Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 05:17 AM EDT

PDB ID	:	5WFS / pdb_00005wfs
EMDB ID	:	EMD-8829
Title	:	70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C4)
Authors	:	Fislage, M.; Frank, J.
Deposited on	:	2017-07-12
Resolution	:	3.00 Å(reported)

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

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

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

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

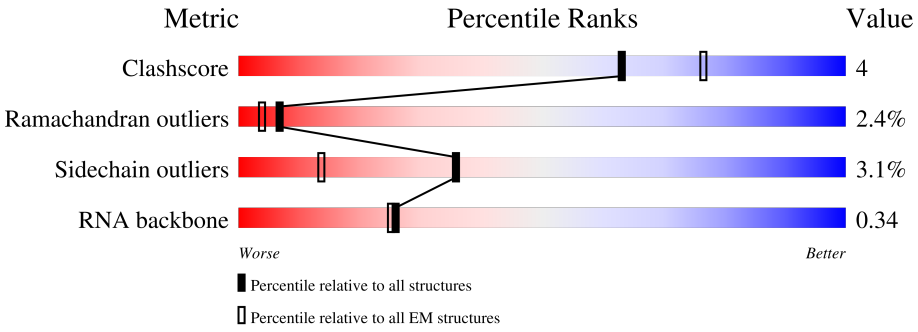
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

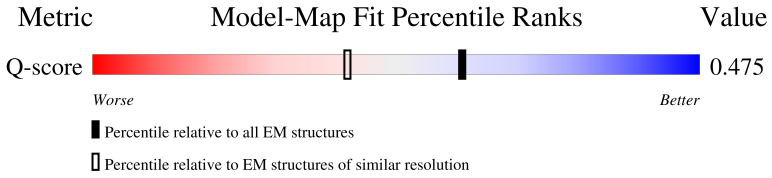
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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





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

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

Mol	Chain	Length	Quality of chain
1	A	2903	59% 33% 7% •
2	B	120	49% 41% 10%
3	C	271	88% 11% •

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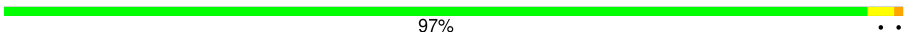
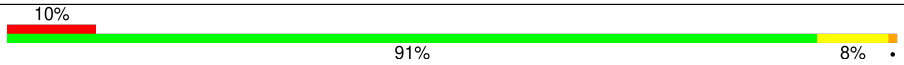
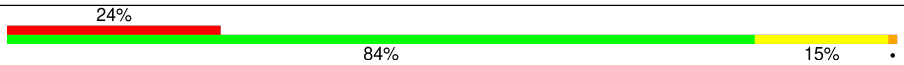
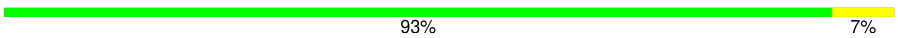
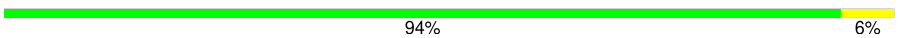
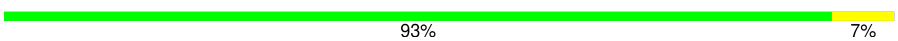
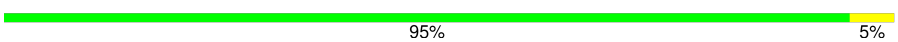
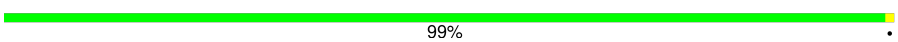
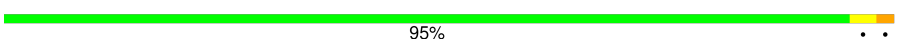
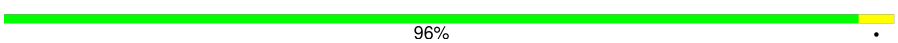
Mol	Chain	Length	Quality of chain
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	
9	I	141	
10	J	141	
11	K	122	
12	L	143	
13	M	136	
14	N	119	
15	O	116	
16	P	114	
17	Q	115	
18	R	102	
19	S	109	
20	T	92	
21	U	102	
22	V	92	
23	W	75	
24	X	77	
25	Y	60	
26	Z	56	
27	0	55	
28	1	51	

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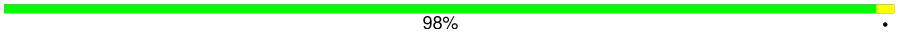
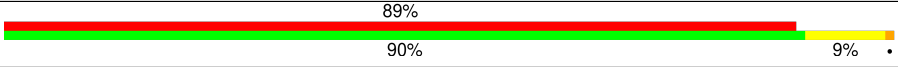
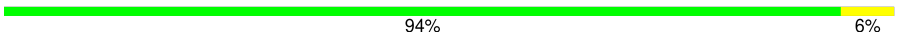
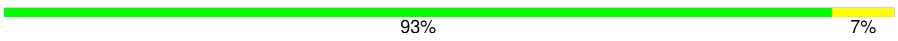
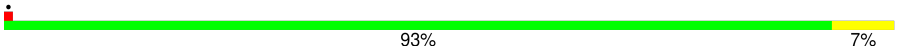
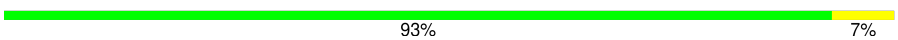
Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	77% 18% 5%
55	v	77	65% 31%
55	w	77	8% 55% 31% 13%
56	x	12	67% 25% 8%
57	y	76	46% 43% 11%
58	z	393	92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	2030	-	-	X	-
63	GTP	z	402	-	-	X	-

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 155100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62277	27788	11459	20130	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1557	974	287	293	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	115	Total	C	N	O	0	0
			933	595	190	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
55	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

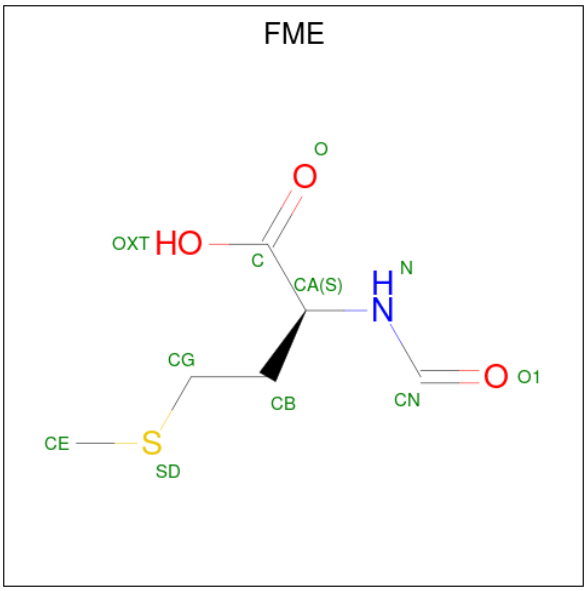
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	1011	Total	Mg	0
			1011	1011	
60	B	37	Total	Mg	0
			37	37	
60	C	1	Total	Mg	0
			1	1	
60	D	2	Total	Mg	0
			2	2	
60	E	1	Total	Mg	0
			1	1	
60	M	2	Total	Mg	0
			2	2	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	T	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	0	3	Total	Mg	0
			3	3	

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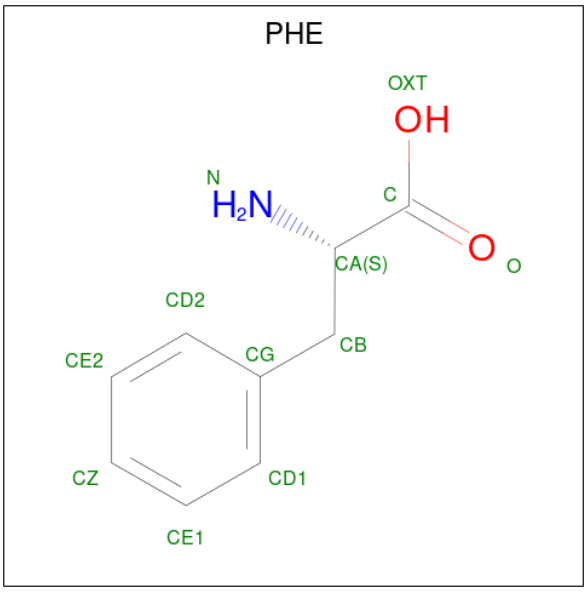
Mol	Chain	Residues	Atoms	AltConf
60	2	1	Total Mg 1 1	0
60	a	392	Total Mg 392 392	0
60	d	1	Total Mg 1 1	0
60	e	1	Total Mg 1 1	0
60	i	1	Total Mg 1 1	0
60	u	1	Total Mg 1 1	0
60	v	6	Total Mg 6 6	0
60	w	2	Total Mg 2 2	0
60	x	1	Total Mg 1 1	0
60	y	2	Total Mg 2 2	0
60	z	2	Total Mg 2 2	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

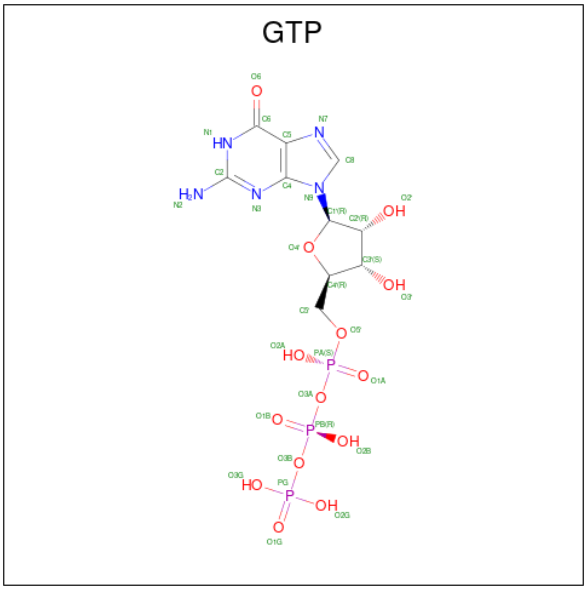
Mol	Chain	Residues	Atoms	AltConf
61	A	6	Total K 6 6	0
61	a	1	Total K 1 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
62	z	1	11	9	1	1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	5	14	3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	828	Total O 828 828	0
64	B	29	Total O 29 29	0
64	C	5	Total O 5 5	0
64	D	6	Total O 6 6	0
64	E	5	Total O 5 5	0
64	J	4	Total O 4 4	0
64	L	5	Total O 5 5	0
64	N	1	Total O 1 1	0
64	O	1	Total O 1 1	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	3	Total O 3 3	0
64	W	2	Total O 2 2	0
64	X	3	Total O 3 3	0
64	Y	1	Total O 1 1	0
64	0	2	Total O 2 2	0
64	1	1	Total O 1 1	0
64	2	2	Total O 2 2	0
64	3	1	Total O 1 1	0
64	a	253	Total O 253 253	0
64	c	1	Total O 1 1	0
64	i	1	Total O 1 1	0

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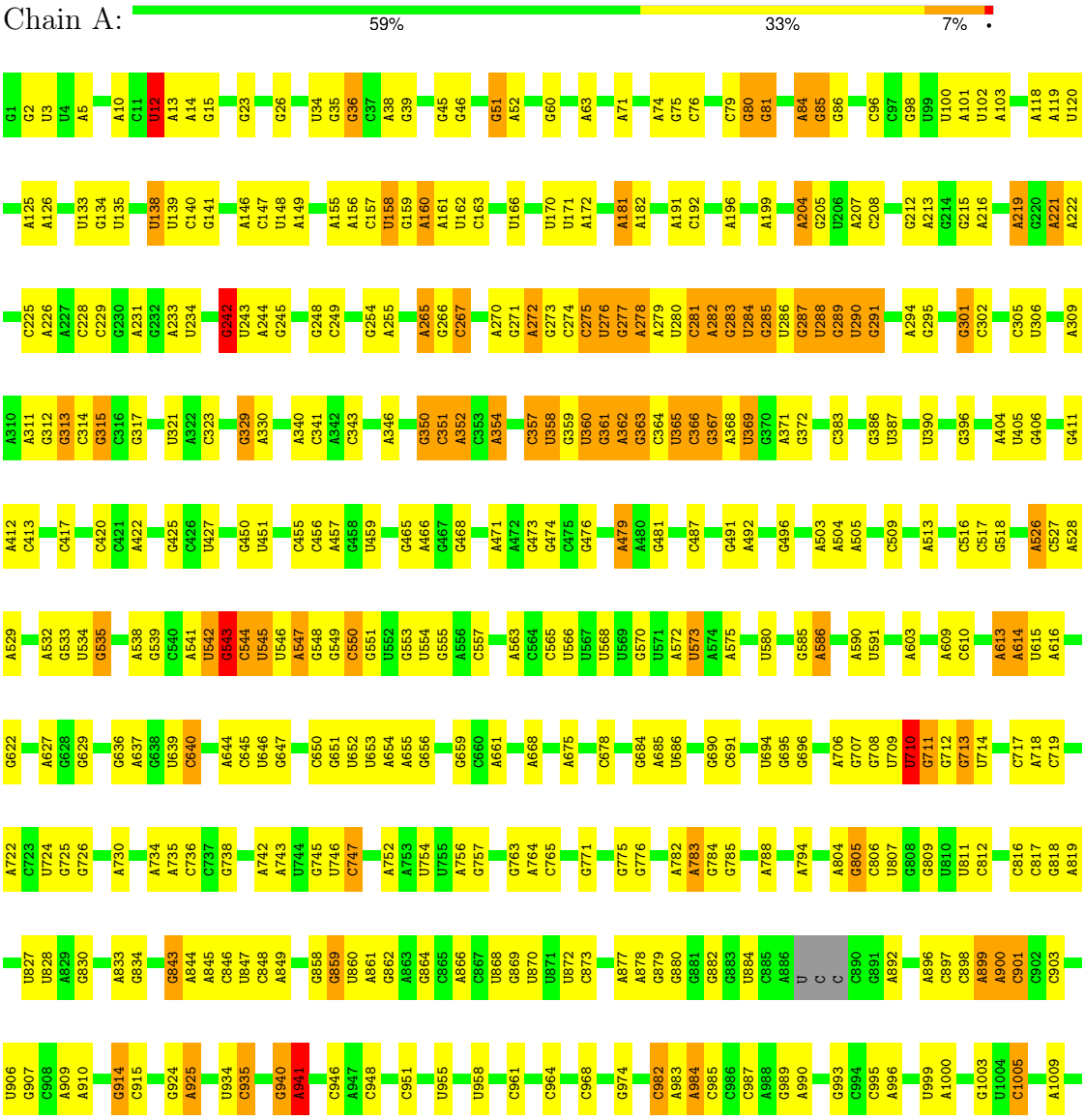
Mol	Chain	Residues	Atoms	AltConf
64	j	1	Total O 1 1	0
64	l	2	Total O 2 2	0
64	m	1	Total O 1 1	0
64	o	1	Total O 1 1	0
64	q	1	Total O 1 1	0
64	s	3	Total O 3 3	0
64	u	1	Total O 1 1	0
64	v	3	Total O 3 3	0
64	w	1	Total O 1 1	0
64	x	1	Total O 1 1	0
64	y	2	Total O 2 2	0

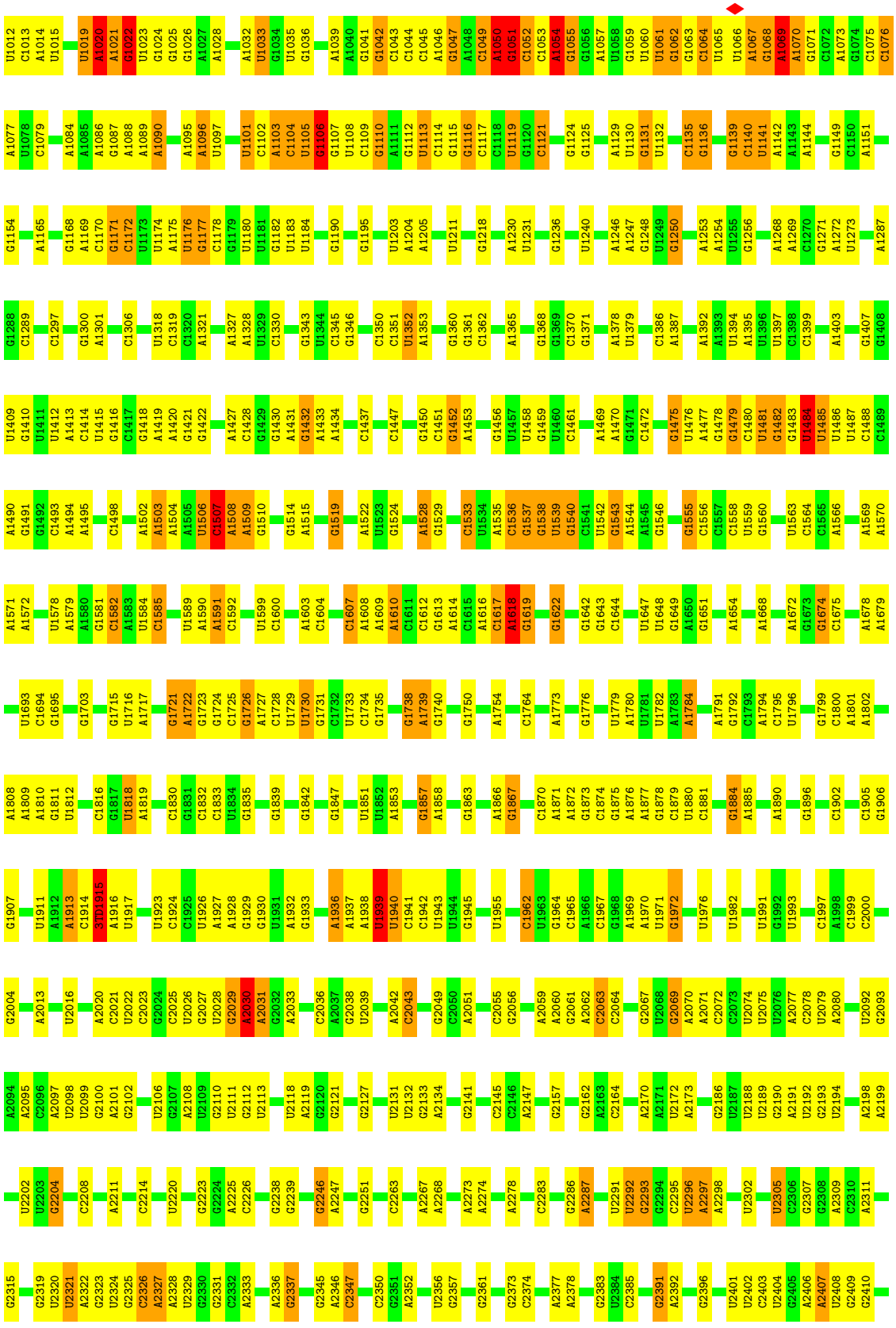
3 Residue-property plots (i)

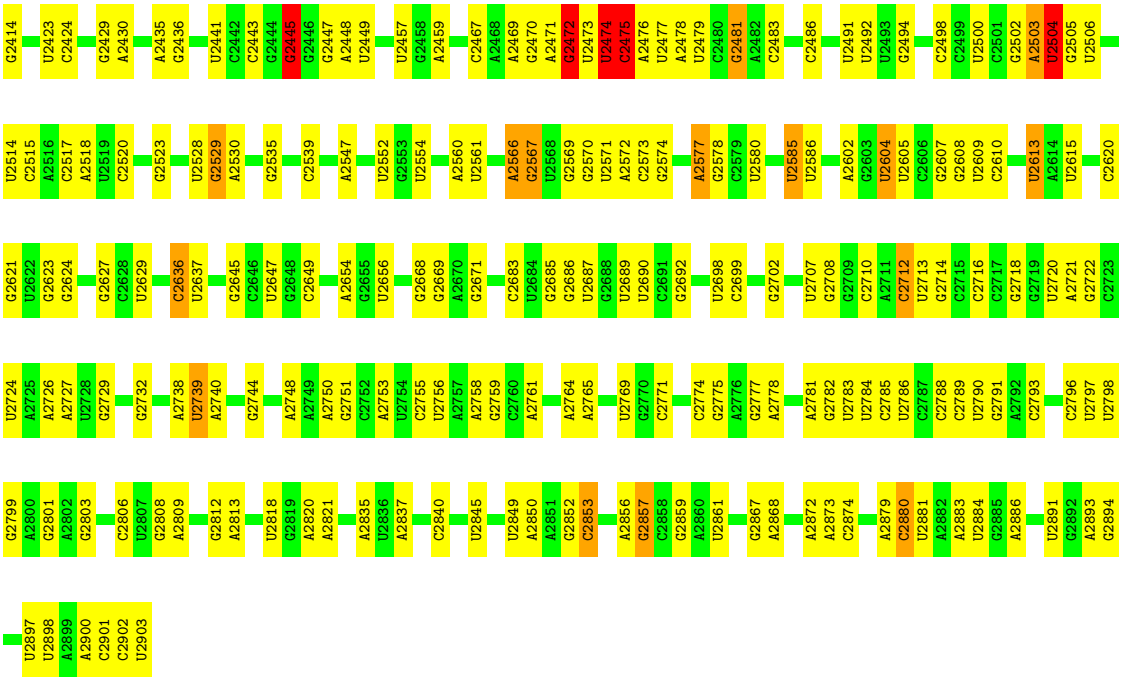
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA

Chain A:

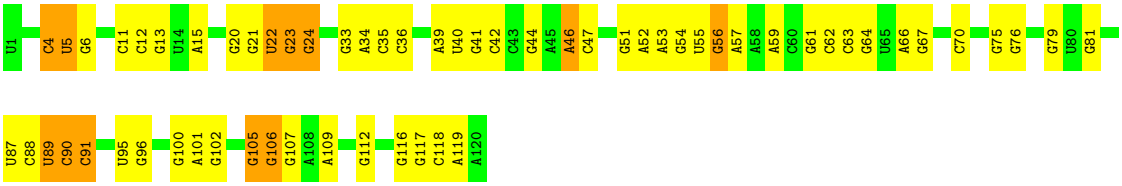






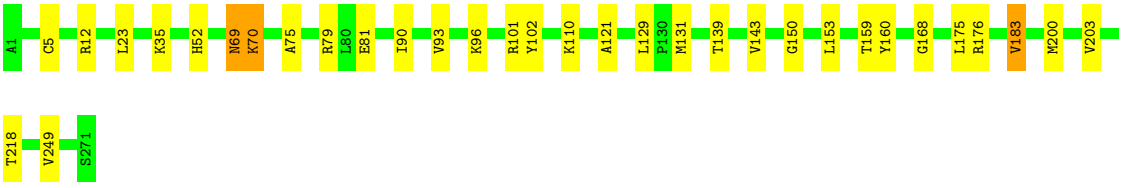
• Molecule 2: 5S rRNA

Chain B:



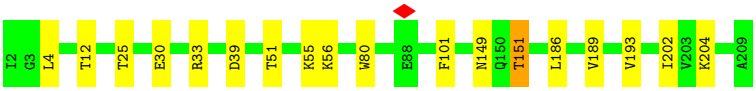
• Molecule 3: 50S ribosomal protein L2

Chain C:



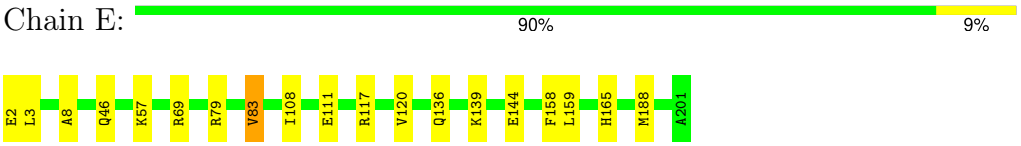
• Molecule 4: 50S ribosomal protein L3

Chain D:



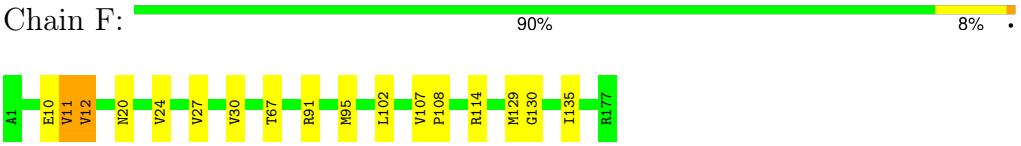
• Molecule 5: 50S ribosomal protein L4

Chain E:



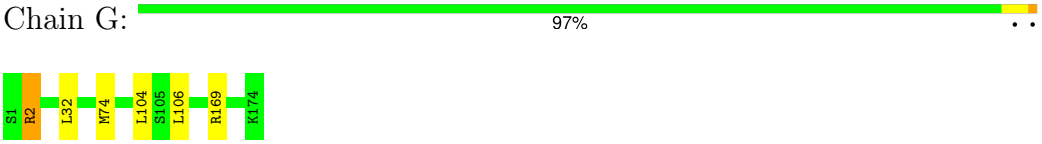
• Molecule 6: 50S ribosomal protein L5

Chain F:



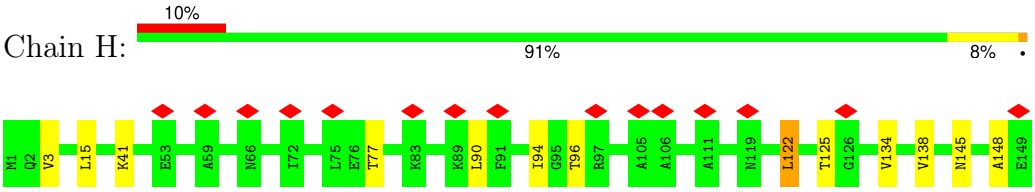
• Molecule 7: 50S ribosomal protein L6

Chain G:



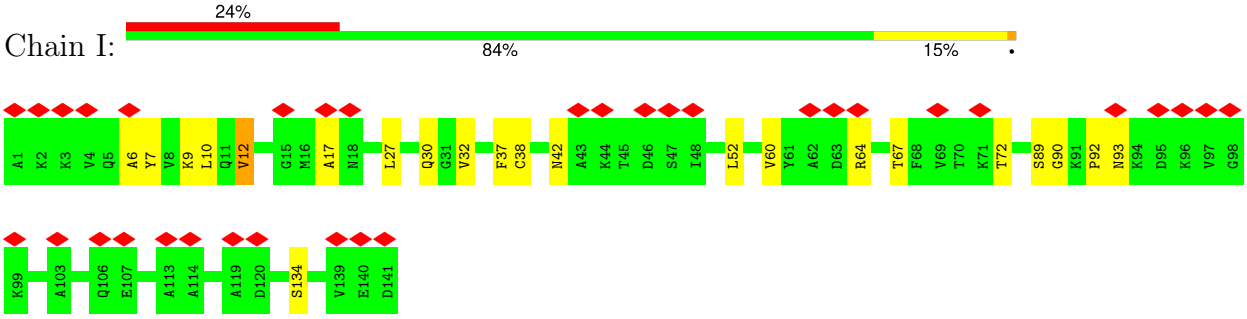
• Molecule 8: 50S ribosomal protein L9

Chain H:



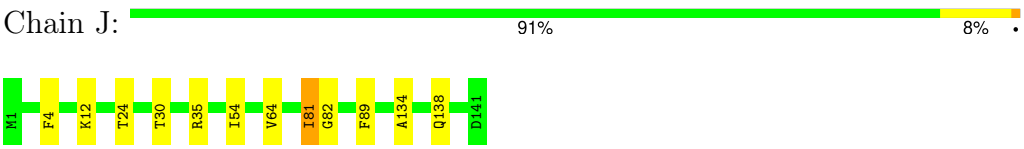
• Molecule 9: 50S ribosomal protein L11

Chain I:



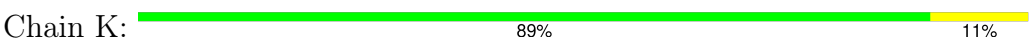
• Molecule 10: 50S ribosomal protein L13

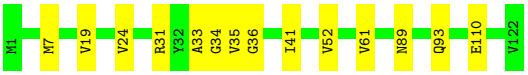
Chain J:



• Molecule 11: 50S ribosomal protein L14

Chain K:





• Molecule 12: 50S ribosomal protein L15

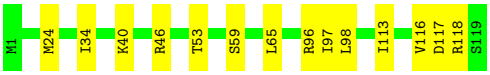
Chain L:

• Molecule 13: 50S ribosomal protein L16

Chain M:

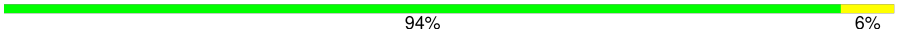
• Molecule 14: 50S ribosomal protein L17

Chain N:



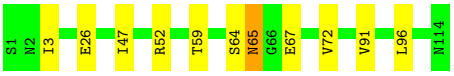
• Molecule 15: 50S ribosomal protein L18

Chain O:



• Molecule 16: 50S ribosomal protein L19

Chain P:

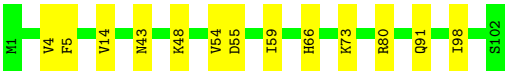


• Molecule 17: 50S ribosomal protein L20

Chain Q:

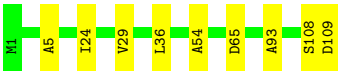
• Molecule 18: 50S ribosomal protein L21

Chain R:



• Molecule 19: 50S ribosomal protein L22

Chain S:

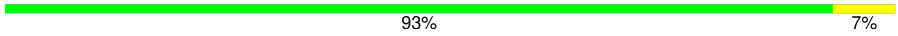


• Molecule 20: 50S ribosomal protein L23

Chain T:

• Molecule 21: 50S ribosomal protein L24

Chain U:

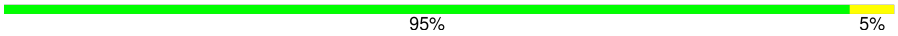


• Molecule 22: 50S ribosomal protein L25

Chain V:

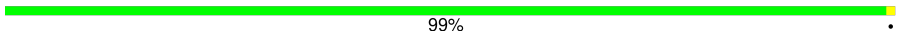
• Molecule 23: 50S ribosomal protein L27

Chain W:



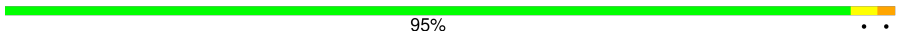
• Molecule 24: 50S ribosomal protein L28

Chain X:



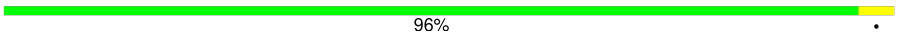
• Molecule 25: 50S ribosomal protein L29

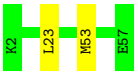
Chain Y:



• Molecule 26: 50S ribosomal protein L30

Chain Z:



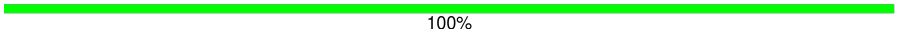


• Molecule 27: 50S ribosomal protein L32

Chain 0:

• Molecule 28: 50S ribosomal protein L33

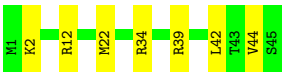
Chain 1:



There are no outlier residues recorded for this chain.

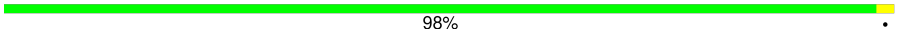
• Molecule 29: 50S ribosomal protein L34

Chain 2:



• Molecule 30: 50S ribosomal protein L35

Chain 3:

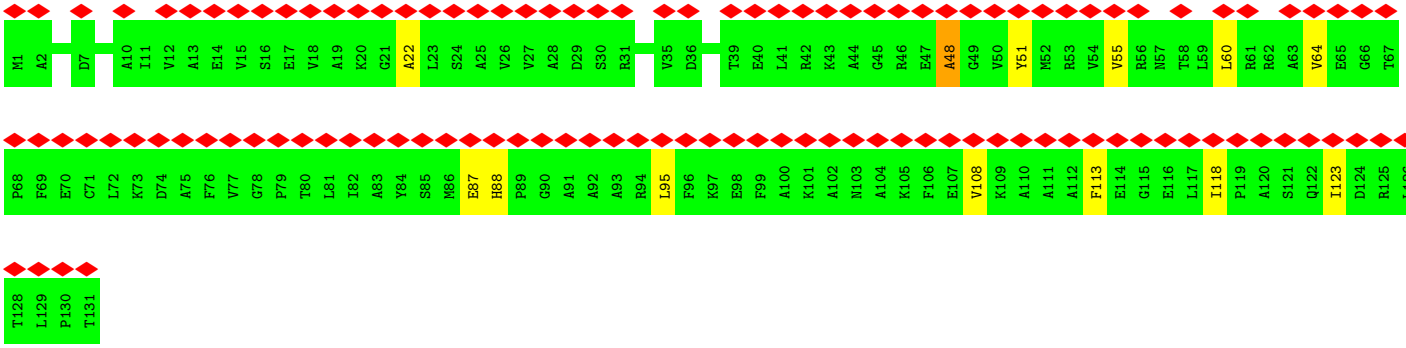


• Molecule 31: 50S ribosomal protein L36 1

Chain 4:

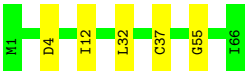
• Molecule 32: 50S ribosomal protein L10

Chain 5:



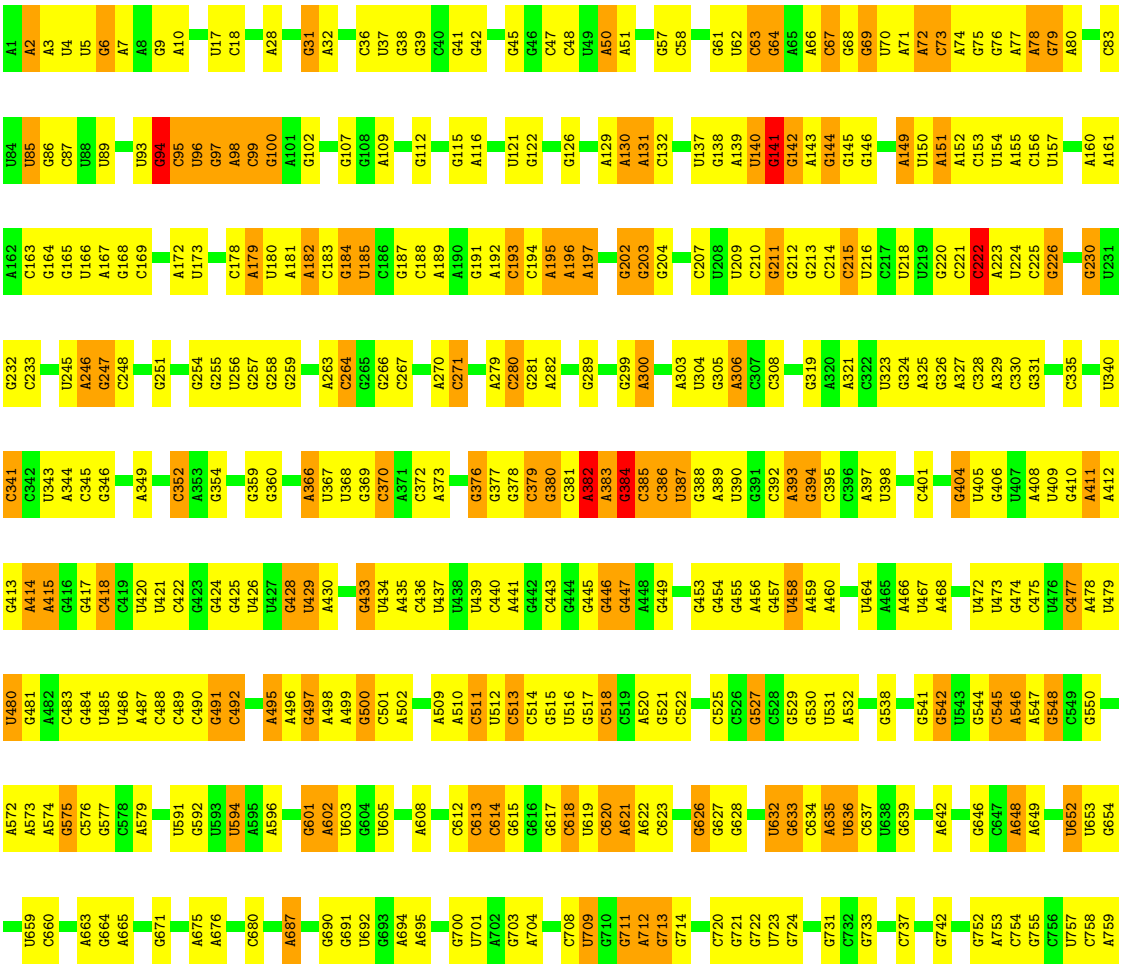
• Molecule 33: 50S ribosomal protein L31

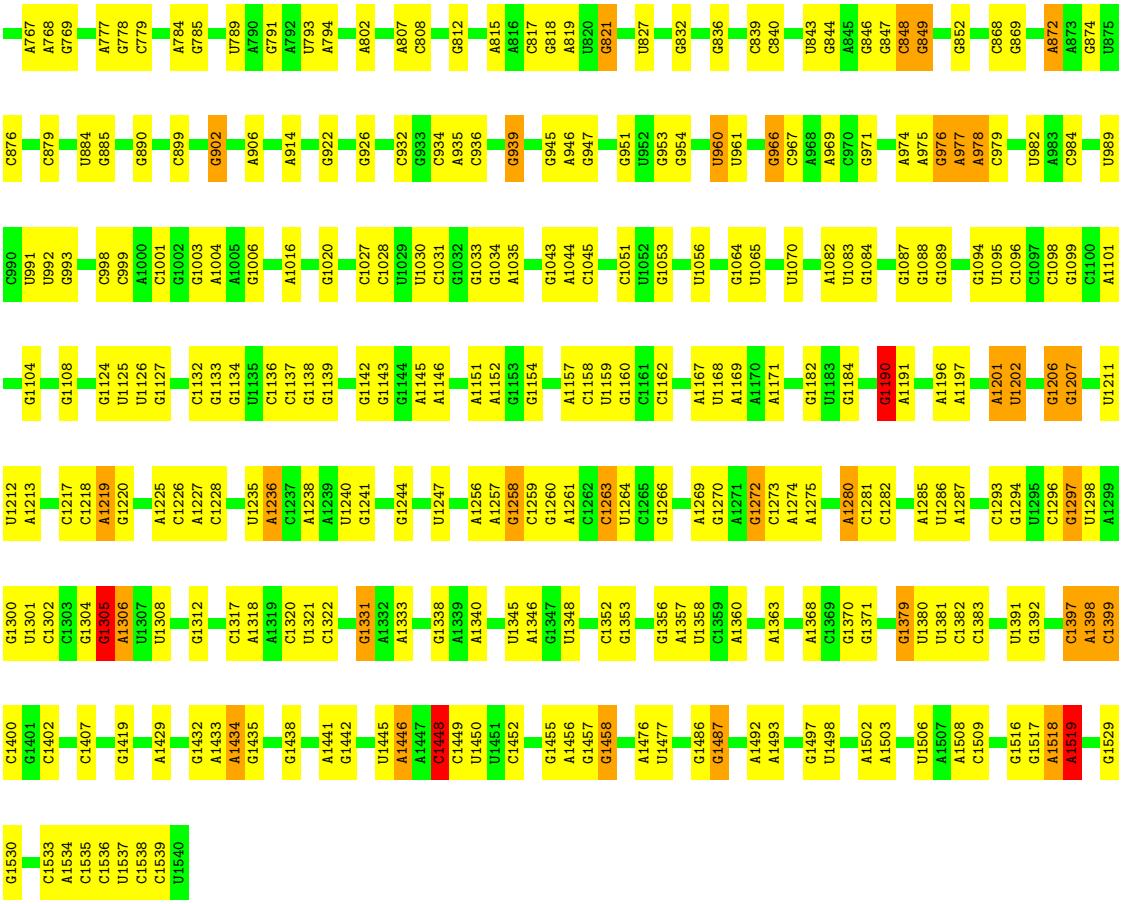
Chain 6:



• Molecule 34: 16S rRNA

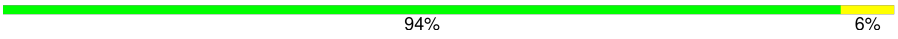
Chain a:

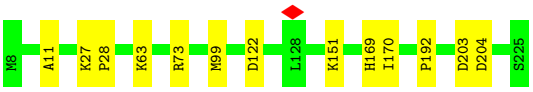




• Molecule 35: 30S ribosomal protein S2

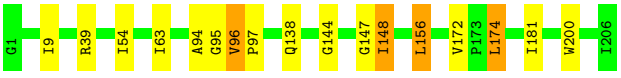
Chain b:





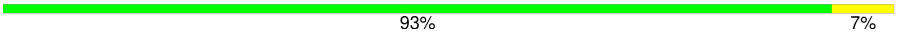
• Molecule 36: 30S ribosomal protein S3

Chain c:



• Molecule 37: 30S ribosomal protein S4

Chain d:

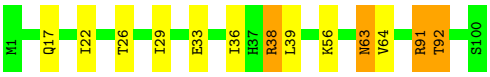


• Molecule 38: 30S ribosomal protein S5

Chain e:

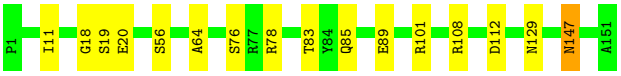
• Molecule 39: 30S ribosomal protein S6

Chain f:



• Molecule 40: 30S ribosomal protein S7

Chain g:

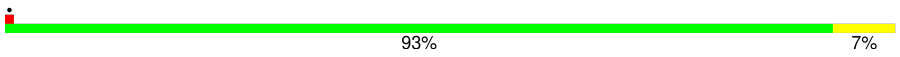


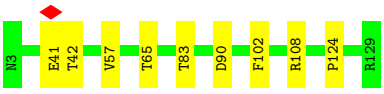
• Molecule 41: 30S ribosomal protein S8

Chain h:

• Molecule 42: 30S ribosomal protein S9

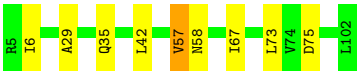
Chain i:





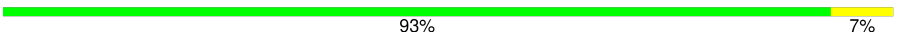
• Molecule 43: 30S ribosomal protein S10

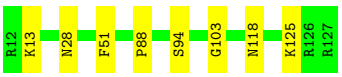
Chain j:



• Molecule 44: 30S ribosomal protein S11

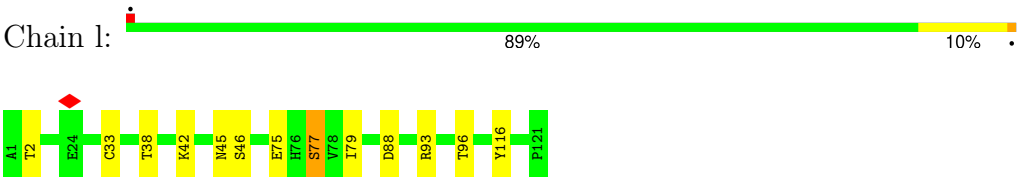
Chain k:





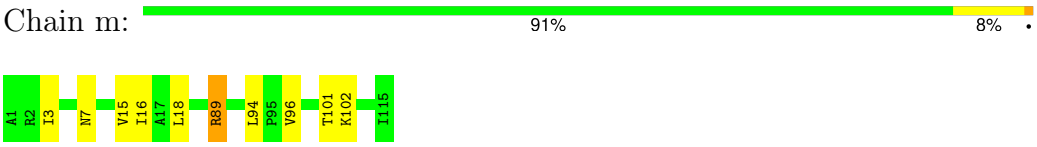
• Molecule 45: 30S ribosomal protein S12

Chain l:



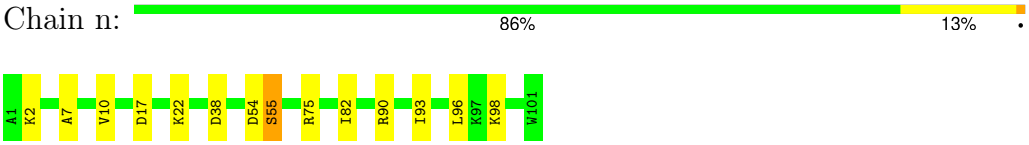
• Molecule 46: 30S ribosomal protein S13

Chain m:



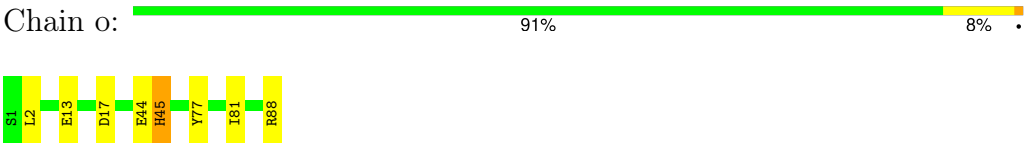
• Molecule 47: 30S ribosomal protein S14

Chain n:



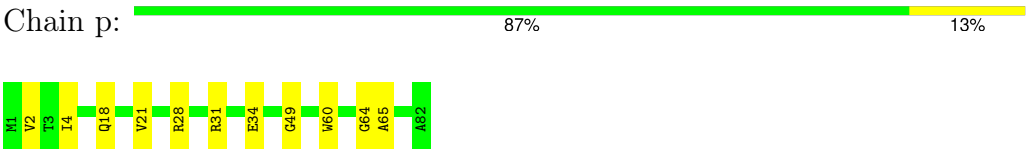
• Molecule 48: 30S ribosomal protein S15

Chain o:



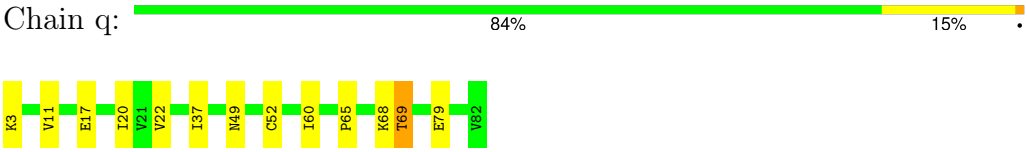
• Molecule 49: 30S ribosomal protein S16

Chain p:



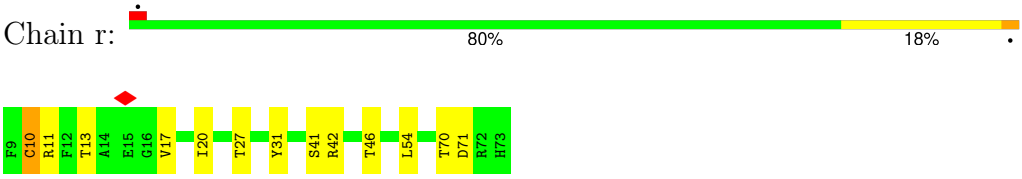
• Molecule 50: 30S ribosomal protein S17

Chain q:



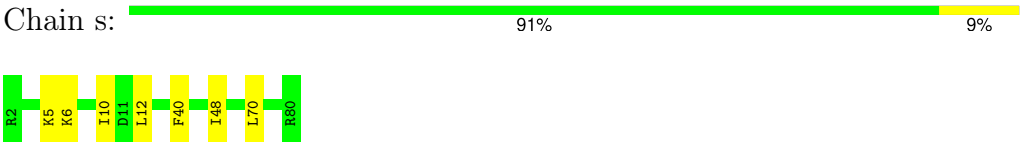
• Molecule 51: 30S ribosomal protein S18

Chain r:



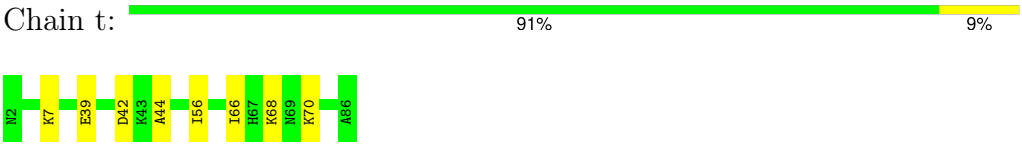
• Molecule 52: 30S ribosomal protein S19

Chain s:



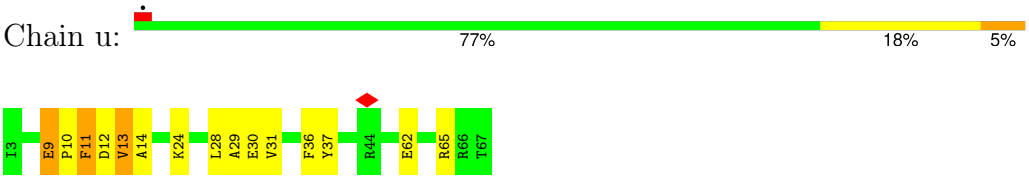
• Molecule 53: 30S ribosomal protein S20

Chain t:



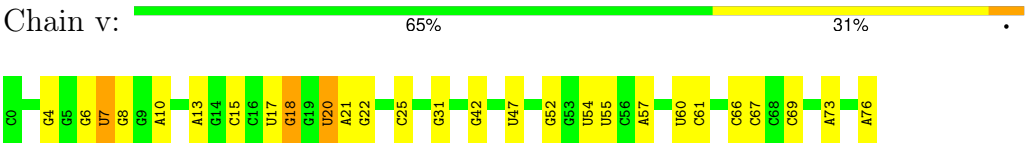
• Molecule 54: 30S ribosomal protein S21

Chain u:



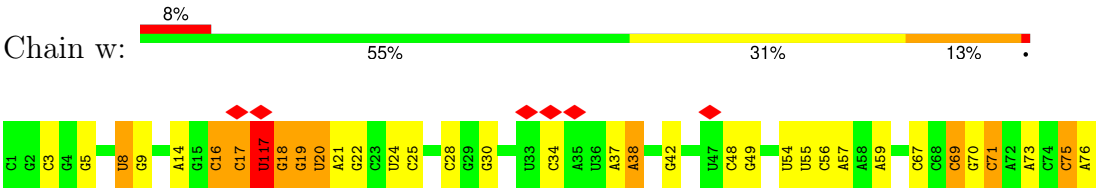
• Molecule 55: tRNA-fMet

Chain v:



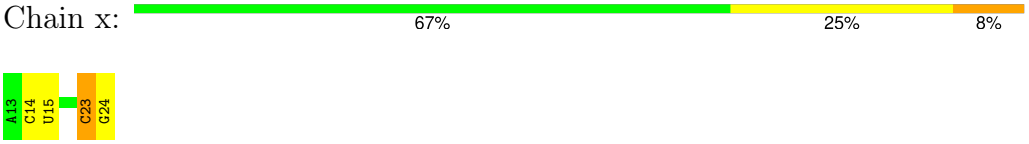
• Molecule 55: tRNA-fMet

Chain w:



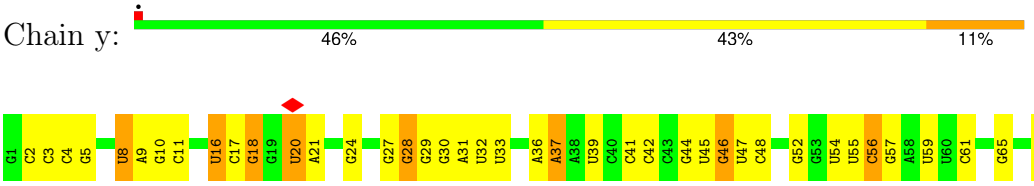
• Molecule 56: mRNA

Chain x:



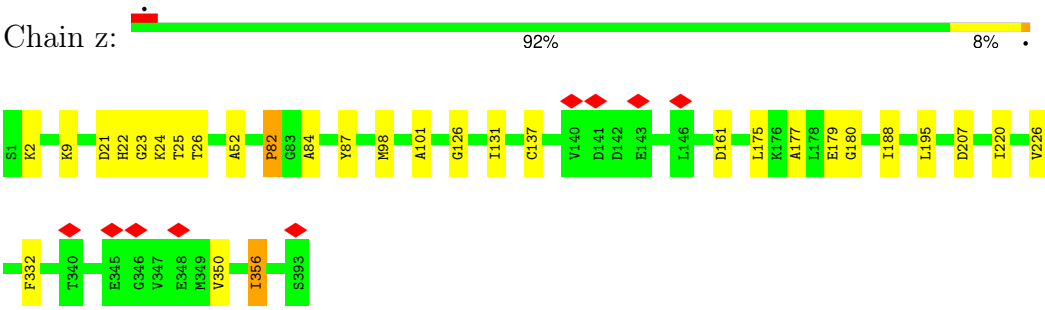
• Molecule 57: Phe-tRNA-Phe

Chain y:



• Molecule 58: Elongation factor Tu 2

Chain z:


92%
8%
S1
K2
K9
D21
H22
G23
K24
T25
T26
A52
P82
G83
A84
Y87
M98
A101
G126
I131
C137
V140
D141
D142
E143
L146
D161
L175
K176
A177
L178
E179
G180
I188
L195
D207
I220
V226
K248
E249
D314
F332
T340
E345
G346
V347
E348
M349
V350
I356
S393

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00532	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	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: OMG, OMC, 3TD, MG, 7MG, MIA, 1MG, GTP, H2U, FME, PSU, MA6, K, 5MU, UR3, 2MA, 6MZ, OMU, 4SU, 2MG, 5MC, 4OC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	0/69174	0.76	48/107907 (0.0%)
2	B	0.39	0/2876	0.77	0/4483
3	C	0.50	0/2121	0.78	0/2852
4	D	0.49	0/1578	0.77	2/2124 (0.1%)
5	E	0.49	0/1563	0.82	0/2103
6	F	0.55	0/1434	0.82	0/1926
7	G	0.53	0/1324	0.74	0/1794
8	H	0.62	0/1122	0.81	0/1515
9	I	0.69	0/1046	0.92	0/1410
10	J	0.49	0/1143	0.80	0/1540
11	K	0.50	0/947	0.76	0/1268
12	L	0.51	0/1052	0.88	0/1401
13	M	0.49	0/1093	0.79	0/1460
14	N	0.53	0/964	0.86	0/1289
15	O	0.52	0/902	0.84	0/1209
16	P	0.48	0/929	0.75	0/1242
17	Q	0.49	0/946	0.88	0/1260
18	R	0.48	0/823	0.70	0/1100
19	S	0.49	0/852	0.83	0/1142
20	T	0.50	0/736	0.76	0/984
21	U	0.47	0/787	0.73	0/1051
22	V	0.49	0/752	0.74	0/1008
23	W	0.47	0/579	0.68	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.53	0/495	0.87	0/658
26	Z	0.52	0/438	0.78	0/586
27	0	0.45	0/440	0.81	0/588
28	1	0.49	0/424	0.69	0/565
29	2	0.52	0/370	0.97	0/487
30	3	0.46	0/513	0.84	0/676
31	4	0.46	0/303	0.75	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	5	0.67	0/1001	0.84	0/1350
33	6	0.57	0/531	0.79	0/709
34	a	0.39	0/36725	0.76	25/57285 (0.0%)
35	b	0.55	0/1735	0.79	0/2338
36	c	0.53	0/1651	0.80	0/2225
37	d	0.60	0/1665	0.82	0/2227
38	e	0.52	0/1180	0.84	0/1587
39	f	0.56	0/835	0.81	2/1128 (0.2%)
40	g	0.53	0/1195	0.82	0/1602
41	h	0.52	0/989	0.80	0/1326
42	i	0.56	0/1034	0.76	0/1375
43	j	0.55	0/796	0.74	0/1077
44	k	0.54	0/885	0.78	0/1195
45	l	0.56	0/954	0.78	0/1282
46	m	0.56	0/900	0.84	0/1204
47	n	0.53	0/822	0.79	0/1095
48	o	0.50	0/722	0.83	0/964
49	p	0.56	0/659	0.78	0/884
50	q	0.56	0/657	0.76	0/881
51	r	0.60	0/544	0.80	0/731
52	s	0.55	0/652	0.75	0/877
53	t	0.54	0/671	0.88	0/888
54	u	0.64	0/550	0.92	0/728
55	v	0.41	1/1747 (0.1%)	0.74	0/2721
55	w	0.40	0/1747	0.98	5/2721 (0.2%)
56	x	0.37	0/280	0.77	0/433
57	y	0.40	0/1607	0.73	1/2501 (0.0%)
58	z	0.57	0/3086	0.78	0/4175
All	All	0.43	1/164181 (0.0%)	0.77	83/245149 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
34	a	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	O3'-P	5.46	1.61	1.56

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	117	U	O3'-P-O5'	23.50	139.25	104.00
55	w	117	U	P-O3'-C3'	22.09	153.34	120.20
34	a	1399	C	C2'-C3'-O3'	10.11	124.67	109.50
34	a	1305	G	C2'-C3'-O3'	9.84	124.27	109.50
1	A	301	G	C4'-C3'-O3'	9.44	123.55	109.40
1	A	242	G	C2'-C3'-O3'	9.35	123.52	109.50
1	A	1022	G	C2'-C3'-O3'	9.15	123.23	109.50
1	A	204	A	C4'-C3'-O3'	9.15	123.12	109.40
1	A	2407	A	C2'-C3'-O3'	8.83	126.94	113.70
1	A	1475	G	C2'-C3'-O3'	8.43	122.15	109.50
1	A	1484	U	N1-C1'-C2'	8.41	124.61	112.00
1	A	614	A	C4'-C3'-O3'	-8.34	96.89	109.40
34	a	1432	G	C2'-C3'-O3'	8.32	121.99	109.50
1	A	859	G	C4'-C3'-O3'	8.31	121.87	109.40
34	a	246	A	C4'-C3'-O3'	8.03	121.44	109.40
55	w	117	U	OP1-P-O3'	-7.89	84.33	108.00
1	A	1730	U	C2'-C3'-O3'	7.89	121.33	109.50
34	a	1201	A	C2'-C3'-O3'	7.58	120.86	109.50
34	a	1190	G	C2'-C3'-O3'	7.56	120.83	109.50
1	A	2296	U	C4'-C3'-O3'	7.55	120.72	109.40
1	A	265	A	C4'-C3'-O3'	7.51	120.66	109.40
34	a	574	A	C4'-C3'-O3'	-7.49	101.76	113.00
1	A	2391	G	C4'-C3'-O3'	7.45	124.17	113.00
34	a	495	A	C4'-C3'-O3'	7.44	120.56	109.40
1	A	1070	A	C2'-C3'-O3'	7.04	120.06	109.50
55	w	75	C	C4'-C3'-O3'	6.96	119.83	109.40
1	A	613	A	C2'-C3'-O3'	-6.79	99.32	109.50
1	A	1051	G	N9-C1'-C2'	6.78	122.17	112.00
1	A	360	U	C4'-C3'-O3'	6.58	119.27	109.40
34	a	280	C	C4'-C3'-O3'	6.51	119.17	109.40
1	A	2566	A	C4'-C3'-O3'	6.46	119.08	109.40
1	A	2475	C	N1-C1'-C2'	6.27	121.40	112.00
34	a	960	U	C4'-C3'-O3'	6.22	118.73	109.40
1	A	51	G	C4'-C3'-O3'	6.15	118.63	109.40
1	A	1940	U	C2'-C3'-O3'	6.11	118.67	109.50
1	A	1113	U	C2'-C3'-O3'	-5.96	104.76	113.70
34	a	1448	C	N1-C1'-C2'	5.95	120.92	112.00
1	A	1694	C	C4'-C3'-O3'	5.94	118.31	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	960	U	C2'-C3'-O3'	5.84	118.26	109.50
34	a	1297	G	C2'-C3'-O3'	5.82	118.23	109.50
34	a	85	U	C2'-C3'-O3'	-5.80	105.00	113.70
34	a	214	C	C4'-C3'-O3'	-5.77	104.35	113.00
1	A	2712	C	C2'-C3'-O3'	5.73	118.10	109.50
1	A	1106	G	C1'-C2'-O2'	5.72	120.38	111.80
1	A	1254	A	C4'-C3'-O3'	-5.71	104.43	113.00
1	A	1945	G	C4'-C3'-O3'	-5.71	104.43	113.00
34	a	94	G	C2'-C3'-O3'	5.64	117.96	109.50
1	A	1050	A	C2'-C3'-O3'	5.62	122.14	113.70
1	A	1020	A	C4'-C3'-O3'	5.61	117.81	109.40
1	A	2712	C	C4'-C3'-O3'	5.58	117.78	109.40
34	a	1084	G	C4'-C3'-O3'	-5.58	104.62	113.00
1	A	1536	C	C2'-C3'-O3'	5.57	122.06	113.70
34	a	1272	G	C4'-C3'-O3'	-5.56	104.67	113.00
1	A	1050	A	O4'-C1'-C2'	-5.53	102.07	107.60
1	A	710	U	C2'-C3'-O3'	5.49	121.93	113.70
1	A	2474	U	N1-C1'-C2'	5.40	120.10	112.00
1	A	2467	C	C4'-C3'-O3'	-5.36	104.96	113.00
34	a	382	A	C4'-C3'-O3'	5.35	121.03	113.00
4	D	151	THR	CA-C-N	-5.33	113.42	118.97
4	D	151	THR	C-N-CA	-5.33	113.42	118.97
1	A	2472	G	N9-C1'-C2'	5.33	119.99	112.00
34	a	384	G	N9-C1'-C2'	5.32	121.98	114.00
1	A	1069	A	C2'-C3'-O3'	-5.28	105.79	113.70
34	a	63	C	C3'-C2'-O2'	5.27	118.61	110.70
1	A	12	U	N1-C1'-C2'	5.25	119.88	112.00
1	A	84	A	C4'-C3'-O3'	5.25	117.27	109.40
1	A	1507	C	C3'-C2'-O2'	5.24	118.56	110.70
34	a	429	U	C4'-C3'-O3'	5.20	117.20	109.40
34	a	379	C	C4'-C3'-O3'	-5.19	105.21	113.00
34	a	635	A	C4'-C3'-O3'	-5.18	105.22	113.00
1	A	1481	U	C2'-C3'-O3'	5.14	121.42	113.70
1	A	941	A	C4'-C3'-O3'	-5.14	105.29	113.00
39	f	17	GLN	CA-C-N	5.13	123.47	120.24
39	f	17	GLN	C-N-CA	5.13	123.47	120.24
1	A	982	C	C2'-C3'-O3'	-5.12	106.01	113.70
1	A	543	G	C2'-C3'-O3'	-5.12	106.02	113.70
34	a	712	A	C4'-C3'-O3'	-5.12	105.33	113.00
1	A	2528	U	C3'-C2'-O2'	5.11	118.37	110.70
1	A	1940	U	C4'-C3'-O3'	5.08	117.01	109.40
57	y	2	C	C2'-C3'-O3'	5.06	121.29	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	783	A	C4'-C3'-O3'	5.04	120.56	113.00
55	w	69	C	C2'-C3'-O3'	5.01	121.22	113.70
1	A	2326	C	C3'-C2'-O2'	5.01	118.21	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	A	Sidechain
34	a	141	G	Sidechain
34	a	222	C	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31337	505	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	12	0
4	D	1557	0	1604	5	0
5	E	1544	0	1607	5	0
6	F	1410	0	1447	7	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	2	0
9	I	1032	0	1088	8	0
10	J	1120	0	1151	7	0
11	K	938	0	1012	3	0
12	L	1043	0	1123	7	0
13	M	1074	0	1157	5	0
14	N	951	0	994	4	0
15	O	892	0	923	4	0
16	P	917	0	965	6	0
17	Q	933	0	1006	7	0
18	R	810	0	834	6	0
19	S	845	0	909	4	0
20	T	730	0	795	2	0
21	U	779	0	834	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	739	0	763	3	0
23	W	572	0	593	2	0
24	X	625	0	655	0	0
25	Y	494	0	530	1	0
26	Z	434	0	477	2	0
27	0	434	0	448	5	0
28	1	417	0	451	0	0
29	2	367	0	405	6	0
30	3	504	0	574	0	0
31	4	302	0	343	5	0
32	5	988	0	1025	3	0
33	6	522	0	524	1	0
34	a	33050	0	16652	300	0
35	b	1704	0	1732	3	0
36	c	1624	0	1699	8	0
37	d	1643	0	1710	5	0
38	e	1164	0	1212	11	0
39	f	817	0	808	15	0
40	g	1181	0	1240	5	0
41	h	979	0	1034	9	0
42	i	1022	0	1070	1	0
43	j	786	0	828	3	0
44	k	869	0	878	0	0
45	l	940	0	1001	3	0
46	m	891	0	955	5	0
47	n	810	0	852	5	0
48	o	714	0	737	2	0
49	p	649	0	666	5	0
50	q	648	0	691	4	0
51	r	535	0	552	4	0
52	s	637	0	665	3	0
53	t	665	0	714	1	0
54	u	544	0	579	4	0
55	v	1644	0	840	1	0
55	w	1644	0	840	14	0
56	x	252	0	130	1	0
57	y	1632	0	843	8	0
58	z	3031	0	3052	19	0
59	A	10	0	10	0	0
60	0	3	0	0	0	0
60	2	1	0	0	0	0
60	A	1011	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	B	37	0	0	0	0
60	C	1	0	0	0	0
60	D	2	0	0	0	0
60	E	1	0	0	0	0
60	M	2	0	0	0	0
60	N	1	0	0	0	0
60	Q	1	0	0	0	0
60	T	1	0	0	0	0
60	W	1	0	0	0	0
60	a	392	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	i	1	0	0	0	0
60	u	1	0	0	0	0
60	v	6	0	0	0	0
60	w	2	0	0	0	0
60	x	1	0	0	0	0
60	y	2	0	0	0	0
60	z	2	0	0	0	0
61	A	6	0	0	0	0
61	a	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	16	0
64	0	2	0	0	0	0
64	1	1	0	0	0	0
64	2	2	0	0	0	0
64	3	1	0	0	0	0
64	A	828	0	0	0	0
64	B	29	0	0	0	0
64	C	5	0	0	0	0
64	D	6	0	0	0	0
64	E	5	0	0	0	0
64	J	4	0	0	0	0
64	L	5	0	0	0	0
64	N	1	0	0	0	0
64	O	1	0	0	0	0
64	Q	3	0	0	0	0
64	R	1	0	0	0	0
64	S	3	0	0	0	0
64	W	2	0	0	0	0
64	X	3	0	0	0	0
64	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	a	253	0	0	1	0
64	c	1	0	0	0	0
64	i	1	0	0	0	0
64	j	1	0	0	0	0
64	l	2	0	0	0	0
64	m	1	0	0	0	0
64	o	1	0	0	0	0
64	q	1	0	0	0	0
64	s	3	0	0	0	0
64	u	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
64	y	2	0	0	0	0
All	All	155100	0	103539	1030	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1030) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:182:A:N1	34:a:185:U:O4	1.63	1.31
1:A:1105:U:N3	1:A:1106:G:N9	1.79	1.28
1:A:1021:A:N1	1:A:1141:U:O4	1.70	1.24
1:A:1054:A:N6	1:A:1106:G:N7	1.91	1.18
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.18
1:A:1054:A:N6	1:A:1106:G:C8	2.10	1.18
34:a:827:U:O4	34:a:872:A:N1	1.79	1.15
34:a:141:G:O6	34:a:222:C:C2	1.99	1.14
39:f:38:ARG:HG3	39:f:63:ASN:HB3	1.32	1.12
34:a:141:G:C6	34:a:222:C:O2	2.01	1.12
1:A:2013:A:N1	1:A:2613:U:O4	1.83	1.11
63:z:402:GTP:H8	63:z:402:GTP:H5"	1.07	1.08
1:A:1042:G:O6	1:A:1113:U:O2	1.74	1.06
34:a:141:G:C6	34:a:222:C:C2	2.43	1.05
1:A:1105:U:C4	1:A:1106:G:N9	2.09	1.05
58:z:25:THR:OG1	63:z:402:GTP:O1B	1.73	1.05
1:A:1050:A:C8	1:A:1051:G:C8	2.45	1.04
39:f:38:ARG:CG	39:f:63:ASN:HB3	1.86	1.04
55:w:17:C:C5	55:w:117:U:H5	1.77	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:18:G:O2'	55:w:19:G:OP1	1.74	1.02
1:A:286:U:O2	1:A:354:A:N6	1.93	1.00
55:w:17:C:C5	55:w:117:U:C5	2.49	1.00
34:a:142:G:N2	34:a:222:C:O4'	1.94	1.00
2:B:4:C:N4	2:B:116:G:O6	1.95	1.00
1:A:1105:U:N3	1:A:1106:G:C1'	2.25	0.99
1:A:1050:A:N6	1:A:2751:G:C6	2.29	0.99
34:a:69:G:N2	34:a:100:G:O6	1.96	0.98
34:a:500:G:O6	34:a:545:C:N3	1.97	0.97
63:z:402:GTP:H5"	63:z:402:GTP:C8	2.00	0.97
34:a:936:C:N3	34:a:1379:G:O6	1.97	0.97
1:A:1472:C:N3	1:A:1519:G:O6	1.98	0.96
1:A:1050:A:C6	1:A:2751:G:C6	2.54	0.95
1:A:1050:A:N6	1:A:2751:G:O6	2.02	0.93
1:A:1105:U:N3	1:A:1106:G:C4	2.24	0.93
1:A:1052:C:O2	1:A:1107:G:N1	2.01	0.93
55:w:17:C:H5	55:w:117:U:C5	1.87	0.92
1:A:843:G:O6	1:A:935:C:N3	2.02	0.92
34:a:605:U:O2	34:a:633:G:N1	2.05	0.89
1:A:713:G:N2	1:A:718:A:N7	2.19	0.89
34:a:153:C:N4	34:a:168:G:O6	2.05	0.89
58:z:23:GLY:HA2	63:z:402:GTP:O1A	1.71	0.88
1:A:1054:A:N6	1:A:1106:G:C5	2.31	0.88
1:A:2471:A:H2'	1:A:2472:G:O4'	1.73	0.88
1:A:1054:A:N1	1:A:1106:G:C2'	2.37	0.88
46:m:15:VAL:HG23	46:m:16:ILE:HD12	1.56	0.87
1:A:708:G:O6	1:A:722:A:N6	2.07	0.86
2:B:39:A:O2'	2:B:46:A:N1	2.09	0.86
58:z:23:GLY:CA	63:z:402:GTP:O1A	2.24	0.86
1:A:272:A:N1	1:A:365:U:O4	2.09	0.85
55:w:117:U:O2'	55:w:18:G:OP1	1.95	0.85
1:A:2030:6MZ:O2'	1:A:2031:A:P	2.34	0.85
1:A:283:G:O6	1:A:357:C:H1'	1.77	0.84
58:z:24:LYS:NZ	63:z:402:GTP:O1G	2.08	0.84
1:A:1050:A:H8	1:A:1051:G:C8	1.91	0.84
34:a:417:G:H2'	34:a:418:C:H5'	1.59	0.84
34:a:1397:C:OP2	56:x:23:C:N4	2.10	0.83
34:a:936:C:O2	34:a:1379:G:N1	2.09	0.83
1:A:1047:G:H2'	1:A:1110:G:N2	1.94	0.83
34:a:601:G:H2'	34:a:602:A:H5'	1.60	0.83
34:a:42:G:N3	34:a:622:A:C2	2.47	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:U:C2	1:A:1106:G:O4’	2.32	0.83
1:A:288:U:O4	1:A:352:A:C6	2.32	0.83
58:z:21:ASP:HA	63:z:402:GTP:O2A	1.77	0.82
1:A:1484:U:H2’	1:A:1485:U:C6	2.14	0.82
34:a:263:A:O2’	34:a:264:C:O2	1.98	0.81
1:A:2474:U:H3’	1:A:2475:C:C5	2.16	0.81
1:A:2320:U:H4’	1:A:2321:U:H5”	1.63	0.81
1:A:2297:A:N1	1:A:2321:U:C4	2.49	0.80
1:A:1021:A:N6	1:A:1141:U:H3	1.80	0.80
1:A:1050:A:C8	1:A:1051:G:H8	1.96	0.80
1:A:278:A:N6	1:A:362:A:O4’	2.15	0.80
34:a:137:U:O2	34:a:226:G:N1	2.15	0.79
1:A:1052:C:N3	1:A:1107:G:O6	2.16	0.79
34:a:137:U:N3	34:a:226:G:O6	2.15	0.79
34:a:141:G:N7	34:a:223:A:C2	2.51	0.79
55:w:18:G:O2’	55:w:19:G:P	2.41	0.78
1:A:1021:A:H61	1:A:1141:U:H3	1.28	0.78
1:A:1485:U:H2’	1:A:1486:U:C6	2.18	0.78
1:A:2840:C:H5”	14:N:53:THR:HG21	1.65	0.77
34:a:401:C:O2’	34:a:621:A:N3	2.18	0.77
1:A:1105:U:C2	1:A:1106:G:C1’	2.67	0.77
1:A:1779:U:C5	1:A:1784:A:N7	2.54	0.76
16:P:59:THR:HG22	16:P:72:VAL:HG22	1.68	0.75
1:A:1054:A:C2	1:A:1106:G:O2’	2.39	0.74
34:a:618:C:C2	34:a:622:A:N6	2.56	0.74
1:A:709:U:C4	1:A:722:A:N1	2.55	0.74
1:A:2292:U:H2’	1:A:2293:G:H5’	1.70	0.74
34:a:404:G:C2	34:a:498:A:N3	2.56	0.74
34:a:42:G:N3	34:a:622:A:N3	2.36	0.73
34:a:605:U:O2	34:a:633:G:C6	2.41	0.73
34:a:632:U:H5”	34:a:633:G:H5”	1.70	0.73
34:a:827:U:H3	34:a:872:A:N6	1.87	0.73
1:A:2028:U:H2’	1:A:2029:G:C8	2.24	0.73
1:A:2472:G:H1	1:A:2475:C:H2’	1.54	0.73
34:a:546:A:HO2’	34:a:548:G:HO2’	1.36	0.73
1:A:80:G:H2’	1:A:81:G:H5’	1.71	0.73
34:a:618:C:O2	34:a:622:A:N6	2.21	0.73
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.70	0.73
1:A:1054:A:C4	1:A:1106:G:C2	2.77	0.72
1:A:568:U:H1’	1:A:2030:6MZ:H9C1	1.72	0.71
34:a:74:A:C2	34:a:97:G:N2	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:202:G:O6	34:a:215:C:N3	2.22	0.71
1:A:2028:U:C4	1:A:2029:G:C6	2.78	0.71
34:a:546:A:O2'	34:a:548:G:O2'	2.09	0.71
1:A:1064:C:N4	1:A:1069:A:OP2	2.23	0.71
1:A:2320:U:H4'	1:A:2321:U:C5'	2.20	0.71
1:A:1483:G:N2	1:A:1484:U:C2	2.59	0.70
1:A:1051:G:O6	1:A:1109:C:C2	2.44	0.70
1:A:1105:U:H3	1:A:1106:G:C1'	1.97	0.70
1:A:1507:C:C4	1:A:1508:A:N6	2.60	0.70
1:A:273:G:C8	1:A:365:U:C4	2.80	0.70
58:z:23:GLY:N	63:z:402:GTP:O1A	2.25	0.70
1:A:2297:A:C6	1:A:2321:U:O4	2.46	0.69
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.26	0.69
34:a:182:A:N3	34:a:184:G:C6	2.61	0.69
1:A:286:U:C2	1:A:354:A:N6	2.60	0.69
1:A:709:U:O4	1:A:722:A:N1	2.25	0.69
1:A:278:A:C6	1:A:361:G:H8	2.11	0.69
39:f:38:ARG:HD2	39:f:63:ASN:ND2	2.08	0.69
34:a:404:G:N3	34:a:498:A:H2	1.91	0.68
39:f:38:ARG:HG3	39:f:63:ASN:CB	2.19	0.68
1:A:288:U:O4	1:A:352:A:N6	2.27	0.68
1:A:1050:A:C6	1:A:2751:G:C5	2.82	0.68
34:a:417:G:C2'	34:a:418:C:H5'	2.22	0.68
34:a:193:C:H2'	34:a:194:C:C6	2.29	0.67
55:w:17:C:C6	55:w:117:U:H5	2.11	0.67
1:A:283:G:C8	1:A:358:U:C4	2.83	0.67
34:a:848:C:H6	34:a:848:C:O5'	1.78	0.67
34:a:454:G:O6	34:a:478:A:N1	2.27	0.67
1:A:1021:A:C2	1:A:1141:U:O4	2.46	0.67
1:A:2298:A:C4	1:A:2321:U:C5	2.83	0.67
34:a:380:G:C2	34:a:384:G:O6	2.48	0.67
1:A:1537:G:N1	1:A:1538:G:N3	2.43	0.66
1:A:2297:A:N1	1:A:2321:U:O4	2.28	0.66
34:a:601:G:C2'	34:a:602:A:H5'	2.24	0.66
1:A:278:A:C2	1:A:279:A:N7	2.64	0.66
1:A:924:G:H2'	1:A:925:A:H5'	1.77	0.66
1:A:2856:A:H2'	1:A:2857:G:H5'	1.76	0.66
1:A:288:U:C4	1:A:352:A:N1	2.63	0.66
1:A:2292:U:C2'	1:A:2293:G:H5'	2.25	0.66
1:A:2030:6MZ:O2'	1:A:2031:A:OP2	2.13	0.66
1:A:2471:A:C2	1:A:2479:U:N3	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:A:C2	1:A:359:G:C2	2.84	0.66
5:E:46:GLN:HB3	5:E:83:VAL:HG11	1.78	0.65
1:A:272:A:N1	1:A:365:U:C4	2.64	0.65
1:A:276:U:H2'	1:A:361:G:O6	1.96	0.65
34:a:31:G:C2	34:a:306:A:O2'	2.49	0.65
34:a:382:A:C5	34:a:383:A:C2	2.85	0.65
34:a:446:G:O6	34:a:488:C:N3	2.29	0.65
34:a:131:A:N1	34:a:230:G:O6	2.29	0.65
1:A:710:U:C2	1:A:711:G:C8	2.84	0.65
1:A:1105:U:C5	1:A:1106:G:C8	2.58	0.65
1:A:219:A:N3	1:A:234:U:O2'	2.30	0.64
1:A:278:A:N7	1:A:362:A:N3	2.44	0.64
1:A:362:A:N7	1:A:363:G:C6	2.64	0.64
1:A:2030:6MZ:OP2	1:A:2031:A:H8	1.80	0.64
34:a:922:G:O2'	34:a:1398:A:N1	2.29	0.64
34:a:64:G:N2	34:a:69:G:N7	2.46	0.64
41:h:10:LEU:HD22	41:h:74:ILE:HD11	1.79	0.64
1:A:221:A:N7	1:A:427:U:H5	1.96	0.64
1:A:1607:C:N4	1:A:1622:G:OP2	2.29	0.64
34:a:454:G:C6	34:a:478:A:N1	2.66	0.64
1:A:543:G:H3'	1:A:544:C:H5"	1.80	0.64
1:A:1050:A:N7	1:A:1051:G:N7	2.46	0.64
39:f:38:ARG:CG	39:f:63:ASN:CB	2.70	0.63
3:C:121:ALA:HB3	3:C:129:LEU:HD21	1.80	0.63
1:A:1068:G:H1	1:A:1095:A:H2'	1.64	0.63
1:A:1109:C:H41	1:A:1110:G:H21	1.46	0.63
1:A:550:C:N4	1:A:551:G:C6	2.67	0.63
1:A:1739:A:H2'	1:A:1740:G:O4'	1.99	0.63
34:a:182:A:N1	34:a:185:U:C4	2.59	0.63
1:A:1297:C:OP1	1:A:2710:C:H4'	1.99	0.62
7:G:32:LEU:HB3	7:G:74:MET:HE3	1.81	0.62
1:A:272:A:C2	1:A:366:C:C2	2.87	0.62
1:A:2020:A:N7	27:0:5:ASN:ND2	2.46	0.62
38:e:106:ALA:HB2	38:e:124:ALA:HB3	1.80	0.62
1:A:2472:G:N1	1:A:2475:C:H2'	2.14	0.62
1:A:363:G:H2'	1:A:364:C:O4'	1.99	0.62
1:A:2030:6MZ:OP2	1:A:2030:6MZ:H4'	1.98	0.62
34:a:404:G:C2	34:a:498:A:C2	2.87	0.62
34:a:632:U:C5'	34:a:633:G:H5"	2.30	0.62
1:A:2030:6MZ:HA	1:A:2031:A:P	2.23	0.62
1:A:290:U:O2'	1:A:291:G:O5'	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:137:U:C2	34:a:226:G:O6	2.52	0.62
1:A:517:C:OP1	27:0:12:ARG:NH2	2.32	0.62
1:A:1054:A:N3	1:A:1106:G:C2	2.68	0.62
1:A:900:A:C2	1:A:901:C:O4'	2.53	0.61
39:f:38:ARG:CD	39:f:63:ASN:CB	2.77	0.61
55:w:17:C:H5	55:w:117:U:C4	2.18	0.61
1:A:278:A:N1	1:A:279:A:N7	2.48	0.61
34:a:456:A:C2	34:a:477:C:C2	2.88	0.61
34:a:203:G:N2	34:a:204:G:O6	2.32	0.61
34:a:377:G:N1	34:a:387:U:O2	2.34	0.61
1:A:1021:A:N1	1:A:1141:U:C4	2.63	0.61
1:A:2627:G:O2'	1:A:2781:A:N1	2.30	0.61
1:A:1328:A:H2'	1:A:1330:C:C5	2.36	0.61
1:A:900:A:H2'	1:A:900:A:N3	2.15	0.61
3:C:79:ARG:NH1	3:C:81:GLU:OE2	2.34	0.61
34:a:132:C:N3	34:a:230:G:O6	2.33	0.60
1:A:287:G:C6	1:A:288:U:C5	2.89	0.60
1:A:1005:C:O2'	10:J:30:THR:HG21	2.02	0.60
34:a:827:U:C4	34:a:872:A:N1	2.67	0.60
1:A:133:U:H2'	1:A:134:G:O4'	2.02	0.60
1:A:1936:A:H2	1:A:1943:U:H3	1.49	0.60
34:a:2:A:N3	34:a:613:C:O2'	2.27	0.60
34:a:141:G:O2'	34:a:142:G:O4'	2.19	0.60
1:A:585:G:N7	17:Q:5:ARG:NH1	2.49	0.60
34:a:827:U:N3	34:a:872:A:N6	2.45	0.60
34:a:1240:U:O4	40:g:108:ARG:NH1	2.35	0.60
1:A:288:U:O4	1:A:352:A:N1	2.35	0.60
1:A:1539:U:H2'	1:A:1540:G:C8	2.36	0.60
1:A:2328:A:H2'	1:A:2329:U:C6	2.37	0.60
1:A:1140:C:O2	1:A:1140:C:O5'	2.20	0.60
1:A:1538:G:H2'	1:A:1539:U:O4'	2.02	0.60
1:A:1867:G:O6	1:A:1874:C:C4	2.55	0.60
34:a:141:G:N3	34:a:141:G:H2'	2.17	0.60
1:A:1721:G:O2'	1:A:1739:A:N6	2.35	0.59
34:a:264:C:O2	34:a:264:C:O4'	2.20	0.59
57:y:29:G:N2	57:y:41:C:N3	2.50	0.59
34:a:473:U:C2	34:a:474:G:C8	2.90	0.59
1:A:314:C:H2'	1:A:315:G:H5'	1.85	0.59
34:a:512:U:H2'	34:a:513:C:C5'	2.32	0.59
34:a:839:C:N3	34:a:847:G:O6	2.34	0.59
1:A:1054:A:H2'	1:A:1106:G:N2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:LEU:HD21	6:F:129:MET:HE1	1.84	0.59
34:a:605:U:C2	34:a:633:G:O6	2.56	0.59
1:A:900:A:C2	1:A:901:C:C1'	2.85	0.59
1:A:1779:U:H5	1:A:1784:A:N7	2.01	0.59
57:y:18:G:O2'	57:y:57:G:N2	2.36	0.59
2:B:105:G:H2'	2:B:106:G:H5'	1.84	0.59
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.68	0.59
1:A:639:U:H2'	1:A:640:C:C6	2.38	0.59
1:A:1054:A:C5	1:A:1106:G:C6	2.90	0.59
34:a:708:C:H2'	34:a:709:U:H5'	1.84	0.59
1:A:710:U:H2'	1:A:711:G:H5"	1.84	0.59
34:a:160:A:H1'	34:a:344:A:N7	2.18	0.58
1:A:2029:G:O5'	1:A:2029:G:H8	1.85	0.58
1:A:283:G:O6	1:A:357:C:O2	2.22	0.58
34:a:455:G:N2	34:a:477:C:N3	2.50	0.58
1:A:80:G:C2'	1:A:81:G:H5'	2.34	0.58
6:F:10:GLU:O	6:F:12:VAL:N	2.36	0.58
34:a:827:U:H3	34:a:872:A:H61	1.43	0.58
1:A:2101:A:N6	1:A:2188:U:C4	2.72	0.58
34:a:73:C:H2'	34:a:74:A:C8	2.39	0.58
1:A:1039:A:N1	1:A:1116:G:O6	2.36	0.58
1:A:528:A:C2	1:A:2043:C:H4'	2.39	0.58
1:A:2472:G:O6	1:A:2475:C:H3'	2.04	0.58
1:A:2474:U:H3'	1:A:2475:C:H5	1.68	0.58
34:a:404:G:N3	34:a:498:A:C2	2.71	0.58
52:s:10:ILE:HD12	52:s:40:PHE:CD2	2.38	0.58
1:A:1617:C:P	1:A:1617:C:H3'	2.44	0.58
1:A:1754:A:N1	1:A:2716:C:O2'	2.34	0.58
36:c:63:ILE:HD13	36:c:94:ALA:HB1	1.85	0.58
43:j:57:VAL:HG12	43:j:58:ASN:H	1.68	0.58
1:A:709:U:H2'	1:A:710:U:O4'	2.03	0.57
34:a:69:G:C2	34:a:100:G:O6	2.56	0.57
54:u:9:GLU:HB2	54:u:10:PRO:CD	2.34	0.57
1:A:138:U:O2	1:A:138:U:H2'	2.03	0.57
1:A:1024:G:H1	1:A:1140:C:H5	1.52	0.57
1:A:2472:G:O2'	1:A:2529:G:N2	2.37	0.57
1:A:1140:C:O2	1:A:1140:C:O4'	2.22	0.57
34:a:633:G:H2'	34:a:634:C:C6	2.39	0.57
1:A:272:A:C6	1:A:365:U:O4	2.56	0.57
1:A:713:G:N2	1:A:719:C:C2	2.72	0.57
1:A:1036:G:O6	1:A:1119:U:C2	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:155:A:C2	34:a:167:A:C6	2.92	0.57
34:a:512:U:H2'	34:a:513:C:H5'	1.87	0.57
34:a:137:U:O2	34:a:226:G:C6	2.57	0.57
63:z:402:GTP:H8	63:z:402:GTP:C5'	1.99	0.57
1:A:287:G:N7	1:A:354:A:C6	2.73	0.57
1:A:1109:C:N4	1:A:1110:G:H21	2.03	0.57
1:A:900:A:H2	1:A:901:C:O4'	1.86	0.57
1:A:2013:A:N1	1:A:2613:U:C4	2.68	0.57
34:a:179:A:H2'	34:a:180:U:O4'	2.04	0.57
34:a:382:A:C8	34:a:383:A:C2	2.93	0.57
1:A:321:U:C2	5:E:159:LEU:HD21	2.40	0.57
1:A:710:U:N3	1:A:711:G:N7	2.52	0.57
1:A:1021:A:H3'	1:A:1022:G:H5"	1.85	0.57
1:A:1170:C:H2'	1:A:1171:G:C8	2.40	0.57
34:a:69:G:N2	34:a:71:A:C6	2.73	0.57
34:a:417:G:O6	34:a:426:U:O2	2.22	0.57
39:f:29:ILE:HG21	39:f:64:VAL:HG21	1.86	0.57
58:z:82:PRO:O	63:z:402:GTP:O3G	2.23	0.56
1:A:1482:G:H2'	1:A:1483:G:H5'	1.87	0.56
3:C:69:ASN:O	3:C:70:LYS:C	2.47	0.56
34:a:382:A:C4	34:a:383:A:C2	2.93	0.56
1:A:1483:G:N3	1:A:1484:U:C6	2.73	0.56
34:a:602:A:N1	34:a:636:U:C2	2.74	0.56
40:g:85:GLN:HB2	40:g:147:ASN:HD22	1.71	0.56
1:A:553:G:H2'	1:A:554:U:O4'	2.05	0.56
1:A:2698:U:H2'	1:A:2699:C:C6	2.41	0.56
34:a:936:C:N3	34:a:1379:G:C6	2.73	0.56
58:z:220:ILE:HD12	58:z:226:VAL:HG21	1.87	0.56
1:A:1483:G:O2'	1:A:1484:U:H6	1.89	0.56
9:I:27:LEU:HD21	9:I:37:PHE:CG	2.40	0.56
1:A:2297:A:C2	1:A:2321:U:C5	2.94	0.56
1:A:1054:A:C8	1:A:1107:G:C2	2.93	0.56
1:A:2030:6MZ:OP2	1:A:2031:A:C8	2.58	0.56
34:a:382:A:C8	34:a:383:A:N3	2.74	0.56
1:A:572:A:OP2	18:R:80:ARG:NH2	2.37	0.56
1:A:1047:G:C2'	1:A:1110:G:N2	2.69	0.56
1:A:1033:U:O2	1:A:2750:A:C6	2.59	0.56
1:A:2298:A:C4	1:A:2321:U:C4	2.94	0.56
1:A:1036:G:O6	1:A:1119:U:O2	2.23	0.55
1:A:708:G:O6	1:A:722:A:C6	2.60	0.55
34:a:417:G:C3'	34:a:418:C:H5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:472:U:H2'	34:a:473:U:C6	2.42	0.55
1:A:413:C:HO2'	1:A:1880:U:HO2'	1.50	0.55
1:A:1450:G:N2	1:A:1452:G:O6	2.37	0.55
34:a:946:A:H2'	34:a:947:G:C8	2.41	0.55
1:A:272:A:C2	1:A:366:C:N3	2.75	0.55
1:A:1021:A:N3	1:A:1022:G:H5"	2.21	0.55
1:A:2471:A:C2	1:A:2478:A:N6	2.74	0.55
1:A:285:G:H2'	1:A:286:U:O4'	2.07	0.55
1:A:1472:C:C2	1:A:1519:G:O6	2.58	0.55
1:A:1932:A:H2'	1:A:1933:G:O4'	2.06	0.55
34:a:602:A:H2'	34:a:603:U:C6	2.42	0.55
1:A:1051:G:O6	1:A:1109:C:O2	2.24	0.55
34:a:62:U:O2'	34:a:379:C:O2'	2.13	0.55
34:a:182:A:C6	34:a:185:U:O4	2.51	0.55
34:a:632:U:C3'	34:a:633:G:H5"	2.36	0.55
1:A:710:U:N3	1:A:711:G:C8	2.75	0.55
1:A:1795:C:H2'	1:A:1796:U:O4'	2.06	0.55
15:O:51:ALA:HB3	15:O:78:VAL:HG22	1.89	0.55
1:A:362:A:H2'	1:A:363:G:O4'	2.07	0.55
1:A:861:A:N3	2:B:79:G:O2'	2.36	0.55
1:A:1528:A:N6	1:A:1543:G:O2'	2.40	0.55
34:a:138:G:O6	34:a:225:C:N3	2.40	0.55
38:e:110:MET:HE2	38:e:124:ALA:HB1	1.89	0.55
39:f:26:THR:HG22	39:f:36:ILE:CD1	2.37	0.55
1:A:2273:A:H2'	1:A:2274:A:C8	2.42	0.55
11:K:19:VAL:HB	11:K:41:ILE:HG23	1.88	0.55
34:a:141:G:O2'	34:a:142:G:O5'	2.25	0.55
1:A:2287:A:N1	1:A:2346:A:N7	2.55	0.54
34:a:876:C:H1'	41:h:11:THR:HG21	1.88	0.54
57:y:29:G:N2	57:y:41:C:C2	2.75	0.54
1:A:528:A:C2	1:A:2042:A:H2'	2.43	0.54
34:a:602:A:N1	34:a:636:U:O2	2.40	0.54
51:r:10:CYS:SG	51:r:11:ARG:N	2.73	0.54
55:w:17:C:H5'	55:w:117:U:H5"	1.89	0.54
1:A:1182:G:H2'	1:A:1183:U:O4'	2.08	0.54
1:A:2472:G:C2	1:A:2475:C:C2	2.95	0.54
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.89	0.54
34:a:42:G:C2	34:a:622:A:N3	2.75	0.54
1:A:1068:G:C2	1:A:1096:A:O4'	2.60	0.54
1:A:2788:C:H2'	1:A:2789:C:C6	2.42	0.54
1:A:2856:A:C2'	1:A:2857:G:H5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:MET:HE1	3:C:183:VAL:HG21	1.88	0.54
46:m:3:ILE:HD11	46:m:18:LEU:HD22	1.90	0.54
1:A:160:A:N3	1:A:2208:C:O2'	2.39	0.54
1:A:360:U:O2'	1:A:361:G:O5'	2.17	0.54
1:A:1923:U:H2'	1:A:1924:C:C6	2.43	0.54
1:A:1139:G:H2'	1:A:1140:C:O2	2.08	0.54
34:a:491:G:H2'	34:a:492:C:H5'	1.89	0.54
36:c:174:LEU:HD12	36:c:181:ILE:HD13	1.89	0.54
1:A:283:G:O6	1:A:357:C:C1'	2.53	0.54
1:A:2013:A:C2	1:A:2613:U:O4	2.60	0.54
2:B:75:G:H2'	2:B:76:G:O4'	2.07	0.54
29:2:12:ARG:NE	29:2:44:VAL:HG21	2.22	0.54
34:a:454:G:O6	34:a:478:A:C6	2.61	0.54
34:a:455:G:C2	34:a:478:A:C2	2.96	0.54
1:A:85:G:O6	1:A:98:G:C6	2.61	0.54
1:A:1421:G:N2	1:A:1495:A:N1	2.56	0.54
3:C:5:CYS:SG	3:C:12:ARG:NH1	2.80	0.54
1:A:710:U:C4	1:A:711:G:N7	2.76	0.53
1:A:1014:A:H2'	1:A:1015:U:O4'	2.08	0.53
1:A:1077:A:H5'	9:I:93:ASN:HB2	1.90	0.53
4:D:80:TRP:CD1	4:D:202:ILE:HD11	2.43	0.53
34:a:156:C:H2'	34:a:157:U:O4'	2.08	0.53
34:a:270:A:C6	34:a:271:C:C4	2.96	0.53
38:e:80:LEU:HD22	38:e:146:MET:HE2	1.90	0.53
41:h:77:VAL:HG11	41:h:124:ILE:HD12	1.88	0.53
34:a:447:G:O2'	34:a:487:A:N6	2.42	0.53
34:a:513:C:N3	34:a:538:G:N2	2.55	0.53
1:A:12:U:H2'	1:A:12:U:O2	2.07	0.53
1:A:465:G:H2'	1:A:466:A:C8	2.43	0.53
2:B:101:A:H2'	2:B:102:G:O4'	2.09	0.53
9:I:17:ALA:HB2	9:I:42:ASN:HD21	1.72	0.53
34:a:455:G:N1	34:a:477:C:N4	2.56	0.53
34:a:591:U:C2	34:a:648:A:N6	2.77	0.53
1:A:277:G:N1	1:A:360:U:O2'	2.37	0.53
1:A:1913:A:N1	34:a:1493:A:H2'	2.23	0.53
1:A:2298:A:C5	1:A:2321:U:C4	2.96	0.53
1:A:221:A:N7	1:A:427:U:C5	2.74	0.53
1:A:1054:A:N1	1:A:1106:G:H2'	2.24	0.53
1:A:2074:U:H2'	1:A:2075:U:C6	2.44	0.53
1:A:1068:G:N1	1:A:1095:A:H2'	2.23	0.53
34:a:1476:A:H2'	34:a:1477:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2898:U:O2'	10:J:134:ALA:O	2.26	0.53
1:A:1487:U:H2'	1:A:1488:C:O4'	2.09	0.53
19:S:5:ALA:HB3	19:S:54:ALA:HB2	1.90	0.53
55:w:17:C:C6	55:w:117:U:C5	2.94	0.53
1:A:2514:U:H2'	1:A:2515:C:C6	2.44	0.52
39:f:29:ILE:HG21	39:f:64:VAL:CG2	2.39	0.52
42:i:83:THR:HG21	42:i:102:PHE:HB3	1.91	0.52
1:A:848:C:H2'	1:A:849:A:C8	2.44	0.52
34:a:185:U:O4	34:a:192:A:N1	2.42	0.52
34:a:384:G:O2'	34:a:385:C:O4'	2.15	0.52
34:a:1486:G:H2'	34:a:1487:G:O4'	2.10	0.52
6:F:24:VAL:O	6:F:27:VAL:HG12	2.09	0.52
34:a:390:U:O2'	49:p:28:ARG:NH2	2.42	0.52
1:A:1050:A:C5	1:A:2751:G:C5	2.97	0.52
40:g:78:ARG:HG2	40:g:83:THR:HG22	1.91	0.52
1:A:1926:U:O2'	1:A:1928:A:N7	2.40	0.52
34:a:132:C:O2	34:a:230:G:N1	2.42	0.52
34:a:378:G:O6	34:a:385:C:N4	2.42	0.52
34:a:708:C:C2'	34:a:709:U:H5'	2.40	0.52
1:A:1129:A:N1	1:A:2569:G:O2'	2.41	0.52
1:A:2812:G:H2'	1:A:2813:A:C8	2.45	0.52
6:F:91:ARG:HA	6:F:95:MET:HB2	1.91	0.52
1:A:1076:C:H2'	1:A:1076:C:O2	2.10	0.52
1:A:2291:U:O2'	1:A:2374:C:O2'	2.11	0.52
19:S:24:ILE:HD11	19:S:36:LEU:HG	1.92	0.52
1:A:1809:A:H2'	1:A:1810:A:C8	2.45	0.52
34:a:36:C:H2'	34:a:37:U:O4'	2.10	0.52
34:a:602:A:N6	34:a:636:U:N3	2.58	0.52
52:s:10:ILE:HD12	52:s:40:PHE:CE2	2.45	0.52
1:A:629:G:H5"	1:A:650:C:O2'	2.10	0.52
34:a:263:A:C2'	34:a:264:C:O2	2.58	0.52
34:a:69:G:H2'	34:a:69:G:N3	2.24	0.51
34:a:459:A:H2'	34:a:460:A:O4'	2.10	0.51
34:a:491:G:H2'	34:a:492:C:C5'	2.40	0.51
1:A:2346:A:H3'	1:A:2347:C:C5'	2.39	0.51
1:A:1052:C:C2	1:A:1107:G:N1	2.77	0.51
1:A:2327:A:H2'	1:A:2328:A:C8	2.46	0.51
13:M:105:MET:HG3	13:M:117:PHE:CZ	2.45	0.51
34:a:849:G:O6	64:a:2001:HOH:O	2.19	0.51
1:A:358:U:C4	1:A:359:G:H1'	2.46	0.51
1:A:987:C:O2'	1:A:1000:A:N3	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:THR:HG23	3:C:176:ARG:HG3	1.92	0.51
34:a:137:U:O2	34:a:226:G:O6	2.29	0.51
51:r:31:TYR:HB3	51:r:54:LEU:HD21	1.93	0.51
1:A:363:G:C6	1:A:364:C:C4	2.99	0.51
1:A:2470:G:C5	1:A:2481:G:N2	2.79	0.51
34:a:415:A:N7	34:a:428:G:O6	2.43	0.51
1:A:709:U:C4	1:A:710:U:C4	2.98	0.51
34:a:827:U:O4	34:a:872:A:C2	2.60	0.51
50:q:22:VAL:HG11	50:q:60:ILE:HD11	1.93	0.51
1:A:273:G:N7	1:A:364:C:C4	2.78	0.51
34:a:257:G:C6	34:a:258:G:C5	2.99	0.51
38:e:93:VAL:HG13	38:e:110:MET:HE3	1.93	0.51
1:A:289:G:C6	1:A:351:C:N3	2.79	0.51
34:a:42:G:N3	34:a:622:A:H2	2.04	0.51
34:a:632:U:H3'	34:a:633:G:H5"	1.93	0.51
2:B:54:G:H2'	2:B:55:U:O4'	2.11	0.51
34:a:488:C:H2'	34:a:489:C:C6	2.46	0.51
1:A:1135:C:H3'	1:A:1136:G:H5'	1.93	0.50
1:A:1483:G:N1	1:A:1507:C:N3	2.58	0.50
17:Q:35:PHE:CZ	17:Q:39:ILE:HD11	2.45	0.50
34:a:626:G:OP1	49:p:18:GLN:NE2	2.44	0.50
1:A:270:A:N6	1:A:369:U:O2'	2.39	0.50
1:A:273:G:N7	1:A:364:C:N4	2.59	0.50
1:A:1533:C:O2	1:A:1538:G:N2	2.44	0.50
34:a:976:G:C8	34:a:1358:U:O2	2.64	0.50
1:A:541:A:H2'	1:A:542:U:O4'	2.12	0.50
1:A:940:G:H5"	1:A:941:A:OP2	2.12	0.50
34:a:1434:A:H2'	34:a:1435:G:O4'	2.11	0.50
58:z:26:THR:OG1	63:z:402:GTP:C5'	2.59	0.50
1:A:2101:A:N6	1:A:2188:U:N3	2.59	0.50
34:a:72:A:C6	34:a:73:C:C6	2.99	0.50
34:a:1448:C:O2	34:a:1448:C:H2'	2.12	0.50
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.94	0.50
63:z:402:GTP:C8	63:z:402:GTP:C5'	2.86	0.50
1:A:804:A:H2'	1:A:806:C:C4	2.46	0.50
1:A:948:C:O2	1:A:984:A:O2'	2.28	0.50
1:A:2013:A:H61	1:A:2613:U:H3	1.57	0.50
39:f:38:ARG:HD2	39:f:63:ASN:CG	2.35	0.50
1:A:1394:U:H4'	1:A:1603:A:H4'	1.93	0.50
1:A:1430:G:H2'	1:A:1431:A:O4'	2.12	0.50
1:A:547:A:H3'	1:A:547:A:N3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:G:C6	1:A:712:G:C5	2.99	0.50
1:A:2520:C:C6	1:A:2567:G:H1'	2.47	0.50
34:a:382:A:C5	34:a:383:A:N1	2.80	0.50
34:a:6:G:O6	38:e:99:SER:N	2.45	0.50
1:A:1482:G:O2'	1:A:1509:A:N1	2.38	0.49
32:5:87:GLU:HG2	32:5:95:LEU:HD12	1.93	0.49
34:a:197:A:N1	34:a:220:G:O2'	2.44	0.49
34:a:1258:G:H2'	34:a:1259:C:C6	2.47	0.49
1:A:272:A:C2	1:A:365:U:C4	2.99	0.49
1:A:573:U:O4	1:A:2029:G:O2'	2.30	0.49
34:a:1457:G:H2'	34:a:1458:G:O4'	2.13	0.49
1:A:709:U:O4	1:A:722:A:C6	2.65	0.49
8:H:90:LEU:CD2	8:H:94:ILE:HD11	2.42	0.49
34:a:17:U:H2'	34:a:18:C:C6	2.46	0.49
34:a:75:G:N2	34:a:96:U:C4	2.79	0.49
39:f:38:ARG:CD	39:f:63:ASN:HB3	2.39	0.49
58:z:175:LEU:HD12	63:z:402:GTP:C2	2.47	0.49
1:A:1047:G:H2'	1:A:1110:G:C2	2.46	0.49
1:A:1090:A:H61	1:A:1101:U:H3	1.61	0.49
34:a:501:C:O2'	34:a:502:A:OP2	2.23	0.49
36:c:174:LEU:HD11	36:c:200:TRP:CD1	2.47	0.49
49:p:21:VAL:HG21	49:p:60:TRP:CD1	2.47	0.49
1:A:1032:A:H1'	31:4:23:ILE:HD13	1.94	0.49
34:a:692:U:O2'	34:a:694:A:N7	2.39	0.49
45:l:79:ILE:HD12	45:l:96:THR:HG22	1.94	0.49
57:y:27:G:N2	57:y:28:G:H1'	2.28	0.49
1:A:242:G:O2'	1:A:254:G:O6	2.29	0.49
2:B:22:U:H2'	2:B:23:G:H5'	1.94	0.49
34:a:1235:U:H2'	34:a:1236:A:O4'	2.13	0.49
34:a:1305:G:O2'	34:a:1306:A:OP2	2.25	0.49
1:A:2474:U:H3'	1:A:2475:C:C6	2.46	0.49
3:C:90:ILE:HD12	3:C:102:TYR:CD1	2.48	0.49
58:z:98:MET:HE3	58:z:101:ALA:HB2	1.95	0.49
34:a:141:G:C6	34:a:223:A:C6	3.01	0.49
36:c:148:ILE:O	36:c:148:ILE:HG23	2.13	0.49
1:A:724:U:H2'	1:A:725:G:C8	2.47	0.49
1:A:1076:C:N4	9:I:89:SER:OG	2.45	0.49
1:A:1171:G:C8	1:A:1172:C:H1'	2.48	0.49
1:A:1361:G:H2'	1:A:1362:C:C6	2.48	0.49
1:A:2474:U:H2'	1:A:2474:U:O2	2.11	0.49
34:a:299:G:H2'	34:a:300:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:C:O2'	1:A:346:A:N3	2.43	0.49
1:A:570:G:H2'	1:A:2030:6MZ:N7	2.28	0.49
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.94	0.49
14:N:96:ARG:NH1	14:N:116:VAL:HG13	2.28	0.49
25:Y:2:LYS:HD2	25:Y:56:LEU:HD11	1.94	0.49
34:a:138:G:H2'	34:a:139:A:O4'	2.13	0.49
34:a:529:G:O6	45:l:45:ASN:HA	2.13	0.49
34:a:2:A:C2	34:a:614:C:O4'	2.66	0.48
34:a:479:U:H2'	34:a:480:U:H5'	1.94	0.48
34:a:620:C:H2'	34:a:621:A:O4'	2.13	0.48
34:a:1356:G:H2'	34:a:1357:A:C8	2.48	0.48
36:c:39:ARG:NH1	36:c:54:ILE:O	2.47	0.48
1:A:272:A:C2	1:A:365:U:O4	2.65	0.48
1:A:1327:A:N6	1:A:1328:A:C2	2.81	0.48
34:a:69:G:N2	34:a:100:G:C6	2.80	0.48
34:a:144:G:O6	34:a:178:C:N3	2.46	0.48
34:a:575:G:O2'	34:a:821:G:H5'	2.12	0.48
34:a:440:C:N3	34:a:497:G:O6	2.47	0.48
34:a:1218:C:H2'	34:a:1219:A:C8	2.49	0.48
1:A:1726:G:H2'	1:A:1727:A:O4'	2.13	0.48
2:B:106:G:H2'	2:B:107:G:O4'	2.13	0.48
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.94	0.48
15:O:51:ALA:HB3	15:O:78:VAL:CG2	2.43	0.48
34:a:1448:C:N4	34:a:1456:A:N1	2.62	0.48
1:A:900:A:C2	1:A:901:C:N1	2.81	0.48
34:a:411:A:OP2	37:d:30:LYS:NZ	2.42	0.48
34:a:945:G:C2	34:a:946:A:C8	3.02	0.48
1:A:2585:U:O2	1:A:2585:U:O4'	2.32	0.48
34:a:64:G:C2	34:a:67:C:N4	2.81	0.48
34:a:594:U:O2	34:a:646:G:C2	2.66	0.48
1:A:2471:A:H2'	1:A:2472:G:C4'	2.43	0.48
1:A:2472:G:C6	1:A:2475:C:C6	3.01	0.48
1:A:1050:A:N7	1:A:1051:G:C8	2.77	0.48
1:A:2627:G:N2	1:A:2777:G:OP2	2.47	0.48
2:B:105:G:C2'	2:B:106:G:H5'	2.44	0.48
58:z:25:THR:CB	63:z:402:GTP:O1B	2.58	0.48
1:A:1054:A:N1	1:A:1106:G:O2'	2.41	0.48
17:Q:93:ILE:HD13	18:R:4:VAL:HG13	1.96	0.48
34:a:541:G:H2'	34:a:542:G:O4'	2.13	0.48
47:n:93:ILE:HG21	47:n:96:LEU:HD22	1.96	0.48
1:A:2615:U:C2	27:0:3:GLN:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:63:ILE:HG12	13:M:105:MET:HE3	1.95	0.48
34:a:141:G:N3	34:a:141:G:C2'	2.76	0.48
1:A:267:C:N3	1:A:425:G:O6	2.47	0.47
1:A:1055:G:C8	1:A:1106:G:N1	2.81	0.47
1:A:1533:C:O2	1:A:1538:G:C2	2.66	0.47
1:A:2472:G:C6	1:A:2475:C:H2'	2.48	0.47
34:a:211:G:N3	34:a:211:G:H2'	2.29	0.47
34:a:511:C:O2'	37:d:40:HIS:CE1	2.67	0.47
1:A:1050:A:N6	1:A:2751:G:C5	2.81	0.47
1:A:274:C:H2'	1:A:275:C:O4'	2.13	0.47
1:A:1086:A:H2'	1:A:1086:A:N3	2.29	0.47
1:A:1102:C:H2'	1:A:1103:A:O4'	2.14	0.47
1:A:2297:A:C2	1:A:2321:U:C4	3.02	0.47
34:a:481:G:O2'	34:a:483:C:N4	2.47	0.47
34:a:1064:G:O2'	34:a:1190:G:N2	2.47	0.47
23:W:55:LEU:HD12	23:W:76:ILE:HD12	1.97	0.47
34:a:946:A:O2'	34:a:1333:A:N3	2.46	0.47
1:A:1141:U:OP2	10:J:24:THR:HG21	2.14	0.47
1:A:1484:U:H2'	1:A:1485:U:H6	1.76	0.47
34:a:149:A:H2'	34:a:150:U:C6	2.48	0.47
34:a:386:C:H3'	34:a:387:U:C5'	2.45	0.47
34:a:456:A:H2'	34:a:457:G:C1'	2.45	0.47
40:g:85:GLN:CB	40:g:147:ASN:HD22	2.26	0.47
1:A:351:C:N4	1:A:352:A:N6	2.63	0.47
1:A:924:G:C2'	1:A:925:A:H5'	2.44	0.47
1:A:1052:C:N3	1:A:1107:G:C6	2.81	0.47
1:A:2101:A:C6	1:A:2188:U:N3	2.82	0.47
1:A:2686:G:H2'	1:A:2687:U:O4'	2.15	0.47
1:A:1832:C:N4	1:A:1833:C:C4	2.83	0.47
1:A:2472:G:C6	1:A:2475:C:N1	2.83	0.47
34:a:141:G:C8	34:a:223:A:C2	3.02	0.47
34:a:142:G:N2	34:a:222:C:C1'	2.77	0.47
1:A:1479:G:HO2'	1:A:1560:G:HO2'	1.53	0.47
34:a:369:G:C6	34:a:370:C:C4	3.03	0.47
10:J:35:ARG:HB2	10:J:54:ILE:HD11	1.96	0.47
54:u:28:LEU:HD13	54:u:29:ALA:N	2.30	0.47
1:A:861:A:H2'	1:A:862:G:O4'	2.15	0.47
1:A:1508:A:H4'	1:A:1509:A:OP1	2.15	0.47
34:a:94:G:H4'	34:a:95:C:O5'	2.15	0.47
34:a:1449:C:C2	34:a:1455:G:C2	3.03	0.47
38:e:93:VAL:HG13	38:e:110:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:G:HO2'	1:A:295:G:HO2'	1.62	0.46
1:A:1052:C:O2	1:A:1107:G:C2	2.68	0.46
1:A:1469:A:H2'	1:A:1470:A:C8	2.50	0.46
34:a:195:A:H2'	34:a:196:A:C8	2.50	0.46
34:a:512:U:H2'	34:a:513:C:H5"	1.97	0.46
34:a:513:C:N4	34:a:538:G:N1	2.63	0.46
34:a:648:A:N6	34:a:649:A:C2	2.83	0.46
55:v:18:G:C6	55:v:57:A:N6	2.83	0.46
1:A:287:G:N7	1:A:354:A:N6	2.63	0.46
1:A:586:A:N1	1:A:809:G:O2'	2.45	0.46
1:A:1067:A:H1'	57:y:56:C:C1'	2.46	0.46
34:a:694:A:O2'	55:w:38:A:O2'	2.33	0.46
1:A:1533:C:C2	1:A:1538:G:N2	2.84	0.46
1:A:1799:G:N2	1:A:1818:U:O2'	2.49	0.46
2:B:4:C:H2'	2:B:5:U:O4'	2.16	0.46
22:V:2:PHE:HA	22:V:50:MET:HE1	1.96	0.46
34:a:784:A:H2'	34:a:785:G:C8	2.51	0.46
1:A:1021:A:H3'	1:A:1021:A:N3	2.30	0.46
11:K:24:VAL:HG13	11:K:33:ALA:HB2	1.96	0.46
34:a:109:A:C6	34:a:326:G:C6	3.03	0.46
34:a:141:G:N1	34:a:222:C:O2	2.44	0.46
34:a:807:A:H2'	34:a:808:C:O4'	2.16	0.46
1:A:864:G:O2'	1:A:914:G:O6	2.29	0.46
1:A:1570:A:H2'	1:A:1571:A:C8	2.51	0.46
1:A:1599:U:H2'	1:A:1600:C:C6	2.51	0.46
4:D:4:LEU:HD13	4:D:101:PHE:CE2	2.51	0.46
7:G:104:LEU:HD13	7:G:106:LEU:HD11	1.97	0.46
34:a:126:G:OP1	34:a:605:U:O2'	2.33	0.46
34:a:141:G:C5	34:a:223:A:C2	3.03	0.46
34:a:514:C:C4	34:a:515:G:N7	2.84	0.46
1:A:181:A:C2	1:A:182:A:C4	3.03	0.46
1:A:1050:A:C8	1:A:1051:G:N7	2.77	0.46
34:a:74:A:C2	34:a:97:G:C2	3.04	0.46
34:a:223:A:H2'	34:a:224:U:O4'	2.16	0.46
1:A:2472:G:C4	1:A:2475:C:C4	3.03	0.46
1:A:2797:U:H2'	1:A:2797:U:O2	2.16	0.46
34:a:591:U:N3	34:a:648:A:N6	2.64	0.46
34:a:1391:U:H2'	34:a:1392:G:C8	2.50	0.46
1:A:312:G:H2'	1:A:313:G:H5'	1.97	0.46
1:A:468:G:N7	29:2:39:ARG:NH2	2.64	0.46
1:A:1721:G:H2'	1:A:1738:G:N2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2323:G:H2'	1:A:2324:U:O4'	2.16	0.46
14:N:97:ILE:CD1	14:N:113:ILE:HD12	2.46	0.46
33:6:12:ILE:HD12	33:6:32:LEU:HD11	1.98	0.46
34:a:359:G:H2'	34:a:360:G:O4'	2.16	0.46
34:a:518:C:H5	34:a:530:G:O5'	1.99	0.46
1:A:675:A:N3	1:A:2443:C:O2'	2.46	0.46
34:a:366:A:O3'	34:a:394:G:N2	2.49	0.46
34:a:713:G:H2'	34:a:714:G:C8	2.50	0.46
1:A:543:G:H3'	1:A:544:C:C5'	2.46	0.46
1:A:1165:A:N1	1:A:1184:U:O4	2.48	0.46
1:A:1370:C:H2'	1:A:1371:G:O4'	2.15	0.46
1:A:2038:G:H2'	1:A:2039:U:O4'	2.16	0.46
34:a:592:G:N2	34:a:648:A:H1'	2.31	0.46
54:u:9:GLU:HB2	54:u:10:PRO:HD3	1.97	0.46
34:a:414:A:H2'	34:a:415:A:O4'	2.16	0.45
57:y:28:G:O6	57:y:42:C:N3	2.49	0.45
16:P:91:VAL:HG11	16:P:96:LEU:CD2	2.47	0.45
34:a:675:A:H2'	34:a:676:A:O4'	2.16	0.45
1:A:2472:G:C5	1:A:2475:C:C5	3.04	0.45
1:A:2483:C:O2	1:A:2483:C:O4'	2.32	0.45
34:a:141:G:N1	34:a:222:C:C2	2.82	0.45
1:A:580:U:O3'	17:Q:30:VAL:HG13	2.16	0.45
1:A:609:A:H2'	1:A:610:C:O4'	2.17	0.45
1:A:1613:G:N1	1:A:1617:C:O2'	2.41	0.45
1:A:2560:A:H2'	1:A:2561:U:O4'	2.17	0.45
13:M:57:VAL:HG11	13:M:105:MET:HE1	1.99	0.45
1:A:278:A:C6	1:A:361:G:C8	2.99	0.45
17:Q:104:ALA:O	18:R:48:LYS:NZ	2.50	0.45
34:a:376:G:C2	34:a:389:A:C2	3.04	0.45
1:A:811:U:H2'	12:L:21:ARG:HA	1.99	0.45
6:F:30:VAL:HG12	6:F:95:MET:CE	2.47	0.45
34:a:149:A:C1'	34:a:1446:A:H2	2.30	0.45
34:a:410:G:H1'	34:a:433:G:C2	2.52	0.45
34:a:428:G:O4'	34:a:430:A:C8	2.68	0.45
41:h:104:SER:HB2	41:h:125:ILE:HD11	1.99	0.45
1:A:710:U:O2'	1:A:711:G:OP1	2.20	0.45
1:A:2028:U:C4	1:A:2029:G:O6	2.69	0.45
1:A:2070:A:H2'	1:A:2071:A:O4'	2.15	0.45
1:A:2305:U:H5"	6:F:130:GLY:HA3	1.98	0.45
1:A:2472:G:O6	1:A:2475:C:C3'	2.64	0.45
34:a:502:A:C2	34:a:544:G:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:A:C2	1:A:172:A:C2	3.05	0.45
1:A:273:G:N7	1:A:364:C:N3	2.64	0.45
1:A:1042:G:N3	1:A:1042:G:H2'	2.31	0.45
1:A:1062:G:N7	1:A:1063:G:N2	2.59	0.45
1:A:1604:C:O2'	1:A:1610:A:N1	2.41	0.45
1:A:2853:C:H5"	1:A:2853:C:H6	1.81	0.45
3:C:75:ALA:HB1	3:C:93:VAL:CG1	2.47	0.45
12:L:91:ASP:O	12:L:125:LEU:HD13	2.17	0.45
34:a:97:G:H2'	34:a:98:A:O4'	2.17	0.45
34:a:264:C:O2'	50:q:65:PRO:O	2.29	0.45
34:a:1448:C:N4	34:a:1455:G:H1	2.15	0.45
39:f:91:ARG:HD2	39:f:92:THR:HG23	1.98	0.45
49:p:4:ILE:HG12	49:p:21:VAL:HG22	1.99	0.45
1:A:1250:G:OP2	12:L:21:ARG:NH2	2.50	0.45
1:A:1447:C:O2'	1:A:1544:A:N3	2.38	0.45
1:A:1915:3TD:O4'	1:A:1915:3TD:C5	2.54	0.45
34:a:386:C:H3'	34:a:387:U:H5'	1.99	0.45
34:a:591:U:N3	34:a:592:G:N7	2.65	0.45
34:a:1127:G:H1'	34:a:1280:A:C6	2.52	0.45
34:a:1456:A:H2'	34:a:1457:G:O4'	2.17	0.45
58:z:84:ALA:HB3	58:z:87:TYR:CD2	2.52	0.45
1:A:568:U:H1'	1:A:2030:6MZ:C9	2.45	0.45
1:A:706:A:H2'	1:A:707:G:O4'	2.17	0.45
1:A:1052:C:O2	1:A:1052:C:C2'	2.63	0.45
1:A:1054:A:C8	1:A:1107:G:N1	2.85	0.45
1:A:1591:A:H2'	1:A:1592:C:O4'	2.17	0.45
1:A:2636:C:H2'	1:A:2637:U:C6	2.52	0.45
34:a:868:C:H2'	34:a:869:G:O4'	2.17	0.45
1:A:900:A:N3	1:A:900:A:C2'	2.80	0.44
1:A:1105:U:N3	1:A:1106:G:H1'	2.27	0.44
1:A:1351:C:H2'	1:A:1352:U:O4'	2.18	0.44
16:P:91:VAL:HG11	16:P:96:LEU:HD21	1.99	0.44
34:a:246:A:H4'	34:a:247:G:OP1	2.17	0.44
58:z:350:VAL:HG13	58:z:356:ILE:HD11	1.98	0.44
1:A:289:G:O6	1:A:351:C:N3	2.49	0.44
1:A:550:C:C4	1:A:551:G:C5	3.04	0.44
1:A:471:A:OP1	5:E:79:ARG:NH2	2.50	0.44
1:A:2539:C:H5'	31:4:3:VAL:HG21	1.99	0.44
34:a:67:C:O2'	34:a:172:A:O4'	2.34	0.44
34:a:455:G:C6	34:a:477:C:N4	2.85	0.44
34:a:812:G:OP1	34:a:902:G:N2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:h:7:ALA:O	41:h:11:THR:HG23	2.17	0.44
1:A:362:A:N7	1:A:363:G:C5	2.86	0.44
1:A:2016:U:H1'	27:0:2:VAL:CG1	2.48	0.44
1:A:2785:C:H2'	1:A:2786:U:O4'	2.17	0.44
1:A:267:C:C4	1:A:425:G:O6	2.71	0.44
1:A:516:C:OP1	27:0:9:ARG:NH1	2.51	0.44
1:A:709:U:N3	1:A:722:A:C2	2.85	0.44
1:A:1047:G:N2	1:A:1110:G:H2'	2.32	0.44
1:A:1867:G:C6	1:A:1874:C:N4	2.85	0.44
1:A:2478:A:OP1	31:4:32:LYS:NZ	2.50	0.44
1:A:2500:U:O2	1:A:2504:PSU:C2	2.71	0.44
1:A:38:A:H2'	1:A:39:G:O4'	2.18	0.44
1:A:155:A:H2'	1:A:156:A:C8	2.52	0.44
1:A:1050:A:N1	1:A:2751:G:N1	2.66	0.44
1:A:1105:U:H3	1:A:1106:G:H1'	1.79	0.44
1:A:1668:A:O2'	1:A:1674:G:N7	2.43	0.44
9:I:89:SER:OG	9:I:90:GLY:N	2.50	0.44
14:N:24:MET:HE1	14:N:40:LYS:HB3	1.99	0.44
34:a:386:C:C3'	34:a:387:U:C5'	2.96	0.44
41:h:11:THR:HG22	41:h:14:ARG:HH12	1.82	0.44
1:A:543:G:C6	1:A:550:C:N4	2.85	0.44
1:A:2880:C:H2'	1:A:2880:C:O2	2.18	0.44
39:f:26:THR:HG22	39:f:36:ILE:HD13	1.99	0.44
1:A:244:A:H2'	1:A:245:G:O4'	2.18	0.44
1:A:312:G:C2'	1:A:313:G:H5'	2.47	0.44
1:A:958:U:H2'	2:B:89:U:C2	2.53	0.44
6:F:107:VAL:N	6:F:108:PRO:HD2	2.33	0.44
34:a:220:G:H2'	34:a:221:C:C6	2.53	0.44
34:a:757:U:O2'	34:a:879:C:H1'	2.17	0.44
34:a:939:G:OP1	40:g:101:ARG:NH2	2.47	0.44
34:a:1508:A:H2'	34:a:1509:C:O4'	2.18	0.44
1:A:362:A:C5	1:A:363:G:C5	3.05	0.44
1:A:964:C:O2'	1:A:2273:A:N3	2.48	0.44
1:A:1104:C:O2	1:A:1104:C:H2'	2.18	0.44
34:a:663:A:H2'	34:a:664:G:O4'	2.18	0.44
1:A:1176:U:H2'	1:A:1177:G:C8	2.53	0.43
1:A:1414:C:H2'	1:A:1415:U:O4'	2.18	0.43
34:a:69:G:C2	34:a:71:A:C6	3.06	0.43
34:a:404:G:N2	34:a:498:A:C2	2.85	0.43
41:h:105:THR:HB	41:h:120:LEU:HD13	1.99	0.43
1:A:309:A:N3	1:A:329:G:O2'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:G:H3'	12:L:128:THR:HG21	2.00	0.43
1:A:1055:G:C5	1:A:1106:G:C6	3.06	0.43
1:A:2607:G:H2'	1:A:2608:G:O4'	2.18	0.43
2:B:20:G:H2'	2:B:21:G:O4'	2.18	0.43
34:a:71:A:N3	34:a:71:A:H2'	2.34	0.43
34:a:767:A:H2'	34:a:768:A:O4'	2.17	0.43
38:e:108:GLY:O	38:e:109:ALA:HB3	2.18	0.43
1:A:879:G:O6	1:A:898:C:N3	2.52	0.43
1:A:1230:A:H2'	1:A:1231:U:O4'	2.18	0.43
1:A:1268:A:H2'	1:A:1269:A:O4'	2.18	0.43
1:A:2063:C:C5	1:A:2064:C:C5	3.06	0.43
1:A:2078:C:H2'	1:A:2079:U:O4'	2.18	0.43
13:M:53:MET:HG3	13:M:120:ALA:HB2	2.00	0.43
34:a:393:A:N3	34:a:394:G:C8	2.87	0.43
1:A:1028:A:N3	1:A:2486:C:O2'	2.39	0.43
1:A:1131:G:OP1	10:J:82:GLY:HA2	2.18	0.43
1:A:1642:G:H2'	1:A:1643:G:O4'	2.19	0.43
1:A:940:G:H3'	1:A:941:A:H5"	2.00	0.43
1:A:993:G:N3	18:R:91:GLN:NE2	2.66	0.43
1:A:1432:G:H2'	1:A:1433:A:C8	2.53	0.43
11:K:34:GLY:O	11:K:36:GLY:N	2.51	0.43
20:T:61:LEU:HG	20:T:82:LYS:HG2	2.01	0.43
34:a:522:C:H5"	45:l:116:TYR:OH	2.18	0.43
54:u:11:PHE:CZ	54:u:13:VAL:HG13	2.54	0.43
1:A:158:U:O2	1:A:158:U:H2'	2.18	0.43
1:A:363:G:C6	1:A:364:C:N4	2.87	0.43
1:A:725:G:C6	1:A:726:G:N1	2.86	0.43
1:A:1483:G:C2	1:A:1484:U:C4	3.06	0.43
1:A:1483:G:O6	1:A:1508:A:N1	2.52	0.43
1:A:1538:G:C2'	1:A:1539:U:O4'	2.65	0.43
1:A:2477:U:O2	31:4:4:ARG:NH2	2.49	0.43
9:I:27:LEU:HD21	9:I:37:PHE:CD2	2.54	0.43
34:a:141:G:O6	34:a:222:C:N3	2.46	0.43
34:a:456:A:H2'	34:a:457:G:C8	2.53	0.43
34:a:457:G:C2	34:a:458:U:H1'	2.53	0.43
34:a:945:G:H2'	34:a:945:G:N3	2.34	0.43
43:j:57:VAL:HG12	43:j:58:ASN:N	2.33	0.43
1:A:212:G:H2'	1:A:213:A:O4'	2.19	0.43
1:A:281:C:C4	1:A:282:A:N7	2.87	0.43
1:A:1874:C:H2'	1:A:1874:C:O2	2.18	0.43
22:V:4:ILE:HD13	22:V:47:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:154:U:H2'	34:a:155:A:O4'	2.19	0.43
34:a:380:G:N3	34:a:384:G:O6	2.52	0.43
34:a:433:G:H4'	34:a:433:G:OP1	2.17	0.43
38:e:33:THR:HG22	38:e:51:LYS:HG3	2.00	0.43
1:A:1619:G:C8	1:A:1619:G:O5'	2.72	0.43
1:A:2025:C:H2'	1:A:2026:U:C6	2.54	0.43
1:A:2774:C:H2'	1:A:2775:G:O4'	2.19	0.43
13:M:50:ARG:HD3	13:M:65:ILE:HD11	1.99	0.43
32:5:64:VAL:HG12	32:5:64:VAL:O	2.19	0.43
34:a:648:A:N6	34:a:649:A:N1	2.67	0.43
36:c:9:ILE:HD12	47:n:98:LYS:HD3	2.01	0.43
1:A:2029:G:H2'	1:A:2031:A:OP1	2.18	0.43
1:A:2472:G:C4	1:A:2475:C:N3	2.87	0.43
1:A:2852:G:H2'	1:A:2853:C:O4'	2.17	0.43
2:B:4:C:C4	2:B:116:G:O6	2.66	0.43
34:a:953:G:H2'	34:a:954:G:O4'	2.19	0.43
58:z:26:THR:OG1	63:z:402:GTP:H5'	2.19	0.43
1:A:1246:A:H2'	1:A:1247:A:O4'	2.18	0.43
1:A:1722:A:C2	1:A:1739:A:O4'	2.72	0.43
1:A:2337:G:N3	1:A:2337:G:H2'	2.34	0.43
1:A:2577:A:H5"	1:A:2578:G:H5'	2.01	0.43
2:B:90:C:H2'	2:B:91:C:O4'	2.18	0.43
9:I:17:ALA:CB	9:I:42:ASN:HD21	2.32	0.43
34:a:839:C:N3	34:a:847:G:C6	2.87	0.43
34:a:1263:C:C4	34:a:1264:U:C4	3.07	0.43
49:p:2:VAL:HG23	49:p:65:ALA:HB2	2.01	0.43
1:A:14:A:C6	1:A:526:A:C2	3.07	0.42
34:a:195:A:N3	34:a:222:C:O2'	2.51	0.42
34:a:532:A:N6	34:a:1206:G:O2'	2.52	0.42
35:b:169:HIS:CE1	35:b:170:ILE:HG23	2.54	0.42
1:A:534:U:H2'	1:A:535:G:H5"	2.01	0.42
1:A:538:A:H2'	1:A:539:G:O4'	2.18	0.42
1:A:1477:A:N6	1:A:1514:G:O2'	2.51	0.42
1:A:1999:C:H2'	1:A:2000:C:O4'	2.19	0.42
1:A:2471:A:N1	1:A:2479:U:O4	2.51	0.42
18:R:14:VAL:HG21	18:R:98:ILE:HG13	2.01	0.42
26:Z:23:LEU:HD11	26:Z:53:MET:CE	2.49	0.42
34:a:140:U:H2'	34:a:141:G:H5'	2.01	0.42
34:a:778:G:H2'	34:a:779:C:O4'	2.19	0.42
1:A:283:G:H2'	1:A:284:U:O4'	2.19	0.42
1:A:287:G:C5	1:A:354:A:N6	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:A:C6	1:A:1102:C:C2	3.07	0.42
1:A:1563:U:H2'	1:A:1564:C:C6	2.55	0.42
2:B:23:G:C6	2:B:24:G:O6	2.71	0.42
5:E:108:ILE:HB	12:L:1:MET:HE3	2.00	0.42
34:a:408:A:C6	34:a:409:U:C4	3.08	0.42
34:a:977:A:O2'	34:a:979:C:OP2	2.34	0.42
38:e:92:ARG:HB2	38:e:127:TYR:HB2	2.02	0.42
58:z:131:ILE:HD12	58:z:195:LEU:HD23	2.00	0.42
1:A:271:G:N1	1:A:367:G:C6	2.88	0.42
1:A:289:G:O6	1:A:351:C:C4	2.72	0.42
1:A:476:G:N1	1:A:479:A:OP2	2.52	0.42
1:A:807:U:H1'	1:A:2445:2MG:OP1	2.20	0.42
1:A:898:C:H2'	1:A:899:A:C8	2.54	0.42
1:A:1352:U:O2'	1:A:1570:A:N3	2.44	0.42
1:A:1519:G:N3	1:A:1519:G:H2'	2.32	0.42
1:A:1857:G:O2'	1:A:1884:G:N2	2.52	0.42
1:A:2320:U:H4'	1:A:2321:U:H5'	1.98	0.42
1:A:2683:C:N3	1:A:2727:A:O2'	2.52	0.42
34:a:325:A:H2'	34:a:326:G:C8	2.54	0.42
1:A:289:G:O6	1:A:350:G:O6	2.37	0.42
1:A:684:G:C2	1:A:794:A:C2	3.08	0.42
1:A:1055:G:C2	1:A:1105:U:C4	3.07	0.42
1:A:1483:G:C2	1:A:1484:U:C5	3.07	0.42
1:A:1851:U:O3'	55:w:71:C:O2'	2.36	0.42
34:a:141:G:O6	34:a:223:A:C6	2.72	0.42
34:a:456:A:H2'	34:a:457:G:N9	2.34	0.42
34:a:680:C:O2	34:a:711:G:C2	2.72	0.42
34:a:690:G:H2'	34:a:691:G:O4'	2.20	0.42
1:A:805:G:OP2	12:L:41:ARG:HG2	2.18	0.42
1:A:1721:G:C2'	1:A:1739:A:N6	2.82	0.42
1:A:2298:A:N3	1:A:2321:U:C5	2.86	0.42
1:A:2472:G:C5	1:A:2475:C:C4	3.07	0.42
22:V:86:LEU:HD13	22:V:89:ILE:HD11	2.01	0.42
58:z:26:THR:OG1	63:z:402:GTP:H5"	2.20	0.42
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.52	0.42
34:a:75:G:N3	34:a:97:G:N2	2.67	0.42
34:a:602:A:N6	34:a:636:U:H3	2.18	0.42
34:a:847:G:H2'	34:a:848:C:C6	2.55	0.42
38:e:37:VAL:HG11	38:e:113:VAL:HA	2.02	0.42
43:j:42:LEU:HD11	43:j:73:LEU:HG	2.02	0.42
1:A:544:C:N3	1:A:545:U:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:C:H5”	1:A:1121:C:H6	1.84	0.42
1:A:1582:C:O2’	1:A:1585:C:N3	2.52	0.42
34:a:99:C:H1’	34:a:100:G:N7	2.35	0.42
55:w:17:C:C5	55:w:117:U:C4	3.00	0.42
1:A:573:U:O4	1:A:2030:6MZ:H3’	2.20	0.42
1:A:1318:U:H2’	1:A:1319:C:C6	2.54	0.42
10:J:64:VAL:HG21	10:J:89:PHE:CZ	2.55	0.42
34:a:109:A:C6	34:a:327:A:C6	3.08	0.42
34:a:380:G:O2’	34:a:382:A:C2	2.54	0.42
34:a:512:U:C2’	34:a:513:C:H5”	2.50	0.42
1:A:1421:G:C2	1:A:1422:G:C8	3.08	0.42
1:A:2755:C:O3’	1:A:2756:U:O2	2.38	0.42
34:a:57:G:H2’	34:a:58:C:C6	2.54	0.42
34:a:142:G:H2’	34:a:143:A:O4’	2.19	0.42
34:a:544:G:OP2	37:d:62:ARG:NH2	2.53	0.42
34:a:827:U:C2	34:a:874:G:N2	2.88	0.42
37:d:23:GLY:HA2	37:d:108:ALA:HB1	2.02	0.42
51:r:20:ILE:HG21	51:r:54:LEU:HA	2.02	0.42
1:A:565:C:H2’	1:A:566:U:O4’	2.20	0.41
1:A:1019:U:OP1	1:A:1035:U:O2’	2.22	0.41
1:A:1067:A:H1’	57:y:56:C:O4’	2.20	0.41
1:A:1614:A:C2	19:S:93:ALA:HB2	2.55	0.41
3:C:52:HIS:CD2	3:C:218:THR:HA	2.55	0.41
34:a:619:U:O2	37:d:129:VAL:HA	2.20	0.41
1:A:36:G:N3	1:A:450:G:O2’	2.50	0.41
1:A:1041:G:N1	1:A:1042:G:C8	2.88	0.41
1:A:1879:C:H2’	1:A:1880:U:O4’	2.20	0.41
2:B:24:G:N7	2:B:56:G:H2’	2.35	0.41
4:D:186:LEU:HD21	16:P:3:ILE:HG23	2.01	0.41
20:T:31:VAL:HG22	20:T:84:TYR:CD2	2.55	0.41
34:a:50:A:N1	34:a:360:G:O2’	2.45	0.41
34:a:150:U:H2’	34:a:151:A:H8	1.85	0.41
34:a:303:A:H2’	34:a:304:U:O4’	2.20	0.41
34:a:394:G:H2’	34:a:395:C:O4’	2.19	0.41
58:z:177:ALA:CB	58:z:188:ILE:HD12	2.50	0.41
12:L:30:THR:O	12:L:32:GLY:N	2.53	0.41
19:S:108:SER:OG	19:S:109:ASP:N	2.53	0.41
21:U:93:ARG:HB2	21:U:102:ILE:HD12	2.03	0.41
29:2:34:ARG:NH1	29:2:42:LEU:O	2.53	0.41
34:a:518:C:C5	34:a:530:G:C8	3.08	0.41
34:a:605:U:C2	34:a:633:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1087:G:C2	34:a:1099:G:C2	3.08	0.41
47:n:54:ASP:O	47:n:55:SER:CB	2.67	0.41
1:A:833:A:H2'	1:A:834:G:C8	2.55	0.41
1:A:1028:A:N6	1:A:1125:G:H2'	2.36	0.41
1:A:1105:U:H2'	1:A:1106:G:H4'	2.01	0.41
1:A:1506:U:N3	1:A:1507:C:N4	2.68	0.41
34:a:75:G:N2	34:a:97:G:N1	2.69	0.41
34:a:75:G:C2	34:a:96:U:C4	3.08	0.41
34:a:256:U:C2	34:a:257:G:N7	2.88	0.41
34:a:890:G:O2'	34:a:906:A:N6	2.53	0.41
57:y:28:G:N1	57:y:42:C:O2	2.51	0.41
1:A:1103:A:C8	1:A:1104:C:C6	3.09	0.41
1:A:1537:G:H3'	1:A:1538:G:C5'	2.50	0.41
1:A:2102:G:C6	1:A:2188:U:C4	3.08	0.41
1:A:2539:C:C5'	31:4:3:VAL:HG21	2.50	0.41
2:B:52:A:N6	15:O:64:TYR:OH	2.51	0.41
2:B:62:C:H2'	2:B:63:C:C6	2.56	0.41
26:Z:23:LEU:HD11	26:Z:53:MET:HE2	2.03	0.41
34:a:455:G:C2	34:a:477:C:N3	2.88	0.41
34:a:622:A:C8	34:a:623:C:C5	3.08	0.41
34:a:1202:U:N3	47:n:82:ILE:HG21	2.36	0.41
48:o:44:GLU:HG2	48:o:45:HIS:CD2	2.56	0.41
1:A:690:G:H2'	1:A:691:C:O4'	2.20	0.41
1:A:1969:A:O2'	1:A:1972:G:N3	2.41	0.41
29:2:34:ARG:HB2	29:2:42:LEU:HD12	2.01	0.41
41:h:10:LEU:HD22	41:h:74:ILE:CD1	2.49	0.41
46:m:94:LEU:HD22	46:m:101:THR:HG21	2.03	0.41
53:t:66:ILE:HG23	53:t:70:LYS:HD2	2.02	0.41
10:J:4:PHE:O	17:Q:63:ARG:NH2	2.52	0.41
34:a:258:G:C6	34:a:259:G:C5	3.09	0.41
34:a:352:C:O2	34:a:352:C:H2'	2.20	0.41
34:a:455:G:N2	34:a:478:A:C2	2.89	0.41
34:a:978:A:O4'	34:a:1322:C:O2	2.39	0.41
36:c:172:VAL:HG12	36:c:174:LEU:HD13	2.03	0.41
38:e:15:ILE:HD13	38:e:37:VAL:HG23	2.01	0.41
39:f:38:ARG:CD	39:f:63:ASN:ND2	2.82	0.41
41:h:24:VAL:HG21	41:h:62:LEU:HD11	2.02	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
1:A:2202:U:O2'	1:A:2204:G:OP1	2.32	0.41
18:R:5:PHE:HB3	18:R:59:ILE:HD12	2.02	0.41
34:a:270:A:H2'	34:a:271:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:C:H2'	1:A:226:A:O4'	2.20	0.41
1:A:340:A:H2'	1:A:341:C:O4'	2.20	0.41
1:A:550:C:C4	1:A:551:G:N7	2.89	0.41
1:A:1063:G:O6	1:A:1076:C:N4	2.53	0.41
1:A:1412:U:O4	1:A:1413:A:N6	2.54	0.41
1:A:1502:A:H2'	1:A:1503:A:O4'	2.21	0.41
1:A:1555:G:H5'	1:A:1555:G:C8	2.56	0.41
1:A:1794:A:H2'	1:A:1795:C:C6	2.55	0.41
9:I:32:VAL:HG21	9:I:60:VAL:HG22	2.03	0.41
29:2:44:VAL:O	29:2:44:VAL:HG13	2.21	0.41
34:a:93:U:H3'	34:a:95:C:C5	2.55	0.41
34:a:142:G:C2	34:a:222:C:C1'	3.04	0.41
34:a:144:G:N1	34:a:178:C:O2	2.53	0.41
46:m:15:VAL:HG23	46:m:16:ILE:CD1	2.37	0.41
50:q:11:VAL:HG21	50:q:20:ILE:HD11	2.02	0.41
1:A:1792:G:O2'	1:A:1830:C:OP1	2.36	0.41
1:A:1857:G:N2	1:A:1884:G:O2'	2.41	0.41
8:H:125:THR:HG21	8:H:148:ALA:HB2	2.03	0.41
32:5:48:ALA:HB3	32:5:51:TYR:HE2	1.86	0.41
34:a:622:A:C8	34:a:623:C:C6	3.09	0.41
34:a:1082:A:H2'	34:a:1083:U:O4'	2.21	0.41
47:n:7:ALA:O	47:n:10:VAL:HG12	2.21	0.41
1:A:1049:C:N4	1:A:1050:A:N1	2.68	0.40
1:A:2356:U:H4'	23:W:16:ARG:HG3	2.03	0.40
34:a:602:A:C2	34:a:636:U:O2	2.75	0.40
35:b:27:LYS:N	35:b:28:PRO:CD	2.83	0.40
48:o:77:TYR:CE1	48:o:81:ILE:HD11	2.56	0.40
55:w:16:C:H5"	55:w:17:C:P	2.61	0.40
58:z:98:MET:CE	58:z:101:ALA:HB2	2.51	0.40
1:A:278:A:N7	1:A:362:A:H1'	2.35	0.40
1:A:754:U:H1'	1:A:1618:6MZ:H2	2.02	0.40
1:A:1939:5MU:OP1	1:A:2604:PSU:O2'	2.39	0.40
1:A:2570:G:H2'	1:A:2571:U:O4'	2.22	0.40
1:A:2751:G:H21	7:G:2:ARG:HD3	1.85	0.40
3:C:143:VAL:HB	3:C:153:LEU:HB2	2.03	0.40
34:a:1051:C:O2	34:a:1207:2MG:HM22	2.21	0.40
46:m:89:ARG:HG2	46:m:96:VAL:HA	2.02	0.40
1:A:713:G:N2	1:A:718:A:C5	2.86	0.40
1:A:817:C:H2'	1:A:818:G:O4'	2.22	0.40
1:A:2246:G:H2'	1:A:2247:A:C8	2.57	0.40
1:A:2620:C:H2'	1:A:2621:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:78:A:H2'	34:a:79:G:O4'	2.21	0.40
34:a:1448:C:N4	34:a:1456:A:C2	2.90	0.40
1:A:191:A:H2'	1:A:192:C:C6	2.56	0.40
1:A:1020:A:H61	1:A:1141:U:HO2'	1.67	0.40
4:D:80:TRP:HD1	4:D:202:ILE:HD11	1.87	0.40
15:O:92:PHE:HB2	15:O:117:PHE:CE1	2.56	0.40
34:a:130:A:N1	34:a:233:C:H1'	2.36	0.40
34:a:340:U:C2'	34:a:341:C:OP1	2.69	0.40
34:a:652:U:C4	34:a:752:G:N3	2.89	0.40
34:a:687:A:H2'	34:a:701:U:O4	2.21	0.40
34:a:789:U:O2'	34:a:791:G:N7	2.44	0.40
34:a:1305:G:N2	34:a:1331:G:H1'	2.37	0.40
34:a:1518:MA6:H92	34:a:1519:MA6:C9	2.51	0.40
39:f:22:ILE:O	39:f:26:THR:HG23	2.21	0.40
1:A:207:A:H2'	1:A:208:C:O4'	2.22	0.40
1:A:590:A:H2'	1:A:591:U:O4'	2.21	0.40
1:A:735:A:C8	1:A:736:C:C5	3.10	0.40
1:A:756:A:H2'	1:A:757:G:O4'	2.21	0.40
1:A:1061:U:O2	1:A:1061:U:H2'	2.21	0.40
1:A:1105:U:H2'	1:A:1106:G:C4'	2.52	0.40
1:A:1107:G:H2'	1:A:1108:U:O4'	2.21	0.40
1:A:2738:A:C2	1:A:2739:U:H1'	2.56	0.40
3:C:139:THR:HG23	3:C:160:TYR:CD2	2.57	0.40
16:P:64:SER:O	16:P:65:ASN:C	2.64	0.40
35:b:203:ASP:OD1	35:b:204:ASP:N	2.55	0.40
50:q:68:LYS:O	50:q:69:THR:OG1	2.30	0.40
51:r:70:THR:OG1	51:r:71:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	269/271 (99%)	239 (89%)	27 (10%)	3 (1%)	11 43
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	24 60
5	E	198/200 (99%)	178 (90%)	18 (9%)	2 (1%)	12 45
6	F	175/177 (99%)	157 (90%)	16 (9%)	2 (1%)	11 43
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100 100
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4 22
9	I	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	1 10
10	J	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18 53
11	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3 17
12	L	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	2 12
13	M	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	18 53
14	N	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7 32
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14 48
16	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14 48
17	Q	113/115 (98%)	111 (98%)	2 (2%)	0	100 100
18	R	100/102 (98%)	85 (85%)	12 (12%)	3 (3%)	3 19
19	S	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14 48
20	T	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5 26
21	U	100/102 (98%)	87 (87%)	9 (9%)	4 (4%)	2 14
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11 43
23	W	73/75 (97%)	68 (93%)	5 (7%)	0	100 100
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100 100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	7 32
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
27	0	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	6 30
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100 100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5 25
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
32	5	129/131 (98%)	99 (77%)	21 (16%)	9 (7%)	1 4
33	6	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	3 19
35	b	216/218 (99%)	186 (86%)	25 (12%)	5 (2%)	5 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	c	204/206 (99%)	183 (90%)	15 (7%)	6 (3%)	3 20
37	d	203/205 (99%)	183 (90%)	17 (8%)	3 (2%)	8 35
38	e	156/157 (99%)	133 (85%)	21 (14%)	2 (1%)	9 38
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2 13
40	g	149/151 (99%)	131 (88%)	11 (7%)	7 (5%)	2 11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100 100
42	i	125/127 (98%)	97 (78%)	24 (19%)	4 (3%)	3 18
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1 9
44	k	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	1 9
45	l	119/121 (98%)	93 (78%)	19 (16%)	7 (6%)	1 7
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6 31
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1 10
48	o	86/88 (98%)	79 (92%)	4 (5%)	3 (4%)	3 16
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4 23
50	q	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1 10
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2 11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100 100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4 24
54	u	63/65 (97%)	41 (65%)	12 (19%)	10 (16%)	0 0
58	z	391/393 (100%)	357 (91%)	22 (6%)	12 (3%)	3 19
All	All	6219/6322 (98%)	5486 (88%)	581 (9%)	152 (2%)	7 24

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	70	LYS
5	E	83	VAL
6	F	11	VAL
11	K	89	ASN
16	P	65	ASN
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
42	i	90	ASP
43	j	57	VAL

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Mol	Chain	Res	Type
44	k	88	PRO
44	k	94	SER
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
5	E	8	ALA
8	H	3	VAL
8	H	122	LEU
9	I	7	TYR
9	I	38	CYS
10	J	81	ILE
12	L	92	LEU
14	N	117	ASP
15	O	66	GLY
18	R	54	VAL
18	R	55	ASP
20	T	37	ASP
32	5	60	LEU
38	e	77	ASN
40	g	20	GLU
40	g	64	ALA
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
44	k	103	GLY
45	l	75	GLU
46	m	7	ASN
47	n	22	LYS
47	n	55	SER
47	n	90	ARG
48	o	2	LEU
51	r	10	CYS
51	r	17	VAL
54	u	9	GLU
54	u	30	GLU
58	z	161	ASP
8	H	15	LEU
8	H	41	LYS
9	I	6	ALA

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Mol	Chain	Res	Type
9	I	64	ARG
11	K	110	GLU
13	M	69	PRO
14	N	59	SER
22	V	58	SER
25	Y	24	GLU
27	0	2	VAL
32	5	48	ALA
32	5	88	HIS
33	6	4	ASP
35	b	63	LYS
35	b	73	ARG
36	c	95	GLY
37	d	191	SER
39	f	33	GLU
42	i	124	PRO
44	k	118	ASN
45	l	42	LYS
45	l	88	ASP
47	n	2	LYS
47	n	38	ASP
50	q	17	GLU
51	r	46	THR
54	u	11	PHE
58	z	249	GLU
3	C	150	GLY
4	D	149	ASN
6	F	20	ASN
9	I	10	LEU
12	L	15	ALA
12	L	29	LYS
12	L	31	GLY
18	R	43	ASN
20	T	38	ALA
21	U	6	ARG
21	U	97	SER
32	5	118	ILE
35	b	151	LYS
36	c	147	GLY
37	d	166	LYS
38	e	93	VAL
39	f	63	ASN

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Mol	Chain	Res	Type
40	g	18	GLY
40	g	19	SER
40	g	112	ASP
43	j	35	GLN
44	k	13	LYS
45	l	46	SER
48	o	13	GLU
50	q	49	ASN
50	q	69	THR
50	q	79	GLU
58	z	332	PHE
9	I	92	PRO
11	K	35	VAL
19	S	65	ASP
29	2	2	LYS
32	5	55	VAL
32	5	113	PHE
35	b	11	ALA
35	b	192	PRO
36	c	144	GLY
37	d	34	GLU
39	f	92	THR
40	g	56	SER
45	l	33	CYS
45	l	77	SER
48	o	45	HIS
49	p	64	GLY
53	t	44	ALA
54	u	12	ASP
54	u	36	PHE
54	u	65	ARG
58	z	9	LYS
58	z	82	PRO
58	z	126	GLY
58	z	137	CYS
58	z	180	GLY
12	L	115	GLU
21	U	75	ALA
32	5	22	ALA
32	5	108	VAL
39	f	56	LYS
43	j	6	ILE

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Mol	Chain	Res	Type
43	j	75	ASP
45	l	2	THR
46	m	102	LYS
49	p	49	GLY
54	u	24	LYS
58	z	2	LYS
58	z	207	ASP
58	z	248	LYS
11	K	93	GLN
12	L	85	VAL
36	c	148	ILE
3	C	168	GLY
58	z	52	ALA
9	I	12	VAL
21	U	38	ILE
33	6	55	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	216/216 (100%)	206 (95%)	10 (5%)	24 58
4	D	163/163 (100%)	153 (94%)	10 (6%)	17 49
5	E	164/164 (100%)	153 (93%)	11 (7%)	15 46
6	F	148/148 (100%)	143 (97%)	5 (3%)	32 66
7	G	135/135 (100%)	133 (98%)	2 (2%)	57 80
8	H	114/114 (100%)	108 (95%)	6 (5%)	20 54
9	I	109/109 (100%)	102 (94%)	7 (6%)	16 48
10	J	115/115 (100%)	112 (97%)	3 (3%)	40 72
11	K	103/103 (100%)	99 (96%)	4 (4%)	28 62
12	L	102/102 (100%)	93 (91%)	9 (9%)	9 35
13	M	109/109 (100%)	108 (99%)	1 (1%)	70 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	99/99 (100%)	94 (95%)	5 (5%)	21 55
15	O	86/86 (100%)	85 (99%)	1 (1%)	63 82
16	P	99/99 (100%)	96 (97%)	3 (3%)	36 69
17	Q	88/88 (100%)	84 (96%)	4 (4%)	24 59
18	R	84/84 (100%)	82 (98%)	2 (2%)	43 73
19	S	92/92 (100%)	91 (99%)	1 (1%)	65 83
20	T	79/79 (100%)	76 (96%)	3 (4%)	29 63
21	U	83/83 (100%)	82 (99%)	1 (1%)	63 82
22	V	77/77 (100%)	76 (99%)	1 (1%)	61 81
23	W	57/57 (100%)	56 (98%)	1 (2%)	51 77
24	X	67/67 (100%)	66 (98%)	1 (2%)	57 80
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51 77
26	Z	47/47 (100%)	47 (100%)	0	100 100
27	0	46/46 (100%)	46 (100%)	0	100 100
28	1	46/46 (100%)	46 (100%)	0	100 100
29	2	37/37 (100%)	36 (97%)	1 (3%)	39 71
30	3	51/51 (100%)	50 (98%)	1 (2%)	48 76
31	4	34/34 (100%)	34 (100%)	0	100 100
32	5	100/100 (100%)	100 (100%)	0	100 100
33	6	59/59 (100%)	58 (98%)	1 (2%)	53 78
35	b	180/180 (100%)	178 (99%)	2 (1%)	65 83
36	c	170/170 (100%)	167 (98%)	3 (2%)	51 77
37	d	172/172 (100%)	167 (97%)	5 (3%)	37 70
38	e	120/119 (101%)	109 (91%)	11 (9%)	8 33
39	f	87/87 (100%)	84 (97%)	3 (3%)	32 66
40	g	124/124 (100%)	120 (97%)	4 (3%)	34 67
41	h	104/104 (100%)	102 (98%)	2 (2%)	50 76
42	i	105/105 (100%)	102 (97%)	3 (3%)	37 70
43	j	86/86 (100%)	85 (99%)	1 (1%)	63 82
44	k	89/89 (100%)	87 (98%)	2 (2%)	45 74
45	l	102/102 (100%)	99 (97%)	3 (3%)	37 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	m	93/93 (100%)	92 (99%)	1 (1%)	65 83
47	n	83/83 (100%)	81 (98%)	2 (2%)	43 73
48	o	76/76 (100%)	74 (97%)	2 (3%)	40 72
49	p	65/65 (100%)	63 (97%)	2 (3%)	35 68
50	q	74/74 (100%)	71 (96%)	3 (4%)	27 61
51	r	56/56 (100%)	52 (93%)	4 (7%)	13 43
52	s	70/70 (100%)	67 (96%)	3 (4%)	26 60
53	t	65/65 (100%)	61 (94%)	4 (6%)	16 49
54	u	55/55 (100%)	53 (96%)	2 (4%)	31 65
58	z	325/325 (100%)	322 (99%)	3 (1%)	70 85
All	All	5165/5164 (100%)	5005 (97%)	160 (3%)	36 68

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	23	LEU
3	C	35	LYS
3	C	69	ASN
3	C	96	LYS
3	C	101	ARG
3	C	110	LYS
3	C	183	VAL
3	C	200	MET
3	C	203	VAL
3	C	249	VAL
4	D	12	THR
4	D	30	GLU
4	D	33	ARG
4	D	39	ASP
4	D	51	THR
4	D	55	LYS
4	D	56	LYS
4	D	151	THR
4	D	189	VAL
4	D	204	LYS
5	E	2	GLU
5	E	57	LYS
5	E	69	ARG

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Mol	Chain	Res	Type
5	E	111	GLU
5	E	117	ARG
5	E	136	GLN
5	E	139	LYS
5	E	144	GLU
5	E	158	PHE
5	E	165	HIS
5	E	188	MET
6	F	11	VAL
6	F	12	VAL
6	F	67	THR
6	F	114	ARG
6	F	135	ILE
7	G	2	ARG
7	G	169	ARG
8	H	77	THR
8	H	96	THR
8	H	122	LEU
8	H	134	VAL
8	H	138	VAL
8	H	145	ASN
9	I	9	LYS
9	I	12	VAL
9	I	30	GLN
9	I	52	LEU
9	I	67	THR
9	I	72	THR
9	I	134	SER
10	J	12	LYS
10	J	81	ILE
10	J	138	GLN
11	K	7	MET
11	K	31	ARG
11	K	52	VAL
11	K	61	VAL
12	L	1	MET
12	L	2	ARG
12	L	3	LEU
12	L	14	LYS
12	L	41	ARG
12	L	60	ARG
12	L	63	LYS

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Mol	Chain	Res	Type
12	L	92	LEU
12	L	125	LEU
13	M	40	ARG
14	N	34	ILE
14	N	46	ARG
14	N	65	LEU
14	N	98	LEU
14	N	118	ARG
15	O	28	VAL
16	P	26	GLU
16	P	47	ILE
16	P	67	GLU
17	Q	8	ILE
17	Q	40	LYS
17	Q	101	ASP
17	Q	108	LEU
18	R	66	HIS
18	R	73	LYS
19	S	29	VAL
20	T	69	ARG
20	T	76	ARG
20	T	91	GLN
21	U	73	ASN
22	V	42	LEU
23	W	8	ASN
24	X	59	ASP
25	Y	2	LYS
29	2	22	MET
30	3	61	LEU
33	6	37	CYS
35	b	99	MET
35	b	122	ASP
36	c	138	GLN
36	c	156	LEU
36	c	174	LEU
37	d	33	ILE
37	d	140	ASP
37	d	158	LEU
37	d	186	GLU
37	d	190	LEU
38	e	11	GLN
38	e	19	ARG

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Mol	Chain	Res	Type
38	e	38	VAL
38	e	45	VAL
38	e	114	LEU
38	e	119	VAL
38	e	121	ASN
38	e	136	VAL
38	e	139	THR
38	e	141	ASP
38	e	146	MET
39	f	38	ARG
39	f	39	LEU
39	f	91	ARG
40	g	11	ILE
40	g	76	SER
40	g	89	GLU
40	g	147	ASN
41	h	41	GLU
41	h	111	THR
42	i	41	GLU
42	i	42	THR
42	i	65	THR
43	j	67	ILE
44	k	28	ASN
44	k	125	LYS
45	l	38	THR
45	l	77	SER
45	l	93	ARG
46	m	89	ARG
47	n	17	ASP
47	n	75	ARG
48	o	17	ASP
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	37	ILE
50	q	52	CYS
51	r	13	THR
51	r	27	THR
51	r	41	SER
51	r	42	ARG
52	s	5	LYS

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Mol	Chain	Res	Type
52	s	6	LYS
52	s	12	LEU
53	t	7	LYS
53	t	42	ASP
53	t	56	ILE
53	t	68	LYS
54	u	31	VAL
54	u	62	GLU
58	z	22	HIS
58	z	179	GLU
58	z	356	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	20	ASN
3	C	59	GLN
3	C	85	ASN
3	C	152	GLN
3	C	259	ASN
5	E	94	GLN
5	E	136	GLN
6	F	80	GLN
6	F	134	GLN
7	G	37	ASN
7	G	103	ASN
8	H	18	GLN
9	I	42	ASN
9	I	104	GLN
9	I	106	GLN
10	J	47	HIS
11	K	3	GLN
12	L	93	ASN
13	M	3	GLN
13	M	13	HIS
14	N	62	ASN
14	N	73	ASN
15	O	100	HIS
15	O	104	GLN
16	P	6	GLN
16	P	11	GLN
17	Q	51	GLN

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Mol	Chain	Res	Type
18	R	6	GLN
18	R	11	GLN
18	R	12	HIS
19	S	102	HIS
20	T	48	GLN
21	U	45	GLN
21	U	53	GLN
21	U	65	GLN
21	U	73	ASN
25	Y	27	ASN
26	Z	8	GLN
31	4	37	GLN
32	5	4	ASN
33	6	61	ASN
33	6	65	ASN
35	b	18	GLN
35	b	23	ASN
35	b	50	ASN
36	c	68	HIS
36	c	122	GLN
36	c	175	HIS
37	d	35	GLN
37	d	39	GLN
37	d	84	ASN
37	d	88	ASN
37	d	151	GLN
37	d	163	GLN
38	e	72	ASN
38	e	131	ASN
39	f	37	HIS
40	g	129	ASN
41	h	3	GLN
42	i	125	GLN
44	k	37	GLN
44	k	39	ASN
44	k	63	GLN
45	l	45	ASN
45	l	111	GLN
46	m	99	GLN
48	o	27	GLN
48	o	34	GLN
49	p	79	ASN

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Mol	Chain	Res	Type
50	q	49	ASN
51	r	51	GLN
53	t	47	GLN
58	z	51	ASN
58	z	273	ASN
58	z	301	HIS
58	z	329	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	830 (28%)	91 (3%)
2	B	119/120 (99%)	46 (38%)	7 (5%)
34	a	1539/1540 (99%)	498 (32%)	0
55	v	76/77 (98%)	24 (31%)	0
55	w	76/77 (98%)	33 (43%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	75/76 (98%)	31 (41%)	0
All	All	4793/4805 (99%)	1466 (30%)	98 (2%)

All (1466) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	5	A
1	A	10	A
1	A	12	U
1	A	13	A
1	A	15	G
1	A	23	G
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	G
1	A	52	A
1	A	60	G
1	A	63	A
1	A	71	A

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Mol	Chain	Res	Type
1	A	74	A
1	A	75	G
1	A	76	C
1	A	80	G
1	A	81	G
1	A	85	G
1	A	86	G
1	A	96	C
1	A	100	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	126	A
1	A	135	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	146	A
1	A	147	C
1	A	148	U
1	A	149	A
1	A	157	C
1	A	158	U
1	A	159	G
1	A	160	A
1	A	161	A
1	A	162	U
1	A	163	C
1	A	166	U
1	A	170	U
1	A	171	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	215	G
1	A	216	A

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Mol	Chain	Res	Type
1	A	219	A
1	A	221	A
1	A	222	A
1	A	228	C
1	A	229	C
1	A	231	A
1	A	233	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	275	C
1	A	276	U
1	A	277	G
1	A	278	A
1	A	280	U
1	A	281	C
1	A	282	A
1	A	283	G
1	A	284	U
1	A	285	G
1	A	287	G
1	A	288	U
1	A	289	G
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C
1	A	305	C
1	A	306	U
1	A	311	A
1	A	313	G
1	A	315	G
1	A	317	G
1	A	323	C
1	A	329	G
1	A	330	A
1	A	343	C

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Mol	Chain	Res	Type
1	A	350	G
1	A	351	C
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	362	A
1	A	363	G
1	A	365	U
1	A	366	C
1	A	367	G
1	A	368	A
1	A	369	U
1	A	371	A
1	A	372	G
1	A	383	C
1	A	386	G
1	A	387	U
1	A	390	U
1	A	396	G
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	417	C
1	A	420	C
1	A	422	A
1	A	451	U
1	A	455	C
1	A	456	C
1	A	457	A
1	A	459	U
1	A	473	G
1	A	474	G
1	A	479	A
1	A	481	G
1	A	487	C
1	A	491	G
1	A	492	A
1	A	496	G

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Mol	Chain	Res	Type
1	A	503	A
1	A	504	A
1	A	505	A
1	A	509	C
1	A	513	A
1	A	518	G
1	A	526	A
1	A	527	C
1	A	529	A
1	A	532	A
1	A	533	G
1	A	535	G
1	A	542	U
1	A	543	G
1	A	544	C
1	A	545	U
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	557	C
1	A	563	A
1	A	573	U
1	A	575	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	637	A
1	A	640	C
1	A	644	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	651	G
1	A	652	U
1	A	653	U

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Mol	Chain	Res	Type
1	A	654	A
1	A	655	A
1	A	656	G
1	A	659	G
1	A	661	A
1	A	668	A
1	A	678	C
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	710	U
1	A	711	G
1	A	713	G
1	A	714	U
1	A	717	C
1	A	730	A
1	A	734	A
1	A	738	G
1	A	747	5MC
1	A	752	A
1	A	763	G
1	A	764	A
1	A	765	C
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	805	G
1	A	812	C
1	A	816	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	843	G
1	A	844	A

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Mol	Chain	Res	Type
1	A	845	A
1	A	846	C
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	868	U
1	A	869	G
1	A	870	U
1	A	872	U
1	A	873	C
1	A	877	A
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	906	U
1	A	907	G
1	A	909	A
1	A	910	A
1	A	914	G
1	A	915	C
1	A	925	A
1	A	934	U
1	A	935	C
1	A	940	G
1	A	941	A
1	A	946	C
1	A	951	C
1	A	961	C
1	A	968	C
1	A	974	G
1	A	982	C
1	A	983	A
1	A	984	A

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Mol	Chain	Res	Type
1	A	985	C
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1003	G
1	A	1005	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1019	U
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1042	G
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1049	C
1	A	1050	A
1	A	1051	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G

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Mol	Chain	Res	Type
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1096	A
1	A	1097	U
1	A	1101	U
1	A	1103	A
1	A	1104	C
1	A	1105	U
1	A	1106	G
1	A	1110	G
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1117	C
1	A	1119	U
1	A	1121	C
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1140	C
1	A	1141	U
1	A	1142	A
1	A	1144	A
1	A	1149	G
1	A	1151	A
1	A	1168	G
1	A	1169	A
1	A	1171	G
1	A	1172	C

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Mol	Chain	Res	Type
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1195	G
1	A	1203	U
1	A	1204	A
1	A	1205	A
1	A	1218	G
1	A	1236	G
1	A	1248	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1287	A
1	A	1289	C
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1321	A
1	A	1343	G
1	A	1345	C
1	A	1346	G
1	A	1350	C
1	A	1352	U
1	A	1353	A
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1386	C
1	A	1387	A
1	A	1392	A
1	A	1395	A
1	A	1397	U
1	A	1403	A

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Mol	Chain	Res	Type
1	A	1407	G
1	A	1409	U
1	A	1410	G
1	A	1416	G
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1434	A
1	A	1437	C
1	A	1451	C
1	A	1452	G
1	A	1453	A
1	A	1456	G
1	A	1458	U
1	A	1459	G
1	A	1461	C
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1480	C
1	A	1481	U
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1494	A
1	A	1498	C
1	A	1503	A
1	A	1504	A
1	A	1506	U
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1519	G
1	A	1522	A
1	A	1524	G

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Mol	Chain	Res	Type
1	A	1528	A
1	A	1529	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1540	G
1	A	1542	U
1	A	1543	G
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1566	A
1	A	1569	A
1	A	1572	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1582	C
1	A	1584	U
1	A	1585	C
1	A	1589	U
1	A	1590	A
1	A	1591	A
1	A	1607	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1612	C
1	A	1616	A
1	A	1617	C
1	A	1618	6MZ
1	A	1619	G
1	A	1622	G
1	A	1644	C
1	A	1647	U
1	A	1648	U
1	A	1649	G

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Mol	Chain	Res	Type
1	A	1651	G
1	A	1654	A
1	A	1672	A
1	A	1674	G
1	A	1675	C
1	A	1678	A
1	A	1679	A
1	A	1693	U
1	A	1695	G
1	A	1703	G
1	A	1715	G
1	A	1716	U
1	A	1717	A
1	A	1721	G
1	A	1722	A
1	A	1723	G
1	A	1724	G
1	A	1725	C
1	A	1726	G
1	A	1728	C
1	A	1729	U
1	A	1731	G
1	A	1733	U
1	A	1734	C
1	A	1735	G
1	A	1738	G
1	A	1739	A
1	A	1750	G
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1784	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1812	U
1	A	1816	C

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Mol	Chain	Res	Type
1	A	1818	U
1	A	1819	A
1	A	1839	G
1	A	1842	G
1	A	1847	G
1	A	1853	A
1	A	1857	G
1	A	1858	A
1	A	1863	G
1	A	1866	A
1	A	1867	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1884	G
1	A	1885	A
1	A	1890	A
1	A	1896	G
1	A	1902	C
1	A	1905	C
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1915	3TD
1	A	1916	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1942	C

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Mol	Chain	Res	Type
1	A	1955	U
1	A	1962	5MC
1	A	1964	G
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2029	G
1	A	2030	6MZ
1	A	2031	A
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2051	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2067	G
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2095	A
1	A	2097	A
1	A	2098	U

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Mol	Chain	Res	Type
1	A	2099	U
1	A	2100	G
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2186	G
1	A	2189	U
1	A	2190	G
1	A	2191	A
1	A	2192	U
1	A	2193	G
1	A	2194	U
1	A	2198	A
1	A	2199	A
1	A	2204	G
1	A	2211	A
1	A	2214	C
1	A	2220	U
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2238	G

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Mol	Chain	Res	Type
1	A	2239	G
1	A	2246	G
1	A	2263	C
1	A	2267	A
1	A	2268	A
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2292	U
1	A	2293	G
1	A	2295	C
1	A	2296	U
1	A	2297	A
1	A	2302	U
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2311	A
1	A	2315	G
1	A	2319	G
1	A	2321	U
1	A	2322	A
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2336	A
1	A	2337	G
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2352	A
1	A	2357	G
1	A	2361	G
1	A	2373	G
1	A	2377	A
1	A	2378	A
1	A	2383	G
1	A	2385	C
1	A	2391	G

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Mol	Chain	Res	Type
1	A	2392	A
1	A	2396	G
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A
1	A	2407	A
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2414	G
1	A	2423	U
1	A	2424	C
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2436	G
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2459	A
1	A	2469	A
1	A	2472	G
1	A	2473	U
1	A	2474	U
1	A	2475	C
1	A	2476	A
1	A	2481	G
1	A	2491	U
1	A	2492	U
1	A	2494	G
1	A	2502	G
1	A	2503	2MA
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2517	C
1	A	2518	A
1	A	2523	G
1	A	2529	G
1	A	2530	A

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Mol	Chain	Res	Type
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2574	G
1	A	2577	A
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2610	C
1	A	2613	U
1	A	2623	G
1	A	2624	G
1	A	2629	U
1	A	2636	C
1	A	2647	U
1	A	2649	C
1	A	2654	A
1	A	2656	U
1	A	2668	G
1	A	2669	G
1	A	2671	G
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2692	G
1	A	2702	G
1	A	2707	U
1	A	2708	G
1	A	2713	U
1	A	2714	G
1	A	2718	G
1	A	2721	A
1	A	2722	G
1	A	2724	U
1	A	2726	A
1	A	2729	G
1	A	2732	G

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Mol	Chain	Res	Type
1	A	2739	U
1	A	2740	A
1	A	2744	G
1	A	2748	A
1	A	2753	A
1	A	2758	A
1	A	2759	G
1	A	2761	A
1	A	2764	A
1	A	2765	A
1	A	2769	U
1	A	2771	C
1	A	2778	A
1	A	2782	G
1	A	2783	U
1	A	2784	U
1	A	2790	U
1	A	2791	G
1	A	2793	C
1	A	2796	C
1	A	2798	U
1	A	2799	G
1	A	2801	G
1	A	2803	G
1	A	2806	C
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2835	A
1	A	2837	A
1	A	2845	U
1	A	2849	U
1	A	2850	A
1	A	2853	C
1	A	2857	G
1	A	2859	G
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A

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Mol	Chain	Res	Type
1	A	2874	C
1	A	2879	A
1	A	2880	C
1	A	2881	U
1	A	2883	A
1	A	2884	U
1	A	2886	A
1	A	2891	U
1	A	2894	G
1	A	2897	U
1	A	2900	A
1	A	2901	C
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	5	U
2	B	6	G
2	B	11	C
2	B	12	C
2	B	13	G
2	B	15	A
2	B	22	U
2	B	23	G
2	B	24	G
2	B	33	G
2	B	34	A
2	B	35	C
2	B	36	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	46	A
2	B	47	C
2	B	51	G
2	B	53	A
2	B	56	G
2	B	57	A
2	B	59	A
2	B	61	G
2	B	64	G
2	B	66	A

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Mol	Chain	Res	Type
2	B	67	G
2	B	70	C
2	B	81	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	95	U
2	B	96	G
2	B	100	G
2	B	105	G
2	B	106	G
2	B	109	A
2	B	112	G
2	B	117	G
2	B	118	C
2	B	119	A
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	10	A
34	a	28	A
34	a	31	G
34	a	32	A
34	a	38	G
34	a	39	G
34	a	41	G
34	a	45	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	61	G
34	a	63	C
34	a	64	G
34	a	66	A
34	a	67	C

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Mol	Chain	Res	Type
34	a	68	G
34	a	69	G
34	a	70	U
34	a	72	A
34	a	73	C
34	a	76	G
34	a	77	A
34	a	78	A
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	98	A
34	a	99	C
34	a	100	G
34	a	102	G
34	a	107	G
34	a	112	G
34	a	115	G
34	a	116	A
34	a	121	U
34	a	122	G
34	a	129	A
34	a	130	A
34	a	131	A
34	a	140	U
34	a	141	G
34	a	142	G
34	a	144	G
34	a	145	G
34	a	146	G
34	a	149	A
34	a	151	A
34	a	152	A
34	a	161	A

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Mol	Chain	Res	Type
34	a	163	C
34	a	164	G
34	a	165	G
34	a	166	U
34	a	169	C
34	a	173	U
34	a	179	A
34	a	181	A
34	a	182	A
34	a	183	C
34	a	184	G
34	a	185	U
34	a	187	G
34	a	188	C
34	a	189	A
34	a	191	G
34	a	193	C
34	a	195	A
34	a	196	A
34	a	197	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	215	C
34	a	216	U
34	a	218	U
34	a	222	C
34	a	226	G
34	a	230	G
34	a	232	G
34	a	245	U
34	a	247	G
34	a	248	C
34	a	251	G
34	a	254	G
34	a	255	G
34	a	264	C

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Mol	Chain	Res	Type
34	a	266	G
34	a	267	C
34	a	271	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	282	A
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	308	C
34	a	319	G
34	a	321	A
34	a	323	U
34	a	324	G
34	a	328	C
34	a	329	A
34	a	330	C
34	a	331	G
34	a	335	C
34	a	341	C
34	a	343	U
34	a	345	C
34	a	346	G
34	a	349	A
34	a	352	C
34	a	354	G
34	a	366	A
34	a	367	U
34	a	368	U
34	a	370	C
34	a	372	C
34	a	373	A
34	a	376	G
34	a	380	G
34	a	381	C
34	a	382	A
34	a	383	A
34	a	384	G
34	a	385	C
34	a	386	C

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Mol	Chain	Res	Type
34	a	387	U
34	a	388	G
34	a	392	C
34	a	393	A
34	a	394	G
34	a	397	A
34	a	398	U
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	414	A
34	a	415	A
34	a	418	C
34	a	420	U
34	a	421	U
34	a	422	C
34	a	424	G
34	a	425	G
34	a	428	G
34	a	429	U
34	a	433	G
34	a	434	U
34	a	435	A
34	a	436	C
34	a	437	U
34	a	439	U
34	a	441	A
34	a	443	C
34	a	445	G
34	a	446	G
34	a	447	G
34	a	449	G
34	a	453	G
34	a	458	U
34	a	464	U
34	a	466	A
34	a	467	U
34	a	468	A
34	a	475	C

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Mol	Chain	Res	Type
34	a	477	C
34	a	480	U
34	a	484	G
34	a	485	U
34	a	486	U
34	a	490	C
34	a	491	G
34	a	492	C
34	a	495	A
34	a	496	A
34	a	497	G
34	a	499	A
34	a	500	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	513	C
34	a	517	G
34	a	518	C
34	a	520	A
34	a	521	G
34	a	525	C
34	a	527	7MG
34	a	531	U
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	548	G
34	a	550	G
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	579	A
34	a	594	U
34	a	596	A
34	a	601	G
34	a	602	A
34	a	608	A
34	a	612	C

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Mol	Chain	Res	Type
34	a	613	C
34	a	614	C
34	a	615	G
34	a	617	G
34	a	618	C
34	a	620	C
34	a	621	A
34	a	626	G
34	a	627	G
34	a	628	G
34	a	632	U
34	a	633	G
34	a	635	A
34	a	636	U
34	a	637	C
34	a	639	G
34	a	642	A
34	a	648	A
34	a	652	U
34	a	653	U
34	a	654	G
34	a	659	U
34	a	660	C
34	a	665	A
34	a	671	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	703	G
34	a	704	A
34	a	709	U
34	a	711	G
34	a	712	A
34	a	713	G
34	a	720	C
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	737	C

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Mol	Chain	Res	Type
34	a	742	G
34	a	753	A
34	a	754	C
34	a	755	G
34	a	758	C
34	a	759	A
34	a	769	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	821	G
34	a	832	G
34	a	836	G
34	a	840	C
34	a	843	U
34	a	844	G
34	a	846	G
34	a	848	C
34	a	849	G
34	a	852	G
34	a	872	A
34	a	884	U
34	a	885	G
34	a	899	C
34	a	902	G
34	a	914	A
34	a	926	G
34	a	932	C
34	a	934	C
34	a	935	A
34	a	939	G
34	a	951	G
34	a	960	U
34	a	961	U
34	a	966	2MG
34	a	969	A
34	a	971	G

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Mol	Chain	Res	Type
34	a	974	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	978	A
34	a	982	U
34	a	984	C
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1088	G
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1096	C
34	a	1098	C
34	a	1101	A
34	a	1104	G
34	a	1108	G

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Mol	Chain	Res	Type
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1145	A
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1157	A
34	a	1158	C
34	a	1159	U
34	a	1160	G
34	a	1162	C
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1171	A
34	a	1182	G
34	a	1184	G
34	a	1190	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1206	G
34	a	1211	U
34	a	1212	U
34	a	1213	A
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A

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Mol	Chain	Res	Type
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1238	A
34	a	1241	G
34	a	1244	G
34	a	1247	U
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1263	C
34	a	1266	G
34	a	1269	A
34	a	1270	G
34	a	1272	G
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1308	U
34	a	1312	G
34	a	1317	C
34	a	1318	A

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Mol	Chain	Res	Type
34	a	1320	C
34	a	1321	U
34	a	1331	G
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1352	C
34	a	1353	G
34	a	1360	A
34	a	1363	A
34	a	1368	A
34	a	1370	G
34	a	1371	G
34	a	1379	G
34	a	1380	U
34	a	1381	U
34	a	1382	C
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1438	G
34	a	1441	A
34	a	1442	G
34	a	1445	U
34	a	1446	A
34	a	1448	C
34	a	1450	U
34	a	1452	C
34	a	1458	G
34	a	1487	G
34	a	1492	A
34	a	1497	G
34	a	1502	A
34	a	1503	A

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Mol	Chain	Res	Type
34	a	1506	U
34	a	1517	G
34	a	1519	MA6
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	10	A
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	25	C
55	v	31	G
55	v	42	G
55	v	47	U
55	v	52	G
55	v	60	U
55	v	61	C
55	v	66	C
55	v	67	C
55	v	69	C
55	v	73	A
55	v	76	A
55	w	3	C
55	w	5	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C

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Mol	Chain	Res	Type
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A
55	w	67	C
55	w	69	C
55	w	70	G
55	w	71	C
55	w	73	A
55	w	75	C
55	w	76	A
56	x	14	C
56	x	15	U
56	x	23	C
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U

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Mol	Chain	Res	Type
57	y	21	A
57	y	24	G
57	y	28	G
57	y	30	G
57	y	31	A
57	y	33	U
57	y	36	A
57	y	37	MIA
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	56	C
57	y	59	U
57	y	61	C
57	y	65	G
57	y	75	C
57	y	76	A

All (98) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	84	A
1	A	85	G
1	A	101	A
1	A	119	A
1	A	141	G
1	A	162	U
1	A	196	A
1	A	204	A
1	A	242	G
1	A	265	A
1	A	282	A
1	A	290	U
1	A	301	G
1	A	362	A
1	A	411	G
1	A	547	A
1	A	555	G

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Mol	Chain	Res	Type
1	A	645	C
1	A	652	U
1	A	653	U
1	A	710	U
1	A	747	5MC
1	A	764	A
1	A	775	G
1	A	784	G
1	A	859	G
1	A	872	U
1	A	884	U
1	A	899	A
1	A	984	A
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1050	A
1	A	1069	A
1	A	1070	A
1	A	1089	A
1	A	1124	G
1	A	1130	U
1	A	1140	C
1	A	1190	G
1	A	1211	U
1	A	1240	U
1	A	1399	C
1	A	1419	A
1	A	1420	A
1	A	1432	G
1	A	1451	C
1	A	1452	G
1	A	1458	U
1	A	1475	G
1	A	1481	U
1	A	1490	A
1	A	1507	C
1	A	1508	A
1	A	1536	C
1	A	1538	G
1	A	1555	G
1	A	1607	C

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Mol	Chain	Res	Type
1	A	1608	A
1	A	1730	U
1	A	1818	U
1	A	1857	G
1	A	1875	G
1	A	1884	G
1	A	1939	5MU
1	A	1940	U
1	A	1964	G
1	A	1976	U
1	A	2099	U
1	A	2192	U
1	A	2296	U
1	A	2326	C
1	A	2391	G
1	A	2401	U
1	A	2407	A
1	A	2430	A
1	A	2517	C
1	A	2529	G
1	A	2566	A
1	A	2645	G
1	A	2712	C
1	A	2790	U
1	A	2808	G
1	A	2820	A
1	A	2849	U
1	A	2873	A
1	A	2893	A
1	A	2900	A
1	A	2902	C
2	B	4	C
2	B	34	A
2	B	41	G
2	B	44	G
2	B	46	A
2	B	56	G
2	B	89	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	747	1	19,22,23	1.84	3 (15%)	26,32,35	1.66	6 (23%)
34	MA6	a	1519	34	23,26,27	1.70	6 (26%)	33,38,41	2.34	12 (36%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
34	7MG	a	527	34	23,26,27	1.45	4 (17%)	27,39,42	2.48	7 (25%)
34	5MC	a	1407	34	19,22,23	1.68	2 (10%)	26,32,35	1.31	4 (15%)
1	PSU	A	2604	1	18,21,22	1.42	3 (16%)	21,30,33	1.99	4 (19%)
55	4SU	v	7	55	18,21,22	1.75	4 (22%)	25,30,33	2.42	5 (20%)
57	4SU	y	8	57	18,21,22	1.81	5 (27%)	25,30,33	2.37	7 (28%)
34	UR3	a	1498	34	19,22,23	1.09	2 (10%)	26,32,35	1.99	5 (19%)
57	MIA	y	37	57	28,31,32	2.44	7 (25%)	38,44,47	2.92	15 (39%)
34	5MC	a	967	34	19,22,23	1.84	2 (10%)	26,32,35	1.26	3 (11%)
1	OMG	A	2251	1,55,60	23,26,27	1.27	3 (13%)	32,38,41	1.94	7 (21%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.58	2 (10%)
1	7MG	A	2069	1,60	23,26,27	1.49	4 (17%)	27,39,42	2.54	10 (37%)
34	PSU	a	516	34	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
1	2MA	A	2503	1,60	22,25,26	1.51	5 (22%)	32,37,40	2.25	9 (28%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.22	5 (20%)
1	OMC	A	2498	1,60	19,22,23	0.88	1 (5%)	25,31,34	1.23	2 (8%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.39	4 (21%)
55	5MU	v	54	55	19,22,23	1.49	5 (26%)	27,32,35	1.91	8 (29%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
34	2MG	a	1207	34,60	23,26,27	1.24	3 (13%)	33,38,41	3.00	10 (30%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.07	5 (23%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	PSU	A	2605	1,60	18,21,22	1.42	2 (11%)	21,30,33	2.21	4 (19%)
1	2MG	A	2445	1	23,26,27	1.32	5 (21%)	33,38,41	2.29	8 (24%)
1	6MZ	A	1618	1	22,25,26	1.54	4 (18%)	29,36,39	2.29	10 (34%)
1	3TD	A	1915	1,60	19,22,23	7.04	13 (68%)	23,32,35	2.05	4 (17%)
1	PSU	A	2457	1	18,21,22	1.55	3 (16%)	21,30,33	2.00	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	2MG	a	1516	34	23,26,27	1.27	5 (21%)	33,38,41	2.42	12 (36%)
55	H2U	v	20	55	18,21,22	0.91	1 (5%)	19,30,33	1.63	4 (21%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
1	2MG	A	1835	1	23,26,27	1.28	3 (13%)	33,38,41	2.18	7 (21%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	27,32,35	2.12	8 (29%)
1	PSU	A	746	1,60	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.04	8 (29%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
1	1MG	A	745	1	23,26,27	1.29	3 (13%)	33,39,42	1.97	7 (21%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.48	4 (21%)
57	PSU	y	39	57	18,21,22	1.45	2 (11%)	21,30,33	2.01	4 (19%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.06	5 (23%)
1	5MC	A	1962	1	19,22,23	1.49	2 (10%)	26,32,35	1.24	3 (11%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.08	11 (40%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
57	7MG	y	46	57	23,26,27	1.43	4 (17%)	27,39,42	2.47	7 (25%)
34	4OC	a	1402	34,60	20,23,24	0.81	0	25,32,35	1.34	5 (20%)
34	2MG	a	966	34	23,26,27	1.28	3 (13%)	33,38,41	2.65	10 (30%)
34	MA6	a	1518	34	23,26,27	1.83	6 (26%)	33,38,41	2.19	10 (30%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)
1	H2U	A	2449	1	18,21,22	1.03	2 (11%)	19,30,33	1.49	3 (15%)
1	OMU	A	2552	1,60	19,22,23	1.39	2 (10%)	25,31,34	2.25	8 (32%)
55	PSU	v	55	55,60	18,21,22	1.38	3 (16%)	21,30,33	1.98	5 (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
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	5/15/33/34	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	1,55,60	-	0/9/27/28	0/3/3/3
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	0/7/25/26	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34,60	-	0/9/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
1	PSU	A	2605	1,60	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
1	6MZ	A	1618	1	-	3/9/27/28	0/3/3/3
1	3TD	A	1915	1,60	-	3/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	1/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	4/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
34	4OC	a	1402	34,60	-	2/9/29/30	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
55	PSU	v	55	55,60	-	2/7/25/26	0/2/2/2

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.11	1.66	1.43
1	A	1915	3TD	C6-C5	16.03	1.53	1.35
1	A	1915	3TD	C2'-C1'	-14.45	1.34	1.53
1	A	1915	3TD	C2-N1	8.02	1.47	1.37
57	y	37	MIA	C13-C14	7.18	1.53	1.32
1	A	747	5MC	C5-C4	6.87	1.49	1.44
57	y	37	MIA	C2-S10	-6.66	1.70	1.75
34	a	967	5MC	C5-C4	6.63	1.49	1.44
1	A	1915	3TD	C2-N3	6.41	1.52	1.38
1	A	1915	3TD	O4'-C4'	-6.03	1.31	1.45
34	a	1407	5MC	C5-C4	5.99	1.48	1.44
34	a	1518	MA6	C5-C4	5.48	1.48	1.39
1	A	1962	5MC	C5-C4	5.27	1.48	1.44
1	A	1915	3TD	C6-N1	4.99	1.44	1.36
57	y	37	MIA	C5-C4	4.97	1.47	1.39
55	w	8	4SU	C4-S4	-4.91	1.60	1.68
57	y	8	4SU	C4-S4	-4.85	1.60	1.68
34	a	1519	MA6	C5-C4	4.78	1.47	1.39
1	A	1618	6MZ	C5-C4	4.76	1.47	1.39
55	v	7	4SU	C4-S4	-4.76	1.60	1.68
1	A	2030	6MZ	C5-C4	4.74	1.47	1.39
1	A	2069	7MG	C4-N9	-4.57	1.32	1.37
34	a	516	PSU	C6-C5	4.48	1.40	1.35
57	y	39	PSU	C6-C5	4.43	1.40	1.35
57	y	55	PSU	C6-C5	4.35	1.40	1.35
1	A	2503	2MA	C5-C4	4.33	1.46	1.39
1	A	1911	PSU	C6-C5	4.28	1.40	1.35
1	A	2457	PSU	C6-C5	4.25	1.40	1.35
55	v	55	PSU	C6-C5	4.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2580	PSU	C6-C5	4.18	1.39	1.35
1	A	1917	PSU	C6-C5	4.18	1.39	1.35
1	A	2605	PSU	C6-C5	4.13	1.39	1.35
57	y	32	PSU	C6-C5	4.11	1.39	1.35
55	w	55	PSU	C6-C5	4.10	1.39	1.35
1	A	2504	PSU	C6-C5	4.00	1.39	1.35
1	A	746	PSU	C6-C5	3.73	1.39	1.35
1	A	955	PSU	C6-C5	3.70	1.39	1.35
34	a	527	7MG	C4-N9	-3.68	1.33	1.37
1	A	2604	PSU	C6-C5	3.64	1.39	1.35
57	y	46	7MG	C5-C4	3.50	1.48	1.37
34	a	967	5MC	C6-C5	3.41	1.40	1.34
34	a	527	7MG	C5-C4	3.36	1.48	1.37
55	v	54	5MU	C6-C5	3.32	1.40	1.34
57	y	46	7MG	C4-N9	-3.31	1.33	1.37
57	y	37	MIA	C5-C6	3.26	1.49	1.41
1	A	2552	OMU	C2-N1	3.24	1.43	1.38
34	a	1518	MA6	C5-C6	3.23	1.49	1.41
1	A	2251	OMG	C5-C4	3.18	1.47	1.38
34	a	966	2MG	C5-C4	3.16	1.47	1.38
55	w	54	5MU	C6-C5	3.15	1.39	1.34
34	a	1407	5MC	C6-C5	3.10	1.39	1.34
55	w	54	5MU	C2-N1	3.08	1.43	1.38
34	a	1207	2MG	C5-C4	3.03	1.47	1.38
57	y	54	5MU	C2-N1	3.03	1.43	1.38
34	a	1519	MA6	C5-N7	-3.03	1.33	1.39
55	w	8	4SU	C2-N1	3.02	1.43	1.38
1	A	2069	7MG	C5-C4	3.01	1.46	1.37
34	a	1519	MA6	C5-C6	3.00	1.49	1.41
34	a	1516	2MG	C5-C4	2.98	1.46	1.38
1	A	745	1MG	C2-N1	2.97	1.42	1.37
1	A	1835	2MG	C5-C4	2.95	1.46	1.38
57	y	8	4SU	C2-N1	2.94	1.43	1.38
1	A	1915	3TD	O2'-C2'	2.93	1.50	1.43
1	A	2251	OMG	C5-N7	-2.92	1.33	1.39
1	A	1915	3TD	O2-C2	-2.91	1.17	1.23
1	A	2552	OMU	C4-N3	-2.91	1.33	1.38
57	y	8	4SU	C4-N3	-2.84	1.34	1.37
55	w	8	4SU	C4-N3	-2.83	1.34	1.37
1	A	1618	6MZ	C5-C6	2.82	1.48	1.41
1	A	2030	6MZ	C5-C6	2.82	1.48	1.41
1	A	1915	3TD	C10-N3	-2.81	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	1MG	C5-C4	2.78	1.46	1.38
55	v	7	4SU	C2-N1	2.76	1.42	1.38
1	A	2445	2MG	C5-C4	2.75	1.46	1.38
57	y	54	5MU	C6-C5	2.73	1.39	1.34
55	w	54	5MU	C4-C5	2.73	1.49	1.44
1	A	2580	PSU	C4-N3	-2.73	1.33	1.38
55	v	7	4SU	C4-N3	-2.72	1.34	1.37
34	a	1518	MA6	C5-N7	-2.72	1.34	1.39
1	A	2604	PSU	C4-N3	-2.71	1.33	1.38
1	A	746	PSU	C4-N3	-2.70	1.33	1.38
1	A	2504	PSU	C4-N3	-2.68	1.33	1.38
34	a	1518	MA6	C4-N9	-2.65	1.32	1.37
1	A	747	5MC	C6-C5	2.65	1.38	1.34
1	A	1915	3TD	C4-N3	2.62	1.45	1.40
55	v	54	5MU	C4-N3	-2.62	1.34	1.38
1	A	2503	2MA	C5-N7	-2.58	1.34	1.39
1	A	745	1MG	C5-N7	-2.58	1.33	1.39
55	v	54	5MU	C2-N1	2.57	1.42	1.38
1	A	2605	PSU	C4-N3	-2.56	1.34	1.38
1	A	2457	PSU	C4-N3	-2.55	1.34	1.38
1	A	1915	3TD	O3'-C3'	-2.55	1.36	1.43
57	y	8	4SU	C5-C4	-2.54	1.39	1.42
1	A	2580	PSU	C2-N3	-2.53	1.33	1.37
1	A	955	PSU	C4-N3	-2.50	1.34	1.38
1	A	2445	2MG	C6-N1	-2.49	1.34	1.38
55	v	54	5MU	C4-C5	2.49	1.48	1.44
1	A	2445	2MG	C5-N7	-2.48	1.34	1.39
34	a	966	2MG	C2-N3	2.47	1.36	1.32
1	A	1939	5MU	C6-C5	2.47	1.38	1.34
1	A	2449	H2U	C2-N3	-2.46	1.33	1.38
1	A	2457	PSU	C2-N3	-2.43	1.33	1.37
55	v	7	4SU	C5-C4	-2.42	1.39	1.42
57	y	54	5MU	C4-C5	2.41	1.48	1.44
1	A	1835	2MG	C5-N7	-2.40	1.34	1.39
1	A	1915	3TD	C3'-C4'	2.40	1.59	1.53
1	A	2449	H2U	C4-N3	-2.40	1.33	1.37
57	y	37	MIA	C8-N7	2.39	1.36	1.31
1	A	1939	5MU	C6-N1	-2.39	1.33	1.38
57	y	37	MIA	C5-N7	-2.39	1.34	1.39
1	A	1835	2MG	C6-N1	-2.39	1.34	1.38
1	A	1618	6MZ	C8-N7	2.39	1.36	1.31
1	A	2030	6MZ	C8-N7	2.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	C4-N3	-2.38	1.34	1.38
1	A	1962	5MC	C6-C5	2.37	1.38	1.34
55	w	8	4SU	C5-C4	-2.37	1.39	1.42
1	A	2503	2MA	C4-N9	-2.35	1.32	1.37
34	a	966	2MG	C5-N7	-2.33	1.34	1.39
1	A	2503	2MA	C8-N7	2.33	1.36	1.31
1	A	2503	2MA	C5-C6	2.32	1.47	1.41
34	a	1519	MA6	C4-N9	-2.32	1.32	1.37
1	A	747	5MC	C6-N1	-2.28	1.34	1.38
57	y	54	5MU	C4-N3	-2.28	1.34	1.38
34	a	516	PSU	C4-N3	-2.27	1.34	1.38
1	A	1917	PSU	C4-N3	-2.26	1.34	1.38
1	A	1618	6MZ	C5-N7	-2.25	1.35	1.39
55	w	54	5MU	C4-N3	-2.24	1.34	1.38
57	y	32	PSU	C4-N3	-2.24	1.34	1.38
1	A	2251	OMG	C6-N1	-2.24	1.34	1.38
1	A	1911	PSU	C4-N3	-2.23	1.34	1.38
1	A	1939	5MU	C4-C5	2.23	1.48	1.44
57	y	55	PSU	C4-N3	-2.22	1.34	1.38
34	a	1518	MA6	C6-N6	2.22	1.42	1.36
55	v	55	PSU	C4-N3	-2.21	1.34	1.38
1	A	2030	6MZ	C5-N7	-2.19	1.35	1.39
34	a	1516	2MG	C2-N3	2.19	1.36	1.32
1	A	746	PSU	C2-N3	-2.18	1.33	1.37
34	a	1519	MA6	C6-N6	2.18	1.42	1.36
55	w	55	PSU	C4-N3	-2.17	1.34	1.38
57	y	37	MIA	C2-N1	2.16	1.37	1.34
1	A	2069	7MG	C5-N7	-2.16	1.32	1.35
1	A	2069	7MG	C6-N1	-2.16	1.34	1.38
34	a	1516	2MG	C5-N7	-2.15	1.34	1.39
34	a	1516	2MG	C4-N9	-2.14	1.32	1.38
34	a	1498	UR3	C2-N1	2.13	1.41	1.38
34	a	1516	2MG	C6-N1	-2.13	1.34	1.38
57	y	20	H2U	C2-N3	-2.13	1.34	1.38
57	y	16	H2U	C2-N3	-2.12	1.34	1.38
57	y	46	7MG	C5-C6	2.12	1.48	1.43
34	a	1498	UR3	C5-C4	-2.11	1.38	1.43
1	A	2604	PSU	C2-N3	-2.10	1.34	1.37
55	v	54	5MU	C2-N3	-2.10	1.34	1.38
34	a	527	7MG	C8-N9	2.09	1.47	1.45
57	y	39	PSU	C4-N3	-2.09	1.34	1.38
34	a	1207	2MG	C4-N9	-2.09	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	y	46	7MG	C8-N9	2.09	1.47	1.45
1	A	1939	5MU	C2-N1	2.08	1.41	1.38
1	A	2445	2MG	C2-N3	2.08	1.35	1.32
55	v	20	H2U	C2-N3	-2.07	1.34	1.38
55	w	8	4SU	C6-C5	2.07	1.39	1.35
1	A	2445	2MG	C4-N9	-2.07	1.32	1.38
34	a	1518	MA6	C8-N7	2.06	1.35	1.31
1	A	955	PSU	C2-N3	-2.06	1.34	1.37
1	A	2498	OMC	C5-C4	-2.04	1.38	1.42
34	a	1519	MA6	C8-N7	2.04	1.35	1.31
55	v	55	PSU	C4-C5	2.03	1.50	1.44
34	a	1207	2MG	C5-N7	-2.02	1.35	1.39
34	a	527	7MG	C6-N1	-2.01	1.35	1.38
55	w	20	H2U	C2-N3	-2.01	1.34	1.38
57	y	8	4SU	C6-C5	2.00	1.39	1.35

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1207	2MG	N1-C2-N2	8.86	125.60	116.56
57	y	37	MIA	C5-C4-N3	-8.39	118.34	127.18
34	a	966	2MG	C2-N3-C4	8.31	122.39	112.00
57	y	37	MIA	C12-C13-C14	-8.22	112.26	127.01
34	a	1207	2MG	C2-N3-C4	8.15	122.19	112.00
57	y	46	7MG	N9-C4-N3	8.06	137.26	125.46
34	a	527	7MG	N9-C4-N3	7.90	137.04	125.46
34	a	1516	2MG	C2-N3-C4	7.62	121.54	112.00
1	A	2445	2MG	C2-N3-C4	7.61	121.51	112.00
1	A	1835	2MG	C2-N3-C4	7.59	121.49	112.00
1	A	2069	7MG	N9-C4-N3	7.34	136.21	125.46
1	A	2503	2MA	C5-C4-N3	-7.23	119.57	127.18
55	v	7	4SU	C4-N3-C2	-6.90	120.70	127.31
34	a	1207	2MG	N2-C2-N3	-6.67	112.02	120.51
34	a	1498	UR3	C4-N3-C2	-6.66	119.22	124.58
1	A	2605	PSU	N1-C2-N3	6.54	122.07	115.17
34	a	966	2MG	C5-C4-N3	-6.44	118.14	128.39
57	y	8	4SU	C4-N3-C2	-6.38	121.20	127.31
1	A	2580	PSU	N1-C2-N3	6.30	121.82	115.17
1	A	2457	PSU	N1-C2-N3	6.21	121.72	115.17
1	A	2504	PSU	N1-C2-N3	6.20	121.71	115.17
1	A	1915	3TD	N1-C2-N3	6.15	120.60	116.13
1	A	2251	OMG	C5-C4-N3	-6.14	118.62	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	55	PSU	N1-C2-N3	6.13	121.64	115.17
1	A	1911	PSU	N1-C2-N3	6.13	121.64	115.17
1	A	1917	PSU	N1-C2-N3	6.13	121.63	115.17
57	y	32	PSU	N1-C2-N3	6.12	121.62	115.17
55	w	8	4SU	C4-N3-C2	-6.10	121.47	127.31
1	A	2503	2MA	N3-C4-N9	6.09	134.72	126.99
1	A	2445	2MG	C5-C4-N3	-6.08	118.71	128.39
34	a	966	2MG	N1-C2-N2	6.07	122.76	116.56
1	A	746	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	1835	2MG	C5-C4-N3	-5.98	118.87	128.39
57	y	37	MIA	N3-C4-N9	5.98	134.58	126.99
57	y	55	PSU	N1-C2-N3	5.93	121.42	115.17
1	A	955	PSU	N1-C2-N3	5.92	121.42	115.17
1	A	2604	PSU	N1-C2-N3	5.91	121.40	115.17
57	y	39	PSU	N1-C2-N3	5.90	121.39	115.17
34	a	1516	2MG	C5-C4-N3	-5.90	119.00	128.39
34	a	1207	2MG	C5-C4-N3	-5.88	119.03	128.39
1	A	2030	6MZ	C5-C4-N3	-5.86	118.65	126.72
55	v	55	PSU	N1-C2-N3	5.84	121.33	115.17
1	A	1618	6MZ	C5-C4-N3	-5.82	118.71	126.72
34	a	516	PSU	N1-C2-N3	5.70	121.18	115.17
1	A	1915	3TD	C4-N3-C2	-5.67	118.61	124.61
34	a	1519	MA6	C5-C4-N3	-5.61	118.99	126.72
55	v	7	4SU	C5-C4-N3	5.59	119.95	114.75
1	A	745	1MG	C5-C4-N3	-5.46	119.71	128.39
1	A	2552	OMU	N3-C2-N1	5.41	121.93	114.89
1	A	2552	OMU	C4-N3-C2	-5.32	120.01	126.61
57	y	8	4SU	C5-C4-N3	5.28	119.66	114.75
55	w	8	4SU	C5-C4-N3	5.25	119.63	114.75
55	v	54	5MU	N3-C2-N1	5.19	121.64	114.89
57	y	46	7MG	C5-C4-N3	-5.03	118.68	128.13
1	A	2069	7MG	C5-C4-N3	-5.01	118.73	128.13
1	A	1939	5MU	N3-C2-N1	4.96	121.34	114.89
34	a	527	7MG	C5-C4-N3	-4.95	118.83	128.13
34	a	1518	MA6	C2-N1-C6	4.92	123.84	111.83
55	w	54	5MU	N3-C2-N1	4.89	121.25	114.89
57	y	8	4SU	N3-C2-N1	4.83	121.17	114.89
1	A	1939	5MU	C4-N3-C2	-4.80	121.05	127.34
1	A	2069	7MG	C2-N3-C4	4.75	120.49	112.30
55	v	7	4SU	N3-C2-N1	4.75	121.08	114.89
1	A	2251	OMG	C2-N3-C4	4.73	120.45	112.30
34	a	1518	MA6	C5-C4-N3	-4.71	120.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1519	MA6	C2-N1-C6	4.70	123.30	111.83
34	a	1519	MA6	C4-C5-N7	-4.67	105.25	110.58
1	A	2251	OMG	N9-C4-N3	4.65	135.25	125.95
55	w	20	H2U	O4'-C1'-N1	4.63	115.61	109.30
1	A	2030	6MZ	N3-C4-N9	4.63	135.04	127.17
1	A	1618	6MZ	N3-C4-N9	4.62	135.03	127.17
57	y	46	7MG	C2-N3-C4	4.61	120.24	112.30
1	A	2069	7MG	N9-C8-N7	-4.60	96.87	103.37
1	A	745	1MG	C2-N3-C4	4.59	122.30	111.98
57	y	54	5MU	N3-C2-N1	4.59	120.87	114.89
1	A	2605	PSU	C4-N3-C2	-4.56	120.09	126.37
57	y	46	7MG	N9-C8-N7	-4.53	96.96	103.37
34	a	966	2MG	N9-C4-N3	4.48	134.91	125.95
55	w	8	4SU	N3-C2-N1	4.46	120.70	114.89
55	w	54	5MU	C4-N3-C2	-4.40	121.58	127.34
57	y	54	5MU	C4-N3-C2	-4.37	121.61	127.34
34	a	527	7MG	N9-C8-N7	-4.34	97.23	103.37
34	a	527	7MG	C2-N3-C4	4.34	119.77	112.30
57	y	37	MIA	C4-C5-N7	-4.30	105.66	110.58
34	a	1207	2MG	C6-C5-N7	4.28	138.07	130.29
57	y	54	5MU	C5-C4-N3	4.27	119.04	115.32
1	A	2445	2MG	N9-C4-N3	4.23	134.41	125.95
1	A	745	1MG	N9-C4-N3	4.22	134.39	125.95
55	v	7	4SU	C5-C4-S4	-4.19	119.52	124.31
55	v	54	5MU	C4-N3-C2	-4.19	121.85	127.34
57	y	39	PSU	O2-C2-N1	-4.18	118.47	122.79
1	A	1835	2MG	N9-C4-N3	4.17	134.29	125.95
1	A	955	PSU	C6-C5-C4	-4.15	115.37	118.17
1	A	2449	H2U	N3-C2-N1	4.15	120.82	116.65
1	A	746	PSU	C4-N3-C2	-4.11	120.70	126.37
1	A	955	PSU	C4-N3-C2	-4.10	120.72	126.37
55	w	54	5MU	C5-C4-N3	4.08	118.87	115.32
1	A	747	5MC	CM5-C5-C6	-4.06	117.36	122.85
57	y	8	4SU	C5-C4-S4	-4.05	119.67	124.31
1	A	1917	PSU	C4-N3-C2	-4.01	120.84	126.37
34	a	1516	2MG	C6-C5-N7	4.00	137.57	130.29
57	y	54	5MU	O4-C4-C5	-3.97	120.37	124.92
1	A	1911	PSU	C4-N3-C2	-3.97	120.90	126.37
55	v	54	5MU	C5-C4-N3	3.95	118.76	115.32
57	y	55	PSU	C4-N3-C2	-3.94	120.94	126.37
1	A	747	5MC	C5-C4-N3	-3.92	117.73	121.75
57	y	37	MIA	N6-C6-N1	3.92	123.58	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	55	PSU	C4-N3-C2	-3.89	121.01	126.37
34	a	966	2MG	N2-C2-N3	-3.88	115.56	120.51
1	A	2604	PSU	C4-N3-C2	-3.88	121.02	126.37
34	a	1518	MA6	O4'-C1'-N9	3.88	115.54	108.09
57	y	32	PSU	C4-N3-C2	-3.83	121.10	126.37
57	y	37	MIA	C16-C14-C13	-3.80	111.25	122.66
34	a	1518	MA6	N1-C2-N3	-3.80	122.83	128.58
34	a	1519	MA6	N3-C4-N9	3.80	133.62	127.17
1	A	1939	5MU	O4-C4-C5	-3.77	120.61	124.92
55	v	55	PSU	C4-N3-C2	-3.75	121.20	126.37
1	A	2030	6MZ	C2-N3-C4	3.70	120.88	111.83
1	A	1618	6MZ	C2-N3-C4	3.70	120.86	111.83
55	w	8	4SU	C5-C4-S4	-3.69	120.09	124.31
1	A	2552	OMU	C1'-N1-C2	3.68	124.19	117.59
1	A	2504	PSU	C4-N3-C2	-3.66	121.32	126.37
34	a	516	PSU	C4-N3-C2	-3.66	121.33	126.37
34	a	1516	2MG	N9-C4-N3	3.66	133.27	125.95
1	A	746	PSU	O2-C2-N1	-3.63	119.04	122.79
1	A	1939	5MU	C5-C4-N3	3.63	118.48	115.32
34	a	1498	UR3	C1'-N1-C2	3.62	122.97	117.04
34	a	1519	MA6	C10-N6-C6	-3.60	111.35	120.52
34	a	1516	2MG	N1-C2-N2	3.59	120.22	116.56
1	A	2552	OMU	C5-C4-N3	3.59	119.83	114.80
1	A	2605	PSU	O2-C2-N1	-3.57	119.11	122.79
57	y	54	5MU	C5M-C5-C4	3.56	122.58	118.78
34	a	1518	MA6	C4-C5-N7	-3.56	106.52	110.58
1	A	955	PSU	O2-C2-N1	-3.53	119.15	122.79
1	A	1911	PSU	O2-C2-N1	-3.53	119.15	122.79
57	y	37	MIA	C2-N3-C4	3.51	121.49	112.29
55	w	55	PSU	O2-C2-N1	-3.51	119.17	122.79
1	A	2580	PSU	C4-N3-C2	-3.50	121.55	126.37
34	a	1207	2MG	C4-C5-N7	-3.48	105.15	110.67
57	y	32	PSU	O2-C2-N1	-3.48	119.20	122.79
1	A	2030	6MZ	C4-C5-N7	-3.48	106.61	110.58
1	A	1618	6MZ	C4-C5-N7	-3.46	106.63	110.58
57	y	39	PSU	C4-N3-C2	-3.45	121.61	126.37
34	a	1518	MA6	C2-N3-C4	3.44	120.24	111.83
34	a	1498	UR3	C5-C4-N3	3.43	119.56	115.04
34	a	1519	MA6	C2-N3-C4	3.43	120.20	111.83
57	y	37	MIA	C15-C14-C13	-3.39	112.49	122.66
57	y	55	PSU	O2-C2-N1	-3.39	119.30	122.79
57	y	39	PSU	C6-C5-C4	-3.38	115.90	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1618	6MZ	C6-C5-N7	3.38	136.11	132.43
1	A	2503	2MA	N6-C6-N1	3.37	121.58	117.03
1	A	2030	6MZ	C6-C5-N7	3.37	136.10	132.43
57	y	37	MIA	C6-C5-N7	3.36	136.09	132.43
1	A	1917	PSU	C6-C5-C4	-3.35	115.91	118.17
1	A	745	1MG	N2-C2-N1	3.34	121.47	118.79
34	a	516	PSU	C3'-C2'-C1'	3.34	105.63	101.69
1	A	2457	PSU	C4-N3-C2	-3.32	121.80	126.37
55	w	54	5MU	C5M-C5-C4	3.32	122.32	118.78
55	v	55	PSU	O2-C2-N1	-3.32	119.37	122.79
1	A	1917	PSU	O2-C2-N1	-3.30	119.39	122.79
1	A	2445	2MG	C6-C5-N7	3.29	136.28	130.29
1	A	2503	2MA	C4-N9-C8	3.29	109.19	105.74
34	a	966	2MG	C6-C5-N7	3.29	136.27	130.29
34	a	1518	MA6	C9-N6-C6	-3.28	112.18	120.52
34	a	1207	2MG	N9-C4-N3	3.26	132.47	125.95
34	a	1519	MA6	N1-C2-N3	-3.25	123.67	128.58
34	a	1519	MA6	C5-N7-C8	3.23	108.53	103.45
34	a	516	PSU	C6-C5-C4	-3.22	116.00	118.17
1	A	1618	6MZ	N1-C2-N3	-3.22	123.71	128.58
1	A	1835	2MG	C6-C5-N7	3.20	136.12	130.29
1	A	1911	PSU	C6-C5-C4	-3.20	116.01	118.17
55	w	54	5MU	O4-C4-C5	-3.20	121.26	124.92
55	v	20	H2U	C3'-C2'-C1'	3.20	107.51	101.46
1	A	2030	6MZ	N1-C2-N3	-3.19	123.76	128.58
1	A	2457	PSU	O2-C2-N1	-3.15	119.54	122.79
1	A	1962	5MC	O2-C2-N3	-3.15	117.37	122.33
34	a	1516	2MG	C4-C5-N7	-3.14	105.70	110.67
57	y	20	H2U	O4'-C1'-N1	3.13	113.57	109.30
55	v	20	H2U	N3-C2-N1	3.13	119.80	116.65
34	a	967	5MC	O2-C2-N3	-3.13	117.40	122.33
34	a	1518	MA6	N3-C4-N9	3.13	132.48	127.17
1	A	2498	OMC	O2-C2-N3	-3.12	117.41	122.33
1	A	1618	6MZ	C9-N6-C6	-3.12	119.96	122.85
1	A	746	PSU	C6-C5-C4	-3.11	116.07	118.17
34	a	1407	5MC	O2-C2-N3	-3.11	117.42	122.33
57	y	37	MIA	C5-N7-C8	3.09	108.31	103.45
1	A	2030	6MZ	C9-N6-C6	-3.08	120.00	122.85
34	a	1407	5MC	C5-C4-N3	-3.06	118.61	121.75
34	a	967	5MC	C5-C4-N3	-3.06	118.62	121.75
57	y	8	4SU	C6-N1-C2	-3.06	117.28	121.00
1	A	2504	PSU	O2-C2-N1	-3.05	119.64	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	55	PSU	C6-C5-C4	-3.03	116.13	118.17
1	A	2069	7MG	C5-C6-N1	2.97	116.16	110.94
1	A	2605	PSU	C6-C5-C4	-2.96	116.18	118.17
55	v	54	5MU	O4-C4-C5	-2.96	121.53	124.92
34	a	527	7MG	C5-C6-N1	2.96	116.14	110.94
1	A	2552	OMU	O4-C4-C5	-2.93	120.10	125.16
57	y	46	7MG	C5-C6-N1	2.92	116.08	110.94
55	v	20	H2U	C5-C4-N3	2.90	119.78	116.69
55	w	55	PSU	C3'-C2'-C1'	2.89	105.10	101.69
34	a	516	PSU	O2-C2-N1	-2.88	119.82	122.79
1	A	1962	5MC	C5-C4-N3	-2.87	118.81	121.75
1	A	2552	OMU	O2-C2-N3	-2.85	116.22	121.49
55	w	20	H2U	C5-C6-N1	-2.85	102.91	111.52
55	v	55	PSU	C6-C5-C4	-2.83	116.26	118.17
1	A	1939	5MU	C5-C6-N1	-2.82	120.25	123.31
1	A	2445	2MG	N1-C2-N2	2.75	119.36	116.56
1	A	2604	PSU	O2-C2-N1	-2.73	119.97	122.79
1	A	2503	2MA	C4-C5-N7	-2.73	107.47	110.58
57	y	20	H2U	C5-C4-N3	2.72	119.58	116.69
1	A	2580	PSU	C3'-C2'-C1'	2.69	104.86	101.69
57	y	37	MIA	O4'-C1'-N9	2.68	113.24	108.09
34	a	1402	4OC	C6-C5-C4	2.67	120.22	117.00
1	A	2251	OMG	O6-C6-C5	-2.67	119.50	126.53
1	A	1618	6MZ	C4-N9-C8	2.67	108.54	105.74
1	A	747	5MC	O2-C2-N3	-2.63	118.18	122.33
34	a	1518	MA6	C3'-C2'-C1'	2.63	106.44	101.46
1	A	2030	6MZ	C4-N9-C8	2.62	108.49	105.74
1	A	2604	PSU	C6-C5-C4	-2.62	116.41	118.17
55	w	8	4SU	C6-N1-C2	-2.62	117.81	121.00
1	A	2580	PSU	O2-C2-N3	-2.59	117.26	121.86
1	A	2445	2MG	C4-C5-N7	-2.59	106.57	110.67
1	A	2552	OMU	C6-N1-C2	-2.57	117.86	121.00
57	y	16	H2U	C5-C4-N3	2.57	119.42	116.69
34	a	1516	2MG	N2-C2-N3	-2.56	117.25	120.51
55	v	20	H2U	O4'-C1'-N1	2.55	112.77	109.30
1	A	1618	6MZ	C5-N7-C8	2.54	107.44	103.45
1	A	2503	2MA	C2-N1-C6	2.54	122.00	118.10
34	a	966	2MG	C4-C5-N7	-2.54	106.65	110.67
34	a	1498	UR3	C3U-N3-C2	2.54	121.75	117.33
34	a	1207	2MG	C2-N1-C6	-2.54	121.48	124.55
1	A	2030	6MZ	C5-N7-C8	2.53	107.42	103.45
1	A	2580	PSU	C6-C5-C4	-2.50	116.49	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	32	PSU	C6-C5-C4	-2.50	116.49	118.17
57	y	37	MIA	C2-N1-C6	2.50	122.28	117.54
55	v	7	4SU	C6-N1-C2	-2.49	117.96	121.00
57	y	37	MIA	C16-C14-C15	-2.49	108.86	114.59
1	A	1618	6MZ	C3'-C2'-C1'	2.48	106.16	101.46
1	A	2030	6MZ	C3'-C2'-C1'	2.48	106.15	101.46
57	y	32	PSU	C3'-C2'-C1'	2.48	104.61	101.69
57	y	16	H2U	O4'-C1'-N1	2.46	112.65	109.30
34	a	1519	MA6	C4-C5-C6	2.46	118.45	115.91
34	a	527	7MG	O4'-C1'-N9	2.45	112.63	109.30
34	a	1402	4OC	O4'-C1'-N1	2.44	113.88	108.36
1	A	1835	2MG	N1-C2-N2	2.44	119.05	116.56
34	a	966	2MG	O6-C6-C5	-2.43	120.12	126.53
1	A	2457	PSU	C6-C5-C4	-2.42	116.54	118.17
1	A	2498	OMC	O4'-C1'-N1	2.41	113.83	108.36
57	y	37	MIA	N3-C2-N1	-2.41	122.59	127.00
1	A	747	5MC	C3'-C2'-C1'	2.41	106.03	101.46
1	A	2069	7MG	O4'-C1'-N9	2.41	112.58	109.30
57	y	20	H2U	C3'-C2'-C1'	2.40	106.00	101.46
1	A	2449	H2U	C5-C4-N3	2.39	119.23	116.69
34	a	1402	4OC	C2'-C1'-N1	-2.38	109.72	114.24
55	w	55	PSU	C6-C5-C4	-2.38	116.57	118.17
1	A	747	5MC	C5-C6-N1	-2.38	120.73	123.31
1	A	1962	5MC	CM5-C5-C6	-2.37	119.64	122.85
34	a	1516	2MG	C2-N1-C6	-2.37	121.69	124.55
1	A	2069	7MG	N2-C2-N3	-2.37	115.05	119.67
34	a	967	5MC	C3'-C2'-C1'	2.36	105.93	101.46
55	v	54	5MU	C6-N1-C2	-2.35	118.96	121.30
34	a	1402	4OC	O2-C2-N3	-2.35	118.62	122.33
1	A	1939	5MU	O2-C2-N1	-2.34	119.75	122.80
1	A	2503	2MA	N9-C8-N7	-2.33	110.63	113.94
1	A	745	1MG	O6-C6-C5	-2.32	118.61	124.59
34	a	1402	4OC	C5-C4-N3	-2.32	118.97	122.60
1	A	2251	OMG	C6-C5-N7	2.32	134.50	130.29
57	y	54	5MU	C1'-N1-C2	2.31	121.74	117.59
1	A	2552	OMU	O4'-C1'-N1	2.30	113.58	108.36
1	A	2445	2MG	O6-C6-C5	-2.30	120.47	126.53
1	A	1835	2MG	O6-C6-C5	-2.30	120.47	126.53
57	y	8	4SU	O2-C2-N3	-2.29	117.26	121.49
34	a	1516	2MG	O6-C6-C5	-2.29	120.48	126.53
34	a	1407	5MC	O4'-C1'-N1	2.29	113.55	108.36
55	w	54	5MU	C5M-C5-C6	-2.29	119.75	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	527	7MG	O6-C6-C5	-2.29	122.01	127.62
1	A	1835	2MG	C4-C5-N7	-2.28	107.06	110.67
1	A	1915	3TD	C3'-C2'-C1'	2.27	104.36	101.69
57	y	16	H2U	C3'-C2'-C1'	2.27	105.75	101.46
1	A	2251	OMG	O2'-C2'-C1'	2.26	113.29	108.99
57	y	54	5MU	C5M-C5-C6	-2.26	119.79	122.85
55	w	54	5MU	C3'-C2'-C1'	2.26	105.73	101.46
34	a	1519	MA6	C9-N6-C6	-2.26	114.78	120.52
1	A	2503	2MA	C5-N7-C8	2.25	106.99	103.45
55	w	54	5MU	O4'-C1'-N1	2.25	113.47	108.36
1	A	2504	PSU	C6-C5-C4	-2.25	116.65	118.17
1	A	1939	5MU	C5M-C5-C4	2.25	121.18	118.78
34	a	966	2MG	C2-N1-C6	-2.24	121.84	124.55
1	A	2445	2MG	C2-N1-C6	-2.24	121.84	124.55
1	A	745	1MG	C4-C5-N7	-2.23	107.14	110.67
57	y	8	4SU	C1'-N1-C2	2.22	121.58	117.59
1	A	745	1MG	C6-C5-N7	2.21	134.28	129.36
1	A	2069	7MG	O6-C6-C5	-2.21	122.19	127.62
34	a	966	2MG	C5-C6-N1	2.21	118.87	113.25
34	a	1519	MA6	C10-N6-C9	-2.20	109.11	116.18
1	A	2069	7MG	N2-C2-N1	2.18	121.37	116.76
34	a	1407	5MC	C5-C6-N1	-2.18	120.94	123.31
34	a	1516	2MG	C2'-C1'-N9	-2.17	107.22	113.25
55	v	54	5MU	C5-C6-N1	-2.17	120.96	123.31
57	y	46	7MG	C6-C5-C4	-2.14	118.63	122.40
1	A	2503	2MA	C6-C5-N7	2.14	136.22	132.09
1	A	747	5MC	N1-C2-N3	2.14	122.51	118.80
34	a	1207	2MG	O6-C6-C5	-2.13	120.91	126.53
57	y	46	7MG	O6-C6-C5	-2.13	122.39	127.62
55	v	54	5MU	O4'-C1'-N1	2.11	113.13	108.36
34	a	1516	2MG	O4'-C1'-N9	2.10	113.12	108.36
55	v	54	5MU	O2-C2-N3	-2.09	117.64	121.49
57	y	54	5MU	C6-N1-C2	-2.09	119.23	121.30
34	a	1518	MA6	C5-N7-C8	2.08	106.72	103.45
34	a	1207	2MG	C8-N7-C5	2.08	107.96	104.26
1	A	2251	OMG	C4-C5-N7	-2.08	107.38	110.67
34	a	1516	2MG	C5-C6-N1	2.07	118.52	113.25
55	w	54	5MU	C5-C6-N1	-2.06	121.07	123.31
57	y	55	PSU	C3'-C2'-C1'	2.06	104.12	101.69
1	A	1915	3TD	O4-C4-C5	-2.06	119.02	122.58
34	a	1519	MA6	N9-C8-N7	-2.06	111.02	113.94
1	A	2449	H2U	O4'-C1'-N1	2.05	112.10	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	16	H2U	C5-C6-N1	-2.05	105.31	111.52
55	w	54	5MU	O2-C2-N3	-2.05	117.71	121.49
57	y	20	H2U	C5-C6-N1	-2.05	105.33	111.52
55	v	55	PSU	C3'-C2'-C1'	2.04	104.09	101.69
1	A	2457	PSU	C3'-C2'-C1'	2.03	104.08	101.69
55	w	54	5MU	C6-N1-C2	-2.01	119.30	121.30
1	A	1939	5MU	C5M-C5-C6	-2.01	120.13	122.85
34	a	1498	UR3	O4-C4-C5	-2.01	118.66	124.35
1	A	2069	7MG	C6-C5-C4	-2.01	118.87	122.40
57	y	37	MIA	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C2'-C1'-C5-C4
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	20	H2U	O4'-C1'-N1-C2
55	v	20	H2U	O4'-C1'-N1-C6
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	O4'-C4'-C5'-O5'
57	y	20	H2U	O4'-C1'-N1-C2
57	y	20	H2U	O4'-C1'-N1-C6
57	y	37	MIA	O4'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
57	y	37	MIA	C12-C13-C14-C16
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	w	8	4SU	C3'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C8
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C4
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
55	w	8	4SU	C2'-C1'-N1-C6
57	y	37	MIA	C3'-C4'-C5'-O5'
1	A	1915	3TD	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C2
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
1	A	2604	PSU	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	20	H2U	C4'-C5'-O5'-P
1	A	1917	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
1	A	1618	6MZ	C3'-C4'-C5'-O5'
55	v	20	H2U	C3'-C4'-C5'-O5'
34	a	527	7MG	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
55	w	8	4SU	O4'-C1'-N1-C2
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	2604	PSU	C3'-C4'-C5'-O5'
34	a	527	7MG	C4'-C5'-O5'-P
34	a	966	2MG	C3'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C4
57	y	32	PSU	O4'-C1'-C5-C4
57	y	39	PSU	O4'-C1'-C5-C4
34	a	1519	MA6	C4'-C5'-O5'-P
1	A	2457	PSU	O4'-C4'-C5'-O5'
55	v	7	4SU	C3'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
1	A	1939	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	w	20	H2U	C2'-C1'-N1-C6
57	y	46	7MG	O4'-C1'-N9-C8
55	w	55	PSU	O4'-C1'-C5-C6
57	y	39	PSU	O4'-C1'-C5-C6
34	a	966	2MG	O4'-C4'-C5'-O5'
57	y	37	MIA	N3-C2-S10-C11
1	A	746	PSU	C2'-C1'-C5-C6
1	A	1915	3TD	C2'-C1'-C5-C6
57	y	8	4SU	C2'-C1'-N1-C2
1	A	1618	6MZ	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1519	MA6	1	0
1	A	2604	PSU	1	0
34	a	1207	2MG	1	0
1	A	2030	6MZ	10	0
1	A	2445	2MG	1	0
1	A	1618	6MZ	1	0
1	A	1915	3TD	2	0
1	A	1939	5MU	1	0
1	A	2504	PSU	1	0
34	a	1518	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1481 ligands modelled in this entry, 1478 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	FME	A	3001	-	8,9,10	0.52	0	8,9,11	1.03	0
62	PHE	z	401	-	10,11,12	0.39	0	8,13,15	0.19	0
63	GTP	z	402	60	33,34,34	1.17	3 (9%)	50,54,54	1.74	7 (14%)

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
59	FME	A	3001	-	-	0/7/9/11	-
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
63	GTP	z	402	60	-	7/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.08	1.47	1.38
63	z	402	GTP	C6-N1	-2.68	1.33	1.38
63	z	402	GTP	C5-N7	-2.14	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	402	GTP	C5-C4-N3	-6.33	118.31	128.39
63	z	402	GTP	C2-N3-C4	5.18	121.22	112.30
63	z	402	GTP	N9-C4-N3	4.80	135.55	125.95
63	z	402	GTP	C6-C5-N7	3.10	135.93	130.29
63	z	402	GTP	C4-C5-N7	-2.40	106.86	110.67
63	z	402	GTP	C3'-C2'-C1'	2.25	105.71	101.46
63	z	402	GTP	O6-C6-C5	-2.18	120.78	126.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C5'-O5'-PA-O3A
63	z	402	GTP	C5'-O5'-PA-O1A
63	z	402	GTP	C5'-O5'-PA-O2A
63	z	402	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
63	z	402	GTP	O4'-C4'-C5'-O5'
63	z	402	GTP	PB-O3B-PG-O1G
63	z	402	GTP	C4'-C5'-O5'-PA

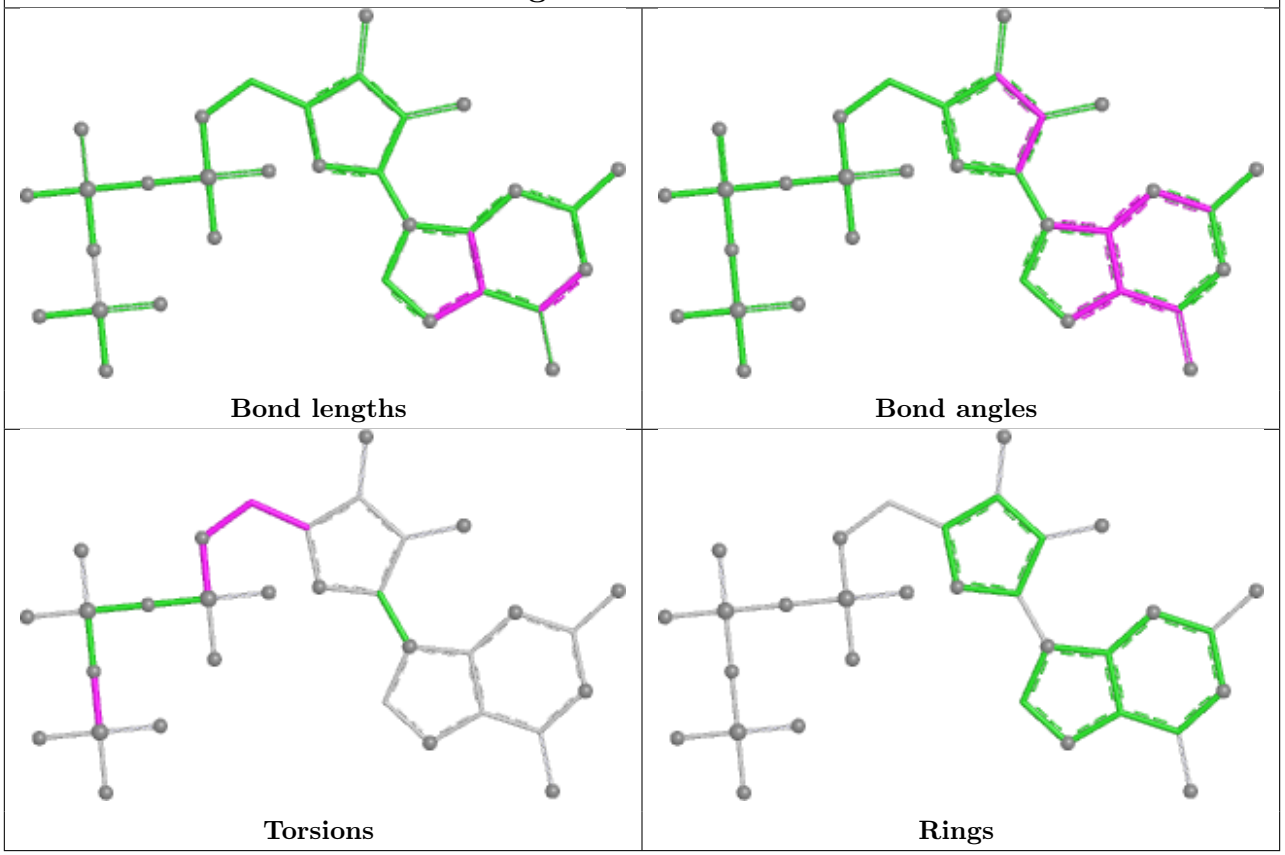
There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	z	402	GTP	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP z 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

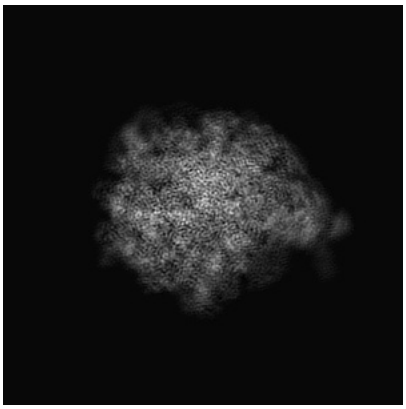
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8829. These allow visual inspection of the internal detail of the map and identification of artifacts.

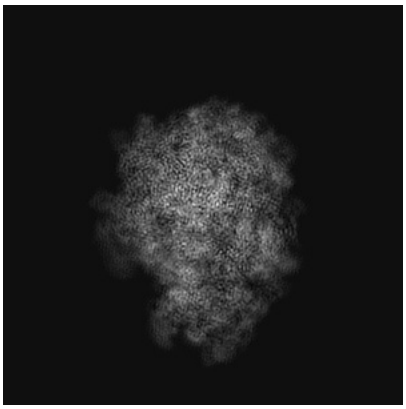
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

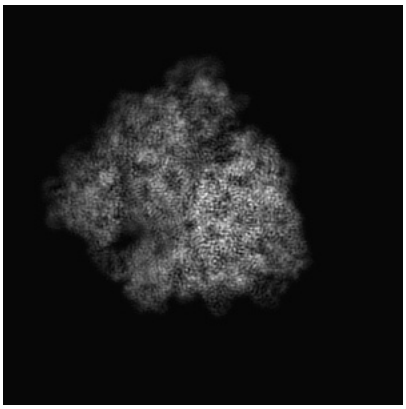
6.1.1 Primary map



X

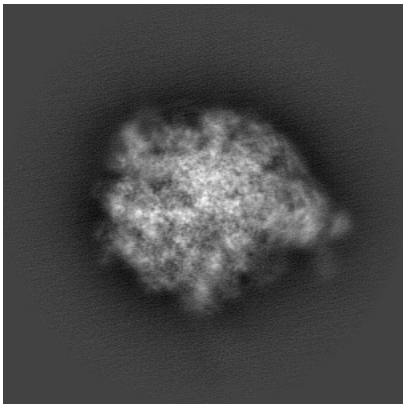


Y

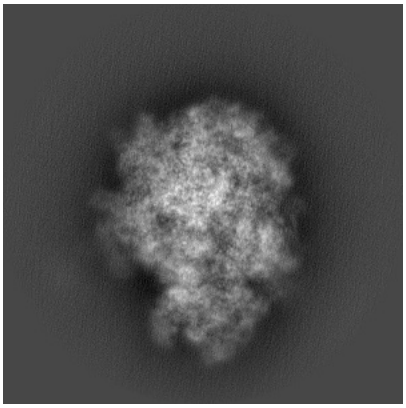


Z

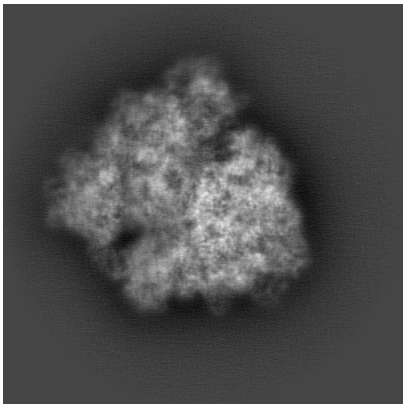
6.1.2 Raw map



X



Y

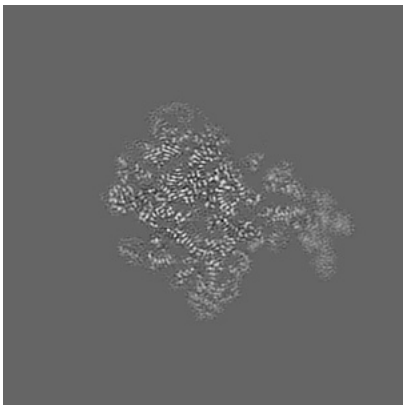


Z

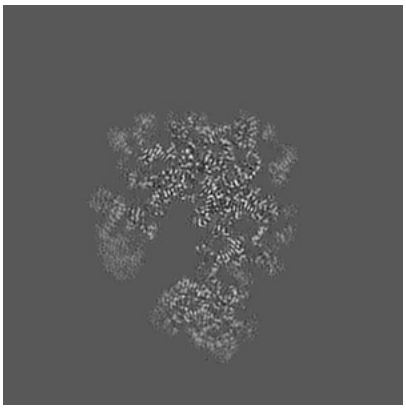
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

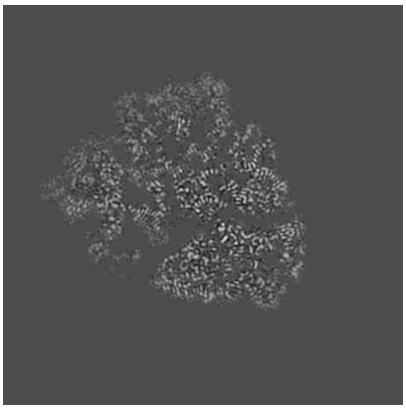
6.2.1 Primary map



X Index: 199

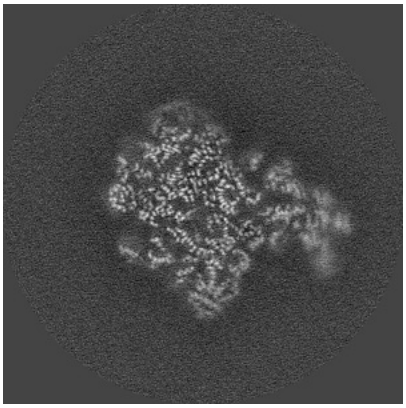


Y Index: 199

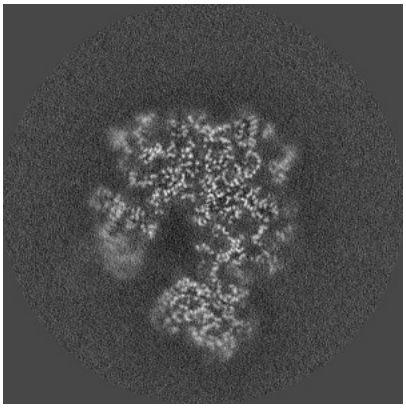


Z Index: 199

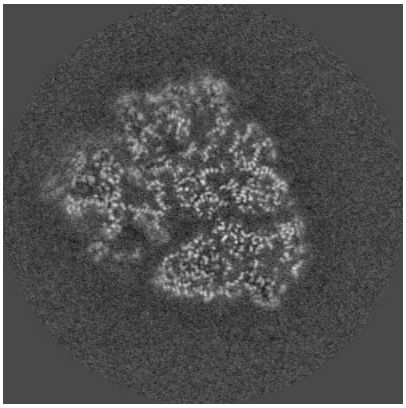
6.2.2 Raw map



X Index: 199



Y Index: 199

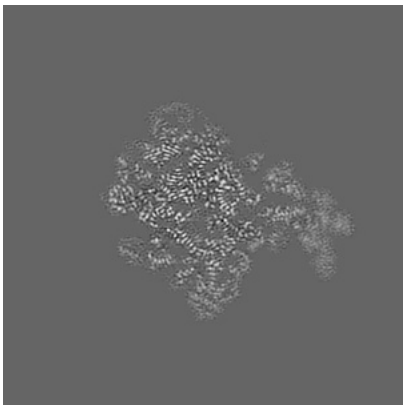


Z Index: 199

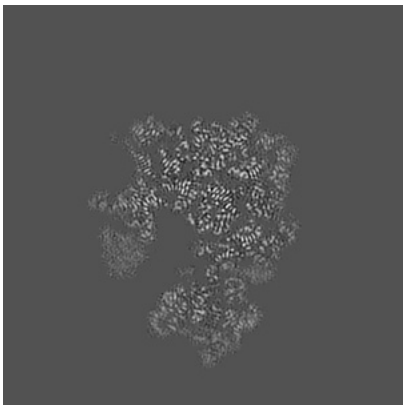
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

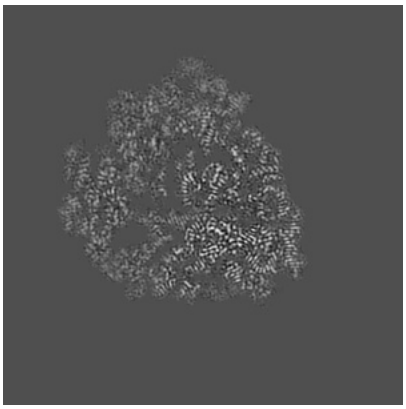
6.3.1 Primary map



X Index: 199

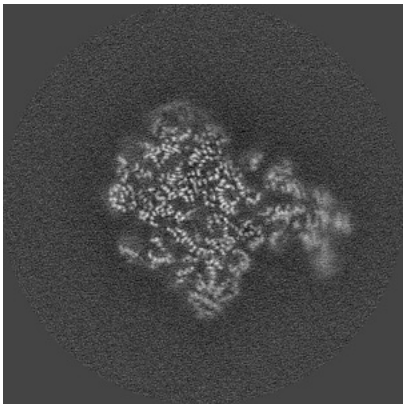


Y Index: 207

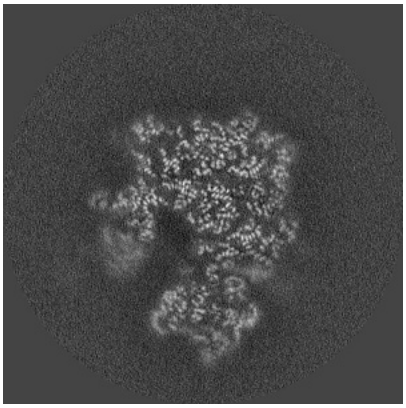


Z Index: 190

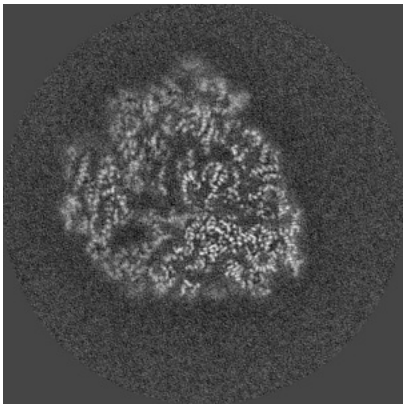
6.3.2 Raw map



X Index: 199



Y Index: 207

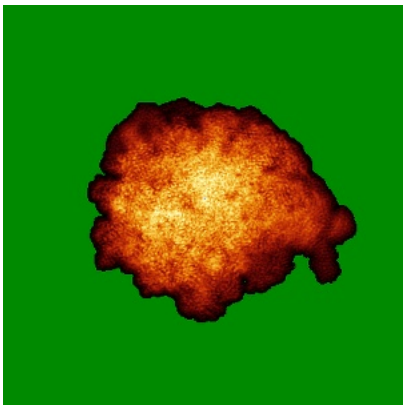


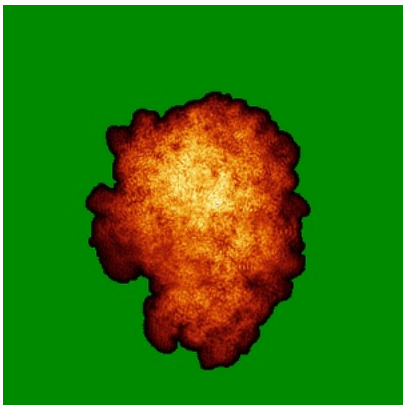
Z Index: 190

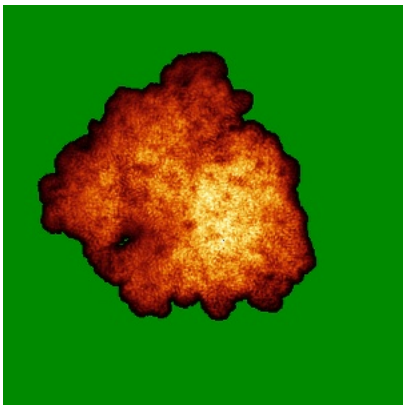
The images above show the largest variance slices of the map in three orthogonal directions.

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

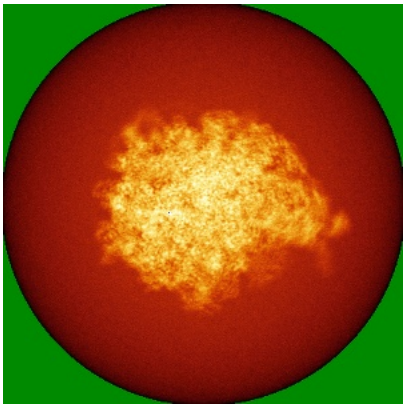
6.4.1 Primary map

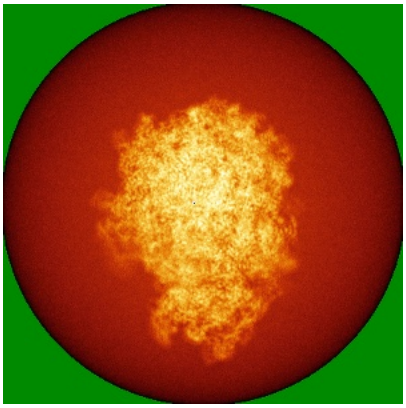

X

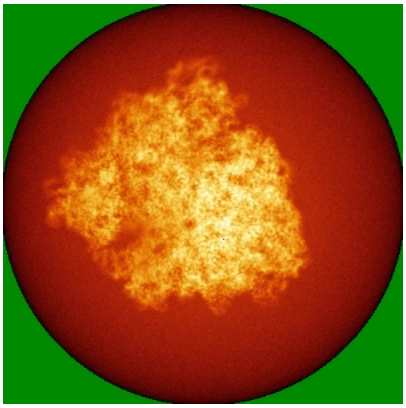

Y


Z

6.4.2 Raw map


X

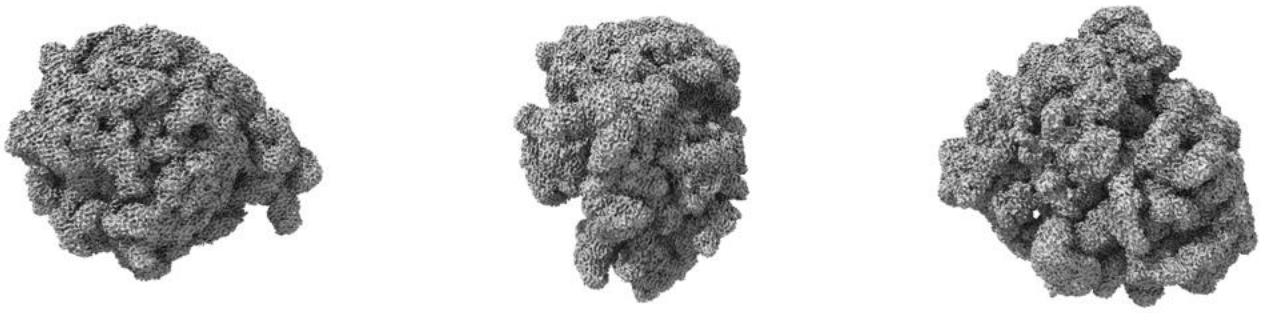

Y


Z

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

6.5 Orthogonal surface views (i)

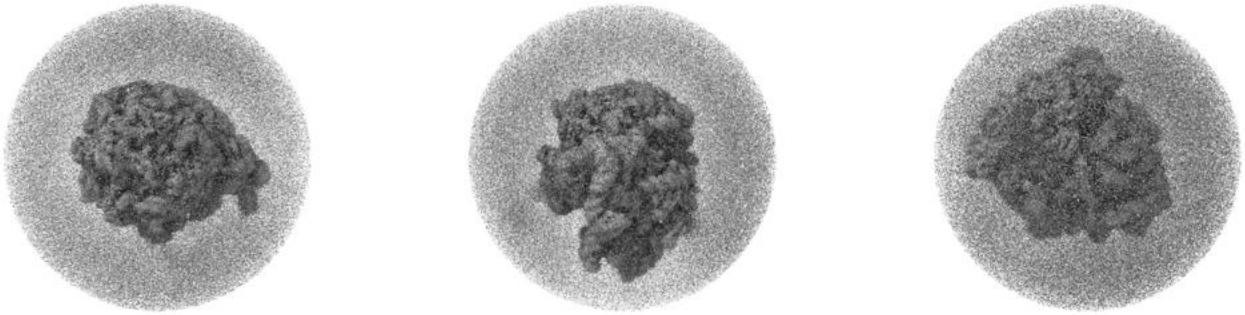
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00532. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

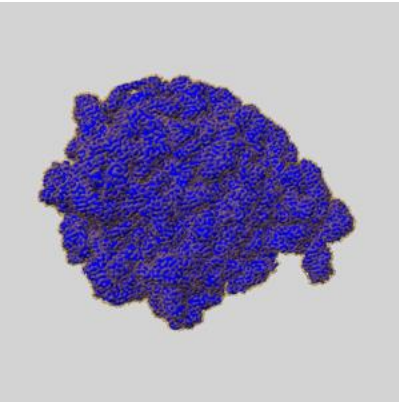
6.6 Mask visualisation (i)

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

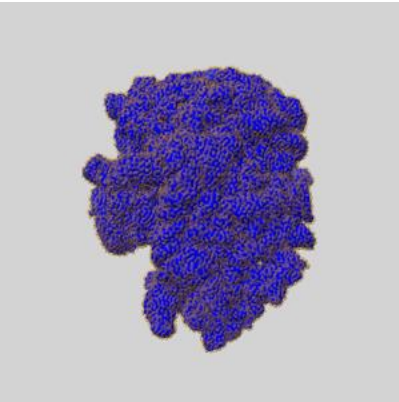
A mask typically either:

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

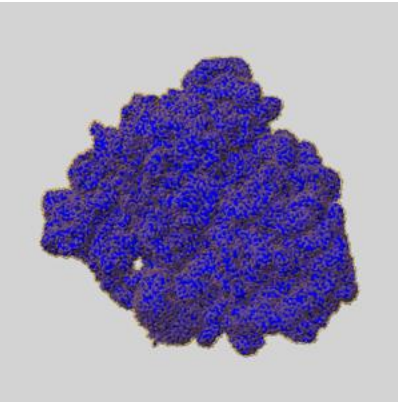
6.6.1 emd_8829_msk_1.map (i)



X



Y

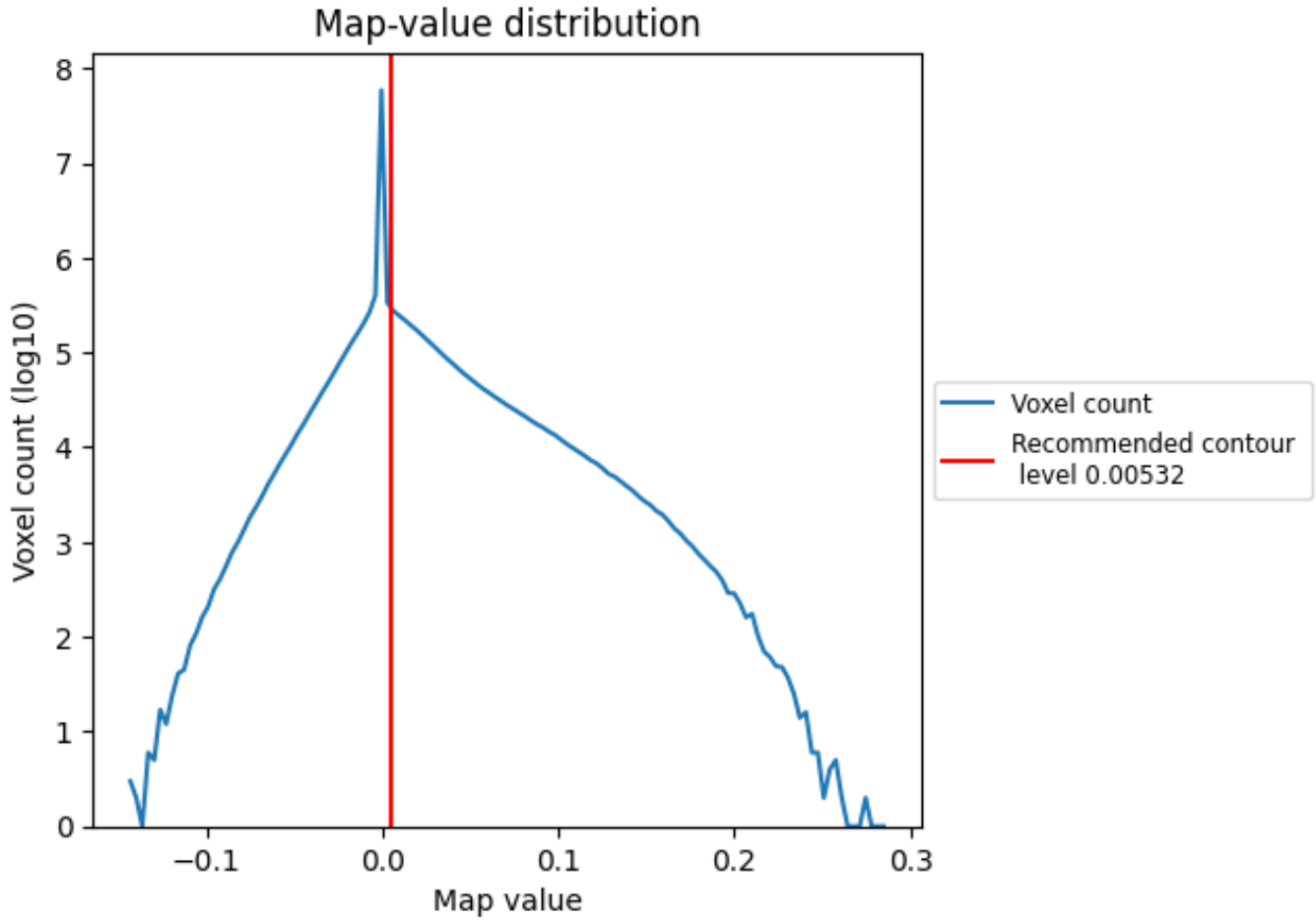


Z

7 Map analysis

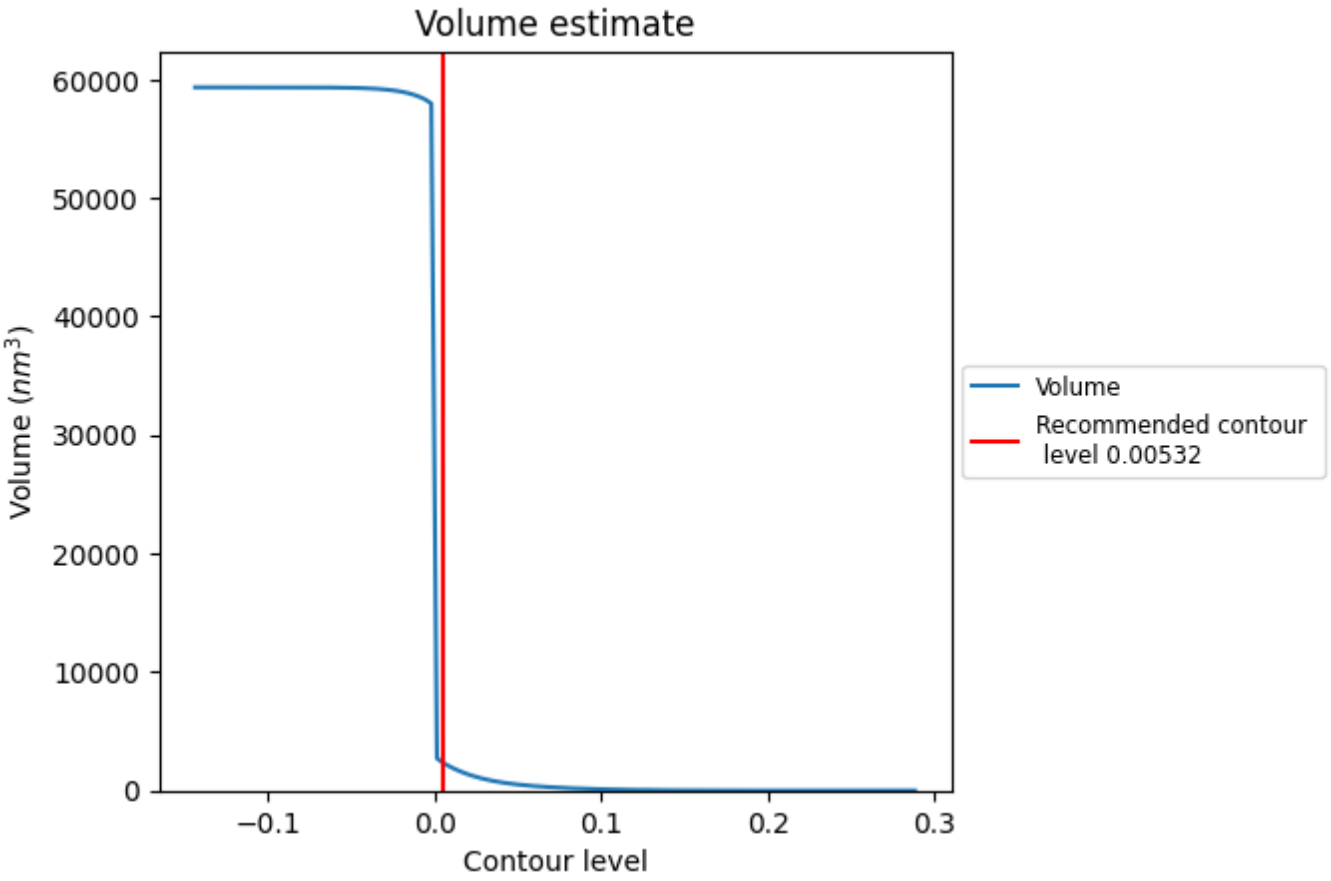
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

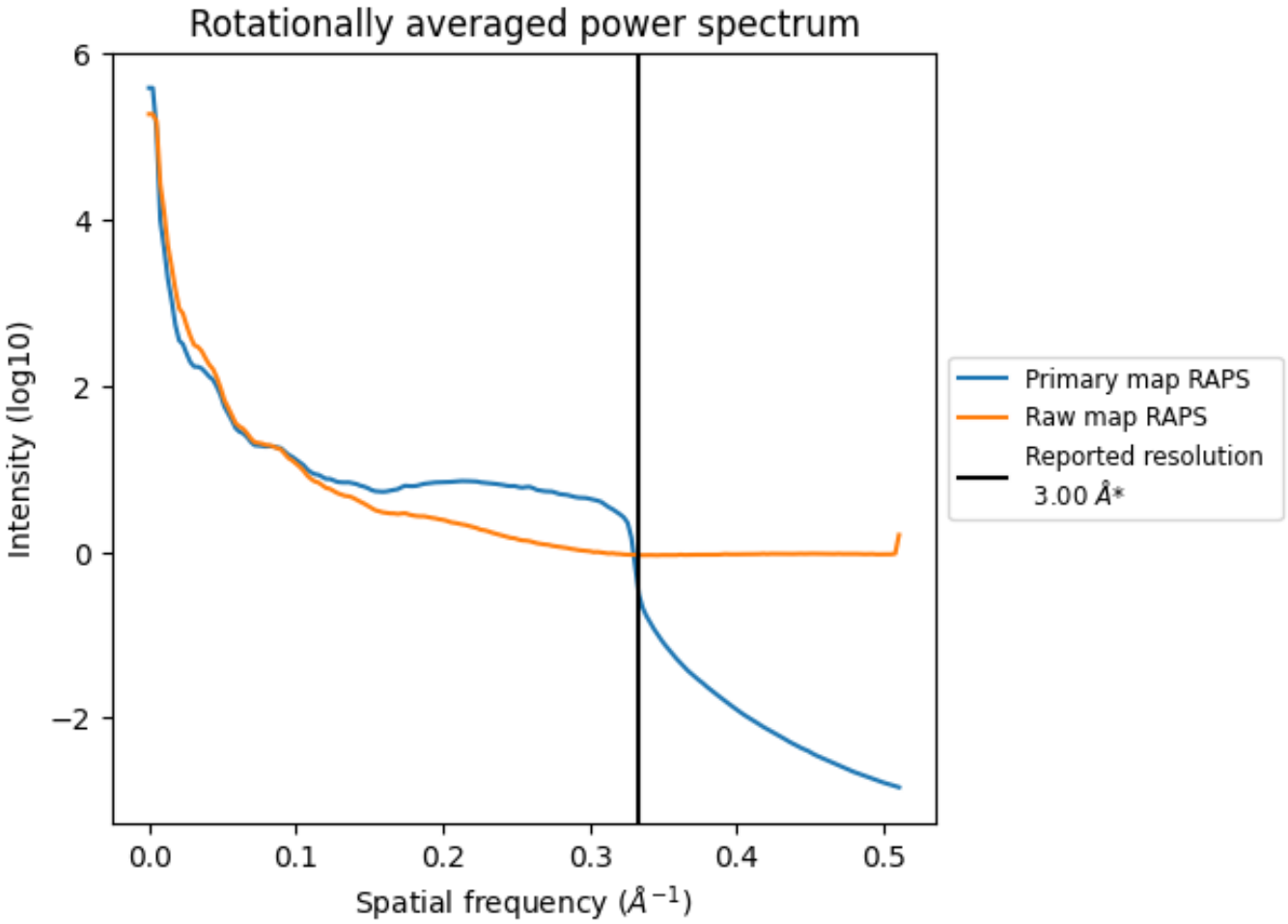
7.2 Volume estimate



The volume at the recommended contour level is 2339 nm^3; this corresponds to an approximate mass of 2113 kDa.

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

7.3 Rotationally averaged power spectrum (i)

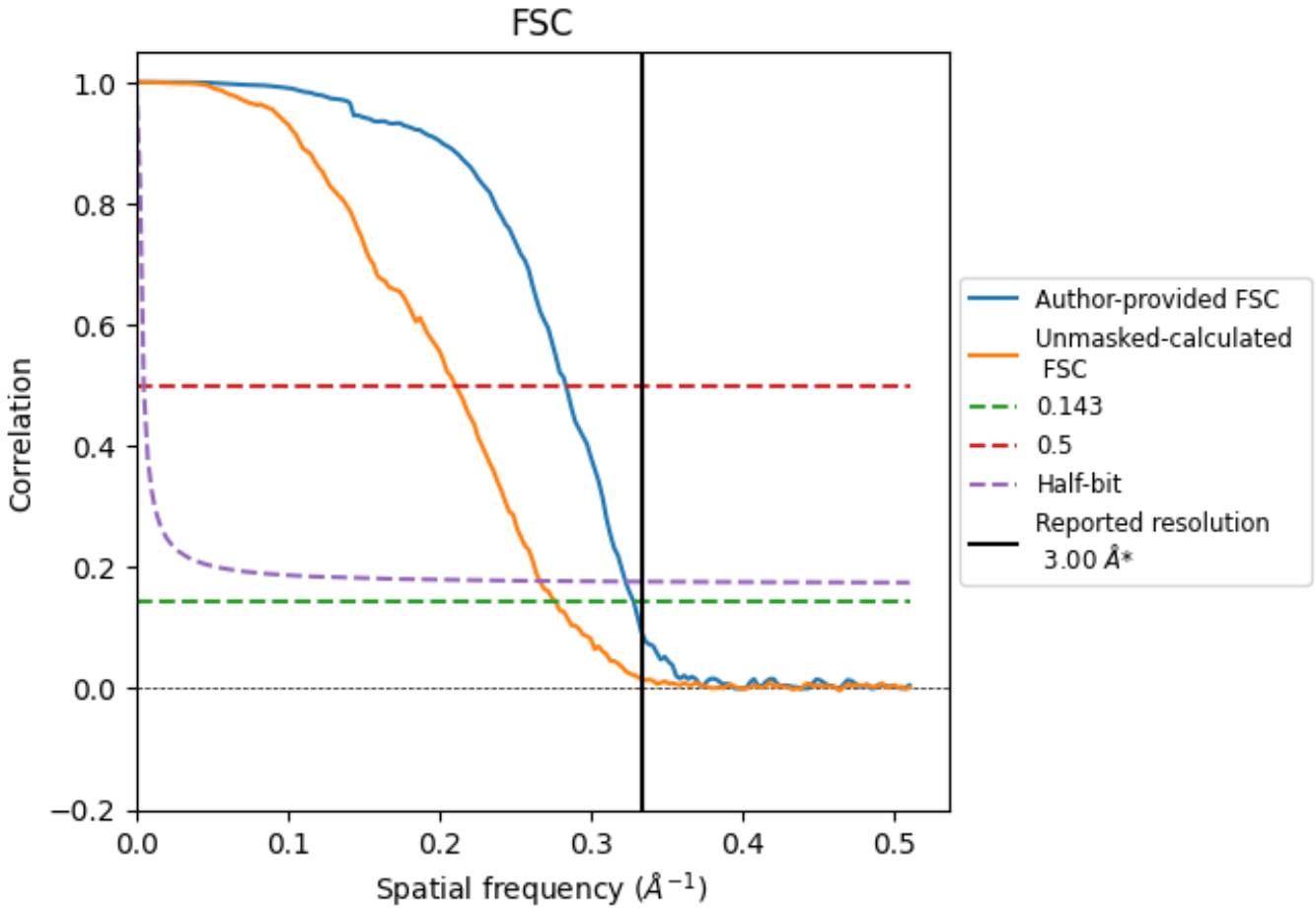


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

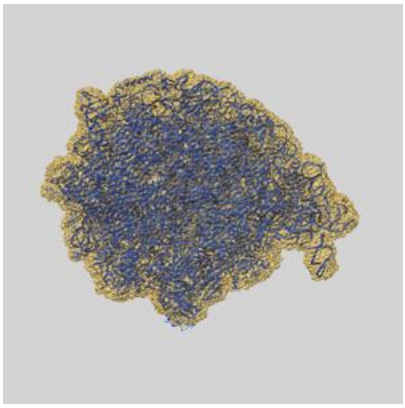
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 3.0 by more than 10 %

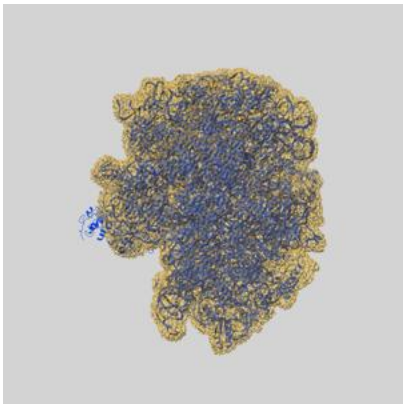
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section 3 on page 20.

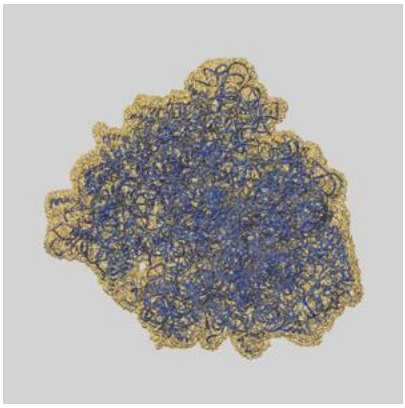
9.1 Map-model overlay



X



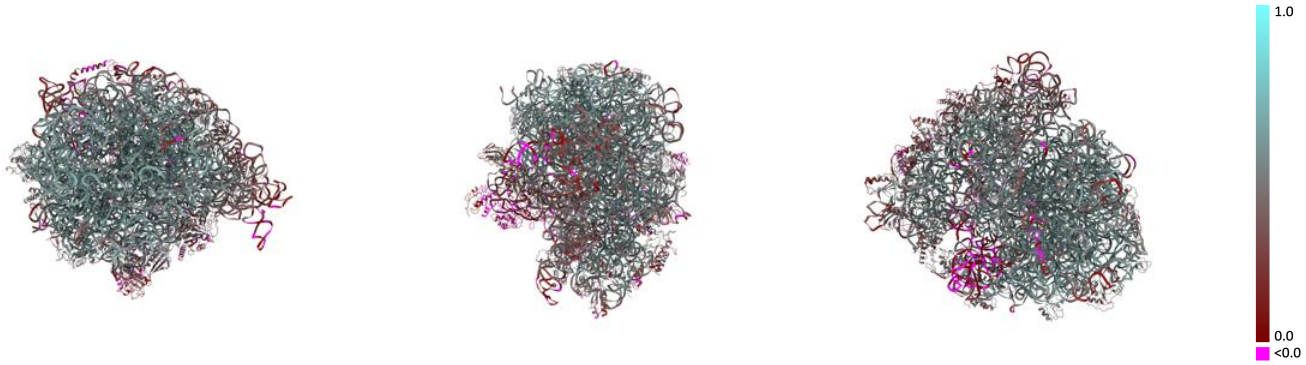
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

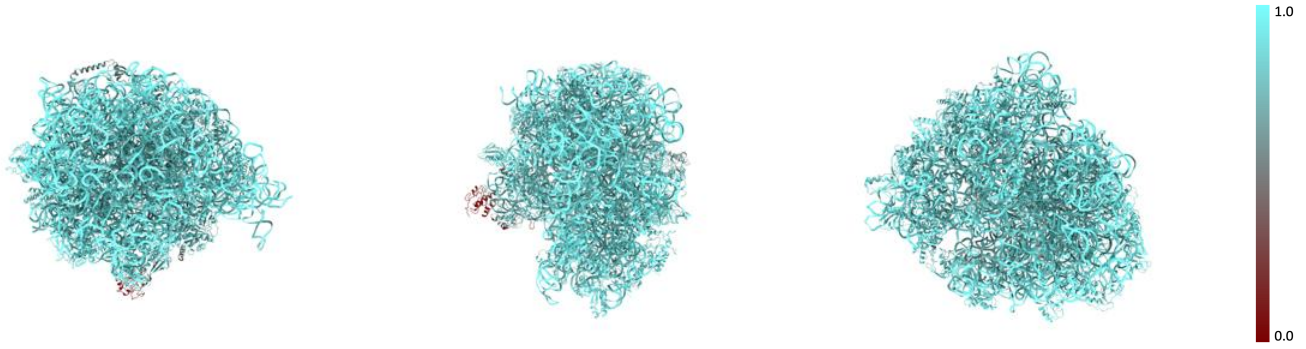
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

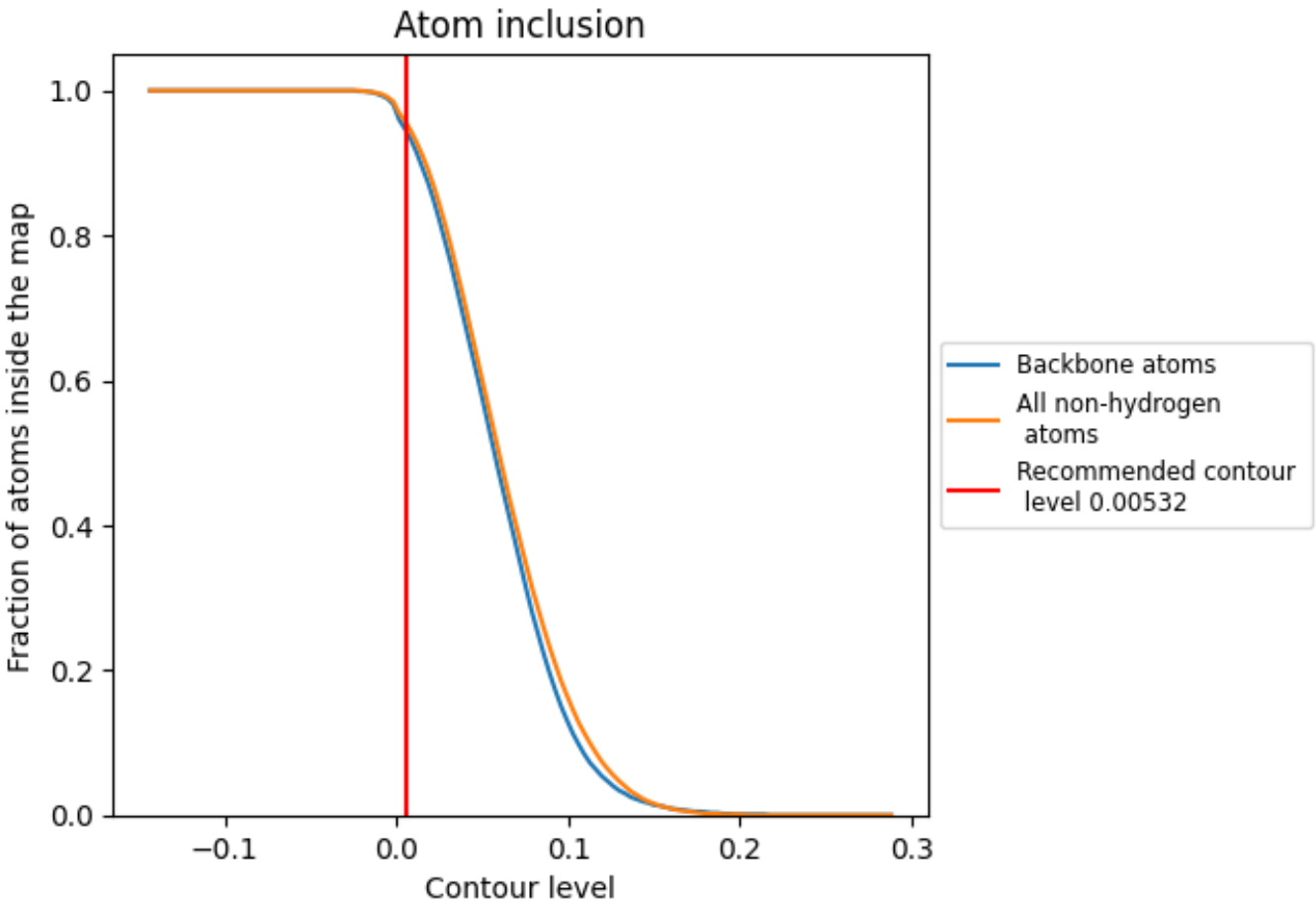
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00532).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00532) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.4750
0	0.9620	0.5080
1	0.9240	0.4640
2	0.9880	0.5860
3	0.9840	0.5760
4	0.9520	0.4940
5	0.1120	-0.0200
6	0.8880	0.3120
A	0.9870	0.5350
B	0.9940	0.5140
C	0.9740	0.5550
D	0.9660	0.5260
E	0.9690	0.5080
F	0.9360	0.4310
G	0.9370	0.3790
H	0.7350	0.2180
I	0.6190	0.0210
J	0.9650	0.5270
K	0.9520	0.5180
L	0.9650	0.5170
M	0.9690	0.5180
N	0.9860	0.5530
O	0.9680	0.4480
P	0.9570	0.5080
Q	0.9560	0.5500
R	0.9390	0.4830
S	0.9520	0.5230
T	0.9340	0.4560
U	0.9450	0.4450
V	0.9490	0.4600
W	0.9640	0.5480
X	0.9550	0.5170
Y	0.9380	0.4430
Z	0.9650	0.5020
a	0.9870	0.4800

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Chain	Atom inclusion	Q-score
b	0.8950	0.3360
c	0.9420	0.4360
d	0.8990	0.2860
e	0.9530	0.4820
f	0.9230	0.4070
g	0.9160	0.3700
h	0.9490	0.4840
i	0.9220	0.3850
j	0.8960	0.3370
k	0.9460	0.4300
l	0.9080	0.4010
m	0.9440	0.4280
n	0.9500	0.4390
o	0.9410	0.4440
p	0.8930	0.2610
q	0.9150	0.3710
r	0.8970	0.4030
s	0.9520	0.4260
t	0.9200	0.3290
u	0.8210	0.2580
v	0.9720	0.4880
w	0.7450	0.0740
x	0.9840	0.4960
y	0.9160	0.2870
z	0.8290	0.2520