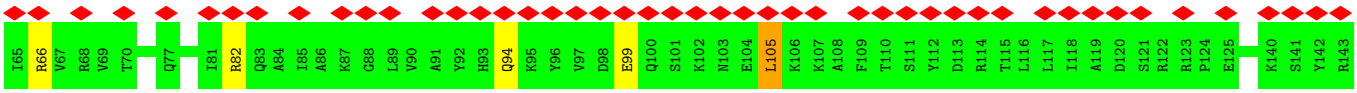




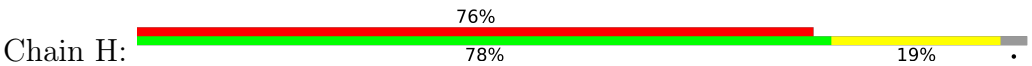
• Molecule 25: 40S ribosomal protein S16-A

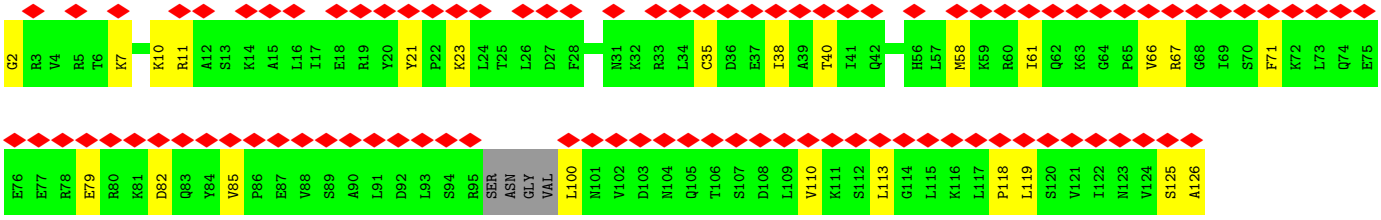






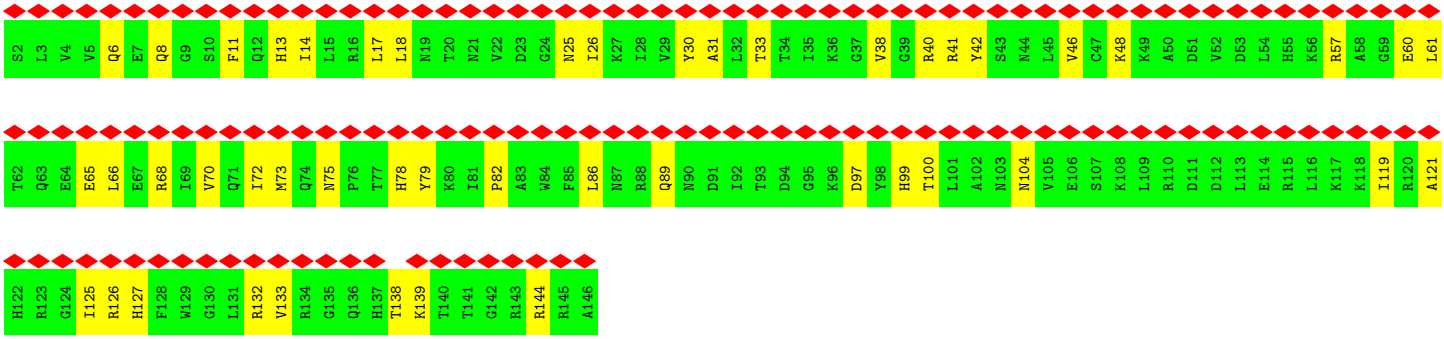
• Molecule 26: 40S ribosomal protein S17-B



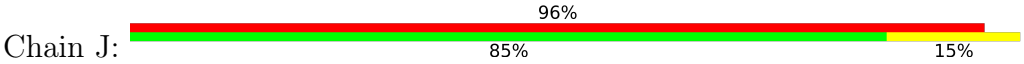


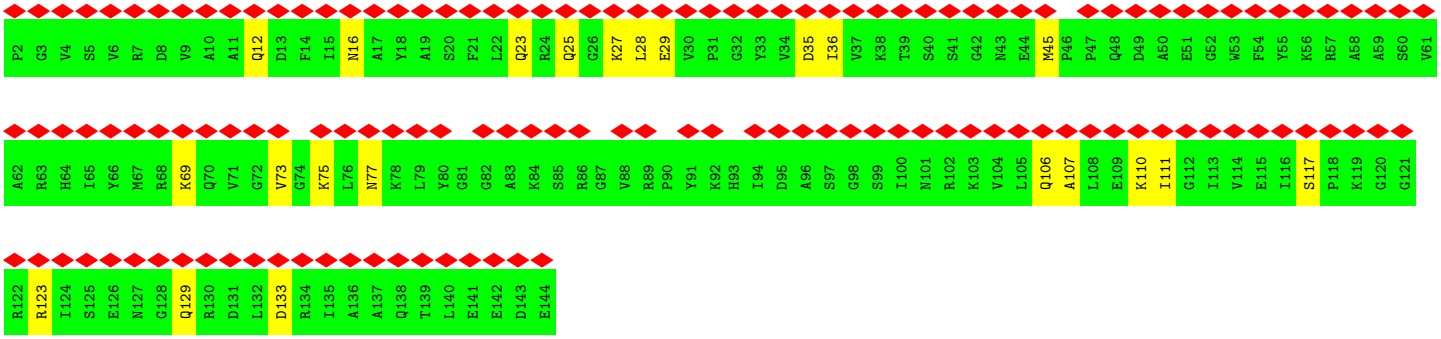
• Molecule 27: 40S ribosomal protein S18-A



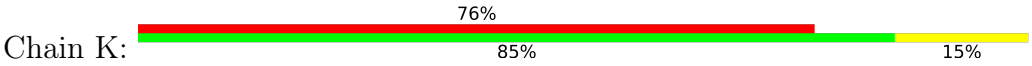


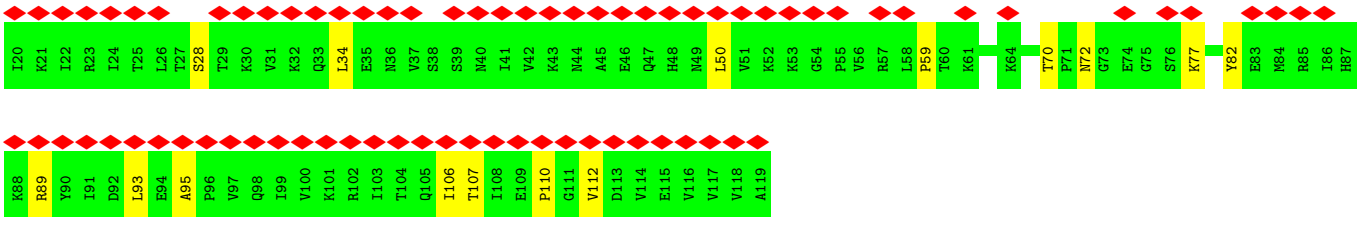
• Molecule 28: 40S ribosomal protein S19-A





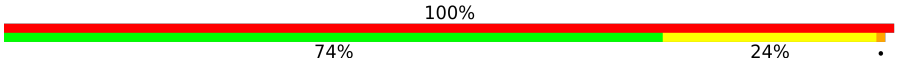
• Molecule 29: 40S ribosomal protein S20

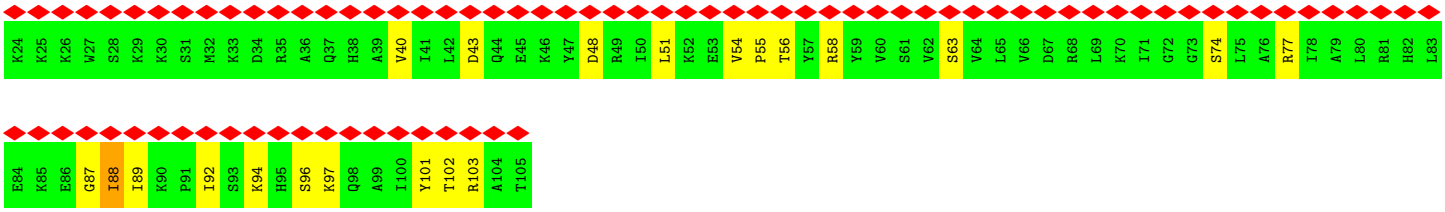




• Molecule 30: 40S ribosomal protein S25-A

Chain L:





• Molecule 31: 40S ribosomal protein S29-A

Chain M:

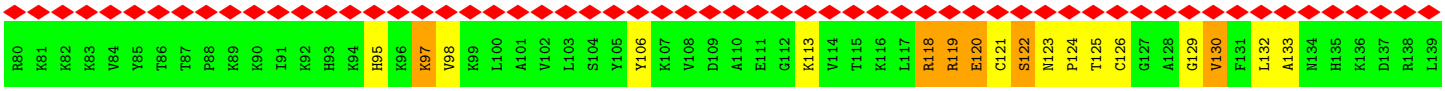




• Molecule 32: Ubiquitin-40S ribosomal protein S31

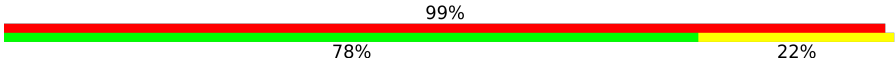
Chain N:

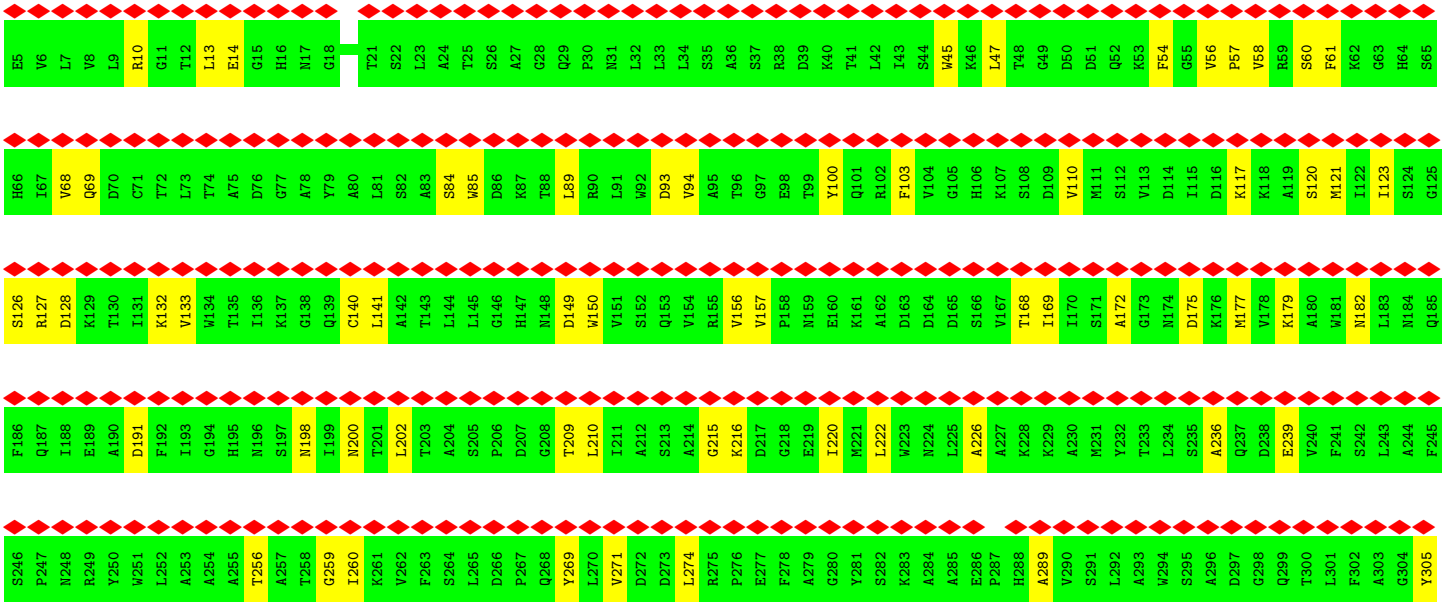




• Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:

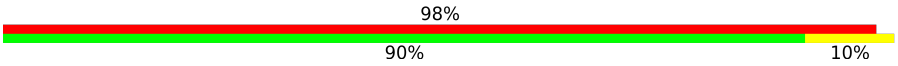


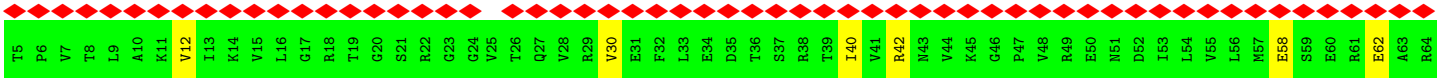




• Molecule 34: 40S ribosomal protein S28-A

Chain h:







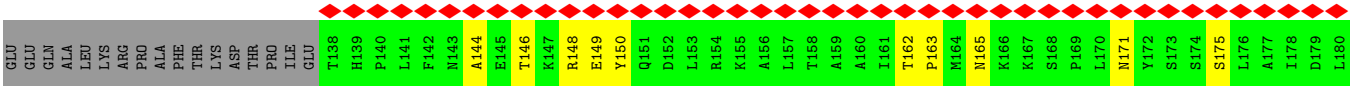
• Molecule 35: Eukaryotic translation initiation factor 3 subunit J

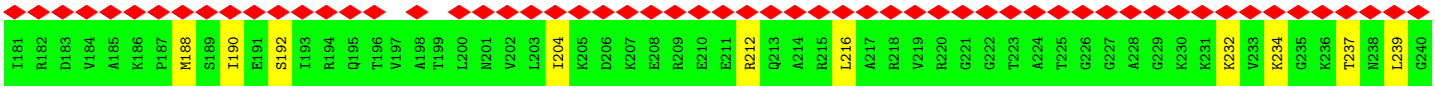
Chain z:

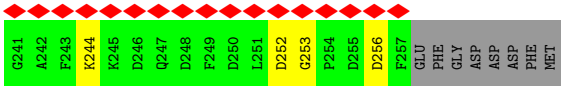












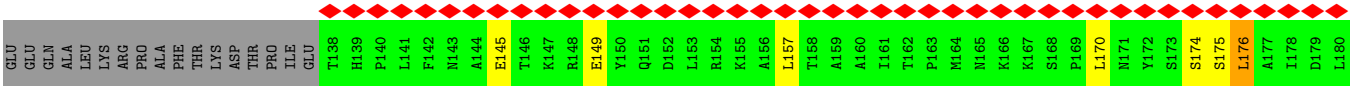
• Molecule 35: Eukaryotic translation initiation factor 3 subunit J

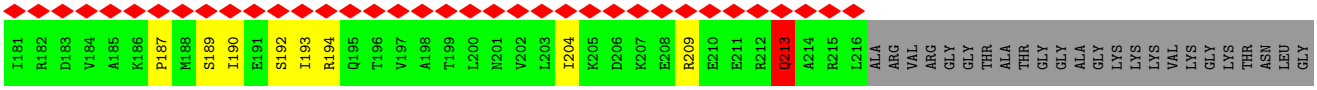
Chain y:











GLY ALA PHE LYS LYS ASP GLN ASP PHE ASP LEU ASP GLY PRO ASP ASP PHE GLU PHE GLY ASP ASP ASP PHE MET

• Molecule 36: Translation initiation factor RLI1

Chain x:



K4 N5 S6 R7 I8 A9 I10 V11 S12 A13 D14 K15 C16 K17 P18 K19 K20 C21 R22 K26 R27 K33 T34 G35 K36 L37 E40 V41 T42 P43 T44 S45 K46 I47 A48 F49 I50 S51 E52 I53 L54 G57 V62 K63 D68 I72 I73 N78 L79 E80 A81 H82

V83 R86 Y87 S88 A89 N90 S91 F92 K93 L94 H95 R96 L97 P98 T99 P100 R101 P102 G103 Q104 V105 L106 G107 L108 V109 G110 T111 N112 G113 I114 G115 K116 S117 T118 A119 L120 K121 I122 L123 A124 G125 K126 Q127 K128 P129 N130 L131 G132 R133 F134 D135 D136 P137 P138 E139 W140 Q141 E142 I143

I144 K145 Y146 F147 R148 G149 S150 E151 L152 Q153 N154 Y155 K158 M159 L160 E161 D162 D163 I164 K165 A166 I167 I168 K169 P170 Q171 Y172 V173 D174 N175 I176 P177 R178 A179 I180 K181 G182 P183 V184 Q185 K186 V187 G188 E189 L190 L191 K192 L193 R194 M195 E196 K197 S198 P199 E200 D201 V202 K203 R204

Y205 I206 K207 I208 L209 Q210 L211 E212 N213 V214 L215 K216 R217 D218 I219 E220 K221 L222 S223 G224 G225 E226 L227 Q228 R229 F230 A231 I232 G233 M234 S235 C236 V237 Q238 E239 A240 D241 V242 Y243 M244 F245 D246 E247 P248 S249 S250 Y251 L252 D253 V254 K255 Q256 R257 L258 N259 A260 A261 Q262 I263 I264

R265 S266 L267 L268 A269 P270 T271 K272 Y273 V274 I275 C276 V277 E278 H279 D280 L281 S282 V283 L284 D285 Y286 L287 S288 D289 F290 V291 C292 I293 I294 Y295 G296 V297 P298 S299 V300 V304 T305 L306 S309 V310 R311 E312 G313 I314 N315 I316 F317 L318 D319 G320 H321 I322 P323 A324 L327 R328

F329 R330 T331 E332 A333 L334 GLN PHE ARG ILE ALA ASP ALA THR GLU ASP LEU GLN ASN ASP SER ALA SER ARG ALA F354 S355 Y356 P357 S358 L359 K360 K361 T362 Q363 G364 D365 F366 V367 L368 N369 V370 E371 E372 G373 E374 F375 S376 D377 S378 E379 I380 L381 V382 M383 M384 G385 E386 N387 G388

T389 G390 K391 T392 T393 L394 I395 K396 L397 L398 A399 G400 A401 L402 K403 P404 D405 E406 G407 Q408 D409 I410 P411 K412 L413 N414 V415 S416 M417 K418 P419 Q420 K421 I422 A423 P424 K425 F426 P427 G428 T429 V430 R431 Q432 L433 F434 F435 K436 K437 I438 R439 G440 Q441 F442 L443 N444 P445 Q446 F447 Q448

T449 D450 V451 V452 K453 P454 L455 R456 I457 D458 D459 I460 I461 D462 Q463 E464 V465 Q466 H467 L468 S469 G470 G471 E472 L473 Q474 R475 V476 A477 I478 V479 L480 A481 L482 G483 I484 P485 A486 D487 I488 Y489 L490 I491 D492 E493 P494 S495 A496 Y497 L498 D499 S500 E501 Q502 R503 I504 I505 C506 S507 K508

V509 I510 R511 R512 F513 I514 L515 H516 N517 K518 K519 T520 A521 F522 I523 V524 E525 H526 D527 F528 I529 M530 A531 T532 Y533 L534 A535 D536 K537 V538 I539 V540 F541 E542 G543 I544 P545 S546 K547 N548 A549 H550 A551 R552 A553 P554 E555 S556 L557 L558 T559 G560 C561 N562 R563 F564 L565 K566 N567 L568

N569 V570 T571 F572 R573 R574 D575 P576 N577 S578 F579 R580 P581 R582 K585 L586 D587 S588 Q589 M590 D591 K592 E593 Q594 K595 S596 S597 G598 N599 Y600 F601 F602 L603 D604

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25245	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 ($e^-/Å^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SF4, 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	2	0.44	0/42211	0.51	10/65773 (0.0%)
2	P	0.43	0/1644	0.76	1/2249 (0.0%)
3	Q	0.43	0/1823	0.88	1/2447 (0.0%)
4	R	0.44	0/1656	0.77	0/2251
5	S	0.48	0/2097	0.78	1/2823 (0.0%)
6	T	0.38	0/1839	0.75	0/2460
7	U	0.41	0/1498	0.77	2/2019 (0.1%)
8	V	0.46	0/1501	0.74	0/2006
9	W	0.44	0/1504	0.77	0/2016
10	X	0.44	0/1168	0.67	0/1575
11	Y	0.44	0/1215	0.83	3/1638 (0.2%)
12	Z	0.40	0/934	0.82	0/1257
13	a	0.44	0/682	0.82	3/921 (0.3%)
14	b	0.48	0/1038	0.79	0/1395
15	c	0.48	0/1139	0.84	0/1518
16	d	0.48	0/1087	0.84	3/1449 (0.2%)
17	e	0.44	0/778	0.81	0/1042
18	f	0.40	0/620	0.82	0/838
19	g	0.40	0/480	0.84	0/639
20	E	0.33	0/936	0.77	0/1259
21	A	0.38	0/1754	0.71	1/2361 (0.0%)
22	B	0.36	0/1625	0.82	1/2197 (0.0%)
23	C	0.39	0/772	0.96	3/1044 (0.3%)
24	D	0.38	0/883	1.04	2/1199 (0.2%)
25	F	0.42	0/1125	0.88	1/1510 (0.1%)
26	H	0.42	0/957	0.90	3/1283 (0.2%)
27	I	0.32	0/1207	0.81	0/1623
28	J	0.36	0/1130	0.81	1/1517 (0.1%)
29	K	0.39	0/807	0.80	0/1091
30	L	0.34	0/661	0.89	2/888 (0.2%)
31	M	0.42	0/452	0.78	1/600 (0.2%)
32	N	0.40	0/571	1.01	2/768 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	O	0.35	0/2436	0.79	2/3318 (0.1%)
34	h	0.37	0/493	0.80	0/663
35	y	0.38	0/631	1.10	4/851 (0.5%)
35	z	0.39	0/905	1.01	2/1213 (0.2%)
36	x	0.39	0/4695	0.90	4/6334 (0.1%)
All	All	0.42	0/86954	0.68	53/126035 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
35	y	0	1

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	y	213	GLN	O-C-N	-13.36	108.31	122.07
35	y	176	LEU	N-CA-C	10.45	122.25	111.07
11	Y	22	ALA	C-N-CD	-7.64	103.80	120.60
35	y	175	SER	N-CA-C	7.58	119.55	111.28
2	P	44	GLY	N-CA-C	-7.42	104.49	114.95
30	L	88	ILE	N-CA-C	7.29	118.05	110.62
23	C	87	VAL	CA-C-N	6.73	126.52	119.05
23	C	87	VAL	C-N-CA	6.73	126.52	119.05
5	S	252	ARG	CA-CB-CG	6.29	126.68	114.10
1	2	1791	A	C2'-C3'-O3'	6.15	118.72	109.50
26	H	125	SER	N-CA-C	6.06	119.48	110.52
30	L	87	GLY	N-CA-C	5.97	127.33	113.18
1	2	59	C	C2'-C3'-O3'	5.89	118.33	109.50
1	2	59	C	P-O3'-C3'	5.83	128.94	120.20
35	z	253	GLY	CA-C-N	5.78	125.46	119.05
35	z	253	GLY	C-N-CA	5.78	125.46	119.05
1	2	1791	A	P-O3'-C3'	5.77	128.85	120.20
13	a	9	VAL	N-CA-C	-5.76	97.37	109.34
23	C	79	TYR	N-CA-C	5.73	117.60	111.36
31	M	36	LEU	CA-CB-CG	5.66	136.11	116.30
36	x	546	SER	CA-C-N	5.66	133.39	121.91
36	x	546	SER	C-N-CA	5.66	133.39	121.91
25	F	105	LEU	CA-CB-CG	5.63	136.01	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	67	THR	CA-C-N	5.61	132.26	121.54
24	D	67	THR	C-N-CA	5.61	132.26	121.54
11	Y	99	ARG	CA-CB-CG	5.59	125.28	114.10
32	N	106	TYR	CA-C-N	5.52	134.89	122.19
32	N	106	TYR	C-N-CA	5.52	134.89	122.19
36	x	557	LEU	N-CA-C	5.47	117.69	111.02
13	a	8	LEU	CA-C-N	5.46	131.79	121.97
13	a	8	LEU	C-N-CA	5.46	131.79	121.97
11	Y	103	GLU	N-CA-C	-5.43	105.44	111.36
1	2	77	U	P-O3'-C3'	5.39	128.29	120.20
36	x	487	ASP	N-CA-C	-5.26	106.92	113.55
21	A	218	LEU	CA-CB-CG	5.21	134.52	116.30
16	d	110	GLN	CA-CB-CG	5.20	124.50	114.10
16	d	50	ALA	CA-C-N	5.19	133.25	122.41
16	d	50	ALA	C-N-CA	5.19	133.25	122.41
28	J	23	GLN	CA-CB-CG	5.15	124.41	114.10
1	2	453	U	C2-N1-C1'	5.14	133.12	117.70
7	U	12	ALA	CA-C-N	5.12	125.33	120.31
7	U	12	ALA	C-N-CA	5.12	125.33	120.31
1	2	1382	A	P-O3'-C3'	5.08	127.83	120.20
1	2	1382	A	C4'-C3'-O3'	5.08	117.02	109.40
1	2	140	A	O5'-P-OP2	5.08	123.22	108.00
3	Q	191	GLU	CA-CB-CG	5.07	124.23	114.10
22	B	148	ARG	CA-CB-CG	5.06	124.22	114.10
35	y	174	SER	CA-C-O	5.03	120.86	117.94
26	H	71	PHE	CA-C-N	5.02	127.71	120.38
26	H	71	PHE	C-N-CA	5.02	127.71	120.38
33	O	307	ASP	CA-C-N	5.02	129.45	122.08
33	O	307	ASP	C-N-CA	5.02	129.45	122.08
1	2	1274	C	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	y	213	GLN	Mainchain

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	2	37739	0	18987	214	0
2	P	1603	0	1610	29	0
3	Q	1798	0	1890	31	0
4	R	1626	0	1715	19	0
5	S	2056	0	2140	24	0
6	T	1815	0	1894	24	0
7	U	1473	0	1555	24	0
8	V	1476	0	1501	16	0
9	W	1479	0	1556	12	0
10	X	1142	0	1209	5	0
11	Y	1192	0	1255	8	0
12	Z	923	0	948	11	0
13	a	673	0	662	10	0
14	b	1021	0	1060	6	0
15	c	1121	0	1196	11	0
16	d	1073	0	1132	12	0
17	e	765	0	814	8	0
18	f	610	0	633	5	0
19	g	472	0	521	6	0
20	E	916	0	941	10	0
21	A	1729	0	1812	26	0
22	B	1605	0	1669	25	0
23	C	754	0	725	13	0
24	D	875	0	878	12	0
25	F	1105	0	1166	9	0
26	H	948	0	990	17	0
27	I	1188	0	1218	33	0
28	J	1112	0	1124	17	0
29	K	797	0	863	12	0
30	L	651	0	682	20	0
31	M	442	0	428	5	0
32	N	560	0	558	43	0
33	O	2383	0	2332	43	0
34	h	491	0	524	3	0
35	y	624	0	645	12	0
35	z	896	0	926	21	0
36	x	4608	0	4755	81	0
37	2	76	0	0	0	0
37	B	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	x	1	0	0	0	0
38	M	1	0	0	0	0
38	N	1	0	0	0	0
39	x	16	0	0	0	0
40	x	27	0	12	5	0
All	All	81866	0	64526	733	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 5.

All (733) 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)
1:2:1235:C:C1'	32:N:140:TYR:HE1	1.40	1.32
1:2:1235:C:C1'	32:N:140:TYR:CE1	2.24	1.20
1:2:1235:C:H1'	32:N:140:TYR:CE1	1.82	1.13
32:N:119:ARG:O	32:N:132:LEU:HG	1.53	1.09
1:2:1235:C:H1'	32:N:140:TYR:HE1	0.92	1.09
32:N:123:ASN:CG	32:N:124:PRO:HD2	1.84	1.02
1:2:1235:C:N1	32:N:140:TYR:CE1	2.30	0.98
1:2:1235:C:C6	32:N:140:TYR:OH	2.17	0.97
1:2:1235:C:C2	32:N:140:TYR:CE1	2.54	0.96
32:N:118:ARG:HG3	32:N:118:ARG:HH11	1.34	0.92
1:2:187:G:H21	1:2:198:A:H62	1.20	0.88
36:x:113:GLY:CA	40:x:703:ADP:O3B	2.26	0.84
32:N:119:ARG:O	32:N:132:LEU:CG	2.26	0.83
30:L:54:VAL:CG2	30:L:88:ILE:HG21	2.08	0.83
1:2:187:G:N2	1:2:198:A:H62	1.76	0.82
13:a:3:ASN:HD21	13:a:7:GLN:NE2	1.77	0.82
32:N:123:ASN:CG	32:N:124:PRO:CD	2.55	0.80
30:L:54:VAL:HG23	30:L:88:ILE:HG21	1.66	0.77
2:P:27:ARG:HD2	2:P:45:VAL:HG12	1.66	0.76
2:P:28:ASN:HA	2:P:46:HIS:NE2	2.01	0.76
36:x:113:GLY:N	40:x:703:ADP:O3B	2.18	0.76
1:2:1235:C:N1	32:N:140:TYR:CZ	2.55	0.74
23:C:13:GLN:O	23:C:17:GLN:HG2	1.88	0.73
32:N:123:ASN:ND2	32:N:124:PRO:HD2	2.03	0.73
32:N:118:ARG:HG3	32:N:118:ARG:NH1	1.97	0.73
13:a:3:ASN:HD21	13:a:7:GLN:HE21	1.36	0.72
23:C:81:ASN:ND2	23:C:81:ASN:O	2.23	0.72
1:2:1235:C:C6	32:N:140:TYR:CZ	2.78	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:119:ALA:O	9:W:124:HIS:ND1	2.24	0.70
2:P:42:PRO:O	26:H:126:ALA:HB2	1.91	0.70
30:L:89:ILE:HG21	30:L:101:TYR:HB3	1.73	0.70
36:x:414:ASN:H	36:x:487:ASP:HB2	1.57	0.69
1:2:1235:C:C1'	32:N:140:TYR:HH	2.05	0.69
36:x:113:GLY:HA2	40:x:703:ADP:O3B	1.92	0.69
2:P:7:PHE:HA	2:P:191:ARG:HH11	1.58	0.68
1:2:1658:G:N1	1:2:1743:U:N3	2.42	0.68
1:2:1658:G:N2	1:2:1743:U:O2	2.27	0.67
36:x:471:GLY:HA2	36:x:497:TYR:HB3	1.74	0.67
7:U:8:ILE:HG13	7:U:9:LEU:HD22	1.76	0.67
1:2:187:G:H21	1:2:198:A:N6	1.91	0.67
1:2:895:G:H1	1:2:917:U:H3	1.42	0.67
32:N:119:ARG:NE	32:N:119:ARG:H	1.93	0.67
11:Y:36:GLN:HE21	11:Y:36:GLN:HA	1.60	0.67
40:x:703:ADP:H5'1	40:x:703:ADP:C8	2.30	0.66
1:2:544:A:H61	35:z:148:ARG:HD2	1.61	0.66
29:K:82:TYR:HB3	31:M:52:PHE:HB3	1.78	0.66
1:2:1235:C:O4'	32:N:140:TYR:OH	2.13	0.66
6:T:98:ARG:HH11	6:T:105:ASP:HB2	1.60	0.65
28:J:73:VAL:O	28:J:77:ASN:ND2	2.30	0.65
30:L:89:ILE:CG2	30:L:101:TYR:HB3	2.27	0.65
6:T:159:ARG:HG2	6:T:172:ALA:HB2	1.79	0.65
1:2:539:G:N3	1:2:540:G:N2	2.42	0.64
7:U:76:LYS:HD3	7:U:79:ARG:HH22	1.60	0.64
20:E:81:ARG:NH2	20:E:120:SER:O	2.30	0.64
33:O:89:LEU:HB2	33:O:103:PHE:HB2	1.78	0.64
22:B:72:HIS:O	25:F:47:LYS:NZ	2.27	0.64
1:2:868:G:H1	1:2:960:U:H3	1.44	0.64
30:L:54:VAL:HG21	30:L:88:ILE:HG21	1.80	0.64
35:z:162:THR:OG1	35:z:163:PRO:HD3	1.98	0.64
32:N:97:LYS:O	32:N:97:LYS:HE2	1.99	0.63
23:C:18:GLU:C	23:C:20:VAL:H	2.07	0.63
6:T:57:ASP:HA	6:T:106:LEU:HA	1.81	0.62
22:B:200:ASN:HB3	22:B:208:SER:HB2	1.81	0.62
1:2:623:A:N6	1:2:970:A:OP1	2.32	0.62
5:S:181:VAL:HG22	5:S:193:GLY:O	1.99	0.62
28:J:117:SER:HB2	28:J:123:ARG:HB2	1.81	0.62
1:2:334:G:O6	8:V:5:ARG:NH2	2.32	0.62
4:R:36:VAL:HG13	4:R:36:VAL:O	2.00	0.61
12:Z:16:VAL:HG12	12:Z:80:HIS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:81:ASN:C	23:C:81:ASN:HD22	2.05	0.61
4:R:87:GLN:HG2	4:R:96:THR:HG22	1.83	0.61
21:A:40:ARG:HG3	29:K:110:PRO:HB3	1.82	0.61
36:x:173:VAL:HB	36:x:227:LEU:HD22	1.81	0.61
36:x:225:GLY:HA2	36:x:251:TYR:HB3	1.81	0.61
36:x:517:ASN:HB3	36:x:519:LYS:HG2	1.82	0.61
3:Q:195:LYS:NZ	3:Q:198:GLU:OE2	2.33	0.61
35:z:165:ASN:ND2	35:y:187:PRO:O	2.33	0.61
1:2:1339:C:O2'	1:2:1341:A:N7	2.32	0.61
3:Q:30:PHE:HB3	3:Q:96:LEU:HD22	1.82	0.60
4:R:78:ASP:HB3	4:R:104:VAL:HG12	1.83	0.60
1:2:1585:U:H3	1:2:1611:A:H2	1.47	0.60
30:L:54:VAL:HG23	30:L:88:ILE:CG2	2.30	0.60
11:Y:36:GLN:HA	11:Y:36:GLN:NE2	2.16	0.60
1:2:400:A:H5"	8:V:25:ARG:HA	1.83	0.60
3:Q:129:THR:OG1	3:Q:179:SER:O	2.19	0.60
7:U:137:GLY:HA3	7:U:153:LEU:HD12	1.84	0.60
12:Z:69:ALA:HA	12:Z:72:LYS:HE2	1.82	0.60
1:2:1303:U:O2'	1:2:1322:A:OP2	2.20	0.60
35:y:145:GLU:HB2	35:y:149:GLU:HG2	1.84	0.60
22:B:94:THR:HG22	22:B:114:ILE:HG13	1.83	0.59
24:D:60:VAL:HG22	24:D:122:VAL:HG23	1.82	0.59
24:D:75:VAL:HG21	24:D:120:VAL:HG21	1.84	0.59
26:H:85:VAL:HG13	26:H:85:VAL:O	2.01	0.59
23:C:60:SER:HB3	23:C:65:TYR:CE1	2.36	0.59
35:z:171:ASN:O	35:z:175:SER:OG	2.19	0.59
22:B:23:VAL:O	22:B:34:GLN:NE2	2.33	0.59
36:x:475:ARG:NH1	36:x:502:GLN:OE1	2.36	0.59
1:2:586:G:OP1	19:g:23:LYS:NZ	2.34	0.59
13:a:21:ASN:HB3	14:b:67:GLY:HA3	1.85	0.59
1:2:126:A:H2	1:2:291:G:H21	1.49	0.59
1:2:65:A:H2	1:2:84:A:H62	1.51	0.59
1:2:998:A:N6	1:2:1004:U:OP2	2.37	0.58
22:B:63:GLN:HE21	22:B:66:GLN:HE21	1.51	0.58
27:I:40:ARG:HB3	28:J:45:MET:HE1	1.83	0.58
1:2:144:U:O4	6:T:137:ARG:NH1	2.36	0.58
1:2:1195:C:OP1	29:K:77:LYS:NZ	2.35	0.58
24:D:63:VAL:HG11	24:D:66:VAL:HG13	1.85	0.58
1:2:2:A:N3	4:R:199:GLN:NE2	2.51	0.58
36:x:454:PRO:O	36:x:456:ARG:NH2	2.37	0.58
4:R:121:VAL:HB	35:z:252:ASP:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:579:A:N6	35:z:237:THR:OG1	2.36	0.58
1:2:1235:C:O4'	32:N:140:TYR:CE1	2.57	0.58
21:A:53:THR:HG21	21:A:94:ARG:HE	1.67	0.58
27:I:75:ASN:OD1	27:I:78:HIS:ND1	2.36	0.58
33:O:210:LEU:HD11	33:O:222:LEU:HD12	1.86	0.58
36:x:186:LYS:HA	36:x:218:ASP:HA	1.86	0.58
35:z:146:THR:OG1	35:z:149:GLU:OE1	2.21	0.58
21:A:162:GLN:N	21:A:163:PRO:HD2	2.19	0.57
33:O:200:ASN:H	33:O:215:GLY:HA2	1.69	0.57
22:B:31:GLU:OE2	22:B:35:GLN:NE2	2.37	0.57
36:x:210:GLN:O	36:x:229:ARG:NH1	2.38	0.57
15:c:74:VAL:HG21	15:c:104:LEU:HD11	1.85	0.57
25:F:55:VAL:HG21	25:F:105:LEU:HD12	1.85	0.57
9:W:106:GLU:O	9:W:112:GLN:NE2	2.36	0.57
6:T:164:LYS:NZ	6:T:169:TYR:OH	2.36	0.57
33:O:216:LYS:HA	33:O:239:GLU:HG2	1.87	0.57
2:P:84:ARG:NH2	26:H:82:ASP:O	2.37	0.57
34:h:12:VAL:HG12	34:h:30:VAL:HG12	1.86	0.57
33:O:56:VAL:CG1	33:O:57:PRO:HD2	2.33	0.57
25:F:50:GLU:OE2	25:F:82:ARG:NH2	2.38	0.57
3:Q:82:ARG:NH2	3:Q:191:GLU:OE2	2.37	0.57
21:A:140:GLY:HA3	21:A:182:LEU:HD13	1.87	0.57
1:2:967:A:OP2	11:Y:124:ARG:NH2	2.38	0.56
1:2:992:A:H2	1:2:1012:U:H3	1.51	0.56
33:O:177:MET:HE2	33:O:179:LYS:HE3	1.86	0.56
20:E:37:ALA:O	20:E:42:ARG:NH1	2.38	0.56
1:2:78:A:O2'	6:T:173:PRO:O	2.21	0.56
1:2:930:A:N3	3:Q:111:ARG:NH2	2.52	0.56
33:O:200:ASN:ND2	33:O:239:GLU:OE1	2.38	0.56
36:x:7:ARG:NH1	36:x:57:GLY:O	2.38	0.56
1:2:1534:G:OP2	30:L:74:SER:OG	2.24	0.56
1:2:1544:U:H5"	27:I:132:ARG:HE	1.70	0.56
19:g:47:VAL:O	19:g:47:VAL:HG13	2.06	0.56
36:x:247:GLU:OE1	36:x:279:HIS:ND1	2.29	0.56
36:x:432:GLN:HA	36:x:435:PHE:HD2	1.70	0.56
1:2:1665:U:O2	1:2:1736:G:O6	2.23	0.56
6:T:2:LYS:HB2	6:T:108:VAL:HG22	1.86	0.56
17:e:32:LYS:O	17:e:37:LYS:NZ	2.34	0.56
22:B:118:LEU:HD22	22:B:129:PRO:HB2	1.88	0.56
1:2:459:G:OP1	16:d:109:LYS:NZ	2.38	0.56
1:2:931:C:H5"	3:Q:116:LYS:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:165:ASN:HD22	35:y:187:PRO:HB2	1.70	0.56
36:x:27:ARG:O	36:x:33:LYS:NZ	2.39	0.56
1:2:653:C:O2	1:2:682:C:N4	2.38	0.56
2:P:13:ASP:OD1	2:P:179:ARG:NH2	2.39	0.55
4:R:139:ILE:HD12	4:R:218:ILE:HB	1.88	0.55
22:B:55:ASP:OD2	22:B:57:SER:OG	2.23	0.55
36:x:385:GLY:HA2	36:x:541:PHE:HB2	1.87	0.55
7:U:9:LEU:HD21	7:U:21:ALA:HB2	1.88	0.55
1:2:332:U:O2'	8:V:5:ARG:NH1	2.40	0.55
24:D:54:ARG:HH21	32:N:129:GLY:HA3	1.72	0.55
25:F:50:GLU:HA	25:F:53:LEU:HB2	1.88	0.55
36:x:133:ARG:NH2	36:x:136:ASP:O	2.40	0.55
1:2:151:G:N3	6:T:13:GLN:NE2	2.54	0.55
1:2:651:G:H1	1:2:683:C:H5	1.55	0.55
1:2:217:A:N1	1:2:844:A:O2'	2.38	0.55
22:B:124:LEU:HD22	22:B:199:ILE:HD13	1.88	0.55
35:z:144:ALA:HB1	35:z:149:GLU:HB3	1.89	0.55
5:S:158:ASP:OD2	5:S:174:LYS:NZ	2.35	0.55
36:x:96:ARG:HB2	36:x:304:VAL:HB	1.88	0.55
13:a:3:ASN:ND2	13:a:7:GLN:HE21	2.02	0.55
30:L:94:LYS:NZ	30:L:101:TYR:OH	2.34	0.55
33:O:127:ARG:HA	33:O:150:TRP:HB2	1.88	0.55
24:D:42:ALA:HB1	24:D:47:GLU:HG2	1.89	0.54
20:E:52:LYS:HD2	20:E:80:MET:HE1	1.89	0.54
36:x:546:SER:O	36:x:546:SER:OG	2.25	0.54
1:2:158:U:O2'	1:2:160:C:OP2	2.25	0.54
15:c:90:ASP:O	15:c:136:TRP:NE1	2.39	0.54
1:2:207:U:O2	8:V:178:ARG:NH2	2.40	0.54
1:2:388:G:OP1	1:2:423:G:O2'	2.25	0.54
1:2:1171:A:H2'	1:2:1172:G:C8	2.42	0.54
21:A:121:GLY:HA2	35:z:256:ASP:CB	2.38	0.54
5:S:44:LEU:HD13	5:S:82:TYR:HB3	1.89	0.54
13:a:38:LYS:HE3	13:a:49:GLU:HB3	1.89	0.54
28:J:107:ALA:HA	28:J:110:LYS:HD2	1.89	0.54
36:x:97:LEU:HD12	36:x:98:PRO:HD2	1.90	0.54
1:2:354:C:H5"	8:V:16:ALA:HB2	1.90	0.54
1:2:1727:G:N2	8:V:32:GLN:OE1	2.28	0.54
36:x:416:SER:HB2	36:x:484:ILE:HG23	1.90	0.54
1:2:696:C:H4'	1:2:697:C:H5'	1.90	0.53
1:2:867:G:OP2	11:Y:3:ARG:NH1	2.41	0.53
1:2:1697:G:O6	1:2:1705:C:N4	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:LYS:O	3:Q:98:THR:OG1	2.26	0.53
4:R:219:GLY:O	13:a:25:LYS:NZ	2.41	0.53
5:S:199:GLU:OE2	5:S:209:HIS:NE2	2.33	0.53
33:O:126:SER:OG	33:O:128:ASP:OD1	2.27	0.53
1:2:1232:U:H5	32:N:97:LYS:HD2	1.71	0.53
1:2:1594:G:OP2	1:2:1596:C:N4	2.41	0.53
1:2:554:C:H1'	1:2:555:A:H2	1.73	0.53
2:P:41:ARG:C	2:P:43:ASP:H	2.17	0.53
8:V:48:THR:OG1	8:V:52:ASN:O	2.26	0.53
21:A:126:VAL:HG11	21:A:188:ILE:HG12	1.89	0.53
27:I:65:GLU:HG2	27:I:68:ARG:HH22	1.72	0.53
1:2:66:U:H5'	6:T:173:PRO:HA	1.89	0.53
1:2:273:G:O6	1:2:283:U:O2	2.27	0.53
1:2:1565:C:OP1	27:I:41:ARG:NH1	2.37	0.53
9:W:113:VAL:HG12	9:W:119:ALA:HB2	1.90	0.53
27:I:25:ASN:HB3	30:L:40:VAL:HG11	1.90	0.53
33:O:132:LYS:NZ	33:O:140:CYS:SG	2.73	0.53
36:x:418:LYS:HD3	36:x:419:PRO:HD2	1.90	0.53
2:P:70:PRO:HB2	2:P:94:GLY:HA3	1.89	0.53
3:Q:23:PRO:HB3	3:Q:26:ARG:HH21	1.73	0.53
6:T:135:PRO:HB3	6:T:140:ASN:HB3	1.91	0.53
26:H:21:TYR:HD1	26:H:58:MET:HE1	1.74	0.53
26:H:61:ILE:HD11	26:H:66:VAL:HG22	1.90	0.53
21:A:28:GLU:OE1	21:A:65:ARG:NH1	2.41	0.53
21:A:39:VAL:HG12	21:A:48:VAL:HG22	1.89	0.53
1:2:805:U:O4	7:U:104:ARG:NH1	2.42	0.53
1:2:1413:U:H3	1:2:1583:A:H5'	1.74	0.53
5:S:251:GLU:OE2	5:S:255:ARG:NH2	2.42	0.53
16:d:57:VAL:HB	16:d:60:PHE:HE2	1.74	0.53
21:A:40:ARG:NH1	21:A:47:GLU:OE1	2.42	0.53
21:A:93:ASP:HB2	21:A:96:LEU:HD12	1.91	0.53
35:z:204:ILE:HD11	35:y:193:ILE:HB	1.91	0.53
36:x:98:PRO:HD3	36:x:304:VAL:HG21	1.91	0.53
7:U:98:ILE:HG12	7:U:121:VAL:HG21	1.91	0.53
1:2:1081:A:H2	1:2:1082:C:H42	1.57	0.52
32:N:119:ARG:H	32:N:119:ARG:HE	1.56	0.52
1:2:459:G:OP2	16:d:105:ARG:NH2	2.36	0.52
5:S:129:VAL:HG22	5:S:139:VAL:HG12	1.91	0.52
21:A:198:GLY:O	21:A:200:LYS:NZ	2.41	0.52
1:2:190:C:N4	1:2:191:C:O2	2.42	0.52
36:x:291:VAL:HG23	36:x:310:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:652:G:O2'	1:2:683:C:N4	2.43	0.52
1:2:992:A:O2'	1:2:1785:U:O2	2.28	0.52
36:x:457:ILE:HD11	36:x:475:ARG:HG2	1.91	0.52
8:V:38:ILE:HG12	8:V:96:LEU:HD11	1.92	0.52
12:Z:17:ALA:HB3	12:Z:81:VAL:HA	1.91	0.52
21:A:115:ILE:HD11	21:A:138:VAL:HG11	1.92	0.52
32:N:120:GLU:HG2	32:N:130:VAL:O	2.10	0.52
10:X:57:LYS:HD3	10:X:131:ILE:HG23	1.92	0.52
13:a:58:TYR:OH	13:a:62:ARG:NH1	2.42	0.52
32:N:133:ALA:HB3	32:N:140:TYR:HB2	1.92	0.52
33:O:61:PHE:HZ	33:O:94:VAL:HA	1.75	0.52
1:2:1645:G:H1	1:2:1755:A:H2	1.56	0.52
2:P:198:MET:HG2	2:P:200:ASP:H	1.75	0.52
22:B:162:VAL:HG13	22:B:166:ARG:HD3	1.91	0.52
25:F:13:LYS:HG3	25:F:14:LYS:H	1.75	0.52
26:H:23:LYS:HA	33:O:198:ASN:HD21	1.73	0.52
1:2:194:U:H2'	1:2:195:G:H4'	1.92	0.52
1:2:1316:G:O2'	26:H:10:LYS:NZ	2.42	0.51
21:A:143:ARG:HH12	35:z:244:LYS:HE2	1.75	0.51
23:C:15:LEU:HG	23:C:68:LEU:HD23	1.92	0.51
33:O:56:VAL:HG13	33:O:57:PRO:HD2	1.91	0.51
1:2:1232:U:H2'	1:2:1233:G:C8	2.46	0.51
7:U:9:LEU:HD11	7:U:17:GLU:HB3	1.91	0.51
31:M:4:GLU:HB3	31:M:6:VAL:HG12	1.90	0.51
1:2:1459:C:OP2	27:I:138:THR:OG1	2.22	0.51
5:S:166:SER:HB2	5:S:168:LYS:HG2	1.92	0.51
27:I:26:ILE:HA	27:I:57:ARG:HH11	1.75	0.51
29:K:70:THR:OG1	29:K:72:ASN:OD1	2.29	0.51
32:N:118:ARG:HH11	32:N:118:ARG:CG	2.13	0.51
36:x:12:SER:OG	36:x:14:ASP:O	2.23	0.51
27:I:26:ILE:HG13	27:I:31:ALA:HB2	1.92	0.51
5:S:252:ARG:NH2	5:S:253:ASP:OD1	2.44	0.51
4:R:35:TRP:CE2	4:R:37:PRO:HB3	2.46	0.51
7:U:163:ASP:OD1	7:U:163:ASP:N	2.43	0.51
15:c:97:ASP:OD1	15:c:97:ASP:N	2.44	0.51
36:x:263:ILE:O	36:x:266:SER:OG	2.27	0.51
1:2:17:C:O2'	1:2:1137:A:N1	2.41	0.51
2:P:89:PHE:O	2:P:93:THR:OG1	2.24	0.51
7:U:153:LEU:HD23	7:U:184:GLU:HB3	1.93	0.51
9:W:109:LEU:HB2	9:W:146:PHE:HB3	1.93	0.51
21:A:162:GLN:N	21:A:163:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:x:86:ARG:HH21	36:x:91:SER:H	1.59	0.51
3:Q:90:GLU:OE1	3:Q:92:GLN:NE2	2.44	0.51
18:f:59:CYS:HG	18:f:61:THR:HG1	1.57	0.51
33:O:156:VAL:HG12	33:O:169:ILE:HG22	1.92	0.51
1:2:480:G:O6	1:2:508:U:O4	2.29	0.50
1:2:1520:U:OP2	28:J:75:LYS:NZ	2.37	0.50
1:2:567:A:OP1	15:c:70:LYS:NZ	2.44	0.50
1:2:1237:G:H2'	1:2:1238:A:H8	1.76	0.50
35:y:190:ILE:HG22	35:y:194:ARG:HH22	1.76	0.50
1:2:1321:A:OP2	2:P:101:ARG:NH2	2.43	0.50
13:a:3:ASN:ND2	13:a:7:GLN:NE2	2.55	0.50
22:B:156:ARG:HH11	22:B:157:ARG:H	1.60	0.50
36:x:281:LEU:HD12	36:x:314:ILE:HG23	1.92	0.50
1:2:639:U:OP1	7:U:112:ARG:NH2	2.45	0.50
4:R:76:LEU:HD13	4:R:104:VAL:HB	1.93	0.50
5:S:103:TYR:O	5:S:182:TYR:OH	2.29	0.50
36:x:116:LYS:HG2	36:x:294:ILE:HD12	1.93	0.50
2:P:41:ARG:C	2:P:43:ASP:N	2.69	0.50
5:S:105:VAL:HG22	5:S:245:LYS:HE2	1.94	0.50
29:K:28:SER:HB3	29:K:112:VAL:HA	1.94	0.50
29:K:50:LEU:HD21	29:K:95:ALA:HB2	1.92	0.50
30:L:92:ILE:HD11	30:L:102:THR:HB	1.94	0.50
1:2:329:G:H5"	8:V:98:LYS:HB3	1.94	0.50
1:2:886:U:OP2	3:Q:216:LYS:NZ	2.45	0.50
33:O:289:ALA:HA	33:O:305:TYR:HA	1.93	0.50
1:2:1489:U:O2'	1:2:1492:A:N3	2.42	0.50
7:U:17:GLU:HG2	7:U:46:ILE:HG12	1.94	0.50
7:U:45:SER:OG	7:U:46:ILE:N	2.43	0.50
21:A:67:ASN:O	21:A:70:THR:OG1	2.26	0.50
35:z:232:LYS:O	35:z:234:LYS:NZ	2.45	0.50
36:x:209:LEU:HD11	36:x:263:ILE:HG12	1.94	0.50
36:x:503:ARG:HB3	36:x:530:MET:HE3	1.93	0.50
1:2:1067:C:H5"	3:Q:150:VAL:HG22	1.94	0.50
24:D:130:THR:HG22	24:D:132:GLU:H	1.77	0.50
30:L:43:ASP:OD1	30:L:43:ASP:N	2.43	0.50
1:2:610:G:HO2'	1:2:613:G:HO2'	1.54	0.49
2:P:88:LYS:NZ	26:H:79:GLU:OE2	2.36	0.49
4:R:89:GLN:NE2	4:R:94:GLN:OE1	2.37	0.49
30:L:96:SER:OG	30:L:97:LYS:NZ	2.39	0.49
2:P:10:THR:OG1	2:P:13:ASP:OD2	2.30	0.49
4:R:120:GLU:HG2	4:R:123:GLY:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:124:LEU:O	30:L:58:ARG:NH1	2.45	0.49
1:2:1083:G:HO2'	1:2:1094:G:HO2'	1.55	0.49
1:2:1235:C:O2	32:N:140:TYR:CE1	2.64	0.49
2:P:105:GLY:N	2:P:135:GLU:OE2	2.34	0.49
32:N:122:SER:O	32:N:122:SER:OG	2.28	0.49
2:P:41:ARG:HG2	2:P:43:ASP:H	1.78	0.49
3:Q:97:LEU:HB3	3:Q:232:HIS:CE1	2.48	0.49
3:Q:136:ARG:HB2	3:Q:218:LEU:HD11	1.94	0.49
19:g:50:VAL:HG22	19:g:52:GLY:H	1.76	0.49
1:2:1040:G:H4'	2:P:32:HIS:CD2	2.47	0.49
14:b:41:MET:HG2	14:b:129:VAL:HG21	1.93	0.49
15:c:60:GLU:HG2	19:g:3:LYS:HB3	1.93	0.49
22:B:63:GLN:HE22	22:B:66:GLN:HB2	1.78	0.49
1:2:845:G:H3'	1:2:846:G:H21	1.77	0.49
21:A:132:LYS:HB3	21:A:189:MET:HG3	1.95	0.49
36:x:265:ARG:NH1	36:x:286:TYR:O	2.42	0.49
22:B:220:VAL:O	22:B:224:ASN:ND2	2.45	0.49
23:C:57:THR:HA	23:C:65:TYR:O	2.13	0.49
2:P:103:THR:HG21	2:P:113:ARG:HH12	1.78	0.49
1:2:1064:G:O2'	3:Q:204:ILE:O	2.30	0.48
12:Z:128:LYS:NZ	17:e:23:CYS:O	2.46	0.48
1:2:29:U:H2'	1:2:30:G:H8	1.77	0.48
1:2:803:A:O2'	7:U:104:ARG:NH1	2.46	0.48
3:Q:144:ARG:HD3	3:Q:208:GLN:HB3	1.95	0.48
17:e:36:ILE:HB	17:e:73:TYR:HB2	1.95	0.48
17:e:44:ILE:HG12	17:e:67:THR:HG23	1.96	0.48
36:x:229:ARG:HG3	36:x:252:LEU:HD21	1.95	0.48
1:2:142:G:H5"	6:T:139:ASN:HD21	1.79	0.48
1:2:332:U:P	8:V:56:ARG:HH22	2.37	0.48
5:S:117:GLU:O	5:S:120:SER:OG	2.31	0.48
23:C:55:VAL:HG12	23:C:68:LEU:HB3	1.94	0.48
33:O:133:VAL:HG13	33:O:141:LEU:HB2	1.94	0.48
36:x:140:TRP:HB3	36:x:160:LEU:HD11	1.94	0.48
1:2:1041:G:H2'	1:2:1042:G:C8	2.47	0.48
27:I:72:ILE:HG12	27:I:79:TYR:HD2	1.78	0.48
36:x:414:ASN:HB2	36:x:487:ASP:OD2	2.13	0.48
5:S:252:ARG:HD2	9:W:71:PHE:HE1	1.77	0.48
15:c:68:ILE:HD13	19:g:7:SER:H	1.78	0.48
7:U:46:ILE:HD12	7:U:60:ILE:HG12	1.94	0.48
33:O:47:LEU:HD12	33:O:54:PHE:CZ	2.47	0.48
1:2:891:A:H2'	1:2:892:A:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:77:GLU:OE1	12:Z:114:ARG:NH2	2.47	0.48
11:Y:36:GLN:HE21	11:Y:36:GLN:CA	2.21	0.48
33:O:120:SER:HB2	33:O:121:MET:HE2	1.96	0.48
35:z:212:ARG:HH12	35:z:216:LEU:HD12	1.79	0.48
36:x:309:SER:O	36:x:313:GLY:N	2.36	0.48
1:2:647:G:H1	1:2:687:G:H22	1.62	0.48
1:2:513:U:H2'	1:2:514:G:C8	2.49	0.48
1:2:891:A:H2'	1:2:892:A:C8	2.49	0.48
3:Q:71:ALA:HB3	12:Z:114:ARG:HH12	1.79	0.48
27:I:89:GLN:HA	27:I:97:ASP:HA	1.96	0.47
36:x:495:SER:O	36:x:503:ARG:NH1	2.47	0.47
1:2:235:G:H5"	1:2:237:C:H41	1.78	0.47
1:2:1681:A:H1'	6:T:66:GLY:HA2	1.96	0.47
5:S:125:LYS:NZ	5:S:225:VAL:O	2.41	0.47
16:d:28:LEU:HD12	16:d:68:LYS:HG2	1.95	0.47
22:B:143:ARG:NH2	22:B:218:GLU:OE1	2.44	0.47
1:2:1533:C:OP2	30:L:77:ARG:NH1	2.45	0.47
36:x:544:ILE:HG21	36:x:547:LYS:HE2	1.96	0.47
1:2:1153:G:OP1	17:e:82:ARG:NH1	2.47	0.47
1:2:1529:C:OP1	22:B:112:ARG:NH2	2.46	0.47
4:R:39:THR:HG22	4:R:41:LEU:H	1.79	0.47
1:2:115:G:H5'	10:X:129:ARG:HD3	1.96	0.47
21:A:207:THR:HG1	26:H:40:THR:HG1	1.57	0.47
1:2:399:A:H4'	5:S:3:ARG:HG2	1.96	0.47
1:2:687:G:OP1	14:b:119:LYS:NZ	2.48	0.47
3:Q:158:SER:HA	3:Q:161:ILE:HD12	1.97	0.47
1:2:472:U:O2'	1:2:769:A:N3	2.46	0.47
1:2:1554:U:OP1	31:M:13:ARG:NH1	2.47	0.47
9:W:59:LEU:HD22	9:W:69:ARG:HA	1.96	0.47
18:f:34:ASP:OD2	18:f:80:ARG:NH1	2.47	0.47
35:y:176:LEU:HD12	35:y:176:LEU:O	2.14	0.47
1:2:918:U:O2'	12:Z:35:GLY:O	2.32	0.47
1:2:1344:A:H2'	1:2:1345:A:C8	2.50	0.47
4:R:180:ALA:HB1	4:R:184:VAL:HG13	1.96	0.47
33:O:68:VAL:HA	33:O:84:SER:HA	1.97	0.47
33:O:69:GLN:OE1	33:O:85:TRP:NE1	2.43	0.47
36:x:368:LEU:HD12	36:x:549:ALA:HB3	1.96	0.47
1:2:1429:G:O2'	29:K:72:ASN:ND2	2.48	0.47
1:2:1466:G:O2'	1:2:1602:C:OP1	2.32	0.47
5:S:19:LEU:HD11	5:S:108:ARG:HD2	1.96	0.47
20:E:86:VAL:HG12	20:E:89:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:702:G:H2'	1:2:703:G:C8	2.49	0.47
1:2:1356:U:H2'	1:2:1357:A:H8	1.80	0.47
1:2:1534:G:N7	30:L:77:ARG:NH2	2.63	0.47
2:P:154:GLU:HA	13:a:63:GLY:HA2	1.96	0.47
4:R:35:TRP:CD1	4:R:35:TRP:C	2.90	0.47
9:W:136:VAL:HG23	9:W:156:ILE:HG12	1.97	0.46
25:F:94:GLN:NE2	33:O:60:SER:OG	2.42	0.46
27:I:48:LYS:HD3	28:J:35:ASP:HB3	1.97	0.46
36:x:414:ASN:HB3	36:x:487:ASP:CG	2.41	0.46
1:2:565:C:H4'	1:2:566:C:H5"	1.96	0.46
8:V:4:SER:HB2	8:V:24:LYS:HD3	1.97	0.46
24:D:41:LEU:HB3	24:D:43:ARG:HG3	1.97	0.46
1:2:1178:G:O6	27:I:139:LYS:NZ	2.47	0.46
6:T:7:TYR:HD1	6:T:113:ILE:HB	1.80	0.46
23:C:35:ILE:HG22	23:C:37:THR:H	1.80	0.46
32:N:141:CYS:SG	32:N:144:CYS:HB2	2.55	0.46
36:x:269:ALA:HB3	36:x:272:LYS:HG3	1.96	0.46
5:S:153:ASN:O	5:S:174:LYS:NZ	2.46	0.46
21:A:18:TYR:HE2	31:M:49:ASP:HB2	1.80	0.46
32:N:119:ARG:O	32:N:132:LEU:CB	2.64	0.46
1:2:898:A:N1	1:2:911:U:O2'	2.47	0.46
1:2:1235:C:C1'	32:N:140:TYR:CZ	2.87	0.46
33:O:110:VAL:HG12	33:O:126:SER:HB3	1.98	0.46
1:2:1432:U:H4'	1:2:1433:G:H5"	1.97	0.46
1:2:1477:G:H5'	28:J:45:MET:HB2	1.97	0.46
1:2:1561:U:H2'	1:2:1562:G:H8	1.81	0.46
18:f:33:LEU:HD23	18:f:81:ARG:HA	1.97	0.46
29:K:34:LEU:HD21	29:K:89:ARG:HD3	1.98	0.46
33:O:209:THR:HB	33:O:226:ALA:HB2	1.97	0.46
35:y:189:SER:O	35:y:192:SER:OG	2.27	0.46
36:x:414:ASN:H	36:x:487:ASP:CB	2.25	0.46
1:2:959:U:H5"	11:Y:14:SER:HB3	1.97	0.46
1:2:424:C:O2'	1:2:426:G:OP1	2.26	0.46
1:2:1515:A:O2'	1:2:1517:U:OP2	2.30	0.46
24:D:29:LYS:HE3	24:D:100:TRP:CD1	2.50	0.46
36:x:166:ALA:HB1	36:x:244:MET:HE1	1.97	0.46
1:2:485:A:N6	1:2:486:G:O6	2.48	0.46
1:2:1537:C:OP2	1:2:1572:G:N2	2.47	0.46
2:P:144:ILE:HG12	2:P:158:VAL:HB	1.97	0.46
33:O:10:ARG:NH2	33:O:314:GLN:HG2	2.30	0.46
1:2:1488:G:O2'	1:2:1494:C:O2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:13:ILE:HD11	16:d:22:GLN:HE21	1.81	0.46
21:A:158:ILE:HG13	21:A:164:VAL:HG12	1.98	0.46
36:x:192:LYS:HD2	36:x:192:LYS:HA	1.82	0.46
23:C:18:GLU:C	23:C:20:VAL:N	2.75	0.45
1:2:405:C:H5"	6:T:93:LYS:HE2	1.98	0.45
3:Q:195:LYS:HD2	3:Q:195:LYS:HA	1.79	0.45
24:D:82:PRO:HD3	32:N:113:LYS:HD2	1.97	0.45
36:x:86:ARG:HG2	36:x:132:GLY:HA2	1.98	0.45
1:2:1699:G:N2	1:2:1700:C:O2'	2.50	0.45
3:Q:128:LYS:NZ	3:Q:132:ASP:OD1	2.44	0.45
1:2:68:A:OP1	6:T:160:ARG:NH2	2.39	0.45
7:U:38:LEU:HB2	7:U:41:LEU:HD22	1.99	0.45
33:O:274:LEU:HD13	33:O:313:TRP:CE2	2.51	0.45
36:x:377:ASP:OD1	36:x:377:ASP:N	2.45	0.45
1:2:31:C:O2'	1:2:547:U:OP1	2.31	0.45
1:2:1357:A:N3	28:J:129:GLN:NE2	2.65	0.45
2:P:119:ARG:NH2	4:R:241:ASP:OD2	2.43	0.45
2:P:183:ARG:HD3	2:P:191:ARG:HH21	1.82	0.45
7:U:22:GLN:HA	7:U:25:VAL:HG22	1.99	0.45
15:c:138:GLU:HB3	35:y:170:LEU:HD11	1.97	0.45
27:I:100:THR:HG22	27:I:104:ASN:HB3	1.98	0.45
33:O:260:ILE:HB	33:O:274:LEU:HD11	1.97	0.45
1:2:298:C:H5"	5:S:38:LEU:HD23	1.98	0.45
1:2:1060:U:H3'	1:2:1061:A:H5"	1.98	0.45
1:2:539:G:H21	1:2:542:A:H62	1.65	0.45
1:2:1658:G:N1	1:2:1743:U:C2	2.79	0.45
6:T:142:ARG:HG2	6:T:147:LEU:HB2	1.98	0.45
12:Z:70:LYS:HA	12:Z:73:GLU:HG2	1.99	0.45
16:d:8:ARG:HH21	16:d:28:LEU:HD13	1.80	0.45
27:I:86:LEU:HD22	27:I:99:HIS:ND1	2.32	0.45
32:N:143:LYS:O	32:N:143:LYS:HG2	2.17	0.45
12:Z:81:VAL:HG11	12:Z:102:LEU:HD13	1.99	0.45
36:x:556:SER:O	36:x:559:THR:OG1	2.30	0.45
1:2:591:A:H2'	1:2:592:A:C8	2.52	0.45
3:Q:28:GLU:HB3	3:Q:50:LYS:HE3	1.99	0.45
3:Q:154:SER:O	3:Q:154:SER:OG	2.30	0.45
14:b:18:GLU:HG2	14:b:65:LEU:HD13	1.99	0.45
36:x:507:SER:OG	36:x:530:MET:SD	2.67	0.45
36:x:585:LYS:HB3	36:x:588:SER:HB3	1.98	0.45
1:2:1672:G:H2'	1:2:1673:G:C8	2.51	0.45
16:d:60:PHE:H	16:d:71:GLY:HA2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:146:THR:O	35:z:150:TYR:N	2.45	0.45
35:y:209:ARG:HB3	35:y:213:GLN:HE22	1.81	0.45
1:2:1650:U:H2'	1:2:1651:A:C8	2.52	0.44
28:J:25:GLN:HG2	28:J:27:LYS:HE2	1.99	0.44
1:2:871:G:H2'	1:2:872:G:C8	2.52	0.44
16:d:135:ASP:HA	36:x:586:LEU:HD13	1.98	0.44
18:f:40:CYS:SG	18:f:58:SER:OG	2.70	0.44
24:D:55:GLY:HA2	24:D:85:LYS:HE2	1.99	0.44
1:2:610:G:O2'	1:2:613:G:O2'	2.26	0.44
7:U:162:ILE:HG22	7:U:165:LYS:HE3	1.99	0.44
11:Y:99:ARG:NH1	11:Y:143:SER:OG	2.50	0.44
1:2:126:A:N6	1:2:263:C:O2'	2.51	0.44
1:2:1500:C:OP1	28:J:106:GLN:NE2	2.39	0.44
7:U:11:GLN:HB3	7:U:12:ALA:H	1.62	0.44
23:C:60:SER:HB3	23:C:65:TYR:HE1	1.82	0.44
36:x:529:ILE:HG12	36:x:581:PRO:HG2	2.00	0.44
1:2:465:G:O2'	36:x:148:ARG:NH1	2.50	0.44
7:U:115:SER:OG	7:U:116:ARG:NH1	2.51	0.44
26:H:100:LEU:N	26:H:118:PRO:O	2.51	0.44
33:O:13:LEU:HB2	33:O:310:ILE:HB	2.00	0.44
36:x:414:ASN:N	36:x:487:ASP:HB2	2.29	0.44
1:2:326:G:OP1	10:X:57:LYS:NZ	2.44	0.44
1:2:851:U:O2'	1:2:852:C:O5'	2.32	0.44
3:Q:129:THR:OG1	3:Q:130:SER:N	2.50	0.44
4:R:35:TRP:CD1	4:R:35:TRP:O	2.70	0.44
9:W:150:LEU:HA	9:W:153:GLU:HG3	2.00	0.44
26:H:7:LYS:O	26:H:11:ARG:N	2.49	0.44
32:N:120:GLU:HB3	32:N:121:CYS:H	1.62	0.44
33:O:126:SER:HG	33:O:128:ASP:CG	2.26	0.44
36:x:370:VAL:HA	36:x:551:ALA:HB3	2.00	0.44
1:2:1477:G:H2'	1:2:1478:G:C8	2.53	0.44
5:S:71:LYS:HG3	5:S:91:THR:HB	2.00	0.44
9:W:107:ARG:NH2	9:W:153:GLU:OE2	2.51	0.44
36:x:384:MET:HE1	36:x:564:PHE:CD2	2.52	0.44
8:V:87:ASN:HB3	8:V:90:LEU:HG	2.00	0.44
1:2:149:C:OP1	16:d:121:THR:OG1	2.31	0.43
16:d:42:GLU:HG2	16:d:52:LYS:HD2	2.00	0.43
20:E:52:LYS:HB3	20:E:80:MET:HE1	2.00	0.43
28:J:12:GLN:O	28:J:16:ASN:ND2	2.51	0.43
1:2:1235:C:O4'	32:N:140:TYR:CZ	2.70	0.43
1:2:1676:U:OP1	8:V:44:HIS:ND1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:45:ILE:HA	5:S:61:VAL:HG11	1.98	0.43
28:J:29:GLU:HG2	28:J:110:LYS:HE2	2.00	0.43
35:z:190:ILE:HA	35:y:204:ILE:HD11	1.99	0.43
35:z:239:LEU:HD23	35:z:239:LEU:HA	1.85	0.43
36:x:185:GLN:NE2	36:x:189:GLU:OE1	2.51	0.43
1:2:498:G:H21	1:2:499:U:H3	1.66	0.43
1:2:1316:G:OP1	26:H:7:LYS:N	2.51	0.43
1:2:1358:G:O2'	28:J:133:ASP:OD2	2.36	0.43
3:Q:55:LYS:HD2	3:Q:55:LYS:HA	1.72	0.43
22:B:57:SER:HB2	22:B:167:ARG:HH22	1.83	0.43
33:O:10:ARG:HH22	33:O:314:GLN:HG2	1.83	0.43
36:x:91:SER:OG	36:x:92:PHE:N	2.50	0.43
36:x:322:ILE:HD12	36:x:327:LEU:HD11	2.01	0.43
1:2:929:A:OP1	1:2:931:C:N4	2.50	0.43
1:2:1662:G:H2'	1:2:1663:G:C8	2.54	0.43
1:2:652:G:O6	1:2:680:U:O2	2.37	0.43
3:Q:46:THR:OG1	3:Q:64:ARG:NH2	2.52	0.43
22:B:133:VAL:HG22	22:B:198:LEU:HD13	2.01	0.43
27:I:18:LEU:N	27:I:18:LEU:HD22	2.33	0.43
27:I:61:LEU:HD23	27:I:61:LEU:HA	1.86	0.43
36:x:22:ARG:HD3	36:x:22:ARG:HA	1.86	0.43
36:x:242:VAL:HG22	36:x:273:TYR:HB2	2.01	0.43
5:S:196:VAL:HG11	5:S:211:LYS:HE3	2.00	0.43
17:e:37:LYS:O	17:e:38:ARG:NH1	2.52	0.43
27:I:17:LEU:HD11	27:I:66:LEU:HD12	2.00	0.43
27:I:17:LEU:HD22	27:I:70:VAL:HG21	2.00	0.43
33:O:149:ASP:H	33:O:175:ASP:HB3	1.84	0.43
36:x:62:VAL:HG21	36:x:72:ILE:HG12	2.01	0.43
36:x:80:GLU:OE2	36:x:93:LYS:NZ	2.50	0.43
36:x:574:ARG:HH22	36:x:581:PRO:HB3	1.84	0.43
1:2:1381:U:H4'	29:K:59:PRO:HG3	2.01	0.43
1:2:1515:A:H4'	1:2:1517:U:H5	1.84	0.43
1:2:1529:C:O2'	28:J:12:GLN:OE1	2.27	0.43
4:R:170:ILE:HB	4:R:197:TYR:HB2	2.01	0.43
8:V:158:SER:O	8:V:161:SER:OG	2.28	0.43
6:T:148:SER:N	6:T:151:ASP:OD2	2.39	0.43
27:I:38:VAL:HG23	27:I:42:TYR:HD2	1.83	0.43
33:O:117:LYS:NZ	33:O:157:VAL:O	2.35	0.43
36:x:244:MET:HG3	36:x:275:ILE:HG23	1.99	0.43
36:x:311:ARG:O	36:x:315:ASN:ND2	2.52	0.43
1:2:1232:U:C5	32:N:97:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1658:G:H2'	1:2:1659:A:C8	2.54	0.43
9:W:105:LEU:HD23	9:W:108:ARG:HD2	2.00	0.43
27:I:82:PRO:HG2	28:J:36:ILE:HG21	2.01	0.43
29:K:50:LEU:HD23	29:K:93:LEU:HD22	2.00	0.43
32:N:119:ARG:O	32:N:132:LEU:HB2	2.19	0.43
34:h:40:ILE:HD11	34:h:62:GLU:HB2	2.01	0.43
35:z:188:MET:HB3	35:z:192:SER:HB3	2.01	0.43
1:2:736:C:H2'	1:2:737:A:H8	1.83	0.42
7:U:71:HIS:ND1	7:U:74:GLN:OE1	2.51	0.42
14:b:15:ASN:ND2	14:b:72:CYS:O	2.41	0.42
20:E:121:ILE:HD11	27:I:125:ILE:HD12	2.01	0.42
27:I:65:GLU:HG2	27:I:68:ARG:NH2	2.33	0.42
30:L:88:ILE:HG22	30:L:89:ILE:CD1	2.48	0.42
32:N:97:LYS:HE2	32:N:97:LYS:HB2	1.29	0.42
2:P:156:VAL:O	13:a:65:SER:OG	2.36	0.42
15:c:92:CYS:HG	15:c:136:TRP:CD1	2.36	0.42
21:A:70:THR:O	21:A:74:GLN:HG3	2.19	0.42
27:I:126:ARG:HB2	27:I:133:VAL:HG12	2.01	0.42
36:x:145:LYS:HA	36:x:148:ARG:HG3	2.01	0.42
1:2:1684:U:H2'	1:2:1685:G:C8	2.54	0.42
19:g:47:VAL:O	19:g:47:VAL:HG22	2.19	0.42
25:F:99:GLU:HG2	33:O:58:VAL:C	2.45	0.42
33:O:13:LEU:HD22	33:O:45:TRP:CE3	2.54	0.42
40:x:703:ADP:H5'1	40:x:703:ADP:H8	1.82	0.42
7:U:49:ILE:HG21	7:U:175:LYS:HG2	2.00	0.42
7:U:143:LEU:HD11	7:U:149:ILE:HD12	2.01	0.42
10:X:109:VAL:HG11	10:X:125:VAL:HG11	2.01	0.42
22:B:114:ILE:HD13	22:B:114:ILE:HA	1.94	0.42
27:I:46:VAL:HG11	27:I:73:MET:HG2	2.00	0.42
1:2:1202:A:N6	1:2:1457:C:OP1	2.46	0.42
20:E:111:MET:HE2	27:I:119:ILE:HB	2.01	0.42
33:O:123:ILE:HG21	33:O:169:ILE:HG21	2.01	0.42
1:2:1383:G:P	29:K:89:ARG:HH12	2.43	0.42
28:J:28:LEU:HA	28:J:111:ILE:HD11	2.00	0.42
1:2:736:C:H2'	1:2:737:A:C8	2.55	0.42
1:2:1487:A:OP2	21:A:8:LYS:NZ	2.51	0.42
3:Q:143:THR:HB	3:Q:205:PHE:HE2	1.85	0.42
7:U:38:LEU:HA	7:U:41:LEU:HD13	2.01	0.42
16:d:55:VAL:HG23	16:d:75:VAL:HG12	2.02	0.42
27:I:13:HIS:HB2	27:I:14:ILE:HD12	2.02	0.42
1:2:475:A:OP2	9:W:126:ARG:NH2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:23:GLU:OE2	21:A:27:ARG:NH2	2.53	0.42
1:2:1316:G:HO2'	1:2:1401:A:HO2'	1.66	0.42
1:2:1357:A:H2'	1:2:1358:G:C8	2.55	0.42
36:x:484:ILE:HG23	36:x:484:ILE:O	2.19	0.42
1:2:241:U:H2'	1:2:242:U:C6	2.55	0.42
1:2:1351:G:H1	1:2:1374:C:H42	1.66	0.42
1:2:1755:A:OP1	15:c:63:GLN:NE2	2.49	0.42
5:S:195:ILE:HD13	5:S:195:ILE:HG21	1.89	0.42
6:T:121:LEU:HD23	6:T:124:LEU:HD12	2.02	0.42
36:x:124:ALA:HB2	36:x:244:MET:HE3	2.02	0.42
1:2:142:G:H5"	6:T:139:ASN:ND2	2.35	0.41
1:2:487:G:H2'	1:2:488:G:C8	2.55	0.41
1:2:939:A:H2'	1:2:940:A:C8	2.55	0.41
1:2:1298:U:O3'	4:R:212:LYS:NZ	2.53	0.41
2:P:3:LEU:HA	2:P:4:PRO:HD3	1.86	0.41
6:T:159:ARG:HB3	6:T:170:THR:HB	2.02	0.41
21:A:23:GLU:HA	21:A:26:THR:HG22	2.01	0.41
21:A:143:ARG:HG2	35:z:239:LEU:HD13	2.01	0.41
22:B:192:GLU:OE1	30:L:63:SER:OG	2.35	0.41
30:L:56:THR:H	30:L:103:ARG:NE	2.18	0.41
33:O:133:VAL:O	33:O:141:LEU:N	2.43	0.41
36:x:52:GLU:OE1	36:x:328:ARG:NH1	2.48	0.41
1:2:219:A:N6	1:2:843:U:O2	2.53	0.41
1:2:225:A:H2'	1:2:226:A:C8	2.55	0.41
1:2:1307:U:O4	1:2:1318:G:N2	2.47	0.41
1:2:1647:U:H2'	1:2:1648:A:C8	2.55	0.41
1:2:1665:U:O2	1:2:1736:G:C6	2.72	0.41
15:c:86:PHE:CE2	15:c:88:PRO:HA	2.55	0.41
1:2:29:U:H2'	1:2:30:G:C8	2.55	0.41
1:2:1235:C:C2	32:N:140:TYR:CZ	3.06	0.41
1:2:1524:A:H2'	1:2:1525:A:C8	2.56	0.41
1:2:1655:A:N6	1:2:1745:G:O2'	2.44	0.41
7:U:27:LEU:HD12	7:U:27:LEU:HA	1.91	0.41
17:e:10:ARG:HB2	17:e:33:ASP:OD1	2.20	0.41
22:B:58:LEU:HG	22:B:138:THR:HG22	2.02	0.41
27:I:6:GLN:O	27:I:8:GLN:NE2	2.53	0.41
33:O:168:THR:HG22	33:O:182:ASN:HA	2.03	0.41
33:O:269:TYR:CE2	33:O:271:VAL:HG12	2.55	0.41
35:z:212:ARG:NH1	35:z:216:LEU:HD12	2.35	0.41
1:2:418:G:O2'	6:T:72:ARG:NH2	2.53	0.41
1:2:585:A:H2'	1:2:586:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1232:U:H2'	1:2:1233:G:H8	1.83	0.41
2:P:147:THR:HG23	2:P:151:SER:OG	2.20	0.41
5:S:198:LYS:HD2	5:S:222:LEU:HD22	2.02	0.41
23:C:7:ASP:HA	23:C:10:LYS:HB2	2.02	0.41
1:2:52:U:H2'	1:2:53:G:C8	2.55	0.41
1:2:898:A:H4'	12:Z:46:MET:HE2	2.03	0.41
2:P:51:GLY:HA3	26:H:113:LEU:HD21	2.03	0.41
22:B:92:ARG:NH2	22:B:169:ASN:OD1	2.52	0.41
32:N:95:HIS:NE2	32:N:97:LYS:HA	2.35	0.41
33:O:172:ALA:HB2	33:O:202:LEU:HD13	2.02	0.41
1:2:474:A:OP1	9:W:145:SER:OG	2.37	0.41
1:2:1237:G:H2'	1:2:1238:A:C8	2.54	0.41
1:2:1414:U:OP2	26:H:2:GLY:N	2.54	0.41
1:2:1628:U:H2'	1:2:1629:G:C8	2.56	0.41
2:P:76:ILE:HD13	2:P:98:ILE:HB	2.02	0.41
3:Q:22:ASP:HA	3:Q:23:PRO:HD3	1.84	0.41
6:T:12:SER:OG	6:T:124:LEU:O	2.29	0.41
8:V:193:LEU:HD23	8:V:193:LEU:HA	1.96	0.41
15:c:56:LYS:HE2	15:c:93:LEU:HG	2.01	0.41
26:H:110:VAL:HG11	26:H:119:LEU:HD11	2.02	0.41
27:I:127:HIS:CE1	27:I:133:VAL:HG11	2.56	0.41
35:y:145:GLU:N	35:y:149:GLU:OE2	2.38	0.41
36:x:414:ASN:CB	36:x:487:ASP:CG	2.93	0.41
1:2:1235:C:O2	32:N:140:TYR:CD1	2.73	0.41
1:2:1319:A:OP1	26:H:67:ARG:NH2	2.40	0.41
4:R:120:GLU:N	4:R:120:GLU:OE1	2.54	0.41
5:S:79:ASP:HB3	5:S:82:TYR:HB2	2.03	0.41
10:X:136:ARG:HH11	10:X:136:ARG:HD2	1.75	0.41
24:D:138:GLU:O	24:D:142:GLN:N	2.43	0.41
27:I:11:PHE:HD1	27:I:60:GLU:HB3	1.85	0.41
1:2:522:U:H5"	16:d:37:LYS:HG3	2.02	0.41
8:V:57:ALA:HB2	8:V:177:GLY:HA2	2.02	0.41
21:A:176:LEU:HD23	35:z:234:LYS:HE3	2.01	0.41
26:H:35:CYS:HA	26:H:38:ILE:HG22	2.02	0.41
1:2:237:C:C5	1:2:834:G:H4'	2.56	0.41
1:2:829:A:O2'	1:2:830:U:O4'	2.36	0.41
1:2:1368:G:H5"	28:J:69:LYS:HG2	2.01	0.41
2:P:103:THR:HA	2:P:104:PRO:HD3	1.98	0.41
3:Q:174:LYS:NZ	3:Q:196:GLU:OE1	2.45	0.41
14:b:70:ASN:ND2	14:b:130:TYR:O	2.40	0.41
20:E:50:THR:HG23	20:E:53:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:213:LYS:HA	22:B:213:LYS:HD3	1.81	0.41
25:F:8:GLN:OE1	25:F:21:HIS:ND1	2.52	0.41
25:F:28:LEU:HD11	25:F:66:ARG:HH22	1.85	0.41
29:K:106:ILE:HG23	29:K:107:THR:HG23	2.03	0.41
30:L:48:ASP:HA	30:L:51:LEU:HB2	2.03	0.41
30:L:55:PRO:HB3	30:L:103:ARG:HE	1.86	0.41
36:x:105:VAL:HG23	36:x:268:LEU:HD11	2.03	0.41
36:x:590:MET:HE2	36:x:590:MET:HB3	1.99	0.41
1:2:968:U:OP1	1:2:1033:C:O2'	2.36	0.41
1:2:1044:U:H5"	3:Q:153:HIS:HE1	1.86	0.41
2:P:116:LYS:HB3	2:P:118:PRO:HD3	2.03	0.41
3:Q:88:VAL:HG11	3:Q:96:LEU:HD12	2.02	0.41
31:M:29:GLY:O	31:M:40:ARG:N	2.54	0.41
32:N:118:ARG:NH1	32:N:118:ARG:CG	2.73	0.41
33:O:93:ASP:HB2	33:O:100:TYR:CE2	2.56	0.41
36:x:574:ARG:HD3	36:x:574:ARG:HA	1.88	0.41
3:Q:70:LEU:HD22	3:Q:84:ILE:HD11	2.03	0.40
23:C:46:LEU:HD13	23:C:66:TYR:CD2	2.56	0.40
27:I:30:TYR:O	27:I:33:THR:OG1	2.39	0.40
35:y:157:LEU:HA	35:y:157:LEU:HD23	1.84	0.40
1:2:1658:G:O6	1:2:1743:U:O4	2.39	0.40
6:T:132:ARG:HG2	6:T:133:LEU:HD12	2.02	0.40
18:f:46:VAL:HG22	18:f:54:VAL:HG11	2.02	0.40
21:A:223:LYS:HB2	33:O:191:ASP:HB2	2.03	0.40
34:h:42:ARG:NH1	34:h:58:GLU:O	2.41	0.40
1:2:629:U:OP1	11:Y:127:ARG:NH2	2.48	0.40
1:2:1340:U:H5"	1:2:1341:A:H5"	2.03	0.40
1:2:1699:G:H3'	1:2:1700:C:H4'	2.02	0.40
6:T:69:LEU:HA	6:T:70:PRO:HD3	1.94	0.40
12:Z:83:ILE:HD11	12:Z:102:LEU:HD22	2.02	0.40
22:B:63:GLN:NE2	22:B:66:GLN:HE21	2.15	0.40
27:I:144:ARG:HD3	27:I:144:ARG:HA	1.82	0.40
33:O:14:GLU:N	33:O:14:GLU:OE1	2.55	0.40
36:x:18:PRO:HA	36:x:21:CYS:SG	2.61	0.40
36:x:280:ASP:HB3	36:x:283:VAL:HG12	2.02	0.40
36:x:523:ILE:HG22	36:x:525:GLU:HG2	2.03	0.40
1:2:1665:U:C2	1:2:1736:G:O6	2.75	0.40
20:E:86:VAL:HG22	20:E:87:PRO:HD2	2.04	0.40
24:D:64:SER:N	24:D:91:VAL:O	2.54	0.40
33:O:220:ILE:HD11	33:O:236:ALA:HB2	2.03	0.40
33:O:256:THR:OG1	33:O:259:GLY:O	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:x:8:ILE:HA	36:x:8:ILE:HD13	1.86	0.40
1:2:1610:G:H5'	22:B:107:LYS:HB2	2.03	0.40
5:S:45:ILE:HB	5:S:80:THR:HG22	2.02	0.40
17:e:22:ARG:HA	17:e:22:ARG:HD2	1.98	0.40
20:E:87:PRO:HA	20:E:90:ILE:HG13	2.03	0.40
27:I:121:ALA:O	27:I:125:ILE:HG13	2.22	0.40
36:x:105:VAL:HB	36:x:288:SER:HA	2.03	0.40
36:x:249:SER:OG	36:x:257:ARG:NE	2.55	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	
2	P	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
3	Q	222/232 (96%)	221 (100%)	1 (0%)	0	100	100
4	R	214/216 (99%)	213 (100%)	1 (0%)	0	100	100
5	S	256/258 (99%)	255 (100%)	1 (0%)	0	100	100
6	T	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
7	U	182/184 (99%)	180 (99%)	2 (1%)	0	100	100
8	V	183/200 (92%)	183 (100%)	0	0	100	100
9	W	182/184 (99%)	181 (100%)	1 (0%)	0	100	100
10	X	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	Y	148/150 (99%)	148 (100%)	0	0	100	100
12	Z	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
13	a	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	b	127/129 (98%)	127 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	c	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
16	d	132/134 (98%)	132 (100%)	0	0	100	100
17	e	95/97 (98%)	95 (100%)	0	0	100	100
18	f	79/81 (98%)	79 (100%)	0	0	100	100
19	g	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
20	E	115/117 (98%)	115 (100%)	0	0	100	100
21	A	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
22	B	204/206 (99%)	204 (100%)	0	0	100	100
23	C	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
24	D	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
25	F	139/141 (99%)	139 (100%)	0	0	100	100
26	H	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
27	I	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
28	J	141/143 (99%)	141 (100%)	0	0	100	100
29	K	98/100 (98%)	98 (100%)	0	0	100	100
30	L	80/82 (98%)	80 (100%)	0	0	100	100
31	M	51/53 (96%)	51 (100%)	0	0	100	100
32	N	71/73 (97%)	57 (80%)	10 (14%)	4 (6%)	1	8
33	O	310/312 (99%)	308 (99%)	2 (1%)	0	100	100
34	h	61/63 (97%)	61 (100%)	0	0	100	100
35	y	77/265 (29%)	76 (99%)	1 (1%)	0	100	100
35	z	118/265 (44%)	117 (99%)	1 (1%)	0	100	100
36	x	578/601 (96%)	577 (100%)	1 (0%)	0	100	100
All	All	5532/5985 (92%)	5484 (99%)	44 (1%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	N	140	TYR
32	N	141	CYS
32	N	120	GLU
32	N	98	VAL

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	
2	P	170/173 (98%)	170 (100%)	0	100	100
3	Q	200/205 (98%)	200 (100%)	0	100	100
4	R	175/175 (100%)	175 (100%)	0	100	100
5	S	220/220 (100%)	220 (100%)	0	100	100
6	T	189/195 (97%)	189 (100%)	0	100	100
7	U	163/165 (99%)	163 (100%)	0	100	100
8	V	148/161 (92%)	148 (100%)	0	100	100
9	W	156/157 (99%)	156 (100%)	0	100	100
10	X	126/127 (99%)	126 (100%)	0	100	100
11	Y	127/127 (100%)	127 (100%)	0	100	100
12	Z	90/96 (94%)	90 (100%)	0	100	100
13	a	71/74 (96%)	71 (100%)	0	100	100
14	b	110/110 (100%)	110 (100%)	0	100	100
15	c	119/119 (100%)	119 (100%)	0	100	100
16	d	112/112 (100%)	112 (100%)	0	100	100
17	e	82/83 (99%)	82 (100%)	0	100	100
18	f	70/70 (100%)	70 (100%)	0	100	100
19	g	50/51 (98%)	50 (100%)	0	100	100
20	E	95/98 (97%)	95 (100%)	0	100	100
21	A	182/182 (100%)	182 (100%)	0	100	100
22	B	172/173 (99%)	172 (100%)	0	100	100
23	C	78/85 (92%)	78 (100%)	0	100	100
24	D	88/98 (90%)	88 (100%)	0	100	100
25	F	117/117 (100%)	117 (100%)	0	100	100
26	H	101/113 (89%)	101 (100%)	0	100	100
27	I	127/128 (99%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	J	115/115 (100%)	115 (100%)	0	100 100
29	K	93/93 (100%)	93 (100%)	0	100 100
30	L	67/73 (92%)	67 (100%)	0	100 100
31	M	47/47 (100%)	47 (100%)	0	100 100
32	N	57/64 (89%)	48 (84%)	9 (16%)	2 13
33	O	250/257 (97%)	250 (100%)	0	100 100
34	h	55/56 (98%)	55 (100%)	0	100 100
35	y	69/221 (31%)	69 (100%)	0	100 100
35	z	90/221 (41%)	90 (100%)	0	100 100
36	x	516/531 (97%)	516 (100%)	0	100 100
All	All	4697/5092 (92%)	4688 (100%)	9 (0%)	85 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	N	97	LYS
32	N	118	ARG
32	N	119	ARG
32	N	122	SER
32	N	125	THR
32	N	126	CYS
32	N	130	VAL
32	N	140	TYR
32	N	145	HIS

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

Mol	Chain	Res	Type
2	P	32	HIS
2	P	69	ASN
2	P	140	ASN
2	P	163	ASN
3	Q	177	GLN
4	R	199	GLN
5	S	96	ASN
5	S	142	HIS
5	S	197	HIS

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Mol	Chain	Res	Type
6	T	176	GLN
6	T	189	HIS
6	T	210	GLN
7	U	11	GLN
7	U	86	GLN
7	U	89	HIS
8	V	94	ASN
9	W	110	GLN
10	X	106	ASN
10	X	110	HIS
10	X	138	ASN
11	Y	36	GLN
11	Y	151	ASN
13	a	7	GLN
14	b	12	ASN
16	d	15	ASN
16	d	63	GLN
16	d	106	GLN
18	f	51	GLN
21	A	165	ASN
22	B	63	GLN
23	C	9	ASN
23	C	81	ASN
24	D	80	ASN
27	I	12	GLN
27	I	19	ASN
27	I	137	HIS
28	J	70	GLN
28	J	101	ASN
30	L	37	GLN
30	L	44	GLN
30	L	82	HIS
33	O	182	ASN
35	z	165	ASN
35	y	213	GLN
36	x	185	GLN
36	x	369	ASN
36	x	584	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1771 (99%)	524 (29%)	18 (1%)

All (524) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	6	G
1	2	11	A
1	2	25	C
1	2	26	A
1	2	34	G
1	2	39	A
1	2	42	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	56	U
1	2	57	G
1	2	59	C
1	2	60	U
1	2	66	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	77	U
1	2	78	A
1	2	100	A
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	117	U
1	2	126	A
1	2	127	G
1	2	129	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	137	U
1	2	138	A

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Mol	Chain	Res	Type
1	2	140	A
1	2	141	U
1	2	142	G
1	2	146	U
1	2	147	A
1	2	156	A
1	2	158	U
1	2	161	U
1	2	168	A
1	2	173	A
1	2	176	C
1	2	178	U
1	2	180	A
1	2	181	A
1	2	187	G
1	2	188	A
1	2	189	C
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	197	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	222	A
1	2	224	C
1	2	225	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	230	C
1	2	231	U
1	2	232	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	239	C
1	2	240	U

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Mol	Chain	Res	Type
1	2	241	U
1	2	249	U
1	2	250	C
1	2	259	U
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	267	U
1	2	272	U
1	2	273	G
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	287	G
1	2	291	G
1	2	299	A
1	2	312	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	321	C
1	2	322	G
1	2	324	U
1	2	328	A
1	2	333	A
1	2	335	U
1	2	336	G
1	2	337	G
1	2	338	C
1	2	351	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	365	G
1	2	387	A
1	2	388	G
1	2	389	G

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Mol	Chain	Res	Type
1	2	393	C
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	417	A
1	2	419	G
1	2	422	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	437	A
1	2	439	U
1	2	441	A
1	2	444	C
1	2	445	A
1	2	448	C
1	2	452	A
1	2	464	A
1	2	468	A
1	2	477	A
1	2	480	G
1	2	482	U
1	2	483	A
1	2	485	A
1	2	487	G
1	2	490	C
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	499	U
1	2	500	C
1	2	501	U
1	2	502	U
1	2	506	A

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Mol	Chain	Res	Type
1	2	507	U
1	2	510	G
1	2	511	A
1	2	514	G
1	2	519	C
1	2	527	A
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	548	G
1	2	549	G
1	2	555	A
1	2	557	G
1	2	559	C
1	2	565	C
1	2	566	C
1	2	568	G
1	2	572	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	583	C
1	2	594	A
1	2	595	G
1	2	606	A
1	2	610	G
1	2	611	U
1	2	613	G
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G

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Mol	Chain	Res	Type
1	2	644	C
1	2	645	C
1	2	647	G
1	2	649	U
1	2	651	G
1	2	654	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	681	U
1	2	682	C
1	2	683	C
1	2	684	A
1	2	688	G
1	2	694	U
1	2	696	C
1	2	698	U
1	2	699	U
1	2	700	C
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	708	C
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	737	A
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	753	A
1	2	765	G

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Mol	Chain	Res	Type
1	2	766	U
1	2	768	C
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	789	A
1	2	795	U
1	2	807	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	826	U
1	2	829	A
1	2	833	U
1	2	834	G
1	2	840	U
1	2	845	G
1	2	846	G
1	2	847	A
1	2	850	A
1	2	852	C
1	2	853	G
1	2	855	A
1	2	856	A
1	2	857	U
1	2	859	A
1	2	863	A
1	2	883	C
1	2	886	U

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Mol	Chain	Res	Type
1	2	902	G
1	2	913	G
1	2	914	G
1	2	921	U
1	2	928	U
1	2	929	A
1	2	933	A
1	2	935	U
1	2	940	A
1	2	942	G
1	2	945	U
1	2	946	U
1	2	951	A
1	2	960	U
1	2	966	A
1	2	969	C
1	2	970	A
1	2	971	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	1001	A
1	2	1004	U
1	2	1005	A
1	2	1021	C
1	2	1023	A
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1032	G
1	2	1039	A
1	2	1052	U
1	2	1053	G
1	2	1054	U
1	2	1057	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1063	U
1	2	1081	A
1	2	1082	C
1	2	1092	A

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Mol	Chain	Res	Type
1	2	1096	C
1	2	1098	U
1	2	1100	G
1	2	1109	G
1	2	1113	A
1	2	1116	A
1	2	1138	A
1	2	1150	G
1	2	1158	C
1	2	1159	C
1	2	1167	G
1	2	1171	A
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1206	U
1	2	1207	C
1	2	1208	A
1	2	1216	C
1	2	1217	A
1	2	1218	G
1	2	1222	C
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1251	U
1	2	1252	C
1	2	1263	G
1	2	1274	C
1	2	1275	A
1	2	1284	C
1	2	1285	U
1	2	1286	U
1	2	1291	G

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Mol	Chain	Res	Type
1	2	1306	C
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1319	A
1	2	1321	A
1	2	1322	A
1	2	1323	C
1	2	1325	A
1	2	1327	C
1	2	1337	A
1	2	1338	C
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1347	U
1	2	1350	U
1	2	1354	G
1	2	1360	A
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1373	C
1	2	1378	U
1	2	1383	G
1	2	1390	U
1	2	1397	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1410	A
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1418	G
1	2	1426	C
1	2	1427	A
1	2	1428	G
1	2	1429	G

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Mol	Chain	Res	Type
1	2	1432	U
1	2	1433	G
1	2	1445	G
1	2	1446	A
1	2	1458	G
1	2	1459	C
1	2	1460	A
1	2	1461	C
1	2	1464	G
1	2	1466	G
1	2	1469	A
1	2	1471	A
1	2	1472	C
1	2	1474	G
1	2	1486	G
1	2	1487	A
1	2	1490	C
1	2	1491	U
1	2	1494	C
1	2	1496	U
1	2	1506	G
1	2	1516	A
1	2	1520	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1531	G
1	2	1534	G
1	2	1535	U
1	2	1537	C
1	2	1539	G
1	2	1540	G
1	2	1543	A
1	2	1548	G
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1565	C
1	2	1573	A
1	2	1582	U
1	2	1583	A
1	2	1584	G

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Mol	Chain	Res	Type
1	2	1590	G
1	2	1597	A
1	2	1601	G
1	2	1607	G
1	2	1610	G
1	2	1611	A
1	2	1616	G
1	2	1619	C
1	2	1631	A
1	2	1634	C
1	2	1635	A
1	2	1637	C
1	2	1639	C
1	2	1640	C
1	2	1641	C
1	2	1642	G
1	2	1651	A
1	2	1654	G
1	2	1656	U
1	2	1657	U
1	2	1658	G
1	2	1667	A
1	2	1669	U
1	2	1680	G
1	2	1681	A
1	2	1682	U
1	2	1685	G
1	2	1686	C
1	2	1688	U
1	2	1692	G
1	2	1693	A
1	2	1695	G
1	2	1696	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1704	U
1	2	1705	C
1	2	1709	C
1	2	1712	A

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Mol	Chain	Res	Type
1	2	1714	A
1	2	1715	G
1	2	1718	G
1	2	1746	A
1	2	1747	G
1	2	1750	A
1	2	1755	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1791	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1797	A
1	2	1799	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	59	C
1	2	77	U
1	2	139	C
1	2	280	U
1	2	387	A
1	2	400	A
1	2	639	U
1	2	640	U
1	2	711	U
1	2	819	G
1	2	928	U
1	2	1226	A
1	2	1274	C
1	2	1344	A

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Mol	Chain	Res	Type
1	2	1382	A
1	2	1636	C
1	2	1694	A
1	2	1791	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 85 ligands modelled in this entry, 82 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	SF4	x	702	36	0,12,12	-	-	-		
39	SF4	x	701	36	0,12,12	-	-	-		
40	ADP	x	703	37	27,29,29	1.35	4 (14%)	42,45,45	1.98	9 (21%)

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
39	SF4	x	701	36	-	-	0/6/5/5
39	SF4	x	702	36	-	-	0/6/5/5
40	ADP	x	703	37	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	703	ADP	C5-C4	4.50	1.47	1.39
40	x	703	ADP	C5-C6	2.71	1.48	1.41
40	x	703	ADP	C8-N7	2.26	1.35	1.31
40	x	703	ADP	C5-N7	-2.14	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	x	703	ADP	C5-C4-N3	-6.34	118.47	126.75
40	x	703	ADP	N3-C4-N9	5.03	135.37	127.08
40	x	703	ADP	C2-N3-C4	3.87	120.89	111.75
40	x	703	ADP	PA-O3A-PB	-3.59	120.49	132.83
40	x	703	ADP	C4-C5-N7	-3.26	106.65	110.62
40	x	703	ADP	N3-C2-N1	-3.02	123.89	128.60
40	x	703	ADP	C5-N7-C8	2.73	107.38	103.51
40	x	703	ADP	C4-N9-C8	2.65	108.60	105.73
40	x	703	ADP	C6-C5-N7	2.07	135.87	132.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	x	703	ADP	C5'-O5'-PA-O3A
40	x	703	ADP	C5'-O5'-PA-O1A
40	x	703	ADP	O4'-C4'-C5'-O5'

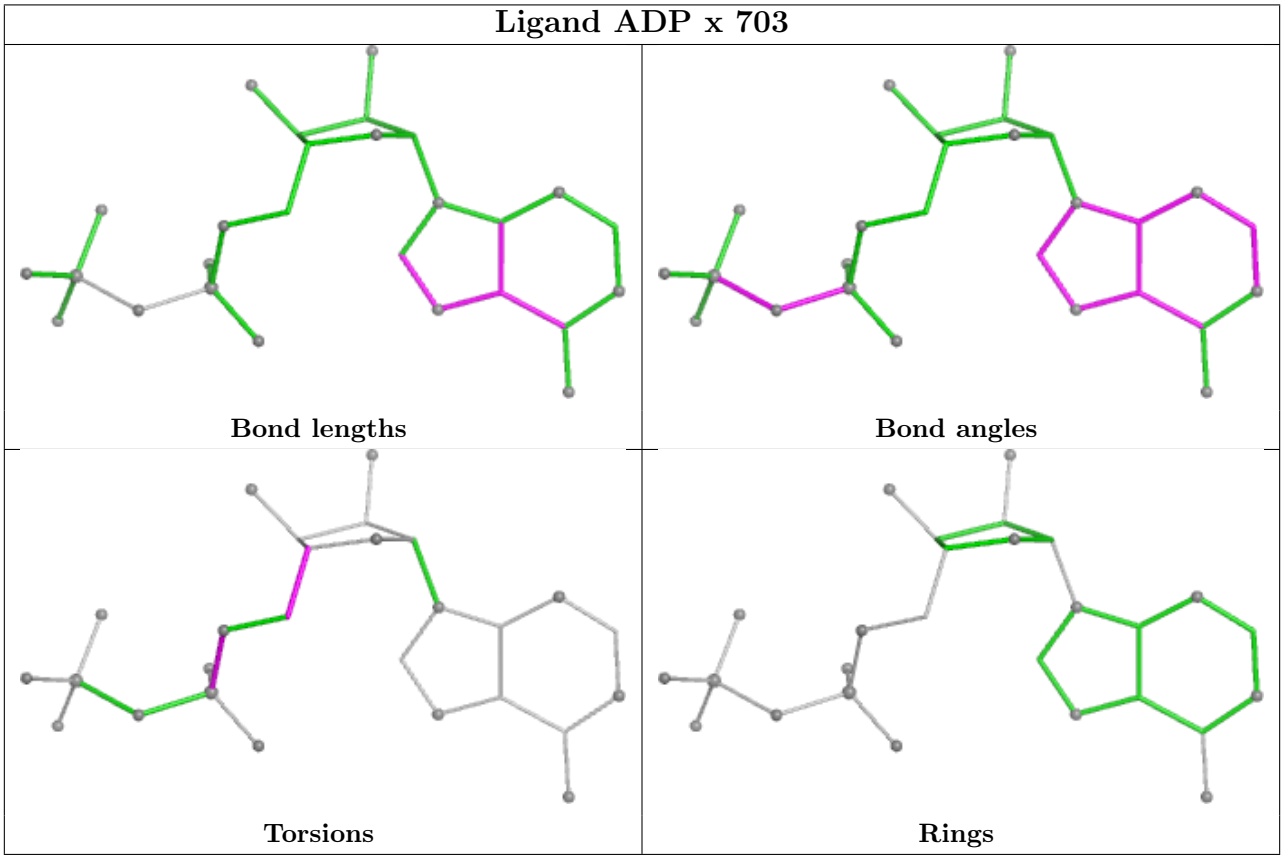
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	x	703	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	714:G	O3'	726:C	P	14.69
1	2	658:C	O3'	676:G	P	14.35

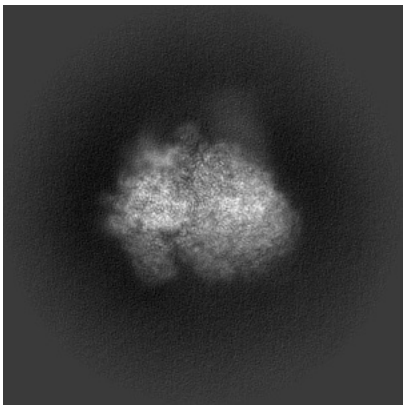
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11608. These allow visual inspection of the internal detail of the map and identification of artifacts.

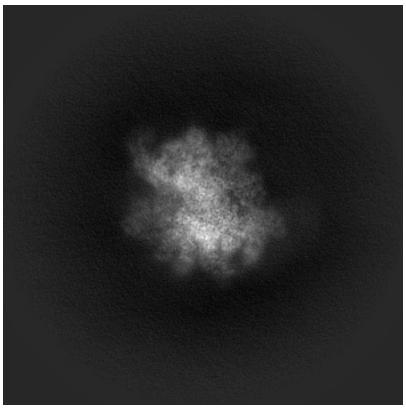
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

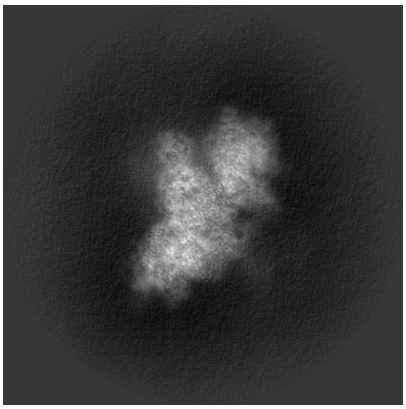
6.1.1 Primary map



X

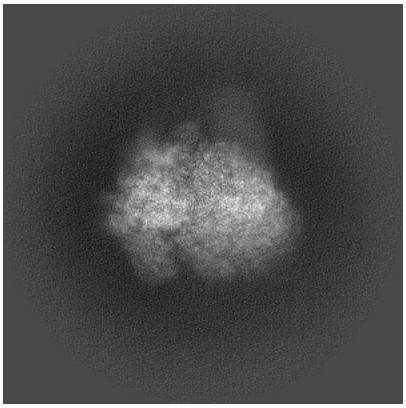


Y

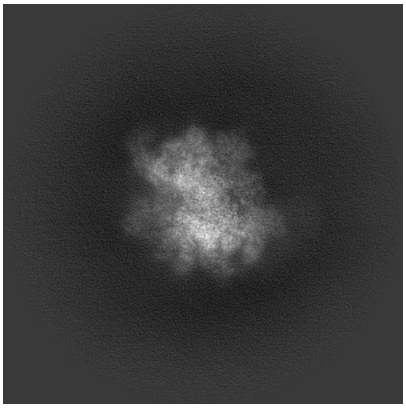


Z

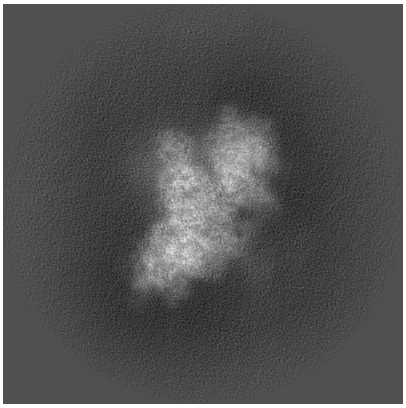
6.1.2 Raw map



X



Y

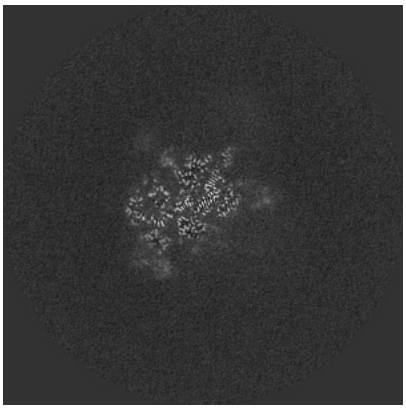


Z

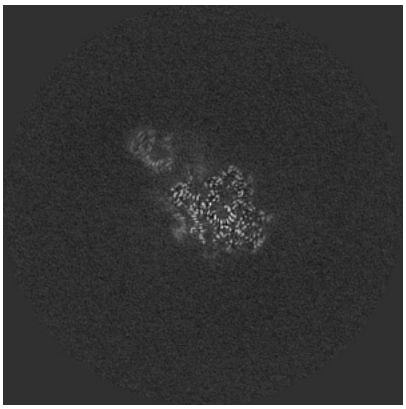
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

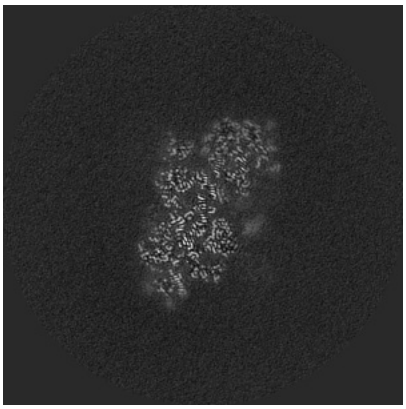
6.2.1 Primary map



X Index: 225

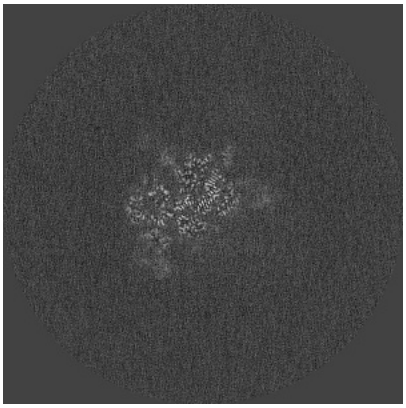


Y Index: 225

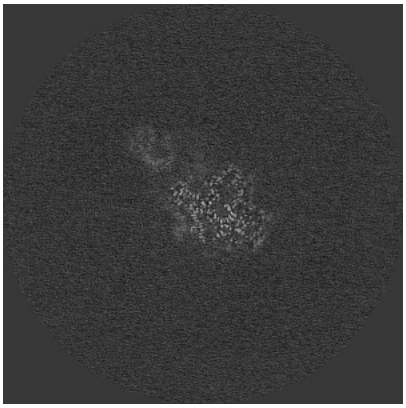


Z Index: 225

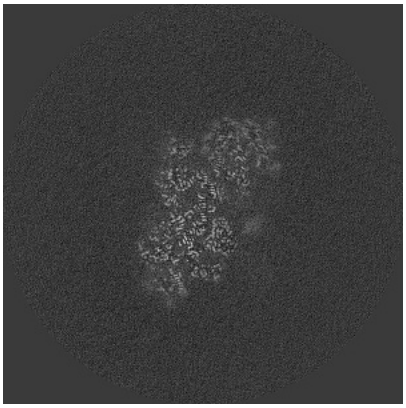
6.2.2 Raw map



X Index: 225



Y Index: 225

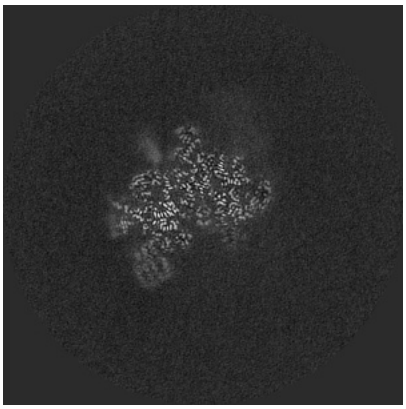


Z Index: 225

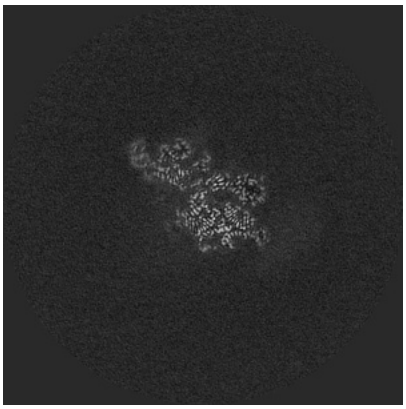
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

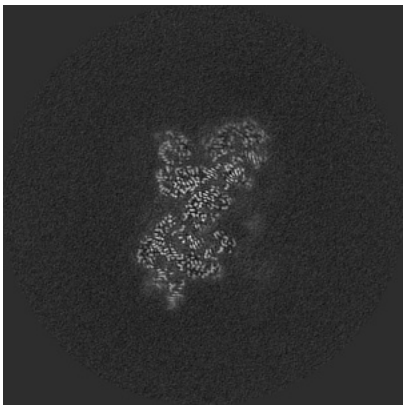
6.3.1 Primary map



X Index: 204

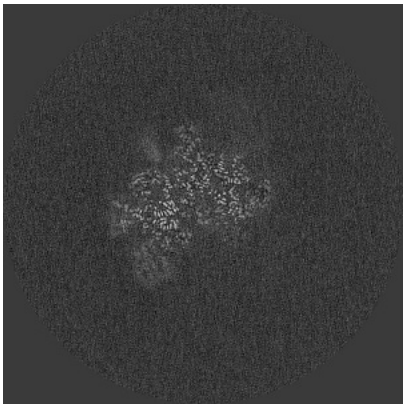


Y Index: 247

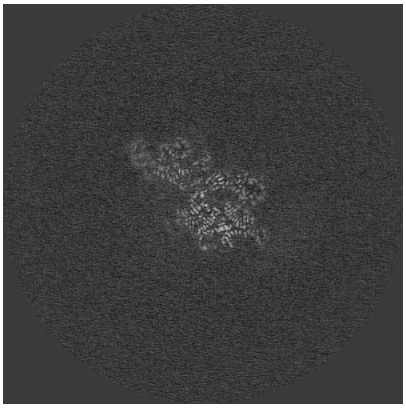


Z Index: 231

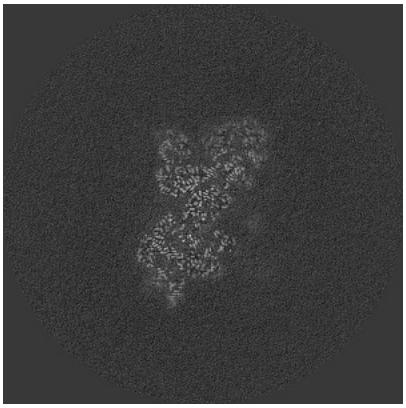
6.3.2 Raw map



X Index: 204



Y Index: 247

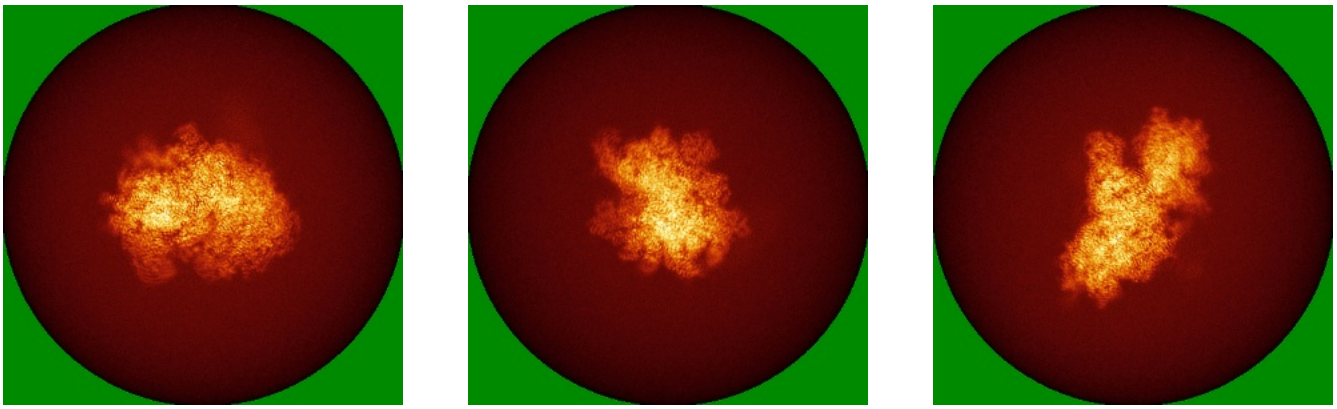


Z Index: 231

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

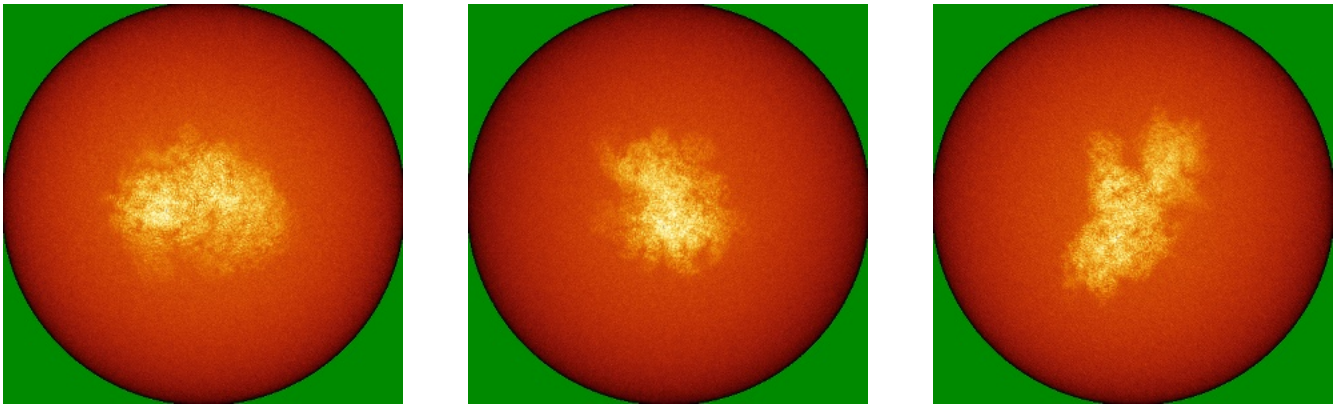
6.4 Orthogonal standard-deviation projections (False-color) (i)

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 0.04. 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.

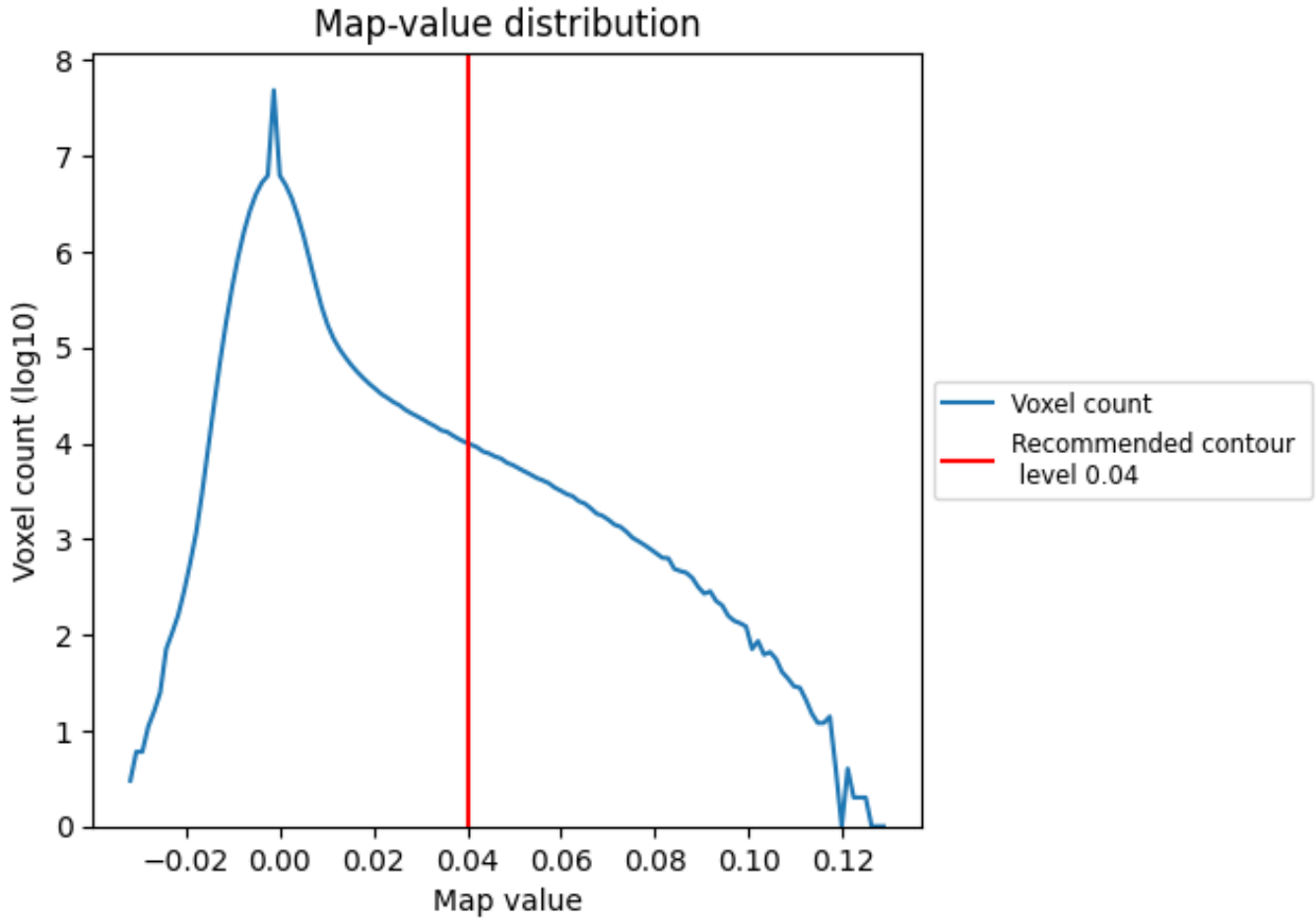
6.6 Mask visualisation (i)

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

7 Map analysis

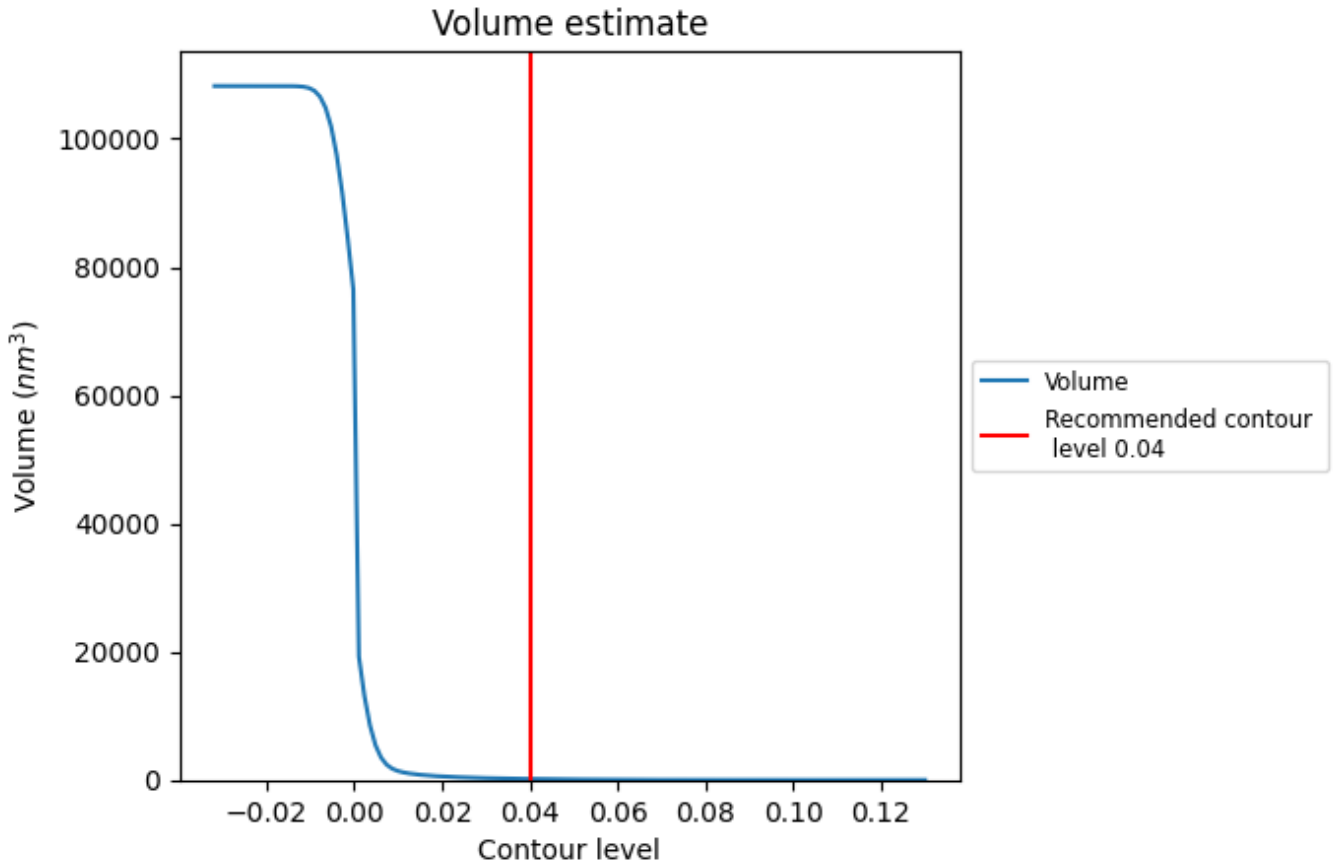
This section contains the results of statistical analysis of the map.

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.

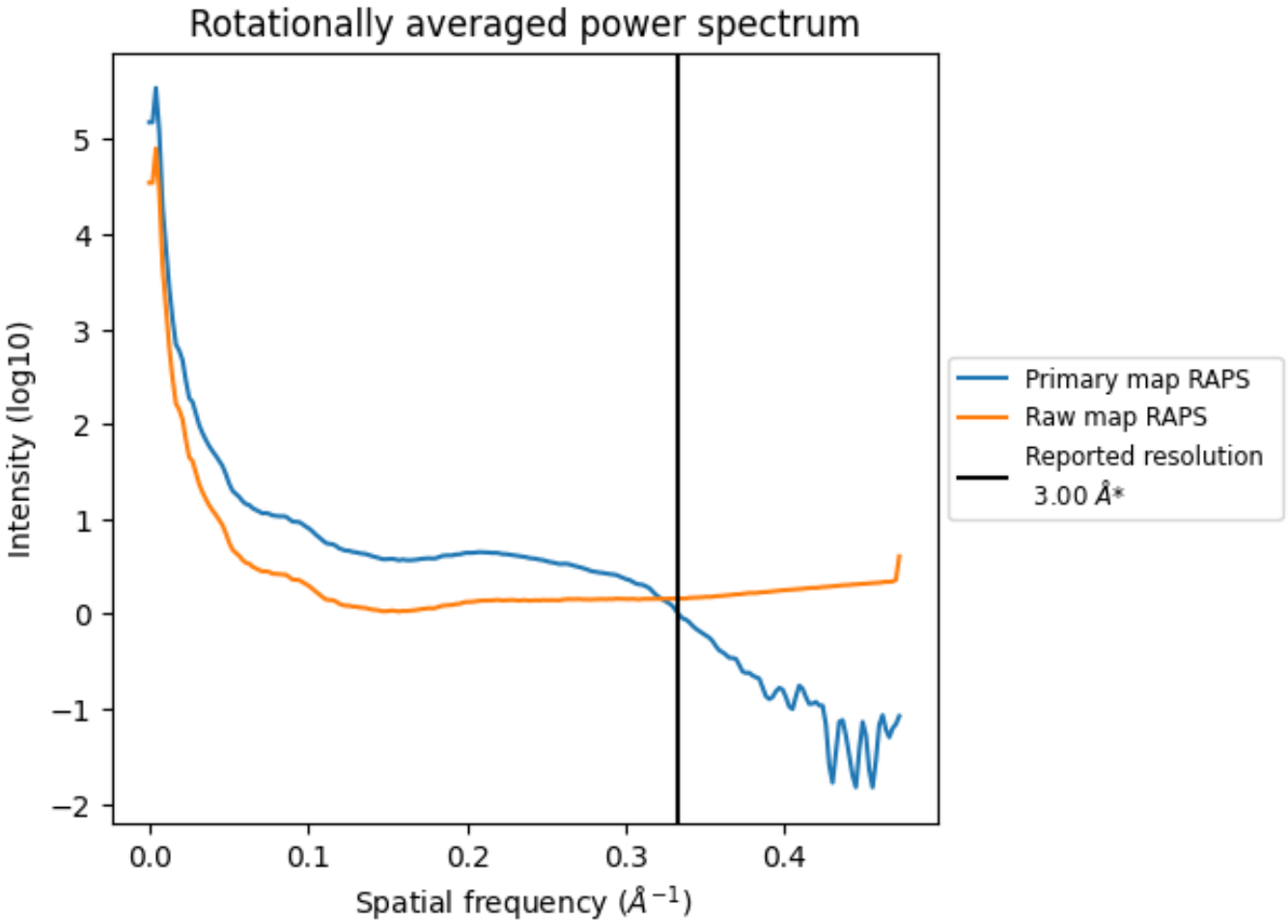
7.2 Volume estimate



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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)

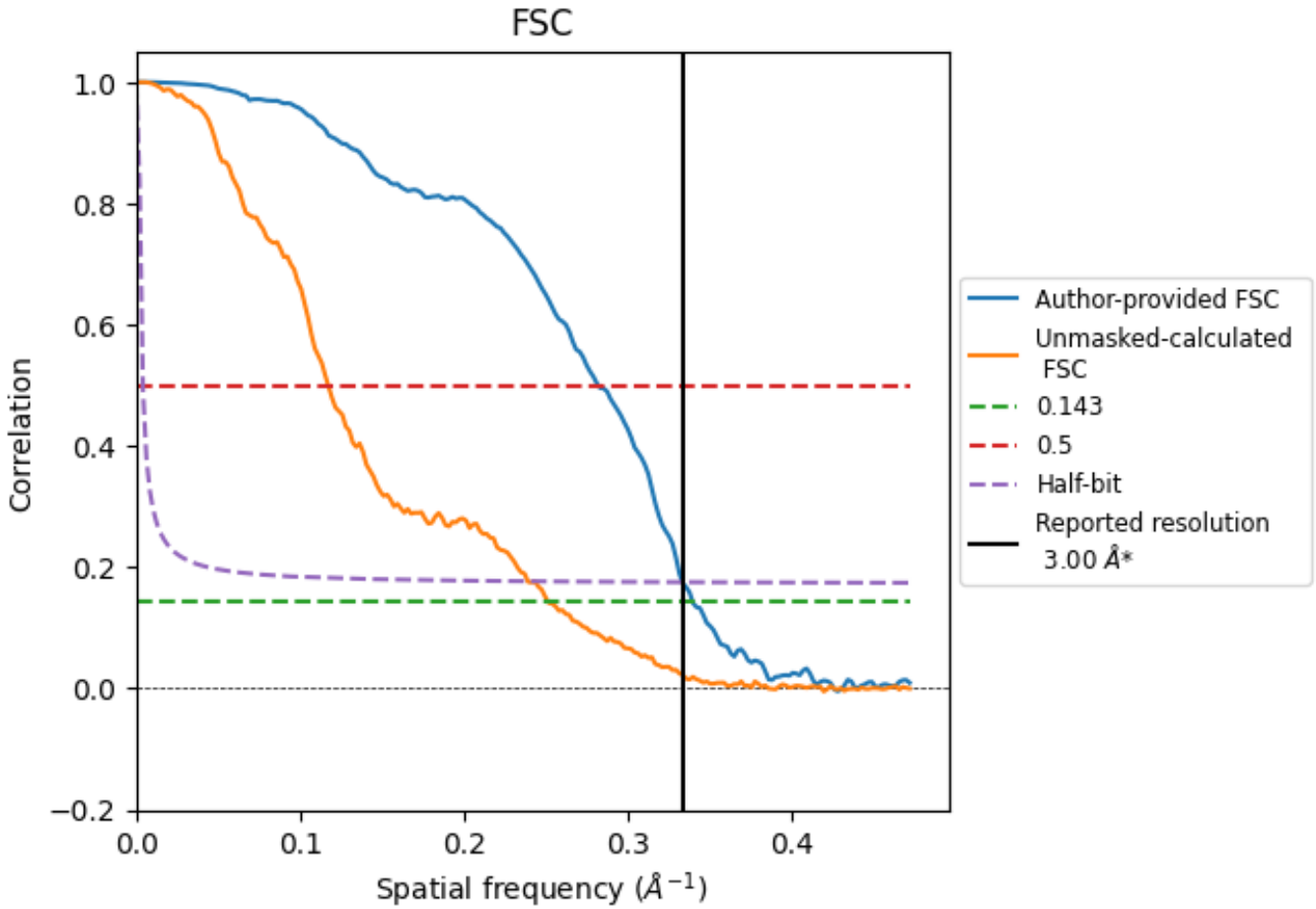


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

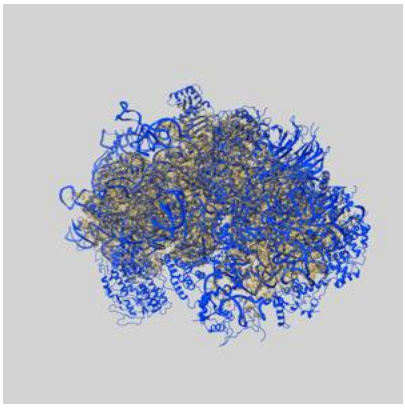
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.94	3.55	3.00
Unmasked-calculated*	3.98	8.53	4.18

*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 3.98 differs from the reported value 3.0 by more than 10 %

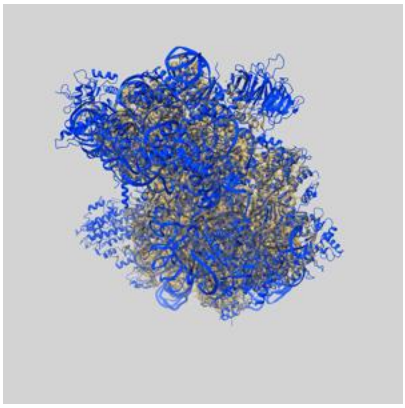
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11608 and PDB model 7A1G. Per-residue inclusion information can be found in section 3 on page 12.

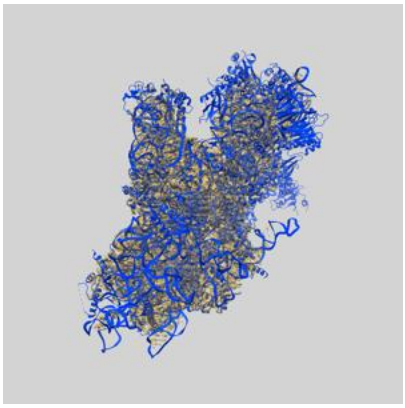
9.1 Map-model overlay



X



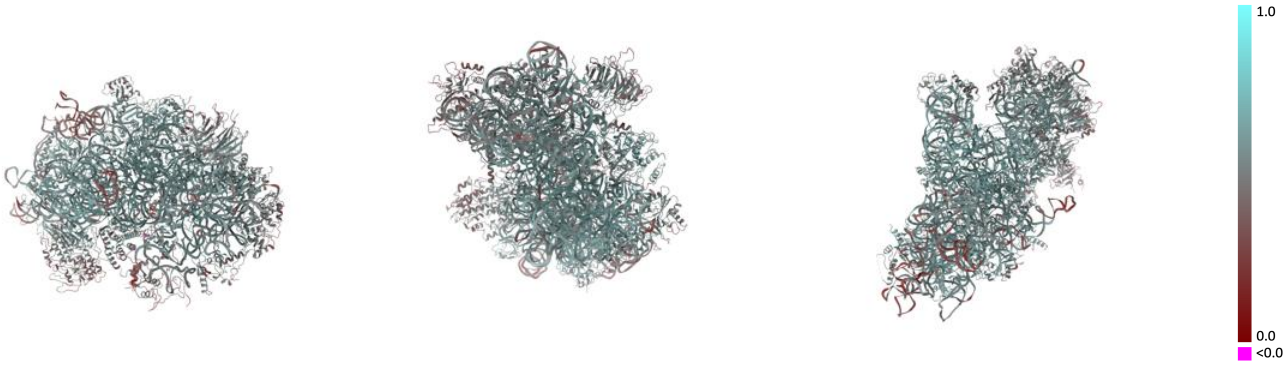
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

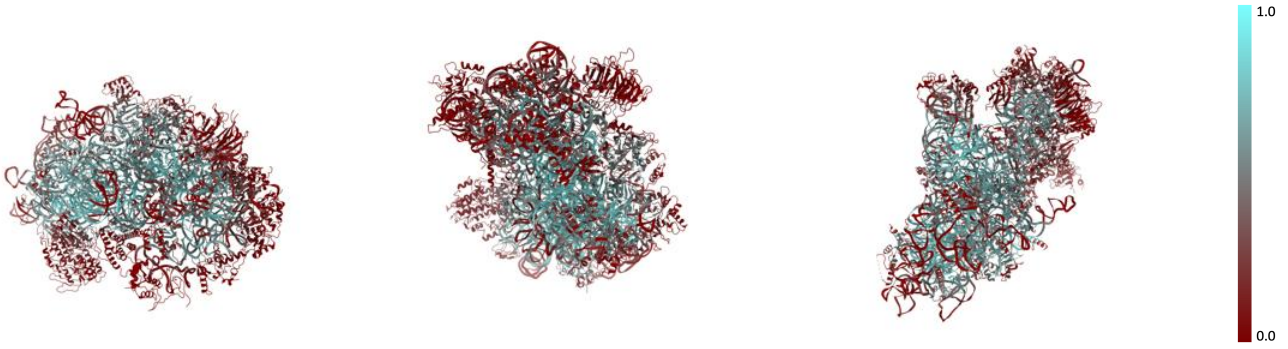
9.2 Q-score mapped to coordinate model (i)



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.

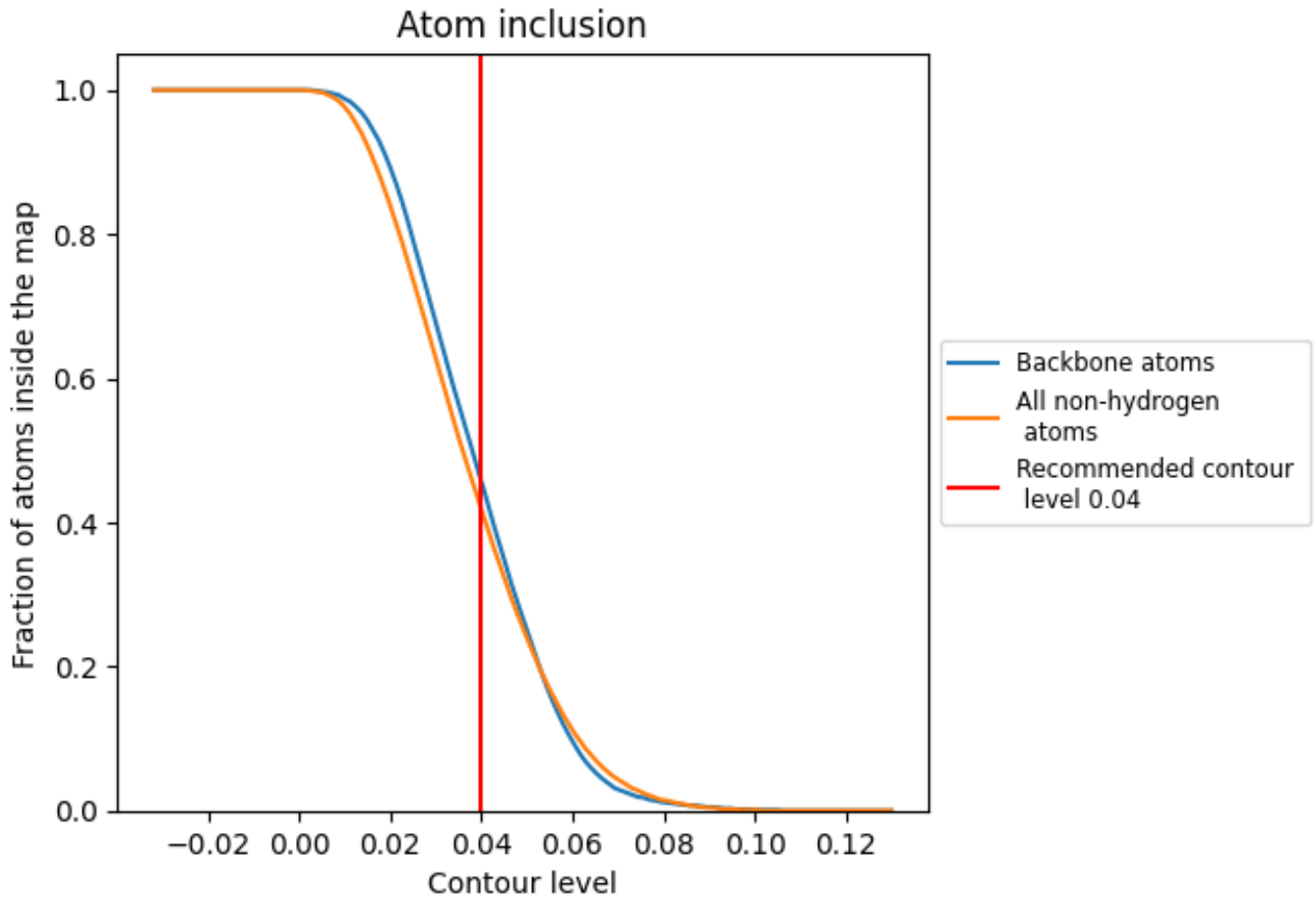
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 42% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4180	0.5470
2	0.5790	0.5630
A	0.2410	0.5320
B	0.1190	0.5070
C	0.1950	0.5040
D	0.0000	0.3700
E	0.0610	0.4790
F	0.2510	0.5580
H	0.2200	0.5180
I	0.0320	0.4750
J	0.1160	0.5140
K	0.2280	0.5180
L	0.0080	0.4330
M	0.4810	0.6070
N	0.0040	0.3590
O	0.0370	0.4870
P	0.4100	0.5840
Q	0.2670	0.5460
R	0.4640	0.5970
S	0.5300	0.6030
T	0.2970	0.5510
U	0.2290	0.5190
V	0.4880	0.5850
W	0.5070	0.5900
X	0.5770	0.6060
Y	0.4490	0.5790
Z	0.3000	0.5650
a	0.4330	0.5830
b	0.6070	0.6170
c	0.5580	0.6020
d	0.4390	0.5600
e	0.4670	0.5970
f	0.3780	0.5760
g	0.3640	0.5370
h	0.0590	0.4960



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Chain	Atom inclusion	Q-score
x	0.1330	0.4760
y	0.0210	0.4770
z	0.0470	0.4800