Full wwPDB EM Validation Report (i)

Dec 7, 2022 – 09:44 AM JST

PDB ID	:	5IMQ
EMDB ID	:	EMD-6584
Title	:	Structure of ribosome bound to cofactor at 3.8 angstrom resolution
Authors	:	Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.
Deposited on	:	2016-03-06
Resolution	:	3.80 Å(reported)
Based on initial models	:	4W2E, 5AA0

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

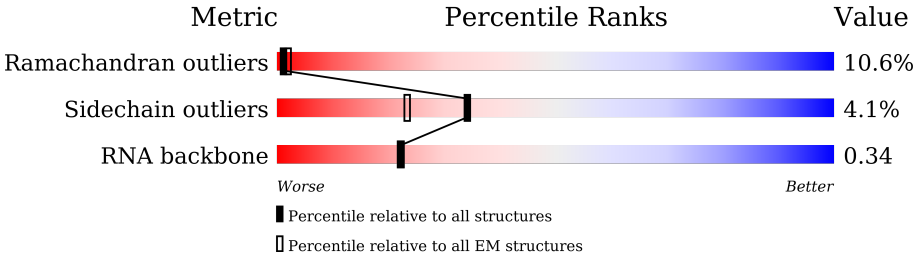
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	37	11%; 84%; 16%
2	2	173	66%; 70%; 5%; 25%
3	3	147	62%; 67%; 21%; •; 9%
4	4	77	12%; 62%; 38%
5	5	76	71%; 55%; 41%; •
6	A	1522	•; 61%; 37%; •
7	D	2893	•; 48%; 44%; 8%
8	E	123	•; 57%; 42%; •

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Mol	Chain	Length	Quality of chain
9	F	256	32% 82% 9% 9%
10	G	239	14% 80% 6% 14%
11	H	209	23% 90% 8%
12	I	162	87% 6% 7%
13	J	101	32% 93% 7%
14	K	156	33% 97%
15	L	138	7% 95% 5%
16	M	128	33% 93% 6%
17	N	105	33% 89% 5% 7%
18	O	129	23% 88% 8%
19	P	132	7% 87% 7% 6%
20	Q	126	46% 71% 17% 10%
21	R	61	11% 87% 10%
22	S	89	15% 96%
23	T	88	14% 90% 5% 6%
24	U	105	18% 93% 6%
25	V	88	33% 78% 5% 17%
26	W	93	47% 40% 41% 14%
27	X	106	10% 90% 7%
28	Y	27	15% 89% 11%
29	Z	229	90% 94% 5%
30	a	276	9% 85% 13%
31	b	206	7% 88% 12%
32	c	210	12% 90% 9%
33	d	182	25% 84% 16%

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Mol	Chain	Length	Quality of chain
34	e	180	12% 83% 13%
35	f	140	9% 88% 11%
36	g	122	11% 85% 15%
37	h	150	21% 79% 16%
38	i	141	9% 84% 13%
39	j	118	5% 93% 6%
40	k	112	16% 88% 10%
41	l	146	14% 66% 12% 20%
42	m	118	96%
43	n	101	19% 86% 14%
44	o	113	89% 8%
45	p	96	8% 91% 6%
46	q	110	16% 78% 22%
47	r	206	31% 77% 10% 13%
48	s	85	7% 91% 7%
49	t	67	93% 7%
50	u	60	88% 8%
51	v	71	11% 77% 21%
52	w	60	7% 77% 15% 5%
53	x	54	7% 56% 33% 9%
54	y	49	10% 88% 12%
55	z	65	11% 80% 14% 5%
56	B	610	30% 54% 37% 6%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 153046 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 L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	37	307	188	68	47	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	2	130	641	381	130	130	0	0

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	134	993	632	175	181	5	0	0

- Molecule 4 is a RNA chain called P- site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	77	1640	732	297	535	76	0	0

- Molecule 5 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	76	1623	723	290	534	76	0	0

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	1515	32554	14490	6022	10527	1515	0	0

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	D	2889	62218	27691	11629	20009	2889	0	0

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	E	123	2641	1175	488	855	123	0	0

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	234	1900	1213	341	341	5	0	0

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	206	1612	1016	314	281	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	208	1703	1066	339	291	7	0	0

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	150	1146	724	217	201	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	101	843	531	155	154	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	155	1257	781	252	218	6	0	0

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	138	1116	705	215	193	3	0	0

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	M	127	1010	639	197	174	0	0

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	98	794	499	156	138	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	119	885	549	168	165	3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	124	970	611	195	163	1	0	0

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	114	914	565	189	158	2	0	0

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	R	60	492	312	104	72	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	88	734	459	147	126	2	0	0

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	T	83	700	443	139	117	1	0	0

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U	104	857	547	161	147	2	0	0

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	V	73	597	380	118	99	0	0

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	80	647	414	119	112	2	0	0

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	X	99	763	470	162	129	2	0	0

- Molecule 28 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	Y	24	208	128	50	30	0	0

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Z	228	1742	1102	318	319	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	a	272	2124	1339	424	358	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	b	206	1578	997	302	273	6	0	0

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	208	1625	1034	303	286	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	d	182	1482	947	269	261	5	0	0

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	e	174	1328	844	248	235	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	139	1113	717	207	186	3	0	0

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	122	932	587	171	170	4	0	0

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	145	1106	688	226	190	2	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	136	1080	688	204	183	5	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	j	117	960	599	202	159	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	k	110	877	553	175	149	0	0

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	117	976	614	197	164	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	117	964	610	202	151	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	n	101	779	501	142	135	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	o	110	876	552	171	151	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	p	94	742	483	133	126	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	q	110	844	539	158	141	6	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	r	180	1435	916	256	260	3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	s	79	625	387	131	106	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	t	67	567	350	116	99	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	u	59	469	298	90	81	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	v	71	581	364	108	104	5	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	w	57	445	279	87	74	5	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	x	49	426	265	87	70	4	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	y	49	430	263	108	57	2	0	0

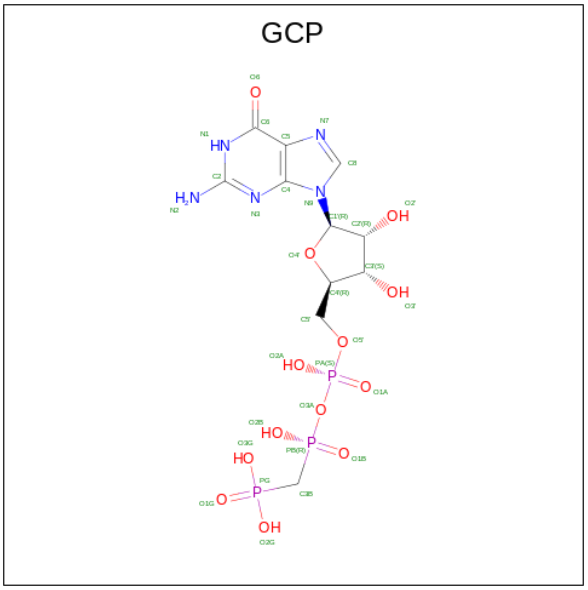
- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	z	64	515	331	102	79	3	0	0

- Molecule 56 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B	591	4628	2968	794	857	9	0	0

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



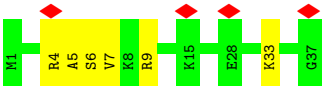
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	B	1	32	11	5	13	3	0

3 Residue-property plots (i)

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

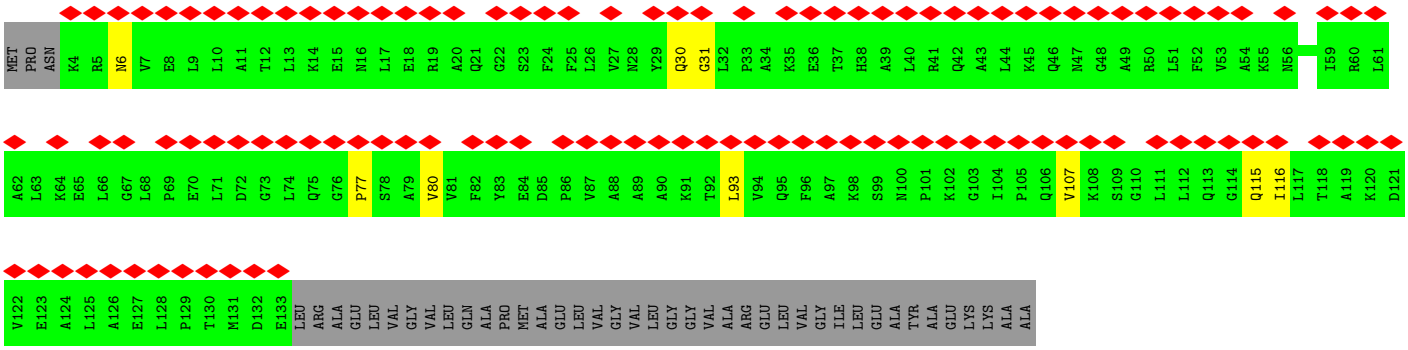
- Molecule 1: 50S ribosomal protein L36

Chain 1:



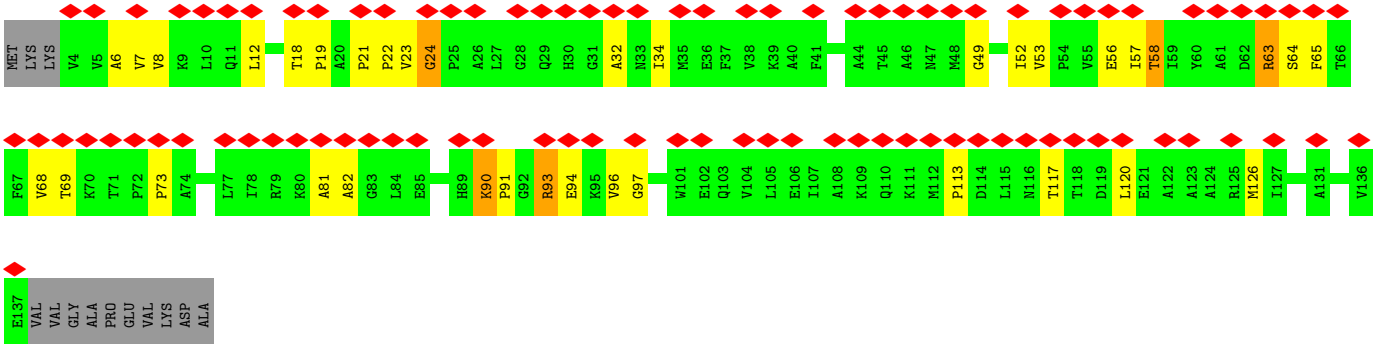
- Molecule 2: 50S ribosomal protein L10

Chain 2:



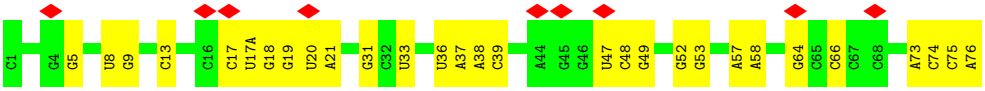
- Molecule 3: 50S ribosomal protein L11

Chain 3:



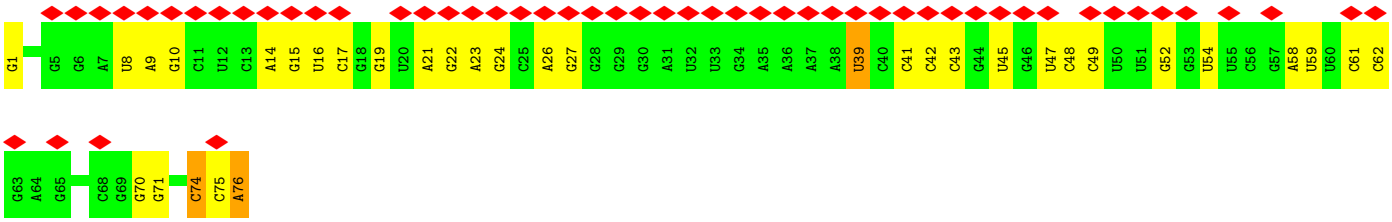
- Molecule 4: P- site tRNA

Chain 4:



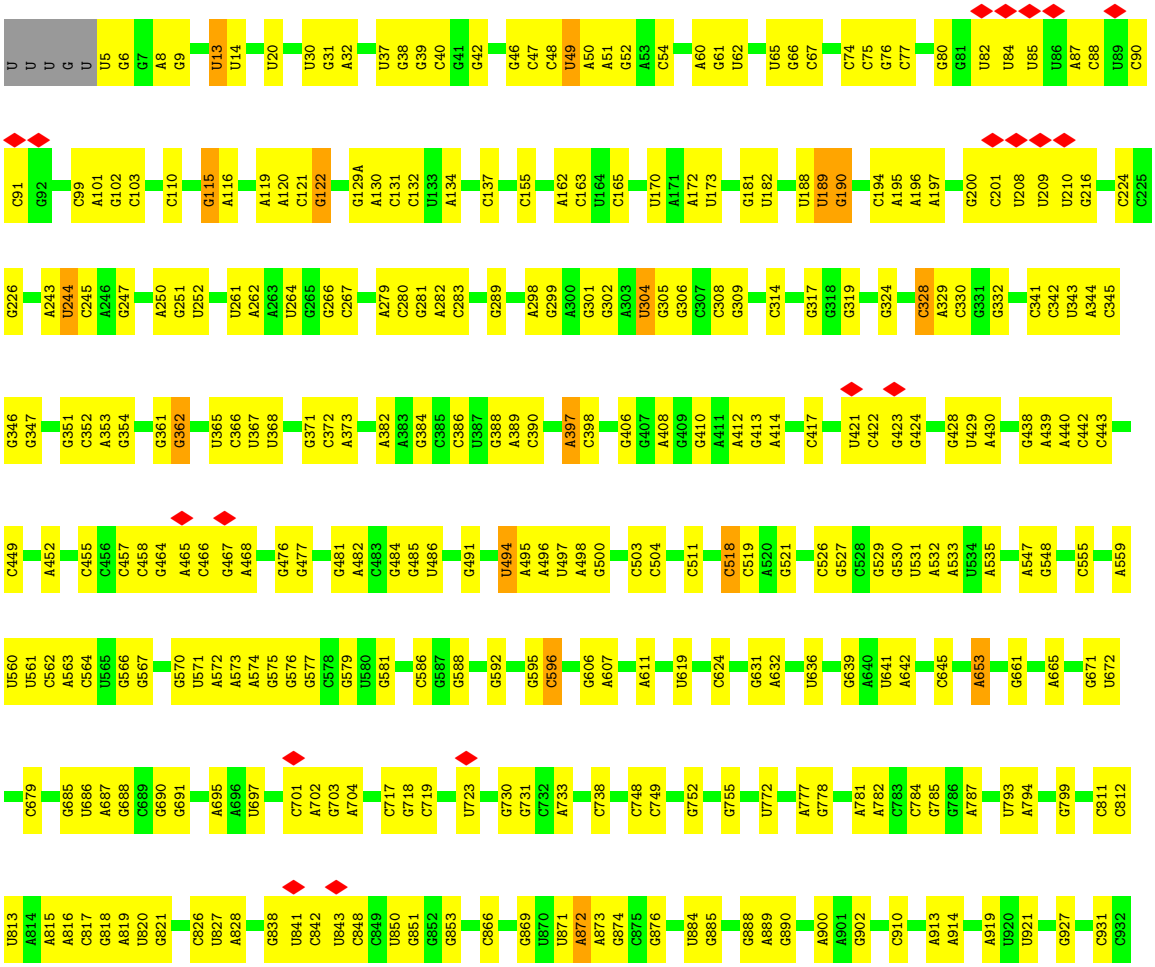
- Molecule 5: E site tRNA

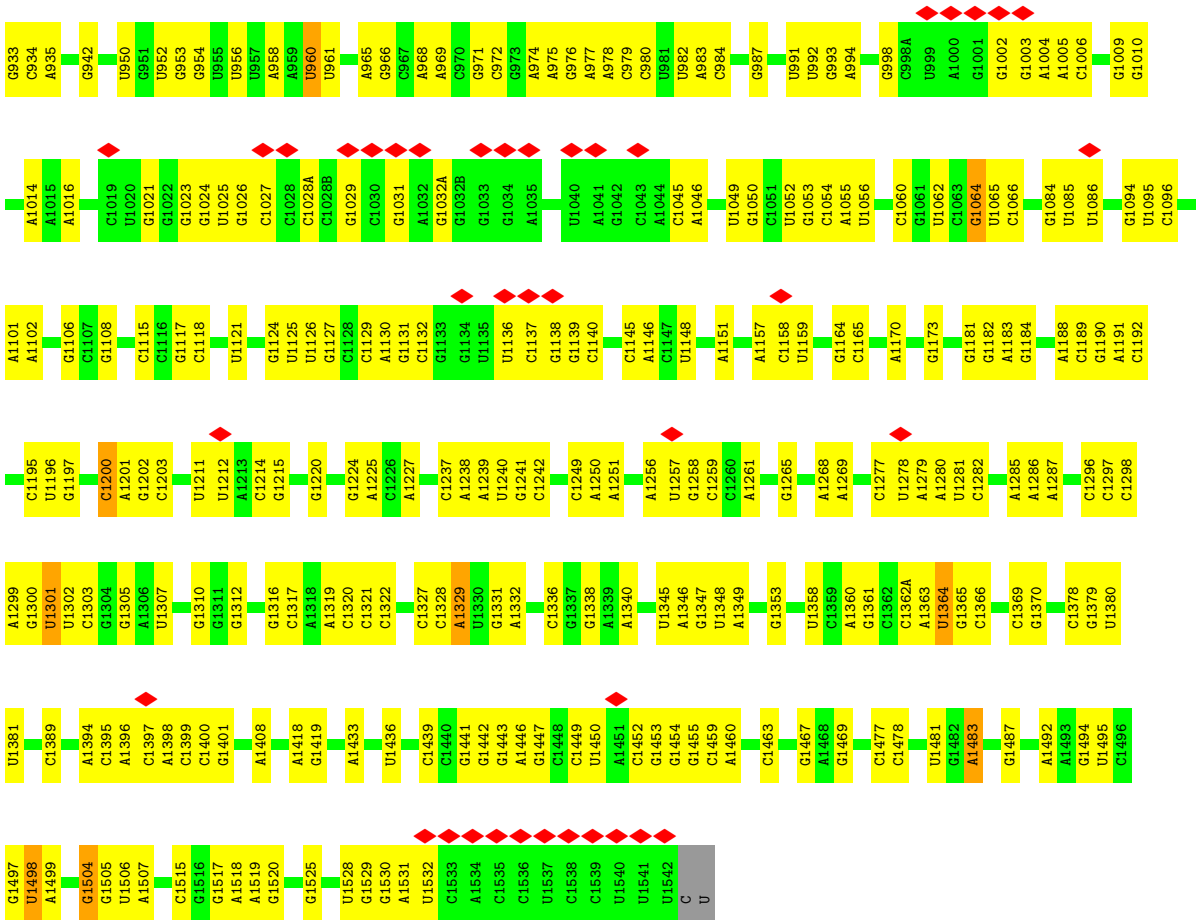
Chain 5:



- Molecule 6: 16S ribosomal RNA

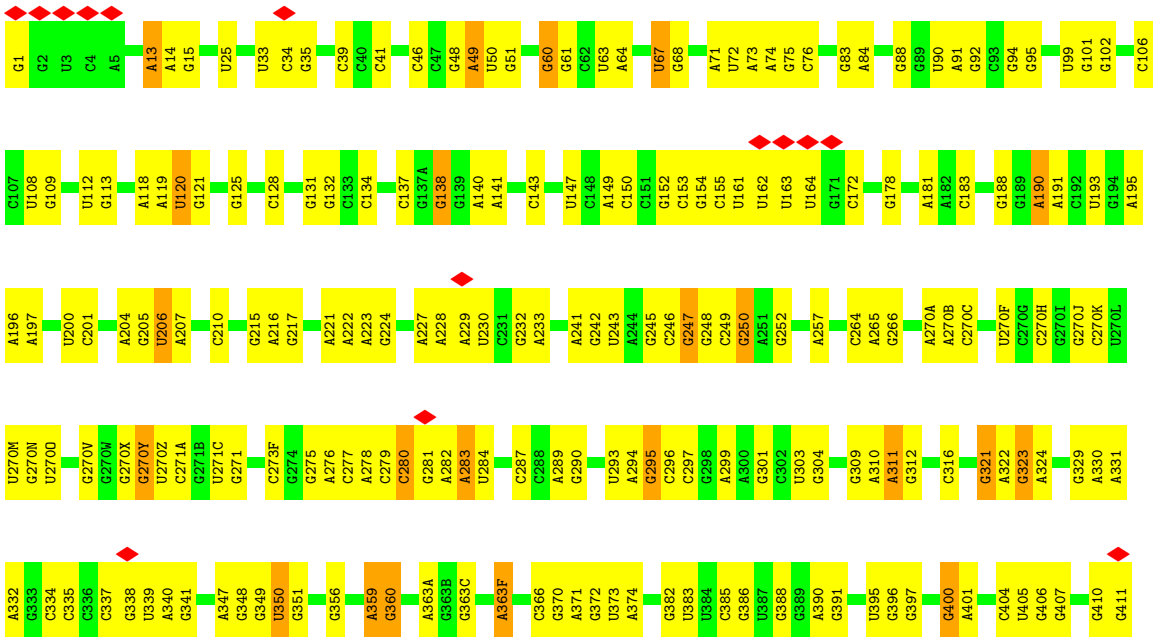
Chain A:

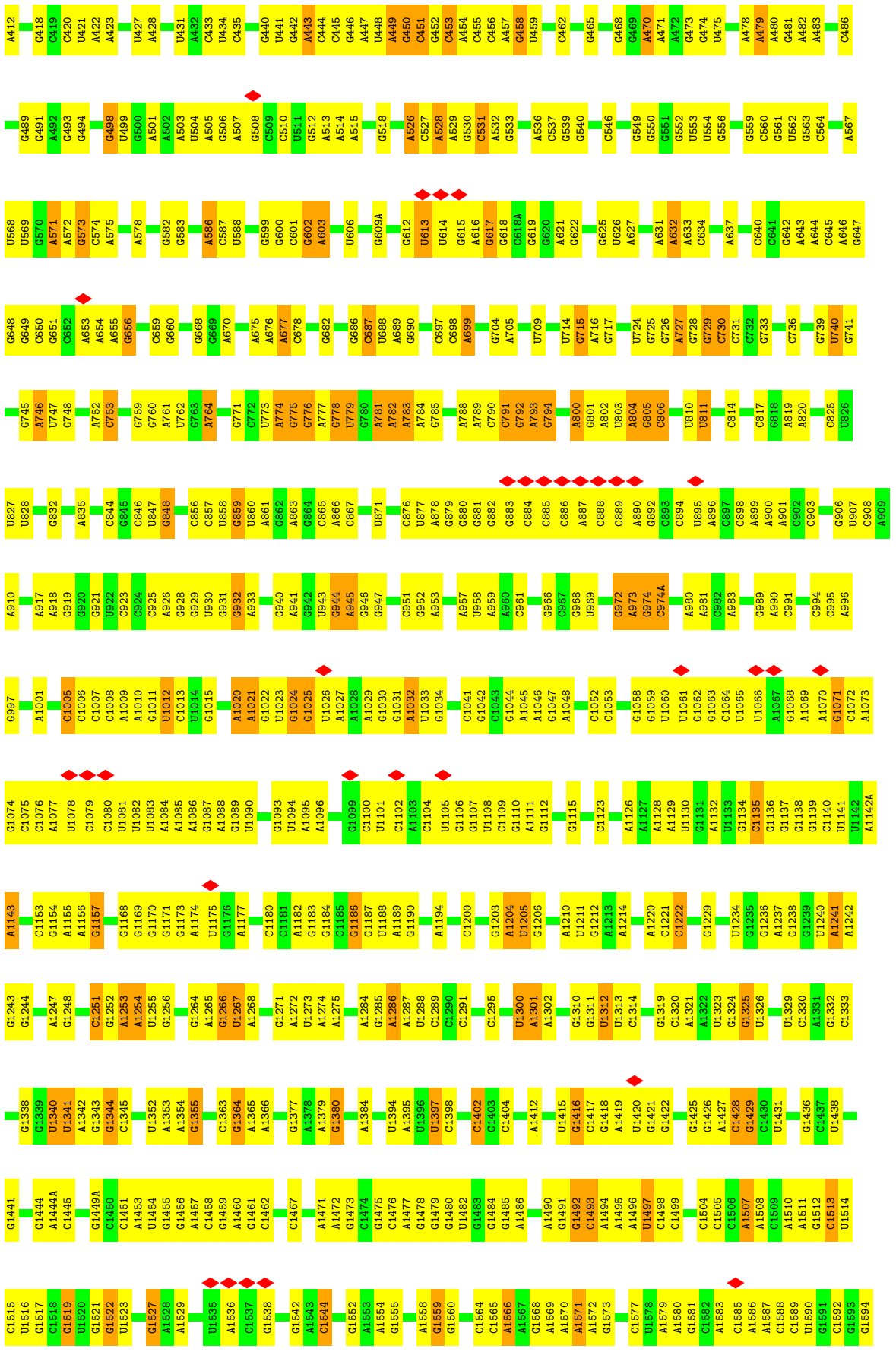




• Molecule 7: 23S ribosomal RNA

Chain D:

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G489 G491 A492 G493 G494 G498 U499 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 A515 G518 A526 C527 A528 A529 G530 C531 A532 G533 A536 C537 G539 G540 C546 G549 G550 G551 G552 U553 U554 G556 G559 C560 G561 U562 G563 C564 A567
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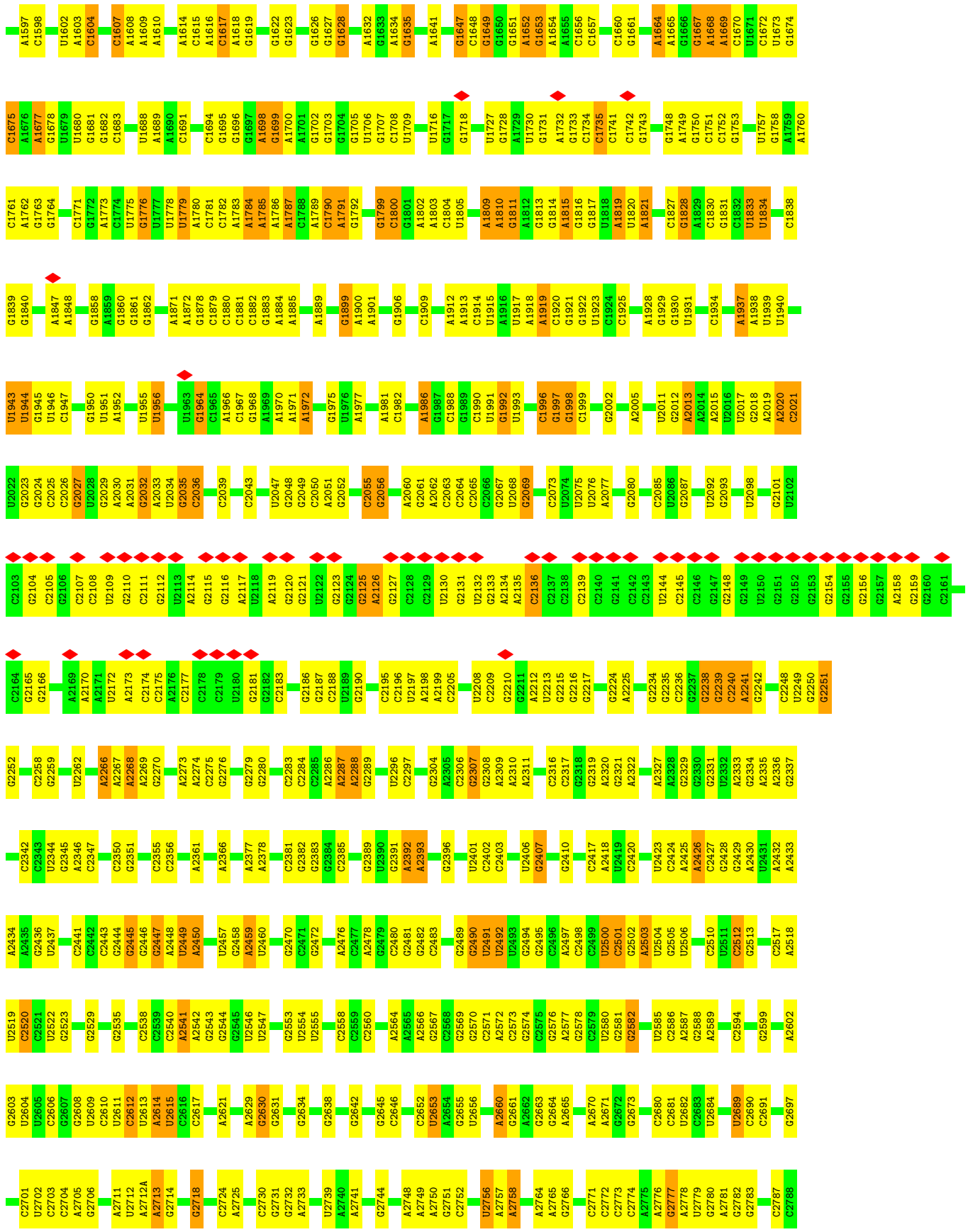
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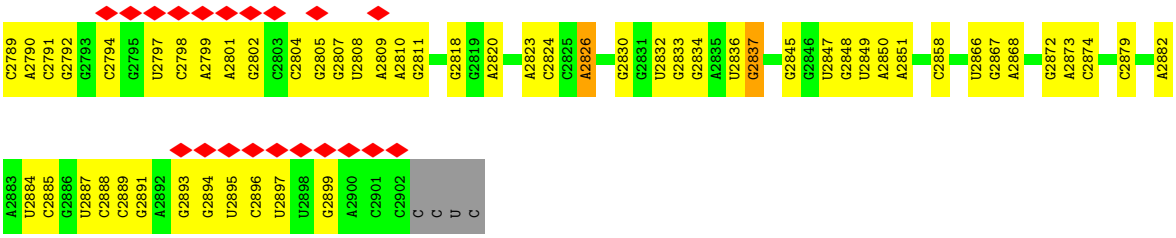
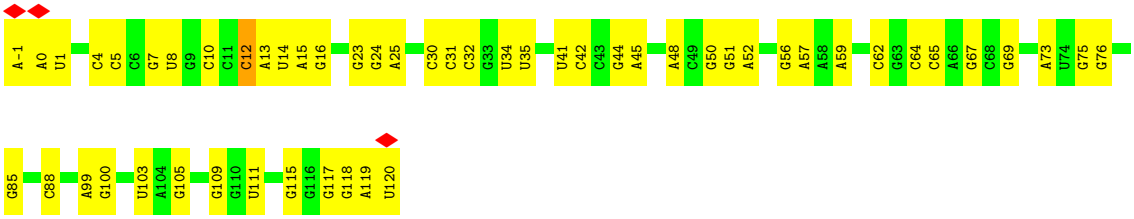


- Molecule 8: 5S ribosomal RNA

Chain E:



- Molecule 9: 30S ribosomal protein S2

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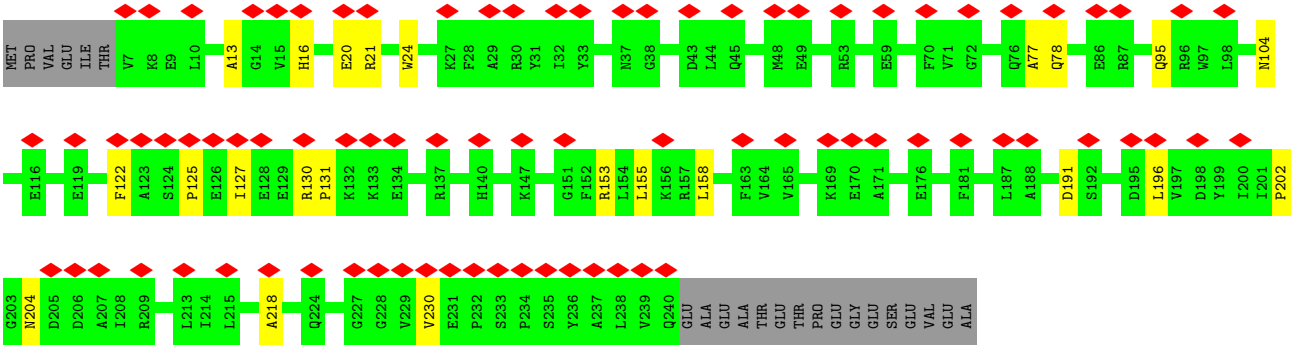

- Molecule 10: 30S ribosomal protein S3

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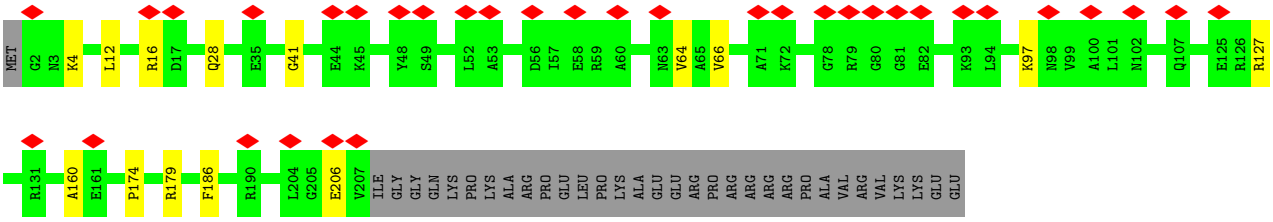
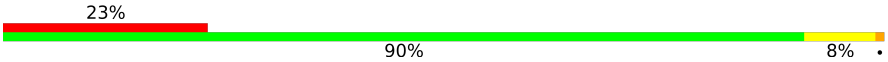
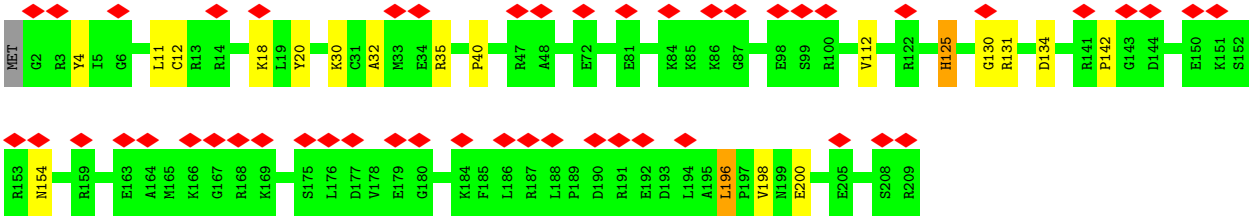


- Molecule 11: 30S ribosomal protein S4

Chain H:





- Molecule 12: 30S ribosomal protein S5

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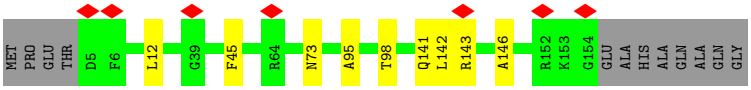

- Molecule 13: 30S ribosomal protein S6

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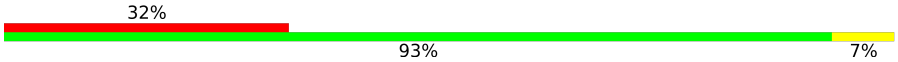

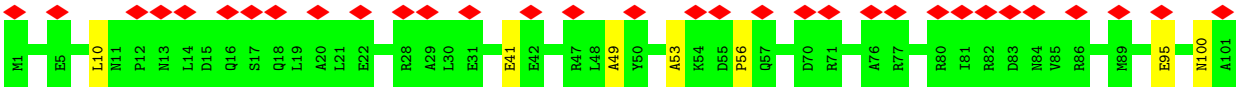

- Molecule 14: 30S ribosomal protein S7

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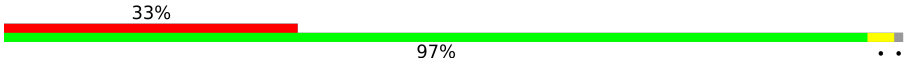
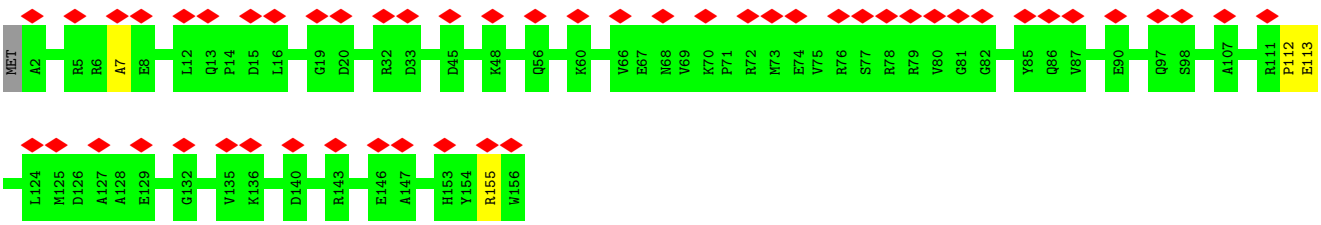
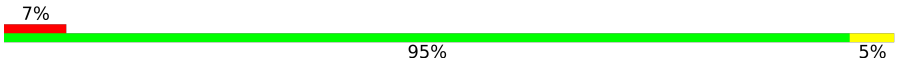
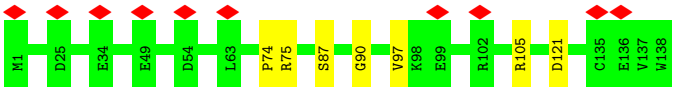




- Molecule 15: 30S ribosomal protein S8

Chain L:





- Molecule 16: 30S ribosomal protein S9

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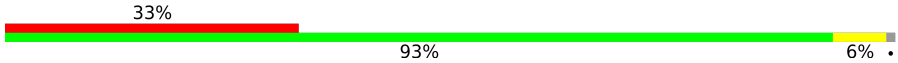

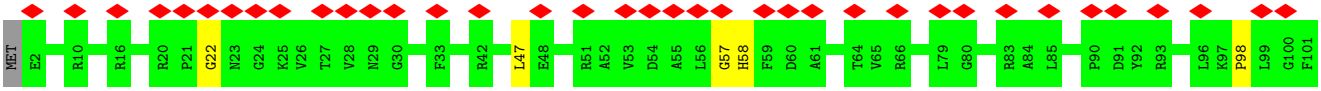

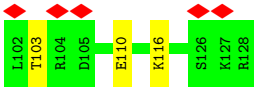

• Molecule 17: 30S ribosomal protein S10

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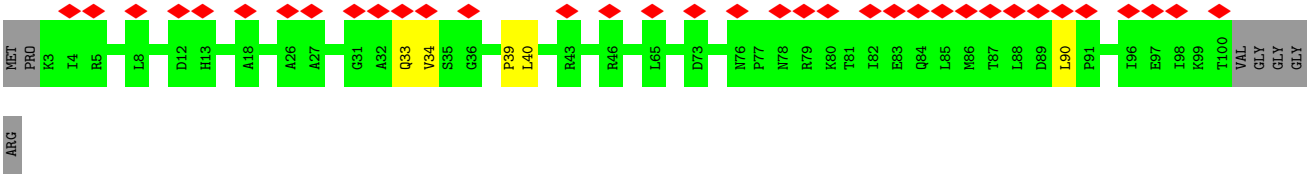

• Molecule 18: 30S ribosomal protein S11

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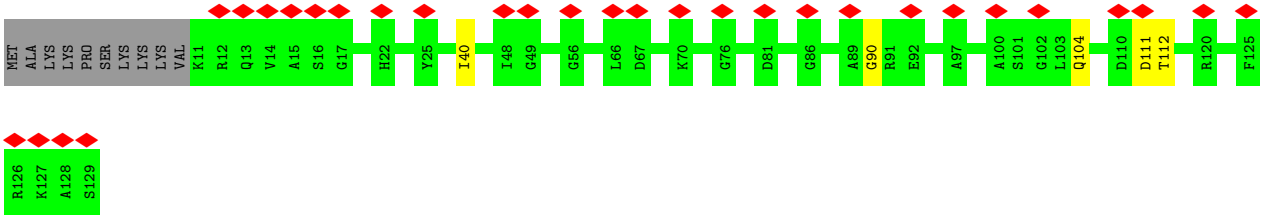
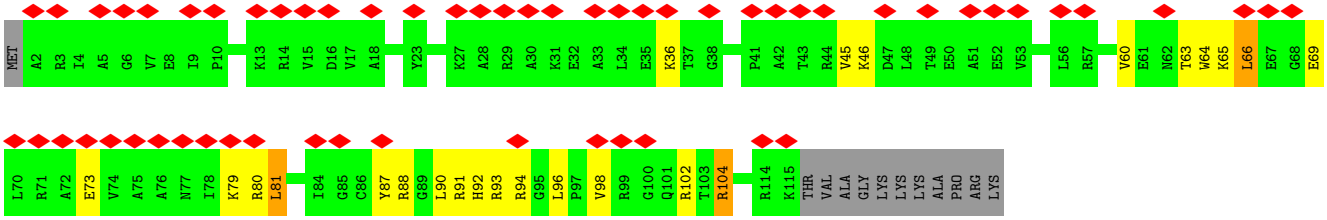


• Molecule 19: 30S ribosomal protein S12

Chain P:

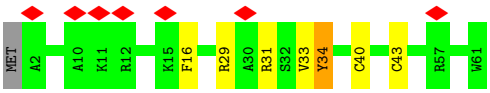
• Molecule 20: 30S ribosomal protein S13

Chain Q:



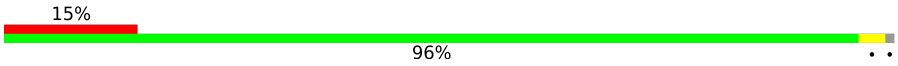
• Molecule 21: 30S ribosomal protein S14 type Z

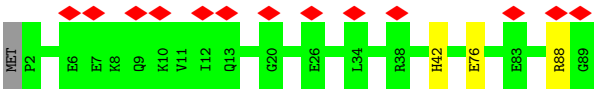
Chain R:



• Molecule 22: 30S ribosomal protein S15

Chain S:





• Molecule 23: 30S ribosomal protein S16

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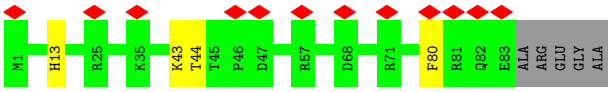
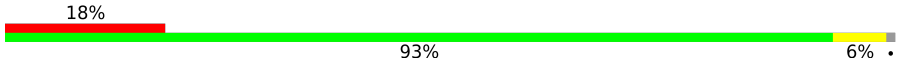
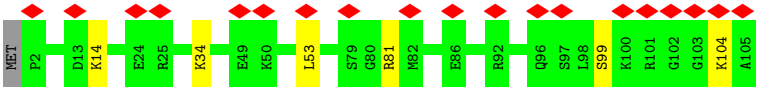


• Molecule 24: 30S ribosomal protein S17

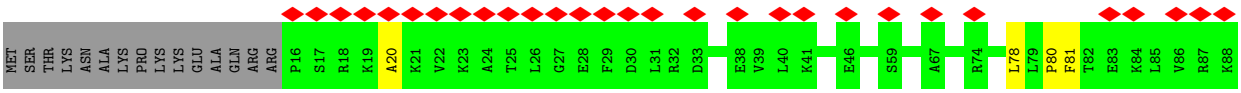
Chain U:





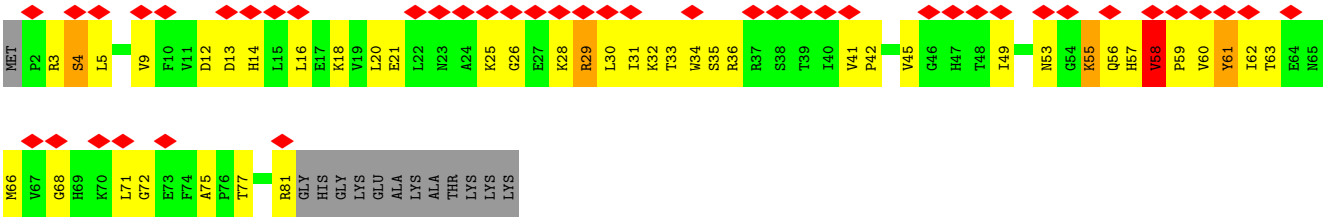
• Molecule 25: 30S ribosomal protein S18

Chain V:



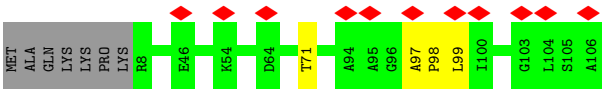
• Molecule 26: 30S ribosomal protein S19

Chain W:



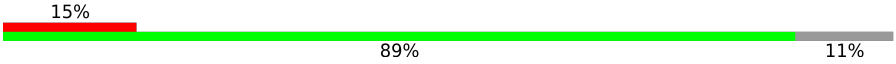
• Molecule 27: 30S ribosomal protein S20

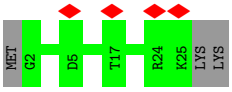
Chain X:



• Molecule 28: 30S ribosomal protein Thx

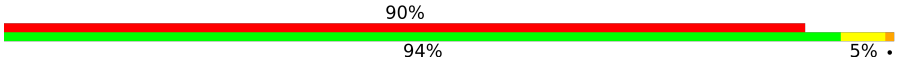
Chain Y:

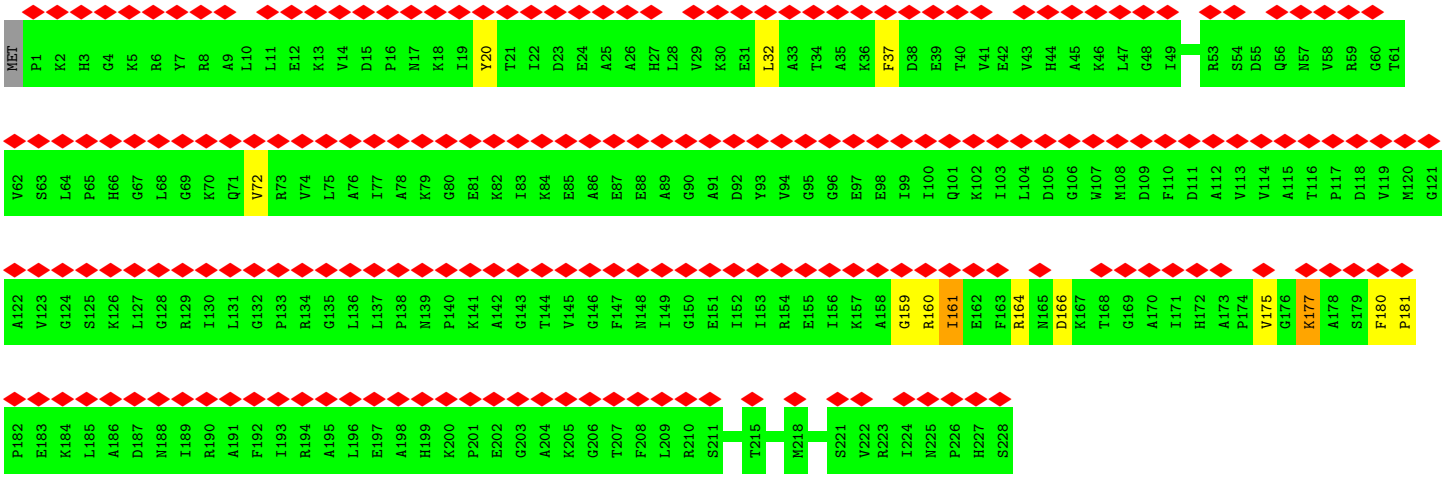




• Molecule 29: 50S ribosomal protein L1

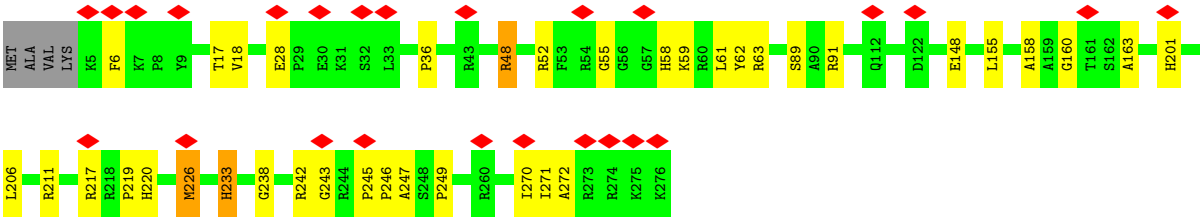
Chain Z:





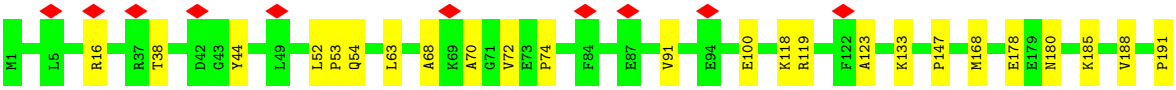
• Molecule 30: 50S ribosomal protein L2

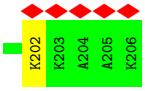
Chain a:



• Molecule 31: 50S ribosomal protein L3

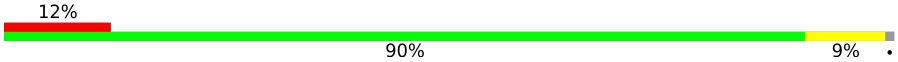
Chain b:

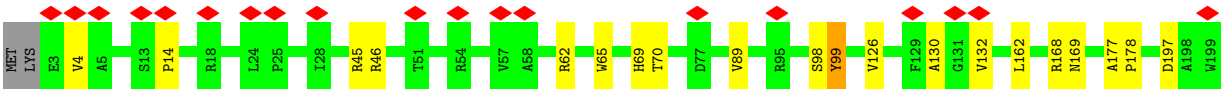


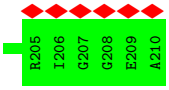


• Molecule 32: 50S ribosomal protein L4

Chain c:

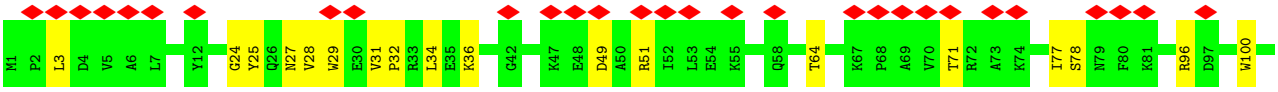


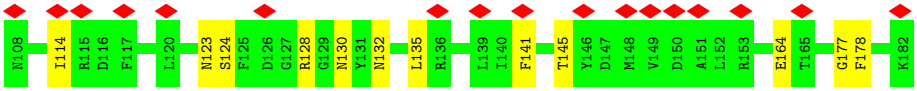




• Molecule 33: 50S ribosomal protein L5

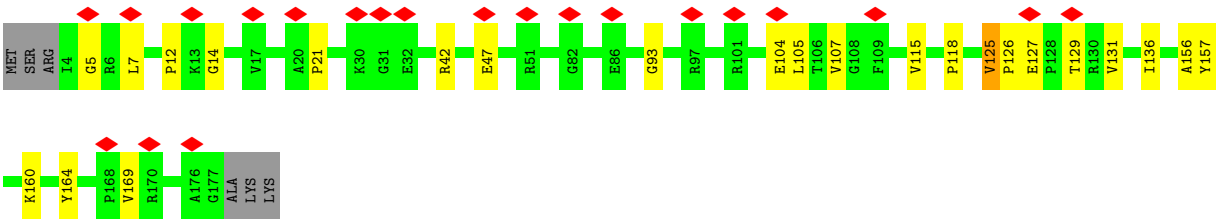
Chain d:





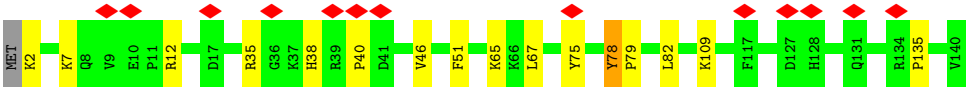
• Molecule 34: 50S ribosomal protein L6

Chain e:



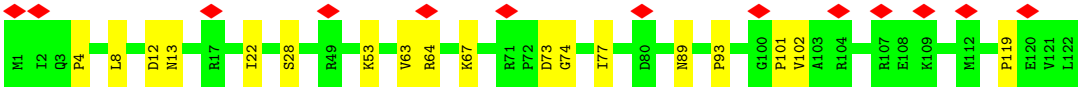
• Molecule 35: 50S ribosomal protein L13

Chain f:



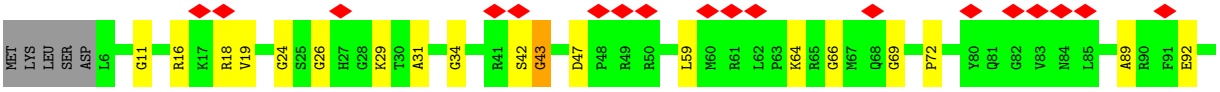
• Molecule 36: 50S ribosomal protein L14

Chain g:



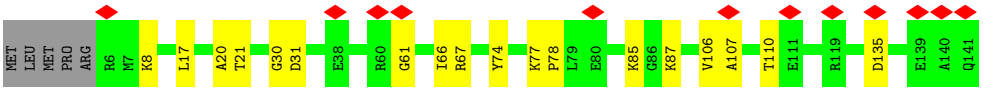
• Molecule 37: 50S ribosomal protein L15

Chain h:



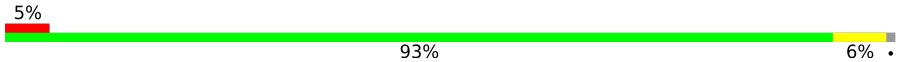
• Molecule 38: 50S ribosomal protein L16

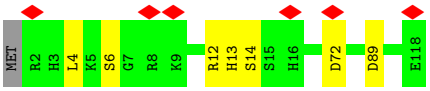
Chain i:



• Molecule 39: 50S ribosomal protein L17

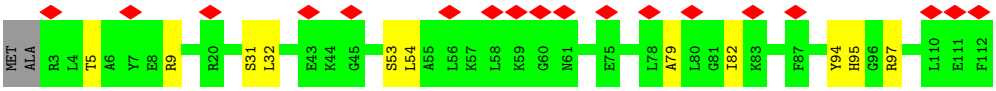
Chain j:





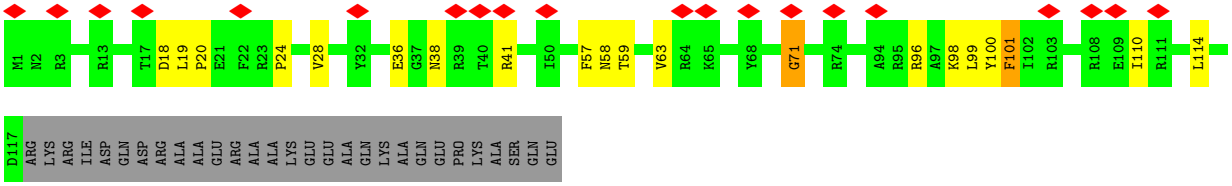
• Molecule 40: 50S ribosomal protein L18

Chain k:



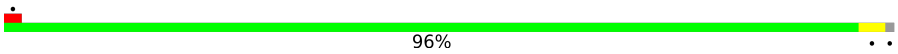
• Molecule 41: 50S ribosomal protein L19

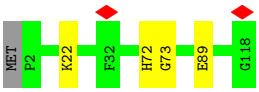
Chain l:



• Molecule 42: 50S ribosomal protein L20

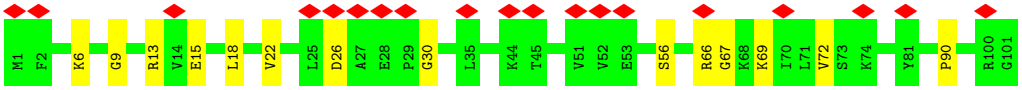
Chain m:





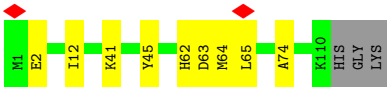
• Molecule 43: 50S ribosomal protein L21

Chain n:



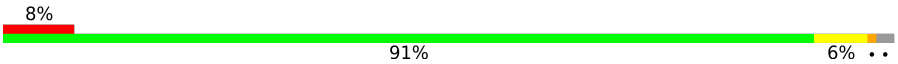
• Molecule 44: 50S ribosomal protein L22

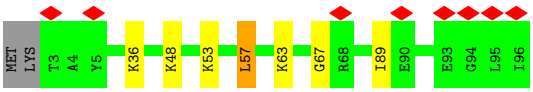
Chain o:



• Molecule 45: 50S ribosomal protein L23

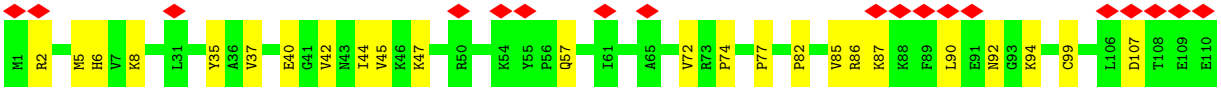
Chain p:





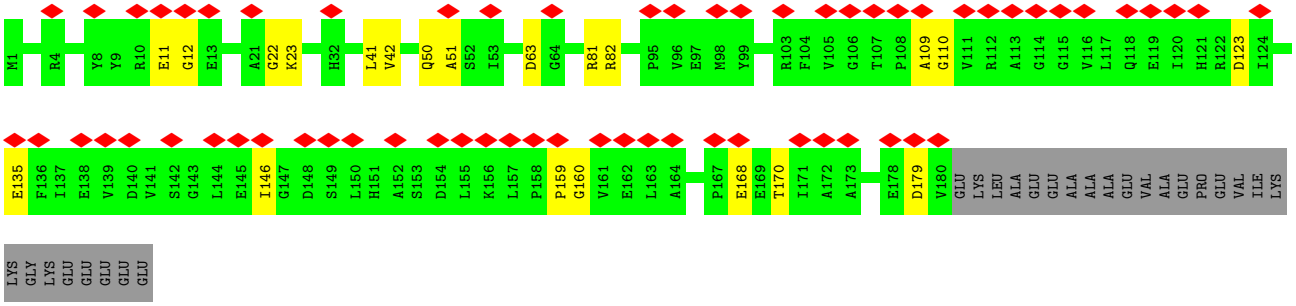
• Molecule 46: 50S ribosomal protein L24

Chain q:



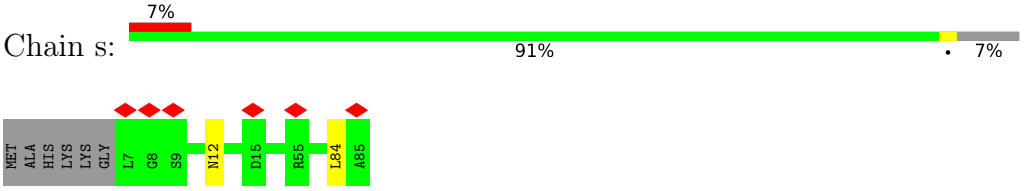
• Molecule 47: 50S ribosomal protein L25

Chain r:



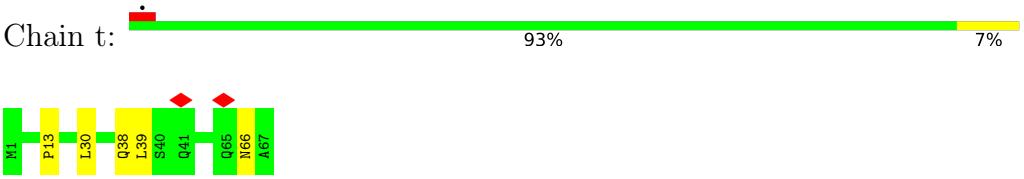
- Molecule 48: 50S ribosomal protein L27

Chain s:



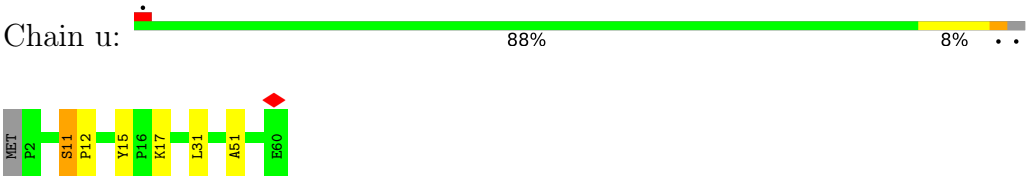
- Molecule 49: 50S ribosomal protein L29

Chain t:



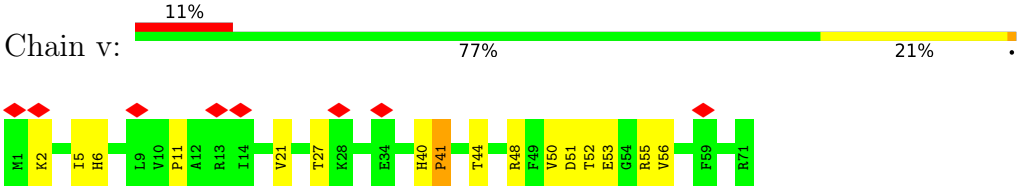
- Molecule 50: 50S ribosomal protein L30

Chain u:



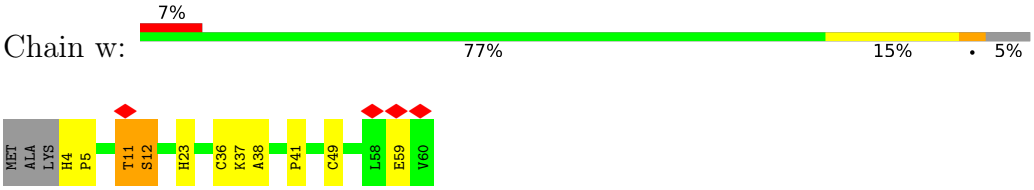
- Molecule 51: 50S ribosomal protein L31

Chain v:



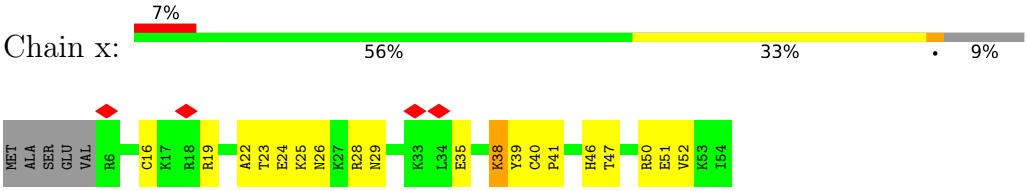
- Molecule 52: 50S ribosomal protein L32

Chain w:



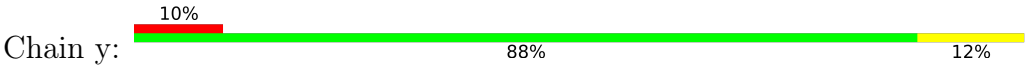
- Molecule 53: 50S ribosomal protein L33

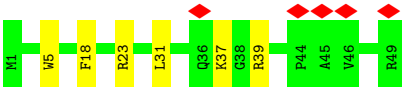
Chain x:



- Molecule 54: 50S ribosomal protein L34

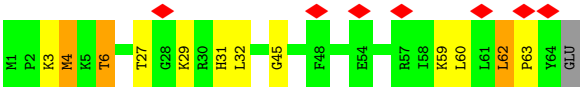
Chain y:





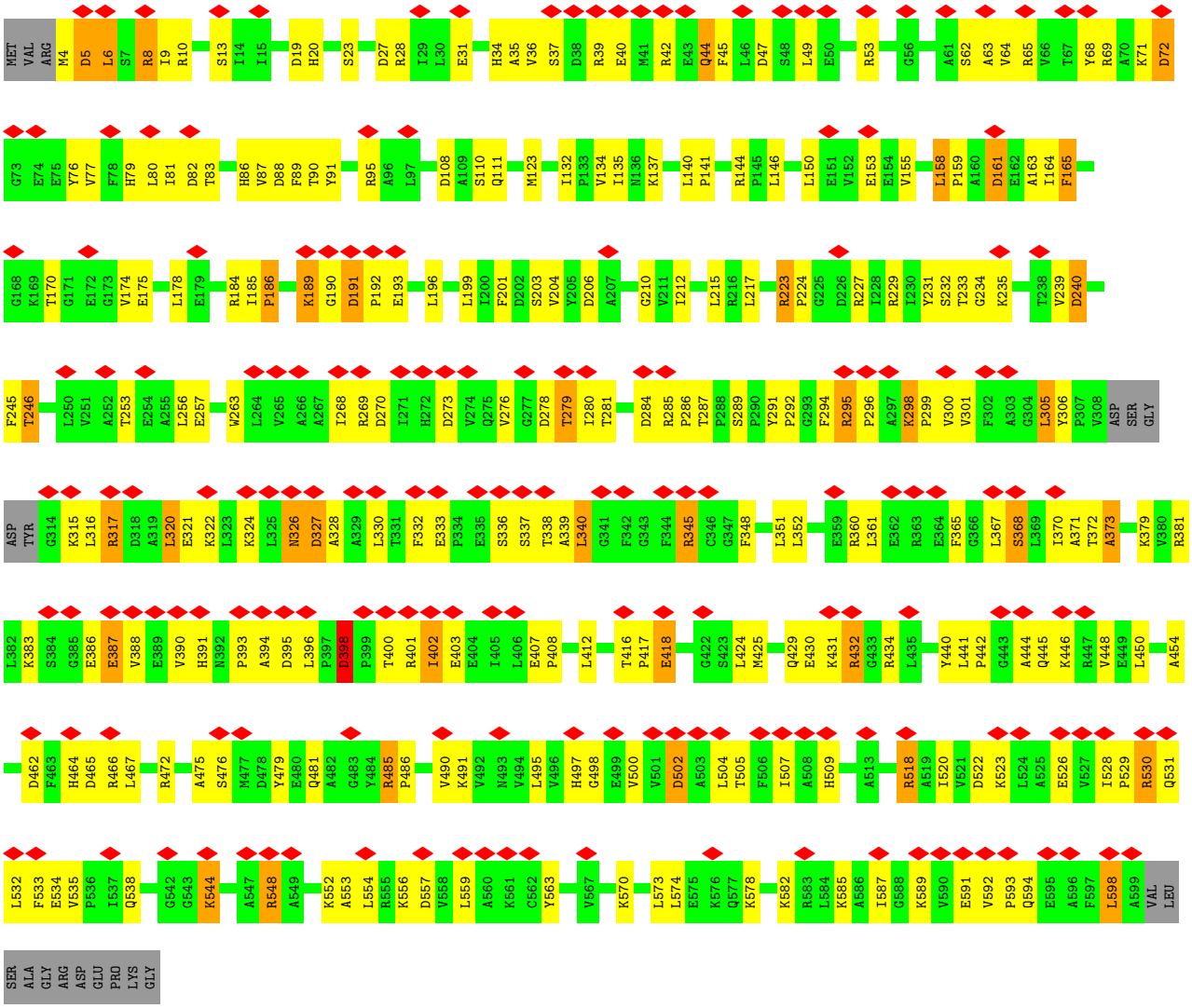
• Molecule 55: 50S ribosomal protein L35

Chain z:



• Molecule 56: Elongation factor 4

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110981	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)	200	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.28, 1.28, 1.28	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: GCP

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	1	0.77	0/310	0.90	0/407
2	2	0.26	0/640	0.50	0/889
3	3	0.54	0/1012	0.82	6/1373 (0.4%)
4	4	0.85	0/1832	1.03	0/2855
5	5	0.62	2/1813 (0.1%)	1.14	7/2823 (0.2%)
6	A	1.00	4/36438 (0.0%)	1.10	59/56869 (0.1%)
7	D	1.40	164/69685 (0.2%)	1.34	623/108786 (0.6%)
8	E	1.10	1/2954 (0.0%)	1.15	6/4606 (0.1%)
9	F	0.50	0/1935	0.74	0/2609
10	G	0.54	0/1636	0.67	0/2205
11	H	0.53	0/1733	0.76	3/2318 (0.1%)
12	I	0.69	0/1162	0.80	0/1564
13	J	0.48	0/856	0.70	1/1154 (0.1%)
14	K	0.47	0/1276	0.66	0/1709
15	L	0.59	0/1136	0.73	0/1527
16	M	0.46	0/1029	0.68	0/1379
17	N	0.49	0/807	0.69	0/1085
18	O	0.51	0/900	0.64	0/1213
19	P	0.67	0/986	0.79	0/1320
20	Q	0.39	0/924	0.66	1/1238 (0.1%)
21	R	0.64	0/501	0.76	1/664 (0.2%)
22	S	0.54	0/745	0.77	0/992
23	T	0.60	0/716	0.73	0/963
24	U	0.54	0/870	0.74	0/1159
25	V	0.44	0/603	0.71	0/799
26	W	0.39	0/661	0.50	2/890 (0.2%)
27	X	0.52	0/765	0.77	0/1007
28	Y	0.51	0/212	0.67	0/277
29	Z	0.37	0/1775	0.63	1/2393 (0.0%)
30	a	0.81	0/2174	0.93	3/2927 (0.1%)
31	b	0.77	0/1611	0.94	1/2171 (0.0%)
32	c	0.77	0/1660	0.90	0/2247

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.55	0/1507	0.81	1/2027 (0.0%)
34	e	0.58	0/1354	0.78	1/1831 (0.1%)
35	f	0.75	0/1140	0.95	2/1537 (0.1%)
36	g	0.79	0/942	0.93	2/1268 (0.2%)
37	h	0.64	0/1123	1.03	3/1493 (0.2%)
38	i	0.75	0/1100	0.90	0/1470
39	j	0.74	0/974	0.91	0/1302
40	k	0.61	0/887	0.95	0/1180
41	l	0.70	0/990	0.93	2/1325 (0.2%)
42	m	0.91	0/982	0.96	0/1306
43	n	0.65	0/790	0.94	1/1057 (0.1%)
44	o	0.78	0/886	0.83	0/1189
45	p	0.71	0/756	0.85	1/1015 (0.1%)
46	q	0.51	0/857	0.84	0/1142
47	r	0.56	0/1467	0.75	0/1992
48	s	0.81	0/633	0.84	0/843
49	t	0.59	0/569	0.82	1/751 (0.1%)
50	u	0.69	0/474	0.93	1/635 (0.2%)
51	v	0.82	0/594	1.11	2/795 (0.3%)
52	w	0.80	0/459	0.99	1/621 (0.2%)
53	x	0.67	0/433	1.00	2/576 (0.3%)
54	y	0.83	0/438	0.98	1/575 (0.2%)
55	z	0.79	0/523	0.96	1/690 (0.1%)
56	B	0.41	0/4718	0.52	25/6392 (0.4%)
All	All	1.09	171/165953 (0.1%)	1.14	761/247430 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
17	N	0	1
19	P	0	1
21	R	0	1
30	a	0	4
32	c	0	2
33	d	0	2
35	f	0	3
37	h	0	1
40	k	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	l	0	3
47	r	0	1
51	v	0	1
52	w	0	5
53	x	0	3
55	z	0	3
All	All	0	34

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1786	A	N9-C4	12.42	1.45	1.37
5	5	1	G	OP3-P	-10.94	1.48	1.61
7	D	1	G	OP3-P	-10.91	1.48	1.61
8	E	-1	A	OP3-P	-10.79	1.48	1.61
7	D	363(F)	A	O3'-P	9.72	1.72	1.61
7	D	1668	A	N9-C4	-8.35	1.32	1.37
7	D	775	G	N9-C4	8.03	1.44	1.38
7	D	783	A	N9-C4	-7.73	1.33	1.37
7	D	1668	A	N3-C4	-7.71	1.30	1.34
7	D	1021	A	N9-C4	-7.52	1.33	1.37
7	D	2019	A	N9-C4	-7.37	1.33	1.37
7	D	603	A	N9-C4	-7.31	1.33	1.37
7	D	781	A	N9-C4	-7.07	1.33	1.37
7	D	792	G	N7-C5	-7.05	1.35	1.39
7	D	792	G	C6-N1	-7.03	1.34	1.39
7	D	1154	G	N7-C5	-6.91	1.35	1.39
7	D	1787	A	N9-C4	-6.78	1.33	1.37
7	D	1791	A	N3-C4	-6.75	1.30	1.34
7	D	1669	A	N3-C4	-6.73	1.30	1.34
7	D	574	C	N1-C6	-6.72	1.33	1.37
7	D	586	A	C5-C4	-6.62	1.34	1.38
5	5	76	A	N9-C4	-6.57	1.33	1.37
7	D	1669	A	C5-C6	-6.56	1.35	1.41
7	D	1670	C	N1-C6	-6.53	1.33	1.37
7	D	2240	C	N1-C6	-6.49	1.33	1.37
7	D	764	A	C5-C4	-6.36	1.34	1.38
7	D	676	A	N3-C4	-6.31	1.31	1.34
7	D	2019	A	N3-C4	-6.28	1.31	1.34
7	D	794	G	N7-C5	-6.27	1.35	1.39
6	A	298	A	N9-C4	-6.21	1.34	1.37
7	D	1791	A	N9-C4	-6.21	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	793	A	N7-C5	-6.18	1.35	1.39
6	A	574	A	N9-C4	-6.16	1.34	1.37
7	D	2589	A	N7-C5	-6.14	1.35	1.39
7	D	793	A	C5-C6	-6.02	1.35	1.41
7	D	2495	G	N7-C5	-6.01	1.35	1.39
7	D	2241	A	N7-C5	-6.00	1.35	1.39
7	D	678	C	N1-C6	-6.00	1.33	1.37
7	D	514	A	N9-C4	-5.98	1.34	1.37
7	D	247	G	C6-N1	-5.97	1.35	1.39
7	D	586	A	N3-C4	-5.97	1.31	1.34
7	D	972	G	C6-N1	-5.97	1.35	1.39
7	D	2444	G	N7-C5	-5.97	1.35	1.39
7	D	190	A	N9-C4	-5.96	1.34	1.37
7	D	687	C	N1-C6	-5.96	1.33	1.37
7	D	1821	A	N9-C4	-5.92	1.34	1.37
7	D	689	A	N9-C4	-5.91	1.34	1.37
7	D	820	A	N3-C4	-5.88	1.31	1.34
7	D	2491	U	C2-N3	5.87	1.41	1.37
7	D	2273	A	N7-C5	-5.83	1.35	1.39
7	D	2503	A	N7-C5	-5.76	1.35	1.39
7	D	1815	A	N3-C4	-5.74	1.31	1.34
7	D	1668	A	C6-N1	-5.73	1.31	1.35
7	D	573	G	N7-C5	-5.68	1.35	1.39
7	D	2242	G	N7-C5	-5.66	1.35	1.39
7	D	2393	A	N9-C4	-5.66	1.34	1.37
7	D	468	G	N7-C5	-5.65	1.35	1.39
7	D	1760	A	N9-C4	-5.64	1.34	1.37
7	D	1819	A	N9-C4	-5.64	1.34	1.37
7	D	2051	A	N9-C4	-5.63	1.34	1.37
7	D	449	A	N7-C5	-5.61	1.35	1.39
7	D	1354	A	N3-C4	-5.59	1.31	1.34
7	D	947	G	N7-C5	-5.58	1.35	1.39
7	D	1677	A	N9-C4	-5.57	1.34	1.37
7	D	675	A	N3-C4	-5.56	1.31	1.34
7	D	2446	G	N7-C5	-5.56	1.35	1.39
7	D	451	C	N1-C6	-5.55	1.33	1.37
7	D	1377	G	C6-N1	-5.55	1.35	1.39
7	D	781	A	N3-C4	-5.52	1.31	1.34
7	D	1986	A	N7-C5	-5.52	1.35	1.39
7	D	2459	A	N7-C5	-5.52	1.35	1.39
7	D	2251	G	N7-C5	-5.51	1.35	1.39
7	D	783	A	N3-C4	-5.51	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	973	A	N9-C4	-5.51	1.34	1.37
7	D	2433	A	N3-C4	-5.48	1.31	1.34
7	D	677	A	N9-C4	-5.48	1.34	1.37
7	D	1787	A	C5-C6	-5.48	1.36	1.41
7	D	526	A	N9-C4	-5.46	1.34	1.37
7	D	1813	G	N7-C5	-5.46	1.35	1.39
7	D	2005	A	N3-C4	-5.46	1.31	1.34
7	D	800	A	N7-C5	-5.44	1.35	1.39
7	D	1977	A	N9-C4	-5.44	1.34	1.37
7	D	2826	A	N9-C4	-5.43	1.34	1.37
7	D	1354	A	N9-C4	-5.43	1.34	1.37
7	D	2274	A	N3-C4	-5.41	1.31	1.34
7	D	2541	A	N9-C4	-5.41	1.34	1.37
7	D	443	A	N9-C4	-5.40	1.34	1.37
7	D	2055	C	N3-C4	-5.39	1.30	1.33
7	D	250	G	C6-N1	-5.38	1.35	1.39
7	D	2021	C	N1-C6	-5.37	1.33	1.37
7	D	806	C	N1-C2	-5.37	1.34	1.40
7	D	1006	C	N1-C2	-5.37	1.34	1.40
7	D	1377	G	N7-C5	-5.36	1.36	1.39
7	D	2052	G	N9-C8	-5.36	1.34	1.37
7	D	1899	G	N3-C4	-5.36	1.31	1.35
7	D	974	G	N7-C5	-5.36	1.36	1.39
7	D	1735	C	O3'-P	5.34	1.67	1.61
7	D	817	C	N1-C6	-5.34	1.33	1.37
7	D	1154	G	C8-N7	-5.34	1.27	1.30
7	D	2443	C	N1-C6	-5.34	1.33	1.37
7	D	2238	G	N7-C5	-5.33	1.36	1.39
6	A	1483	A	N9-C4	-5.33	1.34	1.37
7	D	1783	A	N9-C4	-5.32	1.34	1.37
7	D	2614	A	C5-C4	-5.32	1.35	1.38
7	D	2689	U	C2-N3	-5.31	1.34	1.37
7	D	1998	G	N7-C5	-5.30	1.36	1.39
7	D	775	G	N7-C5	-5.29	1.36	1.39
7	D	2052	G	C5-C4	-5.29	1.34	1.38
7	D	617	G	N9-C4	-5.28	1.33	1.38
7	D	974	G	C8-N7	-5.28	1.27	1.30
7	D	564	C	N1-C6	-5.27	1.33	1.37
7	D	2052	G	N7-C5	-5.27	1.36	1.39
7	D	190	A	C5-C4	-5.27	1.35	1.38
6	A	574	A	N3-C4	-5.26	1.31	1.34
7	D	957	A	N9-C4	-5.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1632	A	C5-C6	-5.26	1.36	1.41
7	D	49	A	N9-C4	-5.25	1.34	1.37
7	D	1301	A	N3-C4	-5.25	1.31	1.34
7	D	2594	C	N1-C6	-5.25	1.34	1.37
7	D	190	A	N3-C4	-5.25	1.31	1.34
7	D	782	A	N9-C4	-5.24	1.34	1.37
7	D	1029	A	N3-C4	-5.24	1.31	1.34
7	D	2013	A	C5-C4	-5.23	1.35	1.38
7	D	1617	C	N1-C6	-5.23	1.34	1.37
7	D	746	A	N9-C4	-5.22	1.34	1.37
7	D	1364	G	N9-C8	-5.22	1.34	1.37
7	D	1952	A	N9-C4	-5.22	1.34	1.37
7	D	1143	A	N7-C5	-5.22	1.36	1.39
7	D	586	A	C6-N1	-5.22	1.31	1.35
7	D	835	A	N9-C4	-5.21	1.34	1.37
7	D	1999	C	N1-C6	-5.21	1.34	1.37
7	D	820	A	C6-N1	-5.21	1.31	1.35
7	D	2024	G	N7-C5	-5.20	1.36	1.39
7	D	515	A	N7-C5	-5.20	1.36	1.39
7	D	1830	C	C4-C5	-5.20	1.38	1.43
7	D	1189	A	N7-C5	-5.18	1.36	1.39
7	D	1937	A	N9-C4	-5.18	1.34	1.37
7	D	1783	A	N3-C4	-5.18	1.31	1.34
7	D	1668	A	C2-N3	-5.17	1.28	1.33
7	D	2589	A	N9-C4	-5.17	1.34	1.37
7	D	578	A	N9-C4	-5.17	1.34	1.37
7	D	2713	A	N9-C4	-5.17	1.34	1.37
7	D	2587	A	N9-C4	-5.16	1.34	1.37
7	D	2392	A	N9-C4	-5.16	1.34	1.37
7	D	1981	A	N3-C4	-5.15	1.31	1.34
7	D	632	A	N9-C4	-5.14	1.34	1.37
7	D	981	A	N3-C4	-5.14	1.31	1.34
7	D	1024	G	N3-C4	-5.12	1.31	1.35
7	D	2242	G	C6-N1	-5.12	1.35	1.39
7	D	1803	A	N9-C4	-5.12	1.34	1.37
7	D	773	U	N1-C2	-5.09	1.33	1.38
7	D	1992	G	C5-C4	-5.08	1.34	1.38
7	D	1287	A	N9-C4	-5.08	1.34	1.37
7	D	806	C	N1-C6	-5.06	1.34	1.37
7	D	514	A	N7-C5	-5.06	1.36	1.39
7	D	863	A	N3-C4	-5.06	1.31	1.34
7	D	2495	G	C8-N7	-5.06	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	778	G	N7-C5	-5.05	1.36	1.39
7	D	2520	C	N1-C6	-5.05	1.34	1.37
7	D	794	G	C6-N1	-5.04	1.36	1.39
7	D	1301	A	N9-C4	-5.04	1.34	1.37
7	D	957	A	N3-C4	-5.04	1.31	1.34
7	D	2588	G	C5-C4	-5.04	1.34	1.38
7	D	810	U	C2-N3	-5.03	1.34	1.37
7	D	2826	A	C5-C6	-5.03	1.36	1.41
7	D	804	A	N9-C4	-5.02	1.34	1.37
7	D	1137	G	C6-N1	-5.02	1.36	1.39
7	D	2697	G	N9-C4	-5.01	1.33	1.38
7	D	2540	C	N1-C6	-5.01	1.34	1.37
7	D	528	A	N3-C4	-5.01	1.31	1.34
7	D	699	A	N3-C4	-5.00	1.31	1.34

All (761) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	775	G	N3-C4-C5	-15.67	120.77	128.60
7	D	2491	U	C6-N1-C2	-13.29	113.03	121.00
7	D	1664	A	C8-N9-C4	-13.09	100.56	105.80
7	D	1779	U	C5-C4-O4	-12.85	118.19	125.90
7	D	775	G	C8-N9-C4	-12.80	101.28	106.40
7	D	791	C	N1-C2-O2	12.50	126.40	118.90
7	D	1786	A	N3-C4-C5	-12.04	118.37	126.80
7	D	1779	U	N3-C4-O4	12.01	127.81	119.40
7	D	1779	U	C5-C6-N1	11.90	128.65	122.70
7	D	1786	A	N3-C4-N9	11.36	136.49	127.40
7	D	775	G	N3-C4-N9	11.33	132.80	126.00
7	D	879	G	N1-C6-O6	-11.33	113.10	119.90
7	D	515	A	C6-C5-N7	-10.49	124.96	132.30
7	D	1786	A	C4-C5-C6	10.46	122.23	117.00
7	D	688	U	C2-N3-C4	-10.30	120.82	127.00
7	D	1664	A	N7-C8-N9	10.24	118.92	113.80
7	D	774	A	C6-N1-C2	-10.15	112.51	118.60
7	D	2490	G	N1-C6-O6	-9.97	113.92	119.90
7	D	341	G	N3-C4-N9	9.94	131.96	126.00
7	D	1668	A	N1-C2-N3	9.92	134.26	129.30
7	D	1786	A	C6-N1-C2	-9.91	112.65	118.60
7	D	2073	C	C6-N1-C2	-9.85	116.36	120.30
7	D	1786	A	C6-C5-N7	-9.76	125.47	132.30
6	A	1086	U	C2-N1-C1'	9.72	129.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	775	G	N3-C2-N2	9.66	126.66	119.90
7	D	775	G	N1-C2-N2	-9.55	107.60	116.20
7	D	775	G	C4-N9-C1'	9.41	138.73	126.50
7	D	1786	A	C8-N9-C4	-9.39	102.04	105.80
7	D	729	G	C8-N9-C4	-9.29	102.68	106.40
7	D	2035	G	N3-C4-N9	9.26	131.56	126.00
7	D	1313	U	N3-C2-O2	-9.25	115.73	122.20
7	D	1025	G	O4'-C1'-N9	9.17	115.54	108.20
7	D	1632	A	N1-C6-N6	9.16	124.09	118.60
7	D	2459	A	C6-N1-C2	-9.09	113.15	118.60
7	D	1313	U	C6-N1-C2	-9.03	115.58	121.00
7	D	2491	U	C5-C6-N1	8.99	127.20	122.70
7	D	775	G	N7-C8-N9	8.95	117.58	113.10
7	D	458	G	O4'-C1'-N9	8.83	115.26	108.20
7	D	1925	C	C2-N1-C1'	8.83	128.51	118.80
7	D	531	C	C6-N1-C2	-8.82	116.77	120.30
7	D	791	C	C6-N1-C1'	-8.81	110.23	120.80
7	D	2251	G	C6-C5-N7	-8.79	125.12	130.40
7	D	1313	U	C5-C6-N1	8.78	127.09	122.70
7	D	2495	G	N3-C4-N9	8.78	131.27	126.00
7	D	531	C	N3-C2-O2	-8.73	115.79	121.90
7	D	2495	G	C6-C5-N7	-8.69	125.19	130.40
7	D	1813	G	C6-C5-N7	-8.67	125.20	130.40
7	D	1668	A	C2-N3-C4	-8.67	106.27	110.60
7	D	1205	U	N1-C2-O2	8.62	128.83	122.80
7	D	341	G	C6-C5-N7	-8.56	125.26	130.40
7	D	363(F)	A	OP2-P-O3'	8.56	124.04	105.20
7	D	1513	C	N1-C2-O2	8.49	124.00	118.90
7	D	1785	A	C8-N9-C4	-8.44	102.42	105.80
7	D	2444	G	C6-C5-N7	-8.44	125.33	130.40
7	D	1617	C	C2-N1-C1'	8.40	128.04	118.80
7	D	2492	U	N3-C2-O2	-8.38	116.34	122.20
7	D	2035	G	N3-C4-C5	-8.38	124.41	128.60
7	D	2460	U	N3-C2-O2	-8.36	116.35	122.20
7	D	778	G	C4-C5-N7	8.34	114.13	110.80
7	D	1377	G	C6-C5-N7	-8.28	125.43	130.40
6	A	1064	G	O4'-C1'-N9	8.27	114.82	108.20
5	5	74	C	N1-C2-O2	8.26	123.85	118.90
7	D	1571	A	C2-N3-C4	8.25	114.72	110.60
7	D	794	G	C6-C5-N7	-8.23	125.46	130.40
7	D	2460	U	C2-N1-C1'	8.21	127.55	117.70
7	D	515	A	N3-C4-N9	8.13	133.91	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	515	A	N9-C4-C5	-8.05	102.58	105.80
7	D	350	U	N3-C2-O2	-8.05	116.57	122.20
7	D	2056	G	C4-N9-C1'	8.05	136.96	126.50
7	D	2288	A	O4'-C1'-N9	8.04	114.63	108.20
7	D	2035	G	C8-N9-C1'	-8.01	116.58	127.00
7	D	687	C	C2-N3-C4	-8.00	115.90	119.90
7	D	1012	U	C2-N1-C1'	-7.98	108.13	117.70
7	D	2056	G	C8-N9-C1'	-7.91	116.72	127.00
7	D	1377	G	C4-N9-C1'	7.85	136.71	126.50
7	D	120	U	N1-C2-O2	7.84	128.29	122.80
6	A	1328	C	C2-N1-C1'	7.83	127.42	118.80
7	D	404	C	N1-C2-O2	7.81	123.59	118.90
7	D	1205	U	C3'-C2'-C1'	-7.81	95.25	101.50
7	D	515	A	C4-C5-C6	7.80	120.90	117.00
7	D	2459	A	C4-C5-C6	7.74	120.87	117.00
7	D	2287	A	C8-N9-C4	7.71	108.88	105.80
6	A	1328	C	N1-C2-O2	7.70	123.52	118.90
7	D	1813	G	N3-C4-N9	7.68	130.61	126.00
7	D	1527	G	C5-C6-N1	-7.64	107.68	111.50
7	D	1313	U	C2-N1-C1'	7.60	126.82	117.70
7	D	1649	G	C6-C5-N7	-7.60	125.84	130.40
7	D	2035	G	C4-N9-C1'	7.57	136.34	126.50
7	D	297	C	N1-C2-O2	7.55	123.43	118.90
7	D	1656	C	C2-N1-C1'	7.54	127.10	118.80
7	D	791	C	C2-N1-C1'	7.54	127.09	118.80
7	D	2495	G	C8-N9-C1'	-7.54	117.20	127.00
7	D	879	G	C5-C6-O6	7.53	133.12	128.60
7	D	150	C	C2-N1-C1'	7.49	127.04	118.80
7	D	2445	G	N3-C4-N9	7.48	130.49	126.00
7	D	1657	C	C5-C6-N1	7.48	124.74	121.00
7	D	2495	G	C4-N9-C1'	7.43	136.16	126.50
7	D	1492	G	C5-C6-O6	-7.43	124.14	128.60
7	D	1786	A	C4-N9-C1'	7.43	139.67	126.30
7	D	1604	C	N3-C2-O2	-7.41	116.71	121.90
7	D	2492	U	C2-N1-C1'	7.38	126.55	117.70
7	D	1698	A	O4'-C1'-N9	7.37	114.09	108.20
6	A	115	G	C4-N9-C1'	7.36	136.07	126.50
7	D	1813	G	C4-C5-N7	7.35	113.74	110.80
7	D	791	C	N3-C4-C5	7.30	124.82	121.90
7	D	1805	U	N3-C2-O2	-7.25	117.12	122.20
7	D	1566	A	O4'-C1'-N9	7.24	114.00	108.20
7	D	341	G	C8-N9-C1'	-7.24	117.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1313	U	N1-C2-O2	7.21	127.85	122.80
7	D	791	C	N3-C2-O2	-7.21	116.85	121.90
5	5	74	C	C2-N1-C1'	7.21	126.73	118.80
7	D	1492	G	N3-C4-N9	7.20	130.32	126.00
7	D	120	U	C2-N1-C1'	7.18	126.32	117.70
7	D	341	G	N1-C2-N2	-7.17	109.74	116.20
7	D	1617	C	C6-N1-C1'	-7.16	112.21	120.80
7	D	2449	U	C5-C6-N1	-7.16	119.12	122.70
7	D	2491	U	N1-C2-N3	7.16	119.19	114.90
7	D	1810	A	O4'-C1'-N9	7.15	113.92	108.20
7	D	1377	G	N3-C4-N9	7.15	130.29	126.00
7	D	2615	U	C2-N1-C1'	7.14	126.27	117.70
7	D	811	U	C5-C6-N1	7.13	126.27	122.70
7	D	341	G	N9-C4-C5	-7.13	102.55	105.40
7	D	1925	C	C6-N1-C1'	-7.11	112.27	120.80
6	A	1328	C	C6-N1-C1'	-7.11	112.27	120.80
6	A	1200	C	C6-N1-C2	-7.08	117.47	120.30
7	D	1656	C	C6-N1-C2	-7.07	117.47	120.30
7	D	1925	C	N1-C2-O2	7.07	123.14	118.90
7	D	981	A	N9-C4-C5	7.06	108.62	105.80
7	D	1021	A	C2-N3-C4	-7.04	107.08	110.60
7	D	2689	U	N3-C2-O2	-7.04	117.27	122.20
7	D	2522	U	C2-N1-C1'	7.04	126.14	117.70
7	D	805	G	O4'-C1'-N9	7.03	113.83	108.20
7	D	1205	U	N1-C1'-C2'	-7.00	104.30	112.00
7	D	2444	G	C4-C5-N7	6.99	113.59	110.80
7	D	2459	A	C4-N9-C1'	6.97	138.85	126.30
7	D	49	A	C8-N9-C4	6.97	108.59	105.80
7	D	687	C	C4-C5-C6	6.96	120.88	117.40
7	D	1204	A	C4-N9-C1'	6.96	138.82	126.30
7	D	1830	C	C2-N1-C1'	6.95	126.45	118.80
7	D	775	G	C6-N1-C2	-6.93	120.94	125.10
7	D	1786	A	C5-C6-N1	6.92	121.16	117.70
7	D	1813	G	N9-C4-C5	-6.91	102.64	105.40
55	z	62	LEU	CA-CB-CG	-6.90	99.42	115.30
7	D	974	G	C2-N3-C4	-6.89	108.45	111.90
7	D	350	U	N1-C2-O2	6.89	127.62	122.80
7	D	515	A	C4-C5-N7	6.88	114.14	110.70
7	D	531	C	N1-C2-O2	6.88	123.03	118.90
7	D	1312	U	C5-C6-N1	-6.88	119.26	122.70
7	D	247	G	C6-C5-N7	-6.87	126.28	130.40
7	D	775	G	C2-N3-C4	6.86	115.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	458	G	C4-N9-C1'	-6.85	117.60	126.50
7	D	775	G	C4-C5-C6	6.85	122.91	118.80
7	D	1377	G	N3-C4-C5	-6.84	125.18	128.60
7	D	341	G	C4-N9-C1'	6.84	135.39	126.50
7	D	2021	C	C5-C6-N1	-6.83	117.59	121.00
6	A	20	U	C2-N1-C1'	6.81	125.87	117.70
7	D	2445	G	C6-C5-N7	-6.81	126.31	130.40
7	D	733	G	C6-C5-N7	-6.80	126.32	130.40
7	D	1222	C	C2-N1-C1'	6.79	126.27	118.80
7	D	1786	A	C2-N3-C4	6.76	113.98	110.60
7	D	67	U	N3-C2-O2	-6.75	117.47	122.20
7	D	1493	C	N1-C2-O2	6.73	122.94	118.90
7	D	1012	U	C5-C6-N1	-6.73	119.33	122.70
7	D	2459	A	C8-N9-C1'	-6.69	115.66	127.70
7	D	783	A	C5-N7-C8	-6.67	100.56	103.90
7	D	2830	G	C6-C5-N7	-6.66	126.40	130.40
7	D	1497	U	C5-C4-O4	-6.66	121.90	125.90
6	A	115	G	C8-N9-C1'	-6.65	118.36	127.00
7	D	753	C	C6-N1-C2	-6.64	117.64	120.30
7	D	2021	C	C2-N1-C1'	-6.63	111.50	118.80
7	D	1527	G	C6-N1-C2	6.63	129.08	125.10
7	D	2612	C	N3-C2-O2	-6.62	117.26	121.90
37	h	59	LEU	CA-CB-CG	6.61	130.49	115.30
7	D	2032	G	C4-C5-N7	6.60	113.44	110.80
7	D	733	G	C8-N9-C1'	-6.59	118.43	127.00
7	D	945	A	O4'-C1'-N9	6.58	113.47	108.20
7	D	2837	G	C4-N9-C1'	6.57	135.04	126.50
7	D	1377	G	C8-N9-C1'	-6.57	118.46	127.00
7	D	1204	A	N7-C8-N9	6.56	117.08	113.80
7	D	1253	A	N9-C4-C5	-6.56	103.18	105.80
7	D	764	A	C8-N9-C4	6.53	108.41	105.80
11	H	12	CYS	CA-CB-SG	6.53	125.75	114.00
7	D	778	G	C6-C5-N7	-6.53	126.48	130.40
6	A	1329	A	N7-C8-N9	6.52	117.06	113.80
7	D	1657	C	C4-C5-C6	-6.52	114.14	117.40
7	D	1813	G	C8-N9-C1'	-6.50	118.55	127.00
7	D	2459	A	N3-C4-N9	6.50	132.60	127.40
7	D	2056	G	N3-C4-N9	6.49	129.89	126.00
6	A	115	G	N3-C4-N9	6.48	129.89	126.00
7	D	1154	G	C4-N9-C1'	6.47	134.91	126.50
7	D	2251	G	C4-C5-N7	6.47	113.39	110.80
7	D	2500	U	O5'-P-OP2	-6.47	99.88	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	794	G	C4-N9-C1'	6.46	134.90	126.50
7	D	917	A	C6-N1-C2	-6.46	114.73	118.60
7	D	764	A	N7-C8-N9	-6.46	110.57	113.80
7	D	2450	A	O5'-P-OP1	-6.45	99.89	105.70
7	D	1787	A	C2-N3-C4	-6.44	107.38	110.60
6	A	244	U	C2-N1-C1'	6.43	125.42	117.70
7	D	2490	G	C5-C6-O6	6.43	132.46	128.60
7	D	1925	C	N3-C2-O2	-6.43	117.40	121.90
6	A	1086	U	C5-C6-N1	6.42	125.91	122.70
7	D	1632	A	C6-C5-N7	-6.42	127.80	132.30
7	D	2449	U	C2-N1-C1'	-6.42	110.00	117.70
7	D	1338	G	C4-C5-N7	6.41	113.36	110.80
7	D	1571	A	O4'-C1'-N9	6.40	113.32	108.20
7	D	879	G	C6-C5-N7	6.40	134.24	130.40
7	D	150	C	C6-N1-C1'	-6.39	113.13	120.80
6	A	324	G	C8-N9-C4	-6.39	103.85	106.40
7	D	733	G	C4-N9-C1'	6.38	134.80	126.50
49	t	30	LEU	CA-CB-CG	-6.37	100.64	115.30
7	D	733	G	N3-C4-N9	6.37	129.82	126.00
7	D	1205	U	N3-C2-O2	-6.37	117.74	122.20
7	D	1628	G	C4-N9-C1'	6.35	134.76	126.50
7	D	396	G	C4-N9-C1'	6.34	134.75	126.50
7	D	2571	C	C2-N1-C1'	-6.33	111.84	118.80
7	D	1776	G	C4-C5-N7	6.32	113.33	110.80
7	D	1222	C	N1-C2-O2	6.30	122.68	118.90
7	D	715	G	C6-C5-N7	-6.28	126.63	130.40
7	D	571	A	N1-C6-N6	-6.28	114.83	118.60
5	5	74	C	C6-N1-C1'	-6.28	113.27	120.80
7	D	848	G	C2-N3-C4	-6.28	108.76	111.90
7	D	1123	C	N1-C2-O2	6.27	122.66	118.90
7	D	2495	G	N9-C4-C5	-6.27	102.89	105.40
7	D	120	U	N3-C2-O2	-6.26	117.81	122.20
7	D	2251	G	C4-N9-C1'	6.26	134.64	126.50
7	D	2251	G	N1-C2-N2	-6.26	110.56	116.20
7	D	1779	U	C2-N1-C1'	6.26	125.21	117.70
7	D	2490	G	N1-C2-N2	-6.26	110.57	116.20
7	D	1429	G	C6-C5-N7	-6.24	126.66	130.40
7	D	1204	A	O5'-P-OP2	-6.24	100.09	105.70
7	D	730	C	N3-C2-O2	-6.23	117.54	121.90
7	D	1566	A	N7-C8-N9	6.23	116.92	113.80
6	A	1369	C	N1-C2-O2	6.22	122.64	118.90
7	D	341	G	N3-C4-C5	-6.22	125.49	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	321	G	C4-N9-C1'	-6.20	118.45	126.50
7	D	396	G	C8-N9-C1'	-6.20	118.94	127.00
7	D	1668	A	N3-C4-N9	-6.19	122.44	127.40
35	f	78	TYR	C-N-CD	-6.18	106.99	120.60
7	D	13	A	N1-C6-N6	-6.17	114.89	118.60
7	D	1344	G	C8-N9-C4	-6.17	103.93	106.40
6	A	494	U	C2-N1-C1'	6.17	125.10	117.70
7	D	2689	U	N1-C2-O2	6.17	127.12	122.80
6	A	13	U	C5-C6-N1	6.17	125.78	122.70
30	a	155	LEU	CA-CB-CG	6.17	129.48	115.30
7	D	2495	G	C4-C5-N7	6.16	113.27	110.80
7	D	283	A	N1-C6-N6	6.16	122.30	118.60
7	D	48	G	C6-C5-N7	-6.15	126.71	130.40
7	D	2036	C	N1-C2-O2	6.14	122.59	118.90
6	A	1498	U	C5-C6-N1	-6.14	119.63	122.70
7	D	1123	C	C2-N1-C1'	6.14	125.55	118.80
7	D	945	A	N1-C6-N6	-6.14	114.92	118.60
6	A	115	G	C6-C5-N7	-6.14	126.72	130.40
6	A	960	U	C2-N1-C1'	6.13	125.06	117.70
7	D	729	G	C5-C6-O6	6.13	132.28	128.60
7	D	2490	G	N3-C2-N2	6.13	124.19	119.90
7	D	2837	G	C6-C5-N7	-6.13	126.72	130.40
7	D	2445	G	N9-C4-C5	-6.13	102.95	105.40
7	D	2837	G	C8-N9-C1'	-6.13	119.03	127.00
7	D	562	U	N1-C2-O2	-6.13	118.51	122.80
7	D	1813	G	C4-N9-C1'	6.12	134.46	126.50
7	D	1492	G	N9-C4-C5	-6.11	102.95	105.40
7	D	270(Y)	G	C8-N9-C4	6.11	108.84	106.40
7	D	774	A	C5-C6-N1	6.11	120.75	117.70
7	D	515	A	N1-C2-N3	6.10	132.35	129.30
7	D	1492	G	C5-C6-N1	6.10	114.55	111.50
7	D	2460	U	C6-N1-C2	-6.10	117.34	121.00
7	D	2289	G	C8-N9-C1'	-6.09	119.08	127.00
45	p	57	LEU	CB-CG-CD1	-6.09	100.64	111.00
7	D	1775	U	C2-N1-C1'	6.08	125.00	117.70
7	D	2035	G	C5-C6-N1	6.08	114.54	111.50
7	D	1005	C	N1-C2-O2	6.08	122.55	118.90
7	D	1006	C	N1-C2-O2	-6.08	115.25	118.90
7	D	2459	A	C6-C5-N7	-6.07	128.05	132.30
7	D	321	G	N3-C4-N9	-6.07	122.36	126.00
7	D	458	G	C8-N9-C1'	6.07	134.89	127.00
7	D	944	G	C4-N9-C1'	6.07	134.39	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1604	C	C2-N1-C1'	6.07	125.48	118.80
7	D	2459	A	N3-C4-C5	-6.06	122.56	126.80
7	D	805	G	C2-N3-C4	-6.05	108.87	111.90
7	D	1429	G	C4-N9-C1'	6.05	134.37	126.50
36	g	74	GLY	N-CA-C	-6.05	97.98	113.10
6	A	872	A	O4'-C1'-N9	6.05	113.04	108.20
7	D	2653	U	C5-C6-N1	6.04	125.72	122.70
7	D	1660	C	N1-C2-O2	-6.04	115.28	118.90
7	D	729	G	N9-C4-C5	6.03	107.81	105.40
7	D	775	G	C6-C5-N7	-6.03	126.78	130.40
7	D	806	C	N1-C2-O2	-6.03	115.28	118.90
7	D	917	A	C5-C6-N1	6.02	120.71	117.70
31	b	63	LEU	CA-CB-CG	6.02	129.15	115.30
6	A	1086	U	C6-N1-C1'	-6.01	112.78	121.20
7	D	247	G	C4-N9-C1'	6.01	134.32	126.50
7	D	2307	G	C4-N9-C1'	6.00	134.30	126.50
7	D	1998	G	C6-C5-N7	-5.99	126.81	130.40
7	D	2491	U	P-O3'-C3'	-5.99	112.52	119.70
7	D	1785	A	N9-C4-C5	5.98	108.19	105.80
7	D	774	A	N1-C2-N3	5.97	132.29	129.30
7	D	2445	G	C8-N9-C1'	-5.97	119.23	127.00
7	D	2268	A	C8-N9-C4	-5.96	103.42	105.80
11	H	196	LEU	CA-CB-CG	5.94	128.97	115.30
7	D	687	C	N3-C2-O2	-5.94	117.74	121.90
7	D	1493	C	C2-N1-C1'	5.94	125.33	118.80
7	D	350	U	C2-N1-C1'	5.94	124.83	117.70
7	D	688	U	N1-C2-N3	5.94	118.46	114.90
7	D	515	A	C6-N1-C2	-5.93	115.04	118.60
7	D	1649	G	C4-N9-C1'	5.93	134.21	126.50
7	D	792	G	C4-N9-C1'	5.93	134.21	126.50
7	D	727	A	N1-C2-N3	5.93	132.26	129.30
6	A	518	C	P-O3'-C3'	5.92	126.81	119.70
7	D	60	G	N1-C2-N2	-5.92	110.87	116.20
7	D	676	A	C5-N7-C8	-5.92	100.94	103.90
7	D	729	G	N7-C8-N9	5.91	116.06	113.10
7	D	297	C	N3-C4-C5	5.91	124.26	121.90
7	D	450	G	N1-C6-O6	5.91	123.45	119.90
7	D	1377	G	N1-C2-N2	-5.91	110.88	116.20
7	D	774	A	O4'-C1'-N9	5.90	112.92	108.20
7	D	1428	C	OP1-P-O3'	5.90	118.18	105.20
7	D	2126	A	O4'-C1'-N9	5.90	112.92	108.20
7	D	2459	A	N1-C2-N3	5.89	132.25	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1251	C	C6-N1-C2	5.89	122.66	120.30
7	D	1380	G	C8-N9-C1'	-5.89	119.34	127.00
7	D	1425	G	C6-C5-N7	-5.88	126.88	130.40
7	D	1632	A	C4-C5-N7	5.88	113.64	110.70
7	D	1598	C	N1-C2-O2	5.87	122.42	118.90
7	D	383	U	N1-C2-O2	5.87	126.91	122.80
7	D	856	C	C2-N1-C1'	5.87	125.26	118.80
7	D	1157	G	C4-N9-C1'	5.87	134.13	126.50
6	A	397	A	N1-C6-N6	-5.87	115.08	118.60
7	D	1253	A	C8-N9-C4	5.87	108.15	105.80
7	D	2289	G	C4-N9-C1'	5.87	134.12	126.50
7	D	1665	A	N7-C8-N9	5.86	116.73	113.80
7	D	682	G	C6-C5-N7	-5.85	126.89	130.40
7	D	531	C	C2-N1-C1'	5.85	125.23	118.80
7	D	311	A	O4'-C1'-N9	5.84	112.87	108.20
7	D	1799	G	O4'-C1'-N9	5.84	112.87	108.20
7	D	2612	C	O5'-P-OP1	-5.83	100.45	105.70
7	D	1566	A	C4-N9-C1'	5.83	136.79	126.30
7	D	761	A	C4-C5-N7	5.83	113.61	110.70
7	D	1325	G	O4'-C1'-N9	5.83	112.86	108.20
7	D	1241	A	N7-C8-N9	5.82	116.71	113.80
6	A	324	G	N7-C8-N9	5.82	116.01	113.10
7	D	972	G	C4-N9-C1'	5.82	134.07	126.50
7	D	1222	C	C6-N1-C1'	-5.82	113.82	120.80
7	D	1649	G	C8-N9-C1'	-5.81	119.44	127.00
7	D	1341	U	O5'-P-OP1	-5.81	100.47	105.70
7	D	659	C	C6-N1-C2	5.81	122.62	120.30
7	D	733	G	C4-C5-N7	5.81	113.12	110.80
33	d	3	LEU	CA-CB-CG	5.81	128.66	115.30
7	D	2002	G	C4-C5-N7	5.80	113.12	110.80
7	D	1972	A	C6-N1-C2	-5.80	115.12	118.60
41	l	114	LEU	CA-CB-CG	-5.80	101.96	115.30
7	D	1513	C	N3-C2-O2	-5.80	117.84	121.90
7	D	1623	G	C4-N9-C1'	5.79	134.03	126.50
7	D	730	C	N1-C2-O2	5.79	122.37	118.90
7	D	1123	C	C6-N1-C1'	-5.79	113.86	120.80
7	D	1667	G	C4-N9-C1'	5.77	134.00	126.50
7	D	1205	U	P-O3'-C3'	-5.77	112.78	119.70
7	D	1204	A	C8-N9-C4	-5.76	103.50	105.80
7	D	295	G	C8-N9-C4	5.75	108.70	106.40
7	D	453	C	N1-C2-O2	5.75	122.35	118.90
7	D	2445	G	C4-C5-N7	5.75	113.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	617	G	N3-C4-C5	5.75	131.47	128.60
7	D	1380	G	C4-N9-C1'	5.75	133.97	126.50
7	D	1475	G	N3-C4-N9	5.74	129.45	126.00
7	D	2501	C	N1-C2-O2	5.74	122.34	118.90
5	5	1	G	N3-C4-C5	5.74	131.47	128.60
7	D	1522	G	C6-C5-N7	-5.74	126.96	130.40
35	f	82	LEU	CA-CB-CG	-5.74	102.11	115.30
7	D	138	G	N3-C4-N9	5.73	129.44	126.00
7	D	1416	G	C2-N3-C4	-5.73	109.03	111.90
7	D	1840	G	C6-C5-N7	-5.73	126.96	130.40
7	D	2758	A	N9-C4-C5	-5.73	103.51	105.80
7	D	1527	G	N7-C8-N9	5.73	115.96	113.10
7	D	776	G	P-O3'-C3'	5.72	126.57	119.70
52	w	12	SER	N-CA-C	5.71	126.42	111.00
6	A	1086	U	C6-N1-C2	-5.71	117.58	121.00
7	D	2582	G	C4-N9-C1'	5.71	133.92	126.50
7	D	341	G	N3-C2-N2	5.70	123.89	119.90
7	D	1377	G	C4-C5-C6	5.69	122.22	118.80
7	D	1790	C	C2-N1-C1'	-5.69	112.54	118.80
7	D	321	G	N3-C4-C5	5.69	131.44	128.60
7	D	792	G	N3-C4-C5	-5.68	125.76	128.60
7	D	2073	C	N3-C2-O2	-5.68	117.92	121.90
7	D	1667	G	C6-C5-N7	-5.68	126.99	130.40
7	D	820	A	N1-C2-N3	5.67	132.14	129.30
7	D	2270	G	C6-C5-N7	-5.67	127.00	130.40
7	D	400	G	N1-C6-O6	5.67	123.30	119.90
7	D	779	U	C5-C6-N1	5.67	125.53	122.70
7	D	2756	U	C6-N1-C2	5.67	124.40	121.00
6	A	1364	U	C2-N1-C1'	5.66	124.49	117.70
7	D	972	G	N3-C4-C5	-5.66	125.77	128.60
7	D	2029	G	N3-C4-N9	-5.66	122.61	126.00
7	D	791	C	C6-N1-C2	5.66	122.56	120.30
7	D	470	A	C6-N1-C2	-5.65	115.21	118.60
7	D	106	C	N1-C2-O2	-5.65	115.51	118.90
7	D	2660	A	O4'-C1'-N9	-5.65	103.68	108.20
7	D	2242	G	C4-N9-C1'	5.64	133.84	126.50
6	A	328	C	C6-N1-C2	-5.64	118.04	120.30
7	D	1661	G	N3-C4-N9	-5.64	122.61	126.00
7	D	1950	G	N1-C6-O6	-5.64	116.51	119.90
7	D	1799	G	C8-N9-C1'	5.64	134.33	127.00
7	D	410	G	C4-N9-C1'	5.63	133.82	126.50
7	D	1204	A	C8-N9-C1'	-5.63	117.56	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1377	G	N1-C2-N3	5.63	127.28	123.90
7	D	1951	U	N3-C2-O2	-5.63	118.26	122.20
7	D	688	U	N3-C4-C5	5.63	117.98	114.60
7	D	1937	A	C5-N7-C8	-5.63	101.08	103.90
6	A	49	U	C5-C6-N1	-5.63	119.88	122.70
7	D	410	G	N3-C4-N9	5.63	129.38	126.00
7	D	1786	A	N7-C8-N9	5.63	116.61	113.80
6	A	38	G	N3-C4-N9	-5.62	122.63	126.00
7	D	775	G	C5-C6-N1	5.61	114.31	111.50
7	D	2035	G	N1-C6-O6	-5.61	116.53	119.90
7	D	2289	G	C6-C5-N7	-5.61	127.03	130.40
7	D	1153	C	C6-N1-C2	-5.60	118.06	120.30
7	D	498	G	C8-N9-C4	-5.60	104.16	106.40
7	D	1012	U	O4'-C1'-N1	5.60	112.68	108.20
8	E	12	C	C6-N1-C2	-5.60	118.06	120.30
7	D	1513	C	C2-N1-C1'	5.60	124.96	118.80
13	J	10	LEU	CA-CB-CG	5.59	128.16	115.30
7	D	793	A	N1-C6-N6	5.59	121.95	118.60
7	D	2025	C	C2-N1-C1'	5.59	124.95	118.80
7	D	1475	G	C6-C5-N7	-5.59	127.05	130.40
7	D	1266	G	N3-C4-N9	-5.58	122.65	126.00
7	D	1632	A	C5-C6-N6	-5.58	119.23	123.70
7	D	2021	C	C4-C5-C6	5.58	120.19	117.40
6	A	1498	U	C2-N1-C1'	-5.58	111.01	117.70
7	D	1669	A	C6-C5-N7	-5.58	128.40	132.30
7	D	582	G	C6-C5-N7	-5.57	127.06	130.40
7	D	1429	G	C8-N9-C1'	-5.56	119.77	127.00
7	D	603	A	C4-C5-C6	-5.56	114.22	117.00
7	D	1840	G	C4-C5-N7	5.56	113.02	110.80
7	D	1267	U	C5-C6-N1	5.56	125.48	122.70
8	E	100	G	C4-N9-C1'	5.56	133.72	126.50
7	D	1397	U	C2-N1-C1'	5.55	124.36	117.70
7	D	2777	G	C8-N9-C4	-5.55	104.18	106.40
7	D	1833	U	N1-C2-N3	5.55	118.23	114.90
7	D	2457	U	N1-C2-O2	5.54	126.68	122.80
5	5	1	G	N3-C4-N9	-5.54	122.67	126.00
7	D	1699	G	N3-C4-N9	-5.54	122.67	126.00
7	D	1899	G	C2-N3-C4	-5.54	109.13	111.90
7	D	1653	G	N1-C2-N2	-5.54	111.22	116.20
7	D	1800	C	C6-N1-C1'	-5.54	114.16	120.80
7	D	2492	U	N1-C2-O2	5.54	126.67	122.80
7	D	2495	G	N3-C4-C5	-5.54	125.83	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	122	G	N3-C4-N9	5.53	129.32	126.00
7	D	2020	A	P-O3'-C3'	5.52	126.33	119.70
7	D	2544	G	C6-C5-N7	-5.52	127.09	130.40
7	D	1025	G	C2-N3-C4	5.52	114.66	111.90
7	D	1559	G	N9-C1'-C2'	-5.52	105.93	112.00
7	D	150	C	O4'-C1'-N1	5.51	112.61	108.20
7	D	120	U	C6-N1-C1'	-5.51	113.49	121.20
6	A	581	G	C6-C5-N7	-5.51	127.09	130.40
7	D	1566	A	C6-C5-N7	-5.51	128.44	132.30
6	A	1296	C	N1-C2-O2	5.51	122.20	118.90
7	D	363(F)	A	O3'-P-O5'	-5.51	93.54	104.00
7	D	1944	U	N3-C2-O2	-5.51	118.34	122.20
7	D	2241	A	N1-C2-N3	5.51	132.05	129.30
5	5	74	C	N3-C2-O2	-5.50	118.05	121.90
6	A	1261	A	N1-C6-N6	5.50	121.90	118.60
7	D	1355	G	C4-C5-N7	5.50	113.00	110.80
7	D	2460	U	N1-C2-O2	5.50	126.65	122.80
6	A	570	G	C4-C5-N7	5.50	113.00	110.80
7	D	1340	U	N1-C2-N3	5.50	118.20	114.90
7	D	1735	C	O3'-P-O5'	-5.50	93.55	104.00
7	D	1668	A	N9-C4-C5	5.50	108.00	105.80
7	D	2025	C	C6-N1-C2	-5.48	118.11	120.30
7	D	1139	G	N1-C6-O6	5.48	123.19	119.90
7	D	2447	G	N3-C4-C5	-5.48	125.86	128.60
7	D	297	C	N3-C2-O2	-5.47	118.07	121.90
7	D	2718	G	C4-N9-C1'	5.47	133.62	126.50
7	D	1154	G	C8-N9-C1'	-5.47	119.89	127.00
7	D	359	A	N9-C1'-C2'	-5.47	105.98	112.00
7	D	848	G	C4-C5-N7	5.47	112.99	110.80
7	D	2612	C	C6-N1-C2	-5.47	118.11	120.30
7	D	2069	G	N3-C4-N9	5.46	129.28	126.00
7	D	1665	A	C5-N7-C8	-5.45	101.17	103.90
7	D	360	G	C4-N9-C1'	5.45	133.59	126.50
7	D	138	G	C4-N9-C1'	5.44	133.58	126.50
7	D	1522	G	C4-C5-N7	5.44	112.98	110.80
7	D	1652	A	C5-N7-C8	-5.44	101.18	103.90
7	D	25	U	C2-N3-C4	-5.44	123.74	127.00
7	D	247	G	C8-N9-C1'	-5.44	119.93	127.00
7	D	1071	G	C6-C5-N7	-5.44	127.14	130.40
7	D	1810	A	C5-C6-N1	5.43	120.42	117.70
7	D	1475	G	C4-N9-C1'	5.43	133.56	126.50
7	D	1604	C	C6-N1-C2	-5.43	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	859	G	C4-C5-N7	5.43	112.97	110.80
7	D	1012	U	C6-N1-C1'	5.43	128.80	121.20
7	D	138	G	C8-N9-C1'	-5.43	119.94	127.00
7	D	1786	A	C5-C6-N6	-5.43	119.36	123.70
7	D	775	G	C8-N9-C1'	-5.42	119.95	127.00
7	D	1632	A	N9-C4-C5	-5.42	103.63	105.80
7	D	2307	G	C8-N9-C1'	-5.42	119.95	127.00
7	D	1007	C	N1-C2-O2	-5.42	115.65	118.90
7	D	2503	A	C6-C5-N7	-5.42	128.50	132.30
7	D	848	G	C6-C5-N7	-5.42	127.15	130.40
7	D	2517	C	C2-N3-C4	-5.42	117.19	119.90
7	D	1660	C	C2-N3-C4	-5.41	117.19	119.90
7	D	1830	C	C6-N1-C2	-5.41	118.14	120.30
6	A	596	C	C5-C6-N1	5.41	123.70	121.00
7	D	1338	G	N9-C4-C5	-5.41	103.24	105.40
7	D	341	G	C4-C5-C6	5.40	122.04	118.80
7	D	283	A	C5-C6-N6	-5.40	119.38	123.70
7	D	1950	G	N9-C4-C5	5.40	107.56	105.40
7	D	2136	C	C2-N1-C1'	5.40	124.74	118.80
7	D	2512	C	C5-C6-N1	5.40	123.70	121.00
7	D	2522	U	C6-N1-C1'	-5.39	113.65	121.20
7	D	1544	C	N1-C2-O2	5.39	122.13	118.90
7	D	2241	A	C6-N1-C2	-5.39	115.37	118.60
7	D	1675	C	N1-C2-O2	5.39	122.13	118.90
7	D	792	G	C6-C5-N7	-5.38	127.17	130.40
6	A	1504	G	O5'-P-OP2	-5.38	100.86	105.70
7	D	1254	A	O4'-C1'-N9	5.38	112.51	108.20
6	A	1301	U	C2-N1-C1'	5.38	124.16	117.70
7	D	1314	C	C6-N1-C2	-5.38	118.15	120.30
7	D	1943	U	P-O3'-C3'	5.38	126.16	119.70
7	D	1649	G	N3-C4-N9	5.38	129.23	126.00
7	D	1828	G	N9-C4-C5	5.38	107.55	105.40
7	D	2444	G	C4-N9-C1'	5.38	133.49	126.50
7	D	859	G	C6-C5-N7	-5.37	127.17	130.40
41	l	63	VAL	N-CA-C	-5.37	96.49	111.00
6	A	1086	U	N1-C2-O2	5.37	126.56	122.80
7	D	759	G	C4-C5-N7	5.37	112.95	110.80
7	D	2307	G	N3-C4-N9	5.37	129.22	126.00
21	R	43	CYS	CA-CB-SG	5.37	123.66	114.00
7	D	656	G	C6-C5-N7	-5.36	127.18	130.40
7	D	1791	A	O5'-P-OP1	-5.36	100.87	105.70
7	D	2251	G	N3-C4-N9	5.36	129.22	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	645	C	C2-N1-C1'	5.35	124.69	118.80
7	D	730	C	C6-N1-C2	-5.35	118.16	120.30
7	D	1205	U	C2-N3-C4	5.35	130.21	127.00
7	D	280	C	C6-N1-C1'	-5.35	114.38	120.80
7	D	1669	A	C4-C5-N7	5.35	113.37	110.70
7	D	2056	G	C6-N1-C2	-5.35	121.89	125.10
7	D	974(A)	C	N3-C4-N4	5.34	121.74	118.00
7	D	2073	C	C5-C6-N1	5.34	123.67	121.00
7	D	1675	C	N3-C2-O2	-5.33	118.17	121.90
7	D	973	A	OP1-P-O3'	5.33	116.92	105.20
7	D	2251	G	O5'-P-OP2	-5.33	100.91	105.70
7	D	2703	C	C6-N1-C2	-5.33	118.17	120.30
7	D	1660	C	C2-N1-C1'	-5.32	112.94	118.80
7	D	67	U	N1-C2-O2	5.31	126.52	122.80
7	D	1810	A	C2-N3-C4	5.31	113.25	110.60
6	A	494	U	N1-C2-O2	5.30	126.51	122.80
7	D	1025	G	C8-N9-C4	-5.30	104.28	106.40
7	D	1964	G	O4'-C1'-N9	-5.30	103.96	108.20
7	D	2426	A	C4-N9-C1'	5.30	135.83	126.30
53	x	39	TYR	N-CA-C	5.30	125.30	111.00
7	D	1143	A	C6-N1-C2	-5.29	115.43	118.60
7	D	2630	G	N3-C4-N9	5.29	129.17	126.00
7	D	940	G	C8-N9-C4	-5.28	104.29	106.40
7	D	2612	C	N1-C2-N3	5.28	122.90	119.20
51	v	40	HIS	C-N-CD	-5.28	108.98	120.60
6	A	244	U	N1-C2-O2	5.28	126.50	122.80
7	D	2073	C	C2-N1-C1'	5.27	124.60	118.80
7	D	2407	G	N1-C6-O6	-5.27	116.74	119.90
7	D	363(F)	A	P-O3'-C3'	-5.27	113.38	119.70
7	D	1604	C	N1-C2-O2	5.27	122.06	118.90
7	D	2447	G	N3-C4-N9	5.27	129.16	126.00
7	D	323	G	N3-C4-C5	-5.27	125.97	128.60
7	D	603	A	C4-N9-C1'	-5.27	116.82	126.30
7	D	1519	G	C8-N9-C1'	-5.27	120.15	127.00
8	E	50	G	C8-N9-C4	5.26	108.50	106.40
7	D	2445	G	C4-N9-C1'	5.26	133.33	126.50
7	D	848	G	N1-C6-O6	5.25	123.05	119.90
36	g	8	LEU	CA-CB-CG	5.25	127.38	115.30
7	D	2472	G	C8-N9-C1'	-5.25	120.17	127.00
7	D	410	G	N3-C4-C5	-5.25	125.98	128.60
7	D	774	A	C8-N9-C4	-5.25	103.70	105.80
7	D	776	G	C6-C5-N7	-5.25	127.25	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	2266	A	P-O3'-C3'	5.24	125.99	119.70
7	D	2136	C	N1-C2-O2	5.24	122.04	118.90
7	D	1771	C	C6-N1-C2	-5.24	118.21	120.30
7	D	2027	G	C8-N9-C1'	-5.24	120.19	127.00
7	D	794	G	N3-C4-N9	5.23	129.14	126.00
7	D	1253	A	O4'-C1'-N9	-5.23	104.01	108.20
7	D	1786	A	C8-N9-C1'	-5.23	118.28	127.70
6	A	244	U	C6-N1-C1'	-5.23	113.88	121.20
7	D	1628	G	C8-N9-C1'	-5.23	120.20	127.00
7	D	1809	A	O4'-C1'-N9	5.23	112.38	108.20
7	D	1667	G	C8-N9-C1'	-5.23	120.20	127.00
7	D	1571	A	C5-C6-N1	5.22	120.31	117.70
5	5	39	U	C2-N1-C1'	5.22	123.96	117.70
7	D	546	C	N1-C2-O2	5.21	122.03	118.90
7	D	1527	G	C2-N3-C4	-5.21	109.30	111.90
51	v	41	PRO	N-CA-C	5.21	125.64	112.10
7	D	2125	G	N3-C4-N9	-5.21	122.88	126.00
7	D	1647	G	O5'-P-OP1	-5.20	101.02	105.70
6	A	1477	C	N1-C2-O2	5.20	122.02	118.90
7	D	856	C	C6-N1-C1'	-5.20	114.57	120.80
7	D	1951	U	C2-N1-C1'	5.20	123.93	117.70
7	D	2606	C	N3-C4-C5	5.19	123.98	121.90
6	A	13	U	N1-C2-O2	5.19	126.44	122.80
7	D	793	A	C6-C5-N7	-5.19	128.67	132.30
7	D	2021	C	C6-N1-C1'	5.19	127.03	120.80
7	D	280	C	C6-N1-C2	5.19	122.38	120.30
7	D	676	A	C2-N3-C4	-5.19	108.01	110.60
7	D	1664	A	C5-N7-C8	-5.19	101.31	103.90
7	D	1776	G	C6-C5-N7	-5.19	127.29	130.40
7	D	778	G	N9-C4-C5	-5.18	103.33	105.40
53	x	23	THR	N-CA-C	5.18	124.99	111.00
7	D	2251	G	C8-N9-C1'	-5.18	120.27	127.00
3	3	21	PRO	C-N-CD	5.18	139.27	128.40
7	D	1784	A	N9-C4-C5	-5.18	103.73	105.80
7	D	60	G	N1-C6-O6	-5.17	116.80	119.90
6	A	137	C	C6-N1-C2	5.17	122.37	120.30
7	D	794	G	C8-N9-C1'	-5.17	120.28	127.00
7	D	1656	C	N3-C2-O2	-5.17	118.28	121.90
7	D	515	A	C4-N9-C1'	5.16	135.59	126.30
7	D	602	G	P-O3'-C3'	5.16	125.90	119.70
7	D	794	G	C4-C5-N7	5.16	112.87	110.80
7	D	2258	C	N3-C4-C5	5.16	123.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	11	LEU	CA-CB-CG	-5.16	103.42	115.30
50	u	11	SER	C-N-CD	-5.16	109.24	120.60
6	A	115	G	N3-C4-C5	-5.16	126.02	128.60
7	D	609(A)	G	N3-C4-N9	-5.16	122.91	126.00
7	D	1800	C	C2-N1-C1'	5.16	124.47	118.80
7	D	687	C	N1-C2-N3	5.15	122.81	119.20
7	D	1834	U	N3-C2-O2	-5.15	118.59	122.20
7	D	277	C	C2-N1-C1'	5.15	124.47	118.80
7	D	1799	G	C4-N9-C1'	-5.15	119.80	126.50
37	h	43	GLY	N-CA-C	-5.15	100.23	113.10
7	D	2472	G	C6-C5-N7	-5.14	127.31	130.40
7	D	1139	G	C4-C5-N7	5.14	112.86	110.80
6	A	362	G	C2-N3-C4	-5.14	109.33	111.90
7	D	2642	G	C6-C5-N7	-5.13	127.32	130.40
7	D	183	C	C2-N3-C4	-5.13	117.33	119.90
7	D	733	G	N9-C4-C5	-5.13	103.35	105.40
7	D	1325	G	N1-C6-O6	5.13	122.98	119.90
7	D	2239	G	C4-N9-C1'	5.13	133.17	126.50
7	D	811	U	C4-C5-C6	-5.13	116.62	119.70
7	D	613	U	O4'-C1'-N1	5.12	112.30	108.20
7	D	1402	C	C6-N1-C2	-5.12	118.25	120.30
6	A	304	U	C2-N1-C1'	5.12	123.85	117.70
56	B	186	PRO	C-N-CD	5.12	139.16	128.40
7	D	321	G	C8-N9-C1'	5.12	133.66	127.00
7	D	462	C	C2-N1-C1'	5.12	124.43	118.80
7	D	295	G	C4-N9-C1'	-5.11	119.85	126.50
7	D	515	A	C8-N9-C1'	-5.11	118.50	127.70
7	D	2056	G	O4'-C1'-N9	-5.11	104.11	108.20
6	A	1106	G	N3-C4-N9	-5.11	122.93	126.00
29	Z	181	PRO	C-N-CD	5.11	139.13	128.40
6	A	1369	C	C2-N1-C1'	5.11	124.42	118.80
7	D	791	C	N3-C4-N4	-5.11	114.42	118.00
37	h	69	GLY	N-CA-C	-5.11	100.33	113.10
7	D	2703	C	N1-C2-O2	5.10	121.96	118.90
7	D	972	G	N3-C4-N9	5.10	129.06	126.00
7	D	1397	U	C5-C6-N1	5.10	125.25	122.70
43	n	15	GLU	C-N-CD	5.10	139.11	128.40
7	D	1519	G	C4-N9-C1'	5.10	133.13	126.50
7	D	247	G	N1-C2-N3	5.10	126.96	123.90
7	D	974	G	N9-C4-C5	-5.10	103.36	105.40
7	D	2242	G	C8-N9-C1'	-5.09	120.38	127.00
7	D	740	U	C5-C6-N1	5.09	125.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	805	G	N3-C4-C5	5.09	131.15	128.60
7	D	1032	A	C8-N9-C4	5.09	107.84	105.80
7	D	1157	G	C8-N9-C1'	-5.09	120.38	127.00
6	A	1369	C	N3-C2-O2	-5.09	118.34	121.90
7	D	2052	G	C6-C5-N7	-5.09	127.35	130.40
7	D	1153	C	C2-N1-C1'	5.09	124.39	118.80
56	B	396	LEU	C-N-CD	5.09	139.08	128.40
7	D	60	G	N3-C4-N9	5.08	129.05	126.00
7	D	1996	C	P-O3'-C3'	5.08	125.80	119.70
8	E	50	G	N9-C4-C5	-5.08	103.37	105.40
7	D	761	A	C5-N7-C8	-5.08	101.36	103.90
7	D	2617	C	N3-C4-C5	5.08	123.93	121.90
8	E	100	G	C6-C5-N7	-5.08	127.35	130.40
56	B	398	ASP	C-N-CD	5.08	139.07	128.40
3	3	90	LYS	C-N-CD	5.08	139.07	128.40
7	D	462	C	N3-C2-O2	-5.08	118.34	121.90
56	B	333	GLU	C-N-CD	5.08	139.06	128.40
3	3	18	THR	C-N-CD	5.08	139.06	128.40
7	D	1635	G	C4-N9-C1'	5.08	133.10	126.50
7	D	1986	A	C8-N9-C4	-5.08	103.77	105.80
20	Q	96	LEU	C-N-CD	5.08	139.06	128.40
30	a	48	ARG	CB-CG-CD	5.08	124.80	111.60
56	B	454	ALA	C-N-CD	5.08	139.06	128.40
6	A	189	U	C2-N1-C1'	5.07	123.79	117.70
7	D	1997	G	C2-N3-C4	-5.07	109.36	111.90
56	B	528	ILE	C-N-CD	5.07	139.06	128.40
7	D	1617	C	N3-C2-O2	-5.07	118.35	121.90
56	B	289	SER	C-N-CD	5.07	139.05	128.40
56	B	373	ALA	C-N-CD	5.07	139.05	128.40
7	D	1919	A	P-O3'-C3'	5.07	125.78	119.70
3	3	53	VAL	C-N-CD	5.07	139.04	128.40
7	D	2653	U	C2-N1-C1'	5.06	123.78	117.70
56	B	223	ARG	C-N-CD	5.06	139.03	128.40
7	D	247	G	N3-C4-N9	5.06	129.04	126.00
7	D	1205	U	C5-C6-N1	5.06	125.23	122.70
56	B	191	ASP	C-N-CD	5.06	139.03	128.40
56	B	246	THR	C-N-CD	5.06	139.03	128.40
7	D	1607	C	N3-C2-O2	5.06	125.44	121.90
7	D	2500	U	P-O3'-C3'	5.06	125.77	119.70
7	D	1571	A	N1-C2-N3	-5.06	126.77	129.30
26	W	75	ALA	C-N-CD	5.06	139.02	128.40
3	3	24	GLY	C-N-CD	5.06	139.02	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1498	U	C2-N3-C4	-5.06	123.97	127.00
7	D	1660	C	C6-N1-C1'	5.06	126.87	120.80
56	B	158	LEU	C-N-CD	5.06	139.02	128.40
56	B	407	GLU	C-N-CD	5.06	139.02	128.40
7	D	2069	G	C6-C5-N7	-5.06	127.37	130.40
56	B	287	THR	C-N-CD	5.06	139.02	128.40
56	B	295	ARG	C-N-CD	5.06	139.02	128.40
56	B	298	LYS	C-N-CD	5.06	139.02	128.40
7	D	297	C	C2-N1-C1'	5.05	124.36	118.80
7	D	1956	U	N3-C2-O2	-5.05	118.66	122.20
34	e	125	VAL	C-N-CD	5.05	139.02	128.40
56	B	416	THR	C-N-CD	5.05	139.01	128.40
56	B	485	ARG	C-N-CD	5.05	139.01	128.40
56	B	592	VAL	C-N-CD	5.05	139.02	128.40
56	B	185	ILE	C-N-CD	5.05	139.01	128.40
6	A	38	G	N3-C4-C5	5.05	131.13	128.60
7	D	1507	A	O4'-C1'-N9	5.05	112.24	108.20
56	B	535	VAL	C-N-CD	5.05	139.01	128.40
7	D	1286	A	C8-N9-C4	5.05	107.82	105.80
56	B	132	ILE	C-N-CD	5.05	139.01	128.40
56	B	212	ILE	C-N-CD	5.05	139.00	128.40
3	3	12	LEU	C-N-CD	5.05	139.00	128.40
7	D	1623	G	C8-N9-C1'	-5.05	120.44	127.00
7	D	2279	G	C6-C5-N7	-5.05	127.37	130.40
56	B	441	LEU	C-N-CD	5.04	139.00	128.40
26	W	58	VAL	C-N-CD	5.04	138.99	128.40
7	D	1628	G	N3-C4-N9	5.04	129.02	126.00
7	D	1669	A	C5-N7-C8	-5.04	101.38	103.90
7	D	676	A	C6-C5-N7	-5.04	128.77	132.30
56	B	83	THR	C-N-CD	5.04	138.98	128.40
7	D	479	A	C8-N9-C4	5.04	107.81	105.80
7	D	1205	U	C2'-C3'-O3'	5.04	121.76	113.70
7	D	1300	U	O4'-C1'-N1	-5.04	104.17	108.20
7	D	1792	G	C6-C5-N7	-5.04	127.38	130.40
7	D	2758	A	C5-C6-N6	-5.03	119.67	123.70
8	E	100	G	C8-N9-C1'	-5.03	120.46	127.00
7	D	1522	G	N1-C6-O6	5.03	122.92	119.90
7	D	206	U	C2-N1-C1'	-5.03	111.67	117.70
7	D	1186	G	C4-C5-N7	-5.03	108.79	110.80
6	A	1086	U	N3-C2-O2	-5.03	118.68	122.20
7	D	433	C	C2-N1-C1'	5.03	124.33	118.80
7	D	659	C	N3-C4-C5	5.03	123.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1833	U	C2-N3-C4	-5.02	123.99	127.00
7	D	2642	G	C4-C5-N7	5.02	112.81	110.80
54	y	31	LEU	CA-CB-CG	-5.02	103.75	115.30
6	A	653	A	O4'-C1'-N9	5.02	112.22	108.20
7	D	410	G	C8-N9-C1'	-5.02	120.47	127.00
7	D	733	G	C5-C6-O6	-5.02	125.59	128.60
30	a	220	HIS	N-CA-C	5.02	124.55	111.00
7	D	753	C	C5-C6-N1	5.02	123.51	121.00
7	D	1021	A	C5-N7-C8	-5.01	101.39	103.90
7	D	246	C	N3-C4-C5	5.01	123.91	121.90
7	D	2703	C	C2-N1-C1'	5.01	124.31	118.80
7	D	2703	C	N3-C2-O2	-5.01	118.39	121.90
7	D	688	U	N1-C2-O2	-5.01	119.29	122.80
7	D	1204	A	C4-C5-C6	5.01	119.50	117.00
7	D	1811	G	C4-C5-N7	5.01	112.80	110.80
7	D	1950	G	O4'-C1'-N9	5.01	112.21	108.20
7	D	13	A	N9-C4-C5	5.01	107.80	105.80
7	D	932	G	N1-C2-N2	-5.01	111.69	116.20
7	D	609(A)	G	N3-C2-N2	-5.00	116.40	119.90
7	D	1020	A	C8-N9-C4	5.00	107.80	105.80
7	D	1135	C	N1-C2-O2	5.00	121.90	118.90
6	A	190	G	C8-N9-C4	-5.00	104.40	106.40
7	D	1950	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	95	GLN	Peptide
17	N	33	GLN	Peptide
19	P	15	ARG	Peptide
21	R	34	TYR	Peptide
30	a	226	MET	Peptide
30	a	233	HIS	Peptide
30	a	238	GLY	Peptide
30	a	246	PRO	Peptide
32	c	177	ALA	Peptide
32	c	98	SER	Peptide
33	d	130	ASN	Peptide
33	d	141	PHE	Peptide
35	f	2	LYS	Peptide
35	f	75	TYR	Peptide

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Mol	Chain	Res	Type	Group
35	f	78	TYR	Peptide
37	h	122	PRO	Peptide
40	k	53	SER	Peptide
40	k	94	TYR	Peptide
41	l	100	TYR	Peptide
41	l	57	PHE	Peptide
41	l	71	GLY	Peptide
47	r	160	GLY	Peptide
51	v	2	LYS	Peptide
52	w	11	THR	Peptide
52	w	4	HIS	Peptide
52	w	41	PRO	Peptide
52	w	49	CYS	Peptide
52	w	5	PRO	Peptide
53	x	22	ALA	Peptide
53	x	26	ASN	Peptide
53	x	38	LYS	Peptide
55	z	29	LYS	Peptide
55	z	4	MET	Peptide
55	z	59	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0 3
2	2	128/173 (74%)	96 (75%)	23 (18%)	9 (7%)	1 17
3	3	132/147 (90%)	68 (52%)	37 (28%)	27 (20%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	232/256 (91%)	179 (77%)	32 (14%)	21 (9%)	1	12
10	G	204/239 (85%)	170 (83%)	21 (10%)	13 (6%)	1	20
11	H	206/209 (99%)	172 (84%)	17 (8%)	17 (8%)	1	13
12	I	148/162 (91%)	125 (84%)	15 (10%)	8 (5%)	2	22
13	J	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	1	20
14	K	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	5	36
15	L	136/138 (99%)	112 (82%)	17 (12%)	7 (5%)	2	23
16	M	125/128 (98%)	90 (72%)	27 (22%)	8 (6%)	1	20
17	N	96/105 (91%)	80 (83%)	12 (12%)	4 (4%)	3	26
18	O	117/129 (91%)	104 (89%)	8 (7%)	5 (4%)	2	26
19	P	122/132 (92%)	91 (75%)	24 (20%)	7 (6%)	1	21
20	Q	112/126 (89%)	77 (69%)	23 (20%)	12 (11%)	0	8
21	R	58/61 (95%)	43 (74%)	9 (16%)	6 (10%)	0	9
22	S	86/89 (97%)	74 (86%)	10 (12%)	2 (2%)	6	38
23	T	81/88 (92%)	69 (85%)	8 (10%)	4 (5%)	2	24
24	U	102/105 (97%)	80 (78%)	16 (16%)	6 (6%)	1	21
25	V	71/88 (81%)	57 (80%)	10 (14%)	4 (6%)	2	21
26	W	78/93 (84%)	30 (38%)	25 (32%)	23 (30%)	0	0
27	X	97/106 (92%)	85 (88%)	8 (8%)	4 (4%)	3	27
28	Y	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
29	Z	226/229 (99%)	187 (83%)	28 (12%)	11 (5%)	2	24
30	a	270/276 (98%)	201 (74%)	38 (14%)	31 (12%)	0	7
31	b	204/206 (99%)	150 (74%)	31 (15%)	23 (11%)	0	7
32	c	206/210 (98%)	165 (80%)	25 (12%)	16 (8%)	1	15
33	d	180/182 (99%)	115 (64%)	42 (23%)	23 (13%)	0	5
34	e	172/180 (96%)	125 (73%)	24 (14%)	23 (13%)	0	4
35	f	137/140 (98%)	107 (78%)	19 (14%)	11 (8%)	1	14
36	g	120/122 (98%)	81 (68%)	24 (20%)	15 (12%)	0	6
37	h	143/150 (95%)	93 (65%)	28 (20%)	22 (15%)	0	4
38	i	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	5
39	j	115/118 (98%)	104 (90%)	6 (5%)	5 (4%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	108/112 (96%)	77 (71%)	22 (20%)	9 (8%)	1	13
41	l	115/146 (79%)	80 (70%)	19 (16%)	16 (14%)	0	4
42	m	115/118 (98%)	100 (87%)	11 (10%)	4 (4%)	3	31
43	n	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	5
44	o	108/113 (96%)	86 (80%)	14 (13%)	8 (7%)	1	16
45	p	92/96 (96%)	71 (77%)	14 (15%)	7 (8%)	1	15
46	q	108/110 (98%)	63 (58%)	21 (19%)	24 (22%)	0	1
47	r	178/206 (86%)	130 (73%)	28 (16%)	20 (11%)	0	7
48	s	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	5	36
49	t	65/67 (97%)	54 (83%)	7 (11%)	4 (6%)	1	20
50	u	57/60 (95%)	44 (77%)	8 (14%)	5 (9%)	1	12
51	v	69/71 (97%)	35 (51%)	21 (30%)	13 (19%)	0	2
52	w	55/60 (92%)	37 (67%)	11 (20%)	7 (13%)	0	5
53	x	47/54 (87%)	16 (34%)	16 (34%)	15 (32%)	0	0
54	y	47/49 (96%)	33 (70%)	9 (19%)	5 (11%)	0	8
55	z	62/65 (95%)	45 (73%)	8 (13%)	9 (14%)	0	4
56	B	587/610 (96%)	267 (46%)	188 (32%)	132 (22%)	0	1
All	All	6536/6972 (94%)	4756 (73%)	1087 (17%)	693 (11%)	1	8

All (693) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	ARG
1	1	33	LYS
2	2	77	PRO
2	2	93	LEU
2	2	107	VAL
3	3	23	VAL
3	3	57	ILE
3	3	69	THR
3	3	73	PRO
3	3	90	LYS
3	3	96	VAL
3	3	117	THR
9	F	16	HIS
9	F	20	GLU

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Mol	Chain	Res	Type
9	F	104	ASN
9	F	127	ILE
9	F	158	LEU
10	G	16	ARG
11	H	20	TYR
11	H	30	LYS
11	H	142	PRO
11	H	198	VAL
12	I	73	ASN
12	I	98	THR
13	J	49	ALA
14	K	113	GLU
15	L	97	VAL
16	M	98	PRO
17	N	90	LEU
19	P	77	LEU
19	P	91	LYS
20	Q	36	LYS
20	Q	60	VAL
20	Q	65	LYS
20	Q	81	LEU
21	R	34	TYR
23	T	44	THR
24	U	99	SER
25	V	78	LEU
25	V	81	PHE
26	W	5	LEU
26	W	53	ASN
26	W	55	LYS
26	W	60	VAL
26	W	61	TYR
26	W	62	ILE
26	W	71	LEU
27	X	71	THR
29	Z	37	PHE
30	a	52	ARG
30	a	58	HIS
30	a	59	LYS
30	a	89	SER
30	a	91	ARG
30	a	211	ARG
30	a	226	MET

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Mol	Chain	Res	Type
30	a	243	GLY
30	a	245	PRO
30	a	249	PRO
31	b	16	ARG
31	b	38	THR
31	b	74	PRO
31	b	100	GLU
31	b	119	ARG
31	b	123	ALA
31	b	147	PRO
31	b	178	GLU
31	b	185	LYS
31	b	191	PRO
32	c	45	ARG
32	c	126	VAL
32	c	169	ASN
33	d	27	ASN
33	d	51	ARG
33	d	114	ILE
33	d	123	ASN
33	d	145	THR
35	f	35	ARG
35	f	51	PHE
35	f	65	LYS
35	f	67	LEU
35	f	79	PRO
36	g	22	ILE
36	g	63	VAL
36	g	89	ASN
36	g	101	PRO
36	g	102	VAL
37	h	18	ARG
37	h	42	SER
37	h	47	ASP
37	h	92	GLU
37	h	111	ARG
37	h	122	PRO
38	i	8	LYS
38	i	31	ASP
38	i	66	ILE
38	i	67	ARG
38	i	77	LYS

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Mol	Chain	Res	Type
38	i	78	PRO
38	i	87	LYS
39	j	6	SER
39	j	12	ARG
40	k	31	SER
40	k	32	LEU
40	k	95	HIS
41	l	24	PRO
41	l	28	VAL
41	l	58	ASN
42	m	22	LYS
42	m	89	GLU
43	n	18	LEU
43	n	22	VAL
43	n	69	LYS
43	n	90	PRO
44	o	12	ILE
44	o	65	LEU
44	o	74	ALA
45	p	36	LYS
45	p	89	ILE
46	q	47	LYS
46	q	72	VAL
46	q	77	PRO
46	q	82	PRO
46	q	94	LYS
46	q	107	ASP
47	r	41	LEU
47	r	63	ASP
47	r	146	ILE
48	s	12	ASN
49	t	13	PRO
49	t	38	GLN
49	t	39	LEU
50	u	12	PRO
50	u	17	LYS
50	u	51	ALA
51	v	11	PRO
51	v	27	THR
51	v	41	PRO
51	v	44	THR
51	v	51	ASP

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Mol	Chain	Res	Type
51	v	56	VAL
52	w	23	HIS
52	w	36	CYS
53	x	19	ARG
53	x	25	LYS
53	x	29	ASN
53	x	52	VAL
54	y	5	TRP
54	y	18	PHE
54	y	23	ARG
55	z	32	LEU
56	B	39	ARG
56	B	68	TYR
56	B	146	LEU
56	B	203	SER
56	B	223	ARG
56	B	233	THR
56	B	280	ILE
56	B	296	PRO
56	B	298	LYS
56	B	320	LEU
56	B	328	ALA
56	B	339	ALA
56	B	340	LEU
56	B	386	GLU
56	B	394	ALA
56	B	444	ALA
56	B	475	ALA
56	B	486	PRO
56	B	490	VAL
56	B	497	HIS
56	B	504	LEU
56	B	531	GLN
56	B	557	ASP
56	B	563	TYR
56	B	585	LYS
56	B	587	ILE
1	1	5	ALA
1	1	9	ARG
2	2	30	GLN
2	2	80	VAL
2	2	116	ILE

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Mol	Chain	Res	Type
3	3	24	GLY
3	3	32	ALA
3	3	34	ILE
3	3	49	GLY
3	3	56	GLU
3	3	58	THR
3	3	82	ALA
3	3	93	ARG
9	F	24	TRP
9	F	155	LEU
9	F	191	ASP
10	G	66	VAL
10	G	179	ARG
11	H	4	TYR
11	H	154	ASN
11	H	196	LEU
11	H	200	GLU
12	I	12	LEU
12	I	95	ALA
13	J	53	ALA
14	K	112	PRO
15	L	74	PRO
15	L	121	ASP
16	M	47	LEU
16	M	110	GLU
16	M	116	LYS
17	N	39	PRO
19	P	6	THR
20	Q	45	VAL
20	Q	46	LYS
20	Q	69	GLU
20	Q	98	VAL
20	Q	104	ARG
21	R	16	PHE
21	R	29	ARG
21	R	31	ARG
23	T	43	LYS
23	T	80	PHE
24	U	104	LYS
25	V	20	ALA
26	W	4	SER
26	W	9	VAL

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Mol	Chain	Res	Type
26	W	13	ASP
26	W	59	PRO
29	Z	20	TYR
29	Z	32	LEU
29	Z	166	ASP
30	a	6	PHE
30	a	18	VAL
30	a	55	GLY
30	a	158	ALA
30	a	160	GLY
30	a	163	ALA
30	a	201	HIS
30	a	217	ARG
30	a	219	PRO
30	a	233	HIS
31	b	44	TYR
31	b	53	PRO
31	b	54	GLN
31	b	202	LYS
32	c	14	PRO
32	c	89	VAL
32	c	168	ARG
33	d	24	GLY
33	d	28	VAL
33	d	36	LYS
33	d	64	THR
33	d	71	THR
33	d	124	SER
34	e	12	PRO
34	e	21	PRO
34	e	93	GLY
34	e	107	VAL
34	e	118	PRO
34	e	131	VAL
34	e	164	TYR
35	f	7	LYS
35	f	38	HIS
36	g	13	ASN
36	g	64	ARG
36	g	67	LYS
36	g	119	PRO
37	h	11	GLY

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Mol	Chain	Res	Type
37	h	16	ARG
37	h	24	GLY
37	h	29	LYS
37	h	31	ALA
37	h	107	LYS
37	h	124	LYS
37	h	127	ALA
38	i	20	ALA
38	i	85	LYS
38	i	107	ALA
39	j	14	SER
39	j	89	ASP
40	k	54	LEU
40	k	79	ALA
40	k	82	ILE
40	k	97	ARG
41	l	38	ASN
41	l	98	LYS
41	l	99	LEU
41	l	101	PHE
42	m	72	HIS
43	n	56	SER
43	n	66	ARG
44	o	2	GLU
44	o	63	ASP
45	p	53	LYS
45	p	67	GLY
46	q	8	LYS
46	q	87	LYS
46	q	90	LEU
47	r	12	GLY
47	r	42	VAL
47	r	109	ALA
47	r	123	ASP
47	r	159	PRO
47	r	179	ASP
49	t	66	ASN
51	v	5	ILE
51	v	6	HIS
52	w	11	THR
52	w	12	SER
53	x	16	CYS

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Mol	Chain	Res	Type
53	x	28	ARG
53	x	38	LYS
53	x	41	PRO
53	x	50	ARG
55	z	27	THR
55	z	31	HIS
56	B	9	ILE
56	B	40	GLU
56	B	47	ASP
56	B	71	LYS
56	B	77	VAL
56	B	79	HIS
56	B	82	ASP
56	B	87	VAL
56	B	88	ASP
56	B	158	LEU
56	B	163	ALA
56	B	165	PHE
56	B	190	GLY
56	B	204	VAL
56	B	227	ARG
56	B	231	TYR
56	B	234	GLY
56	B	239	VAL
56	B	240	ASP
56	B	268	ILE
56	B	273	ASP
56	B	300	VAL
56	B	301	VAL
56	B	338	THR
56	B	371	ALA
56	B	398	ASP
56	B	502	ASP
56	B	522	ASP
56	B	526	GLU
56	B	548	ARG
56	B	593	PRO
56	B	594	GLN
2	2	115	GLN
3	3	22	PRO
9	F	131	PRO
9	F	204	ASN

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Mol	Chain	Res	Type
10	G	12	LEU
10	G	64	VAL
10	G	160	ALA
10	G	206	GLU
11	H	35	ARG
11	H	130	GLY
11	H	131	ARG
12	I	143	ARG
12	I	146	ALA
13	J	41	GLU
13	J	56	PRO
14	K	7	ALA
14	K	155	ARG
15	L	87	SER
16	M	58	HIS
16	M	103	THR
17	N	34	VAL
18	O	104	GLN
18	O	111	ASP
19	P	22	SER
22	S	76	GLU
24	U	14	LYS
27	X	99	LEU
29	Z	161	ILE
29	Z	177	LYS
30	a	17	THR
30	a	247	ALA
30	a	271	ILE
31	b	68	ALA
31	b	72	VAL
31	b	118	LYS
31	b	168	MET
31	b	188	VAL
32	c	46	ARG
32	c	130	ALA
32	c	178	PRO
33	d	29	TRP
33	d	32	PRO
33	d	132	ASN
33	d	135	LEU
33	d	164	GLU
33	d	177	GLY

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Mol	Chain	Res	Type
34	e	47	GLU
34	e	156	ALA
34	e	157	TYR
34	e	160	LYS
34	e	169	VAL
35	f	40	PRO
35	f	135	PRO
36	g	4	PRO
36	g	53	LYS
36	g	73	ASP
36	g	93	PRO
37	h	64	LYS
38	i	21	THR
38	i	135	ASP
40	k	5	THR
41	l	19	LEU
41	l	36	GLU
41	l	41	ARG
41	l	110	ILE
43	n	6	LYS
43	n	26	ASP
45	p	48	LYS
45	p	63	LYS
46	q	2	ARG
46	q	35	TYR
46	q	45	VAL
46	q	86	ARG
47	r	51	ALA
47	r	81	ARG
47	r	135	GLU
51	v	21	VAL
51	v	48	ARG
51	v	50	VAL
51	v	55	ARG
52	w	37	LYS
53	x	47	THR
53	x	51	GLU
56	B	8	ARG
56	B	34	HIS
56	B	36	VAL
56	B	42	ARG
56	B	64	VAL

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Mol	Chain	Res	Type
56	B	81	ILE
56	B	86	HIS
56	B	141	PRO
56	B	159	PRO
56	B	170	THR
56	B	189	LYS
56	B	192	PRO
56	B	253	THR
56	B	299	PRO
56	B	305	LEU
56	B	321	GLU
56	B	332	PHE
56	B	368	SER
56	B	373	ALA
56	B	388	VAL
56	B	393	PRO
56	B	402	ILE
56	B	418	GLU
56	B	442	PRO
56	B	500	VAL
56	B	529	PRO
56	B	530	ARG
56	B	544	LYS
3	3	6	ALA
3	3	7	VAL
3	3	63	ARG
3	3	81	ALA
3	3	126	MET
9	F	13	ALA
9	F	21	ARG
9	F	77	ALA
9	F	202	PRO
10	G	4	LYS
10	G	28	GLN
11	H	32	ALA
11	H	125	HIS
11	H	134	ASP
13	J	95	GLU
13	J	100	ASN
17	N	40	LEU
18	O	90	GLY
18	O	112	THR

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Mol	Chain	Res	Type
19	P	17	LYS
19	P	78	GLN
19	P	92	ASP
20	Q	92	HIS
21	R	33	VAL
24	U	53	LEU
24	U	81	ARG
26	W	29	ARG
26	W	34	TRP
26	W	35	SER
26	W	41	VAL
26	W	72	GLY
29	Z	160	ARG
29	Z	164	ARG
30	a	148	GLU
30	a	272	ALA
31	b	70	ALA
33	d	49	ASP
33	d	78	SER
33	d	96	ARG
33	d	178	PHE
34	e	7	LEU
34	e	14	GLY
34	e	104	GLU
34	e	127	GLU
34	e	136	ILE
36	g	28	SER
37	h	66	GLY
37	h	89	ALA
37	h	119	GLU
38	i	17	LEU
38	i	30	GLY
38	i	61	GLY
40	k	9	ARG
41	l	59	THR
42	m	73	GLY
43	n	13	ARG
43	n	72	VAL
44	o	41	LYS
44	o	62	HIS
45	p	57	LEU
46	q	6	HIS

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Mol	Chain	Res	Type
46	q	42	VAL
46	q	57	GLN
46	q	92	ASN
46	q	99	CYS
47	r	11	GLU
47	r	23	LYS
47	r	82	ARG
47	r	168	GLU
47	r	170	THR
48	s	84	LEU
50	u	11	SER
50	u	31	LEU
51	v	53	GLU
53	x	24	GLU
53	x	46	HIS
54	y	37	LYS
54	y	39	ARG
55	z	4	MET
56	B	6	LEU
56	B	37	SER
56	B	44	GLN
56	B	63	ALA
56	B	134	VAL
56	B	186	PRO
56	B	232	SER
56	B	245	PHE
56	B	279	THR
56	B	317	ARG
56	B	326	ASN
56	B	360	ARG
56	B	372	THR
56	B	387	GLU
56	B	390	VAL
56	B	432	ARG
56	B	498	GLY
56	B	598	LEU
1	1	6	SER
1	1	7	VAL
2	2	6	ASN
3	3	8	VAL
3	3	113	PRO
9	F	78	GLN

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Mol	Chain	Res	Type
9	F	122	PHE
9	F	125	PRO
9	F	218	ALA
10	G	127	ARG
11	H	18	LYS
11	H	112	VAL
12	I	141	GLN
12	I	142	LEU
15	L	75	ARG
15	L	105	ARG
20	Q	63	THR
22	S	88	ARG
24	U	34	LYS
26	W	12	ASP
26	W	31	ILE
29	Z	72	VAL
29	Z	175	VAL
30	a	48	ARG
30	a	63	ARG
31	b	133	LYS
31	b	180	ASN
32	c	62	ARG
32	c	69	HIS
32	c	70	THR
32	c	99	TYR
32	c	162	LEU
33	d	25	TYR
33	d	128	ARG
34	e	42	ARG
34	e	105	LEU
36	g	12	ASP
37	h	26	GLY
37	h	72	PRO
39	j	72	ASP
41	l	18	ASP
41	l	96	ARG
44	o	64	MET
46	q	5	MET
46	q	44	ILE
46	q	74	PRO
46	q	85	VAL
47	r	50	GLN

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Mol	Chain	Res	Type
52	w	59	GLU
53	x	35	GLU
53	x	40	CYS
55	z	6	THR
55	z	62	LEU
55	z	63	PRO
56	B	5	ASP
56	B	35	ALA
56	B	72	ASP
56	B	76	TYR
56	B	137	LYS
56	B	155	VAL
56	B	161	ASP
56	B	286	PRO
56	B	324	LYS
56	B	327	ASP
56	B	345	ARG
56	B	403	GLU
56	B	417	PRO
56	B	446	LYS
56	B	505	THR
56	B	553	ALA
56	B	573	LEU
9	F	153	ARG
9	F	230	VAL
10	G	97	LYS
20	Q	66	LEU
21	R	40	CYS
23	T	13	HIS
27	X	97	ALA
30	a	36	PRO
30	a	62	TYR
32	c	4	VAL
34	e	125	VAL
35	f	109	LYS
38	i	110	THR
43	n	9	GLY
46	q	40	GLU
52	w	38	ALA
55	z	3	LYS
56	B	224	PRO
56	B	408	PRO

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Mol	Chain	Res	Type
56	B	518	ARG
3	3	19	PRO
3	3	91	PRO
10	G	41	GLY
11	H	40	PRO
18	O	40	ILE
25	V	80	PRO
26	W	42	PRO
26	W	68	GLY
27	X	98	PRO
30	a	28	GLU
34	e	126	PRO
35	f	46	VAL
47	r	22	GLY
47	r	110	GLY
55	z	45	GLY
56	B	174	VAL
56	B	507	ILE
2	2	31	GLY
3	3	97	GLY
16	M	57	GLY
26	W	58	VAL
31	b	91	VAL
34	e	5	GLY
37	h	34	GLY
37	h	43	GLY
43	n	30	GLY
56	B	276	VAL
56	B	370	ILE
9	F	130	ARG
10	G	174	PRO
15	L	90	GLY
26	W	26	GLY
26	W	45	VAL
30	a	270	ILE
34	e	115	VAL
38	i	106	VAL
41	l	71	GLY
46	q	37	VAL
56	B	191	ASP
56	B	448	VAL
3	3	52	ILE

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Mol	Chain	Res	Type
16	M	22	GLY
29	Z	159	GLY
32	c	132	VAL
41	l	20	PRO
43	n	67	GLY
56	B	210	GLY
56	B	292	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	34/34 (100%)	34 (100%)	0	100	100
3	3	101/111 (91%)	93 (92%)	8 (8%)	12	42
9	F	202/220 (92%)	201 (100%)	1 (0%)	88	94
10	G	160/188 (85%)	159 (99%)	1 (1%)	86	92
11	H	180/181 (99%)	179 (99%)	1 (1%)	86	92
12	I	115/123 (94%)	114 (99%)	1 (1%)	78	88
13	J	90/90 (100%)	90 (100%)	0	100	100
14	K	126/127 (99%)	126 (100%)	0	100	100
15	L	119/119 (100%)	119 (100%)	0	100	100
16	M	98/99 (99%)	98 (100%)	0	100	100
17	N	88/92 (96%)	88 (100%)	0	100	100
18	O	90/99 (91%)	90 (100%)	0	100	100
19	P	104/109 (95%)	103 (99%)	1 (1%)	76	86
20	Q	92/101 (91%)	78 (85%)	14 (15%)	3	18
21	R	49/50 (98%)	49 (100%)	0	100	100
22	S	79/80 (99%)	78 (99%)	1 (1%)	69	82
23	T	72/74 (97%)	72 (100%)	0	100	100
24	U	96/97 (99%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	V	64/77 (83%)	64 (100%)	0	100	100
26	W	71/80 (89%)	47 (66%)	24 (34%)	0	1
27	X	76/82 (93%)	76 (100%)	0	100	100
28	Y	19/22 (86%)	19 (100%)	0	100	100
29	Z	180/181 (99%)	177 (98%)	3 (2%)	60	78
30	a	215/218 (99%)	212 (99%)	3 (1%)	67	81
31	b	166/166 (100%)	165 (99%)	1 (1%)	86	92
32	c	164/166 (99%)	161 (98%)	3 (2%)	59	77
33	d	156/156 (100%)	152 (97%)	4 (3%)	46	69
34	e	143/148 (97%)	142 (99%)	1 (1%)	84	91
35	f	118/119 (99%)	117 (99%)	1 (1%)	81	89
36	g	100/100 (100%)	99 (99%)	1 (1%)	76	86
37	h	111/116 (96%)	109 (98%)	2 (2%)	59	77
38	i	106/111 (96%)	105 (99%)	1 (1%)	78	88
39	j	100/101 (99%)	98 (98%)	2 (2%)	55	75
40	k	87/88 (99%)	87 (100%)	0	100	100
41	l	105/127 (83%)	104 (99%)	1 (1%)	76	86
42	m	93/94 (99%)	93 (100%)	0	100	100
43	n	82/82 (100%)	82 (100%)	0	100	100
44	o	90/92 (98%)	89 (99%)	1 (1%)	73	85
45	p	76/78 (97%)	76 (100%)	0	100	100
46	q	91/91 (100%)	91 (100%)	0	100	100
47	r	159/179 (89%)	159 (100%)	0	100	100
48	s	63/67 (94%)	63 (100%)	0	100	100
49	t	62/62 (100%)	62 (100%)	0	100	100
50	u	51/52 (98%)	50 (98%)	1 (2%)	55	75
51	v	63/63 (100%)	62 (98%)	1 (2%)	62	79
52	w	50/52 (96%)	50 (100%)	0	100	100
53	x	48/52 (92%)	48 (100%)	0	100	100
54	y	42/42 (100%)	42 (100%)	0	100	100
55	z	54/55 (98%)	52 (96%)	2 (4%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	B	490/505 (97%)	347 (71%)	143 (29%)	0 2
All	All	5390/5618 (96%)	5167 (96%)	223 (4%)	34 59

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	58	THR
3	3	63	ARG
3	3	64	SER
3	3	65	PHE
3	3	68	VAL
3	3	93	ARG
3	3	94	GLU
3	3	120	LEU
9	F	196	LEU
10	G	186	PHE
11	H	125	HIS
12	I	45	PHE
19	P	80	HIS
20	Q	64	TRP
20	Q	66	LEU
20	Q	73	GLU
20	Q	79	LYS
20	Q	80	ARG
20	Q	81	LEU
20	Q	87	TYR
20	Q	88	ARG
20	Q	90	LEU
20	Q	91	ARG
20	Q	93	ARG
20	Q	94	ARG
20	Q	102	ARG
20	Q	104	ARG
22	S	42	HIS
26	W	3	ARG
26	W	4	SER
26	W	14	HIS
26	W	16	LEU
26	W	18	LYS
26	W	20	LEU
26	W	21	GLU
26	W	25	LYS

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Mol	Chain	Res	Type
26	W	28	LYS
26	W	29	ARG
26	W	30	LEU
26	W	32	LYS
26	W	33	THR
26	W	36	ARG
26	W	49	ILE
26	W	55	LYS
26	W	56	GLN
26	W	57	HIS
26	W	58	VAL
26	W	61	TYR
26	W	63	THR
26	W	66	MET
26	W	77	THR
26	W	81	ARG
29	Z	161	ILE
29	Z	177	LYS
29	Z	180	PHE
30	a	61	LEU
30	a	206	LEU
30	a	242	ARG
31	b	52	LEU
32	c	65	TRP
32	c	99	TYR
32	c	197	ASP
33	d	31	VAL
33	d	34	LEU
33	d	77	ILE
33	d	100	TRP
34	e	129	THR
35	f	12	ARG
36	g	77	ILE
37	h	19	VAL
37	h	126	VAL
38	i	74	TYR
39	j	4	LEU
39	j	13	HIS
41	l	101	PHE
44	o	45	TYR
50	u	15	TYR
51	v	52	THR

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Mol	Chain	Res	Type
55	z	6	THR
55	z	60	LEU
56	B	4	MET
56	B	5	ASP
56	B	6	LEU
56	B	8	ARG
56	B	10	ARG
56	B	13	SER
56	B	19	ASP
56	B	20	HIS
56	B	23	SER
56	B	27	ASP
56	B	28	ARG
56	B	31	GLU
56	B	44	GLN
56	B	45	PHE
56	B	49	LEU
56	B	53	ARG
56	B	62	SER
56	B	65	ARG
56	B	69	ARG
56	B	72	ASP
56	B	80	LEU
56	B	89	PHE
56	B	90	THR
56	B	91	TYR
56	B	95	ARG
56	B	108	ASP
56	B	110	SER
56	B	111	GLN
56	B	123	MET
56	B	135	ILE
56	B	140	LEU
56	B	144	ARG
56	B	150	LEU
56	B	153	GLU
56	B	161	ASP
56	B	164	ILE
56	B	165	PHE
56	B	175	GLU
56	B	178	LEU
56	B	184	ARG

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Mol	Chain	Res	Type
56	B	189	LYS
56	B	193	GLU
56	B	196	LEU
56	B	199	LEU
56	B	201	PHE
56	B	206	ASP
56	B	215	LEU
56	B	217	LEU
56	B	229	ARG
56	B	235	LYS
56	B	240	ASP
56	B	246	THR
56	B	256	LEU
56	B	257	GLU
56	B	263	TRP
56	B	269	ARG
56	B	270	ASP
56	B	278	ASP
56	B	279	THR
56	B	281	THR
56	B	284	ASP
56	B	285	ARG
56	B	291	TYR
56	B	294	PHE
56	B	295	ARG
56	B	305	LEU
56	B	306	TYR
56	B	315	LYS
56	B	316	LEU
56	B	317	ARG
56	B	320	LEU
56	B	322	LYS
56	B	326	ASN
56	B	327	ASP
56	B	330	LEU
56	B	336	SER
56	B	337	SER
56	B	340	LEU
56	B	345	ARG
56	B	348	PHE
56	B	351	LEU
56	B	352	LEU

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Mol	Chain	Res	Type
56	B	361	LEU
56	B	365	PHE
56	B	367	LEU
56	B	368	SER
56	B	379	LYS
56	B	381	ARG
56	B	383	LYS
56	B	387	GLU
56	B	391	HIS
56	B	395	ASP
56	B	398	ASP
56	B	400	THR
56	B	401	ARG
56	B	402	ILE
56	B	412	LEU
56	B	418	GLU
56	B	424	LEU
56	B	425	MET
56	B	429	GLN
56	B	430	GLU
56	B	431	LYS
56	B	432	ARG
56	B	434	ARG
56	B	440	TYR
56	B	445	GLN
56	B	450	LEU
56	B	462	ASP
56	B	464	HIS
56	B	465	ASP
56	B	466	ARG
56	B	467	LEU
56	B	472	ARG
56	B	476	SER
56	B	479	TYR
56	B	481	GLN
56	B	485	ARG
56	B	491	LYS
56	B	495	LEU
56	B	502	ASP
56	B	509	HIS
56	B	518	ARG
56	B	520	ILE

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Mol	Chain	Res	Type
56	B	523	LYS
56	B	530	ARG
56	B	532	LEU
56	B	533	PHE
56	B	534	GLU
56	B	538	GLN
56	B	544	LYS
56	B	548	ARG
56	B	552	LYS
56	B	554	LEU
56	B	556	LYS
56	B	559	LEU
56	B	570	LYS
56	B	574	LEU
56	B	578	LYS
56	B	582	LYS
56	B	589	LYS
56	B	591	GLU
56	B	598	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	32	HIS
1	1	36	GLN
3	3	29	GLN
9	F	212	GLN
10	G	6	HIS
10	G	37	GLN
10	G	63	ASN
10	G	69	HIS
10	G	102	ASN
10	G	104	GLN
11	H	62	GLN
11	H	77	ASN
11	H	119	GLN
11	H	125	HIS
11	H	129	ASN
12	I	141	GLN
13	J	73	ASN
14	K	84	ASN
14	K	96	GLN

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Mol	Chain	Res	Type
14	K	97	GLN
14	K	148	ASN
15	L	81	HIS
16	M	34	ASN
17	N	33	GLN
17	N	56	HIS
18	O	117	ASN
19	P	80	HIS
19	P	99	HIS
20	Q	101	GLN
22	S	13	GLN
22	S	37	ASN
22	S	46	HIS
24	U	26	GLN
24	U	45	HIS
24	U	96	GLN
26	W	14	HIS
26	W	69	HIS
27	X	45	GLN
27	X	73	HIS
29	Z	71	GLN
29	Z	165	ASN
30	a	115	GLN
30	a	116	GLN
30	a	201	HIS
30	a	233	HIS
31	b	85	ASN
31	b	129	HIS
31	b	135	HIS
31	b	180	ASN
33	d	130	ASN
34	e	143	GLN
34	e	158	HIS
35	f	94	HIS
36	g	88	ASN
37	h	27	HIS
37	h	84	ASN
37	h	128	HIS
39	j	13	HIS
39	j	50	HIS
40	k	38	GLN
41	l	84	GLN

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Mol	Chain	Res	Type
42	m	94	ASN
42	m	117	GLN
43	n	80	GLN
43	n	87	HIS
44	o	34	ASN
44	o	57	ASN
44	o	61	ASN
45	p	31	HIS
47	r	54	HIS
47	r	73	GLN
49	t	4	GLN
49	t	51	GLN
50	u	19	GLN
51	v	20	ASN
51	v	47	GLN
52	w	23	HIS
53	x	49	HIS
54	y	16	HIS
56	B	17	HIS
56	B	20	HIS
56	B	79	HIS
56	B	127	HIS
56	B	142	ASN
56	B	209	GLN
56	B	248	GLN
56	B	275	GLN
56	B	353	HIS
56	B	358	GLN
56	B	481	GLN
56	B	509	HIS
56	B	577	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	4	76/77 (98%)	29 (38%)	0
5	5	75/76 (98%)	32 (42%)	3 (4%)
6	A	1515/1522 (99%)	529 (34%)	102 (6%)
7	D	2888/2893 (99%)	1316 (45%)	205 (7%)
8	E	122/123 (99%)	48 (39%)	4 (3%)
All	All	4676/4691 (99%)	1954 (41%)	314 (6%)

All (1954) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	4	5	G
4	4	8	U
4	4	9	G
4	4	13	C
4	4	17	C
4	4	17(A)	U
4	4	18	G
4	4	19	G
4	4	20	U
4	4	21	A
4	4	31	G
4	4	33	U
4	4	36	U
4	4	37	A
4	4	38	A
4	4	39	C
4	4	47	U
4	4	48	C
4	4	49	G
4	4	52	G
4	4	53	G
4	4	57	A
4	4	58	A
4	4	64	G
4	4	66	C
4	4	73	A
4	4	74	C
4	4	75	C
4	4	76	A
5	5	8	U
5	5	9	A
5	5	10	G
5	5	14	A
5	5	15	G
5	5	16	U
5	5	17	C
5	5	19	G
5	5	21	A
5	5	22	G
5	5	23	A
5	5	24	G
5	5	26	A

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Mol	Chain	Res	Type
5	5	27	G
5	5	39	U
5	5	41	C
5	5	42	C
5	5	43	C
5	5	45	U
5	5	47	U
5	5	48	C
5	5	49	C
5	5	52	G
5	5	54	U
5	5	59	U
5	5	61	C
5	5	62	C
5	5	70	G
5	5	71	G
5	5	74	C
5	5	75	C
5	5	76	A
6	A	6	G
6	A	8	A
6	A	9	G
6	A	13	U
6	A	14	U
6	A	30	U
6	A	31	G
6	A	32	A
6	A	37	U
6	A	39	G
6	A	40	C
6	A	42	G
6	A	46	G
6	A	47	C
6	A	48	C
6	A	49	U
6	A	50	A
6	A	51	A
6	A	52	G
6	A	54	C
6	A	61	G
6	A	62	U
6	A	65	U

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Mol	Chain	Res	Type
6	A	66	G
6	A	67	C
6	A	74	C
6	A	75	C
6	A	76	G
6	A	77	C
6	A	80	G
6	A	82	U
6	A	84	U
6	A	85	U
6	A	87	A
6	A	88	C
6	A	90	C
6	A	91	C
6	A	99	C
6	A	101	A
6	A	102	G
6	A	103	C
6	A	110	C
6	A	116	A
6	A	120	A
6	A	121	C
6	A	122	G
6	A	130	A
6	A	131	C
6	A	132	C
6	A	134	A
6	A	155	C
6	A	162	A
6	A	163	C
6	A	165	C
6	A	170	U
6	A	172	A
6	A	173	U
6	A	182	U
6	A	188	U
6	A	189	U
6	A	190	G
6	A	194	C
6	A	195	A
6	A	196	A
6	A	197	A

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Mol	Chain	Res	Type
6	A	200	G
6	A	201	C
6	A	208	U
6	A	209	U
6	A	210	U
6	A	216	G
6	A	224	C
6	A	226	G
6	A	244	U
6	A	245	C
6	A	247	G
6	A	250	A
6	A	251	G
6	A	252	U
6	A	261	U
6	A	262	A
6	A	264	U
6	A	266	G
6	A	267	C
6	A	279	A
6	A	280	C
6	A	282	A
6	A	283	C
6	A	289	G
6	A	299	G
6	A	301	G
6	A	302	G
6	A	304	U
6	A	306	G
6	A	308	C
6	A	309	G
6	A	314	C
6	A	317	G
6	A	319	G
6	A	328	C
6	A	329	A
6	A	330	C
6	A	332	G
6	A	341	C
6	A	342	C
6	A	343	U
6	A	344	A

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Mol	Chain	Res	Type
6	A	345	C
6	A	346	G
6	A	347	G
6	A	351	G
6	A	352	C
6	A	353	A
6	A	354	G
6	A	361	G
6	A	362	G
6	A	365	U
6	A	367	U
6	A	368	U
6	A	371	G
6	A	373	A
6	A	382	A
6	A	384	G
6	A	386	C
6	A	388	G
6	A	389	A
6	A	390	C
6	A	397	A
6	A	398	C
6	A	406	G
6	A	408	A
6	A	410	G
6	A	412	A
6	A	413	G
6	A	414	A
6	A	417	C
6	A	421	U
6	A	422	C
6	A	423	G
6	A	424	G
6	A	429	U
6	A	430	A
6	A	438	G
6	A	439	A
6	A	440	A
6	A	442	C
6	A	443	C
6	A	449	C
6	A	452	A

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Mol	Chain	Res	Type
6	A	455	C
6	A	457	C
6	A	458	C
6	A	464	G
6	A	465	A
6	A	466	C
6	A	467	G
6	A	468	A
6	A	476	G
6	A	477	G
6	A	481	G
6	A	482	A
6	A	485	G
6	A	486	U
6	A	491	G
6	A	494	U
6	A	496	A
6	A	497	U
6	A	500	G
6	A	503	C
6	A	504	C
6	A	511	C
6	A	518	C
6	A	519	C
6	A	521	G
6	A	527	G
6	A	529	G
6	A	530	G
6	A	531	U
6	A	532	A
6	A	533	A
6	A	535	A
6	A	548	G
6	A	555	C
6	A	559	A
6	A	560	U
6	A	561	U
6	A	562	C
6	A	563	A
6	A	564	C
6	A	566	G
6	A	567	G

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Mol	Chain	Res	Type
6	A	571	U
6	A	572	A
6	A	573	A
6	A	575	G
6	A	576	G
6	A	577	G
6	A	579	G
6	A	586	C
6	A	588	G
6	A	592	G
6	A	596	C
6	A	606	G
6	A	607	A
6	A	611	A
6	A	619	U
6	A	624	C
6	A	631	G
6	A	632	A
6	A	636	U
6	A	639	G
6	A	641	U
6	A	642	A
6	A	653	A
6	A	661	G
6	A	665	A
6	A	671	G
6	A	672	U
6	A	679	C
6	A	685	G
6	A	687	A
6	A	688	G
6	A	690	G
6	A	691	G
6	A	695	A
6	A	697	U
6	A	701	C
6	A	702	A
6	A	703	G
6	A	704	A
6	A	718	G
6	A	719	C
6	A	723	U

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Mol	Chain	Res	Type
6	A	730	G
6	A	731	G
6	A	733	A
6	A	738	C
6	A	749	C
6	A	752	G
6	A	755	G
6	A	772	U
6	A	777	A
6	A	778	G
6	A	781	A
6	A	782	A
6	A	784	C
6	A	785	G
6	A	787	A
6	A	793	U
6	A	794	A
6	A	799	G
6	A	811	C
6	A	812	C
6	A	813	U
6	A	815	A
6	A	816	A
6	A	817	C
6	A	818	G
6	A	819	A
6	A	820	U
6	A	821	G
6	A	826	C
6	A	827	U
6	A	828	A
6	A	838	G
6	A	841	U
6	A	842	C
6	A	843	U
6	A	848	C
6	A	850	U
6	A	851	G
6	A	853	G
6	A	866	C
6	A	869	G
6	A	871	U

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Mol	Chain	Res	Type
6	A	873	A
6	A	874	G
6	A	876	G
6	A	884	U
6	A	885	G
6	A	888	G
6	A	889	A
6	A	890	G
6	A	900	A
6	A	902	G
6	A	910	C
6	A	913	A
6	A	914	A
6	A	919	A
6	A	921	U
6	A	927	G
6	A	931	C
6	A	933	G
6	A	934	C
6	A	935	A
6	A	942	G
6	A	950	U
6	A	952	U
6	A	953	G
6	A	954	G
6	A	956	U
6	A	958	A
6	A	960	U
6	A	961	U
6	A	965	A
6	A	966	G
6	A	968	A
6	A	969	A
6	A	971	G
6	A	972	C
6	A	974	A
6	A	975	A
6	A	976	G
6	A	977	A
6	A	978	A
6	A	980	C
6	A	982	U

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Mol	Chain	Res	Type
6	A	983	A
6	A	984	C
6	A	987	G
6	A	991	U
6	A	993	G
6	A	994	A
6	A	998	G
6	A	1002	G
6	A	1003	G
6	A	1004	A
6	A	1005	A
6	A	1006	C
6	A	1009	G
6	A	1010	G
6	A	1014	A
6	A	1016	A
6	A	1021	G
6	A	1023	G
6	A	1024	G
6	A	1025	U
6	A	1026	G
6	A	1027	C
6	A	1028(A)	C
6	A	1029	G
6	A	1031	G
6	A	1032(A)	G
6	A	1045	C
6	A	1046	A
6	A	1050	G
6	A	1052	U
6	A	1053	G
6	A	1054	C
6	A	1055	A
6	A	1056	U
6	A	1060	C
6	A	1062	U
6	A	1064	G
6	A	1065	U
6	A	1066	C
6	A	1084	G
6	A	1085	U
6	A	1094	G

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Mol	Chain	Res	Type
6	A	1095	U
6	A	1096	C
6	A	1101	A
6	A	1102	A
6	A	1108	G
6	A	1115	C
6	A	1117	G
6	A	1118	C
6	A	1121	U
6	A	1124	G
6	A	1125	U
6	A	1126	U
6	A	1127	G
6	A	1129	C
6	A	1130	A
6	A	1131	G
6	A	1132	C
6	A	1136	U
6	A	1137	C
6	A	1138	G
6	A	1139	G
6	A	1140	C
6	A	1146	A
6	A	1148	U
6	A	1151	A
6	A	1157	A
6	A	1158	C
6	A	1159	U
6	A	1164	G
6	A	1165	C
6	A	1170	A
6	A	1173	G
6	A	1181	G
6	A	1183	A
6	A	1184	G
6	A	1188	A
6	A	1189	C
6	A	1191	A
6	A	1192	C
6	A	1195	C
6	A	1196	U
6	A	1197	G

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Mol	Chain	Res	Type
6	A	1200	C
6	A	1201	A
6	A	1202	G
6	A	1203	C
6	A	1211	U
6	A	1212	U
6	A	1215	G
6	A	1220	G
6	A	1224	G
6	A	1225	A
6	A	1227	A
6	A	1237	C
6	A	1238	A
6	A	1239	A
6	A	1240	U
6	A	1241	G
6	A	1242	C
6	A	1249	C
6	A	1250	A
6	A	1251	A
6	A	1256	A
6	A	1257	U
6	A	1258	G
6	A	1259	C
6	A	1265	G
6	A	1268	A
6	A	1269	A
6	A	1277	C
6	A	1278	U
6	A	1279	A
6	A	1280	A
6	A	1281	U
6	A	1282	C
6	A	1286	A
6	A	1287	A
6	A	1297	C
6	A	1298	C
6	A	1299	A
6	A	1300	G
6	A	1301	U
6	A	1302	U
6	A	1303	C

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Mol	Chain	Res	Type
6	A	1305	G
6	A	1307	U
6	A	1310	G
6	A	1312	G
6	A	1316	G
6	A	1317	C
6	A	1320	C
6	A	1321	C
6	A	1322	C
6	A	1327	C
6	A	1329	A
6	A	1331	G
6	A	1332	A
6	A	1336	C
6	A	1338	G
6	A	1340	A
6	A	1345	U
6	A	1346	A
6	A	1347	G
6	A	1348	U
6	A	1349	A
6	A	1353	G
6	A	1358	U
6	A	1360	A
6	A	1361	G
6	A	1362(A)	C
6	A	1363	A
6	A	1364	U
6	A	1365	G
6	A	1366	C
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1380	U
6	A	1381	U
6	A	1389	C
6	A	1395	C
6	A	1397	C
6	A	1398	A
6	A	1400	C
6	A	1401	G
6	A	1408	A

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Mol	Chain	Res	Type
6	A	1418	A
6	A	1419	G
6	A	1433	A
6	A	1436	U
6	A	1439	C
6	A	1441	G
6	A	1442	G
6	A	1443	G
6	A	1446	A
6	A	1447	G
6	A	1450	U
6	A	1452	C
6	A	1453	G
6	A	1454	G
6	A	1455	G
6	A	1459	C
6	A	1460	A
6	A	1463	C
6	A	1467	G
6	A	1469	G
6	A	1478	C
6	A	1481	U
6	A	1483	A
6	A	1487	G
6	A	1492	A
6	A	1494	G
6	A	1495	U
6	A	1497	G
6	A	1499	A
6	A	1504	G
6	A	1505	G
6	A	1506	U
6	A	1507	A
6	A	1515	C
6	A	1517	G
6	A	1518	A
6	A	1519	A
6	A	1520	G
6	A	1525	G
6	A	1528	U
6	A	1529	G
6	A	1530	G

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Mol	Chain	Res	Type
6	A	1531	A
6	A	1532	U
7	D	13	A
7	D	14	A
7	D	15	G
7	D	33	U
7	D	34	C
7	D	35	G
7	D	39	C
7	D	41	C
7	D	46	C
7	D	49	A
7	D	50	U
7	D	51	G
7	D	60	G
7	D	61	G
7	D	63	U
7	D	64	A
7	D	68	G
7	D	71	A
7	D	72	U
7	D	73	A
7	D	74	A
7	D	75	G
7	D	76	C
7	D	84	A
7	D	88	G
7	D	90	U
7	D	91	A
7	D	92	G
7	D	94	G
7	D	95	G
7	D	99	U
7	D	101	G
7	D	102	G
7	D	108	U
7	D	109	G
7	D	112	U
7	D	113	G
7	D	118	A
7	D	119	A
7	D	120	U

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Mol	Chain	Res	Type
7	D	121	G
7	D	125	G
7	D	128	C
7	D	131	G
7	D	132	G
7	D	134	C
7	D	137	C
7	D	138	G
7	D	140	A
7	D	141	A
7	D	143	C
7	D	147	U
7	D	149	A
7	D	152	G
7	D	153	C
7	D	154	G
7	D	155	C
7	D	161	U
7	D	162	U
7	D	163	U
7	D	164	U
7	D	172	C
7	D	178	G
7	D	181	A
7	D	188	G
7	D	190	A
7	D	191	A
7	D	193	U
7	D	195	A
7	D	196	A
7	D	197	A
7	D	200	U
7	D	201	C
7	D	204	A
7	D	205	G
7	D	206	U
7	D	207	A
7	D	210	C
7	D	216	A
7	D	217	G
7	D	221	A
7	D	222	A

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Mol	Chain	Res	Type
7	D	223	A
7	D	224	G
7	D	227	A
7	D	228	A
7	D	229	A
7	D	230	U
7	D	232	G
7	D	233	A
7	D	241	A
7	D	242	G
7	D	243	U
7	D	245	G
7	D	248	G
7	D	249	C
7	D	250	G
7	D	252	G
7	D	257	A
7	D	264	C
7	D	265	A
7	D	266	G
7	D	270(A)	A
7	D	270(B)	A
7	D	270(C)	C
7	D	270(F)	U
7	D	270(H)	C
7	D	270(J)	G
7	D	270(K)	C
7	D	270(M)	U
7	D	270(N)	G
7	D	270(O)	U
7	D	270(V)	G
7	D	270(X)	G
7	D	270(Y)	G
7	D	270(Z)	U
7	D	271(A)	C
7	D	271(C)	U
7	D	271	G
7	D	273(F)	C
7	D	275	G
7	D	276	A
7	D	278	A
7	D	279	C

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Mol	Chain	Res	Type
7	D	280	C
7	D	281	G
7	D	282	A
7	D	283	A
7	D	284	U
7	D	287	C
7	D	289	A
7	D	290	G
7	D	293	U
7	D	294	A
7	D	295	G
7	D	296	C
7	D	299	A
7	D	301	G
7	D	303	U
7	D	304	G
7	D	309	G
7	D	310	A
7	D	311	A
7	D	312	G
7	D	316	C
7	D	321	G
7	D	322	A
7	D	323	G
7	D	324	A
7	D	329	G
7	D	330	A
7	D	331	A
7	D	332	A
7	D	335	C
7	D	338	G
7	D	339	U
7	D	340	A
7	D	347	A
7	D	348	G
7	D	349	G
7	D	350	U
7	D	351	G
7	D	356	G
7	D	359	A
7	D	360	G
7	D	363(A)	A

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Mol	Chain	Res	Type
7	D	363(C)	G
7	D	363(F)	A
7	D	370	G
7	D	371	A
7	D	372	G
7	D	373	U
7	D	374	A
7	D	382	G
7	D	385	C
7	D	386	G
7	D	388	G
7	D	390	A
7	D	391	G
7	D	395	U
7	D	397	G
7	D	400	G
7	D	401	A
7	D	405	U
7	D	406	G
7	D	407	G
7	D	411	G
7	D	412	A
7	D	418	G
7	D	420	C
7	D	421	U
7	D	422	A
7	D	423	A
7	D	427	U
7	D	428	A
7	D	431	U
7	D	434	U
7	D	435	C
7	D	440	G
7	D	441	U
7	D	442	G
7	D	443	A
7	D	444	C
7	D	445	C
7	D	446	G
7	D	447	A
7	D	448	U
7	D	449	A

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Mol	Chain	Res	Type
7	D	450	G
7	D	451	C
7	D	452	G
7	D	453	C
7	D	454	A
7	D	455	C
7	D	456	C
7	D	457	A
7	D	458	G
7	D	459	U
7	D	465	G
7	D	471	A
7	D	473	G
7	D	475	U
7	D	478	A
7	D	479	A
7	D	480	A
7	D	481	G
7	D	482	A
7	D	483	A
7	D	486	C
7	D	491	G
7	D	493	G
7	D	494	G
7	D	498	G
7	D	499	U
7	D	501	A
7	D	503	A
7	D	504	U
7	D	505	A
7	D	507	A
7	D	508	G
7	D	510	C
7	D	513	A
7	D	518	G
7	D	526	A
7	D	527	C
7	D	528	A
7	D	529	A
7	D	530	G
7	D	531	C
7	D	532	A

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Mol	Chain	Res	Type
7	D	533	G
7	D	536	A
7	D	539	G
7	D	540	G
7	D	549	G
7	D	550	G
7	D	552	G
7	D	553	U
7	D	554	U
7	D	556	G
7	D	559	G
7	D	560	C
7	D	561	G
7	D	563	G
7	D	568	U
7	D	569	U
7	D	571	A
7	D	572	A
7	D	573	G
7	D	575	A
7	D	583	G
7	D	586	A
7	D	588	U
7	D	599	G
7	D	600	G
7	D	601	C
7	D	603	A
7	D	606	U
7	D	612	G
7	D	613	U
7	D	614	U
7	D	615	G
7	D	616	A
7	D	617	G
7	D	618	G
7	D	619	G
7	D	621	A
7	D	622	G
7	D	625	G
7	D	626	U
7	D	627	A
7	D	631	A

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Mol	Chain	Res	Type
7	D	632	A
7	D	633	A
7	D	634	C
7	D	637	A
7	D	640	C
7	D	642	G
7	D	643	A
7	D	644	A
7	D	645	C
7	D	646	A
7	D	647	G
7	D	648	G
7	D	649	G
7	D	650	C
7	D	651	G
7	D	653	A
7	D	654	A
7	D	655	A
7	D	656	G
7	D	660	G
7	D	668	G
7	D	670	A
7	D	677	A
7	D	687	C
7	D	690	G
7	D	697	C
7	D	698	C
7	D	699	A
7	D	704	G
7	D	705	A
7	D	709	U
7	D	714	U
7	D	715	G
7	D	716	A
7	D	717	G
7	D	724	U
7	D	725	G
7	D	726	G
7	D	727	A
7	D	728	G
7	D	729	G
7	D	730	C

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Mol	Chain	Res	Type
7	D	731	C
7	D	736	C
7	D	739	G
7	D	740	U
7	D	741	G
7	D	745	G
7	D	746	A
7	D	747	U
7	D	748	G
7	D	752	A
7	D	753	C
7	D	760	G
7	D	762	U
7	D	764	A
7	D	771	G
7	D	774	A
7	D	775	G
7	D	776	G
7	D	777	A
7	D	778	G
7	D	779	U
7	D	781	A
7	D	782	A
7	D	783	A
7	D	784	A
7	D	785	G
7	D	789	A
7	D	790	C
7	D	791	C
7	D	792	G
7	D	793	A
7	D	794	G
7	D	800	A
7	D	801	G
7	D	802	A
7	D	803	U
7	D	804	A
7	D	805	G
7	D	806	C
7	D	811	U
7	D	814	C
7	D	819	A

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Mol	Chain	Res	Type
7	D	825	C
7	D	827	U
7	D	828	U
7	D	832	G
7	D	844	C
7	D	846	C
7	D	847	U
7	D	848	G
7	D	857	C
7	D	858	U
7	D	859	G
7	D	860	U
7	D	861	A
7	D	865	C
7	D	866	A
7	D	867	C
7	D	871	U
7	D	876	C
7	D	877	U
7	D	878	A
7	D	880	G
7	D	881	G
7	D	882	G
7	D	883	G
7	D	884	C
7	D	885	C
7	D	886	C
7	D	887	A
7	D	888	C
7	D	889	C
7	D	890	A
7	D	892	G
7	D	894	C
7	D	895	U
7	D	896	A
7	D	898	C
7	D	899	A
7	D	900	A
7	D	901	A
7	D	903	C
7	D	906	G
7	D	907	U

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Mol	Chain	Res	Type
7	D	908	C
7	D	910	A
7	D	918	A
7	D	919	G
7	D	921	G
7	D	923	C
7	D	925	C
7	D	926	A
7	D	928	G
7	D	929	G
7	D	930	U
7	D	931	G
7	D	932	G
7	D	933	A
7	D	941	A
7	D	943	U
7	D	944	G
7	D	945	A
7	D	946	G
7	D	951	C
7	D	952	G
7	D	953	A
7	D	958	U
7	D	959	A
7	D	961	C
7	D	966	G
7	D	968	G
7	D	969	U
7	D	972	G
7	D	973	A
7	D	974	G
7	D	974(A)	C
7	D	980	A
7	D	983	A
7	D	990	A
7	D	991	C
7	D	994	C
7	D	995	C
7	D	996	A
7	D	997	G
7	D	1001	A
7	D	1005	C

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Mol	Chain	Res	Type
7	D	1008	C
7	D	1009	A
7	D	1010	A
7	D	1011	G
7	D	1012	U
7	D	1013	C
7	D	1015	G
7	D	1020	A
7	D	1021	A
7	D	1022	G
7	D	1023	U
7	D	1024	G
7	D	1025	G
7	D	1026	U
7	D	1027	A
7	D	1030	G
7	D	1031	G
7	D	1032	A
7	D	1033	U
7	D	1034	G
7	D	1041	C
7	D	1042	G
7	D	1044	G
7	D	1045	A
7	D	1046	A
7	D	1047	G
7	D	1048	A
7	D	1052	C
7	D	1053	C
7	D	1058	G
7	D	1059	G
7	D	1060	U
7	D	1061	U
7	D	1062	G
7	D	1063	G
7	D	1064	C
7	D	1065	U
7	D	1066	U
7	D	1068	G
7	D	1069	A
7	D	1070	A
7	D	1071	G

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Mol	Chain	Res	Type
7	D	1072	C
7	D	1073	A
7	D	1074	G
7	D	1075	C
7	D	1076	C
7	D	1077	A
7	D	1078	U
7	D	1079	C
7	D	1080	C
7	D	1081	U
7	D	1082	U
7	D	1083	U
7	D	1084	A
7	D	1085	A
7	D	1086	A
7	D	1087	G
7	D	1088	A
7	D	1089	G
7	D	1090	U
7	D	1093	G
7	D	1094	U
7	D	1095	A
7	D	1096	A
7	D	1100	C
7	D	1101	U
7	D	1102	C
7	D	1104	C
7	D	1105	U
7	D	1106	G
7	D	1107	G
7	D	1108	U
7	D	1109	C
7	D	1110	G
7	D	1111	A
7	D	1112	G
7	D	1115	G
7	D	1126	A
7	D	1128	A
7	D	1129	A
7	D	1130	U
7	D	1132	A
7	D	1134	G

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Mol	Chain	Res	Type
7	D	1135	C
7	D	1136	G
7	D	1138	G
7	D	1140	C
7	D	1141	U
7	D	1142(A)	A
7	D	1143	A
7	D	1155	A
7	D	1156	A
7	D	1157	G
7	D	1168	G
7	D	1169	G
7	D	1170	G
7	D	1171	G
7	D	1173	G
7	D	1174	A
7	D	1175	U
7	D	1177	A
7	D	1180	C
7	D	1182	A
7	D	1184	G
7	D	1186	G
7	D	1187	G
7	D	1188	U
7	D	1190	G
7	D	1194	A
7	D	1200	C
7	D	1203	G
7	D	1204	A
7	D	1205	U
7	D	1206	G
7	D	1211	U
7	D	1212	G
7	D	1214	A
7	D	1220	A
7	D	1221	C
7	D	1222	C
7	D	1229	G
7	D	1234	U
7	D	1237	A
7	D	1238	G
7	D	1240	U

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Mol	Chain	Res	Type
7	D	1241	A
7	D	1242	A
7	D	1243	G
7	D	1244	G
7	D	1247	A
7	D	1248	G
7	D	1251	C
7	D	1252	G
7	D	1253	A
7	D	1254	A
7	D	1255	U
7	D	1256	G
7	D	1264	G
7	D	1265	A
7	D	1266	G
7	D	1267	U
7	D	1268	A
7	D	1271	G
7	D	1272	A
7	D	1273	U
7	D	1274	A
7	D	1275	A
7	D	1284	A
7	D	1285	G
7	D	1286	A
7	D	1288	U
7	D	1289	C
7	D	1291	C
7	D	1295	C
7	D	1300	U
7	D	1301	A
7	D	1302	A
7	D	1311	G
7	D	1312	U
7	D	1319	G
7	D	1320	C
7	D	1321	A
7	D	1324	G
7	D	1325	G
7	D	1326	U
7	D	1329	U
7	D	1330	C

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Mol	Chain	Res	Type
7	D	1332	G
7	D	1333	C
7	D	1340	U
7	D	1341	U
7	D	1342	A
7	D	1343	G
7	D	1344	G
7	D	1345	C
7	D	1352	U
7	D	1353	A
7	D	1355	G
7	D	1363	C
7	D	1364	G
7	D	1365	A
7	D	1366	A
7	D	1380	G
7	D	1384	A
7	D	1394	U
7	D	1395	A
7	D	1397	U
7	D	1398	C
7	D	1402	C
7	D	1404	C
7	D	1412	A
7	D	1415	U
7	D	1416	G
7	D	1417	C
7	D	1418	G
7	D	1419	A
7	D	1420	U
7	D	1421	G
7	D	1422	G
7	D	1426	G
7	D	1427	A
7	D	1428	C
7	D	1429	G
7	D	1431	U
7	D	1436	G
7	D	1438	U
7	D	1441	G
7	D	1444(A)	A
7	D	1445	C

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Mol	Chain	Res	Type
7	D	1449(A)	G
7	D	1451	C
7	D	1453	A
7	D	1454	U
7	D	1455	G
7	D	1456	G
7	D	1457	A
7	D	1458	C
7	D	1459	G
7	D	1460	A
7	D	1461	G
7	D	1462	C
7	D	1467	C
7	D	1471	A
7	D	1472	A
7	D	1473	G
7	D	1476	C
7	D	1477	A
7	D	1478	G
7	D	1479	G
7	D	1480	G
7	D	1482	U
7	D	1484	G
7	D	1485	G
7	D	1486	A
7	D	1490	A
7	D	1491	G
7	D	1492	G
7	D	1493	C
7	D	1494	A
7	D	1495	A
7	D	1496	A
7	D	1497	U
7	D	1498	C
7	D	1499	C
7	D	1504	C
7	D	1505	C
7	D	1507	A
7	D	1508	A
7	D	1510	A
7	D	1511	A
7	D	1512	G

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Mol	Chain	Res	Type
7	D	1513	C
7	D	1514	U
7	D	1515	C
7	D	1516	U
7	D	1517	G
7	D	1519	G
7	D	1521	G
7	D	1522	G
7	D	1523	U
7	D	1527	G
7	D	1529	A
7	D	1536	A
7	D	1538	G
7	D	1542	G
7	D	1544	C
7	D	1552	G
7	D	1554	A
7	D	1555	G
7	D	1558	A
7	D	1559	G
7	D	1560	G
7	D	1564	C
7	D	1565	C
7	D	1566	A
7	D	1568	G
7	D	1569	A
7	D	1570	A
7	D	1571	A
7	D	1572	A
7	D	1573	G
7	D	1577	C
7	D	1579	A
7	D	1580	A
7	D	1581	G
7	D	1583	A
7	D	1585	C
7	D	1586	A
7	D	1587	A
7	D	1588	C
7	D	1589	C
7	D	1590	U
7	D	1592	C

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Mol	Chain	Res	Type
7	D	1594	G
7	D	1597	A
7	D	1602	U
7	D	1603	A
7	D	1604	C
7	D	1607	C
7	D	1608	A
7	D	1609	A
7	D	1610	A
7	D	1614	A
7	D	1615	C
7	D	1616	A
7	D	1617	C
7	D	1618	A
7	D	1619	G
7	D	1622	G
7	D	1626	G
7	D	1627	G
7	D	1628	G
7	D	1635	G
7	D	1641	A
7	D	1647	G
7	D	1648	C
7	D	1649	G
7	D	1652	A
7	D	1653	G
7	D	1654	A
7	D	1664	A
7	D	1667	G
7	D	1668	A
7	D	1669	A
7	D	1672	C
7	D	1673	U
7	D	1674	G
7	D	1675	C
7	D	1677	A
7	D	1678	G
7	D	1680	U
7	D	1682	G
7	D	1683	C
7	D	1689	A
7	D	1691	C

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Mol	Chain	Res	Type
7	D	1694	C
7	D	1695	G
7	D	1696	G
7	D	1698	A
7	D	1699	G
7	D	1700	A
7	D	1702	G
7	D	1703	G
7	D	1705	G
7	D	1706	U
7	D	1707	G
7	D	1708	C
7	D	1709	U
7	D	1716	U
7	D	1718	G
7	D	1727	U
7	D	1728	G
7	D	1730	U
7	D	1731	G
7	D	1732	A
7	D	1733	G
7	D	1734	C
7	D	1741	C
7	D	1742	C
7	D	1743	G
7	D	1748	G
7	D	1749	A
7	D	1750	G
7	D	1751	C
7	D	1752	C
7	D	1753	G
7	D	1758	G
7	D	1761	C
7	D	1762	A
7	D	1763	G
7	D	1764	G
7	D	1773	A
7	D	1776	G
7	D	1779	U
7	D	1780	A
7	D	1781	C
7	D	1782	C

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Mol	Chain	Res	Type
7	D	1784	A
7	D	1785	A
7	D	1787	A
7	D	1789	A
7	D	1790	C
7	D	1791	A
7	D	1799	G
7	D	1800	C
7	D	1802	A
7	D	1804	C
7	D	1809	A
7	D	1810	A
7	D	1811	G
7	D	1814	G
7	D	1815	A
7	D	1816	G
7	D	1817	G
7	D	1820	U
7	D	1821	A
7	D	1827	C
7	D	1828	G
7	D	1831	G
7	D	1833	U
7	D	1834	U
7	D	1838	C
7	D	1839	G
7	D	1847	A
7	D	1848	A
7	D	1858	G
7	D	1860	G
7	D	1861	G
7	D	1862	G
7	D	1871	A
7	D	1872	A
7	D	1878	G
7	D	1879	C
7	D	1880	C
7	D	1881	C
7	D	1882	C
7	D	1883	G
7	D	1884	A
7	D	1885	A

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Mol	Chain	Res	Type
7	D	1889	A
7	D	1899	G
7	D	1900	A
7	D	1901	A
7	D	1906	G
7	D	1909	C
7	D	1912	A
7	D	1913	A
7	D	1914	C
7	D	1915	U
7	D	1917	U
7	D	1918	A
7	D	1919	A
7	D	1920	C
7	D	1921	G
7	D	1922	G
7	D	1923	U
7	D	1928	A
7	D	1929	G
7	D	1930	G
7	D	1931	U
7	D	1934	C
7	D	1937	A
7	D	1938	A
7	D	1939	U
7	D	1940	U
7	D	1944	U
7	D	1945	G
7	D	1946	U
7	D	1947	C
7	D	1955	U
7	D	1956	U
7	D	1964	G
7	D	1966	A
7	D	1967	C
7	D	1968	G
7	D	1970	A
7	D	1971	A
7	D	1972	A
7	D	1975	G
7	D	1982	C
7	D	1986	A

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Mol	Chain	Res	Type
7	D	1988	C
7	D	1990	C
7	D	1991	U
7	D	1992	G
7	D	1993	U
7	D	1996	C
7	D	1997	G
7	D	1998	G
7	D	2011	U
7	D	2012	G
7	D	2013	A
7	D	2015	A
7	D	2018	G
7	D	2020	A
7	D	2021	C
7	D	2023	G
7	D	2026	C
7	D	2027	G
7	D	2030	A
7	D	2031	A
7	D	2032	G
7	D	2033	A
7	D	2034	U
7	D	2035	G
7	D	2036	C
7	D	2039	C
7	D	2043	C
7	D	2048	G
7	D	2049	G
7	D	2050	C
7	D	2055	C
7	D	2056	G
7	D	2060	A
7	D	2061	G
7	D	2062	A
7	D	2063	C
7	D	2064	C
7	D	2065	C
7	D	2067	G
7	D	2068	U
7	D	2069	G
7	D	2075	U

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Mol	Chain	Res	Type
7	D	2076	U
7	D	2077	A
7	D	2080	G
7	D	2085	C
7	D	2087	G
7	D	2092	U
7	D	2093	G
7	D	2098	U
7	D	2101	G
7	D	2104	G
7	D	2105	C
7	D	2107	C
7	D	2108	C
7	D	2109	U
7	D	2110	G
7	D	2111	C
7	D	2112	G
7	D	2114	A
7	D	2116	G
7	D	2117	A
7	D	2119	A
7	D	2120	G
7	D	2121	G
7	D	2123	G
7	D	2125	G
7	D	2126	A
7	D	2127	G
7	D	2130	U
7	D	2131	G
7	D	2132	U
7	D	2133	G
7	D	2134	A
7	D	2135	A
7	D	2136	C
7	D	2139	C
7	D	2144	U
7	D	2145	C
7	D	2148	G
7	D	2154	G
7	D	2156	G
7	D	2159	G
7	D	2165	G

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Mol	Chain	Res	Type
7	D	2166	G
7	D	2170	A
7	D	2172	U
7	D	2173	A
7	D	2174	C
7	D	2175	C
7	D	2177	C
7	D	2181	G
7	D	2183	C
7	D	2186	G
7	D	2187	G
7	D	2188	C
7	D	2190	G
7	D	2195	C
7	D	2196	C
7	D	2197	U
7	D	2198	A
7	D	2205	C
7	D	2208	U
7	D	2209	C
7	D	2210	G
7	D	2212	A
7	D	2213	U
7	D	2215	G
7	D	2216	G
7	D	2217	G
7	D	2224	G
7	D	2225	A
7	D	2234	G
7	D	2235	G
7	D	2236	C
7	D	2238	G
7	D	2239	G
7	D	2240	C
7	D	2241	A
7	D	2248	C
7	D	2249	U
7	D	2250	G
7	D	2251	G
7	D	2252	G
7	D	2259	G
7	D	2262	U

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Mol	Chain	Res	Type
7	D	2266	A
7	D	2267	A
7	D	2268	A
7	D	2269	A
7	D	2276	G
7	D	2280	G
7	D	2283	C
7	D	2284	C
7	D	2286	A
7	D	2287	A
7	D	2288	A
7	D	2296	U
7	D	2297	C
7	D	2304	G
7	D	2306	C
7	D	2307	G
7	D	2308	G
7	D	2309	A
7	D	2310	A
7	D	2311	A
7	D	2316	C
7	D	2317	C
7	D	2319	G
7	D	2320	A
7	D	2321	G
7	D	2322	A
7	D	2327	A
7	D	2329	G
7	D	2331	G
7	D	2333	A
7	D	2334	G
7	D	2335	A
7	D	2336	A
7	D	2337	G
7	D	2342	C
7	D	2345	G
7	D	2346	A
7	D	2347	C
7	D	2350	C
7	D	2351	G
7	D	2355	C
7	D	2356	C

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Mol	Chain	Res	Type
7	D	2361	A
7	D	2366	A
7	D	2378	A
7	D	2381	C
7	D	2382	G
7	D	2383	G
7	D	2385	C
7	D	2389	G
7	D	2392	A
7	D	2393	A
7	D	2396	G
7	D	2401	U
7	D	2403	C
7	D	2406	U
7	D	2407	G
7	D	2410	G
7	D	2417	C
7	D	2418	A
7	D	2420	C
7	D	2423	U
7	D	2424	C
7	D	2425	A
7	D	2426	A
7	D	2427	C
7	D	2428	G
7	D	2429	G
7	D	2430	A
7	D	2432	A
7	D	2434	A
7	D	2436	G
7	D	2437	U
7	D	2441	C
7	D	2445	G
7	D	2447	G
7	D	2448	A
7	D	2449	U
7	D	2450	A
7	D	2459	A
7	D	2470	G
7	D	2476	A
7	D	2478	A
7	D	2480	C

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Mol	Chain	Res	Type
7	D	2481	G
7	D	2482	G
7	D	2483	C
7	D	2489	G
7	D	2490	G
7	D	2491	U
7	D	2492	U
7	D	2494	G
7	D	2498	C
7	D	2501	C
7	D	2502	G
7	D	2503	A
7	D	2504	U
7	D	2505	G
7	D	2506	U
7	D	2510	C
7	D	2512	C
7	D	2513	G
7	D	2518	A
7	D	2519	U
7	D	2520	C
7	D	2523	G
7	D	2529	G
7	D	2535	G
7	D	2538	C
7	D	2541	A
7	D	2542	A
7	D	2543	G
7	D	2546	U
7	D	2547	U
7	D	2553	G
7	D	2554	U
7	D	2555	U
7	D	2558	C
7	D	2560	C
7	D	2564	A
7	D	2566	A
7	D	2567	G
7	D	2569	G
7	D	2570	G
7	D	2572	A
7	D	2573	C

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Mol	Chain	Res	Type
7	D	2574	G
7	D	2576	G
7	D	2577	A
7	D	2578	G
7	D	2580	U
7	D	2581	G
7	D	2582	G
7	D	2586	C
7	D	2599	G
7	D	2602	A
7	D	2603	G
7	D	2604	U
7	D	2608	G
7	D	2609	U
7	D	2610	C
7	D	2611	U
7	D	2612	C
7	D	2613	U
7	D	2614	A
7	D	2615	U
7	D	2621	A
7	D	2629	A
7	D	2630	G
7	D	2631	G
7	D	2634	G
7	D	2638	G
7	D	2645	G
7	D	2646	C
7	D	2652	C
7	D	2653	U
7	D	2655	G
7	D	2656	U
7	D	2660	A
7	D	2661	G
7	D	2663	G
7	D	2664	G
7	D	2665	A
7	D	2670	A
7	D	2671	A
7	D	2673	G
7	D	2680	C
7	D	2681	C

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Mol	Chain	Res	Type
7	D	2682	U
7	D	2684	U
7	D	2689	U
7	D	2690	C
7	D	2691	C
7	D	2701	C
7	D	2702	U
7	D	2704	C
7	D	2706	G
7	D	2711	A
7	D	2712	U
7	D	2712(A)	A
7	D	2713	A
7	D	2714	G
7	D	2718	G
7	D	2724	C
7	D	2725	A
7	D	2730	C
7	D	2731	G
7	D	2732	G
7	D	2733	A
7	D	2739	U
7	D	2741	A
7	D	2744	G
7	D	2748	A
7	D	2749	A
7	D	2750	A
7	D	2751	G
7	D	2752	C
7	D	2756	U
7	D	2757	A
7	D	2758	A
7	D	2764	A
7	D	2765	A
7	D	2766	G
7	D	2771	C
7	D	2772	C
7	D	2773	C
7	D	2774	C
7	D	2776	A
7	D	2777	G
7	D	2778	A

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Mol	Chain	Res	Type
7	D	2779	U
7	D	2780	G
7	D	2781	A
7	D	2782	G
7	D	2783	G
7	D	2787	C
7	D	2789	C
7	D	2790	A
7	D	2791	C
7	D	2792	G
7	D	2794	C
7	D	2797	U
7	D	2798	C
7	D	2799	A
7	D	2801	A
7	D	2802	G
7	D	2804	C
7	D	2805	G
7	D	2807	G
7	D	2808	U
7	D	2809	A
7	D	2810	A
7	D	2811	G
7	D	2818	G
7	D	2820	A
7	D	2823	A
7	D	2824	C
7	D	2826	A
7	D	2832	U
7	D	2833	G
7	D	2834	G
7	D	2836	U
7	D	2837	G
7	D	2845	G
7	D	2847	U
7	D	2849	U
7	D	2850	A
7	D	2851	A
7	D	2858	C
7	D	2866	U
7	D	2867	G
7	D	2868	A

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Mol	Chain	Res	Type
7	D	2872	G
7	D	2874	C
7	D	2879	C
7	D	2882	A
7	D	2884	U
7	D	2885	C
7	D	2887	U
7	D	2888	C
7	D	2889	C
7	D	2891	G
7	D	2893	G
7	D	2894	G
7	D	2895	U
7	D	2896	C
7	D	2897	U
7	D	2899	G
8	E	0	A
8	E	1	U
8	E	4	C
8	E	5	C
8	E	7	G
8	E	8	U
8	E	10	C
8	E	12	C
8	E	13	A
8	E	14	U
8	E	15	A
8	E	16	G
8	E	23	G
8	E	24	G
8	E	25	A
8	E	30	C
8	E	31	C
8	E	32	C
8	E	35	U
8	E	41	U
8	E	42	C
8	E	44	G
8	E	45	A
8	E	48	A
8	E	51	G
8	E	52	A

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Mol	Chain	Res	Type
8	E	57	A
8	E	59	A
8	E	62	C
8	E	64	C
8	E	65	C
8	E	67	G
8	E	69	G
8	E	73	A
8	E	75	G
8	E	76	G
8	E	85	G
8	E	88	C
8	E	99	A
8	E	103	U
8	E	105	G
8	E	109	G
8	E	111	U
8	E	115	G
8	E	117	G
8	E	118	G
8	E	119	A
8	E	120	U

All (314) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	5	15	G
5	5	58	A
5	5	74	C
6	A	5	U
6	A	13	U
6	A	30	U
6	A	48	C
6	A	50	A
6	A	51	A
6	A	60	A
6	A	99	C
6	A	115	G
6	A	119	A
6	A	129(A)	G
6	A	130	A
6	A	181	G

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Mol	Chain	Res	Type
6	A	196	A
6	A	208	U
6	A	209	U
6	A	210	U
6	A	243	A
6	A	244	U
6	A	250	A
6	A	251	G
6	A	266	G
6	A	279	A
6	A	281	G
6	A	305	G
6	A	308	C
6	A	328	C
6	A	345	C
6	A	366	C
6	A	367	U
6	A	372	C
6	A	388	G
6	A	413	G
6	A	421	U
6	A	428	G
6	A	429	U
6	A	465	A
6	A	481	G
6	A	484	G
6	A	495	A
6	A	498	A
6	A	518	C
6	A	526	C
6	A	547	A
6	A	559	A
6	A	560	U
6	A	566	G
6	A	575	G
6	A	595	G
6	A	653	A
6	A	686	U
6	A	687	A
6	A	701	C
6	A	703	G
6	A	717	C

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Mol	Chain	Res	Type
6	A	748	C
6	A	781	A
6	A	812	C
6	A	838	G
6	A	872	A
6	A	934	C
6	A	960	U
6	A	975	A
6	A	979	C
6	A	982	U
6	A	992	U
6	A	993	G
6	A	1004	A
6	A	1049	U
6	A	1053	G
6	A	1054	C
6	A	1064	G
6	A	1065	U
6	A	1101	A
6	A	1125	U
6	A	1129	C
6	A	1145	C
6	A	1182	G
6	A	1183	A
6	A	1190	G
6	A	1196	U
6	A	1201	A
6	A	1214	C
6	A	1239	A
6	A	1285	A
6	A	1300	G
6	A	1319	A
6	A	1320	C
6	A	1346	A
6	A	1347	G
6	A	1363	A
6	A	1394	A
6	A	1396	A
6	A	1399	C
6	A	1400	C
6	A	1443	G
6	A	1446	A

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Mol	Chain	Res	Type
6	A	1449	C
6	A	1452	C
6	A	1498	U
6	A	1504	G
6	A	1531	A
7	D	13	A
7	D	67	U
7	D	71	A
7	D	72	U
7	D	83	G
7	D	90	U
7	D	119	A
7	D	120	U
7	D	155	C
7	D	190	A
7	D	205	G
7	D	215	G
7	D	221	A
7	D	227	A
7	D	241	A
7	D	247	G
7	D	270(A)	A
7	D	279	C
7	D	280	C
7	D	311	A
7	D	322	A
7	D	323	G
7	D	334	C
7	D	337	C
7	D	339	U
7	D	350	U
7	D	366	C
7	D	373	U
7	D	390	A
7	D	421	U
7	D	446	G
7	D	447	A
7	D	448	U
7	D	455	C
7	D	458	G
7	D	470	A
7	D	474	G

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Mol	Chain	Res	Type
7	D	481	G
7	D	489	G
7	D	503	A
7	D	506	G
7	D	507	A
7	D	512	G
7	D	526	A
7	D	529	A
7	D	537	C
7	D	559	G
7	D	567	A
7	D	587	C
7	D	602	G
7	D	616	A
7	D	626	U
7	D	643	A
7	D	686	G
7	D	726	G
7	D	728	G
7	D	730	C
7	D	740	U
7	D	747	U
7	D	752	A
7	D	776	G
7	D	784	A
7	D	788	A
7	D	800	A
7	D	805	G
7	D	846	C
7	D	858	U
7	D	860	U
7	D	865	C
7	D	884	C
7	D	899	A
7	D	926	A
7	D	930	U
7	D	944	G
7	D	958	U
7	D	973	A
7	D	989	G
7	D	1060	U
7	D	1062	G

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Mol	Chain	Res	Type
7	D	1105	U
7	D	1134	G
7	D	1183	G
7	D	1204	A
7	D	1205	U
7	D	1210	A
7	D	1221	C
7	D	1236	G
7	D	1265	A
7	D	1266	G
7	D	1267	U
7	D	1300	U
7	D	1310	G
7	D	1320	C
7	D	1323	U
7	D	1324	G
7	D	1329	U
7	D	1340	U
7	D	1341	U
7	D	1342	A
7	D	1379	A
7	D	1397	U
7	D	1416	G
7	D	1427	A
7	D	1428	C
7	D	1444	G
7	D	1459	G
7	D	1515	C
7	D	1521	G
7	D	1554	A
7	D	1568	G
7	D	1571	A
7	D	1616	A
7	D	1618	A
7	D	1626	G
7	D	1634	A
7	D	1651	G
7	D	1653	G
7	D	1668	A
7	D	1672	C
7	D	1681	G
7	D	1688	U

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Mol	Chain	Res	Type
7	D	1698	A
7	D	1735	C
7	D	1757	U
7	D	1778	U
7	D	1780	A
7	D	1784	A
7	D	1790	C
7	D	1815	A
7	D	1819	A
7	D	1820	U
7	D	1838	C
7	D	1900	A
7	D	1913	A
7	D	1919	A
7	D	1920	C
7	D	1930	G
7	D	1938	A
7	D	1939	U
7	D	1943	U
7	D	1944	U
7	D	1955	U
7	D	1967	C
7	D	1996	C
7	D	2012	G
7	D	2017	U
7	D	2020	A
7	D	2030	A
7	D	2033	A
7	D	2047	U
7	D	2049	G
7	D	2067	G
7	D	2076	U
7	D	2092	U
7	D	2107	C
7	D	2115	G
7	D	2125	G
7	D	2126	A
7	D	2158	A
7	D	2199	A
7	D	2215	G
7	D	2238	G
7	D	2249	U

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Mol	Chain	Res	Type
7	D	2266	A
7	D	2267	A
7	D	2275	C
7	D	2287	A
7	D	2288	A
7	D	2308	G
7	D	2319	G
7	D	2334	G
7	D	2336	A
7	D	2344	U
7	D	2377	A
7	D	2391	G
7	D	2402	C
7	D	2425	A
7	D	2426	A
7	D	2427	C
7	D	2436	G
7	D	2447	G
7	D	2449	U
7	D	2458	G
7	D	2481	G
7	D	2497	A
7	D	2500	U
7	D	2519	U
7	D	2572	A
7	D	2585	U
7	D	2610	C
7	D	2614	A
7	D	2664	G
7	D	2689	U
7	D	2690	C
7	D	2705	A
7	D	2732	G
7	D	2749	A
7	D	2756	U
7	D	2777	G
7	D	2779	U
7	D	2848	G
7	D	2849	U
7	D	2867	G
7	D	2873	A
7	D	2893	G

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Mol	Chain	Res	Type
8	E	7	G
8	E	14	U
8	E	34	U
8	E	56	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	GCP	B	701	-	27,34,34	1.53	6 (22%)	34,54,54	1.98	8 (23%)

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
57	GCP	B	701	-	-	4/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	701	GCP	C5-C6	4.19	1.48	1.41
57	B	701	GCP	PG-O3G	2.86	1.61	1.54
57	B	701	GCP	PB-O3A	2.84	1.61	1.58
57	B	701	GCP	PG-O2G	2.84	1.61	1.54
57	B	701	GCP	C5-C4	2.46	1.47	1.40
57	B	701	GCP	PB-O2B	2.12	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	B	701	GCP	C2-N3-C4	4.94	121.00	115.36
57	B	701	GCP	C2-N1-C6	4.02	122.32	115.93
57	B	701	GCP	C5-C6-N1	-3.96	118.01	123.43
57	B	701	GCP	PB-O3A-PA	-3.82	120.45	132.56
57	B	701	GCP	C4-C5-C6	-3.71	117.26	120.80
57	B	701	GCP	C3'-C2'-C1'	3.52	106.27	100.98
57	B	701	GCP	N3-C2-N1	-3.31	122.80	127.22
57	B	701	GCP	C4-C5-N7	-2.72	106.57	109.40

There are no chirality outliers.

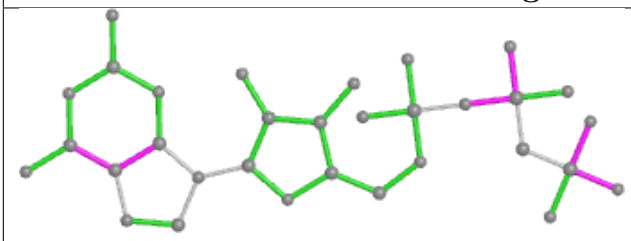
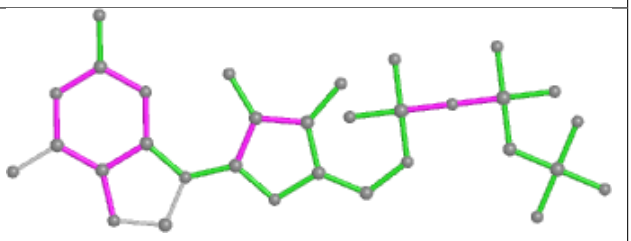
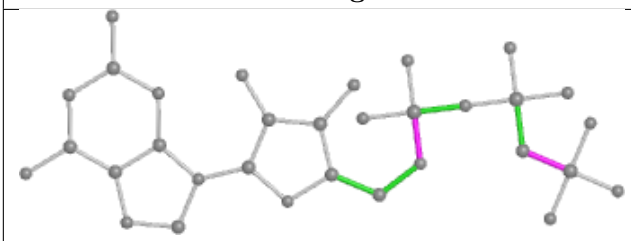
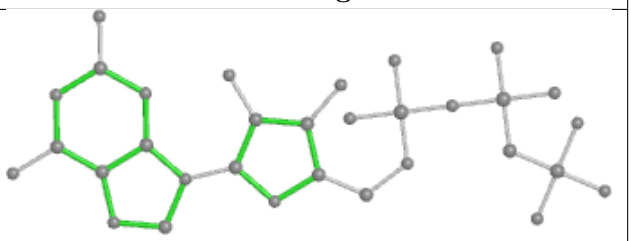
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	701	GCP	C5'-O5'-PA-O3A
57	B	701	GCP	C5'-O5'-PA-O1A
57	B	701	GCP	C5'-O5'-PA-O2A
57	B	701	GCP	PB-C3B-PG-O1G

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 GCP B 701	
 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.

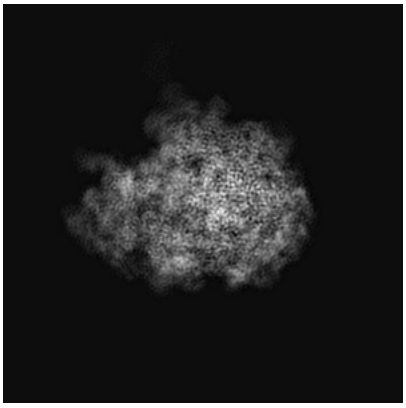
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6584. These allow visual inspection of the internal detail of the map and identification of artifacts.

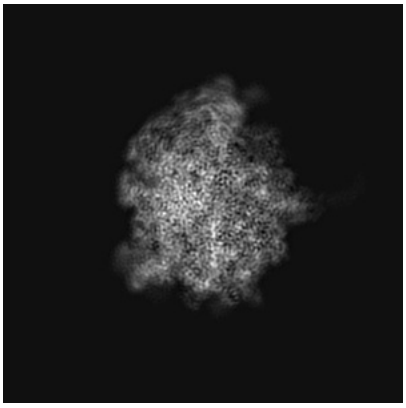
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

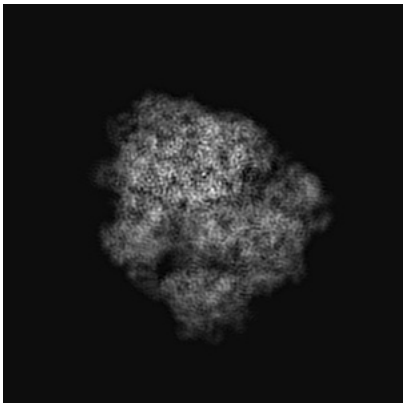
6.1.1 Primary map



X



Y

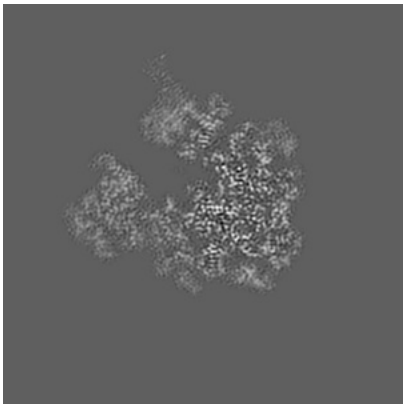


Z

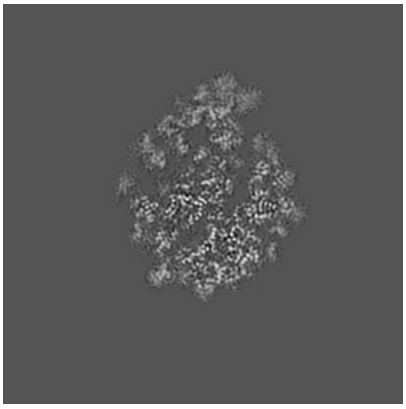
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 162



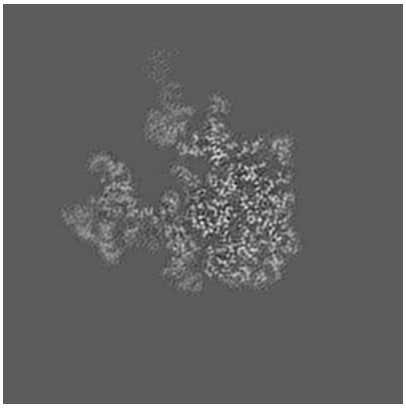
Y Index: 162

Z Index: 162

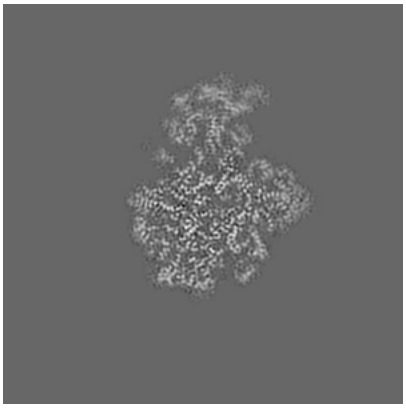
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 168



Y Index: 169

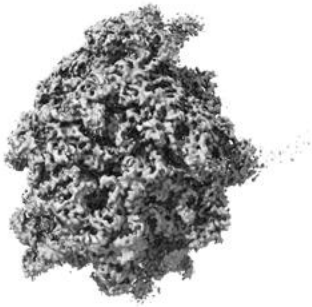
Z Index: 170

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

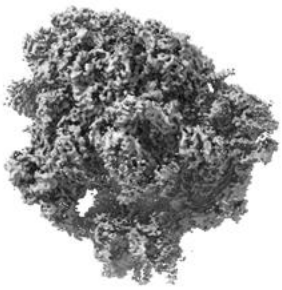
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

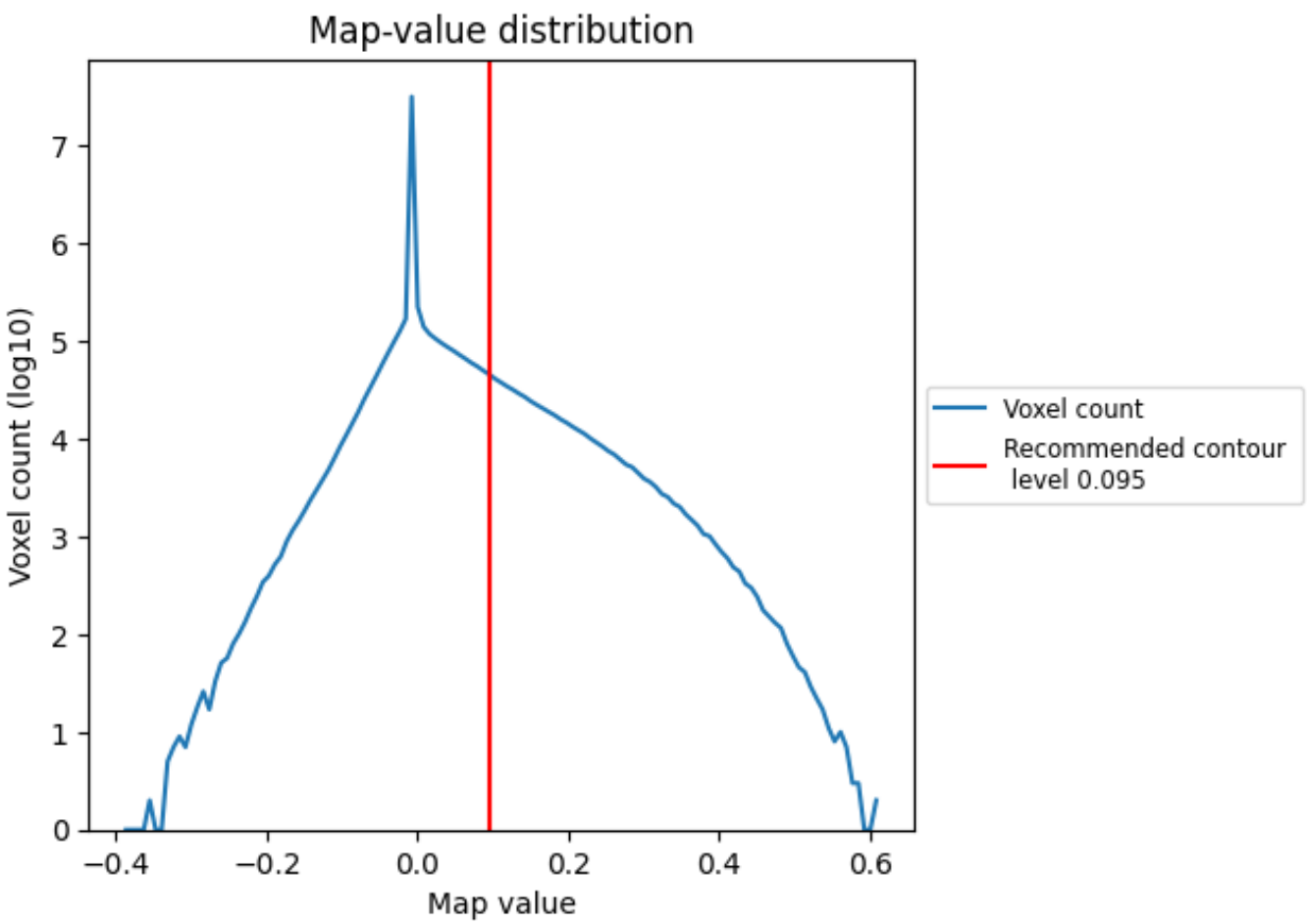
6.5 Mask visualisation (i)

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

7 Map analysis (i)

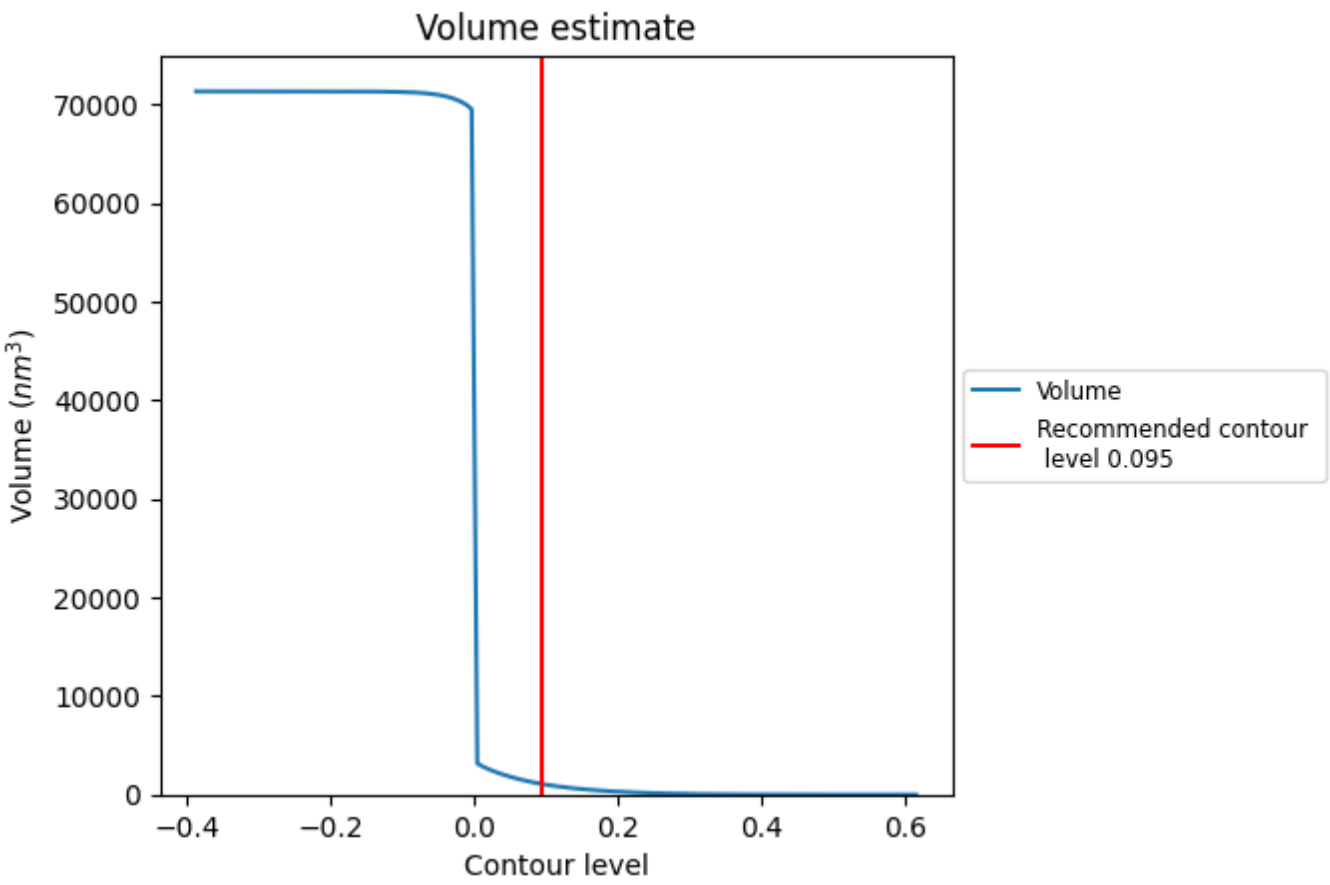
This section contains the results of statistical analysis of the map.

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.

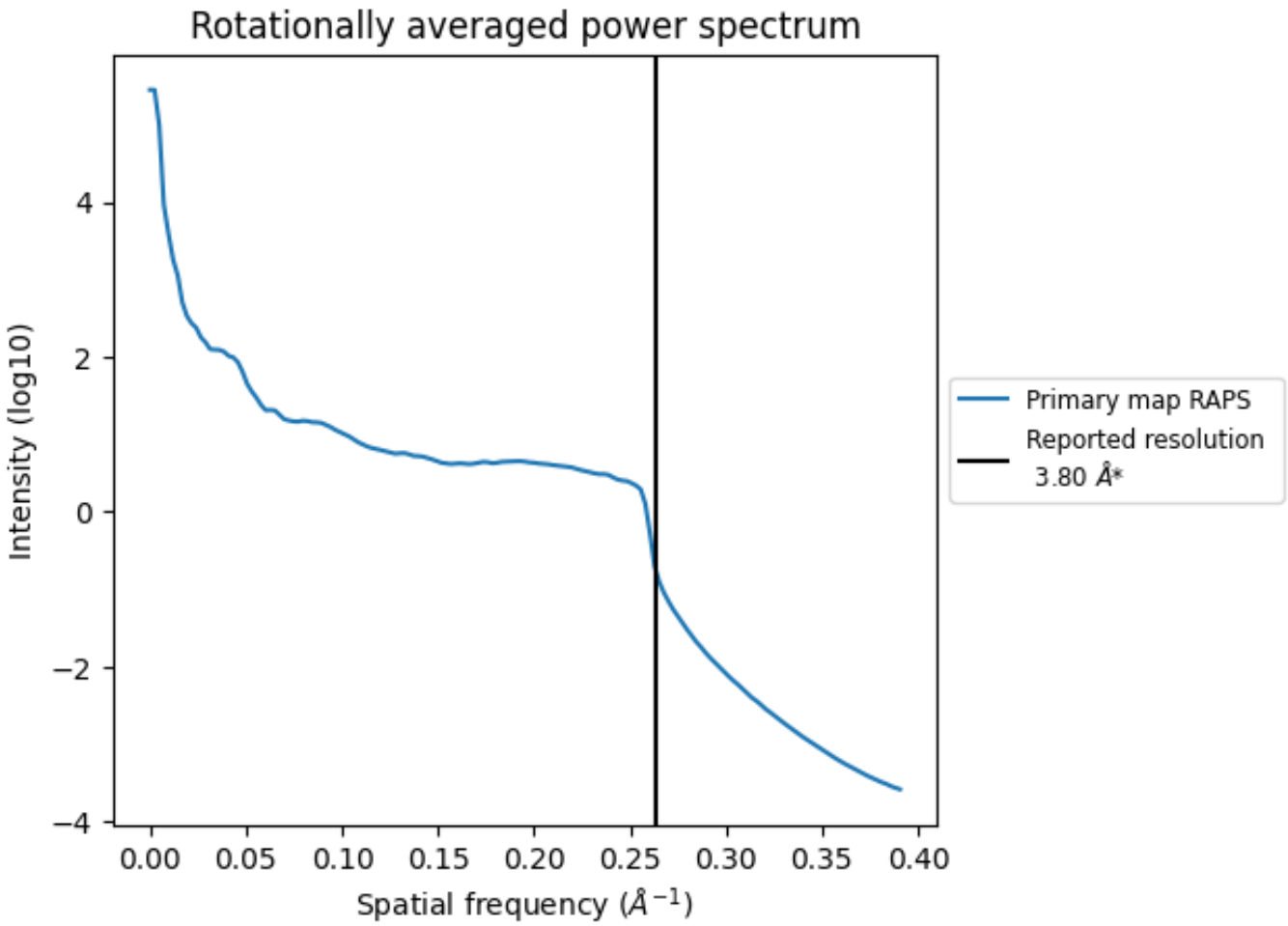
7.2 Volume estimate (i)



The volume at the recommended contour level is 1072 nm^3; this corresponds to an approximate mass of 968 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

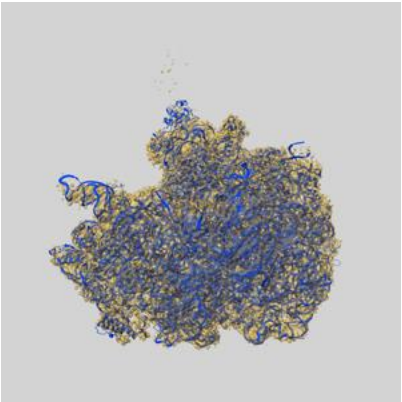
8 Fourier-Shell correlation (i)

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

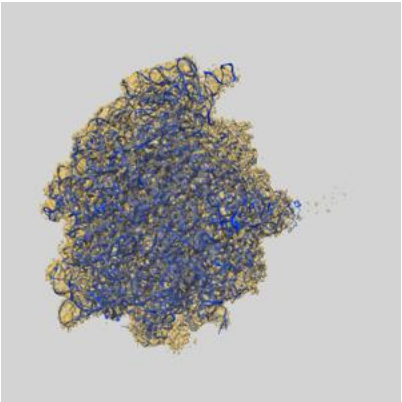
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6584 and PDB model 5IMQ. Per-residue inclusion information can be found in section 3 on page 14.

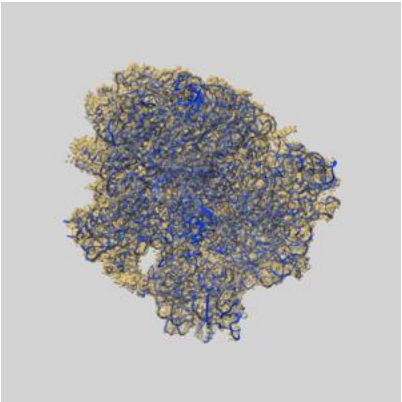
9.1 Map-model overlay (i)



X



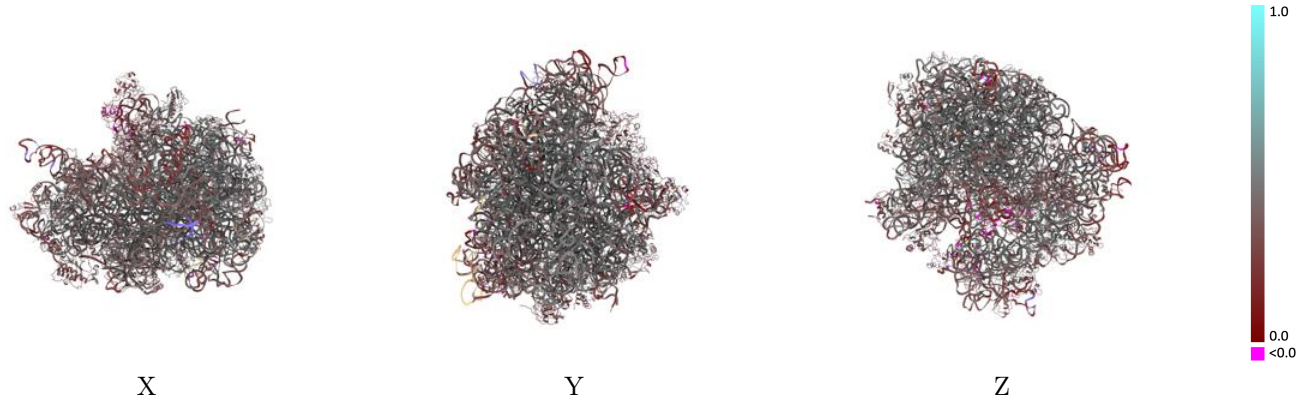
Y



Z

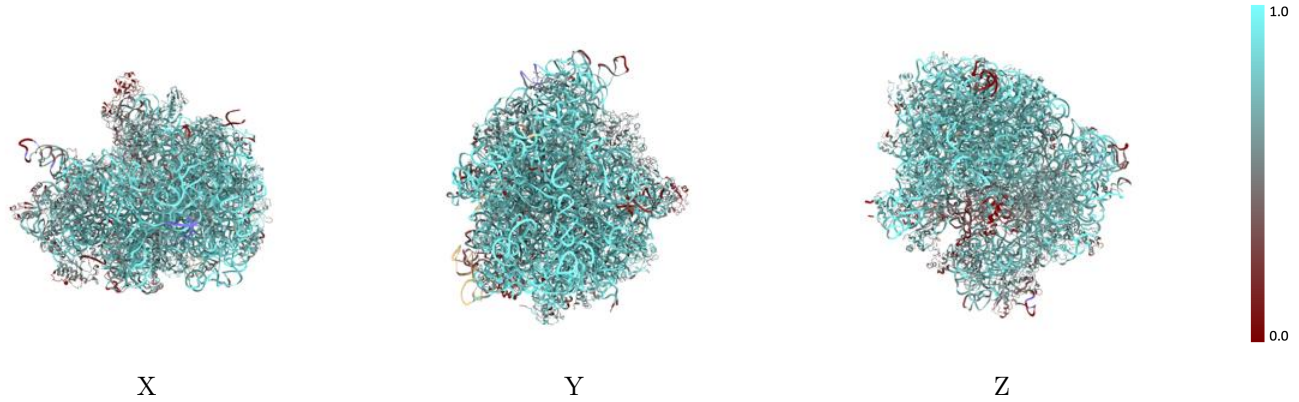
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



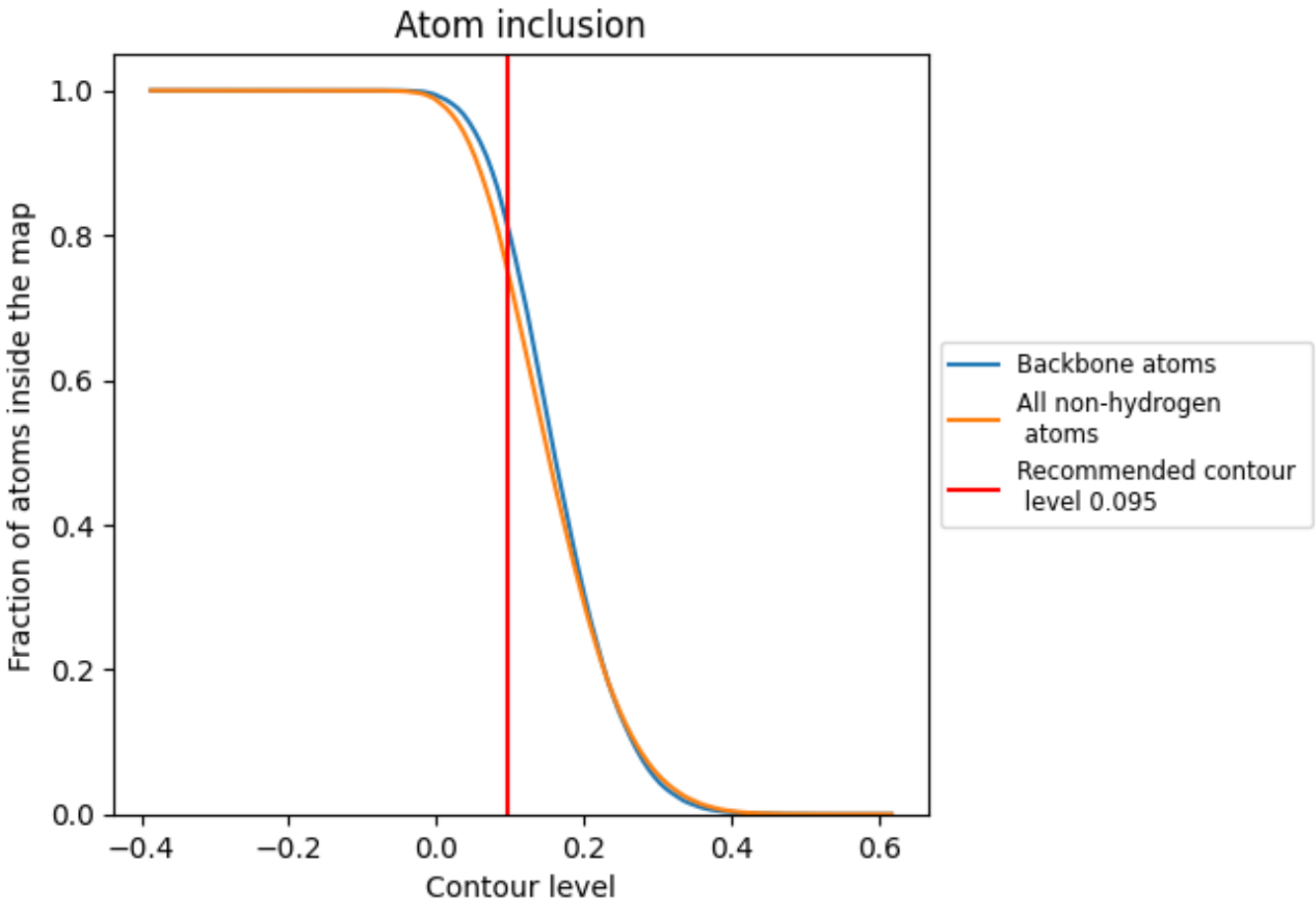
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.095).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7557	0.4020
1	0.7653	0.4810
2	0.1919	0.3240
3	0.3170	0.1780
4	0.6354	0.4010
5	0.2730	0.2430
A	0.8309	0.4030
B	0.5037	0.3030
D	0.8642	0.4290
E	0.8959	0.4250
F	0.5087	0.3650
G	0.5845	0.4070
H	0.6022	0.3710
I	0.6805	0.4430
J	0.5043	0.3330
K	0.4892	0.3660
L	0.6707	0.4270
M	0.5062	0.3610
N	0.4766	0.3540
O	0.5794	0.3990
P	0.6788	0.4600
Q	0.4305	0.2670
R	0.6253	0.4330
S	0.6172	0.3790
T	0.6627	0.3900
U	0.5976	0.3900
V	0.5017	0.3570
W	0.3708	0.1910
X	0.6198	0.3910
Y	0.6806	0.4310
Z	0.1306	0.2160
a	0.6967	0.4310
b	0.7159	0.4330
c	0.6849	0.4010
d	0.5707	0.3180

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Chain	Atom inclusion	Q-score
e	0.6483	0.3860
f	0.6854	0.4130
g	0.6714	0.4210
h	0.6019	0.3350
i	0.6852	0.4220
j	0.7432	0.4460
k	0.6346	0.3260
l	0.6290	0.3950
m	0.7701	0.4360
n	0.6496	0.3650
o	0.7485	0.4560
p	0.6836	0.4190
q	0.6082	0.3660
r	0.5290	0.3770
s	0.7303	0.4570
t	0.7002	0.4210
u	0.7105	0.4390
v	0.6482	0.3690
w	0.7760	0.4230
x	0.6797	0.3610
y	0.7211	0.4510
z	0.6640	0.4210