Full wwPDB EM Validation Report (i)

Sep 17, 2026 – 01:10 AM EDT

PDB ID	:	7RYF / pdb_00007ryf
EMDB ID	:	EMD-24738
Title	:	A. baumannii Ribosome-TP-6076 complex: P-site tRNA 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-08-25
Resolution	:	2.65 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 (i) symbol.

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

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

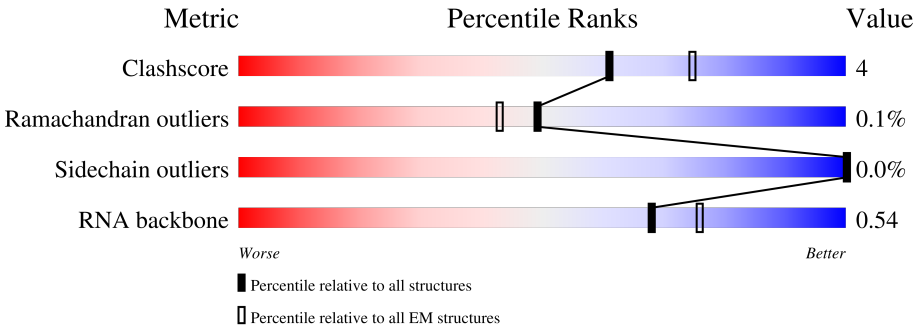
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

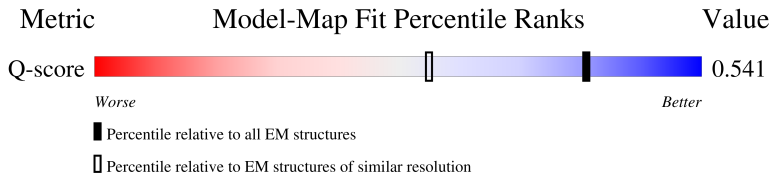
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	0	51	6% 84% 10% 6%
2	1	44	100%
3	2	64	• 88% 11% •

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Mol	Chain	Length	Quality of chain
4	3	38	24% 79% 21%
5	A	2918	9% 68% 20% 8%
6	B	115	32% 80% 11% 9%
7	C	274	90% 9%
8	D	212	93% 6%
9	E	200	6% 94% 6%
10	F	178	95% 55% 42%
11	G	177	72% 78% 20%
12	H	148	26% 36% 59%
13	I	142	89% 10%
14	J	122	97%
15	K	146	93% 5%
16	L	137	88% 11%
17	M	125	93% 5%
18	N	116	23% 81% 17%
19	O	122	7% 88% 7% 5%
20	P	119	93% 5%
21	Q	103	95% 5%
22	R	109	94% 6%
23	S	106	9% 74% 11% 15%
24	T	105	14% 84% 14%
25	U	98	7% 85% 14%
26	V	85	89% 9%
27	W	78	95%
28	X	65	22% 88% 5% 8%

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Mol	Chain	Length	Quality of chain
29	Y	58	95% 5%
30	Z	61	72% 16% 11%
31	a	1544	11% 69% 24% 6%
32	b	250	68% 66% 24% 10%
33	c	250	70% 16% 14%
34	d	208	29% 73% 26%
35	e	165	81% 13% 6%
36	f	127	23% 61% 20% 18%
37	g	156	14% 68% 19% 13%
38	h	131	85% 15%
39	i	128	88% 10%
40	j	103	76% 21%
41	k	128	34% 80% 11% 9%
42	l	124	21% 85% 14%
43	m	118	85% 13%
44	n	101	73% 26%
45	o	89	88% 11%
46	p	101	71% 10% 19%
47	q	85	82% 9% 8%
48	r	75	5% 53% 16% 31%
49	s	91	79% 11% 10%
50	t	88	88% 10%
51	u	71	63% 66% 13% 20%
52	v	77	71% 44% 35% 19%
53	w	3	67% 33%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 137516 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	48	400	256	72	69	3	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	363	222	85	54	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	319	110	76	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	295	179	64	48	4	0	0

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2685	57610	25715	10555	18655	2685	0	0

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	115	2450	1095	440	800	115	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	271	2104	1297	435	364	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	210	1566	969	296	298	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	200	1516	952	281	278	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	174	1370	871	243	248	8	0	0

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	174	1318	832	236	249	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	60	458	287	84	86	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	141	1117	713	199	202	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	122	946	592	180	169	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	K	144	1071	663	213	195	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	137	1087	687	210	185	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	119	942	590	186	163	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	114	857	528	173	155	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	O	116	913	575	176	162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	117	934	589	197	146	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	103	807	506	155	143	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	109	826	514	158	150	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	S	90	702	447	127	128	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	T	103	766	476	142	148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	97	760	477	143	139	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	77	581	360	112	107	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	77	632	395	130	105	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	60	486	302	93	90	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	58	463	286	88	85	4	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	54	447	265	100	81	1	0	0

- Molecule 31 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	a	1528	32782	14631	5994	10630	1527	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	225	1769	1110	328	325	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	215	1690	1065	318	299	8	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	207	1631	1017	313	299	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	155	1129	700	217	207	5	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	104	867	546	158	159	4	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	136	1073	671	201	194	7	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	130	985	615	177	187	6	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	126	991	618	197	175	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	100	801	500	150	148	3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	117	862	535	167	159	1	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l	122	945	580	193	167	5	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	m	115	903	558	184	158	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	100	792	493	158	137	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	88	705	434	144	126	1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	82	644	403	128	112	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	78	614	386	115	112	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	r	52	426	273	74	79	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	82	646	412	125	107	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t	86	663	409	139	113	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	u	57	473	294	96	82	1	0	0

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
52	v	77	1636	733	291	535	76	1	0	0

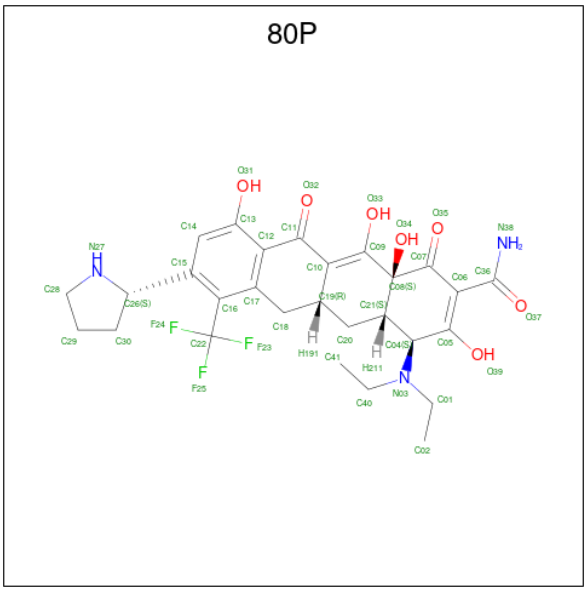
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	w	3	65	29	12	21	3	0	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	3	1	1	1	0

- Molecule 55 is (4S,4aS,5aR,12aS)-4-(diethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-8-[(2S)-pyrrolidin-2-yl]-7-(trifluoromethyl)-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide (CCD ID: 80P) (formula: $C_{28}H_{32}F_3N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

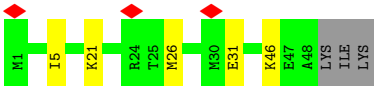
Mol	Chain	Residues	Atoms		AltConf
56	a	4	Total	Mg	0
			4	4	

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.

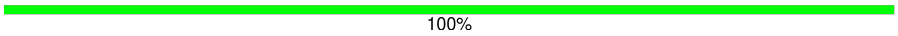
- Molecule 1: 50S ribosomal protein L33

Chain 0:



- Molecule 2: 50S ribosomal protein L34

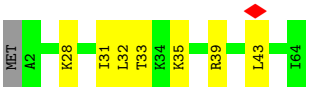
Chain 1:



There are no outlier residues recorded for this chain.

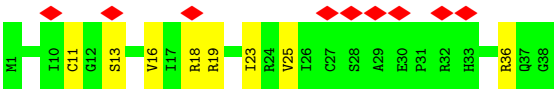
- Molecule 3: 50S ribosomal protein L35

Chain 2:



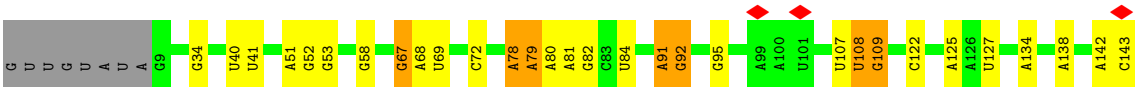
- Molecule 4: 50S ribosomal protein L36

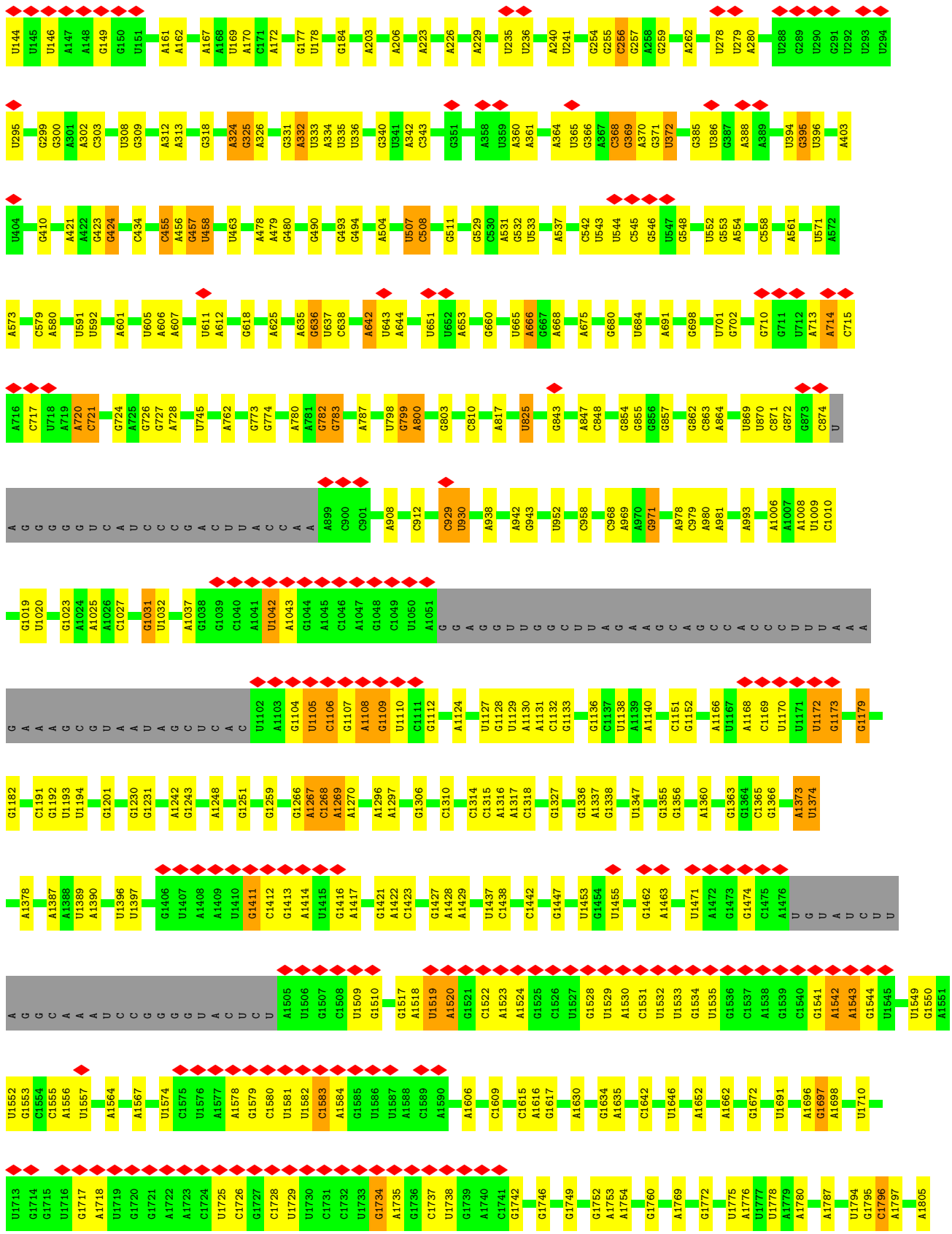
Chain 3:



- Molecule 5: 23S ribosomal RNA

Chain A:

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U295 G299 G300 A301 A302 C303 U308 G309 A312 A313 G318 A324 G325 A326 G331 A332 U333 A334 U335 U336 G340 U341 A342 C343 G351 A358 U359 A360 A361 A364 U365 G366 A367 C368 G369 A370 G371 U372 G385 U386 G387 A388 A389 U394 G395 U396 A403
U404 G410 A421 A422 G423 G424 C434 C455 A456 G457 U458 U463 A478 A479 G480 G490 G493 G494 A504 U507 C508 G511 G529 C530 A531 G532 U533 A537 C542 U543 U544 C545 G546 U547 G548 U552 G553 A554 C558 A561 U571 A572
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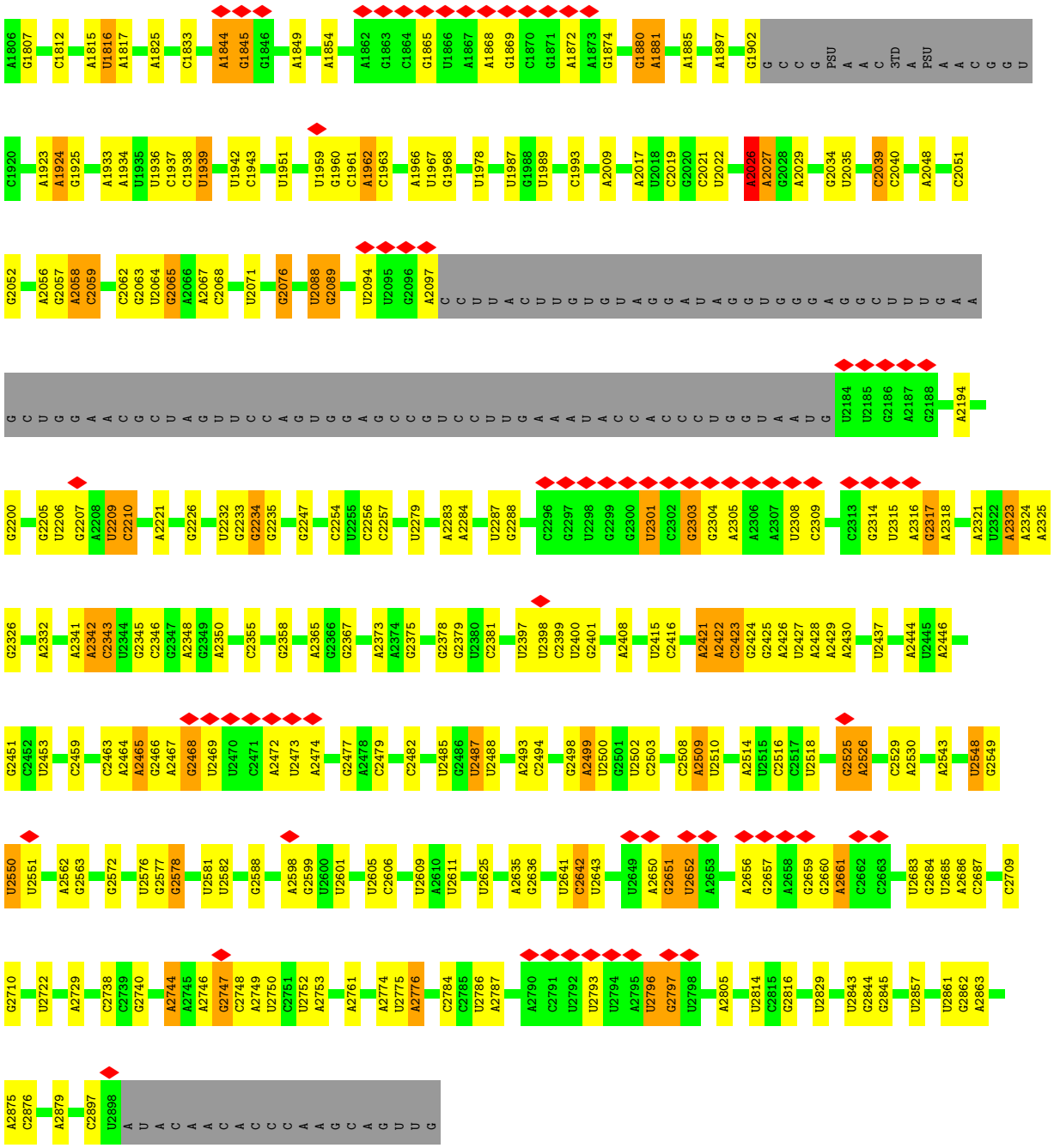
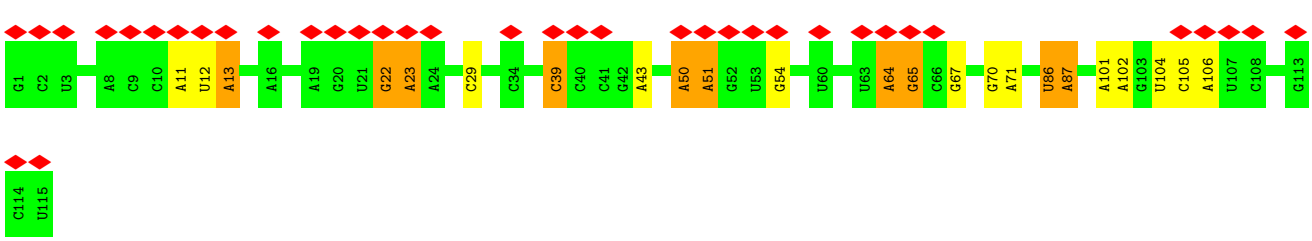


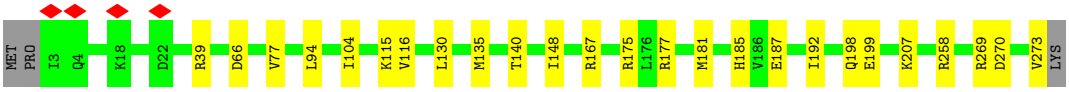
• Molecule 6: 5S ribosomal RNA

Chain B:



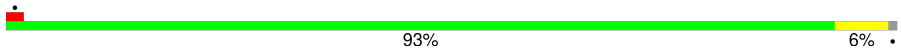
- Molecule 7: 50S ribosomal protein L2

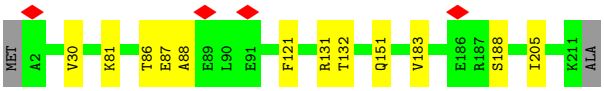
Chain C:



- Molecule 8: 50S ribosomal protein L3

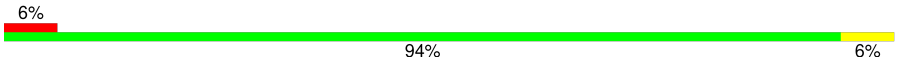
Chain D:

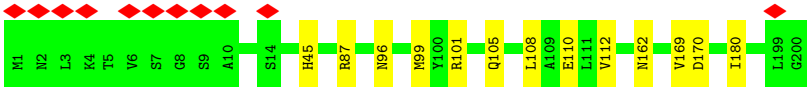




- Molecule 9: 50S ribosomal protein L4

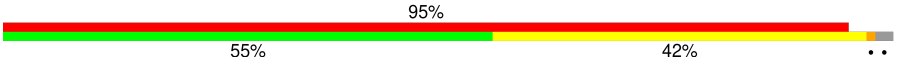
Chain E:

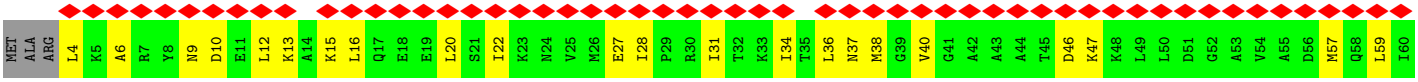


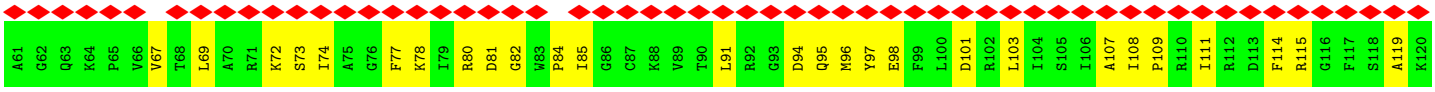


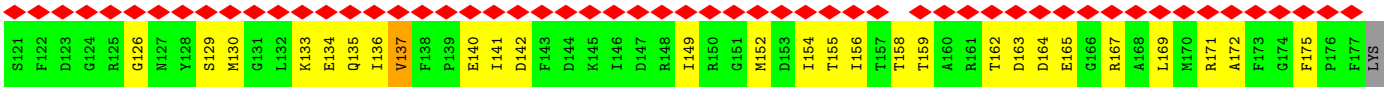
- Molecule 10: 50S ribosomal protein L5

Chain F:



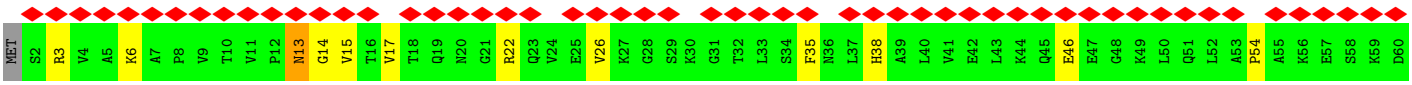


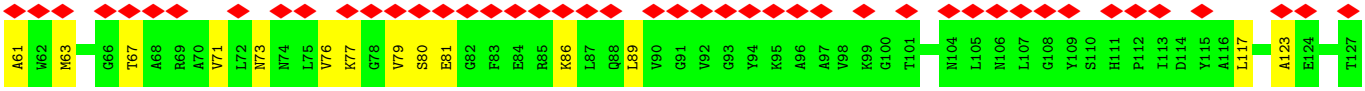


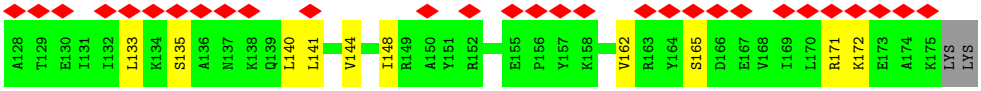


- Molecule 11: 50S ribosomal protein L6

Chain G:

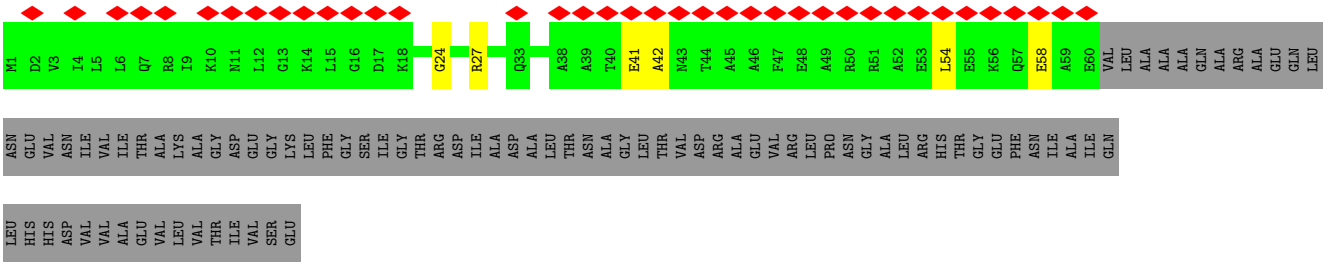






• Molecule 12: 50S ribosomal protein L9

Chain H:

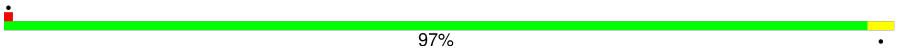


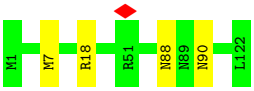
• Molecule 13: 50S ribosomal protein L13

Chain I:

• Molecule 14: 50S ribosomal protein L14

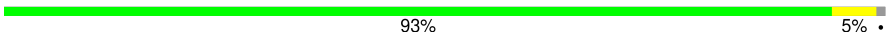
Chain J:





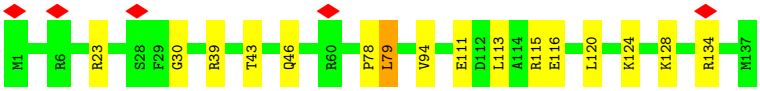
• Molecule 15: 50S ribosomal protein L15

Chain K:



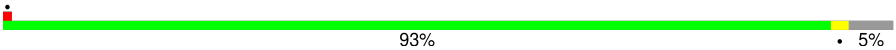
• Molecule 16: 50S ribosomal protein L16

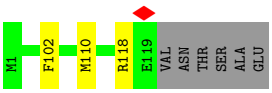
Chain L:



• Molecule 17: 50S ribosomal protein L17

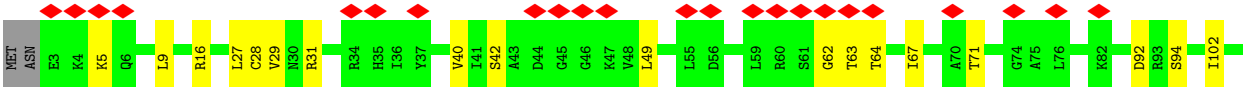
Chain M:

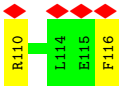




• Molecule 18: 50S ribosomal protein L18

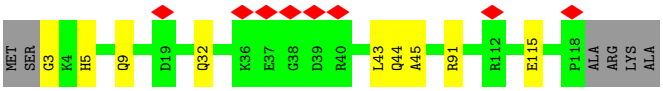
Chain N:





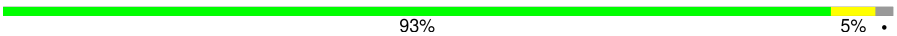
• Molecule 19: 50S ribosomal protein L19

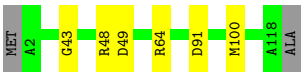
Chain O:



• Molecule 20: 50S ribosomal protein L20

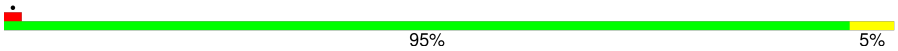
Chain P:

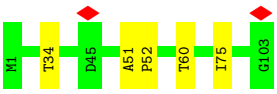




• Molecule 21: 50S ribosomal protein L21

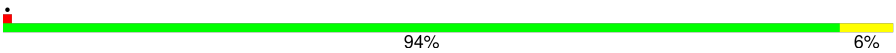
Chain Q:

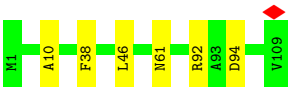




• Molecule 22: 50S ribosomal protein L22

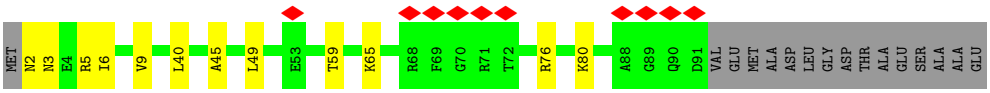
Chain R:





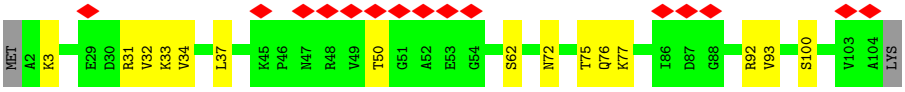
• Molecule 23: 50S ribosomal protein L23

Chain S:



• Molecule 24: 50S ribosomal protein L24

Chain T:

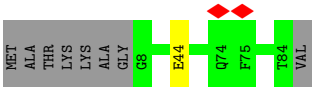


• Molecule 25: 50S ribosomal protein L25

Chain U:

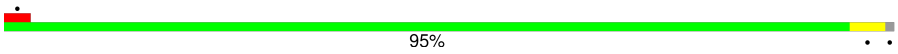
• Molecule 26: 50S ribosomal protein L27

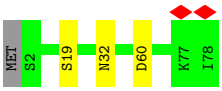
Chain V:



• Molecule 27: 50S ribosomal protein L28

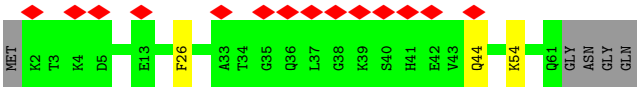
Chain W:





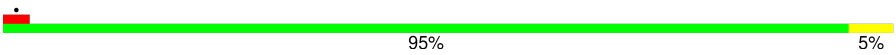
• Molecule 28: 50S ribosomal protein L29

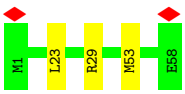
Chain X:



• Molecule 29: 50S ribosomal protein L30

Chain Y:



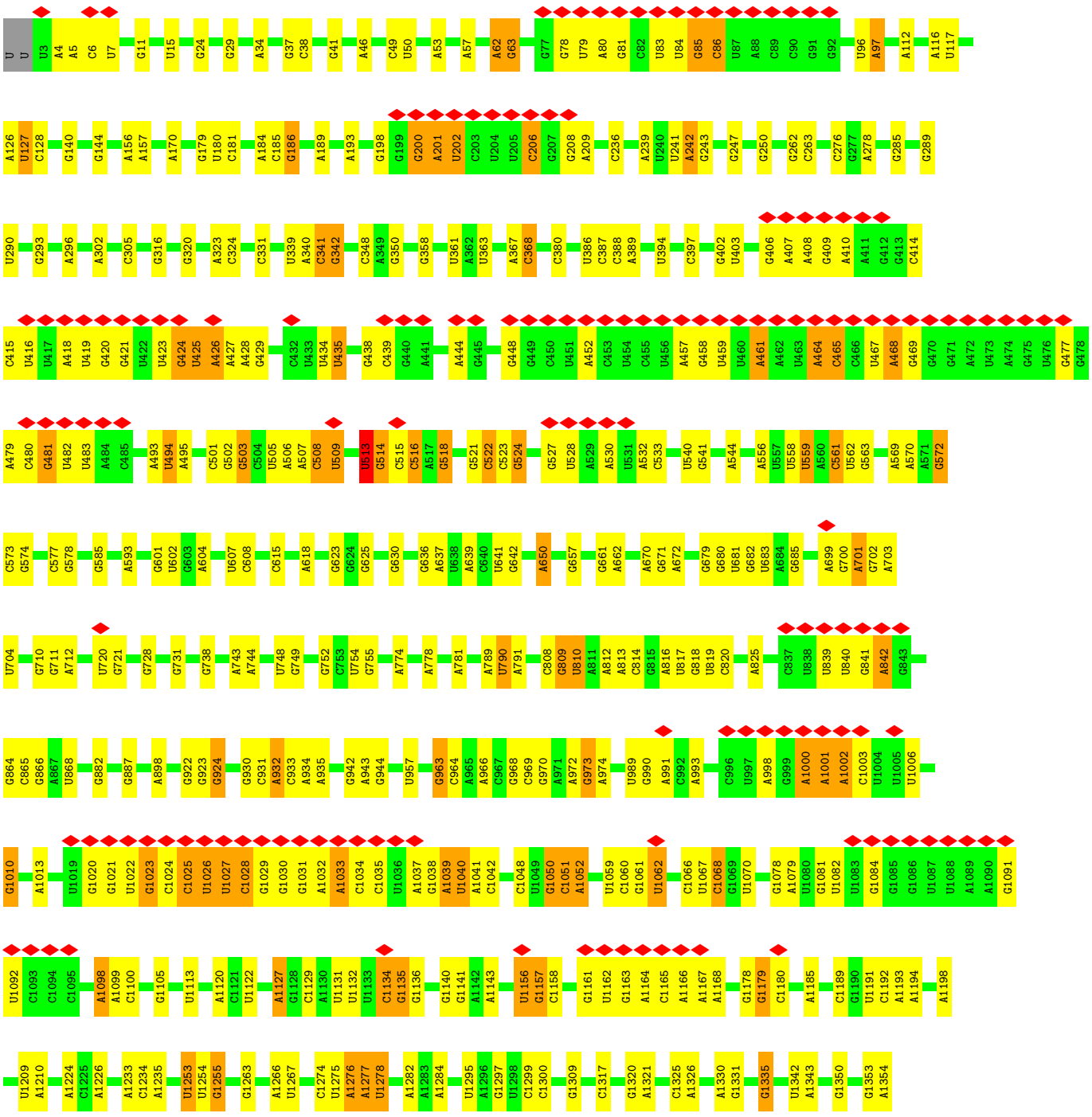


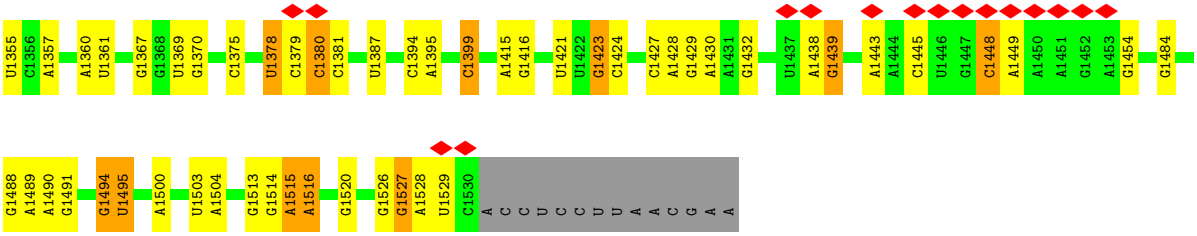
• Molecule 30: 50S ribosomal protein L32

Chain Z:

• Molecule 31: 16S Ribosomal RNA

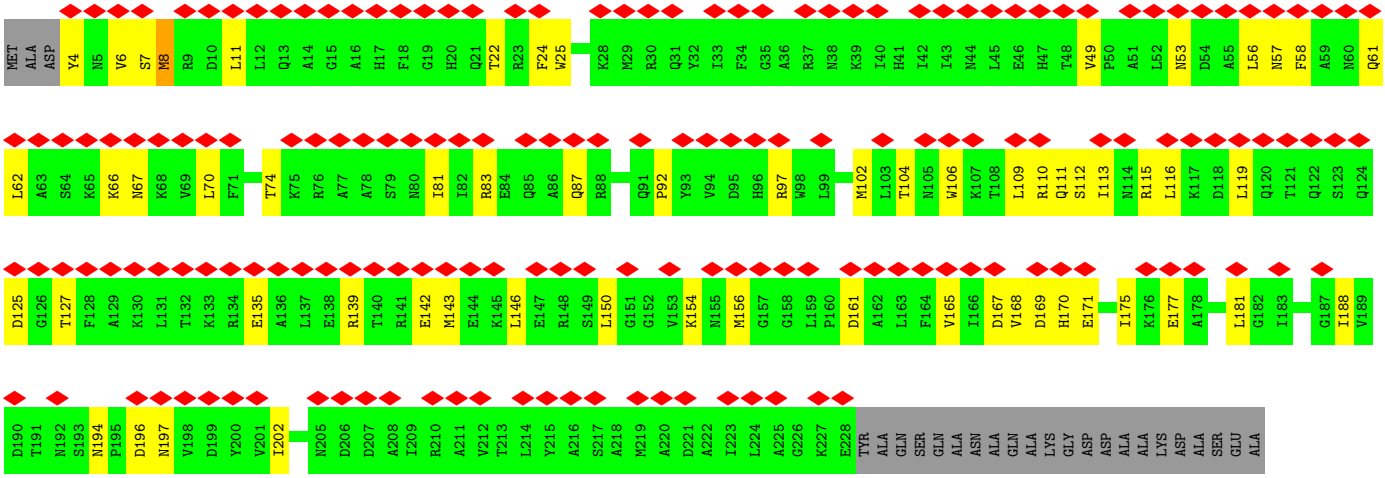
Chain a:





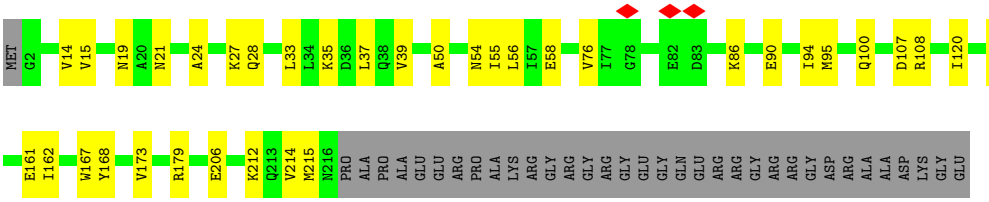
- Molecule 32: 30S ribosomal protein S2

Chain b:



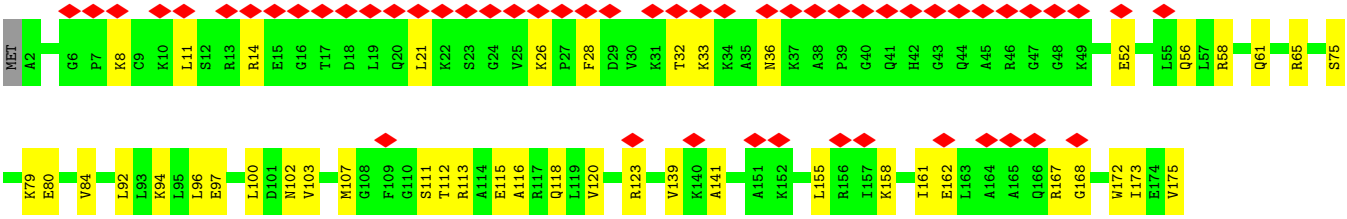
- Molecule 33: 30S ribosomal protein S3

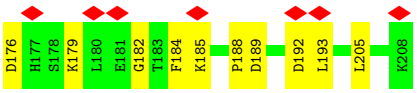
Chain c:



- Molecule 34: 30S ribosomal protein S4

Chain d:



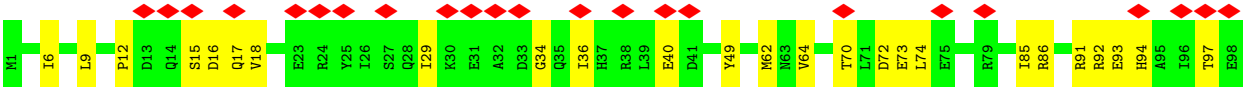


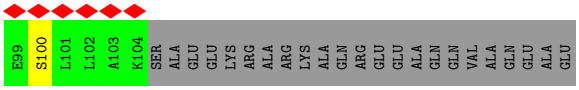
- Molecule 35: 30S ribosomal protein S5

Chain e:

- Molecule 36: 30S ribosomal protein S6

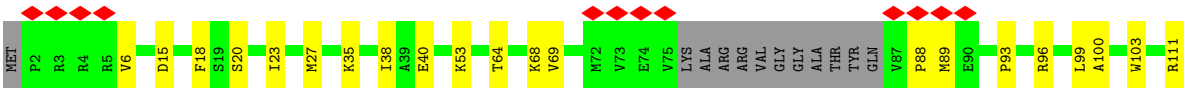
Chain f:

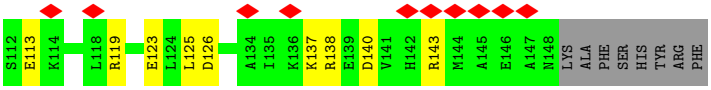




- Molecule 37: 30S ribosomal protein S7

Chain g:





- Molecule 38: 30S ribosomal protein S8

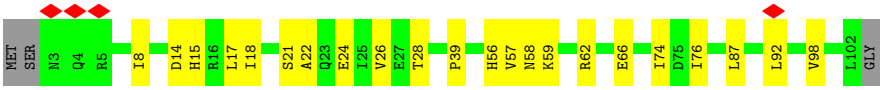
Chain h:

- Molecule 39: 30S ribosomal protein S9

Chain i:

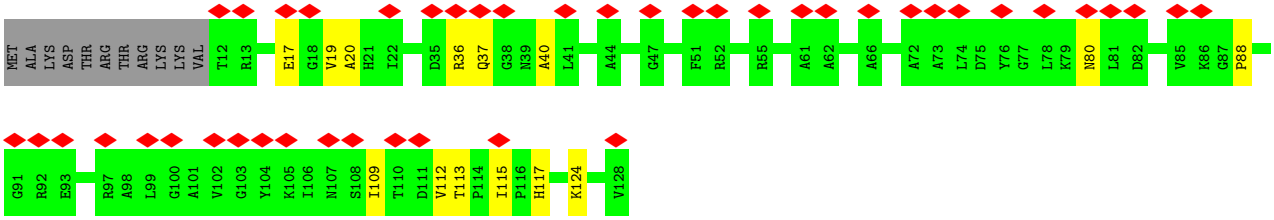
- Molecule 40: 30S ribosomal protein S10

Chain j:



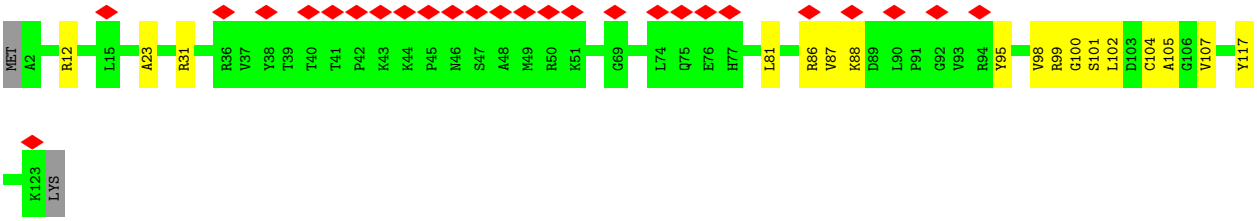
- Molecule 41: 30S ribosomal protein S11

Chain k:



- Molecule 42: 30S ribosomal protein S12

Chain l:

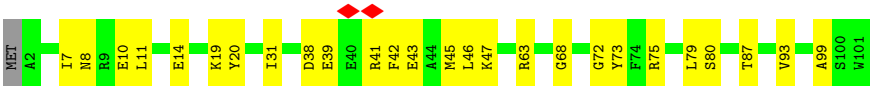


- Molecule 43: 30S ribosomal protein S13

Chain m:

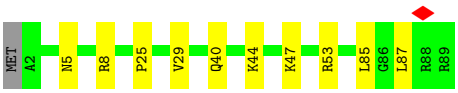
- Molecule 44: 30S ribosomal protein S14

Chain n:



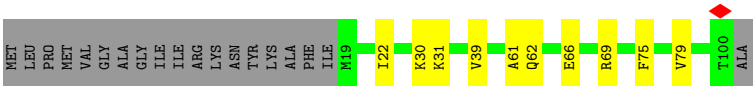
- Molecule 45: 30S ribosomal protein S15

Chain o:



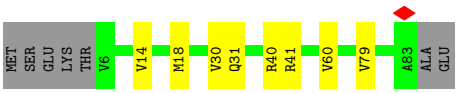
- Molecule 46: 30S ribosomal protein S16

Chain p:



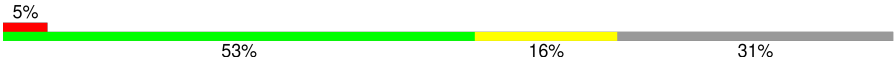
- Molecule 47: 30S ribosomal protein S17

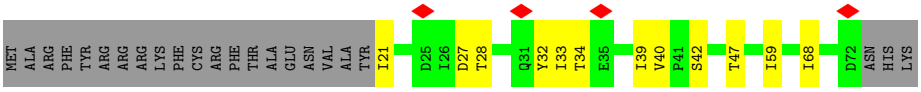
Chain q:



- Molecule 48: 30S ribosomal protein S18

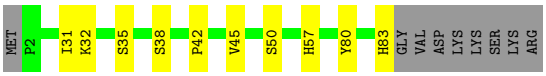
Chain r:





- Molecule 49: 30S ribosomal protein S19

Chain s:

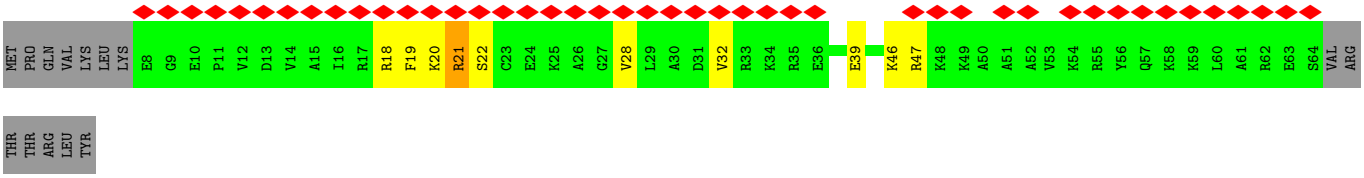


- Molecule 50: 30S ribosomal protein S20

Chain t:

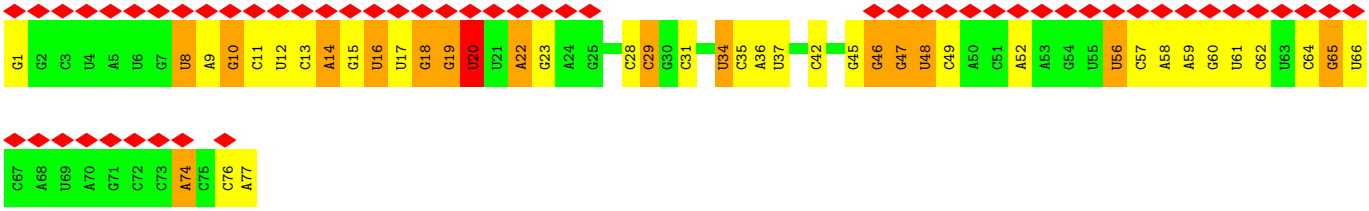
- Molecule 51: 30S ribosomal protein S21

Chain u:



- Molecule 52: tRNA-met

Chain v:



- Molecule 53: mRNA

Chain w:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47011	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.322	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.568, 557.568, 557.568	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.089, 1.089, 1.089	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: 2MA, MA6, 5MC, H2U, MG, 5MU, UR3, ZN, 4OC, PSU, OMU, 6MZ, 80P, 2MG, 4SU, OMG, 7MG

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	0	0.15	0/407	0.31	0/540
2	1	0.15	0/367	0.31	0/481
3	2	0.13	0/515	0.36	0/678
4	3	0.15	0/296	0.31	0/389
5	A	0.11	0/64227	0.28	0/100172
6	B	0.09	0/2739	0.25	0/4266
7	C	0.12	0/2144	0.32	0/2880
8	D	0.13	0/1584	0.32	0/2135
9	E	0.13	0/1537	0.30	0/2073
10	F	0.17	0/1390	0.47	0/1863
11	G	0.18	0/1337	0.40	0/1807
12	H	0.15	0/461	0.39	0/616
13	I	0.13	0/1143	0.34	0/1541
14	J	0.14	0/956	0.31	0/1286
15	K	0.11	0/1079	0.30	0/1439
16	L	0.14	0/1104	0.32	0/1475
17	M	0.14	0/956	0.31	0/1282
18	N	0.14	0/865	0.30	0/1156
19	O	0.15	0/925	0.36	0/1241
20	P	0.14	0/947	0.31	0/1262
21	Q	0.13	0/818	0.32	0/1094
22	R	0.13	0/831	0.29	0/1113
23	S	0.12	0/708	0.31	0/947
24	T	0.11	0/770	0.28	0/1034
25	U	0.12	0/770	0.35	0/1036
26	V	0.11	0/589	0.31	0/788
27	W	0.16	0/642	0.31	0/856
28	X	0.09	0/487	0.23	0/646
29	Y	0.17	0/468	0.33	0/624
30	Z	0.13	0/453	0.29	0/604
31	a	0.14	0/36476	0.28	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.15	0/1799	0.41	0/2429
33	c	0.18	0/1714	0.42	0/2304
34	d	0.16	0/1653	0.39	0/2213
35	e	0.15	0/1141	0.38	0/1537
36	f	0.15	0/882	0.37	0/1189
37	g	0.16	0/1087	0.39	0/1456
38	h	0.13	0/993	0.32	0/1331
39	i	0.17	0/1002	0.37	0/1339
40	j	0.16	0/811	0.35	0/1096
41	k	0.11	0/878	0.25	0/1189
42	l	0.13	0/958	0.31	0/1284
43	m	0.17	0/913	0.39	0/1226
44	n	0.20	0/803	0.42	0/1071
45	o	0.14	0/715	0.28	0/958
46	p	0.13	0/655	0.35	0/879
47	q	0.13	0/621	0.30	0/837
48	r	0.11	0/432	0.28	0/583
49	s	0.17	0/664	0.32	0/897
50	t	0.15	0/669	0.30	0/892
51	u	0.20	0/478	0.50	1/631 (0.2%)
52	v	0.15	0/1739	0.30	0/2709
53	w	0.09	0/72	0.33	0/110
All	All	0.13	0/148670	0.30	1/222379 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	u	21	ARG	CB-CG-CD	6.15	125.44	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	400	0	425	3	0
2	1	363	0	401	0	0
3	2	509	0	566	6	0
4	3	295	0	326	5	0
5	A	57610	0	28970	247	0
6	B	2450	0	1241	11	0
7	C	2104	0	2168	23	0
8	D	1566	0	1605	9	0
9	E	1516	0	1569	8	0
10	F	1370	0	1420	61	0
11	G	1318	0	1373	27	0
12	H	458	0	480	4	0
13	I	1117	0	1136	12	0
14	J	946	0	1007	3	0
15	K	1071	0	1141	7	0
16	L	1087	0	1162	12	0
17	M	942	0	987	3	0
18	N	857	0	899	20	0
19	O	913	0	968	5	0
20	P	934	0	997	5	0
21	Q	807	0	842	5	0
22	R	826	0	894	6	0
23	S	702	0	756	10	0
24	T	766	0	816	8	0
25	U	760	0	783	8	0
26	V	581	0	583	1	0
27	W	632	0	667	4	0
28	X	486	0	528	3	0
29	Y	463	0	488	4	0
30	Z	447	0	435	9	0
31	a	32782	0	16508	224	0
32	b	1769	0	1787	46	0
33	c	1690	0	1774	23	0
34	d	1631	0	1691	40	0
35	e	1129	0	1174	16	0
36	f	867	0	868	23	0
37	g	1073	0	1118	21	0
38	h	985	0	1047	12	0
39	i	991	0	1048	8	0
40	j	801	0	832	14	0
41	k	862	0	877	11	0
42	l	945	0	998	14	0
43	m	903	0	962	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	792	0	833	17	0
45	o	705	0	712	6	0
46	p	644	0	655	5	0
47	q	614	0	658	5	0
48	r	426	0	447	8	0
49	s	646	0	663	6	0
50	t	663	0	715	6	0
51	u	473	0	503	16	0
52	v	1636	0	835	18	0
53	w	65	0	33	1	0
54	3	1	0	0	0	0
55	a	123	0	0	0	0
56	a	4	0	0	0	0
All	All	137516	0	92371	981	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 4.

All (981) 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)
31:a:1025:C:O2'	31:a:1026:U:O5'	1.76	1.00
16:L:43:THR:OG1	16:L:46:GLN:NE2	1.98	0.97
10:F:136:ILE:O	10:F:137:VAL:HG22	1.68	0.93
10:F:108:ILE:HG23	10:F:109:PRO:HD3	1.50	0.93
31:a:572:G:O2'	31:a:818:G:OP2	1.87	0.92
7:C:135:MET:O	7:C:167:ARG:NH2	2.03	0.91
37:g:88:PRO:O	37:g:89:MET:HE2	1.69	0.91
4:3:19:ARG:NH1	5:A:2752:U:OP2	2.04	0.89
11:G:86:LYS:NZ	11:G:165:SER:OG	2.05	0.89
11:G:80:SER:OG	11:G:81:GLU:OE1	1.90	0.89
35:e:106:ALA:O	35:e:111:ARG:NH1	2.06	0.88
5:A:1880:G:O2'	5:A:1881:A:OP1	1.91	0.87
5:A:2373:A:O2'	18:N:116:PHE:OXT	1.92	0.87
5:A:799:G:O2'	5:A:800:A:OP1	1.93	0.87
31:a:1134:C:O2'	31:a:1135:G:N2	2.08	0.87
7:C:269:ARG:NH1	7:C:270:ASP:O	2.08	0.87
52:v:16:U:O2'	52:v:61:U:O2	1.92	0.86
19:O:91:ARG:NE	19:O:115:GLU:OE2	2.07	0.86
10:F:129:SER:C	10:F:130:MET:HE2	2.00	0.86
31:a:1454:G:OP1	50:t:34:ARG:NH1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:34:U:O2'	52:v:36:A:OP2	1.92	0.85
31:a:1098:A:OP2	32:b:97:ARG:NH2	2.10	0.85
5:A:67:G:O2'	5:A:69:U:OP2	1.95	0.84
5:A:1517:G:OP2	5:A:1518:A:O2'	1.97	0.83
34:d:94:LYS:NZ	34:d:188:PRO:O	2.12	0.83
6:B:11:A:O2'	6:B:13:A:OP2	1.97	0.83
31:a:1226:A:O2'	52:v:31:C:OP1	1.96	0.83
5:A:533:U:O2'	20:P:49:ASP:OD1	1.95	0.83
37:g:140:ASP:OD1	37:g:143:ARG:NH2	2.13	0.82
51:u:18:ARG:O	51:u:21:ARG:N	2.12	0.82
5:A:2301:U:O2'	10:F:133:LYS:NZ	2.12	0.82
31:a:514:G:O2'	31:a:516:C:N4	2.14	0.81
52:v:10:G:O6	52:v:46:G:N2	2.13	0.81
31:a:85:G:O2'	31:a:86:C:OP2	1.97	0.81
8:D:30:VAL:O	8:D:188:SER:OG	1.98	0.80
10:F:94:ASP:OD2	10:F:95:GLN:N	2.14	0.80
5:A:2326:G:O2'	26:V:44:GLU:OE2	2.00	0.80
31:a:1025:C:O2'	31:a:1026:U:O4'	1.97	0.80
39:i:104:ARG:NH1	39:i:105:ASP:O	2.14	0.80
32:b:150:LEU:O	32:b:154:LYS:NZ	2.15	0.80
5:A:2467:A:O2'	5:A:2468:G:O5'	2.00	0.79
31:a:1527:G:N7	51:u:46:LYS:NZ	2.31	0.79
34:d:11:LEU:HD21	34:d:65:ARG:HG2	1.64	0.79
37:g:68:LYS:O	37:g:138:ARG:NH1	2.15	0.79
5:A:79:A:OP2	28:X:54:LYS:NZ	2.17	0.78
32:b:74:THR:OG1	32:b:171:GLU:OE2	1.99	0.78
5:A:364:A:OP2	5:A:424:G:O2'	2.02	0.78
31:a:1157:G:O6	31:a:1179:G:O6	2.02	0.78
5:A:184:G:N2	5:A:184:G:OP2	2.17	0.77
31:a:1060:C:OP2	31:a:1061:G:O2'	2.01	0.77
36:f:93:GLU:O	36:f:94:HIS:ND1	2.18	0.77
10:F:12:LEU:HD13	10:F:15:LYS:HE3	1.67	0.77
31:a:1277:A:O2'	31:a:1278:U:OP1	2.00	0.77
5:A:1306:G:OP2	5:A:1306:G:N2	2.13	0.77
34:d:111:SER:OG	34:d:115:GLU:OE1	2.04	0.76
31:a:523:C:OP2	42:l:88:LYS:NZ	2.19	0.76
36:f:72:ASP:OD1	36:f:73:GLU:N	2.19	0.75
6:B:22:G:O6	6:B:54:G:O2'	2.01	0.75
31:a:514:G:HO2'	31:a:516:C:N4	1.84	0.75
10:F:31:ILE:HG21	10:F:96:MET:HE3	1.68	0.75
31:a:1254:U:OP1	33:c:27:LYS:NZ	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2753:A:N1	11:G:67:THR:HG21	2.01	0.74
52:v:1:G:N3	52:v:74:A:N6	2.35	0.74
5:A:713:A:O2'	45:o:40:GLN:OE1	2.04	0.74
5:A:1844:A:O2'	5:A:1845:G:N7	2.17	0.74
31:a:144:G:O6	31:a:170:A:N1	2.21	0.74
36:f:40:GLU:OE1	36:f:100:SER:OG	2.05	0.73
31:a:540:U:OP1	34:d:14:ARG:NE	2.21	0.73
5:A:720:A:O2'	5:A:721:C:OP1	2.07	0.73
32:b:125:ASP:OD2	32:b:127:THR:HG23	1.88	0.73
37:g:111:ARG:NH1	37:g:123:GLU:OE2	2.22	0.72
5:A:78:A:OP1	5:A:79:A:O2'	2.07	0.72
5:A:1519:U:O2'	5:A:1520:A:OP2	2.04	0.72
31:a:189:A:O2'	50:t:59:ASP:OD2	2.06	0.72
5:A:863:C:OP2	16:L:23:ARG:NH1	2.22	0.72
5:A:1962:A:N3	5:A:2588:G:O2'	2.20	0.72
5:A:929:C:O2'	5:A:930:U:O5'	2.07	0.71
25:U:6:LEU:HB2	25:U:67:ILE:HG22	1.70	0.71
52:v:22:A:N6	52:v:48:U:O2	2.20	0.71
35:e:114:LEU:HD13	35:e:122:VAL:HG11	1.72	0.71
5:A:1937:C:N4	5:A:1961:C:O4'	2.24	0.71
6:B:11:A:N1	6:B:67:G:O2'	2.23	0.70
5:A:2465:A:N6	5:A:2477:G:O2'	2.24	0.70
10:F:129:SER:O	10:F:130:MET:HE2	1.90	0.70
52:v:64:C:N4	52:v:65:G:O6	2.24	0.70
5:A:254:G:OP2	5:A:256:C:N4	2.25	0.70
31:a:409:G:N7	34:d:33:LYS:NZ	2.39	0.70
5:A:1816:U:OP1	7:C:177:ARG:NH1	2.24	0.70
5:A:2879:A:OP2	30:Z:49:ARG:NH1	2.25	0.70
37:g:113:GLU:O	37:g:119:ARG:NH1	2.25	0.70
38:h:43:GLU:OE2	38:h:115:ARG:NH2	2.25	0.69
48:r:27:ASP:OD1	48:r:28:THR:N	2.25	0.69
32:b:169:ASP:OD1	32:b:170:HIS:N	2.25	0.69
35:e:59:ILE:O	35:e:63:LEU:HD23	1.93	0.69
43:m:73:ILE:O	43:m:77:ILE:HD12	1.93	0.69
32:b:102:MET:HA	32:b:109:LEU:HD21	1.75	0.69
1:0:31:GLU:OE2	1:0:46:LYS:NZ	2.26	0.69
5:A:1749:G:N2	5:A:1752:G:OP2	2.24	0.68
11:G:89:LEU:HG	11:G:162:VAL:HG22	1.74	0.68
34:d:8:LYS:HG2	34:d:21:LEU:HD23	1.74	0.68
9:E:45:HIS:O	9:E:87:ARG:NH2	2.25	0.68
23:S:5:ARG:O	23:S:9:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:179:ARG:NH1	33:c:206:GLU:OE1	2.27	0.68
3:2:33:THR:OG1	5:A:2416:C:OP1	2.05	0.68
5:A:226:A:N3	5:A:241:U:O2'	2.22	0.68
31:a:423:U:OP2	31:a:424:G:O2'	2.10	0.68
5:A:72:C:O2'	5:A:455:C:N3	2.26	0.68
19:O:44:GLN:NE2	19:O:45:ALA:O	2.27	0.68
38:h:114:ASP:OD2	38:h:118:ARG:NH2	2.26	0.68
31:a:406:G:N2	31:a:427:A:N7	2.42	0.67
7:C:77:VAL:HG22	7:C:115:LYS:NZ	2.09	0.67
1:0:21:LYS:NZ	1:0:26:MET:O	2.26	0.67
32:b:49:VAL:O	32:b:53:ASN:ND2	2.28	0.67
31:a:561:C:OP2	42:l:12:ARG:NH2	2.28	0.66
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.77	0.66
51:u:18:ARG:O	51:u:21:ARG:HD3	1.95	0.66
5:A:1833:C:HO2'	5:A:1923:A:HO2'	1.43	0.66
31:a:200:G:O6	31:a:209:A:N6	2.18	0.66
29:Y:23:LEU:HD11	29:Y:53:MET:CE	2.26	0.66
7:C:185:HIS:NE2	7:C:187:GLU:OE1	2.20	0.65
5:A:1172:U:O2'	5:A:1173:G:OP1	2.08	0.65
13:I:23:LYS:NZ	13:I:142:ILE:O	2.27	0.65
5:A:2526:A:O2'	5:A:2530:A:N6	2.29	0.65
31:a:809:G:O2'	31:a:810:U:OP2	2.15	0.65
31:a:558:U:O2'	31:a:559:U:OP2	2.10	0.64
33:c:86:LYS:O	33:c:90:GLU:OE1	2.15	0.64
37:g:111:ARG:NH2	37:g:126:ASP:OD2	2.30	0.64
49:s:80:TYR:OH	49:s:83:HIS:ND1	2.30	0.64
5:A:2518:U:O2'	5:A:2643:U:OP1	2.15	0.64
34:d:167:ARG:HE	34:d:168:GLY:H	1.45	0.64
5:A:2577:G:OP2	5:A:2577:G:N2	2.26	0.63
31:a:1224:A:N7	43:m:116:ILE:HD12	2.13	0.63
11:G:117:LEU:HD11	11:G:123:ALA:HB3	1.80	0.63
31:a:1098:A:N6	32:b:177:GLU:OE2	2.30	0.63
36:f:36:ILE:HG23	36:f:62:MET:HE1	1.80	0.63
36:f:91:ARG:NH1	36:f:92:ARG:O	2.30	0.63
37:g:99:LEU:HB3	37:g:103:TRP:CH2	2.34	0.63
5:A:2861:U:OP2	5:A:2862:G:O2'	2.07	0.62
6:B:12:U:O3'	6:B:104:U:O2'	2.17	0.62
5:A:1373:A:O2'	5:A:1374:U:OP2	2.14	0.62
5:A:1310:C:O2'	5:A:1387:A:N3	2.30	0.62
24:T:75:THR:OG1	24:T:77:LYS:NZ	2.24	0.62
36:f:29:ILE:HD11	36:f:74:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2401:G:O2'	5:A:2408:A:N6	2.32	0.62
10:F:81:ASP:OD1	10:F:82:GLY:N	2.32	0.62
5:A:2009:A:O2'	22:R:94:ASP:OD2	2.16	0.62
23:S:3:ASN:HA	23:S:6:ILE:HG22	1.82	0.62
6:B:50:A:O2'	6:B:51:A:O5'	2.18	0.61
33:c:161:GLU:HG2	33:c:162:ILE:HD12	1.82	0.61
10:F:46:ASP:OD1	10:F:47:LYS:N	2.33	0.61
31:a:358:G:N2	31:a:361:U:OP2	2.33	0.61
34:d:107:MET:SD	34:d:173:ILE:HG21	2.41	0.61
49:s:80:TYR:HH	49:s:83:HIS:HD1	1.49	0.61
31:a:682:G:O2'	31:a:683:U:O5'	2.19	0.61
3:2:31:ILE:O	3:2:35:LYS:NZ	2.31	0.61
45:o:47:LYS:O	45:o:53:ARG:NH2	2.34	0.61
48:r:34:THR:HG23	48:r:40:VAL:HG22	1.81	0.61
4:3:36:ARG:NH1	5:A:2738:C:OP1	2.34	0.60
31:a:508:C:O2'	31:a:509:U:OP2	2.19	0.60
15:K:98:LYS:NZ	15:K:104:ARG:O	2.35	0.60
18:N:29:VAL:HG21	18:N:102:ILE:HG23	1.84	0.60
31:a:1025:C:HO2'	31:a:1026:U:C4'	2.14	0.60
7:C:77:VAL:HG22	7:C:115:LYS:HZ3	1.65	0.60
10:F:108:ILE:HG23	10:F:109:PRO:CD	2.29	0.60
29:Y:23:LEU:HD11	29:Y:53:MET:HE1	1.82	0.60
36:f:29:ILE:HG22	36:f:34:GLY:HA2	1.84	0.59
5:A:720:A:HO2'	5:A:721:C:P	2.24	0.59
5:A:2508:C:OP2	8:D:131:ARG:NH2	2.36	0.59
11:G:73:ASN:OD1	11:G:77:LYS:NZ	2.35	0.59
30:Z:52:GLN:NE2	30:Z:54:PHE:O	2.27	0.59
5:A:2342:A:H4'	5:A:2343:C:OP2	2.02	0.59
40:j:21:SER:HB3	40:j:92:LEU:HD13	1.85	0.58
52:v:35:C:H42	53:w:3:G:H1	1.51	0.58
5:A:660:G:O2'	15:K:16:ARG:NH1	2.36	0.58
31:a:839:U:O2	31:a:840:U:N3	2.36	0.58
44:n:7:ILE:O	44:n:11:LEU:HD23	2.03	0.58
5:A:537:A:N6	5:A:553:G:O2'	2.36	0.58
5:A:1717:G:O2'	5:A:1735:A:N6	2.37	0.58
31:a:661:G:H22	31:a:738:G:H1	1.51	0.58
23:S:59:THR:HG21	23:S:80:LYS:HE2	1.86	0.58
23:S:49:LEU:HD13	28:X:26:PHE:CZ	2.38	0.58
31:a:1163:G:N2	31:a:1167:A:OP2	2.34	0.58
5:A:1107:G:O2'	5:A:1108:A:N3	2.30	0.57
5:A:1259:G:OP1	30:Z:16:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.17	0.57
5:A:2485:U:O2'	5:A:2487:U:O4	2.17	0.57
10:F:96:MET:SD	10:F:97:TYR:N	2.77	0.57
31:a:434:U:H4'	31:a:435:U:OP2	2.04	0.57
32:b:67:ASN:ND2	32:b:161:ASP:OD1	2.37	0.57
32:b:127:THR:OG1	32:b:139:ARG:NH2	2.37	0.57
5:A:2611:U:H1'	30:Z:4:GLN:HG2	1.87	0.57
10:F:31:ILE:HG21	10:F:96:MET:CE	2.33	0.57
10:F:34:ILE:HG22	10:F:96:MET:HB3	1.87	0.57
31:a:459:U:O2	31:a:464:A:N6	2.38	0.57
31:a:991:A:N3	44:n:8:ASN:ND2	2.52	0.57
31:a:293:G:N2	31:a:296:A:OP2	2.38	0.57
34:d:116:ALA:O	34:d:120:VAL:HG23	2.05	0.57
47:q:60:VAL:HG12	47:q:79:VAL:HG22	1.87	0.57
51:u:18:ARG:O	51:u:21:ARG:CD	2.52	0.57
31:a:1020:G:O2'	31:a:1021:G:O4'	2.20	0.57
18:N:16:ARG:NH1	18:N:92:ASP:OD1	2.37	0.57
31:a:1438:A:O2'	31:a:1439:G:C8	2.58	0.56
31:a:1520:G:OP1	41:k:124:LYS:NZ	2.38	0.56
5:A:714:A:N3	45:o:44:LYS:NZ	2.48	0.56
31:a:341:C:HO2'	31:a:342:G:N2	2.04	0.56
5:A:2843:U:H2'	5:A:2844:G:O4'	2.06	0.56
10:F:171:ARG:NH2	10:F:175:PHE:O	2.37	0.56
31:a:316:G:HO2'	31:a:1432:G:HO2'	1.53	0.56
31:a:933:C:O2'	31:a:1380:C:N4	2.37	0.56
5:A:1106:C:O2'	5:A:1107:G:O4'	2.23	0.56
13:I:140:LEU:CD2	13:I:142:ILE:HG23	2.35	0.56
18:N:110:ARG:NH1	18:N:116:PHE:O	2.38	0.56
31:a:1120:A:O2'	40:j:39:PRO:O	2.21	0.56
3:2:39:ARG:NH2	5:A:2358:G:OP1	2.39	0.56
10:F:31:ILE:CG2	10:F:96:MET:HE3	2.35	0.56
11:G:86:LYS:HD2	11:G:86:LYS:O	2.06	0.56
34:d:112:THR:N	34:d:115:GLU:OE1	2.36	0.56
21:Q:34:THR:HG22	21:Q:60:THR:HG22	1.88	0.56
10:F:162:THR:HG23	10:F:164:ASP:OD1	2.06	0.56
15:K:81:LEU:HD22	15:K:114:LEU:HD12	1.88	0.56
10:F:13:LYS:HE2	10:F:28:ILE:HD12	1.88	0.56
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.87	0.56
31:a:1357:A:OP2	44:n:75:ARG:NH2	2.39	0.56
33:c:173:VAL:HG23	33:c:173:VAL:O	2.05	0.56
39:i:82:THR:HG23	39:i:96:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:396:U:O3'	27:W:32:ASN:ND2	2.39	0.55
44:n:38:ASP:OD1	44:n:39:GLU:N	2.38	0.55
13:I:60:GLU:OE2	13:I:61:GLN:NE2	2.36	0.55
31:a:683:U:O4	31:a:700:G:O2'	2.24	0.55
13:I:73:LYS:NZ	13:I:86:GLU:OE2	2.38	0.55
16:L:30:GLY:O	16:L:134:ARG:NH2	2.40	0.55
30:Z:3:VAL:HG22	30:Z:4:GLN:H	1.71	0.55
32:b:196:ASP:OD1	32:b:197:ASN:N	2.40	0.55
42:l:99:ARG:NH2	42:l:105:ALA:O	2.40	0.55
52:v:19:G:H2'	52:v:20:H2U:H52	1.89	0.55
5:A:1718:A:N6	5:A:1734:G:O2'	2.38	0.55
32:b:70:LEU:HD12	32:b:156:MET:HE1	1.89	0.55
5:A:1037:A:H2	5:A:1112:G:H22	1.54	0.55
32:b:109:LEU:HD11	32:b:110:ARG:CZ	2.37	0.55
37:g:15:ASP:OD1	37:g:18:PHE:N	2.34	0.55
4:3:11:CYS:SG	4:3:13:SER:OG	2.64	0.54
10:F:159:THR:O	10:F:159:THR:HG22	2.08	0.54
31:a:1489:A:H2'	31:a:1490:A:O4'	2.07	0.54
16:L:111:GLU:O	16:L:115:ARG:HG3	2.08	0.54
18:N:16:ARG:NH1	18:N:92:ASP:CG	2.65	0.54
36:f:16:ASP:OD1	36:f:17:GLN:NE2	2.41	0.54
45:o:5:ASN:OD1	45:o:8:ARG:NH2	2.40	0.54
10:F:22:ILE:HD12	10:F:27:GLU:HB2	1.89	0.54
8:D:183:VAL:HG23	8:D:183:VAL:O	2.08	0.54
10:F:36:LEU:HD12	10:F:152:MET:SD	2.47	0.54
31:a:820:C:HO2'	38:h:2:SER:N	2.05	0.54
5:A:1042:U:O4'	5:A:1108:A:N6	2.40	0.54
39:i:114:LEU:HD21	40:j:62:ARG:HB2	1.89	0.54
5:A:552:U:H2'	5:A:553:G:O4'	2.08	0.54
35:e:156:ARG:NH2	38:h:100:LEU:O	2.41	0.54
31:a:341:C:O2'	31:a:342:G:N2	2.41	0.54
38:h:91:ASP:OD1	38:h:92:LYS:NZ	2.40	0.54
34:d:100:LEU:O	34:d:103:VAL:HG12	2.08	0.54
40:j:92:LEU:HD12	40:j:98:VAL:HG21	1.90	0.54
13:I:70:LEU:O	13:I:70:LEU:HD23	2.08	0.53
44:n:63:ARG:NH1	44:n:68:GLY:O	2.42	0.53
51:u:39:GLU:OE1	51:u:47:ARG:NH2	2.41	0.53
31:a:1066:C:H2'	31:a:1067:U:O4'	2.08	0.53
5:A:2467:A:C2'	5:A:2468:G:O5'	2.57	0.53
39:i:11:LYS:O	39:i:12:THR:OG1	2.20	0.53
5:A:2089:G:OP1	12:H:24:GLY:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2226:G:H1'	27:W:32:ASN:OD1	2.08	0.53
31:a:320:G:N1	31:a:323:A:OP2	2.41	0.53
7:C:198:GLN:NE2	7:C:199:GLU:OE1	2.40	0.53
31:a:670:A:H2'	31:a:671:G:C8	2.42	0.53
37:g:40:GLU:OE2	39:i:41:THR:HG21	2.09	0.53
5:A:2071:U:OP2	5:A:2234:G:O2'	2.26	0.53
42:l:81:LEU:O	42:l:98:VAL:HG22	2.09	0.53
1:0:5:ILE:HG21	1:0:21:LYS:HD2	1.90	0.53
5:A:798:U:H4'	5:A:799:G:OP1	2.08	0.53
31:a:1335:G:N3	52:v:42:C:O2'	2.41	0.53
32:b:135:GLU:N	32:b:135:GLU:OE1	2.41	0.53
5:A:1411:G:N2	5:A:1583:C:H42	2.06	0.53
5:A:2467:A:HO2'	5:A:2468:G:C5'	2.21	0.53
11:G:80:SER:HG	11:G:81:GLU:CD	2.12	0.53
16:L:78:PRO:O	16:L:79:LEU:CB	2.55	0.53
31:a:969:C:OP2	40:j:59:LYS:NZ	2.42	0.53
36:f:6:ILE:HB	36:f:62:MET:HB3	1.91	0.53
31:a:754:U:H2'	31:a:755:G:O4'	2.09	0.52
38:h:48:ASN:OD1	38:h:49:VAL:N	2.41	0.52
5:A:68:A:OP1	28:X:44:GLN:NE2	2.42	0.52
10:F:74:ILE:HD12	10:F:77:PHE:HD2	1.74	0.52
34:d:32:THR:HG23	34:d:33:LYS:N	2.24	0.52
41:k:109:ILE:HG21	51:u:19:PHE:HB2	1.91	0.52
34:d:92:LEU:O	34:d:96:LEU:HD12	2.10	0.52
41:k:112:VAL:HG12	41:k:112:VAL:O	2.10	0.52
5:A:1179:G:OP1	29:Y:29:ARG:NH2	2.43	0.52
35:e:60:SER:O	35:e:64:GLU:OE2	2.28	0.52
5:A:2784:C:O2'	5:A:2805:A:N3	2.42	0.52
10:F:34:ILE:HG22	10:F:96:MET:CB	2.39	0.52
32:b:22:THR:O	32:b:24:PHE:N	2.43	0.52
5:A:710:G:H22	5:A:717:C:H42	1.57	0.52
5:A:929:C:HO2'	5:A:930:U:P	2.33	0.52
46:p:61:ALA:O	46:p:62:GLN:NE2	2.43	0.52
5:A:2254:C:O2'	5:A:2423:C:OP2	2.27	0.52
12:H:27:ARG:NH1	27:W:60:ASP:OD2	2.43	0.52
16:L:43:THR:HG22	16:L:94:VAL:HG12	1.92	0.52
32:b:7:SER:O	32:b:8:MET:HB3	2.10	0.52
34:d:172:TRP:CD1	34:d:173:ILE:HD12	2.45	0.52
5:A:2796:U:O2'	5:A:2797:G:OP1	2.22	0.52
10:F:119:ALA:O	10:F:167:ARG:NH2	2.43	0.52
31:a:1025:C:C2'	31:a:1026:U:O4'	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:81:LYS:HD3	8:D:205:ILE:HD11	1.92	0.52
17:M:118:ARG:NH2	30:Z:53:LEU:O	2.42	0.52
34:d:158:LYS:O	34:d:162:GLU:HG3	2.10	0.52
5:A:1442:C:O2'	5:A:1542:A:N3	2.41	0.51
5:A:2315:U:O2'	5:A:2317:G:N7	2.44	0.51
33:c:107:ASP:OD1	33:c:108:ARG:N	2.43	0.51
37:g:27:MET:HE1	37:g:40:GLU:HG2	1.92	0.51
44:n:42:PHE:O	44:n:46:LEU:HD23	2.10	0.51
40:j:22:ALA:O	40:j:26:VAL:HG23	2.11	0.51
7:C:94:LEU:HD11	7:C:104:ILE:HD13	1.93	0.51
48:r:42:SER:OG	48:r:47:THR:O	2.28	0.51
49:s:35:SER:OG	49:s:38:SER:OG	2.24	0.51
52:v:28:C:O2	52:v:45:G:N2	2.43	0.51
6:B:70:G:H21	6:B:101:A:H62	1.58	0.51
31:a:521:G:O3'	42:l:86:ARG:NH2	2.43	0.51
35:e:63:LEU:HB3	35:e:67:ARG:NH1	2.25	0.51
40:j:15:HIS:HA	40:j:18:ILE:HG22	1.92	0.51
51:u:18:ARG:CG	51:u:21:ARG:HD2	2.41	0.51
11:G:22:ARG:NH1	11:G:38:HIS:O	2.44	0.51
31:a:1266:A:N1	31:a:1309:G:O2'	2.41	0.51
36:f:62:MET:HG3	36:f:64:VAL:HG13	1.93	0.51
5:A:1795:G:OP1	7:C:258:ARG:NE	2.40	0.51
31:a:202:U:H2'	31:a:202:U:O2	2.10	0.51
32:b:110:ARG:HD2	32:b:110:ARG:N	2.26	0.51
49:s:42:PRO:O	49:s:45:VAL:HG22	2.11	0.51
10:F:38:MET:HE3	10:F:57:MET:CE	2.40	0.51
31:a:1050:G:H4'	31:a:1051:C:H3'	1.92	0.51
31:a:1092:U:OP1	31:a:1105:G:N2	2.37	0.51
5:A:2048:A:H4'	8:D:151:GLN:O	2.11	0.51
20:P:91:ASP:C	20:P:91:ASP:OD1	2.54	0.51
31:a:681:U:O2'	41:k:40:ALA:O	2.28	0.51
11:G:135:SER:CB	11:G:141:LEU:HD13	2.41	0.51
31:a:198:G:H21	31:a:461:A:H62	1.58	0.51
31:a:562:U:OP2	31:a:563:G:O2'	2.29	0.51
6:B:87:A:OP2	16:L:39:ARG:NE	2.44	0.51
31:a:1113:U:O2'	39:i:108:GLU:OE1	2.28	0.51
34:d:176:ASP:OD2	34:d:179:LYS:NZ	2.44	0.51
5:A:1775:U:OP2	5:A:1780:A:N6	2.38	0.50
31:a:198:G:O2'	31:a:465:C:OP1	2.29	0.50
31:a:406:G:OP1	34:d:26:LYS:NZ	2.34	0.50
31:a:998:A:C6	31:a:1037:A:N6	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:90:GLU:O	33:c:94:ILE:HG13	2.12	0.50
35:e:156:ARG:NH1	35:e:163:ILE:HG23	2.26	0.50
5:A:825:U:O2'	5:A:2064:U:N3	2.43	0.50
5:A:854:G:H2'	5:A:855:G:C8	2.47	0.50
5:A:1474:G:N1	5:A:1509:U:C2	2.79	0.50
10:F:126:GLY:O	10:F:158:THR:OG1	2.27	0.50
31:a:358:G:OP2	42:l:31:ARG:NH2	2.44	0.50
7:C:94:LEU:HD13	7:C:116:VAL:HG21	1.93	0.50
22:R:38:PHE:O	30:Z:38:ARG:NH2	2.44	0.50
31:a:998:A:N1	31:a:1037:A:N6	2.60	0.50
32:b:7:SER:O	32:b:8:MET:CB	2.59	0.50
35:e:63:LEU:HB3	35:e:67:ARG:HH12	1.75	0.50
38:h:79:VAL:HG12	38:h:86:GLN:OE1	2.11	0.50
10:F:38:MET:HE3	10:F:57:MET:HE3	1.93	0.50
18:N:67:ILE:O	18:N:71:THR:HG23	2.11	0.50
10:F:164:ASP:OD1	10:F:165:GLU:N	2.45	0.50
31:a:748:U:H2'	31:a:749:G:O4'	2.11	0.50
34:d:56:GLN:HB3	34:d:205:LEU:HD13	1.92	0.50
10:F:78:LYS:O	10:F:80:ARG:NH1	2.41	0.50
13:I:116:TYR:O	13:I:119:ILE:HG22	2.12	0.50
23:S:2:ASN:OD1	23:S:5:ARG:HB3	2.12	0.50
31:a:513:PSU:OP2	31:a:514:G:N2	2.44	0.50
32:b:119:LEU:HD21	32:b:143:MET:HB2	1.93	0.50
51:u:21:ARG:HG2	51:u:22:SER:N	2.26	0.50
5:A:308:U:H2'	5:A:309:G:O4'	2.12	0.50
11:G:73:ASN:O	11:G:76:VAL:HG12	2.12	0.50
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.41	0.50
40:j:76:ILE:CD1	40:j:87:LEU:HD11	2.42	0.50
42:l:98:VAL:HG23	42:l:101:SER:HB2	1.94	0.50
5:A:727:G:O4'	7:C:207:LYS:NZ	2.45	0.50
37:g:64:THR:HG22	37:g:68:LYS:HZ2	1.76	0.50
40:j:56:HIS:CD2	40:j:57:VAL:HG13	2.46	0.50
44:n:43:GLU:OE1	44:n:47:LYS:NZ	2.45	0.50
5:A:2421:A:H4'	5:A:2422:A:H3'	1.94	0.50
11:G:117:LEU:HD11	11:G:123:ALA:CB	2.42	0.50
10:F:4:LEU:N	10:F:101:ASP:OD1	2.45	0.49
31:a:1528:A:HO2'	31:a:1529:U:C5'	2.25	0.49
38:h:53:GLN:NE2	38:h:58:SER:OG	2.44	0.49
41:k:17:GLU:OE1	41:k:80:ASN:ND2	2.45	0.49
5:A:1471:U:OP2	5:A:1510:G:N1	2.45	0.49
11:G:140:LEU:O	11:G:144:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:54:LEU:O	12:H:58:GLU:OE1	2.30	0.49
16:L:116:GLU:O	16:L:120:LEU:HD23	2.12	0.49
31:a:541:G:OP1	34:d:58:ARG:NH2	2.46	0.49
31:a:1038:G:O2'	31:a:1039:A:O5'	2.30	0.49
32:b:58:PHE:O	32:b:62:LEU:HD23	2.13	0.49
37:g:69:VAL:HG13	37:g:100:ALA:HB1	1.94	0.49
5:A:1474:G:C2	5:A:1509:U:O2	2.66	0.49
14:J:88:ASN:OD1	14:J:90:ASN:N	2.41	0.49
31:a:290:U:OP1	31:a:607:U:O2'	2.22	0.49
31:a:743:A:H2'	31:a:744:A:C8	2.47	0.49
5:A:1413:G:H1'	5:A:1578:A:H61	1.78	0.49
5:A:1428:A:H2'	5:A:1429:A:H8	1.76	0.49
5:A:1524:A:N6	5:A:1541:G:O2'	2.42	0.49
5:A:1583:C:H2'	5:A:1583:C:O2	2.13	0.49
5:A:2324:A:H2'	5:A:2325:A:C8	2.48	0.49
14:J:7:MET:HG3	14:J:18:ARG:HD2	1.93	0.49
18:N:16:ARG:CZ	18:N:92:ASP:OD2	2.60	0.49
24:T:50:THR:O	24:T:50:THR:HG22	2.12	0.49
34:d:75:SER:HB3	34:d:79:LYS:NZ	2.27	0.49
51:u:18:ARG:O	51:u:19:PHE:C	2.56	0.49
5:A:1696:A:H4'	5:A:1697:G:H3'	1.93	0.49
11:G:46:GLU:N	11:G:46:GLU:OE1	2.46	0.49
11:G:171:ARG:O	11:G:172:LYS:HE2	2.12	0.49
31:a:1039:A:H2'	31:a:1040:U:C2	2.47	0.49
10:F:111:ILE:HG23	10:F:111:ILE:O	2.13	0.49
31:a:480:C:OP2	31:a:481:G:O2'	2.26	0.49
33:c:214:VAL:O	33:c:215:MET:SD	2.70	0.49
34:d:80:GLU:O	34:d:84:VAL:HG23	2.13	0.49
36:f:97:THR:HG22	36:f:97:THR:O	2.13	0.49
10:F:12:LEU:HD13	10:F:15:LYS:CE	2.39	0.49
11:G:135:SER:HB3	11:G:141:LEU:HD13	1.94	0.49
31:a:789:A:O2'	31:a:790:U:OP2	2.28	0.49
32:b:22:THR:O	32:b:25:TRP:CD1	2.66	0.49
40:j:14:ASP:OD1	40:j:17:LEU:N	2.34	0.49
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.94	0.49
5:A:394:U:O2'	5:A:395:G:N7	2.43	0.49
10:F:94:ASP:O	10:F:98:GLU:OE1	2.31	0.49
13:I:65:THR:HG22	13:I:66:GLY:N	2.27	0.49
32:b:171:GLU:O	32:b:175:ILE:HD12	2.12	0.49
38:h:48:ASN:N	38:h:63:THR:OG1	2.46	0.49
31:a:1277:A:O2'	31:a:1278:U:P	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1527:G:H3'	31:a:1528:A:C8	2.48	0.48
46:p:30:LYS:O	46:p:31:LYS:HB2	2.12	0.48
5:A:2034:G:H2'	5:A:2035:U:O4'	2.14	0.48
5:A:2796:U:HO2'	5:A:2797:G:P	2.36	0.48
34:d:102:ASN:ND2	34:d:113:ARG:CZ	2.76	0.48
36:f:93:GLU:O	36:f:94:HIS:CG	2.65	0.48
9:E:101:ARG:O	9:E:105:GLN:HG3	2.12	0.48
13:I:140:LEU:HD21	13:I:142:ILE:HG23	1.95	0.48
31:a:1025:C:C2	31:a:1031:G:N2	2.81	0.48
35:e:53:ARG:NH2	35:e:54:GLU:OE2	2.46	0.48
5:A:2549:G:O4'	5:A:2578:G:O2'	2.24	0.48
31:a:414:C:H2'	31:a:415:C:C1'	2.44	0.48
31:a:930:G:N2	31:a:932:A:O4'	2.46	0.48
33:c:35:LYS:O	33:c:39:VAL:HG23	2.13	0.48
34:d:139:VAL:HG12	34:d:184:PHE:CZ	2.49	0.48
5:A:971:G:OP1	5:A:1182:G:O2'	2.15	0.48
33:c:54:ASN:OD1	33:c:55:ILE:N	2.46	0.48
34:d:103:VAL:O	34:d:107:MET:HG2	2.13	0.48
42:l:86:ARG:HD2	42:l:88:LYS:N	2.29	0.48
44:n:31:ILE:O	44:n:41:ARG:NE	2.41	0.48
5:A:1037:A:OP1	25:U:49:ARG:NH2	2.42	0.48
31:a:1025:C:O2	31:a:1031:G:N2	2.46	0.48
31:a:1051:C:H1'	31:a:1052:A:OP2	2.13	0.48
31:a:1378:U:H2'	31:a:1379:C:C6	2.49	0.48
32:b:104:THR:HG22	32:b:181:LEU:HD21	1.95	0.48
36:f:9:LEU:HB2	36:f:85:ILE:O	2.14	0.48
5:A:122:C:HO2'	5:A:134:A:HO2'	1.62	0.48
23:S:40:LEU:C	23:S:40:LEU:HD23	2.39	0.48
10:F:103:LEU:HD12	10:F:107:ALA:HB3	1.96	0.48
10:F:136:ILE:O	10:F:137:VAL:CG2	2.53	0.48
31:a:963:2MG:H2'	31:a:964:5MC:C6	2.49	0.48
31:a:1353:G:H2'	31:a:1354:A:C8	2.49	0.48
10:F:67:VAL:HG12	10:F:84:PRO:HB3	1.96	0.47
18:N:16:ARG:HH22	18:N:94:SER:HA	1.79	0.47
23:S:6:ILE:HD11	23:S:45:ALA:N	2.29	0.47
31:a:1320:G:H2'	31:a:1321:A:C8	2.48	0.47
32:b:104:THR:HG23	32:b:177:GLU:OE1	2.13	0.47
31:a:809:G:H1'	31:a:810:U:OP2	2.15	0.47
35:e:38:VAL:HG23	35:e:66:ALA:HB1	1.97	0.47
37:g:137:LYS:C	37:g:137:LYS:HD2	2.39	0.47
5:A:108:U:O2'	5:A:109:G:OP1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1163:G:N1	31:a:1167:A:OP2	2.46	0.47
31:a:1515:MA6:H93	31:a:1516:MA6:C10	2.43	0.47
32:b:6:VAL:HG21	32:b:11:LEU:HG	1.95	0.47
5:A:542:C:H2'	5:A:543:U:O4'	2.15	0.47
5:A:2747:G:N3	5:A:2747:G:H2'	2.30	0.47
11:G:76:VAL:HG13	11:G:77:LYS:HD3	1.95	0.47
18:N:62:GLY:O	18:N:64:THR:HG23	2.14	0.47
31:a:206:C:OP2	31:a:208:G:O2'	2.32	0.47
5:A:2027:A:N3	5:A:2451:G:O2'	2.37	0.47
7:C:199:GLU:N	7:C:199:GLU:OE2	2.46	0.47
31:a:973:G:OP2	31:a:1355:U:O2'	2.32	0.47
32:b:165:VAL:HG11	32:b:168:VAL:HG12	1.97	0.47
5:A:494:G:H21	22:R:61:ASN:HD21	1.63	0.47
5:A:1027:C:P	16:L:128:LYS:NZ	2.87	0.47
5:A:2287:U:H2'	5:A:2288:G:C8	2.50	0.47
5:A:2301:U:N3	5:A:2303:G:O6	2.48	0.47
7:C:148:ILE:H	7:C:148:ILE:HD12	1.80	0.47
25:U:64:VAL:HG22	25:U:77:LYS:HD3	1.96	0.47
29:Y:23:LEU:HD11	29:Y:53:MET:HE2	1.96	0.47
31:a:416:U:O4'	31:a:416:U:O2	2.31	0.47
31:a:425:U:O2	31:a:426:A:C8	2.67	0.47
31:a:789:A:H1'	31:a:790:U:OP2	2.15	0.47
32:b:116:LEU:HD13	32:b:146:LEU:HB3	1.96	0.47
32:b:142:GLU:HG2	32:b:146:LEU:HD13	1.97	0.47
33:c:124:LEU:HD21	33:c:130:PHE:HB3	1.95	0.47
34:d:36:ASN:OD1	34:d:36:ASN:C	2.58	0.47
34:d:155:LEU:O	34:d:158:LYS:HG3	2.15	0.47
5:A:782:G:H5'	5:A:783:G:OP1	2.15	0.47
50:t:48:THR:O	50:t:52:LYS:HD3	2.14	0.47
18:N:28:CYS:HA	18:N:92:ASP:HB3	1.97	0.47
31:a:1438:A:O2'	31:a:1439:G:P	2.73	0.47
43:m:37:VAL:HG12	43:m:37:VAL:O	2.14	0.47
18:N:16:ARG:NH2	18:N:94:SER:HA	2.30	0.47
31:a:710:G:H2'	31:a:711:G:C8	2.50	0.47
31:a:1010:G:N1	31:a:1013:A:OP2	2.38	0.47
37:g:53:LYS:HD3	37:g:125:LEU:HD11	1.97	0.47
37:g:64:THR:HG22	37:g:68:LYS:NZ	2.30	0.47
5:A:1427:G:H2'	5:A:1428:A:C8	2.50	0.46
30:Z:43:THR:HG1	30:Z:47:PHE:H	1.62	0.46
52:v:13:C:H3'	52:v:14:A:H5"	1.96	0.46
5:A:799:G:C2'	5:A:800:A:OP1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1230:G:O2'	5:A:1231:G:O4'	2.28	0.46
5:A:1138:U:H2'	13:I:65:THR:HG21	1.96	0.46
10:F:136:ILE:HG22	10:F:137:VAL:N	2.30	0.46
25:U:69:VAL:HG13	25:U:69:VAL:O	2.16	0.46
31:a:702:G:C5	31:a:703:A:C8	3.04	0.46
34:d:28:PHE:O	34:d:32:THR:HG22	2.15	0.46
3:2:39:ARG:NH1	5:A:2358:G:OP1	2.48	0.46
5:A:1389:U:H2'	5:A:1390:A:O4'	2.15	0.46
10:F:16:LEU:HD21	10:F:20:LEU:HD12	1.97	0.46
24:T:34:VAL:HG11	24:T:37:LEU:HD12	1.97	0.46
31:a:185:C:H1'	31:a:186:G:OP2	2.15	0.46
33:c:214:VAL:O	33:c:214:VAL:HG12	2.15	0.46
41:k:113:THR:OG1	51:u:28:VAL:HG11	2.15	0.46
42:l:100:GLY:N	42:l:104:CYS:O	2.48	0.46
31:a:637:A:O2'	38:h:108:SER:OG	2.31	0.46
33:c:152:GLU:HG2	33:c:167:TRP:HB3	1.97	0.46
40:j:24:GLU:O	40:j:28:THR:HG23	2.16	0.46
44:n:31:ILE:HD11	44:n:45:MET:HA	1.96	0.46
5:A:1522:C:O2	5:A:1543:A:N6	2.48	0.46
11:G:35:PHE:CE1	11:G:71:VAL:HG11	2.51	0.46
36:f:72:ASP:OD1	36:f:72:ASP:C	2.58	0.46
36:f:85:ILE:O	36:f:85:ILE:HG13	2.15	0.46
42:l:101:SER:OG	42:l:102:LEU:N	2.49	0.46
48:r:33:ILE:HD13	48:r:68:ILE:HG21	1.97	0.46
5:A:1109:G:O2'	5:A:1110:U:O4'	2.34	0.46
31:a:438:G:O6	31:a:439:C:N4	2.49	0.46
43:m:28:HIS:CE1	43:m:32:ASN:OD1	2.68	0.46
48:r:34:THR:CG2	48:r:40:VAL:HG22	2.45	0.46
15:K:95:GLU:OE1	15:K:95:GLU:N	2.48	0.46
16:L:78:PRO:O	16:L:79:LEU:HB3	2.16	0.46
31:a:607:U:N3	31:a:608:C:C5	2.84	0.46
31:a:1000:A:N7	31:a:1032:A:N6	2.64	0.46
32:b:202:ILE:HG13	32:b:202:ILE:O	2.14	0.46
31:a:179:G:OP2	31:a:179:G:N2	2.49	0.46
33:c:120:ILE:HD11	33:c:137:ALA:CB	2.46	0.46
5:A:507:U:C4'	5:A:508:C:OP2	2.64	0.45
13:I:96:LYS:NZ	13:I:99:GLU:OE1	2.32	0.45
18:N:42:SER:HB3	18:N:49:LEU:HD21	1.98	0.45
31:a:435:U:C6	31:a:435:U:OP1	2.68	0.45
46:p:22:ILE:HG12	46:p:39:VAL:HG22	1.97	0.45
5:A:2463:C:H2'	5:A:2464:A:O4'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:38:MET:CE	10:F:57:MET:HE3	2.47	0.45
19:O:5:HIS:O	19:O:9:GLN:NE2	2.49	0.45
31:a:78:G:H2'	31:a:79:U:C6	2.51	0.45
31:a:435:U:H4'	34:d:123:ARG:HD3	1.97	0.45
33:c:138:VAL:HG11	33:c:168:TYR:CE2	2.51	0.45
5:A:715:C:O4'	5:A:715:C:O2	2.34	0.45
5:A:2502:U:H2'	5:A:2572:G:O6	2.16	0.45
10:F:6:ALA:O	10:F:10:ASP:OD1	2.34	0.45
24:T:93:VAL:HG12	24:T:100:SER:HA	1.99	0.45
35:e:106:ALA:HB2	35:e:124:ALA:HB3	1.99	0.45
5:A:368:C:O2	5:A:368:C:O4'	2.33	0.45
5:A:1124:A:N1	5:A:2459:C:O2'	2.45	0.45
5:A:1794:U:OP2	7:C:273:VAL:HG21	2.17	0.45
5:A:2509:A:H2'	5:A:2510:U:C6	2.51	0.45
31:a:1031:G:H2'	31:a:1032:A:O4'	2.16	0.45
31:a:1127:A:C8	31:a:1143:A:C2	3.05	0.45
46:p:75:PHE:O	46:p:79:VAL:HG23	2.17	0.45
5:A:2058:A:O2'	5:A:2059:C:H5'	2.17	0.45
31:a:185:C:H4'	31:a:186:G:O5'	2.17	0.45
31:a:963:2MG:HM22	52:v:35:C:C5'	2.46	0.45
36:f:85:ILE:O	36:f:86:ARG:HB3	2.16	0.45
44:n:43:GLU:HB3	44:n:47:LYS:NZ	2.32	0.45
5:A:605:U:C5	5:A:618:G:C5	3.05	0.45
5:A:1193:U:C2	5:A:1194:U:C5	3.05	0.45
10:F:12:LEU:CD1	10:F:15:LYS:HE3	2.40	0.45
18:N:16:ARG:NH1	18:N:92:ASP:OD2	2.50	0.45
31:a:711:G:H2'	31:a:712:A:C8	2.52	0.45
34:d:61:GLN:O	34:d:65:ARG:HD3	2.17	0.45
35:e:156:ARG:HH11	35:e:163:ILE:HD12	1.82	0.45
42:l:87:VAL:O	42:l:88:LYS:HB3	2.16	0.45
15:K:123:THR:O	15:K:123:THR:HG23	2.15	0.45
16:L:113:LEU:HD12	16:L:116:GLU:OE2	2.15	0.45
31:a:943:A:H2'	31:a:944:G:C8	2.51	0.45
31:a:1253:U:H5'	31:a:1255:G:H1'	1.99	0.45
35:e:36:THR:HG21	35:e:63:LEU:HD22	1.98	0.45
4:3:18:ARG:HG2	4:3:23:ILE:HD13	1.98	0.45
5:A:434:C:O2	5:A:434:C:O4'	2.35	0.45
5:A:666:A:H2'	5:A:668:A:H62	1.81	0.45
31:a:62:A:H1'	31:a:63:G:OP2	2.17	0.45
31:a:1024:C:H2'	31:a:1025:C:C6	2.52	0.45
31:a:1028:C:O2	31:a:1028:C:O4'	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1494:G:O2'	31:a:1515:MA6:H92	2.17	0.45
31:a:1515:MA6:H93	31:a:1516:MA6:N6	2.32	0.45
5:A:726:G:H3'	5:A:727:G:H5'	1.99	0.45
5:A:2651:G:C2'	5:A:2652:U:OP2	2.65	0.45
5:A:2744:A:C2	11:G:63:MET:HE1	2.52	0.45
6:B:86:U:H1'	6:B:87:A:OP2	2.16	0.45
9:E:110:GLU:HB3	15:K:3:LEU:HD11	1.99	0.45
10:F:141:ILE:HG22	10:F:142:ASP:N	2.32	0.45
31:a:1023:G:C2	31:a:1024:C:C6	3.05	0.45
34:d:97:GLU:HG2	34:d:188:PRO:HG3	1.99	0.45
45:o:25:PRO:O	45:o:29:VAL:HG23	2.16	0.45
5:A:325:G:H2'	9:E:162:ASN:HD21	1.82	0.45
9:E:108:LEU:O	9:E:112:VAL:HG23	2.16	0.45
10:F:72:LYS:HG3	10:F:73:SER:N	2.32	0.45
30:Z:3:VAL:HG22	30:Z:4:GLN:N	2.32	0.45
31:a:671:G:H21	41:k:117:HIS:HB2	1.82	0.45
31:a:682:G:O2'	31:a:683:U:C5'	2.65	0.45
32:b:112:SER:HA	32:b:115:ARG:HE	1.81	0.45
33:c:21:ASN:HB3	33:c:58:GLU:HG2	1.98	0.45
5:A:342:A:H2'	5:A:343:C:O4'	2.18	0.44
25:U:23:ARG:O	25:U:27:GLU:OE2	2.35	0.44
31:a:1025:C:O2'	31:a:1026:U:P	2.73	0.44
31:a:1026:U:C6	31:a:1026:U:OP2	2.70	0.44
31:a:1067:U:H2'	31:a:1068:C:C6	2.52	0.44
31:a:1161:G:H2'	31:a:1162:U:O4'	2.17	0.44
5:A:2641:U:H3'	5:A:2642:C:C5'	2.47	0.44
5:A:2651:G:O2'	5:A:2652:U:P	2.75	0.44
31:a:942:G:C2	31:a:943:A:C8	3.05	0.44
40:j:8:ILE:HB	40:j:74:ILE:HB	1.98	0.44
52:v:22:A:O2'	52:v:47:G:O6	2.34	0.44
5:A:299:G:H2'	5:A:300:G:O4'	2.17	0.44
5:A:862:G:H2'	5:A:863:C:C6	2.51	0.44
5:A:2309:C:O4'	10:F:37:ASN:ND2	2.50	0.44
31:a:242:A:C2	31:a:278:A:C5	3.05	0.44
31:a:331:C:O2'	31:a:1430:A:N3	2.48	0.44
31:a:1059:U:H2'	31:a:1060:C:C6	2.51	0.44
32:b:194:ASN:ND2	32:b:196:ASP:OD2	2.50	0.44
37:g:35:LYS:HB3	37:g:38:ILE:HD13	1.99	0.44
5:A:1105:U:O2	5:A:1105:U:C2'	2.65	0.44
5:A:1191:C:C2	5:A:1192:G:C8	3.05	0.44
5:A:1634:G:H2'	5:A:1635:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:14:LEU:C	35:e:14:LEU:HD23	2.43	0.44
5:A:91:A:H1'	5:A:92:G:OP2	2.18	0.44
5:A:1316:A:C4	5:A:1317:A:C8	3.05	0.44
5:A:2323:A:H2'	5:A:2324:A:C8	2.52	0.44
19:O:3:GLY:O	19:O:9:GLN:OE1	2.35	0.44
20:P:64:ARG:NH1	20:P:100:MET:SD	2.90	0.44
31:a:865:C:H2'	31:a:866:G:O4'	2.17	0.44
33:c:212:LYS:O	33:c:215:MET:HA	2.17	0.44
36:f:15:SER:O	36:f:18:VAL:HG13	2.18	0.44
5:A:458:U:OP2	5:A:458:U:H6	2.01	0.44
5:A:1833:C:O2'	5:A:1923:A:O2'	2.17	0.44
5:A:1938:C:OP2	5:A:1939:U:O2'	2.29	0.44
5:A:2744:A:N3	11:G:63:MET:HE1	2.32	0.44
31:a:1026:U:O2'	31:a:1027:U:O2	2.35	0.44
32:b:58:PHE:CZ	32:b:62:LEU:HD21	2.53	0.44
5:A:40:U:O2'	5:A:41:U:C6	2.70	0.44
31:a:1037:A:C2	31:a:1038:G:C5	3.05	0.44
31:a:1277:A:C2'	31:a:1278:U:OP1	2.65	0.44
31:a:1423:G:H2'	31:a:1424:C:O4'	2.18	0.44
34:d:189:ASP:O	34:d:193:LEU:HD23	2.18	0.44
5:A:579:C:H2'	5:A:580:A:H8	1.82	0.44
5:A:1993:C:OP2	8:D:132:THR:OG1	2.30	0.44
5:A:2088:U:H4'	5:A:2089:G:O5'	2.17	0.44
9:E:169:VAL:HG22	9:E:170:ASP:N	2.33	0.44
10:F:59:LEU:HD21	10:F:140:GLU:HA	2.00	0.44
31:a:518:G:O2'	31:a:533:C:O2'	2.04	0.44
31:a:1274:C:O2'	31:a:1276:A:N3	2.49	0.44
51:u:20:LYS:O	51:u:21:ARG:C	2.61	0.44
5:A:1151:C:H2'	5:A:1152:G:O4'	2.18	0.44
5:A:2659:G:H2'	5:A:2660:G:O4'	2.18	0.44
8:D:87:GLU:HG2	8:D:88:ALA:N	2.33	0.44
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.99	0.44
31:a:933:C:C2	31:a:934:A:C8	3.06	0.44
34:d:11:LEU:HD21	34:d:65:ARG:CG	2.43	0.44
34:d:158:LYS:O	34:d:161:ILE:HG12	2.18	0.44
36:f:49:TYR:OH	36:f:86:ARG:NH1	2.51	0.44
41:k:115:ILE:HD11	51:u:28:VAL:HG13	1.99	0.44
5:A:637:U:H2'	5:A:638:C:C6	2.53	0.43
5:A:2067:A:H2'	5:A:2068:C:C6	2.53	0.43
5:A:2641:U:H3'	5:A:2642:C:H5'	2.00	0.43
7:C:94:LEU:HD11	7:C:104:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:108:ILE:HA	10:F:111:ILE:HG22	1.99	0.43
31:a:420:G:H2'	31:a:421:G:C8	2.53	0.43
31:a:1020:G:H2'	31:a:1021:G:C8	2.53	0.43
32:b:116:LEU:HD23	32:b:154:LYS:HE3	2.00	0.43
43:m:53:LEU:O	43:m:57:ARG:HG3	2.18	0.43
5:A:51:A:H2'	5:A:52:G:O4'	2.18	0.43
5:A:122:C:O2'	5:A:134:A:O2'	2.32	0.43
5:A:869:U:H2'	5:A:870:U:C6	2.53	0.43
31:a:1038:G:C2'	31:a:1039:A:O5'	2.66	0.43
32:b:106:TRP:HA	32:b:110:ARG:HD3	2.00	0.43
36:f:12:PRO:O	36:f:15:SER:OG	2.36	0.43
36:f:15:SER:O	36:f:18:VAL:HG22	2.18	0.43
41:k:88:PRO:HG3	51:u:32:VAL:HG11	1.99	0.43
5:A:701:U:H2'	5:A:702:G:O4'	2.18	0.43
5:A:1192:G:C2	5:A:1193:U:C5	3.07	0.43
23:S:6:ILE:HD11	23:S:45:ALA:CA	2.48	0.43
31:a:1023:G:C2	31:a:1024:C:C5	3.05	0.43
31:a:1038:G:H2'	31:a:1039:A:C8	2.53	0.43
31:a:1178:G:O2'	31:a:1179:G:N7	2.48	0.43
32:b:92:PRO:HG3	32:b:156:MET:HE3	1.99	0.43
33:c:33:LEU:O	33:c:37:LEU:HG	2.19	0.43
5:A:2205:G:OP2	5:A:2206:U:O2'	2.34	0.43
6:B:39:C:H41	10:F:69:LEU:HD23	1.83	0.43
31:a:682:G:H2'	31:a:683:U:C6	2.53	0.43
31:a:1263:G:N2	31:a:1266:A:OP2	2.34	0.43
33:c:35:LYS:HD2	33:c:95:MET:HA	1.99	0.43
36:f:70:THR:O	36:f:74:LEU:HD13	2.19	0.43
24:T:32:VAL:HG22	24:T:33:LYS:N	2.34	0.43
31:a:201:A:H4'	31:a:202:U:O5'	2.19	0.43
31:a:397:C:O2'	31:a:618:A:N3	2.50	0.43
31:a:428:A:C4	31:a:429:G:C8	3.07	0.43
18:N:29:VAL:HG21	18:N:102:ILE:CG2	2.48	0.43
24:T:31:ARG:HB3	24:T:62:SER:HB3	2.01	0.43
24:T:72:ASN:O	24:T:76:GLN:N	2.51	0.43
39:i:19:LEU:HD21	39:i:59:TYR:CD1	2.53	0.43
43:m:40:THR:O	43:m:43:THR:HG22	2.18	0.43
5:A:1555:C:OP2	5:A:1556:A:O2'	2.28	0.43
10:F:37:ASN:OD1	10:F:38:MET:N	2.51	0.43
31:a:403:U:O4'	34:d:118:GLN:NE2	2.47	0.43
31:a:701:A:C5	31:a:702:G:C8	3.06	0.43
5:A:2232:U:H2'	5:A:2233:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:40:VAL:N	10:F:85:ILE:O	2.50	0.43
11:G:133:LEU:HD11	11:G:148:ILE:HD12	2.01	0.43
31:a:1131:U:H2'	31:a:1132:U:O4'	2.19	0.43
31:a:1490:A:HO2'	31:a:1491:G:C5'	2.31	0.43
37:g:113:GLU:OE1	37:g:113:GLU:N	2.51	0.43
39:i:89:ASP:HB3	39:i:92:LEU:HD12	2.01	0.43
40:j:66:GLU:HB3	44:n:99:ALA:HB2	2.01	0.43
3:2:32:LEU:HD13	5:A:2415:U:OP2	2.19	0.43
5:A:332:A:H2'	5:A:332:A:N3	2.34	0.43
31:a:156:A:N6	31:a:339:U:O2'	2.52	0.43
31:a:514:G:H4'	31:a:516:C:C5	2.54	0.43
5:A:691:A:OP2	7:C:39:ARG:NH2	2.52	0.43
10:F:34:ILE:HD13	10:F:156:ILE:HG22	2.00	0.43
19:O:32:GLN:HB3	19:O:43:LEU:HD22	2.01	0.43
5:A:369:G:OP2	5:A:369:G:C8	2.72	0.42
5:A:372:U:C6	5:A:372:U:OP2	2.72	0.42
31:a:1033:A:N3	31:a:1033:A:H2'	2.33	0.42
44:n:73:TYR:O	44:n:79:LEU:O	2.37	0.42
5:A:1421:G:OP2	5:A:1422:A:O2'	2.33	0.42
5:A:2400:U:H2'	5:A:2401:G:O4'	2.18	0.42
8:D:86:THR:OG1	8:D:87:GLU:OE1	2.37	0.42
11:G:15:VAL:HG11	11:G:79:VAL:HG23	2.01	0.42
22:R:92:ARG:NH1	22:R:94:ASP:OD1	2.52	0.42
31:a:1078:G:C2	31:a:1079:A:C8	3.07	0.42
31:a:1495:UR3:H6	31:a:1495:UR3:O5'	2.19	0.42
36:f:36:ILE:HD12	36:f:62:MET:HE1	2.00	0.42
50:t:32:ILE:O	50:t:35:THR:HG22	2.19	0.42
51:u:21:ARG:CG	51:u:22:SER:N	2.81	0.42
5:A:825:U:O2'	5:A:2064:U:C2	2.72	0.42
5:A:981:A:N3	5:A:981:A:H2'	2.34	0.42
5:A:1269:A:N1	5:A:1642:C:O2'	2.50	0.42
10:F:154:ILE:HG23	10:F:154:ILE:O	2.19	0.42
31:a:1002:A:O3'	31:a:1035:C:O2'	2.37	0.42
44:n:87:THR:HG22	44:n:93:VAL:HG23	2.00	0.42
48:r:32:TYR:O	48:r:40:VAL:HG23	2.19	0.42
5:A:2466:G:H2'	5:A:2467:A:C8	2.54	0.42
10:F:91:LEU:HD23	10:F:95:GLN:HG3	2.01	0.42
32:b:116:LEU:HD13	32:b:146:LEU:CB	2.49	0.42
37:g:6:VAL:O	37:g:6:VAL:HG13	2.19	0.42
5:A:457:G:H1'	5:A:458:U:OP2	2.19	0.42
5:A:1437:U:H2'	5:A:1438:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:96:ASN:HB2	9:E:99:MET:HG3	2.00	0.42
17:M:102:PHE:CD2	17:M:102:PHE:C	2.97	0.42
31:a:305:C:O2'	31:a:604:A:N1	2.52	0.42
31:a:601:G:H2'	31:a:602:U:O4'	2.20	0.42
31:a:679:G:C2	31:a:680:G:C8	3.07	0.42
34:d:192:ASP:OD1	34:d:192:ASP:C	2.61	0.42
44:n:19:LYS:NZ	44:n:20:TYR:CZ	2.80	0.42
5:A:177:G:H2'	5:A:178:U:C6	2.55	0.42
5:A:1317:A:C5	5:A:1318:C:C5	3.08	0.42
10:F:12:LEU:HD12	10:F:172:ALA:HB1	2.02	0.42
13:I:140:LEU:HD23	13:I:142:ILE:HG23	2.01	0.42
31:a:1157:G:C2	31:a:1158:C:C6	3.08	0.42
31:a:1428:A:H2'	31:a:1429:G:O4'	2.19	0.42
32:b:111:GLN:NE2	32:b:115:ARG:HD2	2.35	0.42
52:v:9:A:O2'	52:v:10:G:N7	2.53	0.42
5:A:665:U:H2'	5:A:666:A:O4'	2.20	0.42
5:A:1025:A:N3	5:A:2482:C:O2'	2.44	0.42
5:A:1168:A:H2'	5:A:1169:C:C6	2.55	0.42
5:A:2479:C:N3	16:L:124:LYS:NZ	2.64	0.42
7:C:130:LEU:HB2	7:C:135:MET:HE2	2.02	0.42
11:G:35:PHE:CD1	11:G:71:VAL:HG11	2.55	0.42
31:a:1448:C:O2	31:a:1448:C:O5'	2.36	0.42
34:d:139:VAL:CG1	34:d:184:PHE:CZ	3.02	0.42
34:d:141:ALA:HB1	34:d:185:LYS:O	2.20	0.42
38:h:75:MET:HE3	38:h:131:SER:OG	2.19	0.42
47:q:14:VAL:HG12	47:q:14:VAL:O	2.20	0.42
5:A:142:A:H2'	5:A:143:C:C6	2.55	0.42
5:A:324:A:H1'	5:A:325:G:OP1	2.19	0.42
5:A:2234:G:H2'	5:A:2234:G:N3	2.35	0.42
41:k:19:VAL:HG22	41:k:20:ALA:N	2.35	0.42
42:l:23:ALA:HB3	42:l:95:TYR:OH	2.19	0.42
43:m:65:THR:HG22	43:m:66:GLU:HG2	2.01	0.42
5:A:591:U:H2'	5:A:592:U:C6	2.54	0.42
5:A:2525:G:C4'	5:A:2526:A:OP2	2.67	0.42
5:A:2529:C:OP1	5:A:2661:A:O2'	2.37	0.42
5:A:2749:A:H2'	5:A:2750:U:O4'	2.20	0.42
7:C:77:VAL:HG22	7:C:115:LYS:HZ1	1.84	0.42
14:J:7:MET:CG	14:J:18:ARG:HD2	2.49	0.42
31:a:388:C:H2'	31:a:389:A:O4'	2.20	0.42
31:a:1156:U:O4'	31:a:1179:G:N2	2.52	0.42
45:o:85:LEU:HB3	45:o:87:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:968:C:H2'	5:A:969:A:O4'	2.19	0.42
5:A:1105:U:O2	5:A:1105:U:H2'	2.20	0.42
5:A:1924:A:H2'	5:A:1925:G:O4'	2.20	0.42
18:N:27:LEU:HD13	18:N:40:VAL:HG22	2.02	0.42
25:U:39:ALA:HB3	25:U:97:ARG:CZ	2.49	0.42
32:b:109:LEU:O	32:b:113:ILE:HG13	2.20	0.42
7:C:135:MET:SD	7:C:192:ILE:HD11	2.60	0.41
7:C:140:THR:HG23	7:C:140:THR:O	2.19	0.41
18:N:29:VAL:O	18:N:94:SER:OG	2.33	0.41
31:a:180:U:C2	31:a:181:C:C5	3.08	0.41
31:a:250:G:O4'	47:q:18:MET:CE	2.68	0.41
34:d:158:LYS:HA	34:d:161:ILE:HG12	2.02	0.41
42:l:107:VAL:HG22	42:l:117:TYR:HB3	2.02	0.41
44:n:10:GLU:O	44:n:14:GLU:HG3	2.20	0.41
52:v:18:G:N2	52:v:59:A:OP1	2.53	0.41
52:v:65:G:C2	52:v:66:U:C6	3.08	0.41
5:A:558:C:O2'	20:P:48:ARG:NH1	2.54	0.41
5:A:1317:A:C6	5:A:1318:C:C5	3.09	0.41
5:A:1365:C:H2'	5:A:1366:G:O4'	2.20	0.41
5:A:1796:C:OP1	7:C:258:ARG:NH2	2.52	0.41
10:F:163:ASP:O	10:F:167:ARG:HD3	2.20	0.41
25:U:4:PHE:HB2	25:U:65:VAL:HG12	2.02	0.41
25:U:68:LYS:HG2	25:U:73:VAL:HG23	2.02	0.41
31:a:435:U:O2	31:a:435:U:H2'	2.19	0.41
31:a:1022:U:H4'	31:a:1023:G:O5'	2.20	0.41
31:a:1023:G:N3	31:a:1023:G:H2'	2.34	0.41
31:a:1038:G:C6	31:a:1039:A:N6	2.88	0.41
31:a:1369:U:H2'	31:a:1370:G:O4'	2.19	0.41
32:b:57:ASN:OD1	32:b:61:GLN:NE2	2.54	0.41
35:e:61:LYS:HA	35:e:64:GLU:OE2	2.19	0.41
5:A:847:A:H2'	5:A:848:C:C6	2.56	0.41
31:a:493:A:C2	31:a:494:U:C5	3.08	0.41
31:a:521:G:H2'	31:a:522:C:C6	2.56	0.41
31:a:808:C:O2'	31:a:898:A:N1	2.53	0.41
31:a:1061:G:H4'	31:a:1062:U:OP1	2.20	0.41
32:b:167:ASP:O	32:b:171:GLU:OE1	2.39	0.41
32:b:175:ILE:HD12	32:b:175:ILE:H	1.86	0.41
33:c:19:ASN:O	33:c:56:LEU:HD12	2.20	0.41
36:f:64:VAL:O	36:f:64:VAL:HG23	2.20	0.41
37:g:93:PRO:HA	37:g:96:ARG:HG2	2.02	0.41
49:s:31:ILE:HG22	49:s:32:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:29:ARG:O	50:t:33:LYS:HG2	2.20	0.41
5:A:698:G:O2'	5:A:1630:A:N3	2.47	0.41
24:T:3:LYS:O	24:T:92:ARG:NH1	2.53	0.41
31:a:127:U:H2'	31:a:128:C:C6	2.55	0.41
31:a:933:C:C4	31:a:934:A:N7	2.88	0.41
31:a:1098:A:H4'	31:a:1099:A:O5'	2.20	0.41
31:a:1488:G:H2'	31:a:1489:A:C8	2.55	0.41
49:s:50:SER:OG	49:s:57:HIS:HB3	2.21	0.41
5:A:368:C:C4'	5:A:369:G:OP2	2.68	0.41
5:A:869:U:H2'	5:A:870:U:H6	1.85	0.41
5:A:1413:G:H1'	5:A:1578:A:N6	2.34	0.41
21:Q:51:ALA:CB	21:Q:52:PRO:CD	2.99	0.41
31:a:1099:A:H2'	31:a:1100:C:C6	2.55	0.41
31:a:1127:A:N7	31:a:1143:A:C6	2.88	0.41
31:a:1330:A:H2'	31:a:1331:G:O4'	2.21	0.41
43:m:30:ALA:O	43:m:33:ILE:HG22	2.21	0.41
5:A:978:A:OP2	5:A:979:C:N4	2.49	0.41
7:C:175:ARG:NH1	7:C:181:MET:HE1	2.36	0.41
17:M:110:MET:HE2	17:M:110:MET:HA	2.01	0.41
31:a:577:C:H2'	31:a:578:G:O4'	2.20	0.41
31:a:809:G:O2'	31:a:810:U:P	2.79	0.41
31:a:1051:C:O2'	31:a:1052:A:OP2	2.30	0.41
33:c:14:VAL:HG12	33:c:15:VAL:HG13	2.03	0.41
47:q:40:ARG:O	47:q:41:ARG:NE	2.51	0.41
50:t:44:TYR:O	50:t:48:THR:HG23	2.20	0.41
5:A:642:A:H2'	5:A:644:A:C8	2.54	0.41
5:A:1355:G:N7	5:A:1356:G:C8	2.89	0.41
5:A:1396:U:H2'	5:A:1397:U:C6	2.56	0.41
10:F:34:ILE:HD12	10:F:155:THR:O	2.21	0.41
32:b:4:TYR:CD2	32:b:56:LEU:HD23	2.56	0.41
41:k:36:ARG:O	41:k:37:GLN:HB2	2.20	0.41
52:v:28:C:H2'	52:v:29:C:O4'	2.21	0.41
5:A:606:A:H2'	5:A:607:A:C8	2.55	0.41
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.66	0.41
6:B:64:A:H5"	6:B:65:G:OP1	2.21	0.41
18:N:5:LYS:O	18:N:9:LEU:HD23	2.20	0.41
31:a:96:U:O2'	31:a:97:A:N7	2.46	0.41
31:a:414:C:H2'	31:a:415:C:C6	2.56	0.41
31:a:657:G:C6	31:a:743:A:N6	2.89	0.41
33:c:50:ALA:HB1	33:c:76:VAL:CG1	2.50	0.41
48:r:39:ILE:HG12	48:r:59:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:28:LYS:HD3	3:2:43:LEU:HD12	2.02	0.41
5:A:34:G:N2	5:A:511:G:H1'	2.35	0.41
5:A:929:C:O2'	5:A:930:U:P	2.77	0.41
5:A:1267:A:O2'	5:A:1268:C:H2'	2.21	0.41
5:A:1652:A:O2'	8:D:121:PHE:O	2.36	0.41
5:A:1737:C:H2'	5:A:1738:U:O4'	2.21	0.41
5:A:1942:U:C2	5:A:1943:C:C5	3.09	0.41
5:A:2039:C:C2	5:A:2040:C:C5	3.09	0.41
5:A:2550:U:O2	5:A:2550:U:O4'	2.39	0.41
5:A:2683:U:H2'	5:A:2684:G:O4'	2.21	0.41
9:E:180:ILE:HG12	15:K:3:LEU:HD22	2.03	0.41
10:F:114:PHE:O	10:F:115:ARG:HG2	2.21	0.41
10:F:133:LYS:O	10:F:134:GLU:HB2	2.21	0.41
13:I:73:LYS:HE3	13:I:86:GLU:OE2	2.20	0.41
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	2.03	0.41
23:S:65:LYS:HB2	23:S:76:ARG:HH21	1.86	0.41
31:a:37:G:H2'	31:a:38:C:C6	2.56	0.41
31:a:386:U:H2'	31:a:387:C:C6	2.56	0.41
31:a:467:U:C2	31:a:468:A:C8	3.09	0.41
31:a:636:G:O6	31:a:637:A:N6	2.53	0.41
31:a:641:U:C2	31:a:642:G:C8	3.09	0.41
31:a:922:G:C2	31:a:924:G:C8	3.09	0.41
31:a:1233:A:H2'	31:a:1234:C:C6	2.56	0.41
31:a:1325:C:C2	31:a:1326:A:C8	3.09	0.41
32:b:66:LYS:HG2	32:b:66:LYS:O	2.21	0.41
34:d:52:GLU:OE1	34:d:52:GLU:N	2.42	0.41
35:e:46:GLY:HA3	35:e:69:ASN:O	2.21	0.41
44:n:72:GLY:O	44:n:80:SER:HA	2.20	0.41
47:q:30:VAL:HG12	47:q:31:GLN:N	2.36	0.41
5:A:458:U:OP2	5:A:458:U:C6	2.73	0.41
5:A:636:G:H2'	5:A:637:U:O4'	2.21	0.41
5:A:1031:G:H2'	5:A:1032:U:O4'	2.20	0.41
5:A:1411:G:N2	5:A:1584:A:N1	2.68	0.41
5:A:2026:6MZ:O2'	5:A:2027:A:P	2.78	0.41
5:A:2076:G:H5'	27:W:19:SER:CB	2.51	0.41
10:F:9:ASN:HA	10:F:13:LYS:CG	2.51	0.41
10:F:135:GLN:H	10:F:149:ILE:HD11	1.86	0.41
31:a:1001:A:C5	31:a:1023:G:H1'	2.56	0.41
31:a:1191:U:H2'	31:a:1192:C:C6	2.56	0.41
32:b:188:ILE:HA	32:b:202:ILE:O	2.21	0.41
48:r:21:ILE:O	48:r:21:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:579:C:H2'	5:A:580:A:C8	2.55	0.40
5:A:605:U:H5	5:A:618:G:C5	2.39	0.40
5:A:1109:G:H2'	5:A:1110:U:O4'	2.21	0.40
5:A:1314:C:O2'	5:A:1315:C:H5'	2.20	0.40
7:C:66:ASP:OD1	7:C:66:ASP:C	2.65	0.40
12:H:41:GLU:HG2	12:H:42:ALA:N	2.37	0.40
18:N:31:ARG:HB2	18:N:102:ILE:HD11	2.03	0.40
18:N:63:THR:O	18:N:64:THR:OG1	2.26	0.40
22:R:92:ARG:CZ	22:R:94:ASP:OD1	2.68	0.40
31:a:703:A:C5	31:a:704:U:C5	3.09	0.40
31:a:1060:C:H3'	31:a:1061:G:H2'	2.03	0.40
32:b:81:ILE:HD12	32:b:81:ILE:H	1.85	0.40
32:b:83:ARG:O	32:b:87:GLN:HG2	2.21	0.40
51:u:18:ARG:O	51:u:20:LYS:N	2.54	0.40
5:A:871:C:C2	5:A:872:G:C8	3.09	0.40
5:A:2345:G:O6	5:A:2365:A:N6	2.54	0.40
23:S:2:ASN:OD1	23:S:2:ASN:O	2.39	0.40
31:a:671:G:H2'	31:a:672:A:H8	1.86	0.40
31:a:1515:MA6:H93	31:a:1516:MA6:H103	2.02	0.40
31:a:1527:G:C3'	31:a:1528:A:C8	3.04	0.40
5:A:161:A:H2'	5:A:162:A:C8	2.56	0.40
5:A:312:A:O2'	5:A:313:A:H2'	2.22	0.40
5:A:1104:G:O2'	5:A:1105:U:C6	2.74	0.40
5:A:1549:U:H2'	5:A:1550:G:O4'	2.21	0.40
5:A:2256:C:C2	5:A:2257:C:C5	3.09	0.40
11:G:3:ARG:HG2	11:G:6:LYS:NZ	2.36	0.40
11:G:13:ASN:OD1	11:G:14:GLY:N	2.48	0.40
31:a:502:G:H2'	31:a:503:G:C8	2.56	0.40
31:a:841:G:H4'	31:a:842:A:O4'	2.21	0.40
33:c:24:ALA:HB1	33:c:28:GLN:HG3	2.04	0.40
37:g:64:THR:O	37:g:68:LYS:HG3	2.21	0.40
43:m:5:ALA:HB1	43:m:65:THR:HG21	2.03	0.40
46:p:66:GLU:OE1	46:p:69:ARG:NH2	2.43	0.40
5:A:1854:A:C2	5:A:1881:A:C1'	3.04	0.40
5:A:2021:C:H2'	5:A:2022:U:C6	2.56	0.40
5:A:2039:C:O2	5:A:2039:C:H2'	2.20	0.40
5:A:2209:U:H4'	5:A:2210:C:OP2	2.21	0.40
6:B:23:A:H2'	6:B:23:A:N3	2.36	0.40
10:F:31:ILE:CD1	10:F:169:LEU:HD21	2.52	0.40
10:F:94:ASP:OD2	10:F:94:ASP:C	2.63	0.40
11:G:17:VAL:HG12	11:G:26:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:367:A:H2'	31:a:368:C:O4'	2.21	0.40
31:a:650:A:O4'	38:h:57:LYS:NZ	2.48	0.40
31:a:754:U:OP1	31:a:819:U:O2'	2.39	0.40
31:a:1025:C:O2'	31:a:1026:U:C5'	2.67	0.40
44:n:42:PHE:CZ	44:n:46:LEU:HD21	2.56	0.40
5:A:1815:A:H4'	5:A:1816:U:H3'	2.04	0.40
5:A:2062:C:O2'	5:A:2063:G:H5'	2.21	0.40
5:A:2775:U:H5"	5:A:2776:A:H2'	2.03	0.40
18:N:16:ARG:HH22	18:N:94:SER:CA	2.35	0.40
31:a:144:G:C6	31:a:170:A:N1	2.90	0.40
31:a:202:U:N3	31:a:208:G:O6	2.54	0.40
31:a:522:C:OP1	42:l:86:ARG:NH2	2.55	0.40
31:a:933:C:O2	31:a:933:C:H2'	2.21	0.40
31:a:1378:U:H3'	31:a:1378:U:O2	2.22	0.40
34:d:175:VAL:HG23	34:d:182:GLY:CA	2.51	0.40
37:g:20:SER:OG	37:g:23:ILE:HB	2.22	0.40
40:j:57:VAL:O	40:j:58:ASN:HB2	2.21	0.40
51:u:18:ARG:C	51:u:20:LYS:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	46/51 (90%)	45 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	C	269/274 (98%)	261 (97%)	8 (3%)	0	100	100
8	D	208/212 (98%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	163 (95%)	8 (5%)	1 (1%)	21	34
11	G	172/177 (97%)	170 (99%)	1 (1%)	1 (1%)	21	34
12	H	58/148 (39%)	56 (97%)	2 (3%)	0	100	100
13	I	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18	30
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	112/116 (97%)	112 (100%)	0	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
23	S	88/106 (83%)	88 (100%)	0	0	100	100
24	T	101/105 (96%)	96 (95%)	5 (5%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	211 (95%)	11 (5%)	1 (0%)	30	45
33	c	213/250 (85%)	202 (95%)	11 (5%)	0	100	100
34	d	205/208 (99%)	198 (97%)	7 (3%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
36	f	102/127 (80%)	96 (94%)	6 (6%)	0	100	100
37	g	132/156 (85%)	130 (98%)	2 (2%)	0	100	100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
42	l	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	76/85 (89%)	76 (100%)	0	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	55/71 (78%)	52 (94%)	3 (6%)	0	100	100
All	All	5399/5872 (92%)	5260 (97%)	135 (2%)	4 (0%)	49	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	137	VAL
11	G	13	ASN
16	L	79	LEU
32	b	8	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	44 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	217/220 (99%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	144 (100%)	0	100	100
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	117/118 (99%)	117 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	59/64 (92%)	59 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	46/50 (92%)	46 (100%)	0	100	100
32	b	185/200 (92%)	185 (100%)	0	100	100
33	c	175/198 (88%)	174 (99%)	1 (1%)	78	88
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	94 (100%)	0	100	100
37	g	113/128 (88%)	113 (100%)	0	100	100
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	70/76 (92%)	70 (100%)	0	100	100
48	r	46/66 (70%)	46 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	48/62 (77%)	48 (100%)	0	100	100
All	All	4470/4756 (94%)	4469 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	c	100	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	53	HIS
7	C	143	ASN
8	D	65	GLN
8	D	176	GLN
9	E	162	ASN
10	F	63	GLN
13	I	58	ASN
15	K	101	ASN
16	L	46	GLN
19	O	15	GLN
19	O	32	GLN
20	P	56	GLN
20	P	101	HIS
22	R	62	ASN
24	T	9	GLN

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Mol	Chain	Res	Type
26	V	29	GLN
26	V	50	ASN
27	W	6	GLN
28	X	25	GLN
29	Y	8	GLN
29	Y	19	HIS
32	b	61	GLN
32	b	67	ASN
33	c	100	GLN
33	c	104	ASN
34	d	56	GLN
34	d	128	ASN
38	h	4	GLN
40	j	56	HIS
40	j	99	GLN
41	k	23	HIS
41	k	39	ASN
41	k	117	HIS
43	m	28	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	268 (17%)	0
5	A	2679/2918 (91%)	414 (15%)	37 (1%)
52	v	76/77 (98%)	30 (39%)	0
53	w	2/3 (66%)	0	0
6	B	114/115 (99%)	15 (13%)	2 (1%)
All	All	4398/4657 (94%)	727 (16%)	39 (0%)

All (727) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	53	G
5	A	58	G
5	A	67	G
5	A	78	A
5	A	80	A
5	A	81	A
5	A	82	G
5	A	92	G

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Mol	Chain	Res	Type
5	A	95	G
5	A	107	U
5	A	108	U
5	A	109	G
5	A	125	A
5	A	127	U
5	A	138	A
5	A	144	U
5	A	146	U
5	A	149	G
5	A	167	A
5	A	169	U
5	A	170	A
5	A	172	A
5	A	203	A
5	A	206	A
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	278	U
5	A	279	U
5	A	280	A
5	A	295	U
5	A	302	A
5	A	303	C
5	A	318	G
5	A	325	G
5	A	326	A
5	A	331	G
5	A	332	A
5	A	333	U
5	A	335	U
5	A	336	U
5	A	340	G
5	A	360	A
5	A	361	A

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Mol	Chain	Res	Type
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	388	A
5	A	395	G
5	A	403	A
5	A	410	G
5	A	421	A
5	A	423	G
5	A	455	C
5	A	456	A
5	A	457	G
5	A	458	U
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	529	G
5	A	531	A
5	A	532	G
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	635	A
5	A	636	G

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Mol	Chain	Res	Type
5	A	643	U
5	A	651	U
5	A	653	A
5	A	666	A
5	A	675	A
5	A	680	G
5	A	684	U
5	A	714	A
5	A	721	C
5	A	724	G
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	787	A
5	A	799	G
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	843	G
5	A	857	G
5	A	864	A
5	A	874	C
5	A	908	A
5	A	912	C
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1006	A
5	A	1008	A

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Mol	Chain	Res	Type
5	A	1009	U
5	A	1010	C
5	A	1019	G
5	A	1020	U
5	A	1023	G
5	A	1031	G
5	A	1042	U
5	A	1043	A
5	A	1105	U
5	A	1106	C
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1136	G
5	A	1140	A
5	A	1166	A
5	A	1170	U
5	A	1172	U
5	A	1173	G
5	A	1179	G
5	A	1201	G
5	A	1242	A
5	A	1243	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1269	A
5	A	1270	A
5	A	1296	A
5	A	1297	A
5	A	1327	G
5	A	1336	G
5	A	1338	G
5	A	1347	U
5	A	1360	A

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Mol	Chain	Res	Type
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1411	G
5	A	1412	C
5	A	1414	A
5	A	1416	G
5	A	1417	A
5	A	1423	C
5	A	1447	G
5	A	1453	U
5	A	1455	U
5	A	1462	G
5	A	1463	A
5	A	1519	U
5	A	1520	A
5	A	1523	A
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1535	U
5	A	1542	A
5	A	1543	A
5	A	1544	G
5	A	1552	U
5	A	1553	G
5	A	1557	U
5	A	1564	A
5	A	1567	A
5	A	1574	U
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1583	C
5	A	1606	A
5	A	1609	C

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Mol	Chain	Res	Type
5	A	1615	C
5	A	1616	A
5	A	1617	G
5	A	1646	U
5	A	1662	A
5	A	1672	G
5	A	1691	U
5	A	1697	G
5	A	1698	A
5	A	1710	U
5	A	1725	U
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1734	G
5	A	1742	G
5	A	1746	G
5	A	1753	A
5	A	1754	A
5	A	1760	G
5	A	1769	A
5	A	1772	G
5	A	1776	A
5	A	1778	U
5	A	1787	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1844	A
5	A	1845	G
5	A	1849	A
5	A	1865	G
5	A	1868	A
5	A	1869	G
5	A	1872	A
5	A	1874	G
5	A	1881	A
5	A	1885	A

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Mol	Chain	Res	Type
5	A	1897	A
5	A	1902	G
5	A	1924	A
5	A	1933	A
5	A	1934	A
5	A	1936	U
5	A	1939	U
5	A	1951	U
5	A	1959	U
5	A	1960	G
5	A	1962	A
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2017	A
5	A	2019	C
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2059	C
5	A	2065	7MG
5	A	2076	G
5	A	2089	G
5	A	2094	U
5	A	2097	A
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2210	C
5	A	2221	A
5	A	2234	G
5	A	2235	G

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Mol	Chain	Res	Type
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2318	A
5	A	2321	A
5	A	2323	A
5	A	2332	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2348	A
5	A	2350	A
5	A	2355	C
5	A	2367	G
5	A	2375	G
5	A	2378	G
5	A	2379	G
5	A	2381	C
5	A	2397	U
5	A	2398	U
5	A	2399	C
5	A	2421	A
5	A	2422	A
5	A	2423	C
5	A	2424	G
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2428	A
5	A	2429	A
5	A	2430	A
5	A	2437	U
5	A	2444	A
5	A	2446	A

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Mol	Chain	Res	Type
5	A	2465	A
5	A	2468	G
5	A	2469	U
5	A	2472	A
5	A	2473	U
5	A	2474	A
5	A	2487	U
5	A	2488	U
5	A	2493	A
5	A	2494	C
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2509	A
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2526	A
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2551	U
5	A	2562	A
5	A	2563	G
5	A	2578	G
5	A	2581	U
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2606	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2636	G
5	A	2642	C
5	A	2650	A
5	A	2651	G
5	A	2652	U
5	A	2656	A
5	A	2657	G
5	A	2661	A

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Mol	Chain	Res	Type
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2740	G
5	A	2744	A
5	A	2746	A
5	A	2748	C
5	A	2761	A
5	A	2774	A
5	A	2776	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2814	U
5	A	2816	G
5	A	2829	U
5	A	2845	G
5	A	2857	U
5	A	2863	A
5	A	2875	A
5	A	2876	C
5	A	2897	C
6	B	13	A
6	B	22	G
6	B	23	A
6	B	29	C
6	B	39	C
6	B	43	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	102	A
6	B	105	C

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Mol	Chain	Res	Type
6	B	106	A
31	a	4	A
31	a	5	A
31	a	6	C
31	a	7	U
31	a	11	G
31	a	15	U
31	a	24	G
31	a	29	G
31	a	34	A
31	a	41	G
31	a	46	A
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	63	G
31	a	80	A
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	97	A
31	a	112	A
31	a	116	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	140	G
31	a	157	A
31	a	184	A
31	a	186	G
31	a	193	A
31	a	200	G
31	a	201	A
31	a	202	U
31	a	206	C
31	a	236	C
31	a	239	A
31	a	241	U

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Mol	Chain	Res	Type
31	a	242	A
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	289	G
31	a	302	A
31	a	324	C
31	a	340	A
31	a	341	C
31	a	342	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	380	C
31	a	394	U
31	a	402	G
31	a	407	A
31	a	408	A
31	a	410	A
31	a	418	A
31	a	419	U
31	a	424	G
31	a	425	U
31	a	426	A
31	a	435	U
31	a	444	A
31	a	448	G
31	a	452	A
31	a	457	A
31	a	458	G
31	a	461	A
31	a	464	A
31	a	465	C
31	a	468	A
31	a	469	G
31	a	477	G
31	a	479	A
31	a	481	G

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Mol	Chain	Res	Type
31	a	482	U
31	a	483	U
31	a	494	U
31	a	495	A
31	a	501	C
31	a	503	G
31	a	505	U
31	a	506	A
31	a	507	A
31	a	508	C
31	a	509	U
31	a	513	PSU
31	a	514	G
31	a	515	C
31	a	516	C
31	a	518	G
31	a	522	C
31	a	524	7MG
31	a	527	G
31	a	528	U
31	a	530	A
31	a	532	A
31	a	544	A
31	a	556	A
31	a	559	U
31	a	561	C
31	a	569	A
31	a	570	A
31	a	572	G
31	a	573	C
31	a	574	G
31	a	585	G
31	a	593	A
31	a	615	C
31	a	623	G
31	a	625	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	685	G
31	a	699	A

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Mol	Chain	Res	Type
31	a	701	A
31	a	720	U
31	a	721	G
31	a	728	G
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	781	A
31	a	790	U
31	a	791	A
31	a	809	G
31	a	810	U
31	a	812	A
31	a	813	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	825	A
31	a	842	A
31	a	864	G
31	a	868	U
31	a	882	G
31	a	887	G
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	935	A
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	968	G
31	a	970	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	993	A
31	a	1000	A
31	a	1001	A

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Mol	Chain	Res	Type
31	a	1002	A
31	a	1003	C
31	a	1006	U
31	a	1010	G
31	a	1023	G
31	a	1025	C
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1033	A
31	a	1034	C
31	a	1039	A
31	a	1040	U
31	a	1041	A
31	a	1042	C
31	a	1048	C
31	a	1050	G
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1068	C
31	a	1070	U
31	a	1081	G
31	a	1082	U
31	a	1084	G
31	a	1091	G
31	a	1098	A
31	a	1122	U
31	a	1127	A
31	a	1129	C
31	a	1134	C
31	a	1135	G
31	a	1136	G
31	a	1140	G
31	a	1141	G
31	a	1156	U
31	a	1157	G
31	a	1164	A
31	a	1165	C
31	a	1166	A

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Mol	Chain	Res	Type
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1185	A
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1198	A
31	a	1209	U
31	a	1210	A
31	a	1235	A
31	a	1253	U
31	a	1255	G
31	a	1267	U
31	a	1275	U
31	a	1276	A
31	a	1277	A
31	a	1278	U
31	a	1282	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1300	C
31	a	1317	C
31	a	1335	G
31	a	1342	U
31	a	1343	A
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1375	C
31	a	1378	U
31	a	1380	C
31	a	1381	C
31	a	1387	U
31	a	1394	C
31	a	1395	A
31	a	1399	4OC
31	a	1415	A
31	a	1416	G

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Mol	Chain	Res	Type
31	a	1421	U
31	a	1423	G
31	a	1427	C
31	a	1439	G
31	a	1443	A
31	a	1445	C
31	a	1448	C
31	a	1449	A
31	a	1484	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1504	A
31	a	1513	G
31	a	1514	G
31	a	1526	G
31	a	1527	G
52	v	8	4SU
52	v	10	G
52	v	11	C
52	v	12	U
52	v	14	A
52	v	15	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	22	A
52	v	23	G
52	v	29	C
52	v	34	U
52	v	37	U
52	v	46	G
52	v	47	G
52	v	48	U
52	v	49	C
52	v	52	A
52	v	56	PSU
52	v	57	C
52	v	58	A
52	v	60	G

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Mol	Chain	Res	Type
52	v	62	C
52	v	65	G
52	v	74	A
52	v	76	C
52	v	77	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	79	A
5	A	84	U
5	A	91	A
5	A	256	C
5	A	324	A
5	A	332	A
5	A	334	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	424	G
5	A	457	G
5	A	463	U
5	A	478	A
5	A	507	U
5	A	642	A
5	A	720	A
5	A	782	G
5	A	799	G
5	A	929	C
5	A	1127	U
5	A	1179	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1337	A
5	A	1519	U
5	A	1697	G
5	A	1816	U
5	A	1880	G
5	A	2088	U
5	A	2209	U
5	A	2342	A

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Mol	Chain	Res	Type
5	A	2422	A
5	A	2525	G
5	A	2651	G
5	A	2747	G
6	B	50	A
6	B	86	U

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PSU	A	952	5	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
31	2MG	a	963	31	23,26,27	0.48	0	33,38,41	0.52	0
52	5MU	v	55	52	19,22,23	0.37	0	27,32,35	0.56	0
5	2MG	A	2441	5	23,26,27	0.44	0	33,38,41	0.50	0
31	UR3	a	1495	31	19,22,23	2.93	6 (31%)	26,32,35	1.61	3 (11%)
31	PSU	a	513	31	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
52	PSU	v	56	52	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
31	MA6	a	1516	31	23,26,27	1.40	4 (17%)	33,38,41	3.34	12 (36%)
5	OMG	A	2247	52,5	23,26,27	0.44	0	32,38,41	0.48	0
31	MA6	a	1515	31	23,26,27	1.37	4 (17%)	33,38,41	3.32	12 (36%)
5	PSU	A	2500	5	18,21,22	1.15	1 (5%)	21,30,33	1.95	5 (23%)
5	PSU	A	2453	5	18,21,22	1.13	1 (5%)	21,30,33	1.97	6 (28%)
5	PSU	A	2601	5	18,21,22	1.10	1 (5%)	21,30,33	1.92	5 (23%)
5	OMU	A	2548	5	19,22,23	3.11	8 (42%)	25,31,34	1.79	5 (20%)
5	6MZ	A	2026	5	22,25,26	2.44	4 (18%)	29,36,39	3.34	12 (41%)
5	PSU	A	2576	5	18,21,22	1.16	1 (5%)	21,30,33	1.91	6 (28%)
52	H2U	v	20	52	18,21,22	0.55	0	19,30,33	1.12	1 (5%)
5	7MG	A	2065	5	23,26,27	1.08	1 (4%)	27,39,42	0.90	2 (7%)
52	4SU	v	8	52	18,21,22	4.51	8 (44%)	25,30,33	2.39	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	5MC	a	964	31	19,22,23	0.53	0	26,32,35	0.61	0
5	5MU	A	1935	5	19,22,23	0.40	0	27,32,35	0.51	0
31	7MG	a	524	31	23,26,27	1.10	1 (4%)	27,39,42	0.88	2 (7%)
5	2MA	A	2499	5	22,25,26	3.97	9 (40%)	32,37,40	2.71	11 (34%)
31	4OC	a	1399	31	20,23,24	3.19	8 (40%)	25,32,35	0.89	1 (4%)
31	2MG	a	1204	31	23,26,27	0.46	0	33,38,41	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	2MG	a	963	31	-	2/9/27/28	0/3/3/3
52	5MU	v	55	52	-	3/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	2/7/25/26	0/2/2/2
52	PSU	v	56	52	-	2/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	5/11/29/30	0/3/3/3
5	OMG	A	2247	52,5	-	1/9/27/28	0/3/3/3
31	MA6	a	1515	31	-	3/11/29/30	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2
5	6MZ	A	2026	5	-	0/9/27/28	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
52	H2U	v	20	52	-	4/7/38/39	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
52	4SU	v	8	52	-	5/7/25/26	0/2/2/2
31	5MC	a	964	31	-	2/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3
5	2MA	A	2499	5	-	5/7/25/26	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
31	2MG	a	1204	31	-	2/9/27/28	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C4-N3	12.19	1.50	1.34
52	v	8	4SU	C2-N1	10.28	1.54	1.38
5	A	2026	6MZ	C6-N6	9.97	1.45	1.34
52	v	8	4SU	C4-N3	8.70	1.46	1.37
5	A	2499	2MA	C2-N3	7.49	1.46	1.34
5	A	2548	OMU	C2-N1	7.36	1.50	1.38
31	a	1495	UR3	C2-N1	7.34	1.48	1.38
52	v	8	4SU	C5-C4	7.19	1.51	1.42
52	v	8	4SU	C2-N3	7.15	1.50	1.38
31	a	1399	4OC	C4-N3	7.14	1.44	1.32
5	A	2499	2MA	C6-N1	6.96	1.44	1.35
5	A	2548	OMU	C2-N3	6.93	1.50	1.38
31	a	1495	UR3	C6-C5	6.73	1.50	1.35
52	v	8	4SU	C6-C5	6.50	1.50	1.35
31	a	1399	4OC	C6-C5	6.31	1.49	1.35
31	a	1399	4OC	C2-N3	6.26	1.48	1.36
5	A	2499	2MA	C2-N1	6.04	1.44	1.34
5	A	2548	OMU	C6-C5	5.77	1.48	1.35
31	a	1495	UR3	C2-N3	5.64	1.50	1.39
31	a	1399	4OC	C4-N4	4.82	1.46	1.36
52	v	8	4SU	C4-S4	-4.80	1.60	1.68
5	A	2499	2MA	C5-C6	4.75	1.54	1.41
31	a	524	7MG	C5-N7	4.53	1.41	1.35
5	A	2065	7MG	C5-N7	4.52	1.41	1.35
5	A	2548	OMU	C4-N3	4.32	1.46	1.38
31	a	1399	4OC	C2-N1	4.19	1.48	1.40
31	a	1515	MA6	C6-N6	3.93	1.47	1.36
31	a	1516	MA6	C6-N6	3.90	1.47	1.36
5	A	2500	PSU	C6-C5	3.88	1.39	1.35
52	v	56	PSU	C6-C5	3.82	1.39	1.35
5	A	2576	PSU	C6-C5	3.80	1.39	1.35
5	A	952	PSU	C6-C5	3.69	1.39	1.35
5	A	2453	PSU	C6-C5	3.68	1.39	1.35
31	a	513	PSU	C6-C5	3.66	1.39	1.35
5	A	2601	PSU	C6-C5	3.63	1.39	1.35
31	a	1399	4OC	C5-C4	3.59	1.48	1.41
31	a	1495	UR3	C6-N1	3.40	1.46	1.38
5	A	2499	2MA	C6-N6	-3.35	1.25	1.34
31	a	1399	4OC	C6-N1	3.32	1.46	1.38
5	A	2026	6MZ	C5-N7	-2.99	1.33	1.39
31	a	1516	MA6	C5-C4	-2.95	1.33	1.39
5	A	2548	OMU	O4-C4	-2.89	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2548	OMU	C6-N1	2.89	1.45	1.38
31	a	1515	MA6	C5-C4	-2.82	1.34	1.39
5	A	2026	6MZ	C5-C4	-2.74	1.34	1.39
52	v	8	4SU	O2-C2	-2.73	1.18	1.23
52	v	8	4SU	C6-N1	2.71	1.44	1.38
31	a	1495	UR3	C4-N3	2.70	1.46	1.40
31	a	1399	4OC	O2-C2	-2.65	1.18	1.23
5	A	2548	OMU	C5-C4	2.54	1.49	1.43
5	A	2499	2MA	C5-N7	-2.51	1.34	1.39
5	A	2548	OMU	O2-C2	-2.40	1.18	1.23
31	a	1516	MA6	C5-N7	-2.37	1.34	1.39
5	A	2026	6MZ	C8-N9	-2.28	1.33	1.37
31	a	1515	MA6	C5-N7	-2.22	1.35	1.39
31	a	1495	UR3	C5-C4	2.21	1.49	1.43
5	A	2499	2MA	C4-N9	-2.21	1.33	1.37
31	a	1516	MA6	C8-N9	-2.17	1.33	1.37
5	A	2499	2MA	C8-N7	2.11	1.35	1.31
31	a	1515	MA6	C8-N9	-2.00	1.34	1.37

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1515	MA6	N1-C6-N6	-12.35	101.81	116.86
31	a	1516	MA6	N1-C6-N6	-12.28	101.89	116.86
5	A	2026	6MZ	C1'-N9-C8	8.59	146.17	127.09
5	A	2026	6MZ	C4-N9-C1'	-8.56	106.61	126.63
31	a	1515	MA6	C5-C6-N6	8.19	138.29	125.33
31	a	1516	MA6	C5-C6-N6	8.14	138.22	125.33
5	A	2499	2MA	C1'-N9-C8	-7.48	110.49	127.09
52	v	8	4SU	C4-N3-C2	-7.19	120.42	127.31
5	A	2026	6MZ	C5-C4-N3	-6.40	117.91	126.72
31	a	1515	MA6	N1-C2-N3	-5.65	120.02	128.58
5	A	2499	2MA	C5-C4-N3	-5.65	121.22	127.18
31	a	1516	MA6	N1-C2-N3	-5.64	120.05	128.58
5	A	2026	6MZ	N1-C2-N3	-5.61	120.08	128.58
5	A	2499	2MA	N9-C8-N7	-5.59	106.00	113.94
31	a	1495	UR3	C4-N3-C2	-5.52	120.14	124.58
5	A	2548	OMU	C4-N3-C2	-5.50	119.78	126.61
5	A	2499	2MA	C4-N9-C1'	5.17	138.73	126.63
52	v	8	4SU	C5-C4-N3	4.96	119.36	114.75
5	A	2453	PSU	C4-N3-C2	-4.94	119.57	126.37
5	A	2500	PSU	N1-C2-N3	4.91	120.34	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	C5-C4-N3	-4.90	119.96	126.72
5	A	2453	PSU	N1-C2-N3	4.90	120.34	115.17
31	a	513	PSU	C4-N3-C2	-4.87	119.66	126.37
52	v	56	PSU	N1-C2-N3	4.86	120.30	115.17
5	A	2601	PSU	C4-N3-C2	-4.86	119.68	126.37
5	A	2500	PSU	C4-N3-C2	-4.82	119.74	126.37
5	A	952	PSU	C4-N3-C2	-4.81	119.75	126.37
5	A	2499	2MA	C4-N9-C8	4.80	110.78	105.74
5	A	952	PSU	N1-C2-N3	4.80	120.23	115.17
52	v	56	PSU	C4-N3-C2	-4.78	119.78	126.37
5	A	2601	PSU	N1-C2-N3	4.76	120.19	115.17
31	a	513	PSU	N1-C2-N3	4.67	120.09	115.17
52	v	8	4SU	C1'-N1-C2	4.66	125.97	117.59
5	A	2576	PSU	C4-N3-C2	-4.66	119.96	126.37
31	a	1515	MA6	C5-C4-N3	-4.65	120.31	126.72
5	A	2576	PSU	N1-C2-N3	4.64	120.06	115.17
5	A	2026	6MZ	C4-C5-C6	4.53	120.55	116.78
31	a	1516	MA6	N9-C8-N7	-4.32	107.81	113.94
5	A	2026	6MZ	N3-C4-N9	4.31	134.49	127.17
31	a	1515	MA6	N9-C8-N7	-4.28	107.86	113.94
5	A	2499	2MA	N3-C4-N9	4.25	132.38	126.99
31	a	1516	MA6	C4-C5-C6	3.97	120.01	115.91
5	A	2026	6MZ	C2-N3-C4	3.94	121.44	111.83
52	v	8	4SU	N3-C2-N1	3.92	120.00	114.89
5	A	2548	OMU	N3-C2-N1	3.90	119.97	114.89
31	a	1515	MA6	C4-C5-C6	3.65	119.68	115.91
31	a	1495	UR3	C5-C4-N3	3.60	119.78	115.04
5	A	2026	6MZ	N9-C8-N7	-3.56	108.88	113.94
52	v	8	4SU	C5-C4-S4	-3.49	120.32	124.31
5	A	2548	OMU	C5-C4-N3	3.48	119.68	114.80
31	a	1515	MA6	C2-N1-C6	3.43	120.20	111.83
31	a	1516	MA6	C2-N1-C6	3.39	120.11	111.83
31	a	1516	MA6	C2-N3-C4	3.34	119.98	111.83
52	v	20	H2U	C5-C4-N3	-3.30	113.18	116.69
31	a	1515	MA6	C2-N3-C4	3.30	119.88	111.83
5	A	2499	2MA	C5-N7-C8	3.29	108.62	103.45
5	A	2499	2MA	N3-C2-N1	-3.28	119.98	125.77
31	a	1516	MA6	N3-C4-N9	3.00	132.28	127.17
52	v	56	PSU	O2-C2-N1	-3.00	119.69	122.79
5	A	2026	6MZ	C5-N7-C8	2.90	108.01	103.45
5	A	2500	PSU	O2-C2-N1	-2.90	119.80	122.79
31	a	1516	MA6	C5-N7-C8	2.88	107.98	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2601	PSU	O2-C2-N1	-2.88	119.82	122.79
31	a	1515	MA6	C5-N7-C8	2.86	107.94	103.45
5	A	2453	PSU	O2-C2-N1	-2.80	119.90	122.79
5	A	2548	OMU	O4-C4-C5	-2.78	120.37	125.16
31	a	513	PSU	O2-C2-N1	-2.75	119.95	122.79
5	A	2576	PSU	O2-C2-N1	-2.72	119.98	122.79
31	a	1515	MA6	N3-C4-N9	2.72	131.79	127.17
5	A	2500	PSU	C6-C5-C4	2.59	119.92	118.17
5	A	2026	6MZ	C5-C6-N1	2.52	120.86	118.15
52	v	56	PSU	C6-N1-C2	-2.51	120.36	122.69
5	A	2065	7MG	C4-C5-N7	2.50	108.33	105.38
31	a	524	7MG	C4-C5-N7	2.50	108.33	105.38
5	A	952	PSU	O2-C2-N1	-2.47	120.24	122.79
31	a	1516	MA6	C4-N9-C8	2.47	108.33	105.74
31	a	1495	UR3	C6-N1-C2	-2.45	119.80	121.80
52	v	8	4SU	C1'-N1-C6	-2.41	115.62	120.78
31	a	1515	MA6	C4-N9-C8	2.40	108.26	105.74
5	A	2576	PSU	O4'-C1'-C2'	2.40	108.47	105.15
5	A	2453	PSU	C6-N1-C2	-2.38	120.48	122.69
5	A	952	PSU	C6-N1-C2	-2.36	120.50	122.69
5	A	2026	6MZ	C9-N6-C6	-2.33	120.69	122.85
5	A	2576	PSU	C6-N1-C2	-2.32	120.53	122.69
5	A	2601	PSU	C6-N1-C2	-2.32	120.54	122.69
5	A	952	PSU	C6-C5-C4	2.30	119.73	118.17
5	A	2500	PSU	C6-N1-C2	-2.27	120.59	122.69
5	A	2453	PSU	C6-C5-C4	2.23	119.68	118.17
31	a	1515	MA6	C4-C5-N7	-2.22	108.04	110.58
31	a	1399	4OC	C6-C5-C4	2.22	119.68	117.00
52	v	56	PSU	O4'-C1'-C2'	2.20	108.20	105.15
31	a	524	7MG	C5-C4-N9	2.20	109.15	106.33
52	v	8	4SU	O2-C2-N3	-2.16	117.50	121.49
31	a	1516	MA6	C4-C5-N7	-2.16	108.11	110.58
5	A	2548	OMU	O2-C2-N1	-2.13	120.02	122.80
52	v	8	4SU	C6-N1-C2	-2.13	118.40	121.00
5	A	2065	7MG	C5-C4-N9	2.11	109.04	106.33
31	a	513	PSU	C6-N1-C2	-2.11	120.74	122.69
5	A	2576	PSU	C6-C5-C4	2.09	119.58	118.17
5	A	2499	2MA	CM2-C2-N1	2.09	120.25	117.13
5	A	2499	2MA	C4-C5-N7	-2.08	108.20	110.58
5	A	2601	PSU	C6-C5-C4	2.05	119.55	118.17
5	A	2453	PSU	O4'-C1'-C2'	2.04	107.98	105.15
5	A	2499	2MA	N6-C6-N1	2.04	119.78	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2026	6MZ	C4-C5-N7	-2.01	108.28	110.58

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
31	a	1515	MA6	C5-C6-N6-C9
31	a	1515	MA6	N1-C6-N6-C9
31	a	1516	MA6	C5-C6-N6-C9
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	56	PSU	C2'-C1'-C5-C4
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2548	OMU	O4'-C4'-C5'-O5'
52	v	8	4SU	C2'-C1'-N1-C6
52	v	8	4SU	C2'-C1'-N1-C2
31	a	513	PSU	C3'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
31	a	1204	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	8	4SU	C3'-C4'-C5'-O5'
5	A	2548	OMU	C3'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	1516	MA6	N1-C6-N6-C9
31	a	524	7MG	O4'-C4'-C5'-O5'
31	a	963	2MG	C3'-C4'-C5'-O5'
31	a	1516	MA6	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
31	a	1204	2MG	C3'-C4'-C5'-O5'
52	v	56	PSU	C4'-C5'-O5'-P
31	a	1515	MA6	C5-C6-N6-C10
31	a	964	5MC	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
31	a	1516	MA6	C5-C6-N6-C10
31	a	964	5MC	O4'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
52	v	8	4SU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
5	A	2499	2MA	C4'-C5'-O5'-P
5	A	2499	2MA	O4'-C1'-N9-C8
5	A	2065	7MG	O4'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C2
52	v	55	5MU	C2'-C1'-N1-C2
31	a	1516	MA6	C3'-C4'-C5'-O5'
5	A	2499	2MA	C2'-C1'-N9-C8

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	963	2MG	2	0
31	a	1495	UR3	1	0
31	a	513	PSU	1	0
31	a	1516	MA6	3	0
5	A	2247	OMG	1	0
31	a	1515	MA6	4	0
5	A	2026	6MZ	2	0
52	v	20	H2U	1	0
31	a	964	5MC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
55	80P	a	1601	56	45,45,45	3.67	21 (46%)	51,72,72	2.47	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	80P	a	1603	56	45,45,45	3.64	22 (48%)	51,72,72	2.46	18 (35%)
55	80P	a	1602	56	45,45,45	4.02	22 (48%)	51,72,72	2.50	19 (37%)

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
55	80P	a	1601	56	-	13/22/87/87	0/5/5/5
55	80P	a	1603	56	-	14/22/87/87	0/5/5/5
55	80P	a	1602	56	-	12/22/87/87	0/5/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	C08-C09	13.07	1.63	1.52
55	a	1603	80P	C08-C09	11.93	1.62	1.52
55	a	1601	80P	C08-C09	11.75	1.62	1.52
55	a	1602	80P	C08-C21	10.04	1.62	1.53
55	a	1601	80P	C21-C04	9.46	1.63	1.54
55	a	1602	80P	C21-C04	8.90	1.62	1.54
55	a	1601	80P	C08-C21	8.42	1.60	1.53
55	a	1603	80P	C08-C21	7.19	1.59	1.53
55	a	1602	80P	C04-N03	7.01	1.54	1.47
55	a	1603	80P	C04-N03	6.95	1.54	1.47
55	a	1602	80P	C06-C36	6.89	1.61	1.47
55	a	1601	80P	C04-N03	6.88	1.54	1.47
55	a	1603	80P	C06-C07	6.73	1.64	1.46
55	a	1603	80P	C21-C04	6.71	1.60	1.54
55	a	1603	80P	C06-C36	6.68	1.61	1.47
55	a	1602	80P	C08-C07	6.66	1.63	1.55
55	a	1602	80P	C06-C07	6.64	1.64	1.46
55	a	1601	80P	C04-C05	5.80	1.63	1.51
55	a	1601	80P	C06-C36	5.74	1.59	1.47
55	a	1601	80P	C08-C07	5.51	1.62	1.55
55	a	1603	80P	C08-C07	5.39	1.62	1.55
55	a	1601	80P	C06-C07	5.31	1.60	1.46
55	a	1603	80P	C04-C05	4.98	1.61	1.51
55	a	1602	80P	C18-C19	4.74	1.65	1.52
55	a	1602	80P	C04-C05	4.69	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1603	80P	C18-C17	4.64	1.58	1.51
55	a	1602	80P	C18-C17	4.50	1.58	1.51
55	a	1603	80P	C18-C19	4.38	1.64	1.52
55	a	1601	80P	C18-C19	3.95	1.63	1.52
55	a	1601	80P	C18-C17	3.89	1.57	1.51
55	a	1602	80P	C16-C17	3.76	1.46	1.40
55	a	1603	80P	C16-C17	3.74	1.46	1.40
55	a	1602	80P	C10-C11	3.73	1.55	1.46
55	a	1603	80P	C12-C11	3.57	1.55	1.46
55	a	1602	80P	C12-C11	3.45	1.55	1.46
55	a	1603	80P	C10-C11	3.43	1.54	1.46
55	a	1601	80P	C16-C17	3.33	1.45	1.40
55	a	1602	80P	C22-C16	3.25	1.59	1.51
55	a	1603	80P	C22-C16	3.18	1.59	1.51
55	a	1601	80P	C12-C11	3.18	1.54	1.46
55	a	1602	80P	C15-C26	3.00	1.56	1.52
55	a	1603	80P	C19-C10	3.00	1.54	1.51
55	a	1602	80P	C12-C13	2.97	1.46	1.41
55	a	1603	80P	C15-C26	2.84	1.56	1.52
55	a	1601	80P	C10-C11	2.81	1.53	1.46
55	a	1601	80P	C15-C26	2.73	1.56	1.52
55	a	1603	80P	C12-C13	2.72	1.45	1.41
55	a	1601	80P	C22-C16	2.63	1.57	1.51
55	a	1602	80P	C19-C10	2.61	1.54	1.51
55	a	1603	80P	C20-C19	2.57	1.59	1.53
55	a	1602	80P	C36-N38	2.53	1.40	1.33
55	a	1603	80P	C40-N03	2.51	1.54	1.47
55	a	1602	80P	C20-C19	2.50	1.58	1.53
55	a	1603	80P	C36-N38	2.48	1.40	1.33
55	a	1601	80P	C12-C13	2.48	1.45	1.41
55	a	1602	80P	C40-N03	2.40	1.54	1.47
55	a	1601	80P	C19-C10	2.36	1.54	1.51
55	a	1601	80P	C36-N38	2.32	1.40	1.33
55	a	1603	80P	C16-C15	2.28	1.43	1.40
55	a	1601	80P	C14-C15	2.23	1.43	1.39
55	a	1602	80P	C14-C15	2.22	1.43	1.39
55	a	1602	80P	C16-C15	2.20	1.43	1.40
55	a	1601	80P	C20-C19	2.20	1.58	1.53
55	a	1601	80P	C40-N03	2.15	1.53	1.47
55	a	1603	80P	C14-C15	2.09	1.43	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1603	80P	C11-C10-C09	8.82	125.77	118.80
55	a	1601	80P	C11-C10-C09	8.68	125.66	118.80
55	a	1602	80P	C11-C10-C09	8.44	125.47	118.80
55	a	1601	80P	C08-C21-C04	5.17	118.71	111.64
55	a	1601	80P	C18-C17-C16	4.91	127.57	119.75
55	a	1603	80P	C36-C06-C07	-4.88	115.19	120.97
55	a	1602	80P	C12-C11-C10	4.81	127.30	118.28
55	a	1602	80P	O33-C09-C08	-4.68	106.59	113.37
55	a	1603	80P	C18-C17-C16	4.59	127.06	119.75
55	a	1602	80P	C36-C06-C07	-4.54	115.60	120.97
55	a	1603	80P	C12-C11-C10	4.52	126.75	118.28
55	a	1602	80P	C08-C21-C04	4.35	117.59	111.64
55	a	1602	80P	C18-C17-C16	4.32	126.64	119.75
55	a	1601	80P	C12-C11-C10	4.31	126.36	118.28
55	a	1601	80P	C13-C12-C17	4.28	123.63	119.03
55	a	1603	80P	O33-C09-C08	-4.27	107.19	113.37
55	a	1602	80P	C13-C12-C17	4.14	123.48	119.03
55	a	1601	80P	C36-C06-C07	-4.12	116.10	120.97
55	a	1603	80P	C13-C12-C17	4.11	123.44	119.03
55	a	1601	80P	O33-C09-C08	-4.02	107.55	113.37
55	a	1603	80P	C08-C21-C04	3.73	116.74	111.64
55	a	1603	80P	O33-C09-C10	3.51	130.34	123.52
55	a	1601	80P	C20-C21-C04	-3.50	108.67	113.73
55	a	1602	80P	O33-C09-C10	3.41	130.14	123.52
55	a	1602	80P	C17-C18-C19	3.37	117.58	113.12
55	a	1602	80P	C20-C21-C04	-3.32	108.94	113.73
55	a	1601	80P	O33-C09-C10	3.28	129.88	123.52
55	a	1603	80P	F25-C22-C16	3.09	119.53	112.32
55	a	1602	80P	C13-C12-C11	-3.08	116.89	121.45
55	a	1602	80P	F25-C22-C16	3.08	119.50	112.32
55	a	1602	80P	O32-C11-C10	-3.06	115.82	121.14
55	a	1603	80P	C13-C12-C11	-3.04	116.95	121.45
55	a	1601	80P	F23-C22-C16	3.03	119.37	112.32
55	a	1601	80P	O32-C11-C10	-3.02	115.88	121.14
55	a	1603	80P	O32-C11-C10	-3.02	115.89	121.14
55	a	1602	80P	C08-C07-C06	2.90	120.36	115.75
55	a	1602	80P	O32-C11-C12	-2.87	116.88	122.06
55	a	1601	80P	C13-C12-C11	-2.82	117.28	121.45
55	a	1601	80P	C14-C13-C12	-2.79	117.79	120.92
55	a	1601	80P	O37-C36-N38	-2.79	116.64	122.89
55	a	1602	80P	O37-C36-N38	-2.67	116.90	122.89
55	a	1603	80P	O37-C36-N38	-2.65	116.95	122.89
55	a	1602	80P	C14-C13-C12	-2.63	117.97	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1603	80P	C14-C13-C12	-2.62	117.98	120.92
55	a	1603	80P	C20-C21-C04	-2.61	109.95	113.73
55	a	1603	80P	O32-C11-C12	-2.60	117.36	122.06
55	a	1603	80P	C08-C07-C06	2.40	119.57	115.75
55	a	1601	80P	O32-C11-C12	-2.38	117.76	122.06
55	a	1603	80P	F23-C22-C16	2.18	117.39	112.32
55	a	1602	80P	F23-C22-C16	2.16	117.35	112.32
55	a	1603	80P	C17-C18-C19	2.11	115.92	113.12
55	a	1602	80P	O35-C07-C08	-2.09	115.14	119.11

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	a	1601	80P	C05-C04-N03-C01
55	a	1601	80P	C21-C04-N03-C40
55	a	1601	80P	C14-C15-C26-N27
55	a	1601	80P	C16-C15-C26-C30
55	a	1601	80P	C16-C15-C26-N27
55	a	1602	80P	C05-C06-C36-N38
55	a	1602	80P	C05-C06-C36-O37
55	a	1602	80P	C07-C06-C36-N38
55	a	1602	80P	C07-C06-C36-O37
55	a	1603	80P	C05-C04-N03-C40
55	a	1603	80P	C05-C06-C36-N38
55	a	1603	80P	C05-C06-C36-O37
55	a	1603	80P	C16-C15-C26-C30
55	a	1601	80P	C21-C04-N03-C01
55	a	1602	80P	C41-C40-N03-C01
55	a	1601	80P	C05-C04-N03-C40
55	a	1602	80P	C05-C04-N03-C40
55	a	1603	80P	C15-C16-C22-F25
55	a	1603	80P	C21-C04-N03-C40
55	a	1603	80P	C17-C16-C22-F25
55	a	1601	80P	C41-C40-N03-C04
55	a	1602	80P	C41-C40-N03-C04
55	a	1603	80P	C14-C15-C26-N27
55	a	1601	80P	C41-C40-N03-C01
55	a	1601	80P	C15-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F25
55	a	1603	80P	C15-C16-C22-F24
55	a	1601	80P	C15-C16-C22-F24

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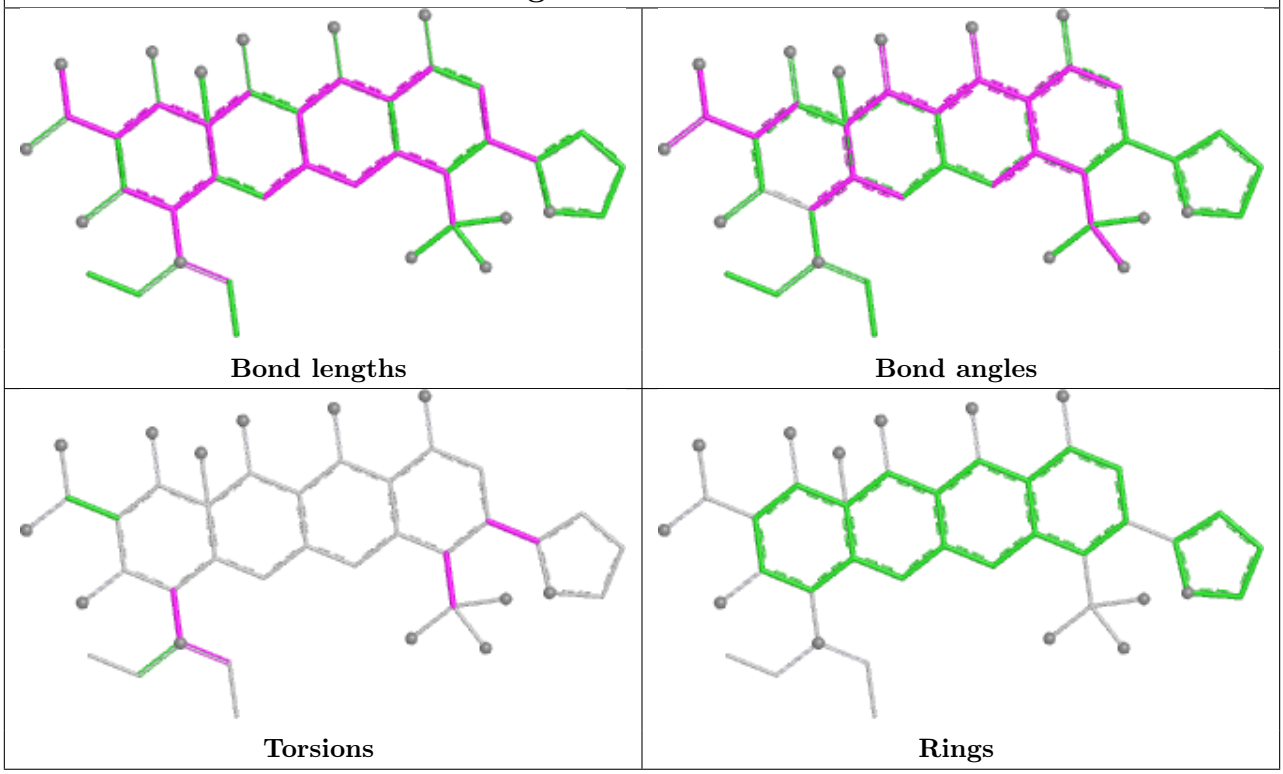
Mol	Chain	Res	Type	Atoms
55	a	1602	80P	C15-C16-C22-F24
55	a	1603	80P	C15-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F23
55	a	1603	80P	C21-C04-N03-C01
55	a	1601	80P	C15-C16-C22-F25
55	a	1603	80P	C17-C16-C22-F24
55	a	1603	80P	C17-C16-C22-F23
55	a	1602	80P	C17-C16-C22-F23
55	a	1601	80P	C14-C15-C26-C30
55	a	1603	80P	C16-C15-C26-N27
55	a	1602	80P	C17-C16-C22-F25

There are no ring outliers.

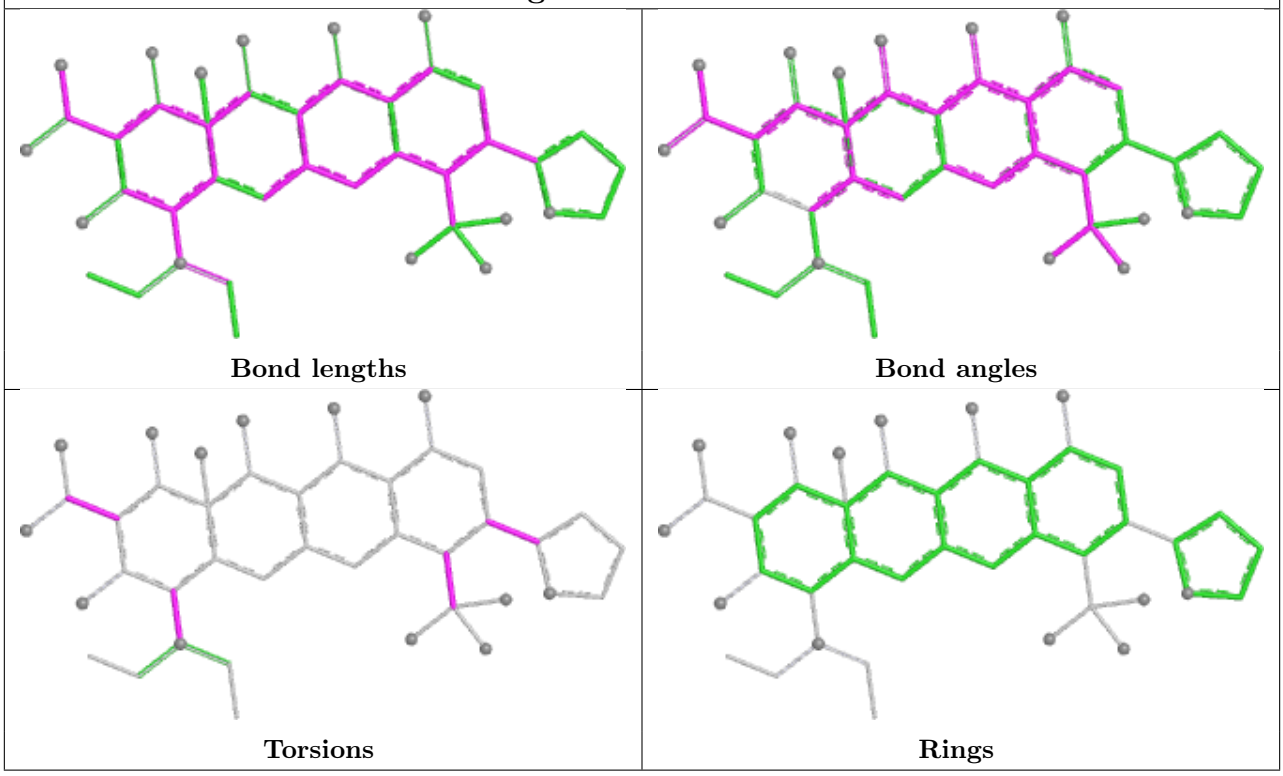
No monomer is involved in short contacts.

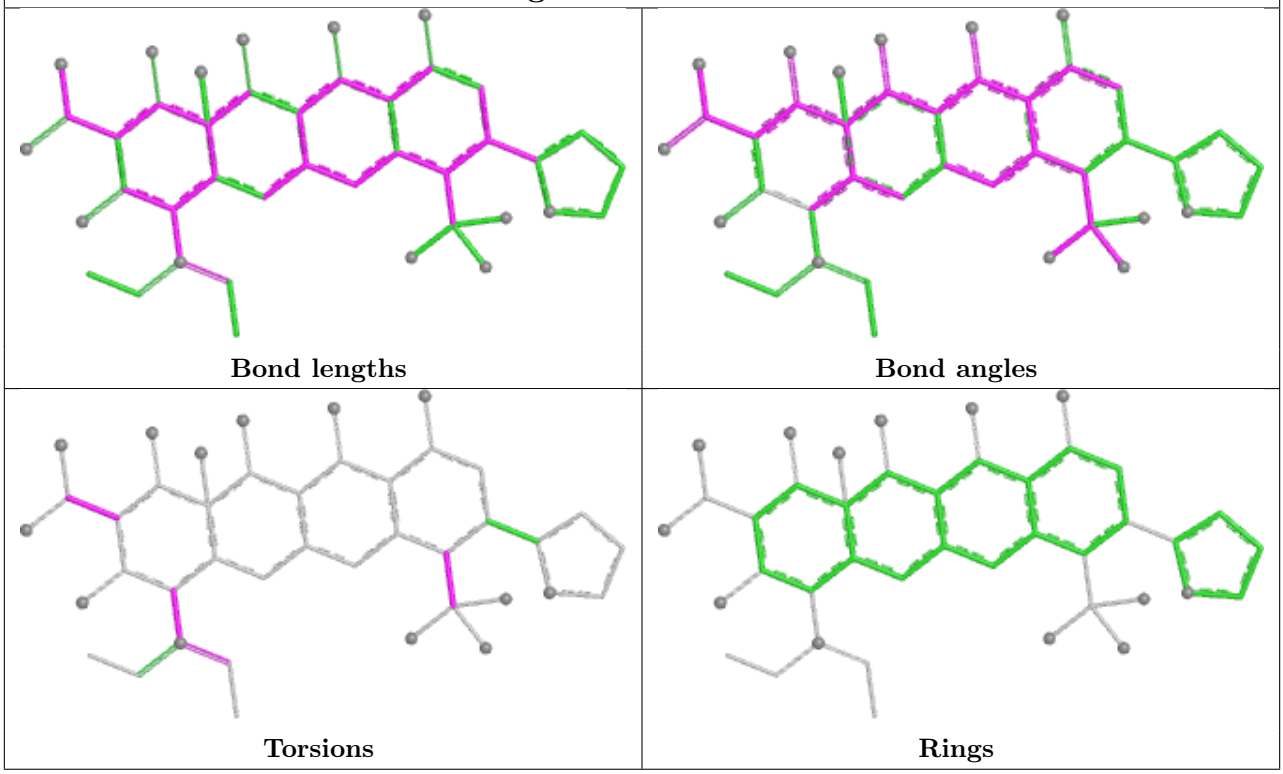
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 80P a 1601



Ligand 80P a 1603



Ligand 80P a 1602	
	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

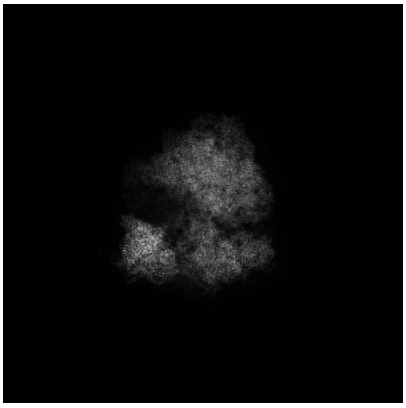
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24738. These allow visual inspection of the internal detail of the map and identification of artifacts.

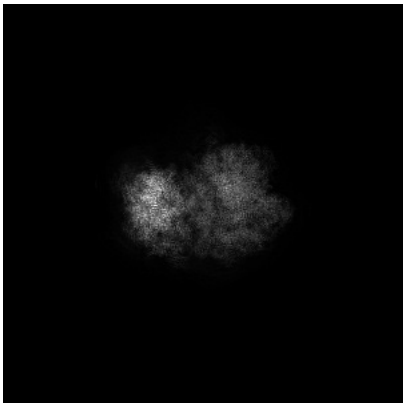
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

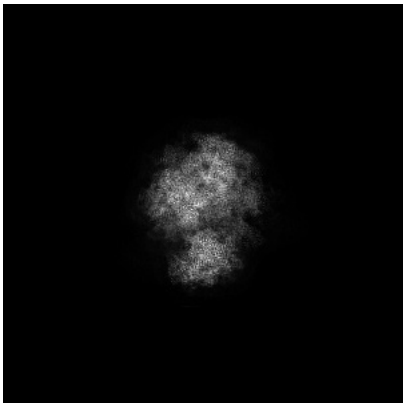
6.1.1 Primary map



X



Y

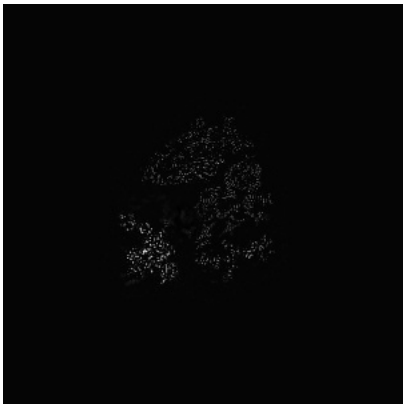


Z

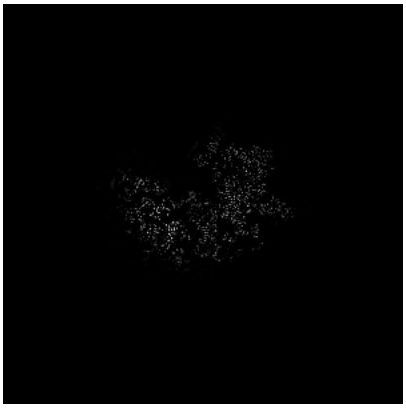
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

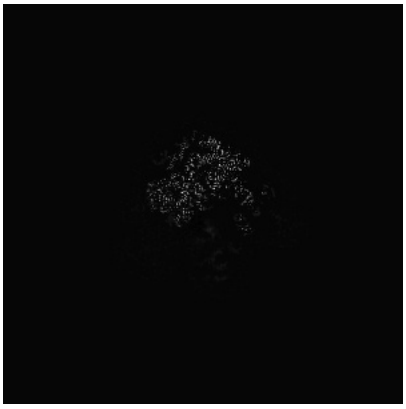
6.2.1 Primary map



X Index: 256



Y Index: 256



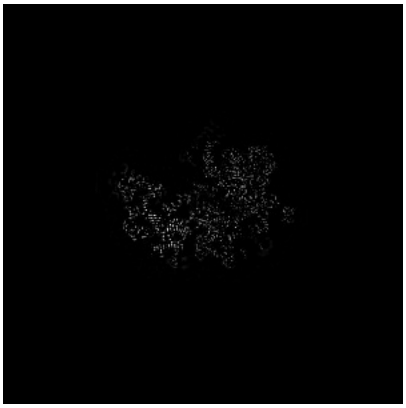
Z Index: 256

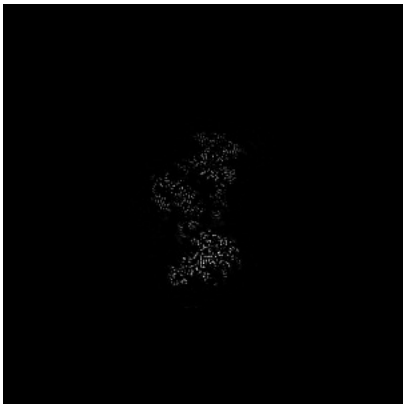
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 263

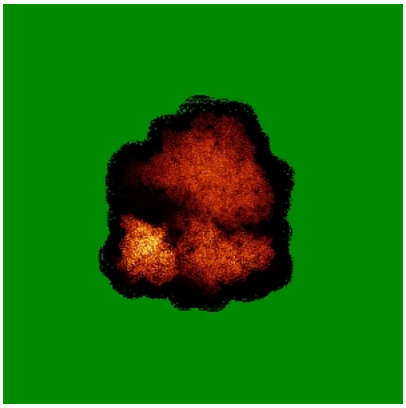

Y Index: 265

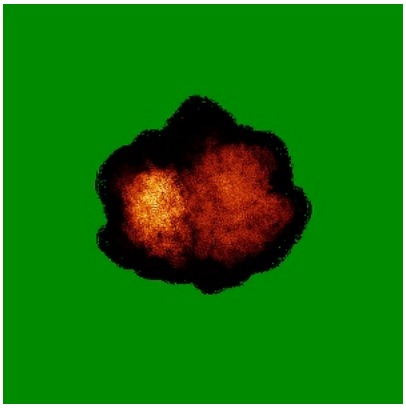

Z Index: 194

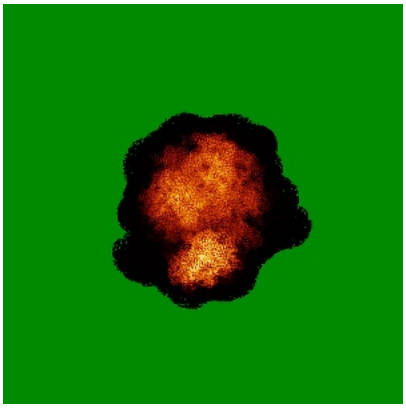
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

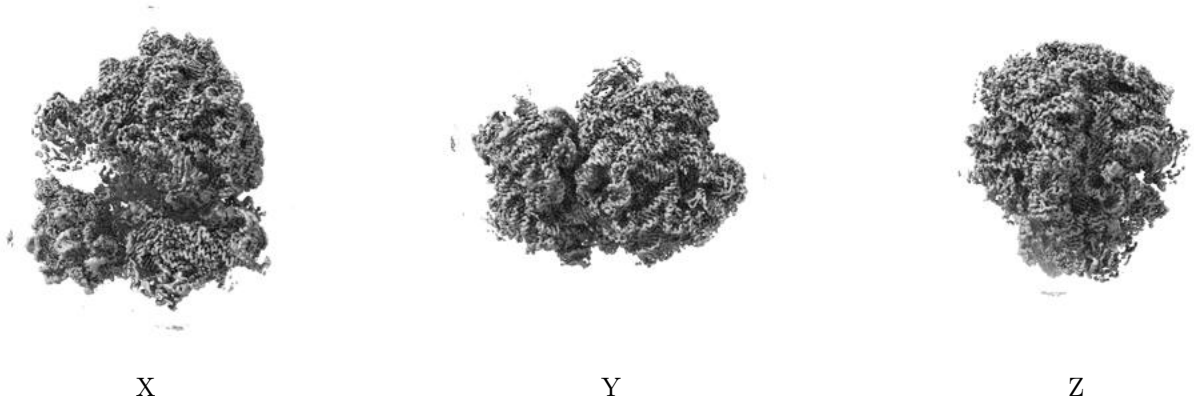

Y


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

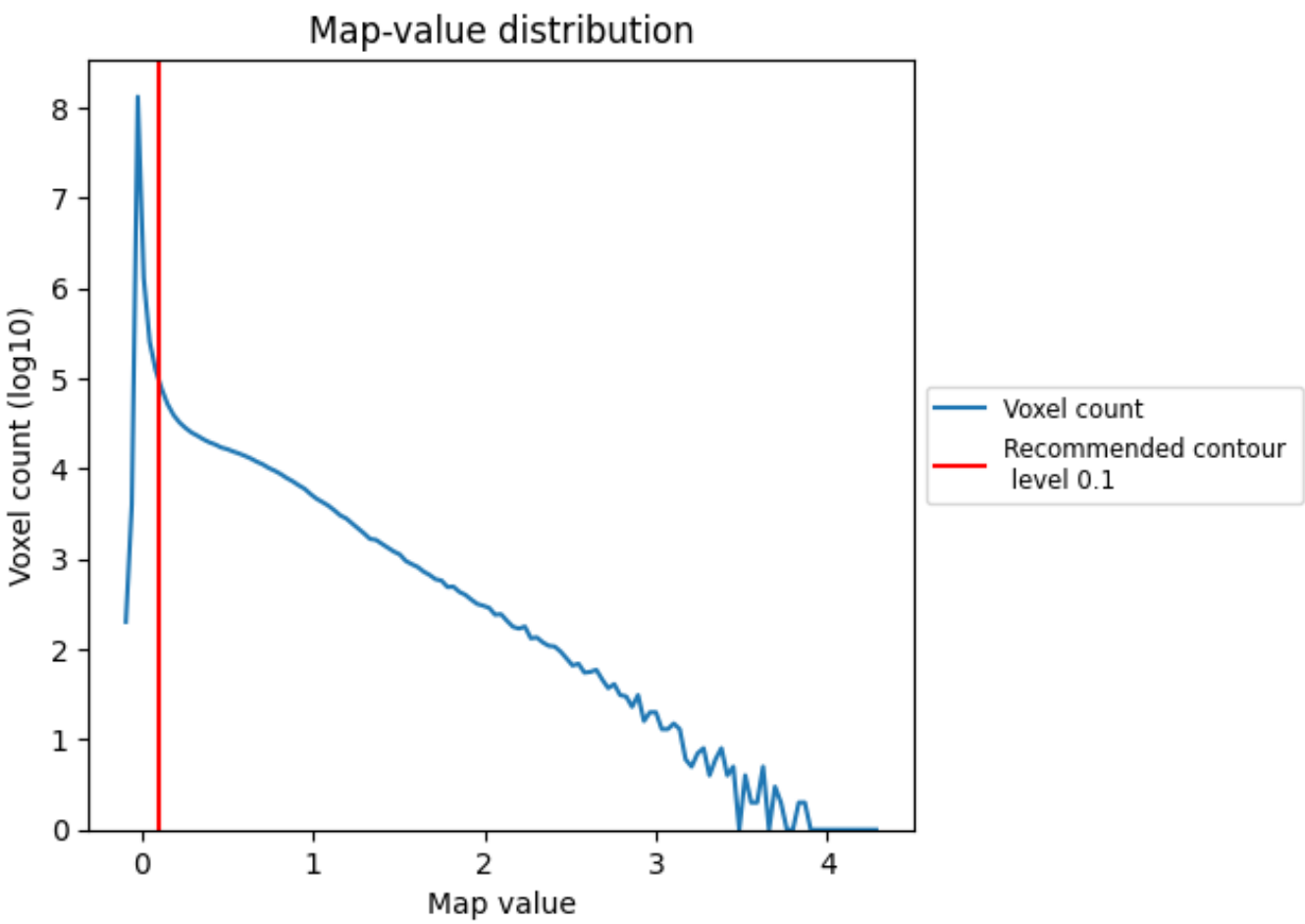
6.6 Mask visualisation (i)

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

7 Map analysis (i)

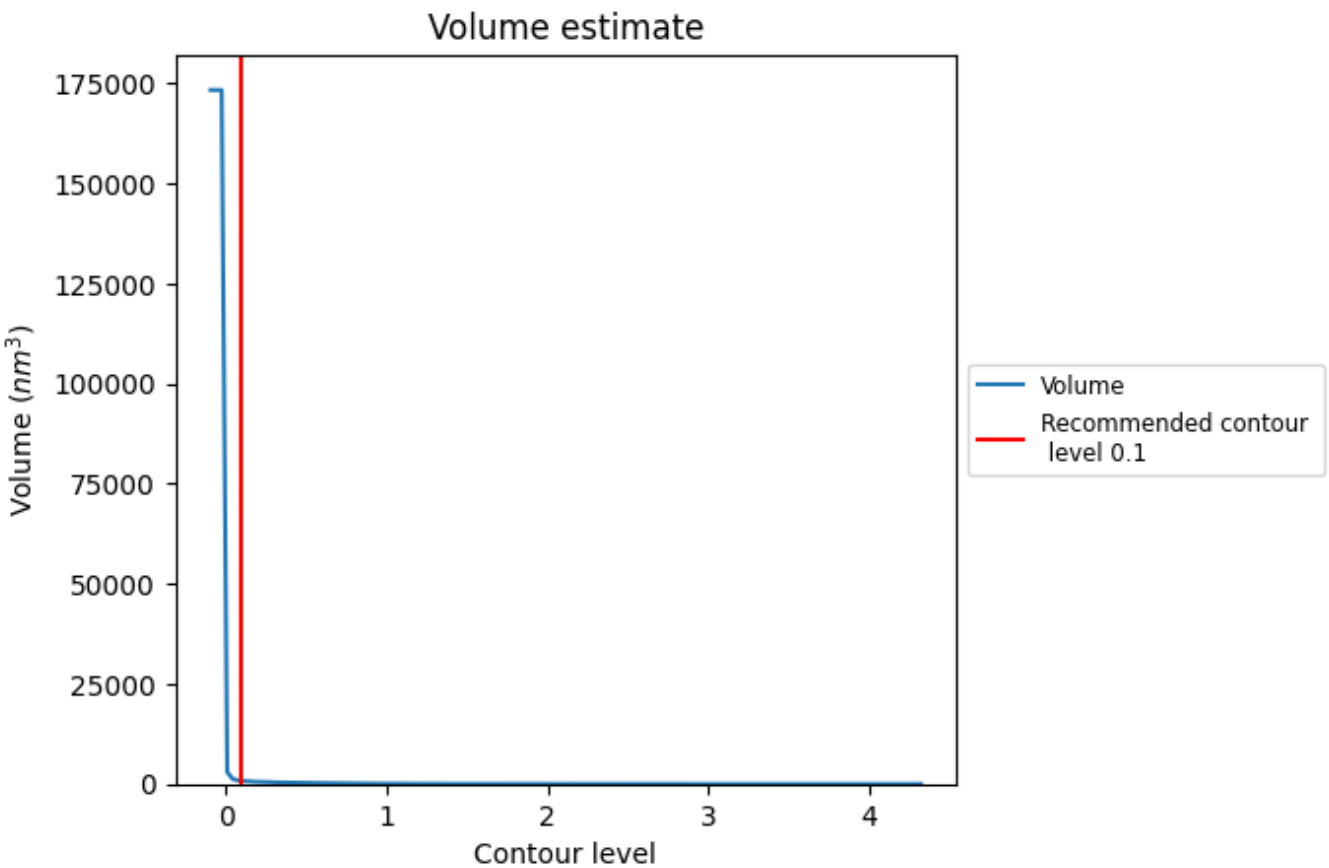
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

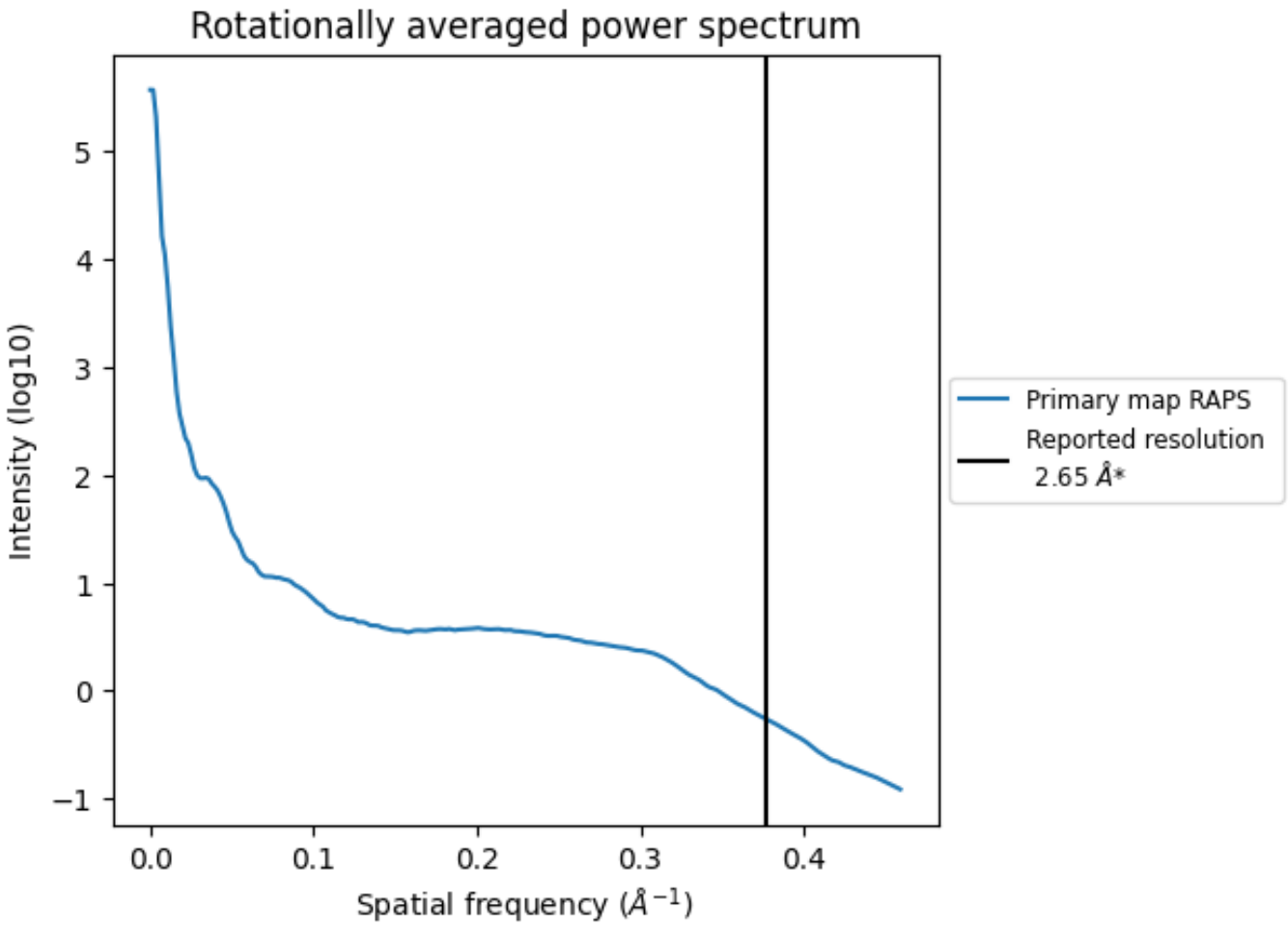
7.2 Volume estimate (i)



The volume at the recommended contour level is 789 nm^3; this corresponds to an approximate mass of 713 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 0.377 Å^{-1}

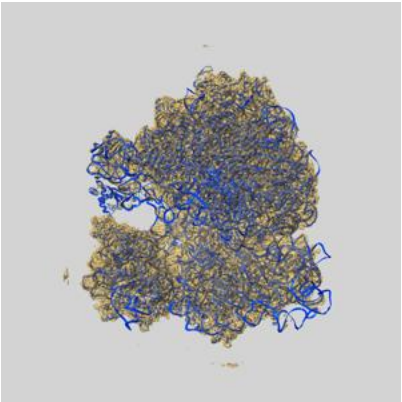
8 Fourier-Shell correlation (i)

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

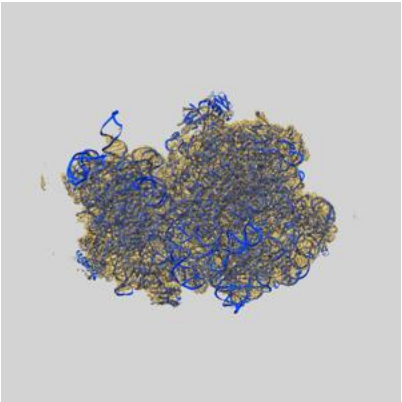
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24738 and PDB model 7RYF. Per-residue inclusion information can be found in section 3 on page 14.

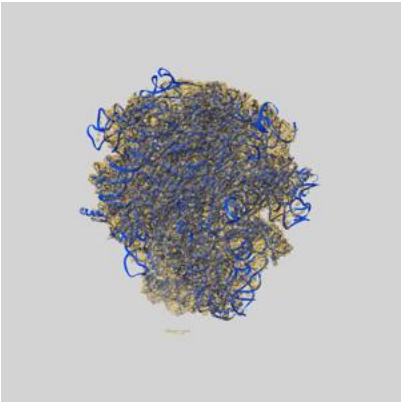
9.1 Map-model overlay (i)



X



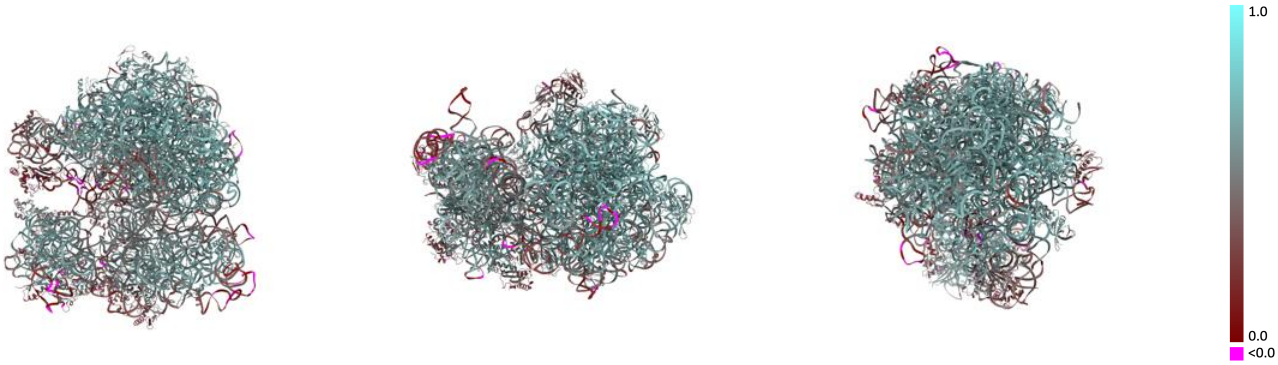
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

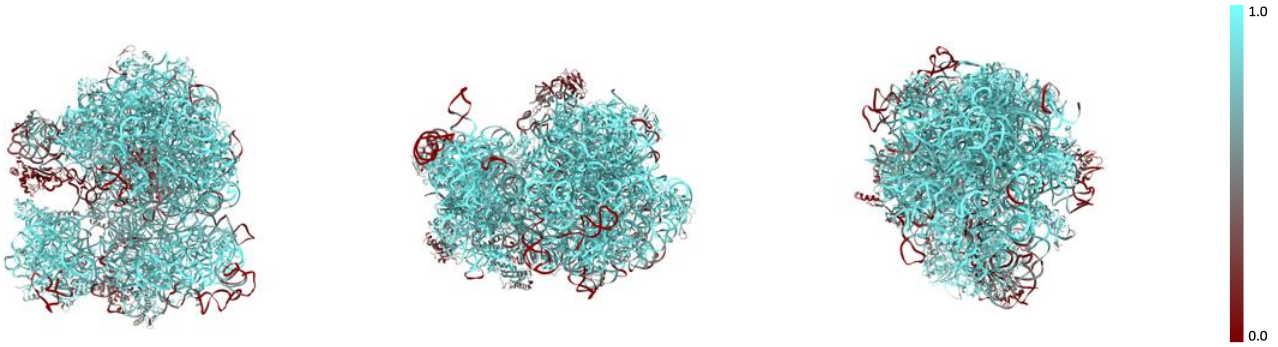
9.2 Q-score mapped to coordinate model (i)



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.

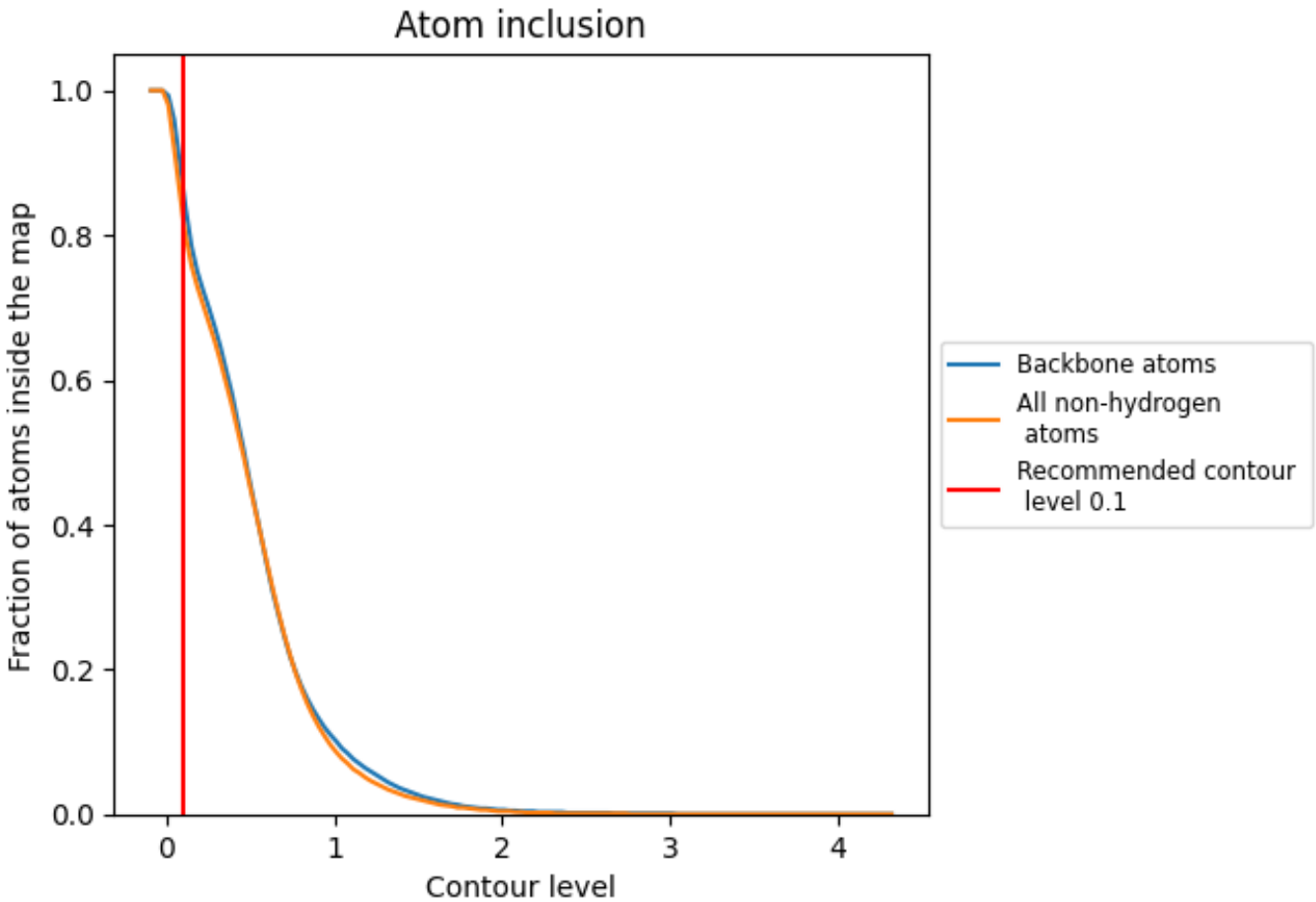
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.5410
0	0.7690	0.5310
1	0.9710	0.6830
2	0.8690	0.5990
3	0.6470	0.4940
A	0.8720	0.5910
B	0.5650	0.4400
C	0.9210	0.6280
D	0.9380	0.6570
E	0.8600	0.6160
F	0.0690	0.2250
G	0.2760	0.3480
H	0.3540	0.3450
I	0.9370	0.6580
J	0.9150	0.6250
K	0.9380	0.6450
L	0.8570	0.5830
M	0.9710	0.6830
N	0.5900	0.4030
O	0.8670	0.5880
P	0.9730	0.6920
Q	0.9050	0.6270
R	0.9260	0.6570
S	0.7700	0.5630
T	0.7100	0.5410
U	0.7990	0.5550
V	0.9140	0.6500
W	0.8860	0.6140
X	0.5900	0.4520
Y	0.8980	0.6240
Z	0.8760	0.6180
a	0.8400	0.5080
b	0.2730	0.2740
c	0.8860	0.5030
d	0.5550	0.3520

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Chain	Atom inclusion	Q-score
e	0.8980	0.5460
f	0.5620	0.3430
g	0.6950	0.3510
h	0.9440	0.5970
i	0.9520	0.5770
j	0.8730	0.5130
k	0.5110	0.3240
l	0.6490	0.4530
m	0.9170	0.5150
n	0.9290	0.5680
o	0.9060	0.5580
p	0.9080	0.5970
q	0.8430	0.5070
r	0.7870	0.4540
s	0.9560	0.5670
t	0.9170	0.5620
u	0.1720	0.2610
v	0.2930	0.1800
w	0.7690	0.3290