



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:59 PM UTC

PDB ID : 9O2Y / pdb_00009o2y
EMDB ID : EMD-70051
Title : Structure of WT E.coli ribosome 70S subunit with complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site (R) beta-2-hydroxy-BocLysine acid charged NH-tRNA^{Pyl}
Authors : Majumdar, C.; Cate, J.H.D.
Deposited on : 2025-04-04
Resolution : 2.14 Å (reported)
Based on initial model : 8EBB

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:

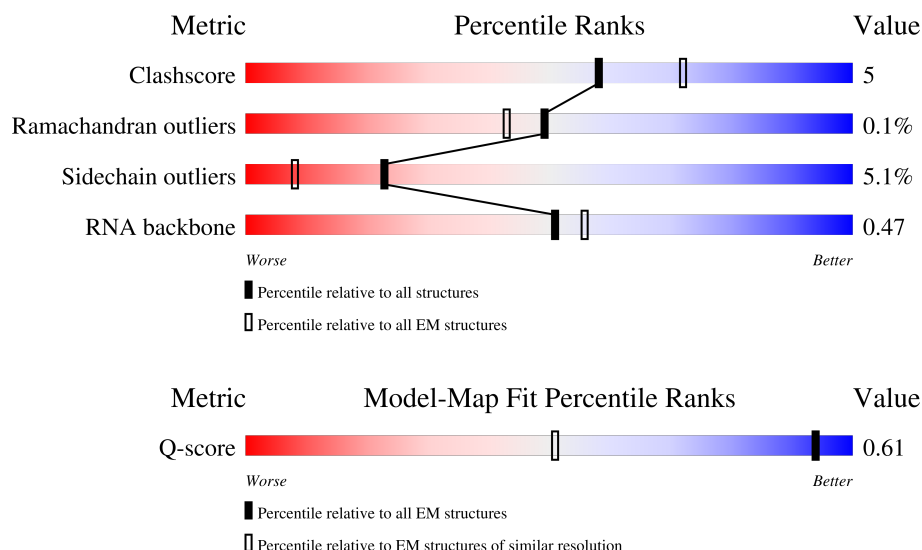
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.14 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	2493 (1.66 - 2.64)

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 $\leq 5\%$. 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	1542	
2	B	241	

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Mol	Chain	Length	Quality of chain
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	X	28	
23	Z	77	
24	a	2904	
25	b	120	
26	c	273	
27	d	209	

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Mol	Chain	Length	Quality of chain
28	e	201	
29	f	179	
30	g	177	
31	h	149	
32	i	142	
33	j	123	
34	k	144	
35	l	136	
36	m	127	
37	n	117	
38	o	115	
39	p	118	
40	q	103	
41	r	110	
42	s	100	
43	t	104	
44	u	94	
45	v	85	
46	w	78	
47	x	63	
48	y	59	
49	z	57	
50	0	55	
51	1	46	
52	2	65	

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Mol	Chain	Length	Quality of chain
53	3	38	<div><div></div><div>29%</div><div></div><div>82%</div><div></div><div>18%</div></div>
54	4	70	<div><div></div><div>81%</div><div></div><div>59%</div><div></div><div>27%</div><div></div><div>14%</div></div>
55	Y	71	<div><div></div><div>76%</div><div></div><div>38%</div><div></div><div>56%</div><div></div><div>..</div></div>

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 145583 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	15	Total	C	N	O	P	0	0
			322	145	61	101	15		

- Molecule 23 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	76	Total	C	N	O	P	0	0
			1622	723	295	528	76		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	76	8AN	-	insertion	GB 1804121330

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 31 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 32 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A1AGK1

- Molecule 36 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 40 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 45 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

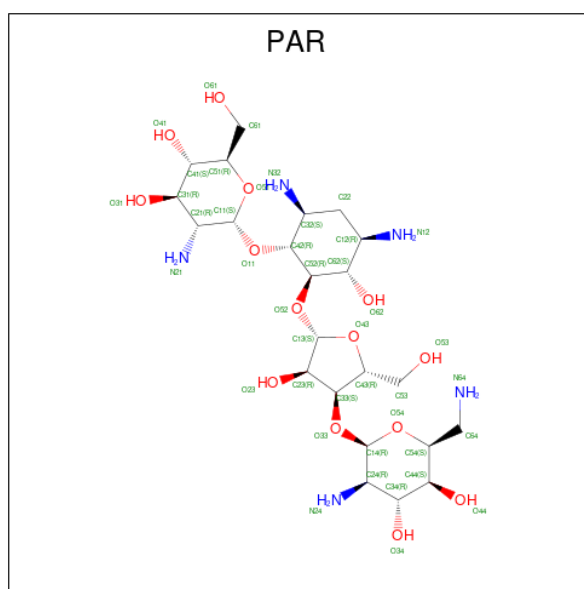
- Molecule 55 is a RNA chain called A-site tRNA^{Pyl}.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	71	Total	C	N	O	P	0	0
			1518	675	276	496	71		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	76	8AN	-	insertion	GB 1721134198

- Molecule 56 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

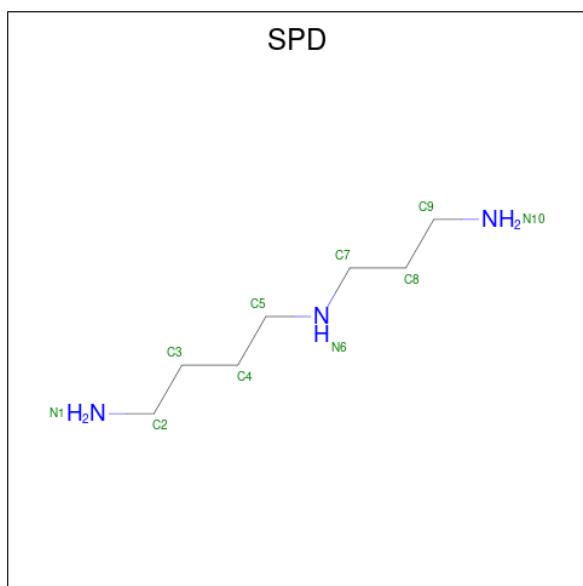
Mol	Chain	Residues	Atoms		AltConf
57	A	92	Total	Mg	0
			92	92	
57	Q	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
57	a	217	Total	Mg	0
			217	217	
57	b	5	Total	Mg	0
			5	5	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	m	1	Total	Mg	0
			1	1	
57	v	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



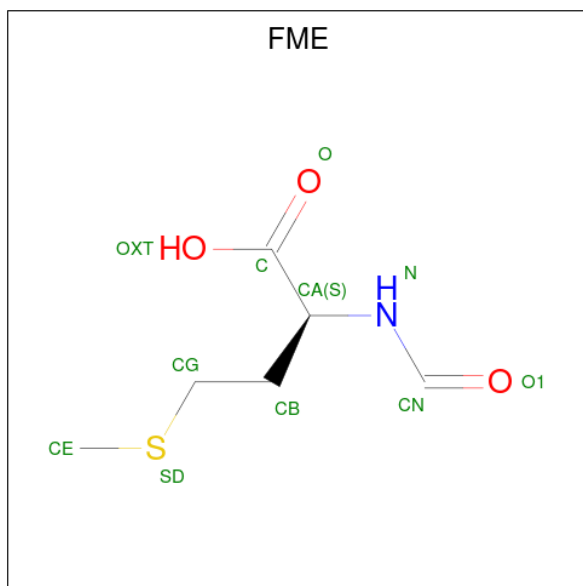
Mol	Chain	Residues	Atoms			AltConf
58	A	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	

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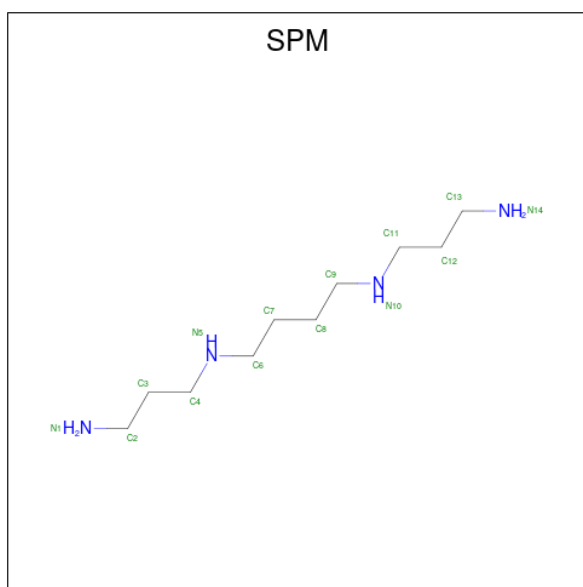
Mol	Chain	Residues	Atoms			AltConf
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	

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



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

- Molecule 60 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
60	a	1	Total	C	N	0
			14	10	4	

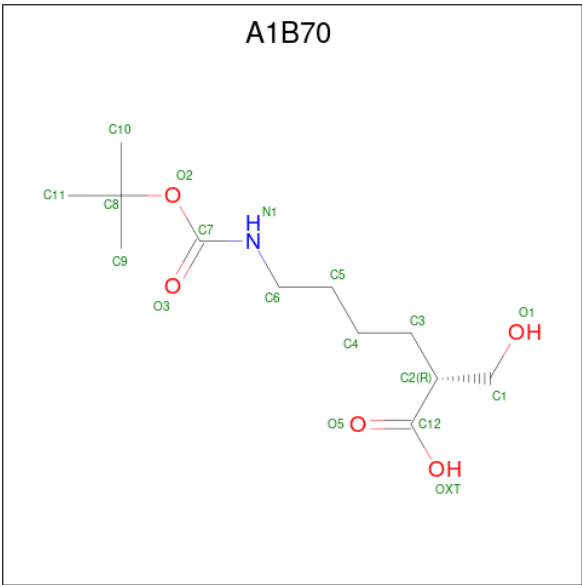
- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	a	9	Total	K	0
			9	9	
61	c	1	Total	K	0
			1	1	

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

- Molecule 63 is (2R)-6-[(tert-butoxycarbonyl)amino]-2-(hydroxymethyl)hexanoic acid (CCD ID: A1B70) (formula: C₁₂H₂₃NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
63	Y	1	Total	C	N	O	0
			17	12	1	4	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	3	Total	O	0
			3	3	
64	Z	1	Total	O	0
			1	1	
64	a	3052	Total	O	0
			3052	3052	
64	b	37	Total	O	0
			37	37	
64	c	90	Total	O	0
			90	90	
64	d	38	Total	O	0
			38	38	
64	e	31	Total	O	0
			31	31	
64	h	1	Total	O	0
			1	1	
64	i	11	Total	O	0
			11	11	
64	j	9	Total	O	0
			9	9	
64	k	36	Total	O	0
			36	36	

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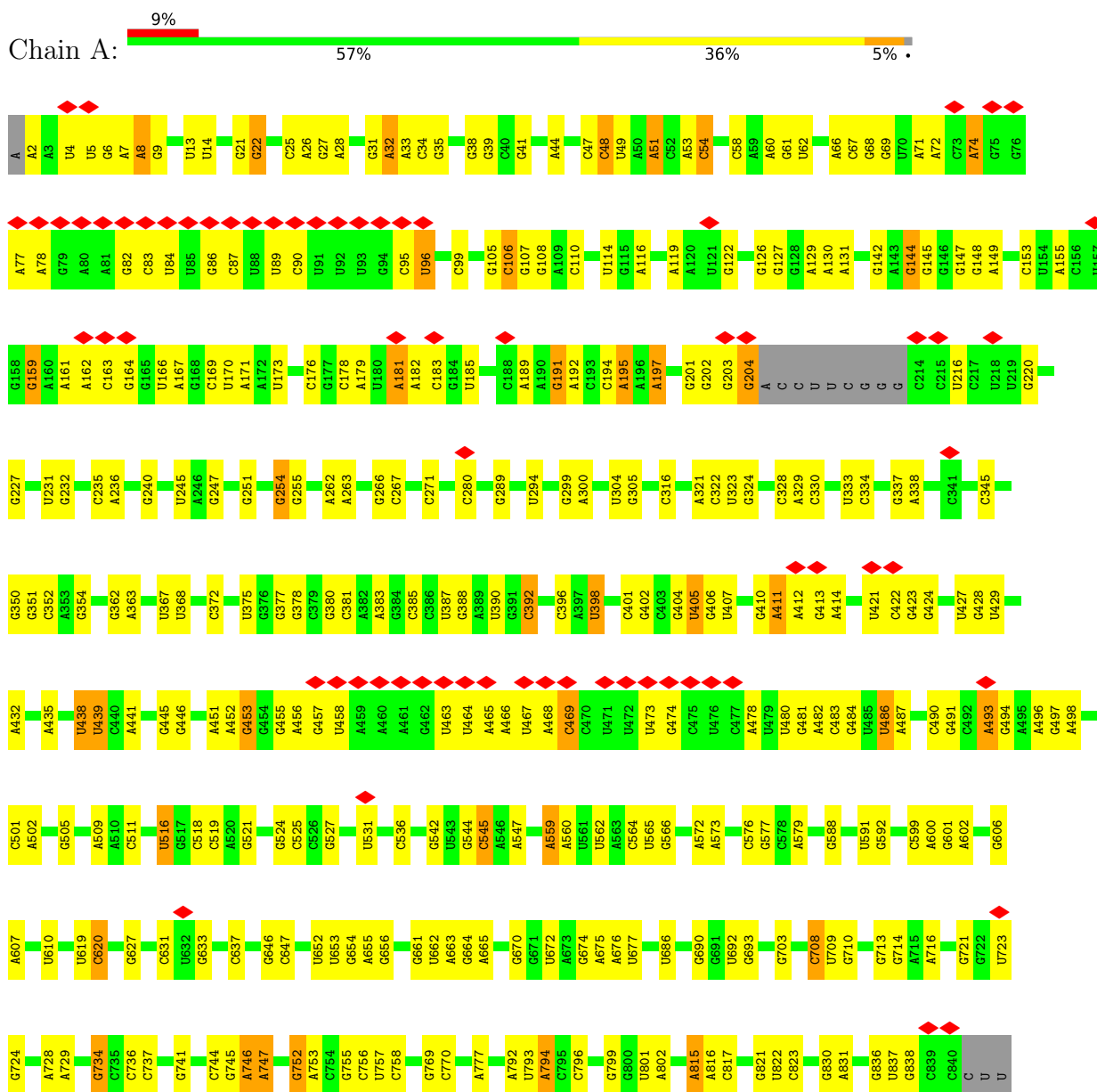
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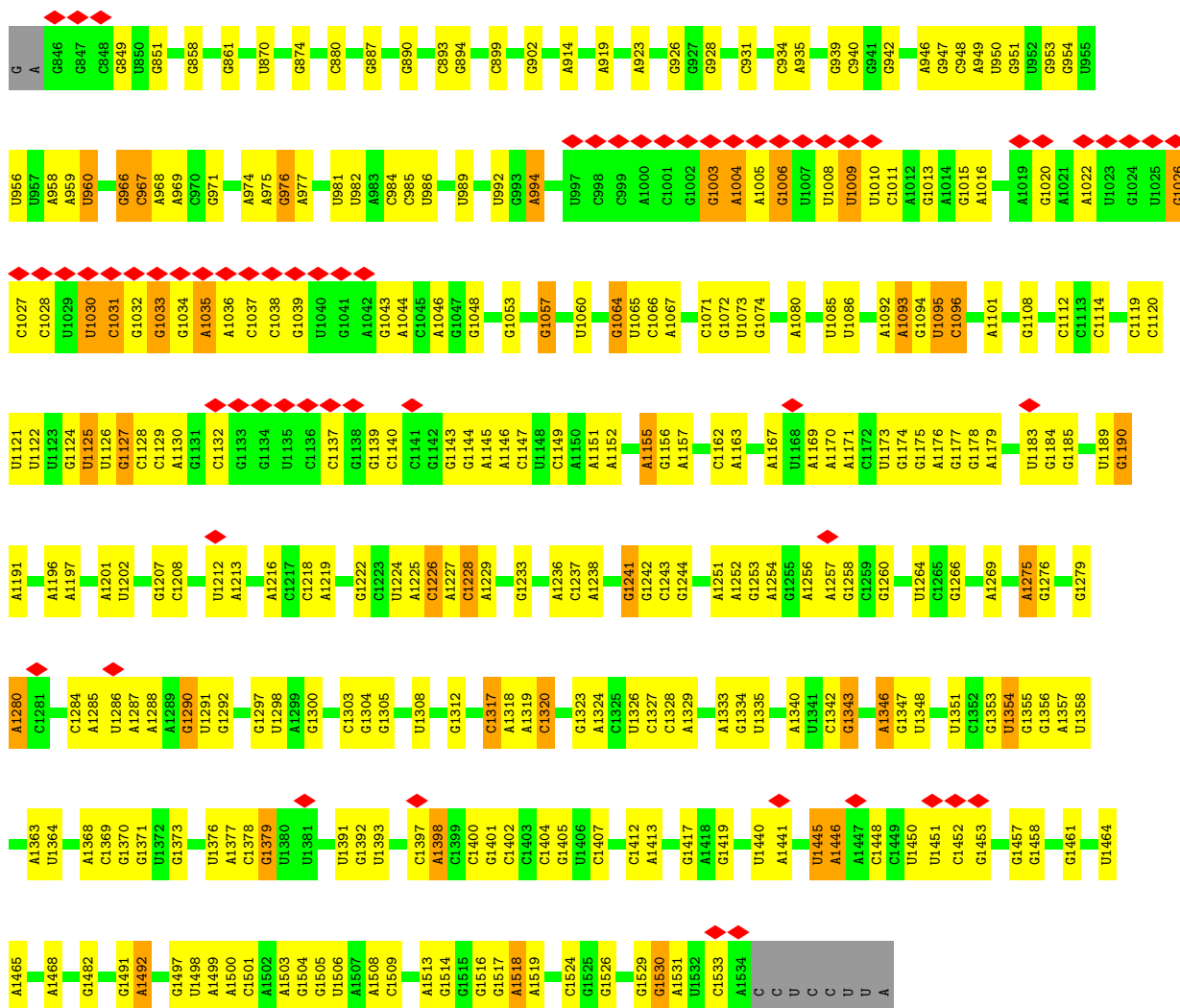
Mol	Chain	Residues	Atoms		AltConf
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64	m	21	Total 21	O 21	0
64	o	12	Total 12	O 12	0
64	p	22	Total 22	O 22	0
64	q	14	Total 14	O 14	0
64	r	21	Total 21	O 21	0
64	s	4	Total 4	O 4	0
64	t	1	Total 1	O 1	0
64	u	5	Total 5	O 5	0
64	v	9	Total 9	O 9	0
64	w	11	Total 11	O 11	0
64	x	1	Total 1	O 1	0
64	y	1	Total 1	O 1	0
64	z	28	Total 28	O 28	0
64	0	1	Total 1	O 1	0
64	1	12	Total 12	O 12	0
64	2	24	Total 24	O 24	0
64	3	2	Total 2	O 2	0
64	Y	2	Total 2	O 2	0

3 Residue-property plots

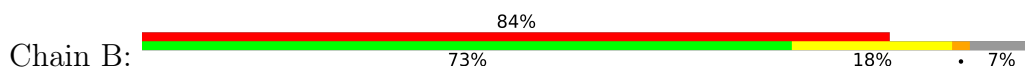
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

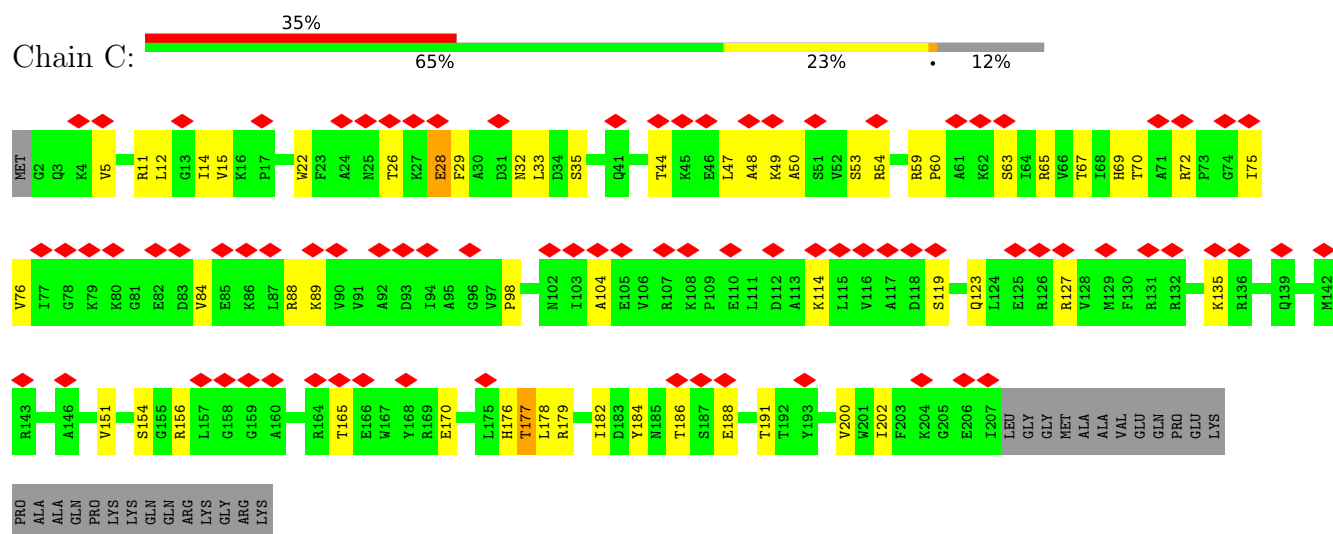




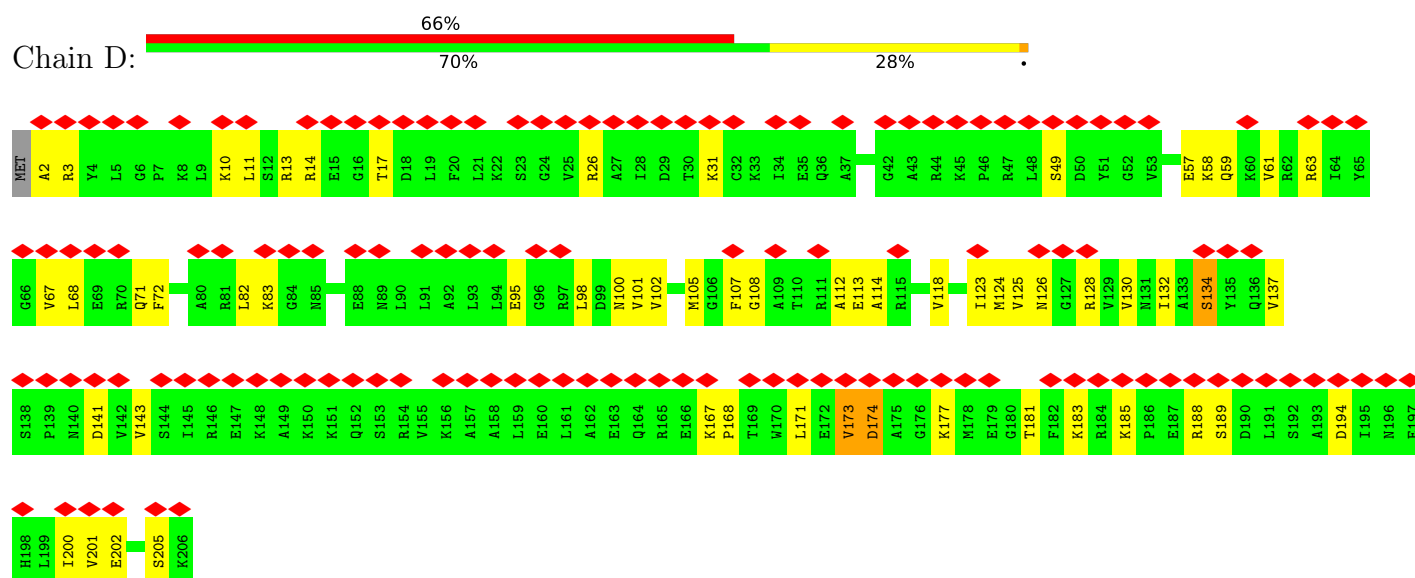
• Molecule 2: 30S ribosomal protein S2



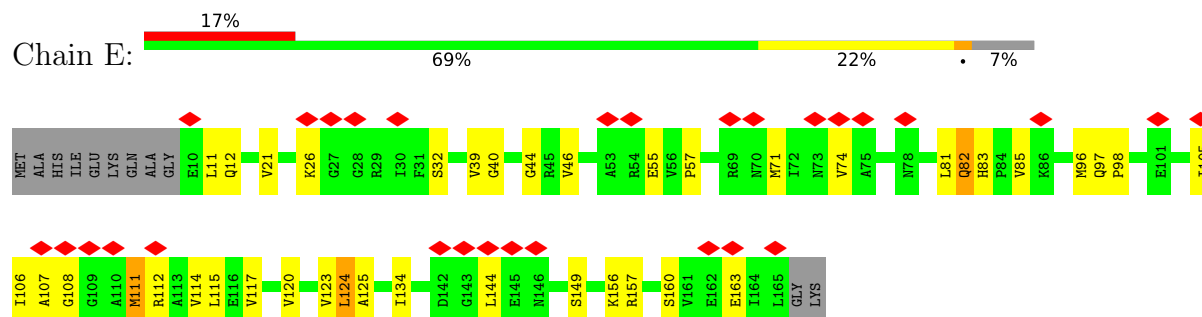
• Molecule 3: Small ribosomal subunit protein uS3



- Molecule 4: Small ribosomal subunit protein uS4

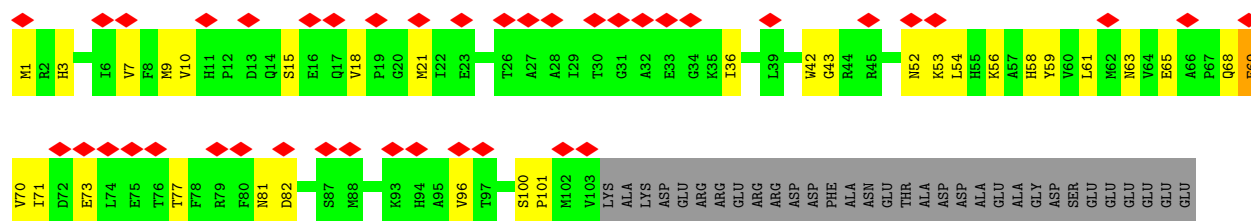


- Molecule 5: Small ribosomal subunit protein uS5

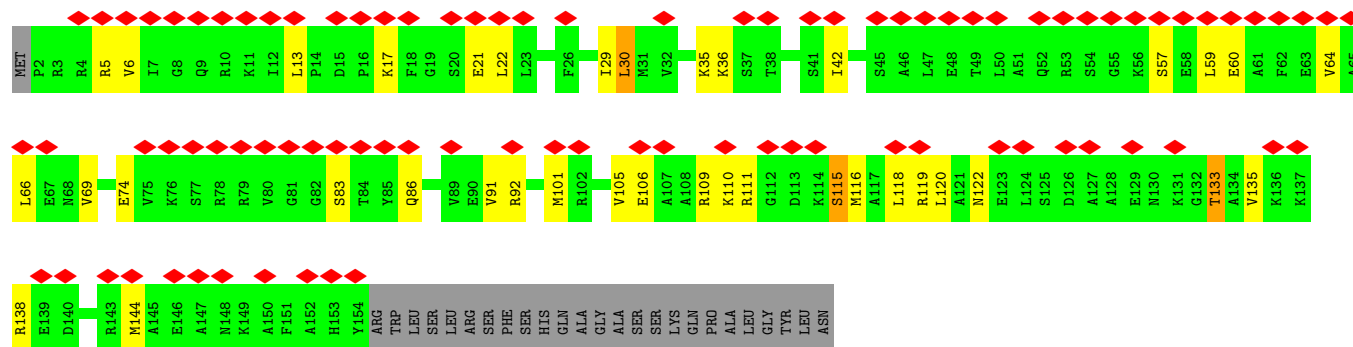


- Molecule 6: Small ribosomal subunit protein bS6

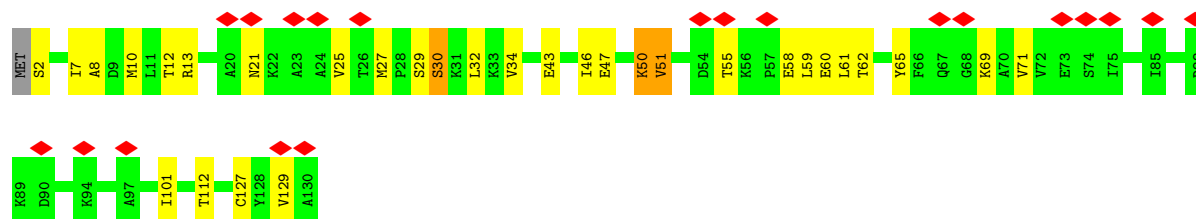
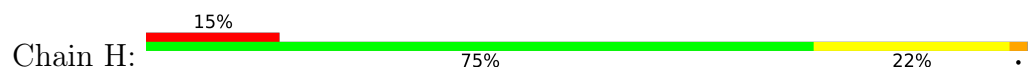




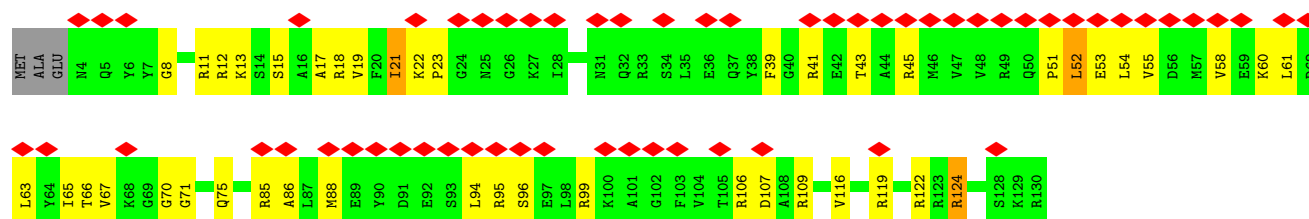
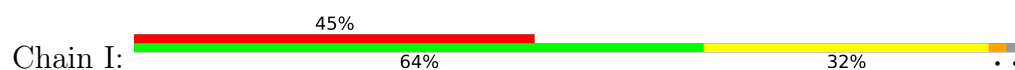
• Molecule 7: Small ribosomal subunit protein uS7



• Molecule 8: Small ribosomal subunit protein uS8

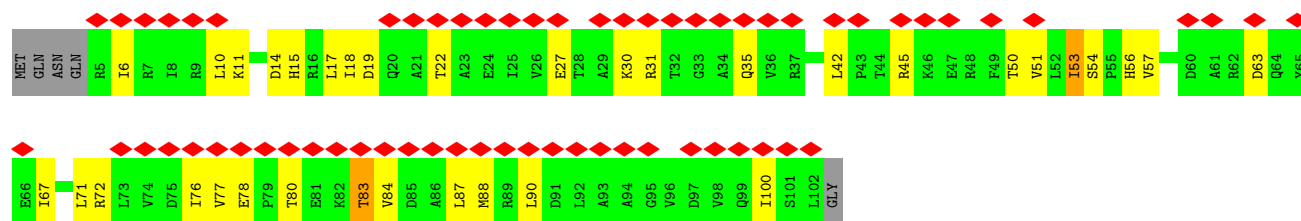


• Molecule 9: Small ribosomal subunit protein uS9

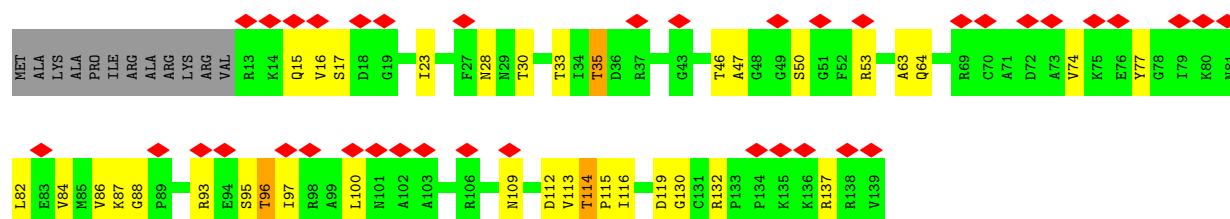


• Molecule 10: Small ribosomal subunit protein uS10

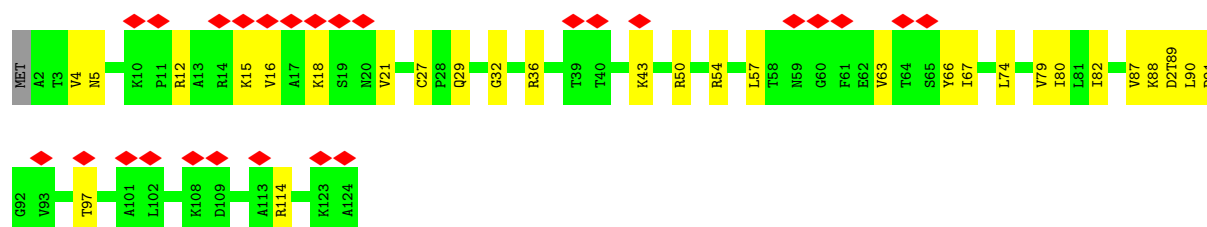
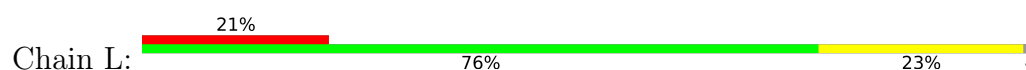




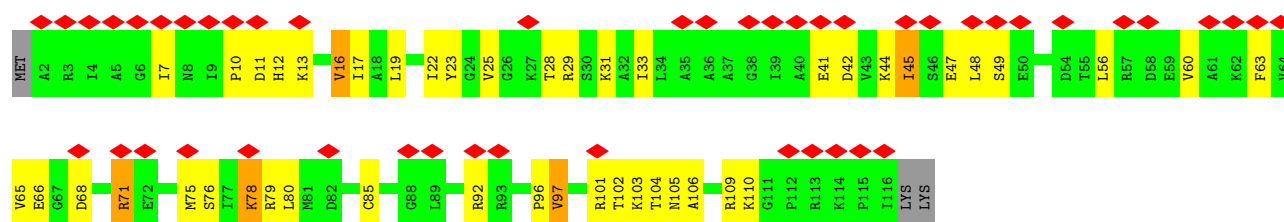
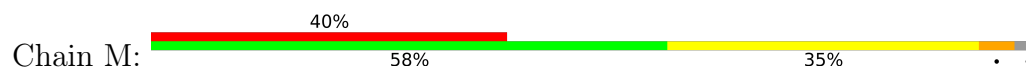
- Molecule 11: Small ribosomal subunit protein uS11



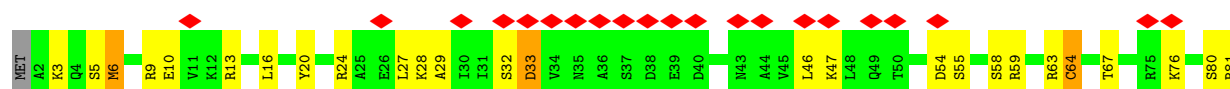
- Molecule 12: Small ribosomal subunit protein uS12

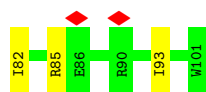


- Molecule 13: Small ribosomal subunit protein uS13

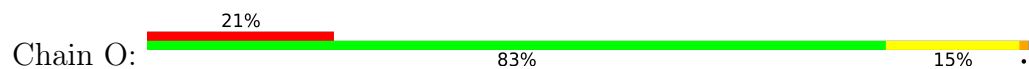


- Molecule 14: Small ribosomal subunit protein uS14

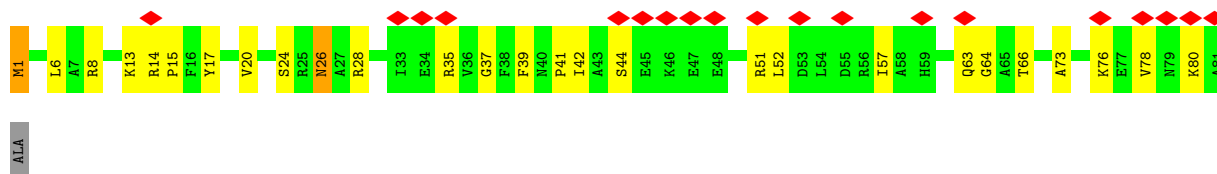




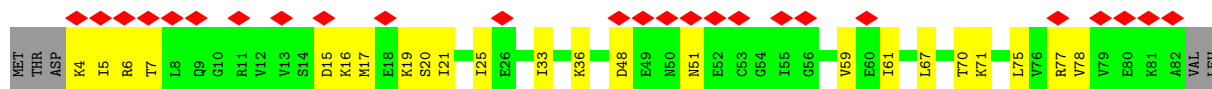
- Molecule 15: Small ribosomal subunit protein uS15



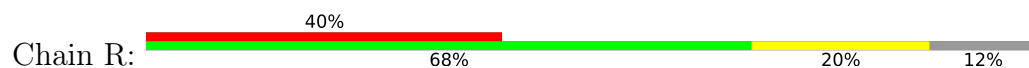
- Molecule 16: Small ribosomal subunit protein bS16



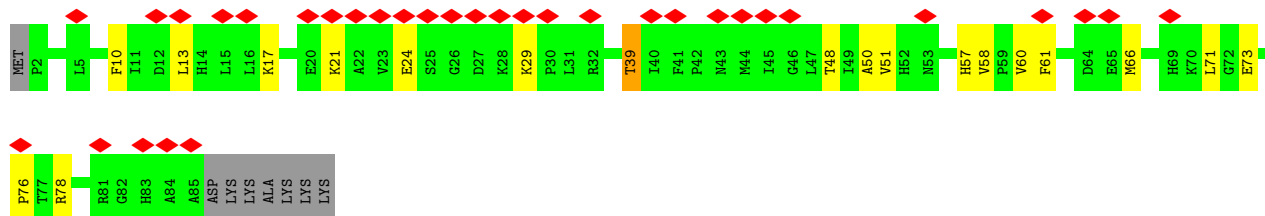
- Molecule 17: Small ribosomal subunit protein uS17



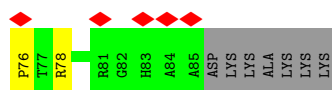
- Molecule 18: Small ribosomal subunit protein bS18

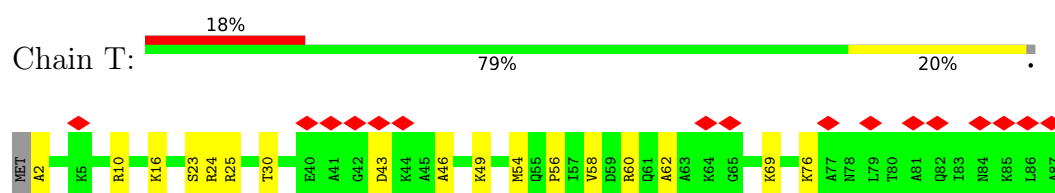


- Molecule 19: Small ribosomal subunit protein uS19

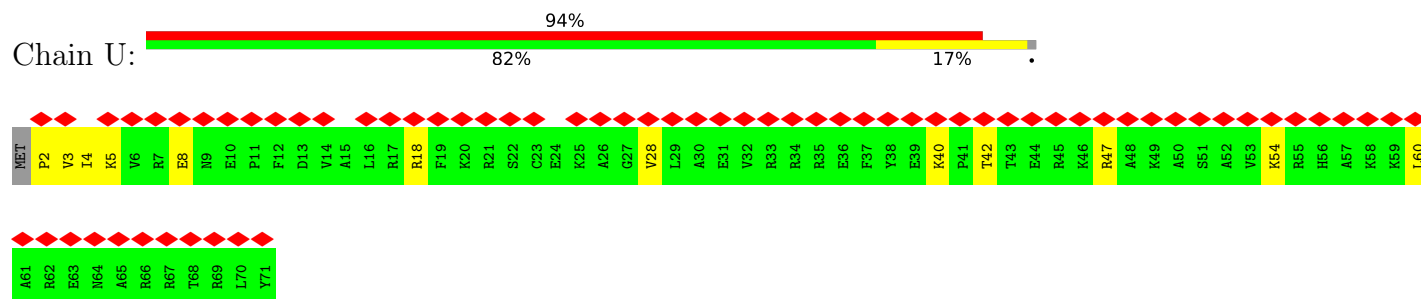


- Molecule 20: Small ribosomal subunit protein bS20

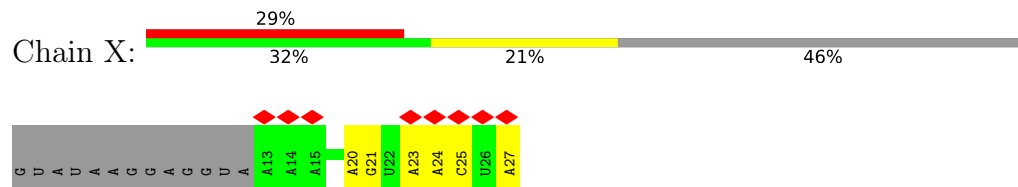




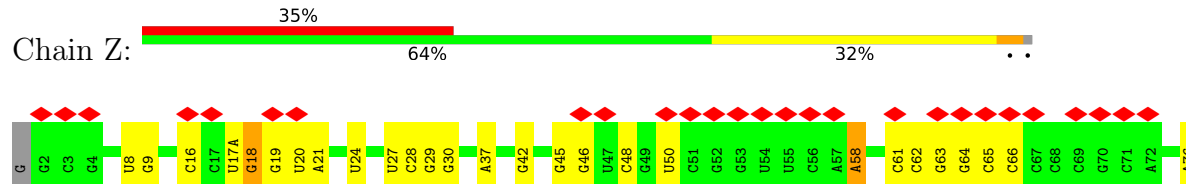
- Molecule 21: Small ribosomal subunit protein bS21



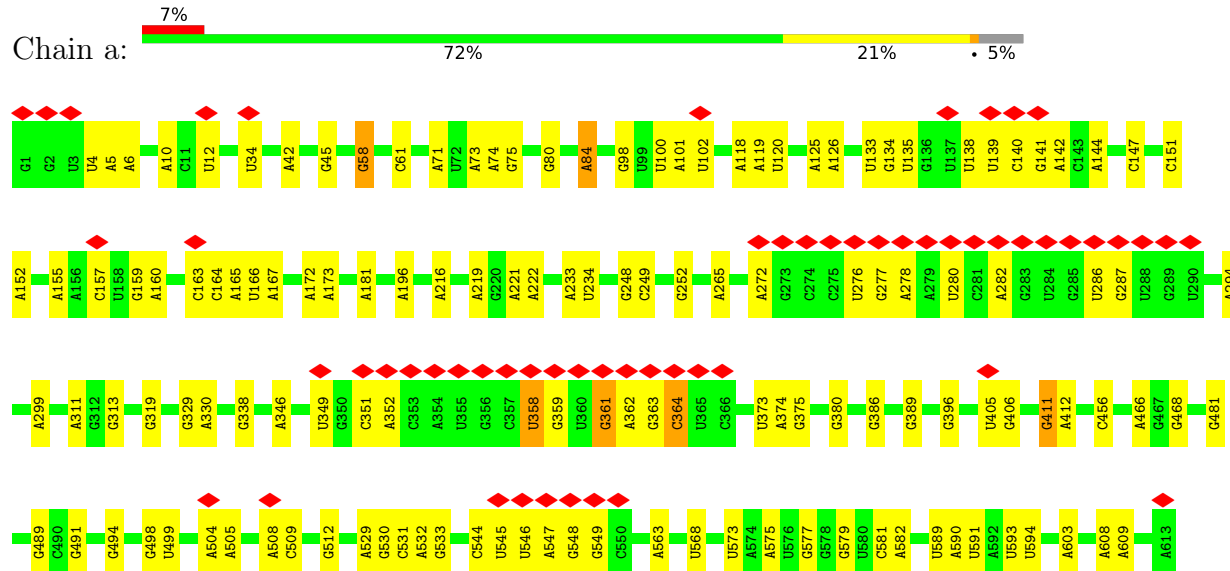
- Molecule 22: mRNA

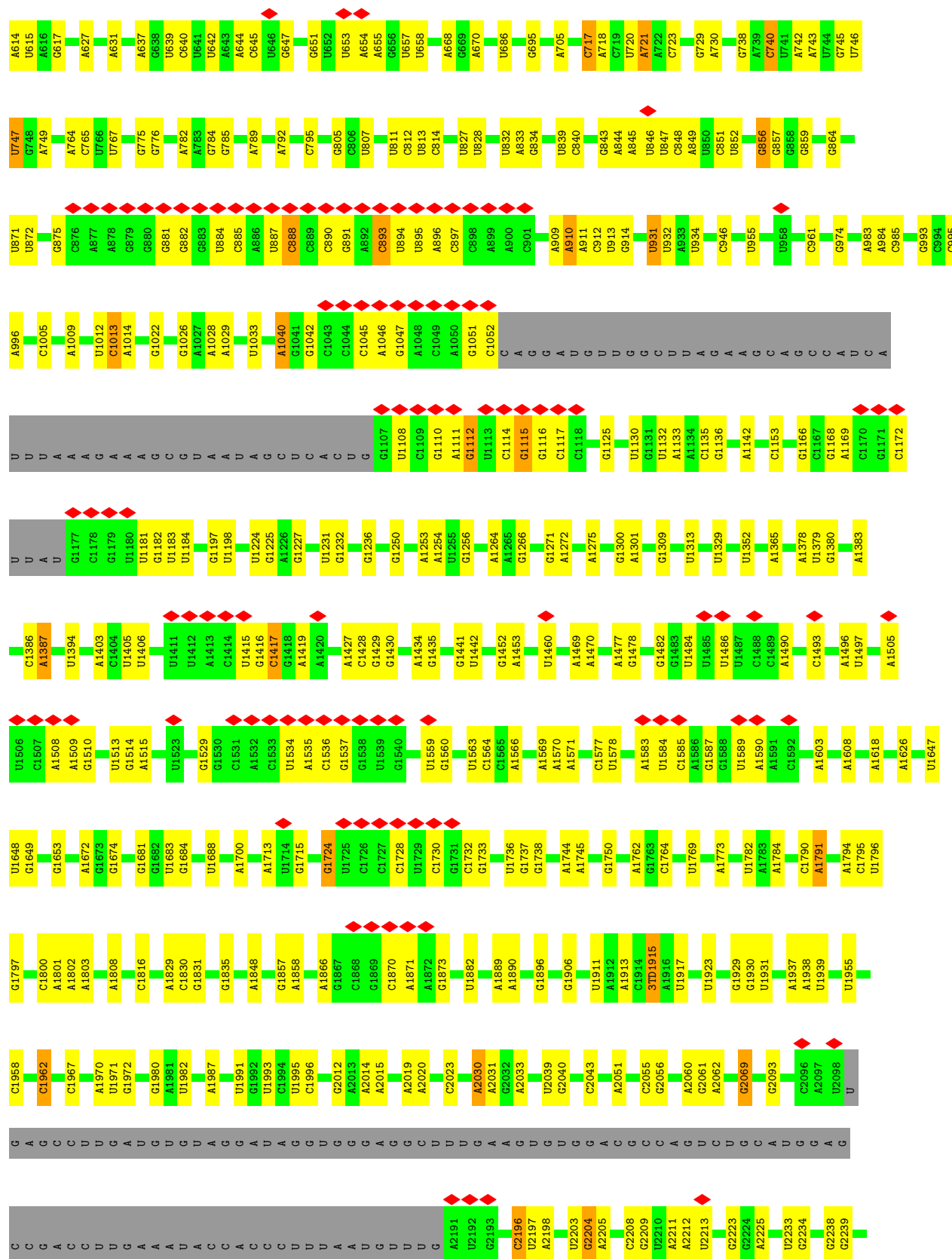


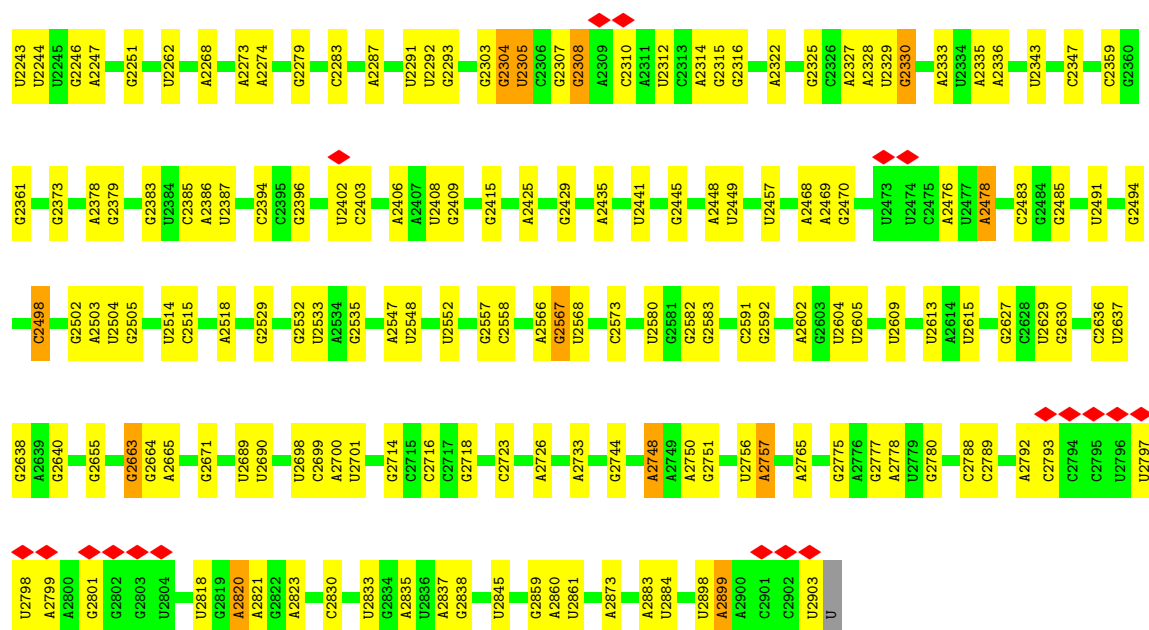
- Molecule 23: P-site tRNA fMet



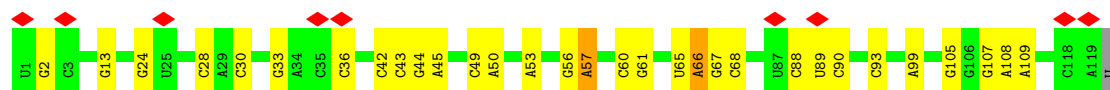
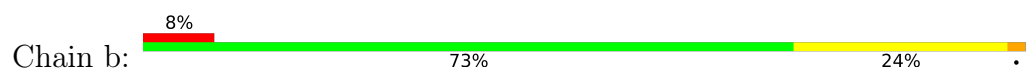
- Molecule 24: 23S rRNA



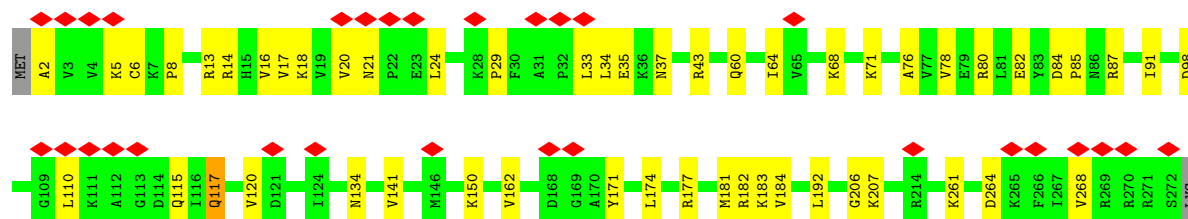
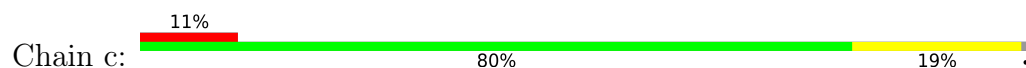




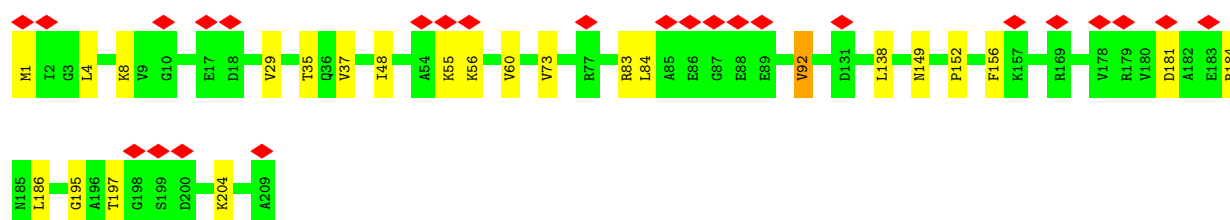
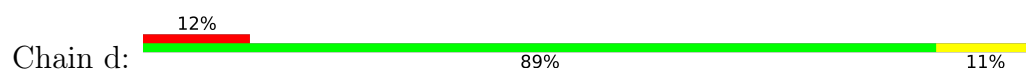
• Molecule 25: 5S rRNA



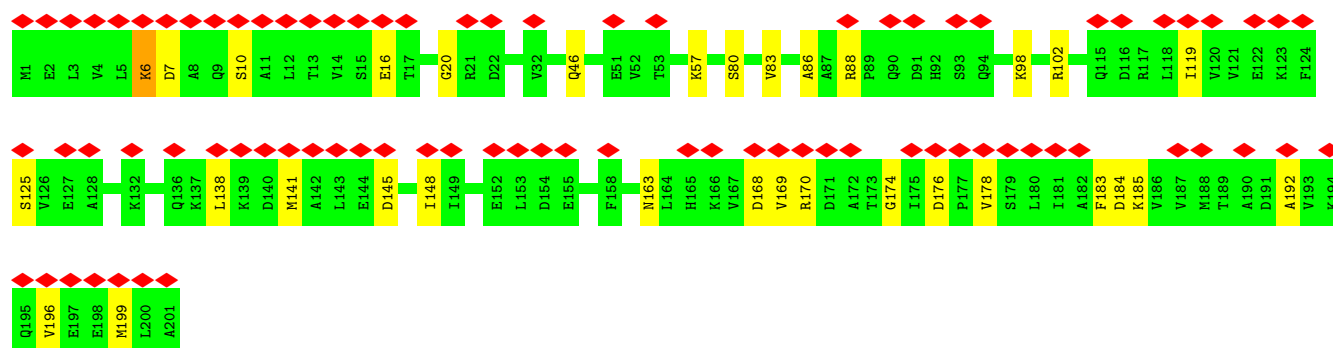
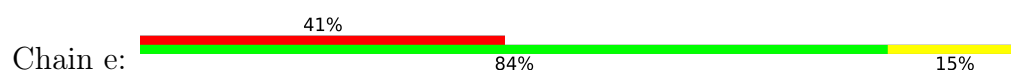
• Molecule 26: 50S ribosomal protein L2



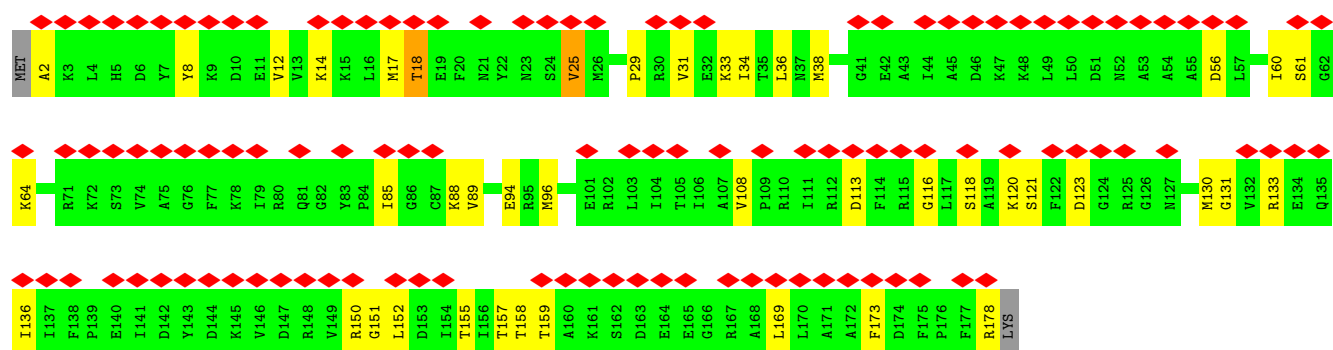
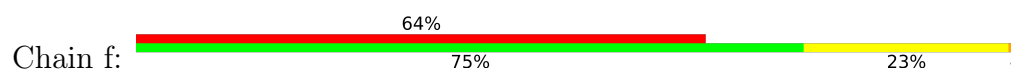
• Molecule 27: 50S ribosomal protein L3



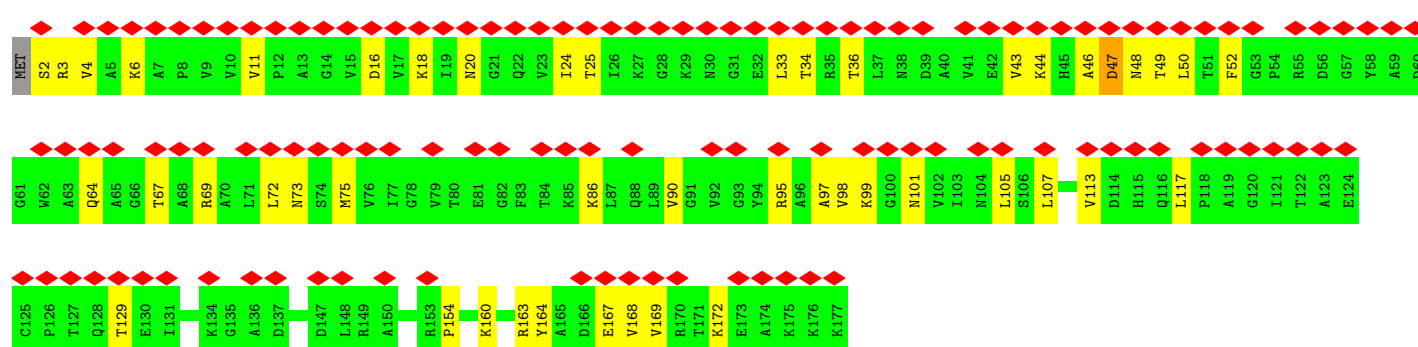
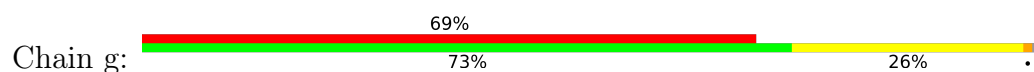
• Molecule 28: Large ribosomal subunit protein uL4



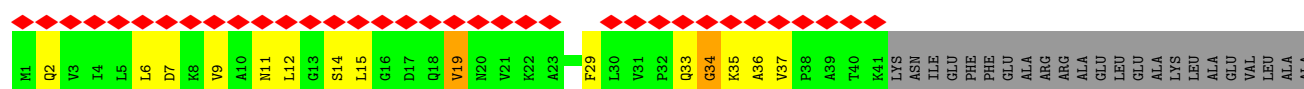
• Molecule 29: Large ribosomal subunit protein uL5



• Molecule 30: Large ribosomal subunit protein uL6

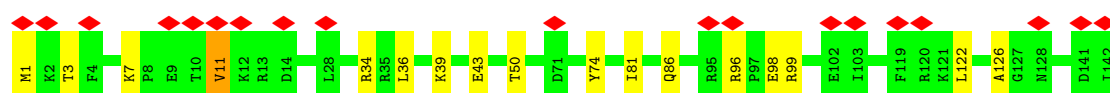
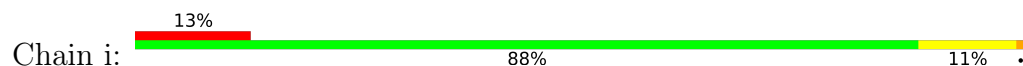


• Molecule 31: Large ribosomal subunit protein bL9

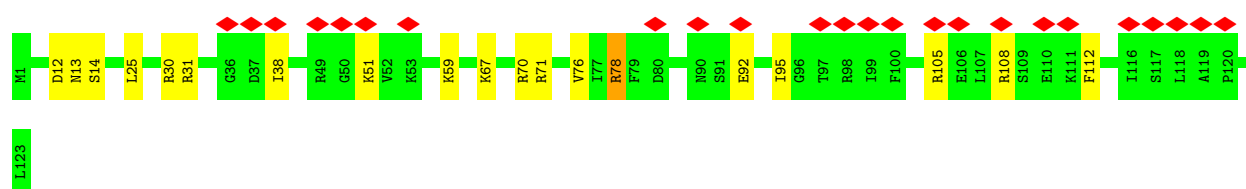
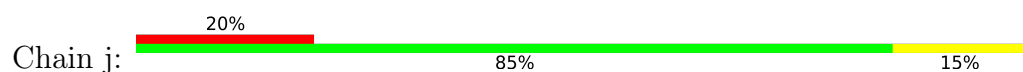


ALA	ASN	ARG	ALA	GLU	LYS	ILE	ASN	GLN	VAL	HIS	LEU	GLU	THR	VAL	THR	ALA	ILE	ALA	LYS	SER	LYS	VAL	ILE	VAL	ASN	GLY	ASP	VAL	GLU	GLY	LYS	LEU	PHE	GLY	SER	ILE	GLY	THR	ARG	ASP	ILE	ALA	ASP	ALA	VAL	THR	ALA	GLY	VAL	VAL	LYS	ALA	LYS	SER	GLU	VAL	ARG	LEU	PRO	ASN	GLY	VAL	LEU	ARG	THR
THR	GLY	HIS	GLU	VAL	SER	PHE	GLN	VAL	HIS	SER	GLU	VAL	PHE	THR	ALA	LYS	VAL	ILE	VAL	ASN	VAL	VAL	VAL	VAL	ALA	GLU	GLY	LYS	LEU	PHE	GLY	SER	ILE	GLY	THR	ARG	ASP	ILE	ALA	ASP	ALA	VAL	THR	ALA	GLY	VAL	VAL	LYS	ALA	LYS	SER	GLU	VAL	ARG	LEU	PRO	ASN	GLY	VAL	LEU	ARG	THR			

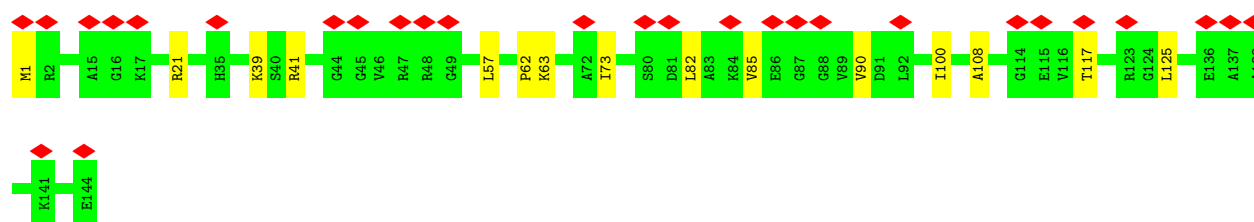
- Molecule 32: Large ribosomal subunit protein uL13



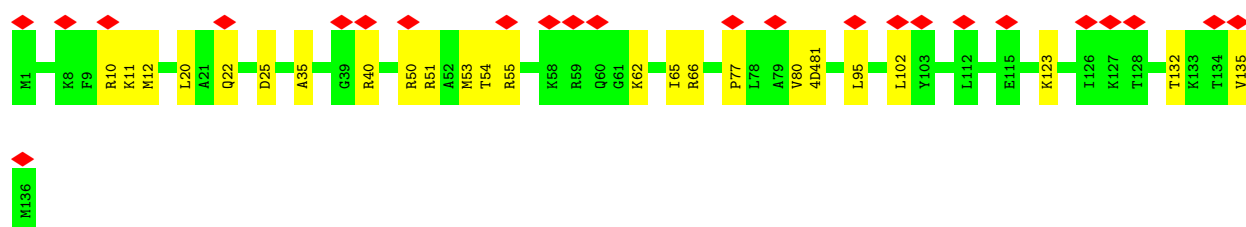
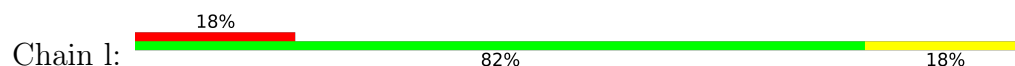
- Molecule 33: Large ribosomal subunit protein uL14



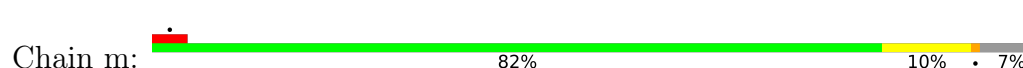
- Molecule 34: Large ribosomal subunit protein uL15



- Molecule 35: 50S ribosomal protein L16

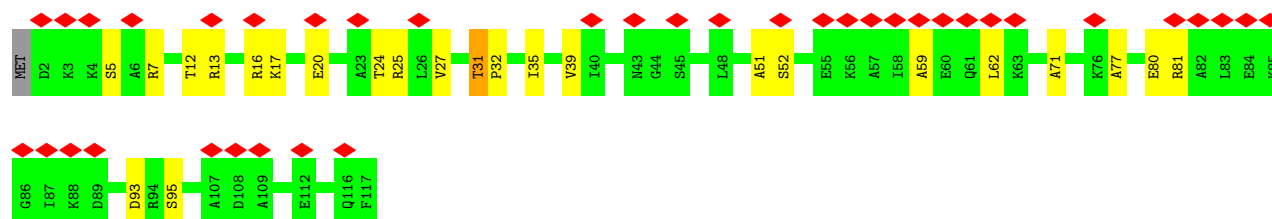
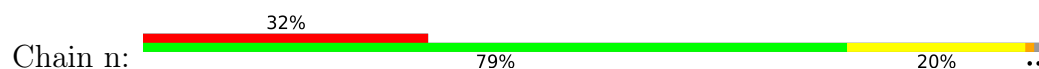


- Molecule 36: Large ribosomal subunit protein bL17

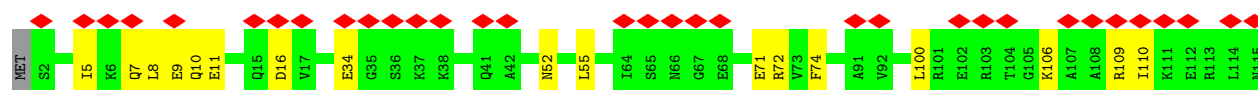
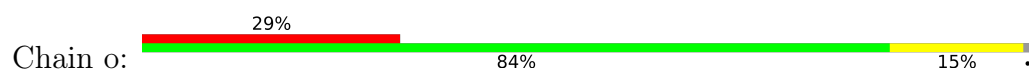




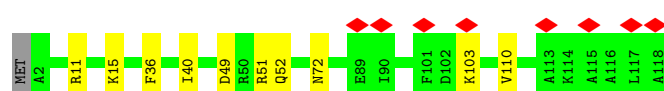
- Molecule 37: Large ribosomal subunit protein uL18



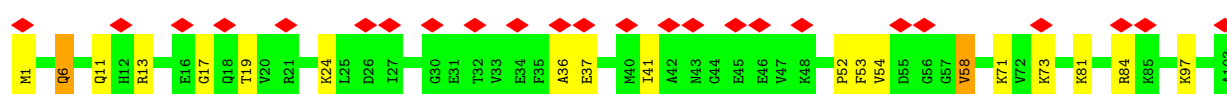
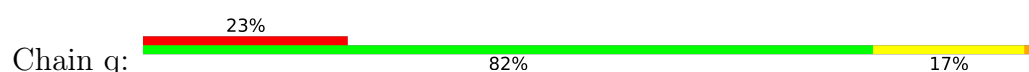
- Molecule 38: Large ribosomal subunit protein bL19



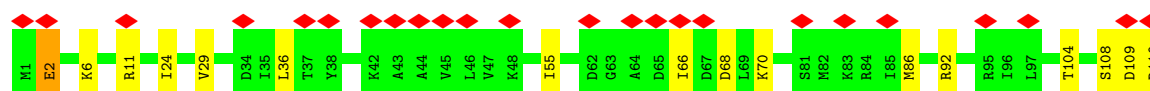
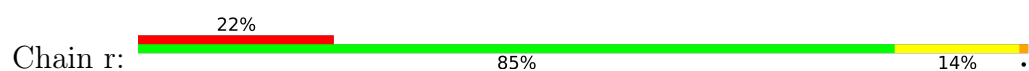
- Molecule 39: 50S ribosomal protein L20



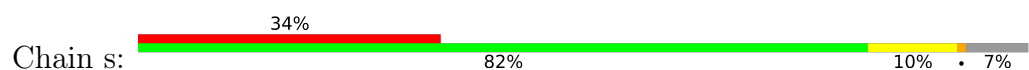
- Molecule 40: Large ribosomal subunit protein bL21

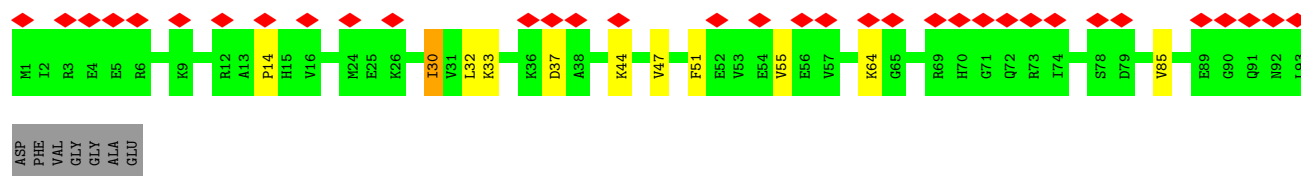


- Molecule 41: Large ribosomal subunit protein uL22

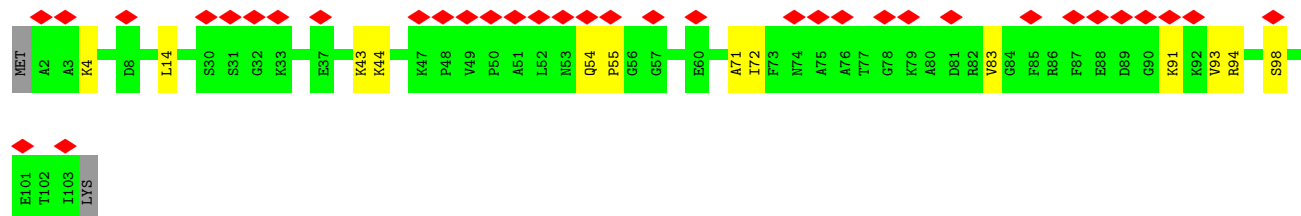
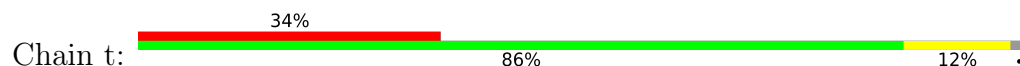


- Molecule 42: 50S ribosomal protein L23

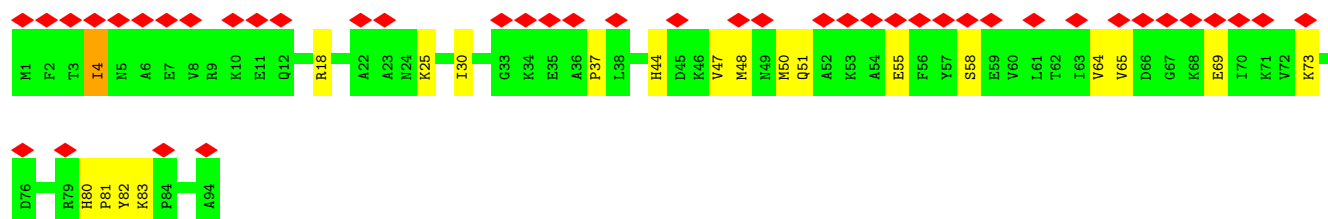
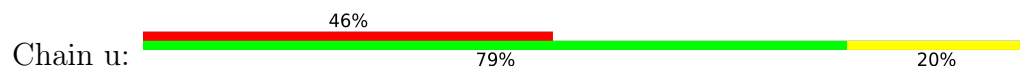




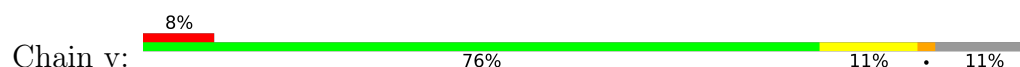
- Molecule 43: 50S ribosomal protein L24



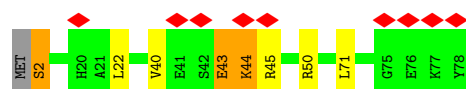
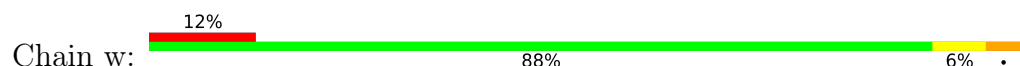
- Molecule 44: Large ribosomal subunit protein bL25



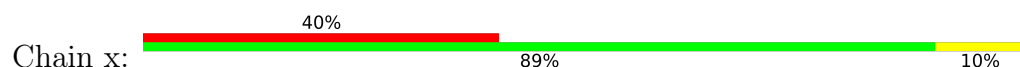
- Molecule 45: Large ribosomal subunit protein bL27



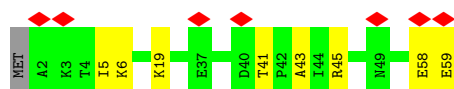
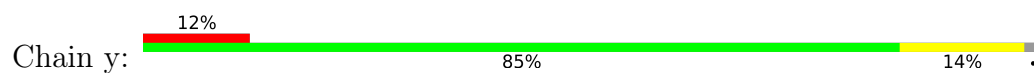
- Molecule 46: 50S ribosomal protein L28



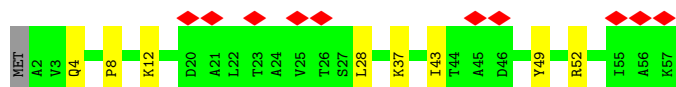
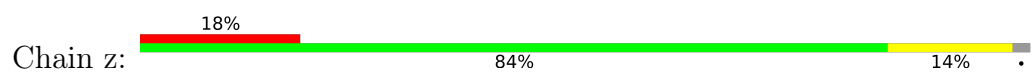
- Molecule 47: Large ribosomal subunit protein uL29



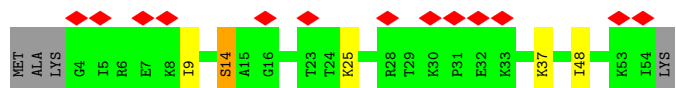
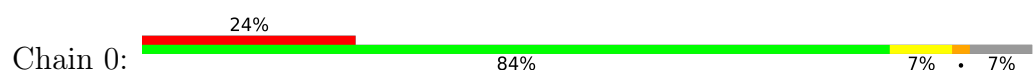
- Molecule 48: 50S ribosomal protein L30



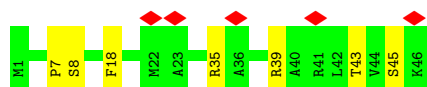
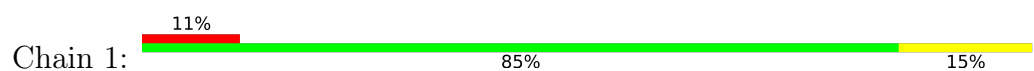
- Molecule 49: 50S ribosomal protein L32



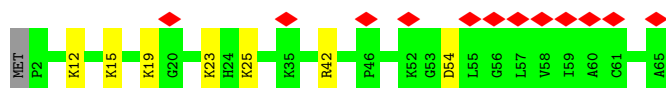
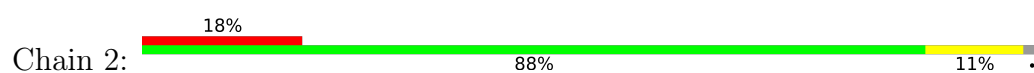
- Molecule 50: 50S ribosomal protein L33



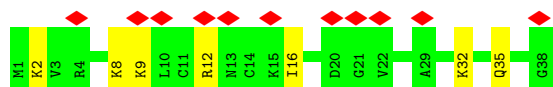
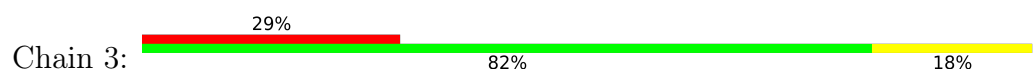
- Molecule 51: 50S ribosomal protein L34



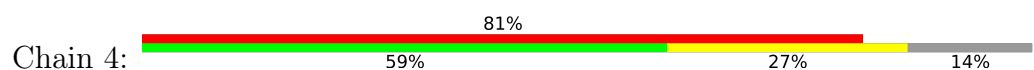
- Molecule 52: 50S ribosomal protein L35

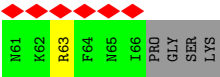
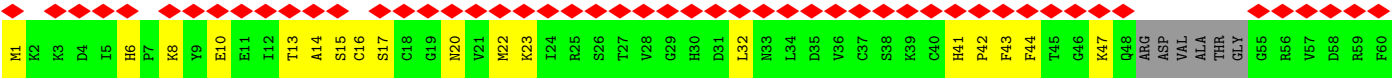


- Molecule 53: 50S ribosomal protein L36

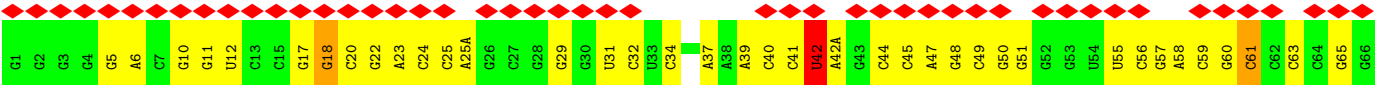
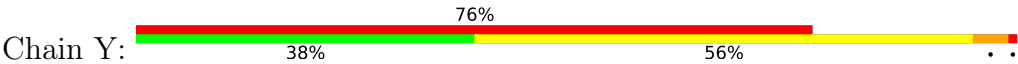


- Molecule 54: 50S ribosomal protein L31





● Molecule 55: A-site tRNAPyl



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86644	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	72.057	Depositor
Minimum map value	-28.133	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.486	Depositor
Recommended contour level	8.25	Depositor
Map size (\AA)	421.632, 421.632, 421.632	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8235, 0.8235, 0.8235	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, 6MZ, MS6, 2MA, OMG, PSU, 5MU, FME, OMC, IAS, OMU, PAR, UR3, H2U, 4D4, MEQ, G7M, ZN, 1MG, 3TD, A1B70, MA6, D2T, SPD, SPM, MG, 8AN, 5MC, 2MG, 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	0.31	1/36236 (0.0%)	0.48	0/56520
2	B	0.25	0/1784	0.53	0/2403
3	C	0.26	0/1651	0.55	0/2225
4	D	0.28	0/1665	0.52	0/2227
5	E	0.31	0/1165	0.55	0/1568
6	F	0.30	0/858	0.63	0/1160
7	G	0.31	0/1219	0.67	1/1635 (0.1%)
8	H	0.30	0/989	0.58	0/1326
9	I	0.43	1/1034 (0.1%)	0.67	0/1375
10	J	0.46	1/796 (0.1%)	0.64	1/1077 (0.1%)
11	K	0.27	0/884	0.55	2/1191 (0.2%)
12	L	0.24	0/960	0.55	0/1286
13	M	0.54	1/900 (0.1%)	0.67	1/1204 (0.1%)
14	N	0.27	0/817	0.49	0/1088
15	O	0.42	1/722 (0.1%)	0.61	1/964 (0.1%)
16	P	0.26	0/653	0.54	0/877
17	Q	0.25	0/650	0.59	0/871
18	R	0.23	0/553	0.58	0/742
19	S	0.21	0/685	0.51	0/922
20	T	0.32	0/676	0.65	0/895
21	U	0.19	0/597	0.38	0/792
22	X	0.36	0/360	0.55	0/556
23	Z	0.31	0/1787	0.53	0/2784
24	a	0.32	0/65651	0.47	5/102413 (0.0%)
25	b	0.29	0/2850	0.47	0/4444
26	c	0.29	0/2121	0.55	0/2852
27	d	0.31	0/1576	0.58	1/2119 (0.0%)
28	e	0.28	0/1571	0.54	0/2113
29	f	0.42	1/1434 (0.1%)	0.65	0/1926
30	g	0.27	0/1343	0.60	0/1816
31	h	0.27	0/306	0.63	0/413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.28	0/1152	0.56	0/1551
33	j	0.34	0/955	0.58	0/1279
34	k	0.28	0/1062	0.55	0/1413
35	l	0.33	0/1073	0.59	0/1433
36	m	0.34	0/958	0.65	1/1281 (0.1%)
37	n	1.21	6/902 (0.7%)	1.28	7/1209 (0.6%)
38	o	0.35	0/929	0.56	0/1242
39	p	0.28	0/960	0.53	0/1278
40	q	0.30	0/829	0.56	0/1107
41	r	0.31	0/864	0.56	0/1156
42	s	0.30	0/744	0.59	0/994
43	t	0.37	0/787	0.68	0/1051
44	u	0.45	0/766	0.66	0/1025
45	v	0.52	2/583 (0.3%)	0.61	0/772
46	w	0.35	0/635	0.63	2/848 (0.2%)
47	x	0.30	0/502	0.57	0/667
48	y	0.30	0/453	0.68	0/605
49	z	0.30	0/450	0.58	0/599
50	0	0.24	0/424	0.52	0/565
51	1	0.25	0/380	0.49	0/498
52	2	0.30	0/513	0.57	0/676
53	3	0.35	0/303	0.56	0/397
54	4	0.22	0/488	0.51	0/649
55	Y	0.34	0/1665	0.71	2/2581 (0.1%)
All	All	0.33	14/152870 (0.0%)	0.52	24/228660 (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
2	B	0	1
11	K	0	1
14	N	0	1
30	g	0	2
31	h	0	1
43	t	0	1
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	32	PRO	N-CD	23.95	1.81	1.47
37	n	32	PRO	CG-CD	-15.80	0.97	1.50
13	M	45	ILE	CG1-CD1	-13.34	0.99	1.51
37	n	32	PRO	CB-CG	-10.64	0.96	1.49
37	n	32	PRO	CA-CB	-10.39	1.39	1.53
29	f	38	MET	C-N	9.66	1.38	1.33
37	n	31	THR	C-O	9.24	1.32	1.24
37	n	32	PRO	CA-C	9.05	1.65	1.52
10	J	53	ILE	CG1-CD1	-8.87	1.17	1.51
9	I	21	ILE	CG1-CD1	-8.38	1.19	1.51
45	v	44	LYS	CE-NZ	-7.79	1.25	1.49
15	O	3	LEU	CG-CD2	-6.03	1.32	1.52
45	v	44	LYS	CD-CE	-5.42	1.36	1.52
1	A	1498	UR3	O3'-P	5.34	1.61	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	32	PRO	CB-CG-CD	23.07	179.91	106.10
37	n	32	PRO	CA-N-CD	-19.48	84.72	112.00
37	n	32	PRO	N-CD-CG	-17.16	77.46	103.20
37	n	32	PRO	CA-CB-CG	-11.08	83.45	104.50
13	M	45	ILE	CG1-CB-CG2	-9.08	83.45	110.70
37	n	31	THR	CA-C-O	-7.40	113.69	120.50
55	Y	42	U	OP2-P-O3'	6.52	119.54	105.20
37	n	31	THR	C-N-CD	6.03	149.71	125.00
55	Y	42	U	P-O3'-C3'	5.98	126.88	119.70
36	m	78	LYS	CB-CG-CD	5.86	124.78	111.30
10	J	53	ILE	CG1-CB-CG2	-5.81	93.28	110.70
7	G	29	ILE	CB-CG1-CD1	5.74	125.86	113.80
46	w	43	GLU	CA-CB-CG	5.54	125.18	114.10
15	O	3	LEU	CD1-CG-CD2	-5.45	98.81	110.80
24	a	12	U	N1-C1'-C2'	5.39	120.08	112.00
46	w	44	LYS	CA-CB-CG	5.34	124.77	114.10
24	a	512	G	O4'-C1'-N9	5.30	116.15	108.20
37	n	31	THR	O-C-N	-5.26	118.34	121.71
24	a	2330	G	C1'-C2'-O2'	-5.22	100.58	108.40
24	a	1313	U	N1-C1'-C2'	5.03	119.55	112.00
11	K	16	VAL	CA-C-N	5.02	131.13	121.54
11	K	16	VAL	C-N-CA	5.02	131.13	121.54
24	a	1114	C	C2'-C3'-O3'	5.02	121.22	113.70
27	d	204	LYS	CG-CD-CE	5.01	122.83	111.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	THR	Peptide
11	K	82	LEU	Peptide
14	N	32	SER	Peptide
30	g	46	ALA	Peptide
30	g	47	ASP	Peptide
31	h	34	GLY	Peptide
43	t	98	SER	Peptide

5.2 Too-close contacts

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	32612	0	16432	286	0
2	B	1753	0	1780	23	0
3	C	1624	0	1696	31	0
4	D	1643	0	1707	41	0
5	E	1152	0	1196	24	0
6	F	839	0	833	16	0
7	G	1203	0	1254	18	0
8	H	979	0	1031	18	0
9	I	1022	0	1070	29	0
10	J	786	0	828	19	0
11	K	877	0	884	22	0
12	L	957	0	1017	17	0
13	M	891	0	952	28	0
14	N	805	0	844	24	0
15	O	714	0	734	6	0
16	P	643	0	661	20	0
17	Q	641	0	682	14	0
18	R	544	0	565	6	0
19	S	668	0	693	13	0
20	T	670	0	719	14	0
21	U	589	0	629	4	0
22	X	322	0	163	1	0
23	Z	1622	0	824	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	59130	0	29763	213	0
25	b	2549	0	1291	9	0
26	c	2082	0	2154	32	0
27	d	1566	0	1618	15	0
28	e	1552	0	1619	18	0
29	f	1410	0	1444	27	0
30	g	1323	0	1371	26	0
31	h	303	0	327	5	0
32	i	1129	0	1162	12	0
33	j	946	0	1023	14	0
34	k	1053	0	1129	8	0
35	l	1075	0	1146	14	0
36	m	945	0	989	9	0
37	n	892	0	923	11	0
38	o	917	0	962	13	0
39	p	947	0	1019	7	0
40	q	816	0	839	11	0
41	r	857	0	922	10	0
42	s	738	0	807	8	0
43	t	779	0	831	7	0
44	u	753	0	780	12	0
45	v	576	0	588	10	0
46	w	625	0	652	2	0
47	x	501	0	531	3	0
48	y	449	0	488	6	0
49	z	444	0	458	5	0
50	0	417	0	451	2	0
51	1	377	0	418	5	0
52	2	504	0	572	7	0
53	3	302	0	340	5	0
54	4	480	0	478	10	0
55	Y	1518	0	776	7	0
56	A	42	0	45	0	0
57	A	92	0	0	0	0
57	Q	1	0	0	0	0
57	a	217	0	0	0	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	m	1	0	0	0	0
57	v	1	0	0	0	0
57	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	A	10	0	19	0	0
58	a	120	0	228	10	0
59	Z	10	0	10	0	0
60	a	14	0	26	1	0
61	a	9	0	0	0	0
61	c	1	0	0	0	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
63	Y	17	0	0	0	0
64	0	1	0	0	0	0
64	1	12	0	0	1	0
64	2	24	0	0	1	0
64	3	2	0	0	0	0
64	A	3	0	0	0	0
64	Y	2	0	0	0	0
64	Z	1	0	0	0	0
64	a	3052	0	0	8	0
64	b	37	0	0	0	0
64	c	90	0	0	2	0
64	d	38	0	0	0	0
64	e	31	0	0	1	0
64	h	1	0	0	0	0
64	i	11	0	0	0	0
64	j	9	0	0	1	0
64	k	36	0	0	1	0
64	l	27	0	0	0	0
64	m	21	0	0	0	0
64	o	12	0	0	0	0
64	p	22	0	0	0	0
64	q	14	0	0	1	0
64	r	21	0	0	0	0
64	s	4	0	0	0	0
64	t	1	0	0	0	0
64	u	5	0	0	0	0
64	v	9	0	0	0	0
64	w	11	0	0	0	0
64	x	1	0	0	0	0
64	y	1	0	0	0	0
64	z	28	0	0	0	0
All	All	145583	0	95393	1050	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1050) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:U:H3	1:A:1457:G:H1	1.04	1.00
1:A:1260:G:N2	1:A:1275:A:H62	1.61	0.96
1:A:1127:G:H1	1:A:1145:A:N6	1.63	0.94
1:A:1260:G:H21	1:A:1275:A:H62	0.92	0.92
1:A:62:U:H3	1:A:105:G:H1	0.90	0.89
24:a:1040:A:H61	24:a:1115:G:H1	1.13	0.88
1:A:1260:G:H21	1:A:1275:A:N6	1.72	0.88
1:A:1127:G:H1	1:A:1145:A:H61	1.17	0.86
24:a:1040:A:N6	24:a:1115:G:H1	1.79	0.81
1:A:202:G:H21	1:A:466:A:H61	1.31	0.78
1:A:959:A:HO2'	1:A:984:C:HO2'	1.32	0.78
29:f:118:SER:HB2	29:f:120:LYS:HE3	1.65	0.77
30:g:95:ARG:HH12	30:g:97:ALA:HB2	1.51	0.76
3:C:182:ILE:HA	3:C:202:ILE:O	1.86	0.76
1:A:861:G:HO2'	1:A:874:G:HO2'	1.35	0.75
24:a:2305:U:H5''	29:f:131:GLY:HA3	1.69	0.74
1:A:672:U:H3	1:A:734:G:H1	1.33	0.74
2:B:134:ALA:HA	2:B:137:ARG:HE	1.53	0.73
4:D:68:LEU:O	4:D:72:PHE:HB2	1.89	0.73
48:y:6:LYS:HB2	48:y:58:GLU:HB2	1.71	0.72
33:j:78:ARG:NH1	38:o:71:GLU:OE1	2.22	0.71
6:F:77:THR:O	6:F:81:ASN:HB2	1.91	0.71
1:A:1320:C:H1'	19:S:73:GLU:HG2	1.71	0.70
37:n:51:ALA:HB2	37:n:81:ARG:HH12	1.56	0.70
1:A:201:G:HO2'	1:A:469:C:HO2'	1.38	0.70
31:h:9:VAL:HG13	31:h:11:ASN:H	1.56	0.69
14:N:29:ALA:O	14:N:33:ASP:HB2	1.92	0.69
1:A:830:G:H4'	2:B:21:ARG:HA	1.75	0.69
32:i:96:ARG:HB2	32:i:99:ARG:HG3	1.74	0.68
24:a:100:U:H3	43:t:91:LYS:HE2	1.60	0.67
8:H:51:VAL:HA	8:H:58:GLU:O	1.95	0.67
55:Y:29:G:N1	55:Y:42:U:N3	2.42	0.67
3:C:70:THR:HG22	3:C:72:ARG:H	1.60	0.67
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.77	0.67
16:P:1:MET:HE2	16:P:66:THR:HG21	1.77	0.66
50:O:14:SER:HB3	50:O:48:ILE:O	1.96	0.66
1:A:837:U:H2'	1:A:838:G:H8	1.59	0.66
4:D:132:ILE:HG22	4:D:134:SER:H	1.60	0.66
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.78	0.66
3:C:69:HIS:HA	3:C:104:ALA:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HB	10:J:76:ILE:HB	1.78	0.65
36:m:22:ARG:HG3	36:m:70:THR:HA	1.79	0.65
1:A:1128:C:H1'	1:A:1147:C:H42	1.62	0.64
33:j:13:ASN:O	33:j:51:LYS:NZ	2.28	0.64
64:a:6309:HOH:O	39:p:11:ARG:NH1	2.28	0.64
13:M:23:TYR:HB3	13:M:66:GLU:HA	1.80	0.64
14:N:54:ASP:HA	14:N:59:ARG:HG3	1.80	0.64
17:Q:77:ARG:HH21	17:Q:78:VAL:HG12	1.62	0.64
36:m:78:LYS:NZ	36:m:82:GLU:OE2	2.31	0.64
1:A:71:A:H61	1:A:99:C:H1'	1.63	0.64
16:P:14:ARG:HH12	16:P:42:ILE:HD13	1.61	0.64
8:H:10:MET:HA	8:H:27:MET:HE1	1.80	0.64
28:e:57:LYS:NZ	64:e:302:HOH:O	2.31	0.64
9:I:71:GLY:O	9:I:75:GLN:HB2	1.97	0.63
27:d:184:ARG:NH1	38:o:7:GLN:OE1	2.31	0.63
1:A:756:C:HO2'	8:H:2:SER:N	1.96	0.63
1:A:677:U:H3	1:A:713:G:H22	1.45	0.63
24:a:749:A:H5''	58:a:6213:SPD:H82	1.79	0.63
3:C:65:ARG:NH1	3:C:67:THR:OG1	2.31	0.63
30:g:2:SER:OG	30:g:3:ARG:N	2.31	0.63
4:D:201:VAL:O	4:D:205:SER:HB2	1.98	0.63
8:H:13:ARG:HE	8:H:27:MET:HE2	1.64	0.62
41:r:24:ILE:HD13	41:r:36:LEU:HD11	1.80	0.62
1:A:216:U:H4'	1:A:464:U:H4'	1.81	0.62
23:Z:50:U:H3	23:Z:64:G:H1	1.47	0.62
13:M:101:ARG:HH12	13:M:103:LYS:HB3	1.63	0.62
1:A:51:A:N7	1:A:114:U:O2'	2.33	0.62
13:M:106:ALA:O	13:M:110:LYS:HB2	2.00	0.62
30:g:48:ASN:HB3	30:g:50:LEU:HG	1.81	0.62
1:A:148:G:HO2'	1:A:1446:A:HO2'	1.48	0.61
1:A:176:C:OP1	20:T:24:ARG:NH1	2.33	0.61
33:j:59:LYS:NZ	33:j:92:GLU:OE2	2.30	0.61
1:A:294:U:OP1	1:A:610:U:O2'	2.16	0.61
1:A:516:PSU:O2'	1:A:519:C:N3	2.33	0.61
1:A:77:A:H2'	1:A:78:A:H8	1.64	0.61
40:q:71:LYS:HG2	40:q:73:LYS:HE2	1.82	0.61
1:A:375:U:H4'	16:P:6:LEU:HD12	1.82	0.61
1:A:1009:U:H3	1:A:1020:G:H1	0.76	0.61
19:S:21:LYS:HA	19:S:24:GLU:HG2	1.81	0.61
1:A:823:C:HO2'	8:H:2:SER:N	1.98	0.61
19:S:48:THR:HA	19:S:60:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:THR:HA	10:J:63:ASP:O	2.00	0.61
24:a:468:G:N7	51:1:39:ARG:NH2	2.43	0.61
2:B:218:ALA:HB1	2:B:222:ARG:HH21	1.66	0.60
1:A:1127:G:N1	1:A:1145:A:N6	2.34	0.60
1:A:674:G:H2'	1:A:675:A:H8	1.67	0.60
3:C:151:VAL:HG22	3:C:200:VAL:HG22	1.83	0.60
29:f:2:ALA:HB2	29:f:94:GLU:OE2	2.01	0.60
1:A:1526:G:N7	21:U:40:LYS:NZ	2.49	0.60
4:D:98:LEU:HD21	4:D:123:ILE:HG21	1.82	0.60
4:D:125:VAL:HG22	4:D:143:VAL:HG22	1.83	0.60
7:G:110:LYS:HD2	7:G:133:THR:HG21	1.84	0.60
26:c:171:TYR:HB3	26:c:183:LYS:HD2	1.84	0.60
1:A:185:U:O2'	20:T:76:LYS:NZ	2.34	0.59
24:a:1478:G:H1	24:a:1513:U:H3	1.50	0.59
1:A:1057:G:O2'	3:C:188:GLU:OE2	2.20	0.59
7:G:57:SER:HB3	7:G:60:GLU:HB3	1.85	0.59
16:P:1:MET:N	16:P:24:SER:OG	2.36	0.59
24:a:1236:G:N7	58:a:6207:SPD:N6	2.42	0.59
35:l:20:LEU:HD13	44:u:81:PRO:HG2	1.84	0.59
2:B:100:MET:HA	2:B:107:VAL:HG21	1.85	0.59
4:D:174:ASP:OD1	4:D:174:ASP:N	2.36	0.59
5:E:107:ALA:O	5:E:112:ARG:NH2	2.35	0.59
31:h:7:ASP:HB3	31:h:35:LYS:HB2	1.84	0.59
1:A:255:G:OP1	17:Q:71:LYS:NZ	2.36	0.59
29:f:56:ASP:OD2	29:f:150:ARG:NH1	2.36	0.59
44:u:80:HIS:CE1	44:u:82:TYR:H	2.20	0.59
14:N:6:MET:HB3	14:N:63:ARG:HH12	1.68	0.58
1:A:31:G:O2'	1:A:48:C:N4	2.36	0.58
1:A:392:C:H4'	16:P:13:LYS:HZ3	1.68	0.58
1:A:1343:G:OP1	9:I:124:ARG:NH2	2.36	0.58
1:A:1440:U:H3	1:A:1461:G:H1	1.50	0.58
4:D:26:ARG:HE	4:D:31:LYS:HG2	1.68	0.58
14:N:64:CYS:HB2	14:N:80:SER:H	1.68	0.58
26:c:84:ASP:HB2	26:c:91:ILE:HG12	1.86	0.58
33:j:108:ARG:HH21	38:o:34:GLU:HB3	1.68	0.58
1:A:1149:C:O2'	1:A:1280:A:N1	2.36	0.58
1:A:1290:G:HO2'	9:I:41:ARG:HH12	1.50	0.58
1:A:1222:G:H5''	19:S:78:ARG:HE	1.69	0.58
9:I:18:ARG:NH1	9:I:66:THR:OG1	2.37	0.58
58:a:6215:SPD:H42	27:d:138:LEU:HB2	1.85	0.58
24:a:2378:A:N1	37:n:13:ARG:NH2	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:4:13:THR:HG22	54:4:23:LYS:HG2	1.85	0.57
9:I:106:ARG:NH1	9:I:107:ASP:O	2.37	0.57
13:M:96:PRO:HB3	13:M:109:ARG:HG3	1.85	0.57
1:A:2:A:H4'	4:D:83:LYS:HE2	1.84	0.57
1:A:1530:G:H2'	1:A:1531:A:H8	1.69	0.57
11:K:23:ILE:HD13	11:K:96:THR:HB	1.86	0.57
1:A:427:U:OP1	4:D:13:ARG:NH1	2.38	0.57
49:z:43:ILE:HG22	49:z:49:TYR:HB2	1.85	0.57
24:a:61:C:OP2	47:x:47:ARG:NH2	2.38	0.57
24:a:84:A:N1	24:a:98:G:O2'	2.38	0.57
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.52	0.57
13:M:11:ASP:HA	13:M:45:ILE:HD11	1.87	0.57
24:a:568:U:H1'	24:a:2030:6MZ:H9C1	1.86	0.57
44:u:64:VAL:HG22	44:u:69:GLU:HG3	1.87	0.57
26:c:181:MET:HB2	26:c:268:VAL:HB	1.86	0.57
1:A:8:A:N6	4:D:202:GLU:O	2.33	0.56
16:P:26:ASN:OD1	16:P:26:ASN:N	2.36	0.56
31:h:12:LEU:HD22	31:h:19:VAL:HG21	1.85	0.56
1:A:796:C:O2'	11:K:137:ARG:NH2	2.38	0.56
10:J:18:ILE:HG23	10:J:72:ARG:HH21	1.70	0.56
17:Q:21:ILE:HG12	17:Q:48:ASP:HB2	1.86	0.56
4:D:95:GLU:O	4:D:100:ASN:ND2	2.38	0.56
5:E:157:ARG:NH2	8:H:43:GLU:OE1	2.38	0.56
27:d:35:THR:HG22	27:d:73:VAL:HG21	1.87	0.56
28:e:7:ASP:OD1	28:e:7:ASP:N	2.37	0.56
3:C:72:ARG:HB3	3:C:75:ILE:HB	1.88	0.56
8:H:47:GLU:HB2	8:H:62:THR:HB	1.88	0.56
46:w:43:GLU:HG3	46:w:45:ARG:HB2	1.87	0.56
1:A:1124:G:N2	1:A:1125:U:O4	2.38	0.56
14:N:13:ARG:HD3	14:N:59:ARG:HB3	1.86	0.56
1:A:1218:C:H2'	1:A:1219:A:H8	1.71	0.56
11:K:88:GLY:O	11:K:93:ARG:NH1	2.38	0.56
12:L:5:ASN:OD1	17:Q:36:LYS:NZ	2.38	0.56
1:A:380:G:N2	1:A:383:A:OP2	2.37	0.56
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.56
29:f:61:SER:HB3	29:f:89:VAL:HG21	1.88	0.56
44:u:44:HIS:O	44:u:48:MET:HB2	2.06	0.56
52:2:42:ARG:NH2	64:2:102:HOH:O	2.38	0.56
5:E:82:GLN:HB2	5:E:83:HIS:HD2	1.70	0.56
5:E:156:LYS:HG3	8:H:71:VAL:HG13	1.87	0.56
1:A:1028:C:N4	1:A:1033:G:O6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:52:LEU:HD22	16:P:57:ILE:HD11	1.88	0.55
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.39	0.55
2:B:42:ASN:HB3	2:B:45:LYS:HB2	1.87	0.55
2:B:31:ILE:HD11	2:B:189:THR:HB	1.88	0.55
4:D:102:VAL:HG13	4:D:107:PHE:HB2	1.88	0.55
14:N:6:MET:HG2	14:N:63:ARG:HH22	1.72	0.55
9:I:63:LEU:HD23	9:I:65:ILE:HD11	1.88	0.55
54:4:41:HIS:HB3	54:4:44:PHE:HB2	1.88	0.55
1:A:619:U:O2'	4:D:128:ARG:NH2	2.40	0.55
4:D:105:MET:HG3	4:D:171:LEU:HD13	1.87	0.55
10:J:11:LYS:HG3	10:J:71:LEU:HD13	1.89	0.55
38:o:5:ILE:HA	38:o:8:LEU:HD12	1.89	0.55
1:A:486:U:H2'	1:A:487:A:H8	1.71	0.55
3:C:119:SER:OG	3:C:123:GLN:OE1	2.20	0.55
4:D:168:PRO:HG2	4:D:171:LEU:HD12	1.88	0.55
24:a:2308:G:O2'	24:a:2310:C:N4	2.39	0.55
35:l:25:ASP:O	35:l:66:ARG:NH1	2.38	0.55
1:A:1009:U:O2	1:A:1020:G:N2	2.26	0.55
24:a:2532:G:N2	24:a:2663:G:O2'	2.39	0.55
28:e:46:GLN:O	28:e:88:ARG:NH2	2.39	0.55
1:A:54:C:OP1	1:A:351:G:N2	2.40	0.55
1:A:880:C:OP1	12:L:5:ASN:ND2	2.36	0.55
1:A:1346:A:OP1	9:I:122:ARG:NH1	2.40	0.55
24:a:1724:G:O6	24:a:1736:U:O4	2.25	0.55
41:r:109:ASP:OD2	41:r:110:ARG:HG3	2.06	0.55
1:A:545:C:OP1	4:D:58:LYS:NZ	2.39	0.54
1:A:721:G:OP2	18:R:43:ARG:NH1	2.40	0.54
1:A:1236:A:H4'	1:A:1304:G:H4'	1.89	0.54
10:J:87:LEU:HA	10:J:90:LEU:HD13	1.89	0.54
20:T:56:PRO:HB2	20:T:60:ARG:HH12	1.72	0.54
24:a:568:U:O4	40:q:81:LYS:NZ	2.40	0.54
45:v:37:ILE:HG21	45:v:80:ILE:HG21	1.89	0.54
1:A:919:A:O2'	1:A:1080:A:N1	2.38	0.54
24:a:1796:U:H2'	24:a:1797:G:H8	1.72	0.54
1:A:664:G:H22	1:A:741:G:H1	1.54	0.54
3:C:184:TYR:HA	3:C:200:VAL:O	2.07	0.54
24:a:1434:A:H2'	24:a:1435:G:C8	2.42	0.54
1:A:181:A:N6	1:A:195:A:OP2	2.39	0.54
1:A:1003:G:N2	1:A:1004:A:O2'	2.41	0.54
18:R:37:GLY:O	18:R:63:ARG:NH2	2.39	0.54
24:a:2640:G:OP1	32:i:99:ARG:NH2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:31:VAL:HA	29:f:158:THR:HG22	1.88	0.54
48:y:5:ILE:HG22	48:y:59:GLU:HA	1.89	0.54
24:a:1469:A:H2'	24:a:1470:A:C8	2.42	0.54
1:A:675:A:O2'	11:K:116:ILE:O	2.23	0.54
4:D:105:MET:HG2	4:D:173:VAL:HG22	1.89	0.54
30:g:33:LEU:HD23	30:g:75:MET:HG3	1.90	0.54
1:A:410:G:H21	1:A:432:A:H62	1.56	0.54
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.88	0.54
16:P:17:TYR:HB2	16:P:39:PHE:HB3	1.89	0.54
24:a:2305:U:N3	29:f:151:GLY:O	2.40	0.54
26:c:35:GLU:HG3	26:c:64:ILE:HD11	1.89	0.54
26:c:87:ARG:NH1	64:c:404:HOH:O	2.39	0.54
1:A:1354:U:H2'	1:A:1355:G:H8	1.73	0.54
21:U:5:LYS:O	21:U:18:ARG:NH2	2.37	0.54
36:m:78:LYS:HG3	36:m:82:GLU:OE2	2.08	0.54
1:A:1064:G:O3'	1:A:1190:G:N2	2.41	0.53
1:A:1342:C:H2'	1:A:1343:G:H8	1.73	0.53
2:B:15:HIS:HB3	2:B:43:LEU:HD11	1.89	0.53
5:E:40:GLY:HA2	5:E:71:MET:HE1	1.91	0.53
24:a:2305:U:OP1	29:f:133:ARG:NH1	2.36	0.53
6:F:101:PRO:HG2	18:R:24:LYS:HB3	1.91	0.53
13:M:16:VAL:HG23	13:M:17:ILE:HG12	1.90	0.53
24:a:1724:G:H1	24:a:1736:U:H3	1.55	0.53
24:a:2830:C:H5''	27:d:56:LYS:HE3	1.89	0.53
1:A:405:U:O4	4:D:3:ARG:N	2.36	0.53
1:A:1348:U:H4'	9:I:122:ARG:HG3	1.90	0.53
9:I:17:ALA:HB2	9:I:67:VAL:HG23	1.89	0.53
13:M:71:ARG:NH1	29:f:113:ASP:OD1	2.34	0.53
9:I:52:LEU:HD23	9:I:58:VAL:HG13	1.90	0.53
16:P:1:MET:N	16:P:1:MET:SD	2.72	0.53
55:Y:29:G:C6	55:Y:42:U:N3	2.75	0.53
1:A:1096:C:O2	1:A:1170:A:O2'	2.26	0.53
2:B:32:PHE:HB3	2:B:40:ILE:HG22	1.90	0.53
3:C:47:LEU:HD22	3:C:76:VAL:HG22	1.90	0.53
24:a:1386:C:H2'	24:a:1387:A:C8	2.43	0.53
24:a:2469:A:H4'	35:l:55:ARG:HD3	1.88	0.53
39:p:36:PHE:O	39:p:40:ILE:HG12	2.09	0.53
24:a:351:C:H2'	24:a:352:A:C8	2.44	0.53
24:a:2012:G:OP1	41:r:11:ARG:NH2	2.36	0.53
30:g:18:LYS:HD3	30:g:25:THR:HG23	1.90	0.53
1:A:74:A:H2	1:A:96:U:H3	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:U:H1'	12:L:12:ARG:HG3	1.91	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.89	0.53
9:I:60:LYS:HE3	9:I:61:LEU:HG	1.91	0.53
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.91	0.53
12:L:36:ARG:HG2	12:L:54:ARG:HB2	1.90	0.53
24:a:278:A:OP2	24:a:361:G:N2	2.39	0.53
1:A:1189:U:H5''	3:C:5:VAL:HG21	1.90	0.53
17:Q:59:VAL:HG12	17:Q:78:VAL:HA	1.90	0.53
28:e:170:ARG:NH1	28:e:174:GLY:O	2.38	0.53
30:g:24:ILE:HD11	30:g:43:VAL:HG21	1.91	0.53
1:A:392:C:OP1	16:P:8:ARG:NH2	2.42	0.52
1:A:453:G:OP1	16:P:76:LYS:NZ	2.37	0.52
3:C:22:TRP:HB3	3:C:59:ARG:H	1.75	0.52
6:F:7:VAL:HG22	6:F:61:LEU:HG	1.90	0.52
17:Q:25:ILE:HD11	17:Q:61:ILE:HD11	1.92	0.52
41:r:2:GLU:OE2	41:r:108:SER:OG	2.26	0.52
1:A:815:A:N7	1:A:1509:C:O2'	2.38	0.52
26:c:71:LYS:NZ	26:c:98:ASP:OD2	2.38	0.52
55:Y:18:G:O4'	55:Y:57:G:N2	2.42	0.52
43:t:4:LYS:O	43:t:94:ARG:NH1	2.41	0.52
54:4:15:SER:HA	54:4:20:ASN:O	2.09	0.52
1:A:1233:G:OP1	9:I:119:ARG:NH2	2.37	0.52
2:B:86:SER:O	2:B:222:ARG:NH1	2.41	0.52
1:A:692:U:OP2	11:K:28:ASN:ND2	2.40	0.52
5:E:107:ALA:HB1	5:E:111:MET:HB3	1.91	0.52
29:f:116:GLY:O	29:f:178:ARG:NH1	2.42	0.52
33:j:105:ARG:NH2	38:o:34:GLU:OE2	2.39	0.52
1:A:404:G:O2'	1:A:498:A:N1	2.41	0.52
3:C:32:ASN:OD1	3:C:59:ARG:NH1	2.42	0.52
24:a:2204:G:H4'	26:c:150:LYS:HG3	1.91	0.52
37:n:7:ARG:NH1	37:n:95:SER:O	2.43	0.52
42:s:44:LYS:HZ2	42:s:55:VAL:HB	1.75	0.52
1:A:1241:G:H2'	1:A:1242:G:H8	1.74	0.52
45:v:37:ILE:HD11	45:v:82:ILE:HD11	1.92	0.52
24:a:219:A:N3	24:a:234:U:O2'	2.37	0.52
24:a:277:G:H21	24:a:361:G:H2'	1.74	0.52
38:o:7:GLN:HA	38:o:10:GLN:HG3	1.90	0.52
2:B:119:THR:O	2:B:123:ASP:HB3	2.09	0.51
3:C:26:THR:HG23	14:N:76:LYS:HD2	1.92	0.51
24:a:1769:U:O2'	24:a:1958:C:OP1	2.28	0.51
24:a:1995:U:O3'	33:j:31:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:2638:G:OP2	27:d:83:ARG:NH2	2.44	0.51
1:A:62:U:O4	1:A:105:G:O6	2.27	0.51
1:A:401:C:H2'	1:A:402:G:C8	2.45	0.51
1:A:544:G:OP2	4:D:63:ARG:NH2	2.42	0.51
1:A:1183:U:O2'	1:A:1185:G:OP2	2.29	0.51
2:B:95:ARG:NH1	2:B:96:TRP:O	2.43	0.51
12:L:67:ILE:HD13	12:L:74:LEU:HD12	1.92	0.51
1:A:438:U:H1'	1:A:439:U:H5	1.76	0.51
1:A:690:G:O6	11:K:53:ARG:NH2	2.43	0.51
24:a:1889:A:H2'	24:a:1890:A:C8	2.46	0.51
40:q:37:GLU:HB3	40:q:53:PHE:CE1	2.46	0.51
42:s:30:ILE:HG13	42:s:85:VAL:HB	1.92	0.51
1:A:1290:G:O2'	9:I:41:ARG:NH1	2.41	0.51
5:E:21:VAL:HG23	5:E:32:SER:HB3	1.93	0.51
40:q:84:ARG:NH2	64:q:202:HOH:O	2.43	0.51
1:A:1067:A:H2'	1:A:1093:A:H4'	1.93	0.51
1:A:1175:G:H2'	1:A:1176:A:H8	1.75	0.51
24:a:1589:U:H2'	24:a:1590:A:H8	1.75	0.51
24:a:1653:G:H3'	36:m:2:ARG:HG2	1.93	0.51
42:s:47:VAL:HG13	42:s:51:PHE:HD2	1.76	0.51
1:A:652:U:O4	1:A:752:G:O2'	2.28	0.51
11:K:84:VAL:HG21	11:K:97:ILE:HD13	1.93	0.51
19:S:10:PHE:O	19:S:39:THR:OG1	2.26	0.51
24:a:1744:A:H3'	24:a:1745:A:H8	1.76	0.51
1:A:1005:A:H3'	1:A:1006:G:H8	1.76	0.51
11:K:15:GLN:NE2	11:K:77:TYR:O	2.44	0.51
35:l:10:ARG:HE	35:l:11:LYS:HE3	1.76	0.51
44:u:80:HIS:CD2	44:u:83:LYS:HD2	2.46	0.51
54:4:16:CYS:SG	54:4:17:SER:N	2.83	0.51
1:A:197:A:N1	1:A:220:G:O2'	2.38	0.50
1:A:227:G:O2'	16:P:63:GLN:OE1	2.28	0.50
1:A:1222:G:OP1	19:S:78:ARG:NH2	2.43	0.50
10:J:10:LEU:O	10:J:71:LEU:HA	2.11	0.50
10:J:19:ASP:HA	10:J:22:THR:HG22	1.93	0.50
24:a:2205:A:OP1	26:c:68:LYS:NZ	2.44	0.50
1:A:1291:U:H2'	1:A:1292:G:H8	1.77	0.50
24:a:1688:U:O2'	24:a:1700:A:N7	2.38	0.50
25:b:93:C:OP2	44:u:18:ARG:NH1	2.44	0.50
32:i:36:LEU:HD11	32:i:122:LEU:HB2	1.93	0.50
38:o:9:GLU:HA	38:o:55:LEU:HD22	1.92	0.50
1:A:1130:A:H61	1:A:1144:G:H1'	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.92	0.50
24:a:1796:U:H2'	24:a:1797:G:C8	2.46	0.50
26:c:16:VAL:HG22	26:c:206:GLY:HA3	1.92	0.50
1:A:542:G:O3'	4:D:14:ARG:NH2	2.43	0.50
10:J:42:LEU:HB2	10:J:71:LEU:HG	1.93	0.50
1:A:77:A:H2'	1:A:78:A:C8	2.45	0.50
1:A:1491:G:H5''	12:L:43:LYS:HG3	1.94	0.50
1:A:601:G:H2'	1:A:602:A:H8	1.76	0.50
24:a:249:C:O2	52:2:12:LYS:NZ	2.40	0.50
24:a:1394:U:H4'	24:a:1603:A:H4'	1.93	0.50
64:a:6537:HOH:O	41:r:92:ARG:NH1	2.45	0.50
45:v:59:LEU:HD12	45:v:80:ILE:HD12	1.94	0.50
10:J:84:VAL:O	10:J:88:MET:HB2	2.11	0.50
12:L:87:VAL:HB	12:L:90:LEU:HB2	1.93	0.50
14:N:64:CYS:SG	14:N:67:THR:N	2.77	0.50
24:a:651:G:H5'	52:2:19:LYS:HG3	1.94	0.50
26:c:2:ALA:N	26:c:20:VAL:O	2.44	0.50
1:A:473:U:H2'	1:A:474:G:H8	1.77	0.50
1:A:1149:C:OP2	9:I:11:ARG:NH2	2.45	0.50
1:A:1356:G:H2'	1:A:1357:A:C8	2.46	0.50
9:I:15:SER:OG	9:I:70:GLY:N	2.43	0.50
24:a:2291:U:H2'	24:a:2292:U:C6	2.47	0.50
42:s:37:ASP:OD1	42:s:37:ASP:N	2.45	0.50
43:t:4:LYS:HD3	43:t:83:VAL:HB	1.94	0.50
51:l:35:ARG:NH1	64:l:102:HOH:O	2.44	0.50
1:A:1513:A:H2'	1:A:1514:G:C8	2.47	0.50
24:a:1434:A:H2'	24:a:1435:G:H8	1.77	0.50
53:3:2:LYS:HB2	53:3:35:GLN:HB3	1.93	0.50
1:A:1290:G:HO2'	9:I:41:ARG:NH1	2.10	0.49
4:D:126:ASN:ND2	4:D:141:ASP:OD1	2.44	0.49
6:F:3:HIS:NE2	6:F:65:GLU:OE1	2.45	0.49
31:h:29:PHE:O	31:h:33:GLN:HB2	2.11	0.49
42:s:44:LYS:NZ	42:s:55:VAL:O	2.45	0.49
10:J:14:ASP:HB3	10:J:17:LEU:HB2	1.94	0.49
20:T:54:MET:HE2	20:T:58:VAL:HG13	1.94	0.49
25:b:49:C:H2'	25:b:50:A:C8	2.46	0.49
1:A:662:U:O2'	1:A:836:G:O5'	2.30	0.49
24:a:848:C:H2'	24:a:849:A:C8	2.47	0.49
1:A:662:U:H2'	1:A:663:A:C8	2.48	0.49
24:a:172:A:H2'	24:a:173:A:C8	2.47	0.49
27:d:4:LEU:HD13	27:d:29:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:12:ASP:OD1	33:j:14:SER:OG	2.27	0.49
1:A:451:A:OP1	1:A:481:G:N1	2.41	0.49
1:A:1032:G:N2	1:A:1033:G:N3	2.60	0.49
4:D:108:GLY:HA2	4:D:113:GLU:HG2	1.94	0.49
5:E:105:ILE:O	5:E:112:ARG:NH1	2.41	0.49
13:M:7:ILE:HD11	13:M:22:ILE:HG12	1.94	0.49
1:A:599:C:H2'	1:A:600:A:H8	1.78	0.49
1:A:1009:U:O4	1:A:1020:G:O6	2.30	0.49
1:A:1379:G:OP2	7:G:5:ARG:NE	2.40	0.49
24:a:2394:C:H5''	34:k:63:LYS:HE2	1.94	0.49
58:a:6213:SPD:H51	41:r:86:MET:HE3	1.95	0.49
55:Y:58:A:O2'	55:Y:61:C:N4	2.45	0.49
1:A:620:C:C2	4:D:132:ILE:HG21	2.48	0.49
1:A:1237:C:OP1	1:A:1303:C:O2'	2.31	0.49
15:O:15:PHE:HB3	15:O:26:GLU:HB3	1.94	0.49
25:b:66:A:H61	25:b:107:G:H2'	1.76	0.49
10:J:54:SER:OG	10:J:56:HIS:O	2.31	0.49
41:r:29:VAL:HB	41:r:55:ILE:HD11	1.94	0.49
1:A:323:U:OP1	20:T:25:ARG:NH2	2.33	0.49
40:q:17:GLY:O	40:q:97:LYS:NZ	2.38	0.49
24:a:1405:U:H2'	24:a:1406:U:C6	2.48	0.49
44:u:80:HIS:CE1	44:u:83:LYS:H	2.31	0.49
1:A:728:A:H2'	1:A:729:A:C8	2.48	0.48
1:A:981:U:OP1	14:N:9:ARG:NH1	2.41	0.48
24:a:351:C:H2'	24:a:352:A:H8	1.78	0.48
24:a:871:U:H2'	24:a:872:U:C6	2.48	0.48
24:a:911:A:N6	35:l:11:LYS:O	2.45	0.48
24:a:1181:U:H2'	24:a:1182:G:C8	2.48	0.48
24:a:2638:G:O2'	24:a:2775:G:N2	2.43	0.48
1:A:1317:C:O5'	14:N:24:ARG:NH2	2.46	0.48
24:a:1429:G:H2'	24:a:1430:G:H8	1.78	0.48
26:c:21:ASN:HB3	26:c:24:LEU:HG	1.95	0.48
30:g:163:ARG:HD3	30:g:169:VAL:HG21	1.95	0.48
1:A:159:G:N2	1:A:162:A:OP2	2.46	0.48
24:a:581:C:H2'	24:a:582:A:C8	2.47	0.48
1:A:235:C:H2'	1:A:236:A:H8	1.77	0.48
1:A:405:U:O4	4:D:2:ALA:N	2.46	0.48
3:C:14:ILE:HG22	3:C:15:VAL:HG23	1.94	0.48
9:I:39:PHE:O	9:I:45:ARG:NE	2.41	0.48
24:a:2243:U:H2'	24:a:2244:U:C6	2.48	0.48
28:e:176:ASP:N	28:e:176:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:35:ILE:HG21	37:n:71:ALA:HA	1.95	0.48
9:I:12:ARG:HD3	9:I:13:LYS:HG3	1.94	0.48
16:P:37:GLY:HA3	16:P:51:ARG:O	2.14	0.48
24:a:1112:G:O3'	30:g:3:ARG:NH2	2.47	0.48
24:a:1378:A:O2'	24:a:1380:G:N7	2.47	0.48
24:a:2312:U:H5'	29:f:85:ILE:HD11	1.96	0.48
42:s:47:VAL:O	42:s:51:PHE:HB2	2.14	0.48
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.48
4:D:67:VAL:HG13	4:D:71:GLN:HB3	1.95	0.48
13:M:25:VAL:HG13	13:M:29:ARG:HB3	1.95	0.48
16:P:15:PRO:HB2	16:P:41:PRO:HG3	1.94	0.48
24:a:668:A:H2'	24:a:670:A:H62	1.79	0.48
28:e:168:ASP:HB2	28:e:183:PHE:CZ	2.48	0.48
37:n:27:VAL:HA	37:n:93:ASP:HB3	1.95	0.48
1:A:676:A:H5''	11:K:115:PRO:HB3	1.95	0.48
47:x:42:LEU:O	47:x:46:VAL:HG12	2.13	0.48
1:A:201:G:H2'	1:A:202:G:C8	2.49	0.48
5:E:46:VAL:HG11	5:E:114:VAL:HG13	1.96	0.48
6:F:42:TRP:HB2	6:F:59:TYR:HB2	1.95	0.48
19:S:48:THR:HG22	19:S:61:PHE:HA	1.96	0.48
1:A:411:A:P	4:D:26:ARG:HH12	2.37	0.48
1:A:1524:C:OP1	11:K:132:ARG:NH2	2.47	0.48
24:a:494:G:H4'	41:r:6:LYS:HB2	1.95	0.48
33:j:70:ARG:HD2	33:j:76:VAL:HB	1.96	0.48
34:k:82:LEU:HD22	34:k:90:VAL:HG21	1.95	0.48
1:A:948:C:H2'	1:A:949:A:H8	1.79	0.48
1:A:1279:G:OP2	10:J:11:LYS:NZ	2.46	0.48
53:3:9:LYS:HE3	53:3:16:ILE:HD12	1.96	0.48
1:A:928:G:O2'	1:A:1533:C:OP1	2.32	0.47
1:A:1342:C:H2'	1:A:1343:G:C8	2.49	0.47
2:B:54:LEU:HD22	2:B:220:THR:HG21	1.95	0.47
3:C:11:ARG:NH2	3:C:177:THR:O	2.47	0.47
24:a:617:G:H5'	28:e:199:MET:HE3	1.96	0.47
24:a:2478:A:H5'	53:3:32:LYS:HE2	1.95	0.47
24:a:2748:A:H5'	30:g:4:VAL:HG21	1.95	0.47
30:g:86:LYS:HE3	30:g:86:LYS:HB2	1.75	0.47
1:A:637:C:H5'	17:Q:4:LYS:HD3	1.96	0.47
1:A:1355:G:H2'	1:A:1356:G:C8	2.49	0.47
2:B:111:ILE:HD13	2:B:111:ILE:HA	1.74	0.47
19:S:58:VAL:HG21	19:S:76:PRO:HD2	1.95	0.47
24:a:1136:G:N7	64:a:6439:HOH:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:2262:U:OP1	24:a:2387:U:O2'	2.32	0.47
37:n:77:ALA:HB1	37:n:81:ARG:HH22	1.79	0.47
1:A:710:G:OP1	6:F:53:LYS:NZ	2.33	0.47
1:A:1071:C:H2'	1:A:1072:G:H8	1.78	0.47
14:N:27:LEU:HD11	14:N:47:LYS:HE2	1.96	0.47
24:a:767:U:C4	60:a:6216:SPM:H132	2.50	0.47
28:e:145:ASP:HB3	28:e:184:ASP:HB2	1.96	0.47
45:v:10:THR:OG1	45:v:11:ARG:N	2.47	0.47
1:A:559:A:H4'	1:A:560:A:H3'	1.95	0.47
27:d:48:ILE:HG23	27:d:84:LEU:HD11	1.95	0.47
24:a:2533:U:OP1	24:a:2665:A:O2'	2.27	0.47
40:q:41:ILE:HD12	40:q:54:VAL:HG11	1.97	0.47
1:A:62:U:OP1	1:A:385:C:O2'	2.32	0.47
1:A:410:G:N2	1:A:432:A:H62	2.13	0.47
1:A:1404:C:H2'	1:A:1405:G:C8	2.49	0.47
9:I:85:ARG:HA	9:I:88:MET:HG3	1.97	0.47
15:O:26:GLU:HG3	15:O:81:LEU:HD22	1.95	0.47
24:a:593:U:H2'	24:a:594:U:C6	2.50	0.47
24:a:631:A:N3	24:a:2415:G:O2'	2.43	0.47
35:l:50:ARG:O	35:l:54:THR:OG1	2.27	0.47
44:u:58:SER:O	44:u:73:LYS:NZ	2.47	0.47
52:2:15:LYS:HB2	52:2:23:LYS:HG2	1.96	0.47
1:A:147:G:H2'	1:A:148:G:C8	2.49	0.47
1:A:493:A:H2'	1:A:494:G:C8	2.50	0.47
1:A:693:G:HO2'	7:G:83:SER:HG	1.62	0.47
6:F:10:VAL:HG12	6:F:58:HIS:HB3	1.96	0.47
13:M:19:LEU:HD11	13:M:56:LEU:HD22	1.97	0.47
18:R:33:ILE:HG21	18:R:68:LEU:HD21	1.95	0.47
30:g:164:TYR:HB2	30:g:167:GLU:HB2	1.96	0.47
1:A:801:U:H2'	1:A:802:A:H8	1.80	0.47
1:A:1333:A:H3'	1:A:1334:G:H8	1.80	0.47
7:G:86:GLN:HE22	7:G:144:MET:HE2	1.79	0.47
14:N:64:CYS:HB2	14:N:80:SER:N	2.30	0.47
18:R:29:LEU:HD13	18:R:59:ILE:HD12	1.97	0.47
1:A:792:A:O2'	1:A:794:A:N7	2.44	0.47
1:A:816:A:OP1	1:A:1526:G:O2'	2.24	0.47
1:A:1356:G:H2'	1:A:1357:A:H8	1.79	0.47
3:C:28:GLU:O	3:C:32:ASN:ND2	2.44	0.47
5:E:96:MET:HE1	5:E:144:LEU:HG	1.97	0.47
6:F:56:LYS:HB3	6:F:56:LYS:HE3	1.80	0.47
24:a:1496:A:N3	24:a:1577:C:O2'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:2640:G:OP1	32:i:96:ARG:NH1	2.48	0.47
26:c:5:LYS:HD3	26:c:17:VAL:HG22	1.97	0.47
40:q:6:GLN:HG2	40:q:11:GLN:HG2	1.96	0.47
9:l:8:GLY:HA3	9:l:86:ALA:HB2	1.96	0.47
13:M:10:PRO:HB2	13:M:13:LYS:HG3	1.97	0.47
24:a:639:U:H2'	24:a:640:C:C6	2.50	0.47
24:a:1009:A:N3	24:a:1153:C:O2'	2.45	0.47
24:a:2273:A:H2'	24:a:2274:A:C8	2.50	0.47
24:a:2483:C:N3	35:l:123:LYS:NZ	2.62	0.47
28:e:192:ALA:O	28:e:196:VAL:HG23	2.15	0.47
30:g:16:ASP:C	30:g:18:LYS:HZ2	2.22	0.47
30:g:101:ASN:HB2	30:g:117:LEU:HB2	1.95	0.47
38:o:5:ILE:O	38:o:9:GLU:HG2	2.15	0.47
1:A:1060:U:H5''	10:J:53:ILE:HD13	1.96	0.46
3:C:44:THR:O	3:C:48:ALA:HB2	2.15	0.46
5:E:12:GLN:O	5:E:39:VAL:HA	2.15	0.46
13:M:68:ASP:HA	13:M:71:ARG:HG2	1.96	0.46
13:M:78:LYS:NZ	24:a:888:C:N3	2.62	0.46
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.97	0.46
16:P:20:VAL:HG12	16:P:35:ARG:HA	1.96	0.46
24:a:375:G:N2	64:a:6709:HOH:O	2.46	0.46
24:a:1051:G:O6	24:a:1108:U:O2	2.33	0.46
58:a:6215:SPD:N6	27:d:138:LEU:O	2.41	0.46
54:4:8:LYS:HG2	54:4:10:GLU:HG2	1.97	0.46
1:A:1048:G:H5''	14:N:3:LYS:HD2	1.97	0.46
4:D:183:LYS:HA	4:D:183:LYS:HD3	1.74	0.46
24:a:813:U:H2'	24:a:814:C:C6	2.50	0.46
33:j:38:ILE:HD11	33:j:112:PHE:HZ	1.79	0.46
1:A:32:A:H2'	1:A:33:A:H8	1.81	0.46
1:A:375:U:O2	16:P:28:ARG:NH1	2.46	0.46
1:A:501:C:H2'	1:A:502:A:H8	1.81	0.46
1:A:1218:C:H2'	1:A:1219:A:C8	2.49	0.46
13:M:44:LYS:O	13:M:47:GLU:C	2.58	0.46
24:a:1570:A:H2'	24:a:1571:A:C8	2.50	0.46
24:a:2751:G:OP2	30:g:3:ARG:NH1	2.40	0.46
1:A:757:U:OP1	1:A:822:U:O2'	2.25	0.46
1:A:770:C:O2'	1:A:899:C:N3	2.42	0.46
7:G:135:VAL:HA	7:G:138:ARG:HB3	1.98	0.46
14:N:64:CYS:HG	14:N:67:THR:H	1.63	0.46
24:a:172:A:H2'	24:a:173:A:H8	1.81	0.46
24:a:832:U:H2'	24:a:833:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:2304:G:OP1	29:f:121:SER:OG	2.30	0.46
27:d:181:ASP:HB3	27:d:186:LEU:HB2	1.97	0.46
32:i:34:ARG:HG3	32:i:39:LYS:HB2	1.97	0.46
38:o:16:ASP:OD1	38:o:16:ASP:N	2.46	0.46
1:A:713:G:H2'	1:A:714:G:C8	2.51	0.46
9:I:22:LYS:HD2	9:I:23:PRO:HD2	1.97	0.46
24:a:2039:U:H2'	24:a:2040:G:C8	2.51	0.46
28:e:98:LYS:O	28:e:102:ARG:HG3	2.15	0.46
35:l:35:ALA:HB2	35:l:102:LEU:HD11	1.98	0.46
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.15	0.46
58:a:6210:SPD:HN11	58:a:6210:SPD:H42	1.47	0.46
32:i:98:GLU:OE1	32:i:126:ALA:N	2.49	0.46
36:m:54:LEU:HD23	36:m:66:ALA:HB2	1.96	0.46
55:Y:29:G:N1	55:Y:42:U:C2	2.84	0.46
12:L:82:ILE:HG22	12:L:97:THR:HG22	1.96	0.46
24:a:4:U:H2'	24:a:5:A:H8	1.81	0.46
1:A:107:G:O6	20:T:10:ARG:NE	2.49	0.46
1:A:501:C:OP1	12:L:114:ARG:NH2	2.49	0.46
3:C:72:ARG:HG3	3:C:75:ILE:HD12	1.98	0.46
5:E:108:GLY:O	5:E:112:ARG:HB2	2.16	0.46
7:G:42:ILE:HG21	7:G:116:MET:HB3	1.98	0.46
24:a:58:G:O2'	24:a:73:A:N1	2.46	0.46
24:a:1028:A:N6	24:a:1125:G:H2'	2.31	0.46
37:n:12:THR:O	37:n:16:ARG:HG2	2.15	0.46
1:A:231:U:H2'	1:A:232:G:C8	2.50	0.46
3:C:35:SER:OG	3:C:59:ARG:NH2	2.48	0.46
24:a:577:G:O2'	24:a:1254:A:OP1	2.34	0.46
24:a:856:G:H2'	24:a:857:G:C8	2.50	0.46
33:j:71:ARG:HA	33:j:71:ARG:HD3	1.76	0.46
1:A:441:A:H61	1:A:494:G:H22	1.64	0.46
5:E:44:GLY:O	5:E:74:VAL:N	2.49	0.46
24:a:2343:U:O2'	24:a:2373:G:O2'	2.32	0.46
1:A:262:A:H2'	1:A:263:A:C8	2.50	0.45
1:A:1127:G:N2	1:A:1145:A:N1	2.50	0.45
14:N:46:LEU:HB3	19:S:13:LEU:HD22	1.98	0.45
24:a:931:U:O4	24:a:1166:G:N2	2.49	0.45
24:a:1589:U:H2'	24:a:1590:A:C8	2.51	0.45
39:p:15:LYS:HB3	39:p:15:LYS:HE3	1.79	0.45
53:3:8:LYS:HB3	53:3:8:LYS:HE2	1.80	0.45
1:A:127:G:O2'	17:Q:6:ARG:NH1	2.50	0.45
1:A:178:C:H2'	1:A:179:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:G:H2'	1:A:1254:A:H8	1.81	0.45
7:G:116:MET:O	7:G:120:LEU:HB2	2.16	0.45
37:n:25:ARG:O	37:n:39:VAL:HA	2.16	0.45
1:A:299:G:H2'	1:A:300:A:C8	2.51	0.45
9:I:19:VAL:HG22	9:I:65:ILE:HG12	1.99	0.45
26:c:120:VAL:HG23	26:c:134:ASN:HD21	1.81	0.45
41:r:6:LYS:HG2	41:r:104:THR:HG23	1.98	0.45
1:A:1266:G:N2	1:A:1269:A:OP2	2.36	0.45
6:F:52:ASN:HB2	6:F:54:LEU:HD12	1.98	0.45
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.98	0.45
24:a:252:G:N7	64:a:6462:HOH:O	2.36	0.45
24:a:742:A:H2'	24:a:743:A:C8	2.51	0.45
24:a:1794:A:H2'	24:a:1795:C:C6	2.52	0.45
25:b:60:C:H2'	25:b:61:G:H8	1.81	0.45
26:c:18:LYS:HG3	26:c:20:VAL:HG23	1.99	0.45
26:c:141:VAL:HG12	26:c:192:LEU:HA	1.98	0.45
27:d:37:VAL:HG23	27:d:92:VAL:HG23	1.98	0.45
9:I:107:ASP:OD1	9:I:109:ARG:NE	2.41	0.45
12:L:43:LYS:HD3	12:L:91:PRO:HG3	1.99	0.45
35:l:50:ARG:HG3	35:l:65:ILE:HD11	1.97	0.45
1:A:745:G:H2'	1:A:746:A:C8	2.52	0.45
1:A:1226:C:H2'	13:M:102:THR:HB	1.99	0.45
1:A:1251:A:O2'	1:A:1369:C:O3'	2.35	0.45
24:a:499:U:H5''	43:t:43:LYS:HD2	1.98	0.45
24:a:1683:U:H2'	24:a:1684:G:C8	2.51	0.45
33:j:25:LEU:HD12	33:j:38:ILE:HG22	1.99	0.45
40:q:36:ALA:HA	40:q:58:VAL:HG23	1.98	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.51	0.45
6:F:70:VAL:HA	6:F:73:GLU:HB2	1.99	0.45
7:G:111:ARG:HH12	7:G:122:ASN:HB3	1.82	0.45
20:T:16:LYS:HD2	20:T:16:LYS:HA	1.74	0.45
24:a:1264:A:H5'	49:z:8:PRO:HG2	1.99	0.45
24:a:2314:A:H2'	24:a:2315:G:C8	2.51	0.45
24:a:2788:C:H2'	24:a:2789:C:C6	2.52	0.45
58:a:6208:SPD:HN11	58:a:6208:SPD:H41	1.54	0.45
30:g:69:ARG:NH1	30:g:73:ASN:OD1	2.49	0.45
47:x:34:SER:O	47:x:34:SER:OG	2.30	0.45
1:A:144:G:H2'	1:A:145:G:C8	2.51	0.45
24:a:2898:U:H2'	24:a:2899:A:C8	2.52	0.45
28:e:16:GLU:O	28:e:20:GLY:C	2.60	0.45
29:f:17:MET:SD	29:f:25:VAL:HG13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:U:O2'	7:G:35:LYS:NZ	2.38	0.45
2:B:114:LEU:HD22	2:B:148:LEU:HD11	1.99	0.45
3:C:63:SER:HA	3:C:98:PRO:HG2	1.98	0.45
4:D:137:VAL:O	4:D:185:LYS:NZ	2.50	0.45
8:H:21:ASN:HA	8:H:65:TYR:OH	2.17	0.45
24:a:126:A:OP1	51:1:45:SER:OG	2.26	0.45
26:c:6:CYS:SG	26:c:18:LYS:NZ	2.67	0.45
26:c:117:GLN:HE21	26:c:117:GLN:HB3	1.59	0.45
1:A:191:G:H2'	1:A:192:A:C8	2.52	0.44
1:A:1173:U:H2'	1:A:1174:G:C8	2.52	0.44
3:C:88:ARG:HH21	3:C:89:LYS:HG3	1.83	0.44
7:G:118:LEU:O	7:G:122:ASN:ND2	2.45	0.44
9:I:51:PRO:HA	9:I:54:LEU:HG	1.99	0.44
10:J:80:THR:O	10:J:83:THR:OG1	2.35	0.44
14:N:16:LEU:O	14:N:20:TYR:HB2	2.17	0.44
24:a:807:U:OP2	34:k:41:ARG:NH2	2.48	0.44
24:a:1672:A:C2	24:a:2582:G:H5'	2.52	0.44
24:a:1802:A:H2'	24:a:1803:A:C8	2.51	0.44
44:u:30:ILE:O	44:u:37:PRO:HA	2.17	0.44
1:A:1013:G:N2	1:A:1016:A:OP2	2.49	0.44
1:A:1071:C:H2'	1:A:1072:G:C8	2.51	0.44
1:A:1228:C:N4	13:M:103:LYS:O	2.41	0.44
3:C:33:LEU:HD21	14:N:93:ILE:HA	1.99	0.44
24:a:1266:G:O2'	24:a:2012:G:O6	2.30	0.44
24:a:1441:G:H2'	24:a:1442:U:C6	2.53	0.44
24:a:2327:A:H2'	24:a:2328:A:C8	2.53	0.44
26:c:8:PRO:HB3	26:c:14:ARG:HG3	2.00	0.44
1:A:1005:A:H3'	1:A:1006:G:C8	2.53	0.44
1:A:1323:G:H2'	1:A:1324:A:C8	2.53	0.44
8:H:50:LYS:HA	8:H:50:LYS:HD3	1.70	0.44
25:b:30:C:H1'	25:b:57:A:H61	1.82	0.44
28:e:170:ARG:NH1	28:e:176:ASP:OD1	2.47	0.44
32:i:74:TYR:O	32:i:86:GLN:HA	2.18	0.44
1:A:89:U:H2'	1:A:90:C:C6	2.52	0.44
1:A:1010:U:H2'	1:A:1011:C:H6	1.83	0.44
1:A:1108:G:H5'	3:C:176:HIS:CD2	2.53	0.44
1:A:1121:U:H2'	1:A:1122:U:C6	2.52	0.44
2:B:119:THR:O	2:B:123:ASP:CB	2.66	0.44
15:O:31:LEU:HD23	15:O:31:LEU:HA	1.82	0.44
24:a:717:C:H3'	24:a:718:A:H8	1.82	0.44
29:f:14:LYS:O	29:f:18:THR:OG1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:A:H2'	1:A:33:A:C8	2.53	0.44
1:A:1179:A:H5''	9:I:99:ARG:HH22	1.82	0.44
24:a:720:U:H2'	24:a:721:A:C8	2.53	0.44
24:a:833:A:H2'	24:a:834:G:C8	2.52	0.44
24:a:2386:A:H4'	45:v:56:ASP:HA	1.99	0.44
24:a:2591:C:H2'	24:a:2592:G:C8	2.53	0.44
33:j:67:LYS:NZ	64:j:202:HOH:O	2.43	0.44
36:m:28:LEU:HD23	36:m:48:VAL:HG21	1.99	0.44
39:p:72:ASN:HB3	39:p:110:VAL:HG11	1.98	0.44
1:A:483:C:O2	16:P:13:LYS:NZ	2.37	0.44
1:A:601:G:H2'	1:A:602:A:C8	2.53	0.44
1:A:1093:A:O2'	1:A:1095:U:OP1	2.24	0.44
1:A:1412:C:H2'	1:A:1413:A:C8	2.52	0.44
6:F:71:ILE:HD13	6:F:71:ILE:HA	1.90	0.44
11:K:47:ALA:HA	11:K:50:SER:HB2	1.99	0.44
12:L:18:LYS:HE2	12:L:18:LYS:HB3	1.88	0.44
12:L:54:ARG:HA	12:L:63:VAL:O	2.17	0.44
13:M:31:LYS:NZ	13:M:41:GLU:OE2	2.44	0.44
24:a:893:C:H2'	24:a:894:U:C6	2.52	0.44
24:a:1309:G:H4'	51:l:7:PRO:HG2	2.00	0.44
24:a:2292:U:H2'	24:a:2293:G:C8	2.53	0.44
24:a:2328:A:H2'	24:a:2329:U:C6	2.52	0.44
34:k:57:LEU:HD22	52:2:54:ASP:HB3	2.00	0.44
1:A:967:5MC:H3'	1:A:968:A:H2'	2.00	0.44
1:A:1015:G:HO2'	1:A:1218:C:HO2'	1.65	0.44
4:D:59:GLN:HE21	4:D:63:ARG:HH21	1.66	0.44
11:K:46:THR:O	11:K:50:SER:OG	2.27	0.44
11:K:64:GLN:HB2	11:K:95:SER:HB3	1.99	0.44
13:M:45:ILE:HA	13:M:48:LEU:HB2	2.00	0.44
20:T:43:ASP:HB3	20:T:46:ALA:HB3	1.99	0.44
24:a:2051:A:N6	64:a:6599:HOH:O	2.42	0.44
25:b:60:C:H2'	25:b:61:G:C8	2.53	0.44
28:e:148:ILE:HB	28:e:169:VAL:HG22	1.99	0.44
32:i:43:GLU:OE2	39:p:103:LYS:NZ	2.45	0.44
1:A:736:C:H2'	1:A:737:C:C6	2.52	0.44
1:A:746:A:H2'	1:A:747:A:C8	2.52	0.44
24:a:151:C:H2'	24:a:152:A:C8	2.52	0.44
58:a:6207:SPD:H72	58:a:6207:SPD:H41	1.77	0.44
27:d:156:PHE:CE1	32:i:81:ILE:HD13	2.53	0.44
1:A:203:G:N2	1:A:204:G:O6	2.51	0.44
1:A:946:A:H2'	1:A:947:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:U:H2'	1:A:1392:G:C8	2.52	0.44
5:E:55:GLU:HB3	5:E:57:PRO:HD2	1.99	0.44
5:E:160:SER:OG	5:E:163:GLU:OE1	2.35	0.44
8:H:8:ALA:O	8:H:12:THR:OG1	2.30	0.44
17:Q:16:LYS:HE2	17:Q:16:LYS:HB3	1.80	0.44
24:a:299:A:N3	24:a:319:G:O2'	2.39	0.44
24:a:993:G:OP2	39:p:51:ARG:NH2	2.47	0.44
30:g:43:VAL:HG13	30:g:52:PHE:HE1	1.83	0.44
1:A:445:G:H2'	1:A:446:G:C8	2.53	0.43
1:A:946:A:H2'	1:A:947:G:C8	2.53	0.43
7:G:101:MET:O	7:G:105:VAL:HG22	2.18	0.43
24:a:2315:G:H2'	24:a:2316:G:H8	1.83	0.43
29:f:33:LYS:HG2	29:f:157:THR:HB	1.99	0.43
39:p:49:ASP:HA	39:p:52:GLN:HB2	2.00	0.43
1:A:1032:G:C2	1:A:1033:G:H1'	2.53	0.43
1:A:1178:G:OP1	9:I:95:ARG:NH2	2.51	0.43
3:C:127:ARG:HA	3:C:127:ARG:HD2	1.78	0.43
11:K:87:LYS:HB2	11:K:113:VAL:HG23	2.00	0.43
14:N:3:LYS:HB2	14:N:6:MET:HB2	1.99	0.43
24:a:2233:U:H2'	24:a:2234:G:C8	2.53	0.43
24:a:2898:U:H2'	24:a:2899:A:H8	1.83	0.43
28:e:119:ILE:HD11	28:e:185:LYS:HD2	1.99	0.43
34:k:62:PRO:HG2	52:2:25:LYS:HB3	2.00	0.43
44:u:25:LYS:HE3	44:u:25:LYS:HB3	1.90	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.54	0.43
1:A:106:C:H2'	1:A:107:G:C8	2.53	0.43
1:A:716:A:N3	11:K:130:GLY:N	2.66	0.43
1:A:1500:A:H5''	1:A:1508:A:H5''	2.01	0.43
4:D:114:ALA:O	4:D:118:VAL:HG23	2.18	0.43
23:Z:18:G:H21	23:Z:58:A:H5'	1.82	0.43
32:i:1:MET:HE1	40:q:13:ARG:H	1.83	0.43
1:A:363:A:N6	12:L:27:CYS:SG	2.91	0.43
1:A:1284:C:H3'	1:A:1285:A:H8	1.83	0.43
12:L:32:GLY:HA3	12:L:57:LEU:HD23	2.00	0.43
12:L:74:LEU:HD13	12:L:80:ILE:HD13	2.00	0.43
17:Q:71:LYS:HB3	17:Q:71:LYS:HE2	1.77	0.43
23:Z:62:C:H2'	23:Z:63:G:H8	1.83	0.43
24:a:851:C:O2'	48:y:43:ALA:O	2.32	0.43
24:a:2615:U:C2	49:z:4:GLN:HA	2.53	0.43
34:k:108:ALA:HB3	34:k:125:LEU:HD22	2.00	0.43
1:A:501:C:H2'	1:A:502:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:A:H2'	1:A:1156:G:C8	2.54	0.43
4:D:26:ARG:HH21	4:D:31:LYS:HA	1.84	0.43
10:J:35:GLN:HE22	10:J:78:GLU:HG3	1.83	0.43
20:T:49:LYS:HE2	20:T:49:LYS:HB2	1.89	0.43
20:T:62:ALA:HB1	20:T:69:LYS:HA	2.01	0.43
30:g:105:LEU:HB2	30:g:113:VAL:HB	2.00	0.43
33:j:25:LEU:O	33:j:30:ARG:NH1	2.50	0.43
35:l:77:PRO:HG2	35:l:80:VAL:HG21	1.99	0.43
37:n:59:ALA:HA	37:n:62:LEU:HD12	1.99	0.43
1:A:159:G:N2	1:A:161:A:H3'	2.34	0.43
1:A:923:A:H5''	5:E:26:LYS:HD3	2.00	0.43
1:A:1119:C:H2'	1:A:1120:C:H6	1.83	0.43
11:K:63:ALA:HB1	11:K:96:THR:HG23	2.00	0.43
18:R:35:GLU:H	18:R:35:GLU:HG3	1.67	0.43
24:a:1182:G:H2'	24:a:1183:U:O4'	2.19	0.43
26:c:261:LYS:HA	26:c:264:ASP:OD2	2.19	0.43
40:q:24:LYS:HB3	40:q:24:LYS:HE3	1.71	0.43
43:t:14:LEU:HD11	43:t:71:ALA:HB2	2.00	0.43
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.33	0.43
3:C:47:LEU:HB3	3:C:50:ALA:HB3	2.01	0.43
10:J:51:VAL:HB	14:N:81:ARG:HB2	1.99	0.43
15:O:64:ARG:HH22	15:O:89:ARG:HG3	1.84	0.43
16:P:37:GLY:CA	16:P:51:ARG:O	2.66	0.43
24:a:1231:U:H2'	24:a:1232:G:H8	1.83	0.43
26:c:80:ARG:NE	26:c:82:GLU:OE2	2.45	0.43
36:m:33:ILE:HD12	36:m:114:GLU:HB3	2.01	0.43
54:4:42:PRO:HB3	54:4:47:LYS:HB2	1.99	0.43
1:A:170:U:H2'	1:A:171:A:C8	2.54	0.43
6:F:69:GLU:H	6:F:69:GLU:HG3	1.46	0.43
15:O:54:ARG:HG3	15:O:54:ARG:HH11	1.82	0.43
24:a:589:U:H2'	24:a:590:A:C8	2.54	0.43
24:a:695:G:OP1	24:a:1380:G:O2'	2.31	0.43
24:a:1980:G:O2'	24:a:1982:U:OP2	2.35	0.43
24:a:2359:C:O2'	52:2:54:ASP:OD2	2.30	0.43
24:a:2820:A:N6	27:d:197:THR:OG1	2.52	0.43
45:v:38:VAL:HG12	45:v:59:LEU:HB2	2.00	0.43
48:y:41:THR:HG22	48:y:43:ALA:H	1.84	0.43
49:z:12:LYS:HD3	49:z:12:LYS:HA	1.71	0.43
1:A:591:U:H2'	1:A:592:G:H8	1.84	0.43
1:A:744:C:H2'	1:A:745:G:H8	1.84	0.43
1:A:1312:G:OP2	54:4:63:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:15:ASP:HA	17:Q:21:ILE:HG22	2.00	0.43
24:a:729:G:C6	26:c:207:LYS:HB2	2.53	0.43
24:a:1013:C:H2'	24:a:1014:A:C8	2.54	0.43
1:A:956:U:H3	1:A:960:U:H3	1.65	0.43
15:O:56:LEU:HD23	15:O:57:LEU:HD13	2.01	0.43
24:a:151:C:H2'	24:a:152:A:H8	1.83	0.43
24:a:286:U:H2'	24:a:287:G:C8	2.54	0.43
24:a:358:U:H2'	24:a:359:G:H8	1.83	0.43
26:c:177:ARG:HA	26:c:177:ARG:HD2	1.85	0.43
30:g:154:PRO:HG3	30:g:163:ARG:HB3	2.00	0.43
1:A:33:A:O2'	12:L:29:GLN:NE2	2.52	0.42
2:B:105:LYS:H	2:B:105:LYS:HG2	1.45	0.42
5:E:106:ILE:HB	5:E:124:LEU:HA	2.01	0.42
24:a:705:A:H1'	26:c:13:ARG:HH12	1.84	0.42
24:a:1197:G:H2'	24:a:1198:U:H6	1.84	0.42
24:a:1830:C:H2'	24:a:1831:G:H8	1.84	0.42
38:o:72:ARG:HD2	38:o:74:PHE:CE2	2.53	0.42
1:A:565:U:OP2	1:A:566:G:O2'	2.37	0.42
4:D:202:GLU:OE2	5:E:112:ARG:NH1	2.52	0.42
24:a:5:A:H2'	24:a:6:A:C8	2.55	0.42
24:a:1040:A:N1	24:a:1115:G:N2	2.60	0.42
24:a:2314:A:H2'	24:a:2315:G:H8	1.84	0.42
25:b:28:C:H5''	37:n:31:THR:HG21	2.02	0.42
26:c:78:VAL:HG21	26:c:110:LEU:HD13	2.01	0.42
29:f:36:LEU:HB3	29:f:152:LEU:HD12	2.01	0.42
44:u:4:ILE:HG23	44:u:50:MET:HE1	2.00	0.42
1:A:25:C:H2'	1:A:26:A:C8	2.54	0.42
1:A:1074:G:O2'	2:B:102:THR:OG1	2.29	0.42
1:A:1228:C:H2'	1:A:1229:A:H8	1.84	0.42
11:K:112:ASP:HB3	21:U:2:PRO:HD2	2.02	0.42
24:a:1013:C:H2'	24:a:1014:A:H8	1.84	0.42
24:a:1724:G:O6	24:a:1736:U:C4	2.72	0.42
24:a:2557:G:H2'	24:a:2558:C:C6	2.54	0.42
24:a:2636:C:H2'	24:a:2637:U:C6	2.54	0.42
24:a:2700:A:H2'	24:a:2701:U:C6	2.54	0.42
25:b:42:C:O2'	29:f:64:LYS:O	2.28	0.42
30:g:64:GLN:HA	30:g:67:THR:HG22	2.02	0.42
30:g:105:LEU:HD12	30:g:107:LEU:HD21	2.01	0.42
38:o:106:LYS:HA	38:o:109:ARG:HD3	2.01	0.42
1:A:227:G:H21	16:P:64:GLY:HA3	1.84	0.42
1:A:254:G:OP1	17:Q:70:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:U:H2'	1:A:802:A:C8	2.53	0.42
1:A:1202:U:C2	14:N:82:ILE:HG21	2.55	0.42
1:A:1308:U:H5''	13:M:97:VAL:HG13	2.02	0.42
1:A:1398:A:H5'	1:A:1401:G:H4'	2.02	0.42
3:C:114:LYS:HA	3:C:114:LYS:HD2	1.76	0.42
13:M:104:THR:OG1	13:M:105:ASN:N	2.53	0.42
24:a:657:U:H2'	24:a:658:U:C6	2.54	0.42
24:a:909:A:H2'	24:a:912:C:C5	2.55	0.42
24:a:1790:C:H2'	24:a:1791:A:C5	2.54	0.42
24:a:2723:C:H5''	36:m:1:MET:HE2	2.00	0.42
1:A:231:U:H2'	1:A:232:G:H8	1.84	0.42
1:A:985:C:H2'	1:A:986:U:C6	2.54	0.42
5:E:46:VAL:HG13	5:E:117:VAL:HG23	2.01	0.42
23:Z:18:G:N2	23:Z:58:A:OP2	2.53	0.42
24:a:1681:G:N3	24:a:1762:A:H2'	2.35	0.42
24:a:2756:U:H1'	24:a:2757:A:H5''	2.01	0.42
29:f:8:TYR:OH	29:f:29:PRO:O	2.29	0.42
30:g:90:VAL:HG23	30:g:160:LYS:HA	2.01	0.42
40:q:52:PRO:HG2	40:q:53:PHE:CE2	2.54	0.42
50:0:9:ILE:HD13	50:0:25:LYS:HD2	2.01	0.42
54:4:14:ALA:HA	54:4:32:LEU:O	2.19	0.42
1:A:708:C:H2'	1:A:709:U:C6	2.55	0.42
1:A:1243:C:H2'	1:A:1244:G:H8	1.84	0.42
1:A:1464:U:H2'	1:A:1465:A:H8	1.84	0.42
4:D:11:LEU:HB3	4:D:63:ARG:HD3	2.01	0.42
5:E:81:LEU:HB2	5:E:98:PRO:HG3	2.01	0.42
6:F:68:GLN:O	6:F:68:GLN:NE2	2.52	0.42
24:a:2655:G:O2'	24:a:2664:G:O6	2.35	0.42
29:f:36:LEU:O	29:f:88:LYS:HA	2.20	0.42
1:A:452:A:H2'	1:A:453:G:O4'	2.20	0.42
1:A:1417:G:N2	1:A:1482:G:H2'	2.35	0.42
2:B:6:MET:HA	2:B:9:MET:SD	2.60	0.42
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.94	0.42
7:G:115:SER:O	7:G:119:ARG:HB2	2.19	0.42
13:M:92:ARG:NH1	24:a:887:U:OP1	2.52	0.42
23:Z:24:U:O2'	24:a:1923:U:OP1	2.26	0.42
24:a:466:A:N1	24:a:795:C:O2'	2.47	0.42
24:a:608:A:H2'	24:a:609:A:C8	2.55	0.42
24:a:839:U:H2'	24:a:840:C:C6	2.55	0.42
24:a:1417:C:HO2'	24:a:1587:G:HO2'	1.61	0.42
36:m:77:ALA:O	36:m:81:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:u:47:VAL:O	44:u:51:GLN:HG3	2.20	0.42
1:A:490:C:H2'	1:A:491:G:H8	1.85	0.42
1:A:953:G:H2'	1:A:954:G:H8	1.85	0.42
1:A:1377:A:OP1	7:G:92:ARG:NH1	2.52	0.42
5:E:97:GLN:HG2	5:E:98:PRO:HD2	2.01	0.42
10:J:77:VAL:HG12	10:J:78:GLU:HG2	2.02	0.42
29:f:29:PRO:HB2	29:f:169:LEU:HD22	2.02	0.42
1:A:1030:U:H5'	1:A:1031:C:H5''	2.02	0.42
1:A:1326:U:H2'	1:A:1327:C:H6	1.84	0.42
4:D:57:GLU:O	4:D:61:VAL:HG23	2.20	0.42
10:J:30:LYS:HB3	10:J:30:LYS:HE3	1.76	0.42
24:a:1183:U:H2'	24:a:1184:U:C6	2.54	0.42
24:a:1429:G:H2'	24:a:1430:G:C8	2.53	0.42
24:a:2583:G:O2'	55:Y:76:8AN:N1	2.49	0.42
1:A:166:U:H2'	1:A:167:A:C8	2.55	0.42
1:A:950:U:H2'	1:A:951:G:C8	2.55	0.42
1:A:1458:G:O2'	20:T:23:SER:OG	2.32	0.42
5:E:96:MET:HE3	5:E:96:MET:HB2	1.91	0.42
8:H:101:ILE:HG13	8:H:129:VAL:HB	2.01	0.42
13:M:33:ILE:HD11	13:M:63:PHE:HE2	1.84	0.42
24:a:2246:G:H2'	24:a:2247:A:C8	2.54	0.42
26:c:182:ARG:HG3	26:c:184:VAL:HG23	2.02	0.42
27:d:55:LYS:HD3	27:d:60:VAL:HG22	2.02	0.42
27:d:152:PRO:HG3	27:d:156:PHE:CZ	2.55	0.42
35:l:51:ARG:HE	35:l:51:ARG:HB3	1.63	0.42
1:A:350:G:OP1	20:T:2:ALA:N	2.53	0.41
1:A:377:G:H2'	1:A:378:G:C8	2.55	0.41
1:A:646:G:H2'	1:A:647:C:C6	2.54	0.41
1:A:1162:C:H2'	1:A:1163:A:C8	2.55	0.41
8:H:7:ILE:HD11	8:H:32:LEU:HG	2.01	0.41
11:K:33:THR:HG22	11:K:35:THR:HG22	2.02	0.41
13:M:71:ARG:O	13:M:75:MET:HG2	2.20	0.41
24:a:740:C:H5'	24:a:1784:A:H3'	2.02	0.41
24:a:851:C:OP1	48:y:19:LYS:HE3	2.20	0.41
24:a:2408:U:H2'	24:a:2409:G:C8	2.54	0.41
24:a:2627:G:N2	24:a:2777:G:OP2	2.51	0.41
27:d:8:LYS:NZ	27:d:195:GLY:O	2.43	0.41
1:A:1347:G:O2'	1:A:1373:G:O6	2.36	0.41
3:C:53:SER:OG	3:C:54:ARG:N	2.51	0.41
13:M:33:ILE:HD13	13:M:60:VAL:HG22	2.02	0.41
24:a:1477:A:N6	24:a:1514:G:O2'	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:37:ASN:OD1	26:c:37:ASN:N	2.53	0.41
26:c:43:ARG:NH1	64:c:418:HOH:O	2.52	0.41
1:A:323:U:H2'	1:A:324:G:O4'	2.20	0.41
1:A:591:U:H2'	1:A:592:G:C8	2.55	0.41
1:A:1303:C:H2'	1:A:1304:G:C8	2.56	0.41
2:B:9:MET:HG3	2:B:43:LEU:HD22	2.02	0.41
3:C:154:SER:HB3	3:C:165:THR:HG23	2.02	0.41
8:H:25:VAL:O	8:H:60:GLU:HA	2.20	0.41
8:H:46:ILE:HG21	8:H:61:LEU:HD21	2.03	0.41
11:K:114:THR:HA	11:K:115:PRO:HD3	1.92	0.41
14:N:6:MET:HB2	14:N:6:MET:HE2	1.80	0.41
24:a:1962:5MC:N4	64:a:6543:HOH:O	2.40	0.41
26:c:60:GLN:HG2	26:c:85:PRO:HB2	2.01	0.41
35:l:40:ARG:HG2	35:l:95:LEU:HD23	2.02	0.41
1:A:1026:G:O6	1:A:1035:A:N1	2.54	0.41
13:M:12:HIS:C	13:M:44:LYS:HZ1	2.27	0.41
24:a:160:A:N3	24:a:2208:C:O2'	2.52	0.41
24:a:363:G:H2'	24:a:364:C:C6	2.55	0.41
24:a:1168:G:H2'	24:a:1169:A:C8	2.56	0.41
28:e:6:LYS:HE2	28:e:6:LYS:HB2	1.86	0.41
42:s:33:LYS:NZ	42:s:33:LYS:HB3	2.36	0.41
1:A:176:C:H5''	20:T:24:ARG:NH2	2.34	0.41
1:A:1216:A:H5''	14:N:5:SER:HB3	2.02	0.41
1:A:1457:G:H5''	20:T:30:THR:HG21	2.01	0.41
4:D:11:LEU:HD13	4:D:63:ARG:HG2	2.03	0.41
8:H:27:MET:HG3	8:H:59:LEU:HB3	2.01	0.41
9:I:19:VAL:HG13	9:I:65:ILE:HG12	2.02	0.41
24:a:913:U:O4	58:a:6214:SPD:H22	2.21	0.41
26:c:33:LEU:HD23	26:c:33:LEU:HA	1.93	0.41
30:g:6:LYS:HD2	30:g:6:LYS:HA	1.77	0.41
41:r:109:ASP:OD2	41:r:110:ARG:N	2.53	0.41
1:A:428:G:H3'	4:D:10:LYS:NZ	2.36	0.41
4:D:167:LYS:NZ	4:D:171:LEU:O	2.53	0.41
7:G:30:LEU:HD13	7:G:109:ARG:HH21	1.86	0.41
24:a:579:G:O2'	24:a:2019:A:OP1	2.39	0.41
24:a:1996:C:P	33:j:31:ARG:HH21	2.43	0.41
24:a:2859:G:H2'	24:a:2860:A:C8	2.56	0.41
31:h:34:GLY:O	31:h:36:ALA:N	2.54	0.41
55:Y:29:G:O6	55:Y:42:U:O4	2.38	0.41
1:A:407:U:H5''	4:D:112:ALA:HB1	2.02	0.41
1:A:445:G:H2'	1:A:446:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:N3	1:A:1369:C:O2'	2.46	0.41
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.88	0.41
24:a:995:C:O2	32:i:3:THR:OG1	2.31	0.41
24:a:2330:G:O3'	45:v:44:LYS:HE2	2.20	0.41
24:a:2485:G:N3	64:a:6486:HOH:O	2.37	0.41
26:c:174:LEU:O	26:c:181:MET:HA	2.21	0.41
30:g:99:LYS:HB2	30:g:99:LYS:HE2	1.83	0.41
46:w:2:SER:O	46:w:50:ARG:NH1	2.54	0.41
51:1:18:PHE:HA	51:1:43:THR:HG21	2.02	0.41
1:A:304:U:H2'	1:A:305:G:C8	2.55	0.41
1:A:939:G:H2'	1:A:940:C:C6	2.56	0.41
1:A:1492:A:H1'	22:X:20:A:O2'	2.21	0.41
24:a:1224:U:H2'	24:a:1225:G:C8	2.56	0.41
24:a:2196:C:H2'	24:a:2197:U:C6	2.56	0.41
24:a:2330:G:O2'	45:v:41:ARG:O	2.30	0.41
30:g:95:ARG:NH1	30:g:97:ALA:HB2	2.29	0.41
32:i:11:VAL:HG21	32:i:50:THR:HG22	2.02	0.41
34:k:39:LYS:NZ	64:k:208:HOH:O	2.39	0.41
43:t:54:GLN:HG2	43:t:55:PRO:HD3	2.03	0.41
54:4:41:HIS:CD2	54:4:43:PHE:HB3	2.56	0.41
1:A:178:C:H2'	1:A:179:A:C8	2.56	0.41
2:B:152:LYS:H	2:B:152:LYS:HG2	1.63	0.41
4:D:105:MET:SD	4:D:171:LEU:HD22	2.61	0.41
6:F:63:ASN:HD22	6:F:96:VAL:HB	1.86	0.41
8:H:43:GLU:HG3	8:H:101:ILE:HD13	2.03	0.41
11:K:100:LEU:HD23	11:K:100:LEU:HA	1.91	0.41
16:P:73:ALA:HA	16:P:76:LYS:HE2	2.01	0.41
19:S:13:LEU:HG	19:S:17:LYS:HE3	2.01	0.41
24:a:411:G:N7	58:a:6208:SPD:N10	2.52	0.41
24:a:642:U:O2'	24:a:644:A:N7	2.43	0.41
24:a:910:A:H2'	24:a:911:A:C8	2.56	0.41
24:a:1417:C:O2'	24:a:1587:G:O2'	2.31	0.41
24:a:2208:C:H2'	24:a:2209:G:C8	2.56	0.41
24:a:2567:G:H2'	24:a:2568:U:C6	2.56	0.41
24:a:2837:A:H2'	24:a:2838:G:C8	2.55	0.41
26:c:76:ALA:O	26:c:115:GLN:HA	2.21	0.41
29:f:8:TYR:HA	29:f:12:VAL:HB	2.02	0.41
30:g:44:LYS:HD2	30:g:44:LYS:HA	1.88	0.41
45:v:41:ARG:HD3	45:v:41:ARG:HA	1.82	0.41
1:A:333:U:H2'	1:A:334:C:H6	1.86	0.41
1:A:947:G:H2'	1:A:948:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:G:H2'	1:A:1144:G:C8	2.56	0.41
1:A:1251:A:H2'	1:A:1252:A:C8	2.56	0.41
5:E:111:MET:HE3	5:E:125:ALA:HB1	2.02	0.41
6:F:15:SER:OG	6:F:58:HIS:ND1	2.54	0.41
11:K:109:ASN:ND2	21:U:4:ILE:O	2.54	0.41
17:Q:17:MET:HE2	17:Q:20:SER:HB2	2.03	0.41
19:S:73:GLU:H	19:S:73:GLU:HG3	1.65	0.41
24:a:851:C:H2'	24:a:852:U:C6	2.55	0.41
24:a:2330:G:O2'	45:v:44:LYS:HE3	2.21	0.41
25:b:43:C:OP1	54:4:6:HIS:NE2	2.48	0.41
29:f:34:ILE:HD12	29:f:96:MET:HG3	2.02	0.41
53:3:12:ARG:H	53:3:12:ARG:CD	2.34	0.41
1:A:34:C:H2'	1:A:35:G:C8	2.56	0.40
1:A:337:G:H2'	1:A:338:A:C8	2.56	0.40
1:A:606:G:H21	1:A:631:C:H3'	1.85	0.40
1:A:994:A:C4	1:A:1216:A:H4'	2.55	0.40
4:D:188:ARG:O	4:D:188:ARG:NH1	2.53	0.40
8:H:29:SER:OG	8:H:30:SER:N	2.53	0.40
24:a:166:U:H2'	24:a:167:A:H8	1.86	0.40
24:a:811:U:H2'	34:k:21:ARG:HA	2.03	0.40
24:a:2014:A:H2'	24:a:2015:A:C8	2.56	0.40
28:e:141:MET:H	28:e:141:MET:HG2	1.72	0.40
38:o:100:LEU:HD11	38:o:110:ILE:HD11	2.02	0.40
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.40
1:A:893:C:H2'	1:A:894:G:H8	1.87	0.40
1:A:1064:G:O2'	1:A:1190:G:N2	2.55	0.40
12:L:50:ARG:HB3	12:L:66:TYR:HE1	1.86	0.40
13:M:76:SER:HA	13:M:79:ARG:HG2	2.03	0.40
23:Z:65:C:H2'	23:Z:66:C:H6	1.86	0.40
24:a:864:G:OP1	35:l:22:GLN:NE2	2.55	0.40
29:f:116:GLY:HA3	29:f:178:ARG:HB3	2.03	0.40
30:g:47:ASP:N	30:g:47:ASP:OD1	2.54	0.40
37:n:17:LYS:NZ	37:n:20:GLU:OE2	2.54	0.40
48:y:45:ARG:HH22	48:y:59:GLU:HG2	1.86	0.40
2:B:129:LEU:HD13	2:B:133:GLU:HB2	2.03	0.40
4:D:68:LEU:HD23	4:D:68:LEU:HA	1.87	0.40
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.56	0.40
11:K:84:VAL:N	11:K:109:ASN:O	2.48	0.40
24:a:590:A:H2'	24:a:591:U:C6	2.56	0.40
24:a:843:G:H2'	24:a:844:A:C8	2.57	0.40
24:a:1563:U:H2'	24:a:1564:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:29:PRO:HG2	26:c:34:LEU:HD11	2.02	0.40
29:f:60:ILE:HA	29:f:60:ILE:HD13	1.78	0.40
1:A:396:C:O2'	1:A:398:U:OP1	2.32	0.40
1:A:1288:A:N1	1:A:1371:G:H1'	2.36	0.40
9:I:55:VAL:HG12	9:I:94:LEU:HD22	2.03	0.40
13:M:80:LEU:HD23	13:M:80:LEU:HA	1.86	0.40
17:Q:19:LYS:H	17:Q:51:ASN:ND2	2.19	0.40
24:a:373:U:H2'	24:a:374:A:H8	1.86	0.40
24:a:2514:U:H2'	24:a:2515:C:C6	2.57	0.40
24:a:2845:U:H5''	38:o:52:ASN:O	2.21	0.40
29:f:34:ILE:HA	29:f:155:THR:O	2.21	0.40
29:f:120:LYS:HE2	29:f:120:LYS:HB3	1.90	0.40
35:l:53:MET:HE3	35:l:53:MET:HB2	1.87	0.40
43:t:72:ILE:HD12	43:t:72:ILE:HA	1.89	0.40
1:A:1073:U:O2	2:B:103:ASN:ND2	2.54	0.40
1:A:1144:G:N2	1:A:1146:A:H62	2.20	0.40
7:G:66:LEU:HD13	7:G:66:LEU:HA	1.81	0.40
9:I:21:ILE:HD13	9:I:86:ALA:HB1	2.04	0.40
24:a:133:U:H2'	24:a:134:G:C8	2.57	0.40
24:a:1028:A:H2'	24:a:1029:A:C8	2.56	0.40
24:a:2303:G:H1'	29:f:123:ASP:OD1	2.22	0.40
24:a:2698:U:H2'	24:a:2699:C:C6	2.56	0.40
28:e:83:VAL:HB	28:e:86:ALA:HB2	2.03	0.40
28:e:138:LEU:HD23	28:e:138:LEU:HA	1.89	0.40
42:s:14:PRO:HA	42:s:32:LEU:HD23	2.02	0.40
49:z:28:LEU:HB2	49:z:37:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	C	204/233 (88%)	191 (94%)	12 (6%)	1 (0%)	24	19
4	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
6	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
7	G	151/179 (84%)	137 (91%)	14 (9%)	0	100	100
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	7
11	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	M	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
14	N	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
17	Q	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
18	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
19	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
26	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
27	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	19
28	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
29	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
30	g	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
31	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
32	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
33	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
34	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
35	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
36	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
37	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	o	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
39	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
40	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
41	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
42	s	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
43	t	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
44	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	v	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
46	w	75/78 (96%)	75 (100%)	0	0	100	100
47	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
48	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
49	z	54/57 (95%)	54 (100%)	0	0	100	100
50	0	49/55 (89%)	49 (100%)	0	0	100	100
51	1	44/46 (96%)	44 (100%)	0	0	100	100
52	2	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	3	36/38 (95%)	36 (100%)	0	0	100	100
54	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
All	All	5479/5913 (93%)	5248 (96%)	228 (4%)	3 (0%)	49	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
27	d	149	ASN
3	C	60	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	168 (90%)	18 (10%)	8	3
3	C	170/190 (90%)	159 (94%)	11 (6%)	15	10
4	D	172/173 (99%)	158 (92%)	14 (8%)	11	6
5	E	119/126 (94%)	111 (93%)	8 (7%)	15	10
6	F	90/116 (78%)	82 (91%)	8 (9%)	9	4
7	G	126/147 (86%)	114 (90%)	12 (10%)	8	4
8	H	104/105 (99%)	96 (92%)	8 (8%)	12	7
9	I	105/107 (98%)	99 (94%)	6 (6%)	18	14
10	J	86/90 (96%)	80 (93%)	6 (7%)	14	8
11	K	89/98 (91%)	82 (92%)	7 (8%)	11	7
12	L	102/103 (99%)	96 (94%)	6 (6%)	18	13
13	M	93/96 (97%)	84 (90%)	9 (10%)	8	3
14	N	83/84 (99%)	77 (93%)	6 (7%)	13	8
15	O	76/77 (99%)	71 (93%)	5 (7%)	15	10
16	P	65/65 (100%)	60 (92%)	5 (8%)	12	7
17	Q	73/78 (94%)	68 (93%)	5 (7%)	14	9
18	R	57/65 (88%)	51 (90%)	6 (10%)	6	3
19	S	72/79 (91%)	69 (96%)	3 (4%)	26	23
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	53 (88%)	7 (12%)	5	2
26	c	216/218 (99%)	214 (99%)	2 (1%)	70	77
27	d	163/163 (100%)	161 (99%)	2 (1%)	63	69
28	e	165/165 (100%)	159 (96%)	6 (4%)	31	30
29	f	148/150 (99%)	141 (95%)	7 (5%)	23	19
30	g	137/138 (99%)	127 (93%)	10 (7%)	13	8
31	h	32/114 (28%)	26 (81%)	6 (19%)	1	0
32	i	116/116 (100%)	114 (98%)	2 (2%)	53	58
33	j	104/104 (100%)	102 (98%)	2 (2%)	50	55
34	k	103/103 (100%)	98 (95%)	5 (5%)	22	18
35	l	107/107 (100%)	103 (96%)	4 (4%)	30	29
36	m	98/103 (95%)	98 (100%)	0	100	100
37	n	86/87 (99%)	82 (95%)	4 (5%)	23	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	o	99/100 (99%)	98 (99%)	1 (1%)	68	74
39	p	89/90 (99%)	89 (100%)	0	100	100
40	q	84/84 (100%)	80 (95%)	4 (5%)	23	18
41	r	93/93 (100%)	89 (96%)	4 (4%)	26	23
42	s	80/84 (95%)	78 (98%)	2 (2%)	42	44
43	t	83/85 (98%)	81 (98%)	2 (2%)	43	45
44	u	78/78 (100%)	75 (96%)	3 (4%)	29	28
45	v	57/63 (90%)	55 (96%)	2 (4%)	32	31
46	w	67/68 (98%)	62 (92%)	5 (8%)	12	7
47	x	54/55 (98%)	52 (96%)	2 (4%)	30	29
48	y	48/49 (98%)	48 (100%)	0	100	100
49	z	47/48 (98%)	46 (98%)	1 (2%)	47	51
50	0	46/49 (94%)	44 (96%)	2 (4%)	26	23
51	1	38/38 (100%)	37 (97%)	1 (3%)	40	42
52	2	51/52 (98%)	51 (100%)	0	100	100
53	3	34/34 (100%)	34 (100%)	0	100	100
54	4	55/62 (89%)	53 (96%)	2 (4%)	31	30
All	All	4571/4825 (95%)	4340 (95%)	231 (5%)	23	17

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	SER
2	B	8	ASP
2	B	9	MET
2	B	23	TRP
2	B	41	ILE
2	B	46	THR
2	B	64	LYS
2	B	73	LYS
2	B	105	LYS
2	B	111	ILE
2	B	114	LEU
2	B	129	LEU
2	B	138	THR
2	B	167	ASP

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Mol	Chain	Res	Type
2	B	169	GLU
2	B	204	ASP
2	B	207	ILE
2	B	212	LEU
3	C	28	GLU
3	C	29	PHE
3	C	49	LYS
3	C	84	VAL
3	C	135	LYS
3	C	156	ARG
3	C	170	GLU
3	C	177	THR
3	C	178	LEU
3	C	186	THR
3	C	191	THR
4	D	17	THR
4	D	49	SER
4	D	82	LEU
4	D	101	VAL
4	D	124	MET
4	D	130	VAL
4	D	134	SER
4	D	173	VAL
4	D	174	ASP
4	D	177	LYS
4	D	181	THR
4	D	189	SER
4	D	194	ASP
4	D	200	ILE
5	E	11	LEU
5	E	82	GLN
5	E	85	VAL
5	E	111	MET
5	E	120	VAL
5	E	124	LEU
5	E	134	ILE
5	E	149	SER
6	F	1	MET
6	F	9	MET
6	F	18	VAL
6	F	21	MET
6	F	36	ILE

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Mol	Chain	Res	Type
6	F	69	GLU
6	F	82	ASP
6	F	100	SER
7	G	6	VAL
7	G	13	LEU
7	G	17	LYS
7	G	21	GLU
7	G	22	LEU
7	G	30	LEU
7	G	59	LEU
7	G	64	VAL
7	G	69	VAL
7	G	106	GLU
7	G	115	SER
7	G	133	THR
8	H	30	SER
8	H	34	VAL
8	H	50	LYS
8	H	51	VAL
8	H	55	THR
8	H	69	LYS
8	H	112	THR
8	H	127	CYS
9	I	43	THR
9	I	52	LEU
9	I	53	GLU
9	I	96	SER
9	I	116	VAL
9	I	124	ARG
10	J	27	GLU
10	J	31	ARG
10	J	45	ARG
10	J	67	ILE
10	J	83	THR
10	J	100	ILE
11	K	17	SER
11	K	30	THR
11	K	35	THR
11	K	74	VAL
11	K	86	VAL
11	K	96	THR
11	K	114	THR

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Mol	Chain	Res	Type
12	L	4	VAL
12	L	15	LYS
12	L	16	VAL
12	L	21	VAL
12	L	79	VAL
12	L	88	LYS
13	M	16	VAL
13	M	28	THR
13	M	42	ASP
13	M	49	SER
13	M	65	VAL
13	M	71	ARG
13	M	78	LYS
13	M	85	CYS
13	M	97	VAL
14	N	6	MET
14	N	28	LYS
14	N	33	ASP
14	N	55	SER
14	N	58	SER
14	N	64	CYS
15	O	6	GLU
15	O	8	THR
15	O	57	LEU
15	O	75	VAL
15	O	79	THR
16	P	1	MET
16	P	26	ASN
16	P	44	SER
16	P	78	VAL
16	P	80	LYS
17	Q	5	ILE
17	Q	7	THR
17	Q	33	ILE
17	Q	67	LEU
17	Q	75	LEU
18	R	14	THR
18	R	20	GLU
18	R	21	ILE
18	R	36	SER
18	R	47	THR
18	R	60	LYS

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Mol	Chain	Res	Type
19	S	29	LYS
19	S	39	THR
19	S	66	MET
21	U	3	VAL
21	U	8	GLU
21	U	28	VAL
21	U	42	THR
21	U	47	ARG
21	U	54	LYS
21	U	60	LEU
26	c	117	GLN
26	c	162	VAL
27	d	1	MET
27	d	92	VAL
28	e	6	LYS
28	e	10	SER
28	e	80	SER
28	e	125	SER
28	e	163	ASN
28	e	178	VAL
29	f	18	THR
29	f	25	VAL
29	f	108	VAL
29	f	130	MET
29	f	136	ILE
29	f	159	THR
29	f	173	PHE
30	g	11	VAL
30	g	20	ASN
30	g	34	THR
30	g	36	THR
30	g	49	THR
30	g	72	LEU
30	g	98	VAL
30	g	129	THR
30	g	168	VAL
30	g	172	LYS
31	h	2	GLN
31	h	6	LEU
31	h	14	SER
31	h	15	LEU
31	h	19	VAL

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Mol	Chain	Res	Type
31	h	37	VAL
32	i	7	LYS
32	i	11	VAL
33	j	78	ARG
33	j	95	ILE
34	k	1	MET
34	k	73	ILE
34	k	85	VAL
34	k	100	ILE
34	k	117	THR
35	l	12	MET
35	l	62	LYS
35	l	132	THR
35	l	135	VAL
37	n	5	SER
37	n	24	THR
37	n	52	SER
37	n	80	GLU
38	o	11	GLU
40	q	1	MET
40	q	6	GLN
40	q	19	THR
40	q	58	VAL
41	r	2	GLU
41	r	66	ILE
41	r	68	ASP
41	r	70	LYS
42	s	30	ILE
42	s	64	LYS
43	t	44	LYS
43	t	93	VAL
44	u	4	ILE
44	u	55	GLU
44	u	65	VAL
45	v	10	THR
45	v	30	SER
46	w	2	SER
46	w	22	LEU
46	w	40	VAL
46	w	44	LYS
46	w	71	LEU
47	x	11	VAL

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Mol	Chain	Res	Type
47	x	56	LEU
49	z	52	ARG
50	0	14	SER
50	0	37	LYS
51	1	8	SER
54	4	1	MET
54	4	22	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	24	ASN
2	B	39	HIS
3	C	41	GLN
3	C	176	HIS
4	D	54	GLN
4	D	74	ASN
4	D	164	GLN
4	D	196	ASN
5	E	73	ASN
5	E	132	ASN
5	E	146	ASN
7	G	52	GLN
7	G	86	GLN
11	K	24	HIS
11	K	40	ASN
11	K	109	ASN
14	N	60	GLN
15	O	40	GLN
16	P	40	ASN
18	R	52	GLN
21	U	9	ASN
26	c	25	HIS
29	f	37	ASN
29	f	63	GLN
30	g	104	ASN
31	h	11	ASN
32	i	47	HIS
32	i	86	GLN
33	j	5	GLN
33	j	93	GLN
35	l	60	GLN

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Mol	Chain	Res	Type
36	m	9	GLN
36	m	107	ASN
37	n	29	HIS
37	n	98	GLN
38	o	10	GLN
39	p	72	ASN
39	p	81	ASN
41	r	31	GLN
42	s	72	GLN
44	u	12	GLN
45	v	57	HIS
46	w	36	HIS
47	x	15	ASN
54	4	33	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1516/1542 (98%)	317 (20%)	8 (0%)
22	X	13/28 (46%)	5 (38%)	0
23	Z	74/77 (96%)	19 (25%)	0
24	a	2749/2904 (94%)	374 (13%)	0
25	b	118/120 (98%)	21 (17%)	0
55	Y	67/71 (94%)	37 (55%)	8 (11%)
All	All	4537/4742 (95%)	773 (17%)	16 (0%)

All (773) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U
1	A	22	G
1	A	27	G
1	A	28	A
1	A	32	A

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Mol	Chain	Res	Type
1	A	38	G
1	A	39	G
1	A	41	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	53	A
1	A	54	C
1	A	58	C
1	A	60	A
1	A	61	G
1	A	66	A
1	A	69	G
1	A	72	A
1	A	74	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	86	G
1	A	87	C
1	A	95	C
1	A	96	U
1	A	106	C
1	A	108	G
1	A	110	C
1	A	116	A
1	A	119	A
1	A	122	G
1	A	126	G
1	A	129	A
1	A	130	A
1	A	131	A
1	A	142	G
1	A	144	G
1	A	149	A
1	A	153	C
1	A	155	A
1	A	159	G
1	A	163	C
1	A	164	G

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Mol	Chain	Res	Type
1	A	169	C
1	A	173	U
1	A	181	A
1	A	182	A
1	A	183	C
1	A	189	A
1	A	191	G
1	A	194	C
1	A	195	A
1	A	197	A
1	A	204	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	254	G
1	A	266	G
1	A	267	C
1	A	271	C
1	A	280	C
1	A	289	G
1	A	316	C
1	A	321	A
1	A	322	C
1	A	328	C
1	A	329	A
1	A	330	C
1	A	345	C
1	A	352	C
1	A	354	G
1	A	362	G
1	A	367	U
1	A	368	U
1	A	372	C
1	A	381	C
1	A	388	G
1	A	390	U
1	A	392	C
1	A	398	U
1	A	405	U
1	A	406	G
1	A	411	A

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Mol	Chain	Res	Type
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	435	A
1	A	439	U
1	A	453	G
1	A	455	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	480	U
1	A	482	A
1	A	484	G
1	A	486	U
1	A	493	A
1	A	496	A
1	A	497	G
1	A	505	G
1	A	509	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	525	C
1	A	531	U
1	A	536	C
1	A	545	C
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A

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Mol	Chain	Res	Type
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	588	G
1	A	607	A
1	A	620	C
1	A	627	G
1	A	633	G
1	A	653	U
1	A	654	G
1	A	655	A
1	A	656	G
1	A	661	G
1	A	665	A
1	A	670	G
1	A	686	U
1	A	703	G
1	A	708	C
1	A	723	U
1	A	724	G
1	A	734	G
1	A	746	A
1	A	747	A
1	A	752	G
1	A	753	A
1	A	755	G
1	A	758	C
1	A	777	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	815	A
1	A	817	C
1	A	821	G
1	A	831	A
1	A	849	G
1	A	851	G
1	A	870	U
1	A	887	G
1	A	890	G
1	A	902	G

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Mol	Chain	Res	Type
1	A	914	A
1	A	926	G
1	A	931	C
1	A	934	C
1	A	935	A
1	A	942	G
1	A	958	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	989	U
1	A	992	U
1	A	994	A
1	A	1003	G
1	A	1004	A
1	A	1006	G
1	A	1008	U
1	A	1009	U
1	A	1022	A
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1039	G
1	A	1043	G
1	A	1044	A
1	A	1046	A
1	A	1053	G
1	A	1057	G
1	A	1064	G
1	A	1065	U
1	A	1066	C

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Mol	Chain	Res	Type
1	A	1085	U
1	A	1086	U
1	A	1092	A
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1132	C
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1151	A
1	A	1152	A
1	A	1155	A
1	A	1157	A
1	A	1167	A
1	A	1169	A
1	A	1171	A
1	A	1177	G
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	A
1	A	1197	A
1	A	1201	A
1	A	1208	C
1	A	1212	U
1	A	1213	A
1	A	1224	U
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	A

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Mol	Chain	Res	Type
1	A	1258	G
1	A	1264	U
1	A	1275	A
1	A	1276	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1297	G
1	A	1298	U
1	A	1300	G
1	A	1305	G
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1328	C
1	A	1335	U
1	A	1340	A
1	A	1343	G
1	A	1346	A
1	A	1353	G
1	A	1354	U
1	A	1363	A
1	A	1364	U
1	A	1368	A
1	A	1370	G
1	A	1376	U
1	A	1378	C
1	A	1379	G
1	A	1397	C
1	A	1398	A
1	A	1400	C
1	A	1419	G
1	A	1441	A
1	A	1445	U
1	A	1446	A
1	A	1448	C
1	A	1450	U
1	A	1451	U
1	A	1452	C
1	A	1453	G

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Mol	Chain	Res	Type
1	A	1468	A
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
22	X	21	G
22	X	23	A
22	X	24	A
22	X	25	C
22	X	27	A
23	Z	8	U
23	Z	9	G
23	Z	16	C
23	Z	17(A)	U
23	Z	18	G
23	Z	19	G
23	Z	20	U
23	Z	21	A
23	Z	27	U
23	Z	28	C
23	Z	29	G
23	Z	30	G
23	Z	37	A
23	Z	42	G
23	Z	45	G
23	Z	46	G
23	Z	48	C
23	Z	58	A
23	Z	61	C
24	a	10	A
24	a	34	U
24	a	42	A
24	a	45	G
24	a	58	G
24	a	71	A
24	a	74	A

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Mol	Chain	Res	Type
24	a	75	G
24	a	80	G
24	a	84	A
24	a	101	A
24	a	102	U
24	a	118	A
24	a	119	A
24	a	120	U
24	a	125	A
24	a	135	U
24	a	138	U
24	a	139	U
24	a	140	C
24	a	141	G
24	a	142	A
24	a	144	A
24	a	147	C
24	a	155	A
24	a	157	C
24	a	159	G
24	a	163	C
24	a	164	C
24	a	165	A
24	a	181	A
24	a	196	A
24	a	216	A
24	a	221	A
24	a	222	A
24	a	233	A
24	a	248	G
24	a	265	A
24	a	272	A
24	a	276	U
24	a	280	U
24	a	282	A
24	a	294	A
24	a	311	A
24	a	313	G
24	a	329	G
24	a	330	A
24	a	338	G
24	a	346	A

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Mol	Chain	Res	Type
24	a	349	U
24	a	358	U
24	a	361	G
24	a	362	A
24	a	364	C
24	a	380	G
24	a	386	G
24	a	389	G
24	a	396	G
24	a	405	U
24	a	406	G
24	a	411	G
24	a	412	A
24	a	456	C
24	a	481	G
24	a	489	G
24	a	491	G
24	a	498	G
24	a	504	A
24	a	505	A
24	a	508	A
24	a	509	C
24	a	529	A
24	a	530	G
24	a	531	C
24	a	532	A
24	a	533	G
24	a	544	C
24	a	545	U
24	a	546	U
24	a	547	A
24	a	548	G
24	a	549	G
24	a	563	A
24	a	573	U
24	a	575	A
24	a	603	A
24	a	614	A
24	a	615	U
24	a	627	A
24	a	637	A
24	a	645	C

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Mol	Chain	Res	Type
24	a	647	G
24	a	653	U
24	a	654	A
24	a	655	A
24	a	686	U
24	a	717	C
24	a	721	A
24	a	723	C
24	a	730	A
24	a	738	G
24	a	740	C
24	a	747	5MU
24	a	764	A
24	a	765	C
24	a	775	G
24	a	776	G
24	a	782	A
24	a	784	G
24	a	785	G
24	a	789	A
24	a	792	A
24	a	805	G
24	a	812	C
24	a	827	U
24	a	828	U
24	a	845	A
24	a	846	U
24	a	847	U
24	a	856	G
24	a	859	G
24	a	875	G
24	a	881	G
24	a	882	G
24	a	884	U
24	a	885	C
24	a	888	C
24	a	890	C
24	a	891	G
24	a	893	C
24	a	895	U
24	a	896	A
24	a	897	C

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Mol	Chain	Res	Type
24	a	910	A
24	a	914	G
24	a	931	U
24	a	932	U
24	a	934	U
24	a	946	C
24	a	961	C
24	a	974	G
24	a	983	A
24	a	984	A
24	a	985	C
24	a	996	A
24	a	1005	C
24	a	1012	U
24	a	1013	C
24	a	1022	G
24	a	1026	G
24	a	1033	U
24	a	1040	A
24	a	1042	G
24	a	1045	C
24	a	1046	A
24	a	1047	G
24	a	1052	C
24	a	1110	G
24	a	1111	A
24	a	1112	G
24	a	1115	G
24	a	1116	G
24	a	1117	C
24	a	1130	U
24	a	1132	U
24	a	1133	A
24	a	1135	C
24	a	1142	A
24	a	1172	C
24	a	1227	G
24	a	1250	G
24	a	1253	A
24	a	1256	G
24	a	1271	G
24	a	1272	A

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Mol	Chain	Res	Type
24	a	1275	A
24	a	1300	G
24	a	1301	A
24	a	1329	U
24	a	1352	U
24	a	1365	A
24	a	1379	U
24	a	1383	A
24	a	1387	A
24	a	1403	A
24	a	1415	U
24	a	1416	G
24	a	1417	C
24	a	1419	A
24	a	1427	A
24	a	1428	C
24	a	1452	G
24	a	1453	A
24	a	1460	U
24	a	1482	G
24	a	1484	U
24	a	1486	U
24	a	1490	A
24	a	1493	C
24	a	1497	U
24	a	1505	A
24	a	1508	A
24	a	1509	A
24	a	1510	G
24	a	1515	A
24	a	1529	G
24	a	1534	U
24	a	1535	A
24	a	1536	C
24	a	1537	G
24	a	1559	U
24	a	1560	G
24	a	1566	A
24	a	1569	A
24	a	1578	U
24	a	1583	A
24	a	1584	U

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Mol	Chain	Res	Type
24	a	1585	C
24	a	1608	A
24	a	1626	A
24	a	1647	U
24	a	1648	U
24	a	1649	G
24	a	1674	G
24	a	1713	A
24	a	1715	G
24	a	1724	G
24	a	1728	C
24	a	1730	C
24	a	1732	C
24	a	1733	G
24	a	1737	G
24	a	1738	G
24	a	1750	G
24	a	1764	C
24	a	1773	A
24	a	1782	U
24	a	1791	A
24	a	1800	C
24	a	1801	A
24	a	1808	A
24	a	1816	C
24	a	1829	A
24	a	1848	A
24	a	1857	G
24	a	1858	A
24	a	1866	A
24	a	1870	C
24	a	1871	A
24	a	1873	G
24	a	1882	U
24	a	1896	G
24	a	1906	G
24	a	1913	A
24	a	1915	3TD
24	a	1929	G
24	a	1930	G
24	a	1931	U
24	a	1937	A

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Mol	Chain	Res	Type
24	a	1938	A
24	a	1955	U
24	a	1967	C
24	a	1970	A
24	a	1971	U
24	a	1972	G
24	a	1987	A
24	a	1991	U
24	a	1993	U
24	a	2020	A
24	a	2023	C
24	a	2031	A
24	a	2033	A
24	a	2043	C
24	a	2055	C
24	a	2056	G
24	a	2060	A
24	a	2061	G
24	a	2062	A
24	a	2069	G7M
24	a	2093	G
24	a	2196	C
24	a	2198	A
24	a	2203	U
24	a	2204	G
24	a	2211	A
24	a	2212	A
24	a	2213	U
24	a	2223	G
24	a	2225	A
24	a	2238	G
24	a	2239	G
24	a	2268	A
24	a	2279	G
24	a	2283	C
24	a	2287	A
24	a	2304	G
24	a	2305	U
24	a	2307	G
24	a	2308	G
24	a	2322	A
24	a	2325	G

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Mol	Chain	Res	Type
24	a	2333	A
24	a	2335	A
24	a	2336	A
24	a	2347	C
24	a	2361	G
24	a	2379	G
24	a	2383	G
24	a	2385	C
24	a	2396	G
24	a	2402	U
24	a	2403	C
24	a	2406	A
24	a	2425	A
24	a	2429	G
24	a	2435	A
24	a	2441	U
24	a	2448	A
24	a	2468	A
24	a	2470	G
24	a	2476	A
24	a	2478	A
24	a	2491	U
24	a	2494	G
24	a	2498	OMC
24	a	2502	G
24	a	2505	G
24	a	2518	A
24	a	2529	G
24	a	2535	G
24	a	2547	A
24	a	2548	U
24	a	2566	A
24	a	2567	G
24	a	2573	C
24	a	2602	A
24	a	2609	U
24	a	2613	U
24	a	2629	U
24	a	2630	G
24	a	2663	G
24	a	2671	G
24	a	2689	U

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Mol	Chain	Res	Type
24	a	2690	U
24	a	2714	G
24	a	2716	C
24	a	2718	G
24	a	2726	A
24	a	2733	A
24	a	2744	G
24	a	2748	A
24	a	2750	A
24	a	2757	A
24	a	2765	A
24	a	2778	A
24	a	2780	G
24	a	2792	A
24	a	2793	C
24	a	2797	U
24	a	2798	U
24	a	2799	A
24	a	2801	G
24	a	2818	U
24	a	2820	A
24	a	2821	A
24	a	2823	A
24	a	2833	U
24	a	2835	A
24	a	2861	U
24	a	2873	A
24	a	2883	A
24	a	2884	U
24	a	2899	A
24	a	2903	U
25	b	2	G
25	b	13	G
25	b	24	G
25	b	33	G
25	b	36	C
25	b	44	G
25	b	45	A
25	b	53	A
25	b	56	G
25	b	57	A
25	b	65	U

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Mol	Chain	Res	Type
25	b	66	A
25	b	67	G
25	b	68	C
25	b	88	C
25	b	89	U
25	b	90	C
25	b	99	A
25	b	105	G
25	b	108	A
25	b	109	A
55	Y	5	G
55	Y	6	A
55	Y	10	G
55	Y	12	U
55	Y	18	G
55	Y	20	C
55	Y	22	G
55	Y	23	A
55	Y	24	C
55	Y	25	C
55	Y	25(A)	A
55	Y	32	C
55	Y	34	C
55	Y	37	A
55	Y	39	A
55	Y	40	C
55	Y	41	C
55	Y	42	U
55	Y	42(A)	A
55	Y	44	C
55	Y	45	C
55	Y	47	A
55	Y	48	G
55	Y	49	C
55	Y	50	G
55	Y	51	G
55	Y	55	U
55	Y	56	C
55	Y	59	C
55	Y	60	G
55	Y	61	C
55	Y	63	C

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Mol	Chain	Res	Type
55	Y	65	G
55	Y	67	U
55	Y	71	U
55	Y	72	C
55	Y	74	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	387	U
1	A	438	U
1	A	858	G
1	A	1026	G
1	A	1035	A
1	A	1085	U
1	A	1114	C
1	A	1139	G
55	Y	11	G
55	Y	17	G
55	Y	31	U
55	Y	42	U
55	Y	47	A
55	Y	48	G
55	Y	49	C
55	Y	71	U

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

42 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	G7M	A	527	1	23,26,27	1.49	4 (17%)	34,39,42	1.83	5 (14%)
24	PSU	a	955	24	18,21,22	1.47	4 (22%)	21,30,33	2.10	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	a	1917	24	18,21,22	1.38	3 (16%)	21,30,33	1.98	4 (19%)
24	5MU	a	747	24	19,22,23	1.52	5 (26%)	27,32,35	1.97	6 (22%)
1	2MG	A	1516	1	23,26,27	1.19	2 (8%)	33,38,41	2.33	8 (24%)
24	PSU	a	2457	24	18,21,22	1.43	3 (16%)	21,30,33	2.13	3 (14%)
24	3TD	a	1915	24	19,22,23	1.63	4 (21%)	23,32,35	2.27	5 (21%)
1	2MG	A	1207	1	23,26,27	1.24	3 (13%)	33,38,41	2.24	8 (24%)
35	MS6	l	82	35	5,7,8	0.19	0	2,7,9	0.12	0
24	G7M	a	2069	24	23,26,27	1.46	4 (17%)	34,39,42	1.75	5 (14%)
24	PSU	a	2605	24	18,21,22	1.32	3 (16%)	21,30,33	2.04	4 (19%)
55	8AN	Y	76	24,55,63	21,24,25	1.75	6 (28%)	26,35,38	2.35	8 (30%)
12	D2T	L	89	12	8,9,10	3.92	3 (37%)	6,11,13	1.65	1 (16%)
1	MA6	A	1518	1	23,26,27	1.60	4 (17%)	33,38,41	2.09	9 (27%)
24	5MC	a	1962	24	19,22,23	1.60	3 (15%)	26,32,35	1.16	3 (11%)
1	MA6	A	1519	1	23,26,27	1.57	4 (17%)	33,38,41	2.25	10 (30%)
24	OMU	a	2552	24,57	19,22,23	1.17	3 (15%)	25,31,34	1.80	6 (24%)
24	6MZ	a	2030	24	22,25,26	1.45	5 (22%)	29,36,39	2.44	11 (37%)
24	PSU	a	2580	24	18,21,22	1.46	3 (16%)	21,30,33	2.03	4 (19%)
24	OMG	a	2251	24,61,23	23,26,27	1.20	3 (13%)	32,38,41	1.91	5 (15%)
27	MEQ	d	150	27	8,9,10	0.46	0	5,10,12	0.43	0
24	1MG	a	745	24	23,26,27	1.18	4 (17%)	33,39,42	1.66	6 (18%)
11	IAS	K	119	11	6,7,8	1.41	1 (16%)	3,8,10	1.24	0
1	2MG	A	966	1	23,26,27	1.27	4 (17%)	33,38,41	2.47	9 (27%)
23	8AN	Z	76	59,23	21,24,25	1.52	4 (19%)	26,35,38	2.32	9 (34%)
24	OMC	a	2498	24,57	19,22,23	0.83	0	25,31,34	1.01	1 (4%)
24	2MG	a	1835	24	23,26,27	1.21	3 (13%)	33,38,41	2.50	9 (27%)
24	2MG	a	2445	24	23,26,27	1.23	4 (17%)	33,38,41	2.16	7 (21%)
24	PSU	a	746	24,57	18,21,22	1.44	3 (16%)	21,30,33	1.85	4 (19%)
1	5MC	A	1407	1	19,22,23	1.67	3 (15%)	26,32,35	1.35	3 (11%)
24	H2U	a	2449	24	18,21,22	1.06	2 (11%)	19,30,33	1.11	3 (15%)
1	4OC	A	1402	1	20,23,24	0.72	0	25,32,35	1.09	2 (8%)
24	PSU	a	2604	24	18,21,22	1.34	3 (16%)	21,30,33	2.07	4 (19%)
1	UR3	A	1498	1	19,22,23	1.11	2 (10%)	26,32,35	2.13	7 (26%)
24	2MA	a	2503	24,61,57	22,25,26	1.45	4 (18%)	32,37,40	2.38	11 (34%)
24	PSU	a	2504	24,61	18,21,22	1.51	3 (16%)	21,30,33	1.99	4 (19%)
24	5MU	a	1939	24	19,22,23	1.46	5 (26%)	27,32,35	2.22	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	a	1911	24	18,21,22	1.48	3 (16%)	21,30,33	1.95	3 (14%)
1	PSU	A	516	1,57	18,21,22	1.41	2 (11%)	21,30,33	2.16	5 (23%)
1	5MC	A	967	1	19,22,23	1.51	2 (10%)	26,32,35	1.11	2 (7%)
35	4D4	l	81	35	9,11,12	1.99	2 (22%)	7,13,15	1.17	1 (14%)
24	6MZ	a	1618	24	22,25,26	1.47	4 (18%)	29,36,39	2.27	10 (34%)

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	G7M	A	527	1	-	1/7/25/26	0/3/3/3
24	PSU	a	955	24	-	0/7/25/26	0/2/2/2
24	PSU	a	1917	24	-	1/7/25/26	0/2/2/2
24	5MU	a	747	24	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
24	PSU	a	2457	24	-	0/7/25/26	0/2/2/2
24	3TD	a	1915	24	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
35	MS6	l	82	35	-	1/4/6/8	-
24	G7M	a	2069	24	-	1/7/25/26	0/3/3/3
24	PSU	a	2605	24	-	0/7/25/26	0/2/2/2
55	8AN	Y	76	24,55,63	-	0/7/25/26	0/3/3/3
12	D2T	L	89	12	-	5/7/12/14	-
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
24	5MC	a	1962	24	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
24	OMU	a	2552	24,57	-	0/9/27/28	0/2/2/2
24	6MZ	a	2030	24	-	2/9/27/28	0/3/3/3
24	PSU	a	2580	24	-	0/7/25/26	0/2/2/2
24	OMG	a	2251	24,61,23	-	0/9/27/28	0/3/3/3
27	MEQ	d	150	27	-	3/8/9/11	-
24	1MG	a	745	24	-	0/7/25/26	0/3/3/3
11	IAS	K	119	11	-	2/7/7/8	-
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
23	8AN	Z	76	59,23	-	1/7/25/26	0/3/3/3
24	OMC	a	2498	24,57	-	0/9/27/28	0/2/2/2
24	2MG	a	1835	24	-	0/9/27/28	0/3/3/3
24	2MG	a	2445	24	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	a	746	24,57	-	3/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
24	H2U	a	2449	24	-	0/7/38/39	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
24	PSU	a	2604	24	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
24	2MA	a	2503	24,61,57	-	1/7/25/26	0/3/3/3
24	PSU	a	2504	24,61	-	1/7/25/26	0/2/2/2
24	5MU	a	1939	24	-	0/7/25/26	0/2/2/2
24	PSU	a	1911	24	-	1/7/25/26	0/2/2/2
1	PSU	A	516	1,57	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
35	4D4	l	81	35	-	1/11/12/14	-
24	6MZ	a	1618	24	-	0/9/27/28	0/3/3/3

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	89	D2T	CB-CA	9.46	1.57	1.54
1	A	1407	5MC	C5-C4	5.87	1.48	1.44
24	a	1962	5MC	C5-C4	5.83	1.48	1.44
1	A	967	5MC	C5-C4	5.22	1.48	1.44
1	A	1518	MA6	C5-C4	5.11	1.48	1.39
1	A	1519	MA6	C5-C4	4.68	1.47	1.39
12	L	89	D2T	CB-CG	4.65	1.59	1.52
24	a	1618	6MZ	C5-C4	4.57	1.47	1.39
55	Y	76	8AN	C5-C4	4.52	1.47	1.39
24	a	2503	2MA	C5-C4	4.39	1.46	1.39
24	a	2069	G7M	C5-N7	-4.37	1.34	1.39
1	A	527	G7M	C5-N7	-4.34	1.34	1.39
23	Z	76	8AN	C5-C4	4.29	1.46	1.39
24	a	2030	6MZ	C5-C4	4.09	1.46	1.39
35	l	81	4D4	CZ-NE	3.92	1.40	1.33
24	a	1911	PSU	C6-C5	3.82	1.39	1.35
24	a	2504	PSU	C6-C5	3.82	1.39	1.35
24	a	955	PSU	C6-C5	3.60	1.39	1.35
24	a	2580	PSU	C6-C5	3.55	1.39	1.35
24	a	746	PSU	C6-C5	3.55	1.39	1.35
24	a	747	5MU	C4-N3	-3.35	1.32	1.38
1	A	1519	MA6	C5-C6	3.31	1.49	1.41
24	a	1915	3TD	C4-N3	-3.29	1.33	1.40
1	A	966	2MG	C5-C4	3.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C5-C4	3.26	1.46	1.38
24	a	745	1MG	C5-C4	3.17	1.47	1.38
24	a	2605	PSU	C6-C5	3.13	1.38	1.35
24	a	2457	PSU	C6-C5	3.11	1.38	1.35
1	A	967	5MC	C6-C5	3.11	1.39	1.34
24	a	1939	5MU	C4-N3	-3.10	1.33	1.38
24	a	1915	3TD	C10-N3	3.09	1.52	1.47
24	a	747	5MU	C6-C5	3.08	1.39	1.34
24	a	1939	5MU	C6-C5	3.07	1.39	1.34
1	A	516	PSU	C6-C5	3.04	1.38	1.35
1	A	1518	MA6	C5-C6	3.04	1.49	1.41
24	a	2251	OMG	C5-C4	3.03	1.47	1.38
24	a	1835	2MG	C5-C4	3.03	1.47	1.38
1	A	1207	2MG	C5-C4	3.02	1.47	1.38
24	a	2069	G7M	C5-C4	2.99	1.45	1.38
55	Y	76	8AN	C5-N7	-2.96	1.33	1.39
24	a	2604	PSU	C6-C5	2.95	1.38	1.35
24	a	2457	PSU	C4-N3	-2.95	1.33	1.38
24	a	2445	2MG	C5-C4	2.93	1.46	1.38
24	a	1915	3TD	C6-C5	2.93	1.38	1.35
24	a	746	PSU	C4-N3	-2.92	1.33	1.38
1	A	1516	2MG	C5-C4	2.91	1.46	1.38
1	A	1407	5MC	C6-C5	2.91	1.39	1.34
24	a	1917	PSU	C6-C5	2.90	1.38	1.35
24	a	2449	H2U	C2-N3	-2.88	1.33	1.38
24	a	1915	3TD	C2-N1	-2.84	1.33	1.37
24	a	2030	6MZ	C4-N9	-2.83	1.31	1.37
24	a	747	5MU	C2-N3	-2.82	1.33	1.38
24	a	955	PSU	C4-N3	-2.79	1.33	1.38
1	A	516	PSU	C4-N3	-2.77	1.33	1.38
24	a	2604	PSU	C4-N3	-2.76	1.33	1.38
24	a	1911	PSU	C4-N3	-2.76	1.33	1.38
24	a	2251	OMG	C6-N1	-2.75	1.33	1.38
1	A	1498	UR3	C2-N1	2.73	1.42	1.38
35	l	81	4D4	CZ-NH2	2.72	1.42	1.32
55	Y	76	8AN	C4-N9	-2.70	1.32	1.37
24	a	2504	PSU	C4-N3	-2.69	1.33	1.38
24	a	2030	6MZ	C5-N7	-2.67	1.34	1.39
12	L	89	D2T	CB-SB	2.65	1.84	1.82
24	a	1618	6MZ	C5-C6	2.64	1.48	1.41
24	a	2605	PSU	C4-N3	-2.64	1.33	1.38
24	a	1917	PSU	C4-N3	-2.62	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	1962	5MC	C6-C5	2.59	1.38	1.34
24	a	2552	OMU	C4-N3	-2.58	1.34	1.38
24	a	2580	PSU	C4-N3	-2.57	1.34	1.38
1	A	966	2MG	C6-N1	-2.57	1.34	1.38
24	a	745	1MG	C2-N1	2.53	1.41	1.37
24	a	1835	2MG	C6-N1	-2.49	1.34	1.38
55	Y	76	8AN	C3'-N3'	-2.49	1.43	1.47
24	a	1939	5MU	C2-N3	-2.46	1.33	1.38
23	Z	76	8AN	C5-N7	-2.44	1.34	1.39
24	a	2503	2MA	C5-C6	2.43	1.47	1.41
1	A	1516	2MG	C6-N1	-2.42	1.34	1.38
24	a	2449	H2U	C4-N3	-2.42	1.33	1.37
24	a	2069	G7M	C6-N1	-2.42	1.34	1.38
1	A	1207	2MG	C6-N1	-2.41	1.34	1.38
24	a	2445	2MG	C6-N1	-2.40	1.34	1.38
24	a	2503	2MA	C5-N7	-2.39	1.34	1.39
1	A	527	G7M	C6-N1	-2.38	1.34	1.38
1	A	1518	MA6	C5-N7	-2.38	1.34	1.39
24	a	1618	6MZ	C5-N7	-2.38	1.34	1.39
24	a	747	5MU	C2-N1	2.36	1.42	1.38
11	K	119	IAS	CB-CG	2.36	1.56	1.50
1	A	966	2MG	C2-N3	2.35	1.36	1.32
23	Z	76	8AN	C5-C6	2.34	1.47	1.41
55	Y	76	8AN	C5-C6	2.34	1.47	1.41
1	A	1519	MA6	C8-N7	2.33	1.36	1.31
24	a	2503	2MA	C8-N7	2.32	1.36	1.31
24	a	2030	6MZ	C5-C6	2.31	1.47	1.41
24	a	1939	5MU	C4-C5	2.31	1.48	1.44
24	a	2552	OMU	C5-C4	-2.29	1.38	1.43
24	a	1911	PSU	C2-N3	-2.27	1.33	1.37
24	a	1962	5MC	C6-N1	-2.21	1.34	1.38
24	a	1618	6MZ	C8-N7	2.18	1.35	1.31
24	a	1835	2MG	C5-N7	-2.18	1.34	1.39
24	a	2580	PSU	O4'-C1'	-2.15	1.40	1.43
24	a	2605	PSU	C2-N3	-2.14	1.33	1.37
24	a	1917	PSU	C2-N1	-2.14	1.33	1.36
24	a	2552	OMU	C2-N3	-2.14	1.34	1.38
1	A	1407	5MC	C6-N1	-2.13	1.34	1.38
24	a	2069	G7M	C4-N9	-2.13	1.32	1.38
1	A	1519	MA6	C5-N7	-2.12	1.35	1.39
24	a	2457	PSU	C2-N3	-2.11	1.34	1.37
1	A	966	2MG	C5-N7	-2.11	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C5-C6	2.11	1.49	1.43
24	a	2604	PSU	C2-N3	-2.09	1.34	1.37
24	a	955	PSU	C2-N1	-2.09	1.33	1.36
24	a	2445	2MG	C4-N9	-2.08	1.32	1.38
24	a	2504	PSU	C2-N1	-2.08	1.34	1.36
24	a	2251	OMG	C5-N7	-2.07	1.34	1.39
24	a	746	PSU	C2-N3	-2.07	1.34	1.37
24	a	2445	2MG	C5-N7	-2.07	1.34	1.39
55	Y	76	8AN	C4'-C3'	2.07	1.57	1.52
23	Z	76	8AN	C4-N9	-2.07	1.33	1.37
24	a	747	5MU	C6-N1	-2.07	1.34	1.38
24	a	955	PSU	C2-N3	-2.06	1.34	1.37
1	A	1207	2MG	C5-N7	-2.06	1.34	1.39
24	a	745	1MG	C4-N9	-2.02	1.32	1.38
24	a	1939	5MU	C6-N1	-2.02	1.34	1.38
1	A	1518	MA6	C4-N9	-2.02	1.33	1.37
1	A	1498	UR3	C5-C4	-2.02	1.38	1.43
24	a	2030	6MZ	C8-N7	2.01	1.35	1.31
24	a	745	1MG	C5-N7	-2.00	1.35	1.39

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	1835	2MG	C2-N3-C4	8.27	122.35	112.00
24	a	2503	2MA	C5-C4-N3	-8.17	118.57	127.18
24	a	1915	3TD	N1-C2-N3	8.16	122.06	116.13
1	A	966	2MG	C2-N3-C4	8.13	122.17	112.00
1	A	1516	2MG	C2-N3-C4	7.65	121.57	112.00
1	A	966	2MG	C5-C4-N3	-7.29	116.79	128.39
24	a	2445	2MG	C2-N3-C4	7.19	121.00	112.00
1	A	1207	2MG	C2-N3-C4	7.08	120.86	112.00
24	a	2503	2MA	N3-C4-N9	6.85	135.68	126.99
24	a	2457	PSU	N1-C2-N3	6.84	122.38	115.17
1	A	516	PSU	N1-C2-N3	6.70	122.23	115.17
24	a	955	PSU	N1-C2-N3	6.63	122.16	115.17
24	a	2030	6MZ	C9-N6-C6	-6.60	116.73	122.85
24	a	1835	2MG	C5-C4-N3	-6.59	117.90	128.39
24	a	2604	PSU	N1-C2-N3	6.40	121.92	115.17
24	a	1911	PSU	N1-C2-N3	6.30	121.81	115.17
1	A	1498	UR3	C4-N3-C2	-6.26	119.54	124.58
24	a	1939	5MU	N3-C2-N1	6.17	122.92	114.89
24	a	2580	PSU	N1-C2-N3	6.05	121.55	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	2605	PSU	N1-C2-N3	6.05	121.55	115.17
24	a	1618	6MZ	C5-C4-N3	-5.98	118.48	126.72
24	a	746	PSU	N1-C2-N3	5.94	121.44	115.17
24	a	1917	PSU	N1-C2-N3	5.94	121.44	115.17
1	A	1516	2MG	C5-C4-N3	-5.91	118.99	128.39
24	a	2504	PSU	N1-C2-N3	5.80	121.29	115.17
24	a	2251	OMG	C5-C4-N3	-5.74	119.25	128.39
23	Z	76	8AN	C5-C4-N3	-5.69	118.88	126.72
1	A	1207	2MG	C5-C4-N3	-5.65	119.39	128.39
1	A	527	G7M	C5-C4-N3	-5.55	117.67	128.15
24	a	2445	2MG	C5-C4-N3	-5.55	119.56	128.39
1	A	1519	MA6	C5-C4-N3	-5.46	119.20	126.72
24	a	747	5MU	N3-C2-N1	5.46	122.00	114.89
1	A	966	2MG	N9-C4-N3	5.39	136.74	125.95
1	A	527	G7M	N9-C4-N3	5.39	136.72	125.95
1	A	1498	UR3	C1'-N1-C2	5.38	125.85	117.04
24	a	1939	5MU	C4-N3-C2	-5.37	120.30	127.34
1	A	1518	MA6	C5-C4-N3	-5.31	119.41	126.72
1	A	527	G7M	C2-N3-C4	5.30	121.44	112.30
23	Z	76	8AN	N3-C4-N9	5.22	136.04	127.17
24	a	2069	G7M	C2-N3-C4	5.12	121.12	112.30
1	A	1519	MA6	C4-C5-N7	-5.10	104.75	110.58
55	Y	76	8AN	O4'-C4'-C3'	5.07	111.59	104.22
55	Y	76	8AN	C5-C4-N3	-5.04	119.77	126.72
55	Y	76	8AN	C2'-C3'-C4'	-4.98	95.88	102.70
24	a	2251	OMG	C2-N3-C4	4.96	120.85	112.30
24	a	2069	G7M	C5-C4-N3	-4.93	118.84	128.15
24	a	745	1MG	C5-C4-N3	-4.84	120.68	128.39
24	a	1618	6MZ	N3-C4-N9	4.81	135.35	127.17
1	A	1518	MA6	C2-N1-C6	4.74	123.41	111.83
24	a	2030	6MZ	C5-C4-N3	-4.64	120.33	126.72
24	a	2069	G7M	N9-C4-N3	4.60	135.14	125.95
24	a	1915	3TD	C1'-C5-C4	4.55	124.51	117.61
24	a	1835	2MG	N9-C4-N3	4.51	134.96	125.95
1	A	1519	MA6	C2-N1-C6	4.49	122.80	111.83
24	a	747	5MU	C4-N3-C2	-4.48	121.47	127.34
24	a	745	1MG	C2-N3-C4	4.40	121.86	111.98
1	A	1518	MA6	C4-C5-N7	-4.30	105.67	110.58
24	a	2552	OMU	C4-N3-C2	-4.28	121.30	126.61
24	a	1835	2MG	N1-C2-N2	4.28	120.93	116.56
1	A	1498	UR3	C6-N1-C2	-4.27	118.31	121.80
24	a	2604	PSU	C4-N3-C2	-4.27	120.49	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	C4-N3-C2	-4.26	120.50	126.37
55	Y	76	8AN	N3-C4-N9	4.23	134.36	127.17
24	a	2605	PSU	C4-N3-C2	-4.23	120.55	126.37
24	a	1939	5MU	C5-C4-N3	4.19	118.97	115.32
24	a	2030	6MZ	C6-C5-N7	4.19	137.00	132.43
24	a	955	PSU	O2-C2-N1	-4.16	118.49	122.79
1	A	1518	MA6	N3-C4-N9	4.12	134.17	127.17
24	a	2445	2MG	N9-C4-N3	4.09	134.13	125.95
24	a	2552	OMU	N3-C2-N1	4.05	120.16	114.89
24	a	2251	OMG	N9-C4-N3	4.01	133.98	125.95
24	a	2457	PSU	C4-N3-C2	-4.01	120.85	126.37
1	A	1207	2MG	N9-C4-N3	3.98	133.90	125.95
24	a	2504	PSU	O2-C2-N1	-3.95	118.72	122.79
1	A	1516	2MG	N9-C4-N3	3.94	133.83	125.95
24	a	2457	PSU	O2-C2-N1	-3.92	118.75	122.79
24	a	2030	6MZ	N3-C4-N9	3.89	133.79	127.17
1	A	1516	2MG	C6-C5-N7	3.87	137.34	130.29
24	a	1618	6MZ	C2-N3-C4	3.87	121.28	111.83
24	a	955	PSU	C4-N3-C2	-3.84	121.08	126.37
24	a	2030	6MZ	C4-N9-C8	3.84	109.77	105.74
24	a	2552	OMU	C5-C4-N3	3.84	120.18	114.80
1	A	1407	5MC	O2-C2-N3	-3.84	116.28	122.33
24	a	1917	PSU	C4-N3-C2	-3.84	121.08	126.37
24	a	2580	PSU	C4-N3-C2	-3.83	121.09	126.37
23	Z	76	8AN	C4-N9-C8	3.82	109.75	105.74
24	a	1917	PSU	O2-C2-N1	-3.81	118.86	122.79
24	a	746	PSU	C4-N3-C2	-3.79	121.15	126.37
24	a	2251	OMG	C6-C5-N7	3.76	137.13	130.29
1	A	516	PSU	O2-C2-N1	-3.75	118.92	122.79
24	a	747	5MU	C5-C4-N3	3.74	118.57	115.32
1	A	1519	MA6	C2-N3-C4	3.74	120.96	111.83
1	A	1519	MA6	N3-C4-N9	3.64	133.36	127.17
24	a	1939	5MU	C5-C6-N1	-3.63	119.37	123.31
24	a	2504	PSU	C4-N3-C2	-3.60	121.41	126.37
1	A	1207	2MG	C6-C5-N7	3.59	136.82	130.29
24	a	1835	2MG	C6-C5-N7	3.57	136.79	130.29
24	a	1911	PSU	C4-N3-C2	-3.55	121.48	126.37
24	a	2445	2MG	C6-C5-N7	3.54	136.74	130.29
24	a	1618	6MZ	C6-C5-N7	3.54	136.29	132.43
23	Z	76	8AN	C2-N3-C4	3.53	120.45	111.83
24	a	747	5MU	C5-C6-N1	-3.52	119.49	123.31
1	A	1519	MA6	C5-N7-C8	3.49	108.94	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	745	1MG	N9-C4-N3	3.49	132.94	125.95
24	a	2580	PSU	O2-C2-N1	-3.49	119.19	122.79
24	a	1915	3TD	C4-N3-C2	-3.46	120.95	124.61
24	a	1618	6MZ	C4-C5-N7	-3.45	106.63	110.58
24	a	1618	6MZ	N1-C2-N3	-3.42	123.41	128.58
24	a	2030	6MZ	C4-C5-N7	-3.40	106.69	110.58
1	A	1519	MA6	N1-C2-N3	-3.39	123.45	128.58
24	a	2552	OMU	O4-C4-C5	-3.36	119.36	125.16
24	a	2030	6MZ	N1-C2-N3	-3.36	123.49	128.58
1	A	1518	MA6	C2-N3-C4	3.34	119.98	111.83
24	a	1939	5MU	O2-C2-N1	-3.32	118.47	122.80
1	A	1207	2MG	N1-C2-N2	3.32	119.95	116.56
24	a	2604	PSU	O2-C2-N1	-3.27	119.42	122.79
24	a	1618	6MZ	C9-N6-C6	-3.26	119.82	122.85
24	a	2030	6MZ	C2-N3-C4	3.25	119.78	111.83
24	a	747	5MU	O4-C4-C5	-3.25	121.20	124.92
24	a	2504	PSU	C6-C5-C4	-3.23	116.00	118.17
1	A	1518	MA6	N1-C2-N3	-3.22	123.70	128.58
24	a	1939	5MU	O4-C4-C5	-3.18	121.28	124.92
1	A	1516	2MG	N1-C2-N2	3.18	119.80	116.56
1	A	1519	MA6	C6-C5-N7	3.17	138.49	133.43
23	Z	76	8AN	N1-C2-N3	-3.10	123.89	128.58
24	a	2552	OMU	O2-C2-N1	-3.08	118.78	122.80
24	a	1962	5MC	C5-C6-N1	-3.08	119.97	123.31
24	a	1835	2MG	N2-C2-N3	-3.05	116.63	120.51
24	a	2503	2MA	C4-N9-C8	3.04	108.92	105.74
1	A	1407	5MC	C5-C4-N3	-3.03	118.65	121.75
24	a	1911	PSU	O2-C2-N1	-3.00	119.69	122.79
1	A	967	5MC	C5-C4-N3	-2.97	118.71	121.75
24	a	745	1MG	C6-C5-N7	2.92	135.85	129.36
24	a	2503	2MA	C2-N1-C6	2.90	122.56	118.10
24	a	2498	OMC	O2-C2-N3	-2.90	117.76	122.33
1	A	1518	MA6	C5-N7-C8	2.89	108.00	103.45
1	A	967	5MC	C5-C6-N1	-2.89	120.18	123.31
24	a	1835	2MG	C4-C5-N7	-2.88	106.11	110.67
24	a	2605	PSU	O2-C2-N1	-2.86	119.84	122.79
24	a	2503	2MA	C4-C5-N7	-2.85	107.33	110.58
1	A	1498	UR3	C5-C4-N3	2.84	118.78	115.04
24	a	1618	6MZ	C4-N9-C8	2.81	108.69	105.74
24	a	2503	2MA	N6-C6-N1	2.80	120.80	117.03
24	a	2030	6MZ	N9-C8-N7	-2.79	109.97	113.94
1	A	1516	2MG	C4-C5-N7	-2.79	106.25	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	76	8AN	C4-C5-N7	-2.76	107.43	110.58
24	a	747	5MU	O2-C2-N3	-2.75	116.41	121.49
55	Y	76	8AN	C2-N3-C4	2.74	118.52	111.83
55	Y	76	8AN	C4-C5-N7	-2.74	107.45	110.58
24	a	2449	H2U	C5-C4-N3	2.74	119.60	116.69
1	A	966	2MG	C6-C5-N7	2.73	135.26	130.29
24	a	2251	OMG	C4-C5-N7	-2.70	106.40	110.67
24	a	2030	6MZ	C5-N7-C8	2.69	107.67	103.45
24	a	1962	5MC	C5-C4-N3	-2.68	119.01	121.75
1	A	1519	MA6	C4-N9-C8	2.66	108.53	105.74
1	A	1402	4OC	O2-C2-N3	-2.65	118.15	122.33
24	a	2445	2MG	N1-C2-N2	2.64	119.26	116.56
24	a	1618	6MZ	C5-N7-C8	2.58	107.51	103.45
1	A	1207	2MG	C4-C5-N7	-2.57	106.60	110.67
12	L	89	D2T	OD1-CG-CB	-2.57	117.07	122.44
35	l	81	4D4	CG-CD-NE	-2.57	104.84	111.88
24	a	2580	PSU	O4'-C1'-C2'	2.55	108.67	105.15
1	A	1519	MA6	N9-C8-N7	-2.55	110.32	113.94
1	A	966	2MG	C4-C5-N7	-2.55	106.64	110.67
1	A	1207	2MG	N2-C2-N3	-2.50	117.33	120.51
24	a	1917	PSU	C6-C5-C4	-2.50	116.49	118.17
1	A	966	2MG	C2-N1-C6	-2.47	121.56	124.55
24	a	2605	PSU	C6-C5-C4	-2.47	116.51	118.17
24	a	745	1MG	C4-C5-N7	-2.47	106.76	110.67
24	a	746	PSU	O2-C2-N1	-2.46	120.25	122.79
23	Z	76	8AN	N9-C8-N7	-2.44	110.47	113.94
23	Z	76	8AN	C5-N7-C8	2.43	107.27	103.45
1	A	527	G7M	C5-C6-N1	2.43	116.85	111.84
1	A	516	PSU	O4'-C1'-C2'	2.41	108.49	105.15
24	a	1962	5MC	O2-C2-N3	-2.41	118.53	122.33
24	a	2445	2MG	C4-C5-N7	-2.41	106.86	110.67
23	Z	76	8AN	O4'-C4'-C3'	2.40	107.71	104.22
1	A	1518	MA6	C4-N9-C8	2.39	108.25	105.74
55	Y	76	8AN	C4-N9-C8	2.39	108.24	105.74
24	a	2069	G7M	C5-C6-N1	2.35	116.69	111.84
1	A	516	PSU	C5-C6-N1	-2.33	118.91	122.14
1	A	1498	UR3	C1'-N1-C6	-2.33	115.81	120.78
24	a	2503	2MA	C5-N7-C8	2.31	107.08	103.45
24	a	745	1MG	C6-C5-C4	-2.28	117.38	119.97
24	a	2449	H2U	N3-C2-N1	2.25	118.91	116.65
24	a	2503	2MA	N3-C2-N1	-2.24	121.82	125.77
24	a	2030	6MZ	C2-N1-C6	2.23	122.64	115.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	2503	2MA	C6-C5-N7	2.20	136.34	132.09
1	A	1516	2MG	N2-C2-N3	-2.18	117.74	120.51
24	a	2445	2MG	O6-C6-C5	-2.17	120.81	126.53
24	a	2069	G7M	O6-C6-C5	-2.17	123.17	128.01
1	A	1498	UR3	O2-C2-N3	-2.16	118.35	121.33
24	a	746	PSU	C5-C6-N1	-2.15	119.15	122.14
1	A	966	2MG	O6-C6-C5	-2.15	120.85	126.53
1	A	1207	2MG	O6-C6-C5	-2.15	120.86	126.53
24	a	1915	3TD	O4'-C1'-C2'	2.14	108.12	105.15
24	a	2503	2MA	N9-C8-N7	-2.12	110.92	113.94
24	a	2449	H2U	O2-C2-N1	-2.10	120.58	123.10
1	A	966	2MG	N1-C2-N2	2.10	118.70	116.56
24	a	1835	2MG	CM2-N2-C2	-2.09	119.15	123.65
1	A	1407	5MC	C5-C6-N1	-2.09	121.04	123.31
24	a	2604	PSU	C6-C5-C4	-2.08	116.77	118.17
1	A	1402	4OC	C6-C5-C4	2.07	119.50	117.00
24	a	1618	6MZ	N9-C8-N7	-2.07	111.00	113.94
1	A	1518	MA6	C6-C5-N7	2.06	136.72	133.43
24	a	1835	2MG	C2-N1-C6	-2.05	122.07	124.55
24	a	2552	OMU	C6-N1-C2	-2.03	118.52	121.00
1	A	1498	UR3	C3U-N3-C2	2.03	120.87	117.33
1	A	1516	2MG	C5-C6-N1	2.02	118.41	113.25
24	a	1915	3TD	C6-C5-C4	-2.02	116.84	118.19
55	Y	76	8AN	N6-C6-N1	2.02	122.87	118.38
24	a	2503	2MA	C2-N3-C4	2.01	121.90	115.02
1	A	966	2MG	C5-C6-N1	2.00	118.35	113.25
1	A	527	G7M	O6-C6-C5	-2.00	123.55	128.01

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	CG-CB-SB-CB1
11	K	119	IAS	N-CA-CB-CG
24	a	746	PSU	O4'-C1'-C5-C6
1	A	1519	MA6	O4'-C4'-C5'-O5'
24	a	1915	3TD	O4'-C4'-C5'-O5'
27	d	150	MEQ	NE2-CD-CG-CB
27	d	150	MEQ	OE1-CD-CG-CB
24	a	1915	3TD	C3'-C4'-C5'-O5'
24	a	2030	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C3'-C4'-C5'-O5'
24	a	2030	6MZ	C3'-C4'-C5'-O5'
24	a	2445	2MG	C3'-C4'-C5'-O5'
23	Z	76	8AN	C4'-C5'-O5'-P
24	a	2504	PSU	O4'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-CG-OD2
27	d	150	MEQ	C-CA-CB-CG
35	l	82	MS6	CB-CG-SD-CE
11	K	119	IAS	CA-CB-CG-OD1
24	a	746	PSU	O4'-C1'-C5-C4
1	A	527	G7M	C4'-C5'-O5'-P
24	a	1911	PSU	O4'-C4'-C5'-O5'
24	a	1917	PSU	O4'-C4'-C5'-O5'
12	L	89	D2T	SB-CB-CG-OD2
1	A	1519	MA6	C4'-C5'-O5'-P
12	L	89	D2T	CA-CB-CG-OD1
24	a	746	PSU	C2'-C1'-C5-C6
35	l	81	4D4	O-C-CA-CB
24	a	2503	2MA	C4'-C5'-O5'-P
24	a	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Y	76	8AN	1	0
1	A	1518	MA6	1	0
24	a	1962	5MC	1	0
24	a	2030	6MZ	1	0
1	A	516	PSU	1	0
1	A	967	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 332 are monoatomic - leaving 17 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$
58	SPD	a	6214	-	9,9,9	0.32	0	8,8,8	0.87	0
58	SPD	a	6213	-	9,9,9	0.34	0	8,8,8	1.14	1 (12%)
58	SPD	a	6209	-	9,9,9	0.32	0	8,8,8	0.99	0
58	SPD	a	6206	-	9,9,9	0.36	0	8,8,8	0.61	0
58	SPD	a	6215	-	9,9,9	0.29	0	8,8,8	1.02	0
58	SPD	a	6212	-	9,9,9	0.33	0	8,8,8	0.88	0
56	PAR	A	1601	-	44,45,45	0.57	0	63,67,67	0.95	1 (1%)
58	SPD	a	6211	-	9,9,9	0.25	0	8,8,8	0.92	0
58	SPD	a	6208	-	9,9,9	0.30	0	8,8,8	0.51	0
58	SPD	a	6217	-	9,9,9	0.33	0	8,8,8	0.64	0
59	FME	Z	101	23	8,9,10	1.08	1 (12%)	8,9,11	1.16	1 (12%)
60	SPM	a	6216	-	13,13,13	0.29	0	12,12,12	0.83	0
58	SPD	a	6205	-	9,9,9	0.32	0	8,8,8	1.01	0
58	SPD	a	6210	-	9,9,9	0.33	0	8,8,8	0.96	0
58	SPD	a	6207	-	9,9,9	0.31	0	8,8,8	0.85	0
63	A1B70	Y	101	55	16,16,17	0.86	2 (12%)	16,20,22	2.21	3 (18%)
58	SPD	A	1692	-	9,9,9	0.35	0	8,8,8	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	a	6214	-	-	3/7/7/7	-
58	SPD	a	6213	-	-	3/7/7/7	-
58	SPD	a	6209	-	-	5/7/7/7	-
58	SPD	a	6206	-	-	2/7/7/7	-
58	SPD	a	6215	-	-	2/7/7/7	-
58	SPD	a	6212	-	-	2/7/7/7	-
56	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
58	SPD	a	6211	-	-	5/7/7/7	-
58	SPD	a	6208	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	a	6217	-	-	4/7/7/7	-
59	FME	Z	101	23	-	3/7/9/11	-
60	SPM	a	6216	-	-	6/11/11/11	-
58	SPD	a	6205	-	-	3/7/7/7	-
58	SPD	a	6210	-	-	5/7/7/7	-
58	SPD	a	6207	-	-	4/7/7/7	-
63	A1B70	Y	101	55	-	4/17/17/19	-
58	SPD	A	1692	-	-	7/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Z	101	FME	CA-N	-2.55	1.42	1.46
63	Y	101	A1B70	C1-C2	-2.03	1.48	1.52
63	Y	101	A1B70	C3-C2	-2.02	1.50	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	Y	101	A1B70	O1-C1-C2	-7.11	96.43	111.24
63	Y	101	A1B70	O5-C12-C2	-3.03	118.31	125.24
63	Y	101	A1B70	C8-O2-C7	2.56	124.85	120.97
56	A	1601	PAR	C14-O33-C33	-2.30	112.54	117.98
59	Z	101	FME	C-CA-N	2.29	113.92	109.50
58	a	6213	SPD	C7-C8-C9	-2.18	106.39	114.17

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	A	1601	PAR	C44-C54-C64-N64
56	A	1601	PAR	O54-C54-C64-N64
58	a	6210	SPD	N1-C2-C3-C4
63	Y	101	A1B70	O5-C12-C2-C3
58	a	6217	SPD	N6-C7-C8-C9
58	a	6206	SPD	C3-C4-C5-N6
58	a	6211	SPD	C3-C4-C5-N6
58	a	6208	SPD	N6-C7-C8-C9
58	a	6211	SPD	N6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
58	a	6208	SPD	N1-C2-C3-C4
58	A	1692	SPD	N6-C7-C8-C9
60	a	6216	SPM	C2-C3-C4-N5
58	a	6207	SPD	N6-C7-C8-C9
58	a	6210	SPD	C4-C5-N6-C7
58	a	6210	SPD	C8-C7-N6-C5
60	a	6216	SPM	N5-C6-C7-C8
58	A	1692	SPD	C3-C4-C5-N6
58	a	6205	SPD	C4-C5-N6-C7
58	a	6214	SPD	C4-C5-N6-C7
58	a	6215	SPD	C8-C7-N6-C5
58	A	1692	SPD	C4-C5-N6-C7
58	a	6209	SPD	C8-C7-N6-C5
58	a	6209	SPD	C7-C8-C9-N10
58	a	6213	SPD	C8-C7-N6-C5
58	a	6214	SPD	C7-C8-C9-N10
58	A	1692	SPD	C2-C3-C4-C5
58	a	6209	SPD	C3-C4-C5-N6
58	a	6211	SPD	N1-C2-C3-C4
60	a	6216	SPM	C8-C9-N10-C11
58	a	6215	SPD	C2-C3-C4-C5
63	Y	101	A1B70	O1-C1-C2-C12
59	Z	101	FME	CB-CG-SD-CE
58	a	6208	SPD	C8-C7-N6-C5
58	A	1692	SPD	N1-C2-C3-C4
58	a	6211	SPD	C2-C3-C4-C5
58	a	6210	SPD	C2-C3-C4-C5
58	a	6207	SPD	C2-C3-C4-C5
58	a	6208	SPD	C2-C3-C4-C5
58	a	6207	SPD	C7-C8-C9-N10
58	a	6213	SPD	C2-C3-C4-C5
58	a	6214	SPD	C8-C7-N6-C5
59	Z	101	FME	CB-CA-N-CN
58	a	6212	SPD	C2-C3-C4-C5
58	a	6217	SPD	C2-C3-C4-C5
58	A	1692	SPD	C8-C7-N6-C5
58	A	1692	SPD	C7-C8-C9-N10
58	a	6205	SPD	C7-C8-C9-N10
58	a	6212	SPD	C7-C8-C9-N10
60	a	6216	SPM	C11-C12-C13-N14
60	a	6216	SPM	N10-C11-C12-C13
56	A	1601	PAR	C23-C33-O33-C14

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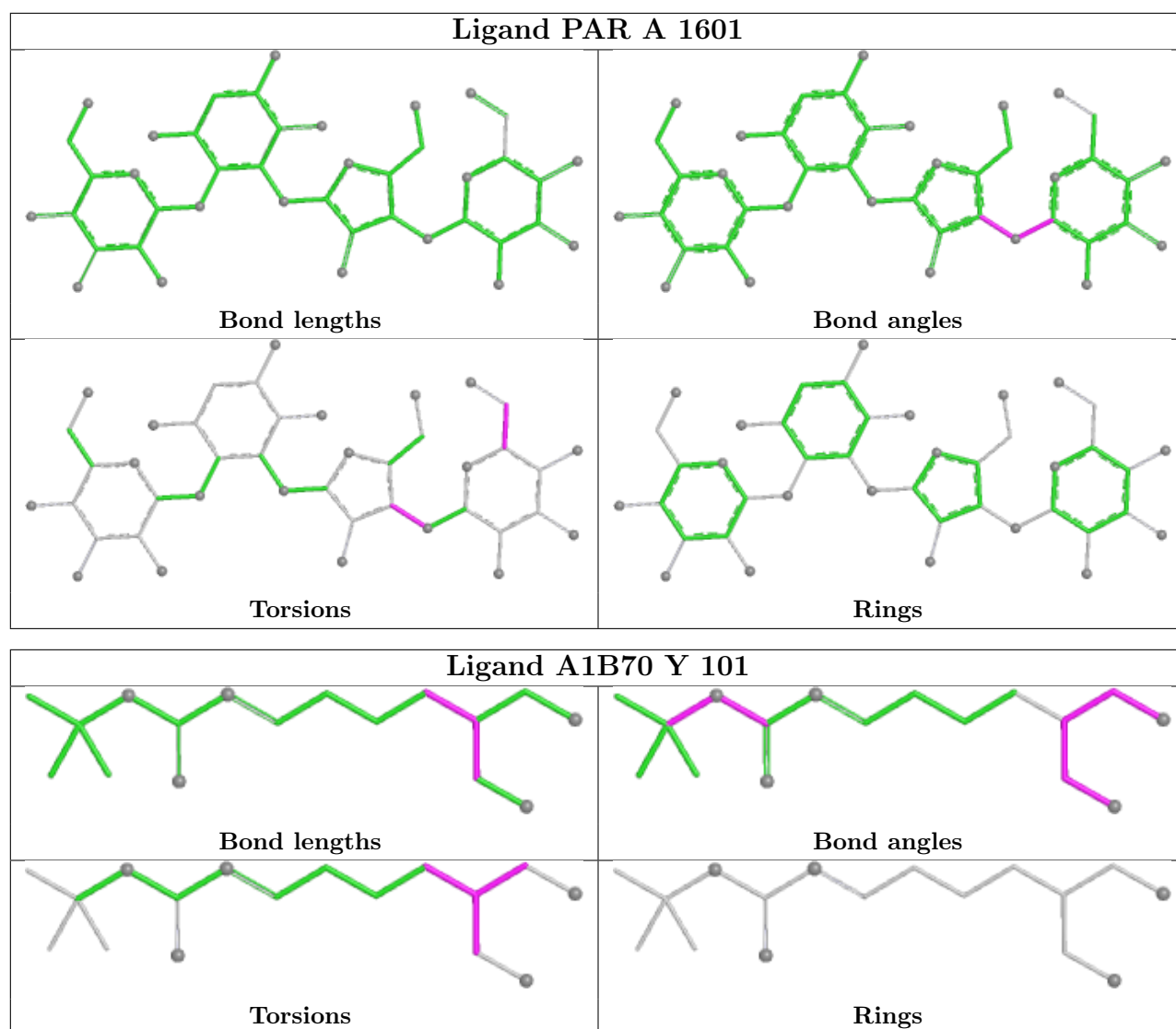
Mol	Chain	Res	Type	Atoms
58	a	6217	SPD	N1-C2-C3-C4
58	a	6209	SPD	C2-C3-C4-C5
58	a	6213	SPD	C3-C4-C5-N6
58	a	6206	SPD	C7-C8-C9-N10
58	a	6208	SPD	C7-C8-C9-N10
58	a	6211	SPD	C4-C5-N6-C7
58	a	6217	SPD	C4-C5-N6-C7
58	a	6208	SPD	C4-C5-N6-C7
60	a	6216	SPM	C3-C4-N5-C6
58	a	6209	SPD	N1-C2-C3-C4
59	Z	101	FME	N-CA-CB-CG
58	a	6207	SPD	C3-C4-C5-N6
63	Y	101	A1B70	C12-C2-C3-C4
58	a	6210	SPD	C7-C8-C9-N10
63	Y	101	A1B70	O1-C1-C2-C3
58	a	6205	SPD	C2-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	a	6214	SPD	1	0
58	a	6213	SPD	2	0
58	a	6215	SPD	2	0
58	a	6208	SPD	2	0
60	a	6216	SPM	1	0
58	a	6210	SPD	1	0
58	a	6207	SPD	2	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Y	5
22	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	13:C	O3'	15:C	P	5.51
1	Y	27:C	O3'	28:G	P	4.79
1	Y	15:C	O3'	17:G	P	4.65
1	X	19:U	O3'	20:A	P	4.07
1	Y	10:G	O3'	11:G	P	3.88
1	Y	43:G	O3'	44:C	P	3.36

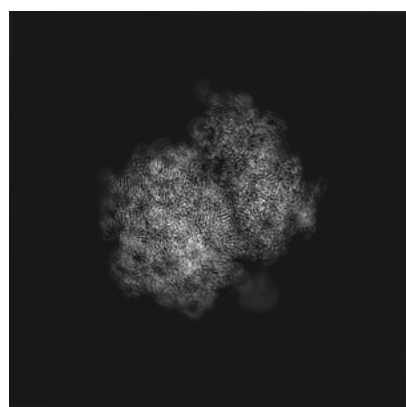
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70051. These allow visual inspection of the internal detail of the map and identification of artifacts.

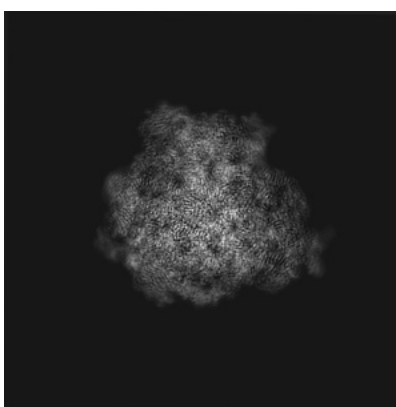
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

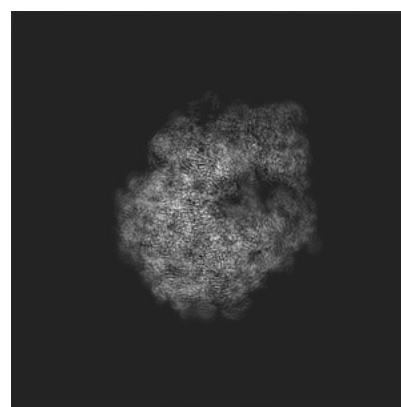
6.1.1 Primary map



X



Y

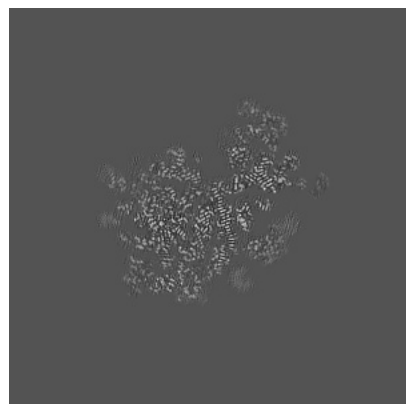


Z

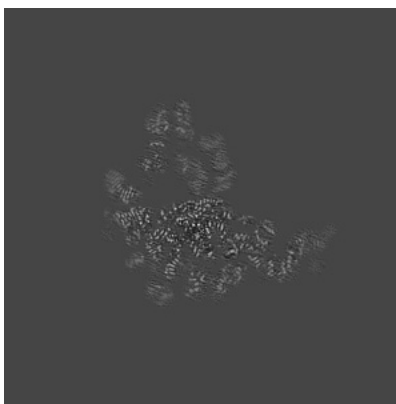
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

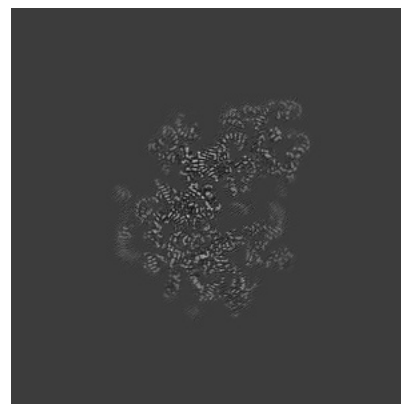
6.2.1 Primary map



X Index: 256



Y Index: 256

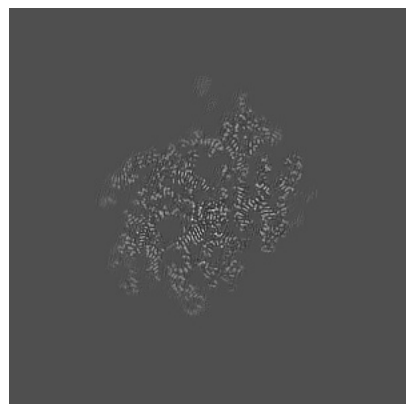


Z Index: 256

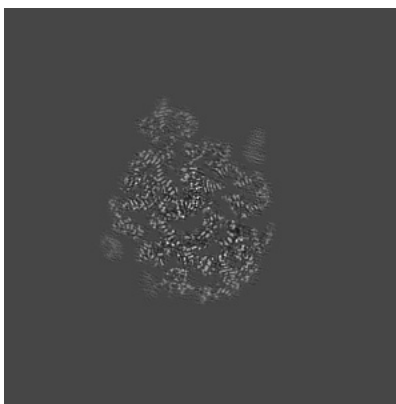
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

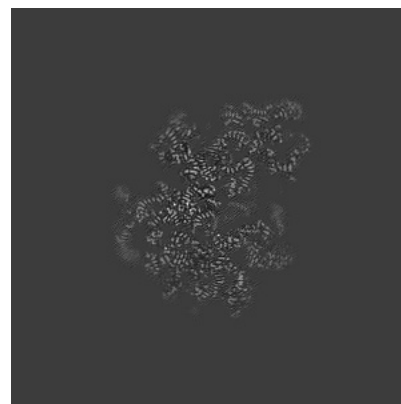
6.3.1 Primary map



X Index: 226



Y Index: 219

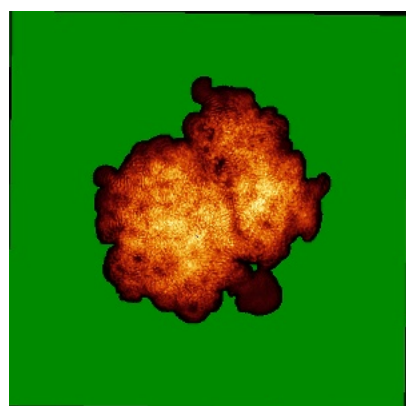


Z Index: 253

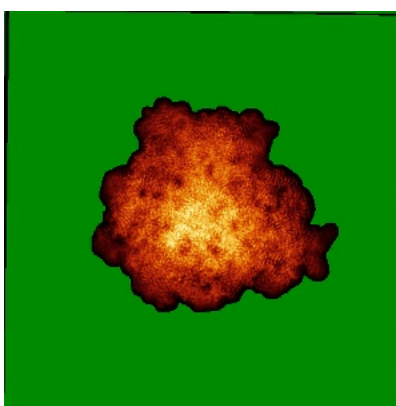
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

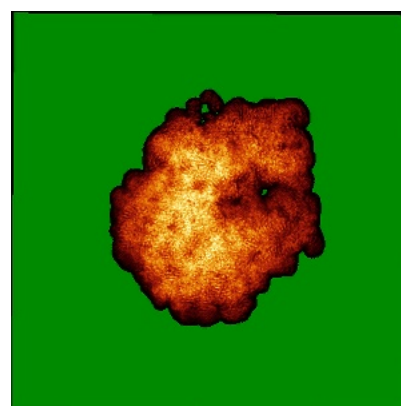
6.4.1 Primary map



X



Y

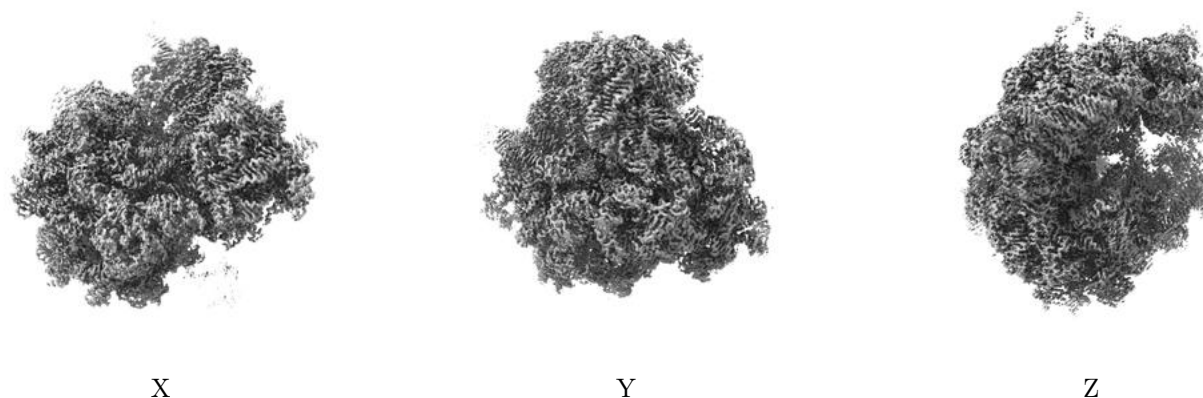


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

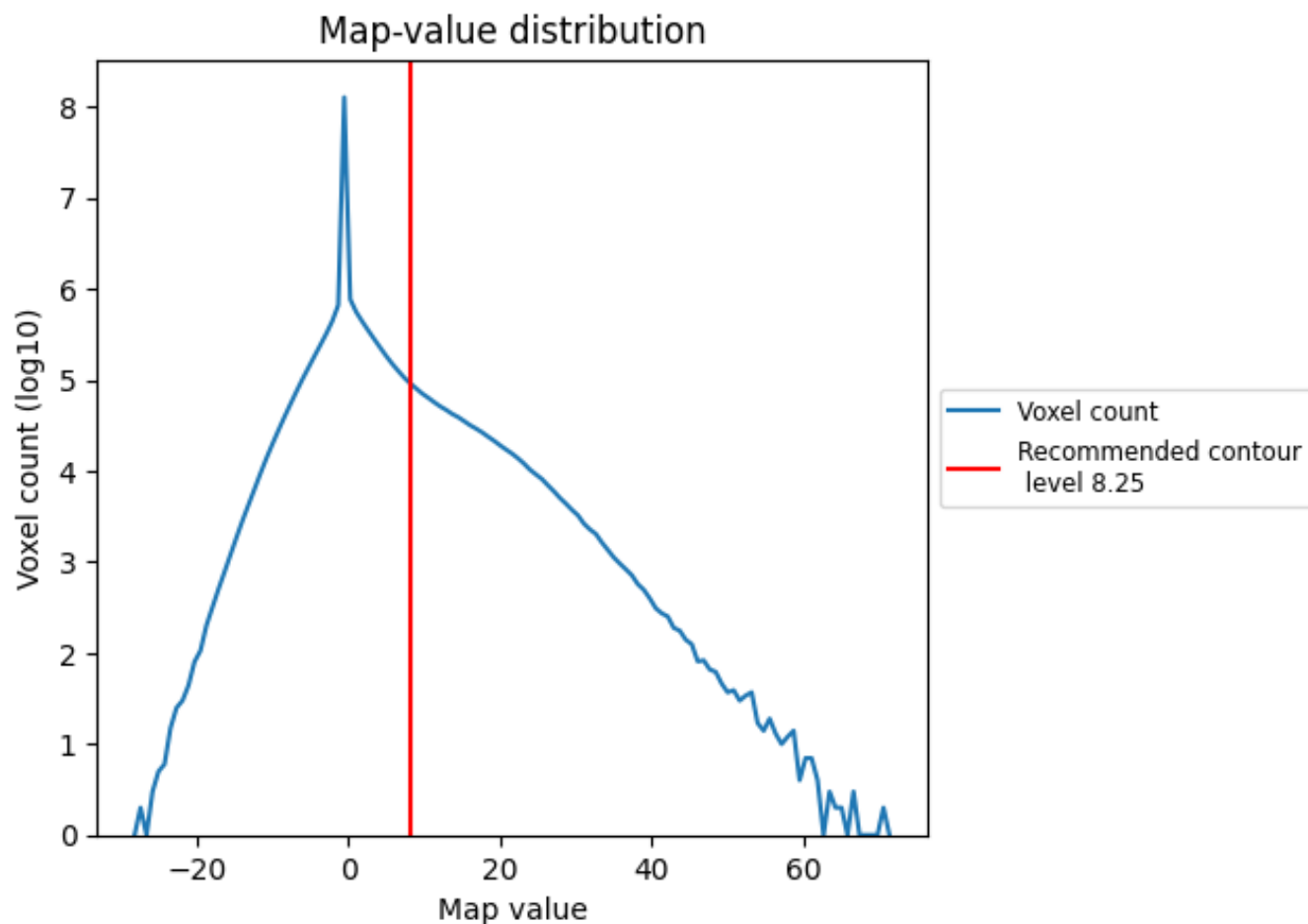
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

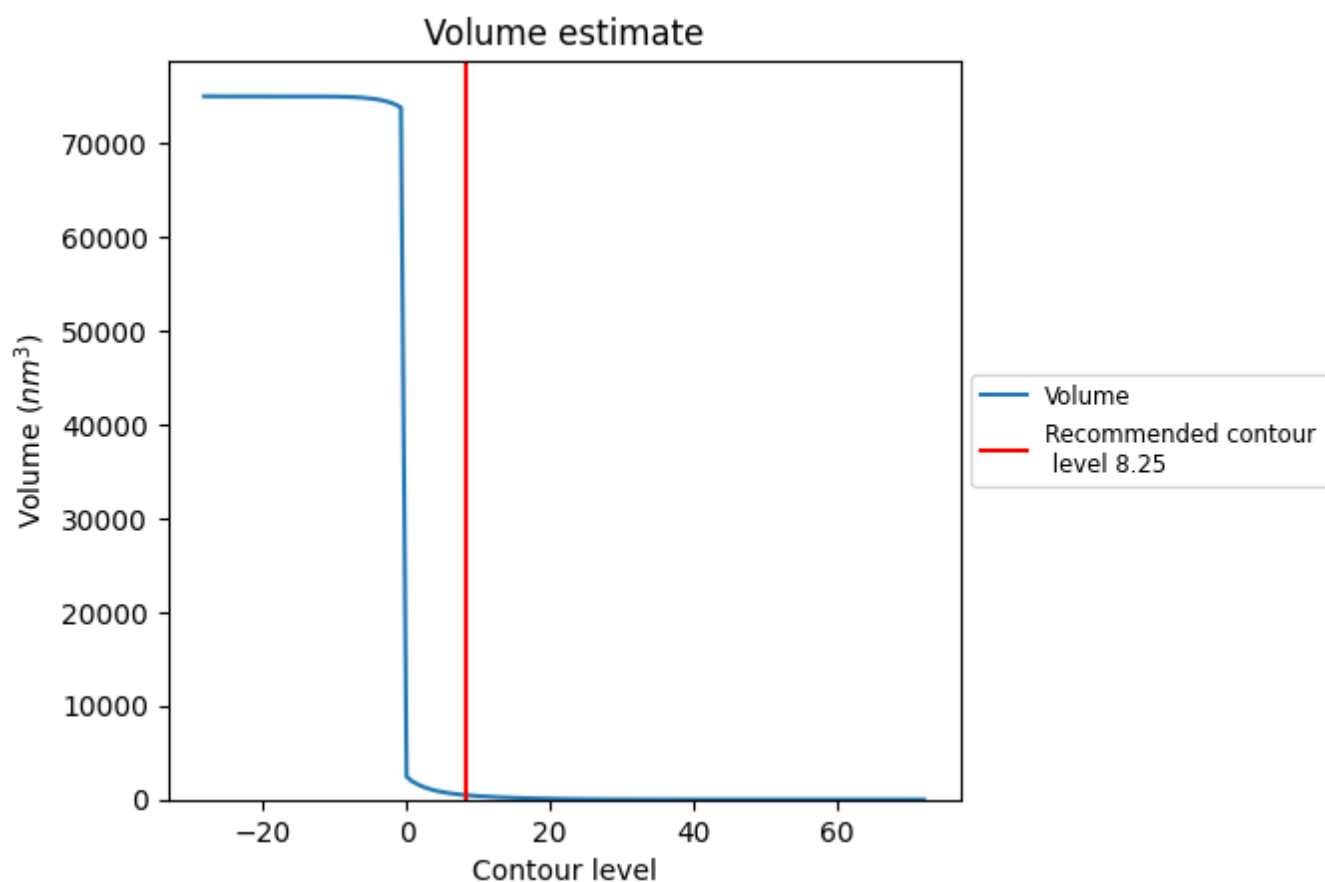
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

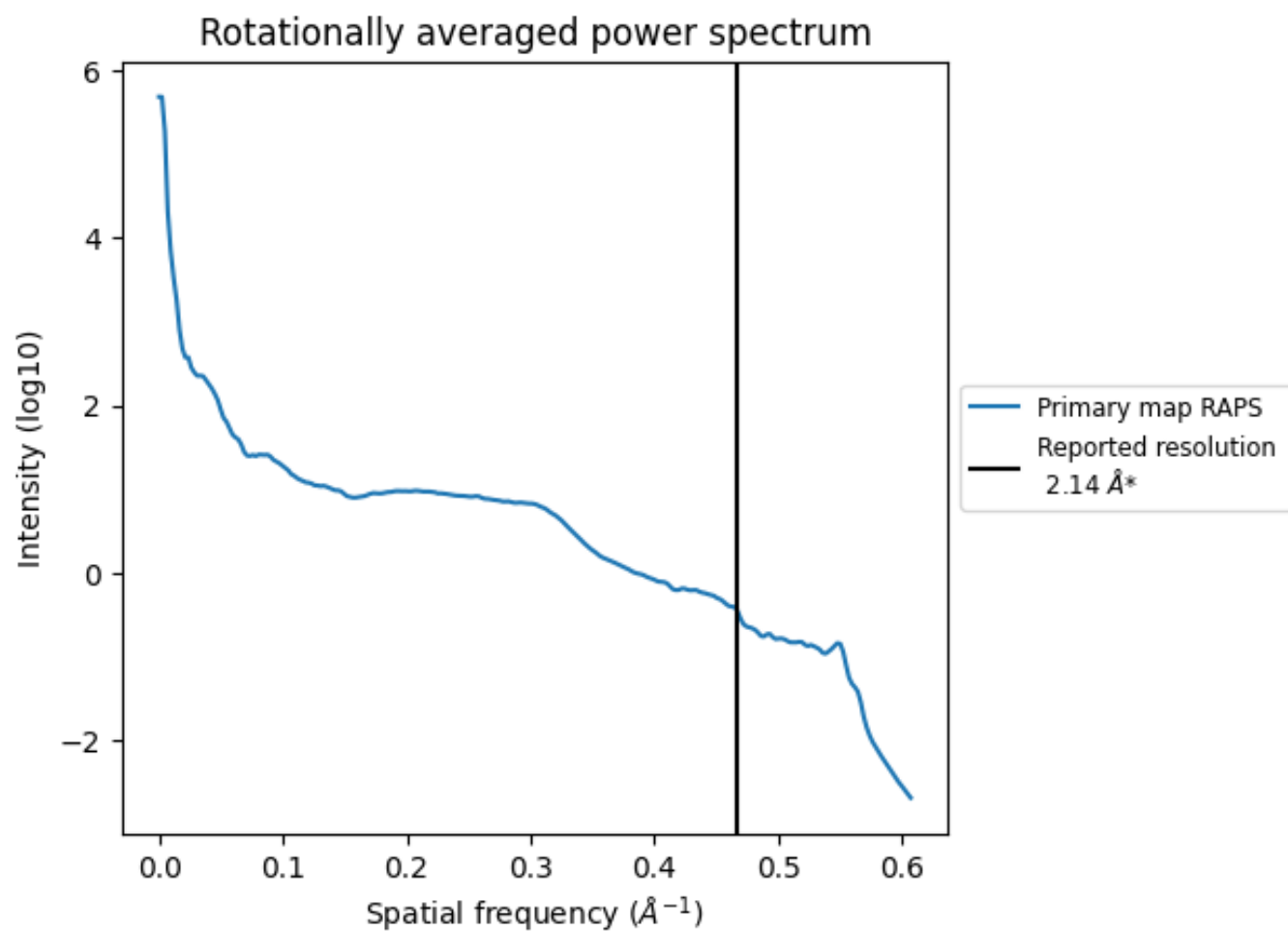
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm^3 ; this corresponds to an approximate mass of 431 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 ⓘ

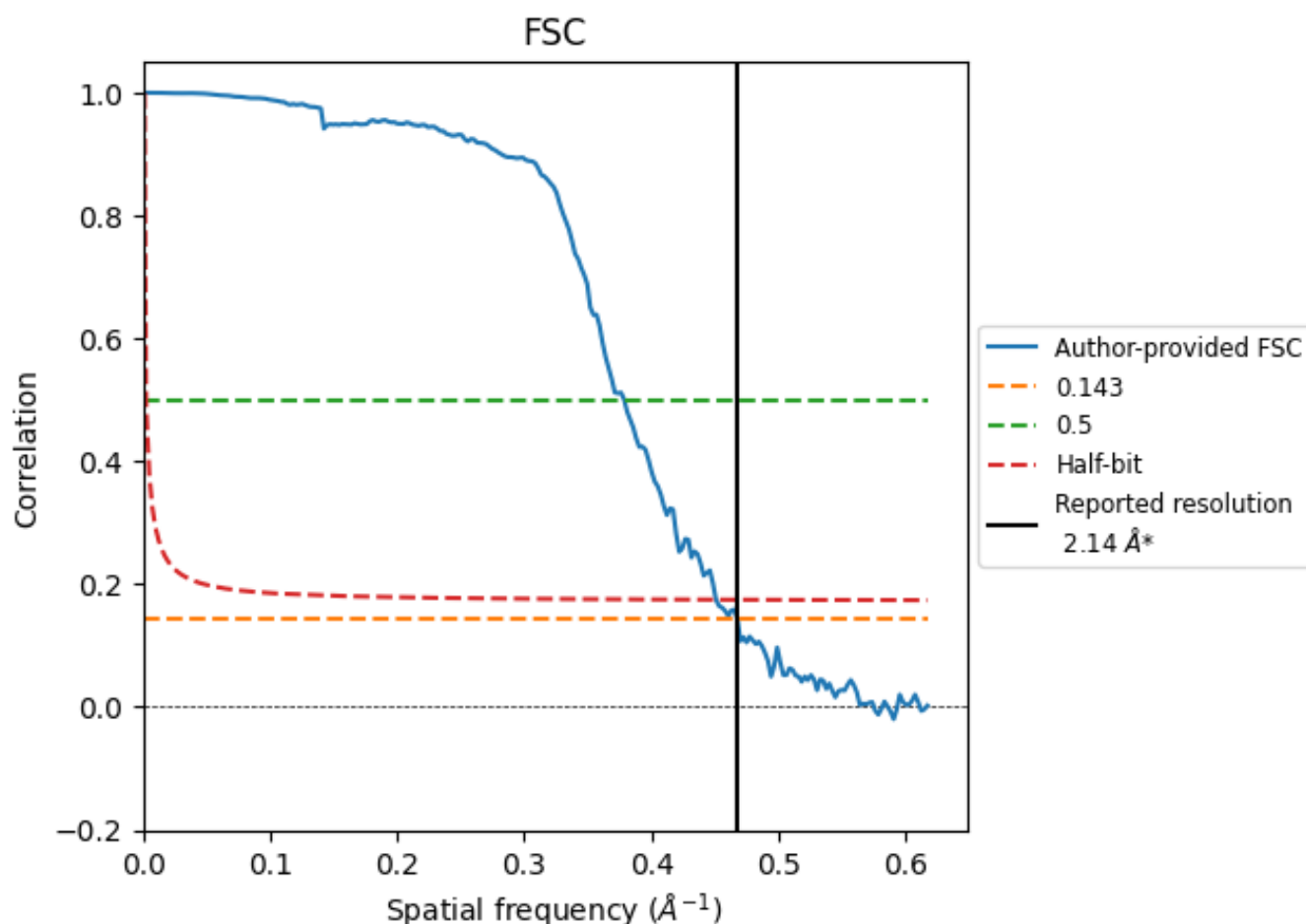


*Reported resolution corresponds to spatial frequency of 0.467 Å^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

8.2 Resolution estimates [i](#)

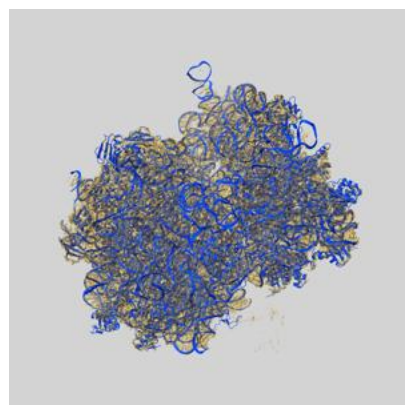
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.64	2.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

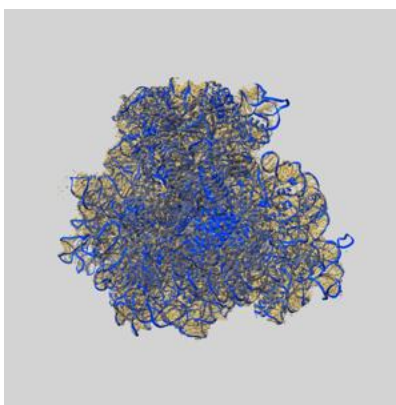
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70051 and PDB model 9O2Y. Per-residue inclusion information can be found in section 3 on page 20.

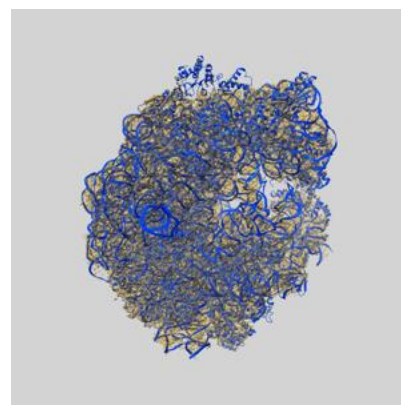
9.1 Map-model overlay [i](#)



X



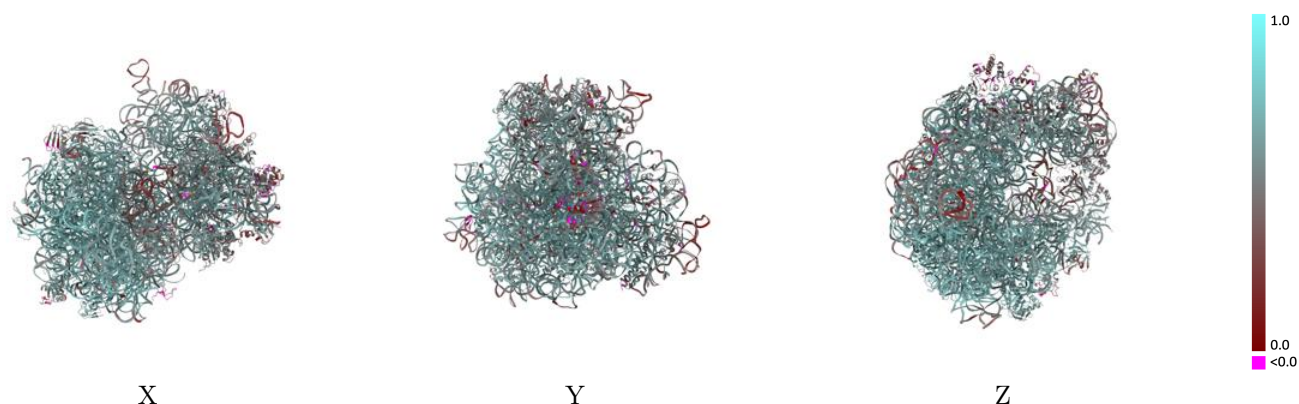
Y



Z

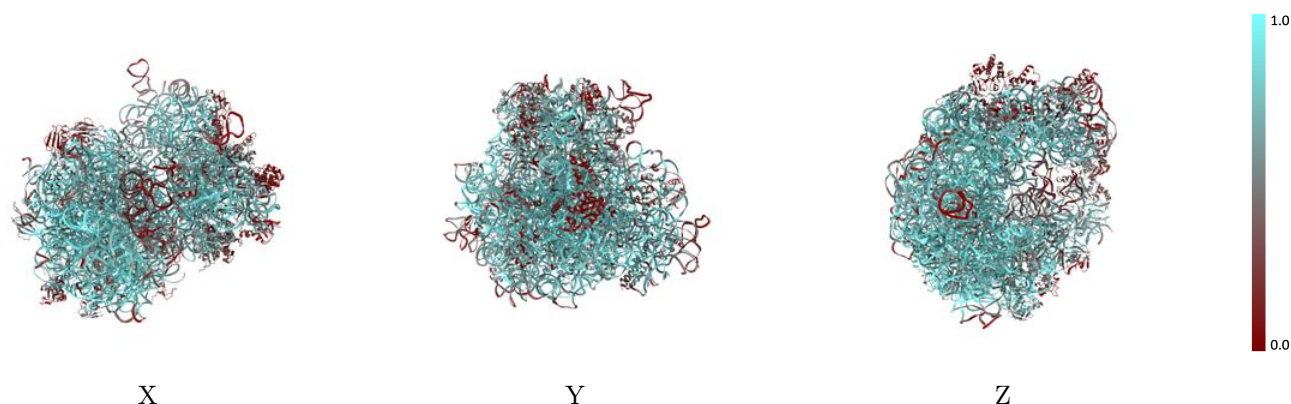
The images above show the 3D surface view of the map at the recommended contour level 8.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



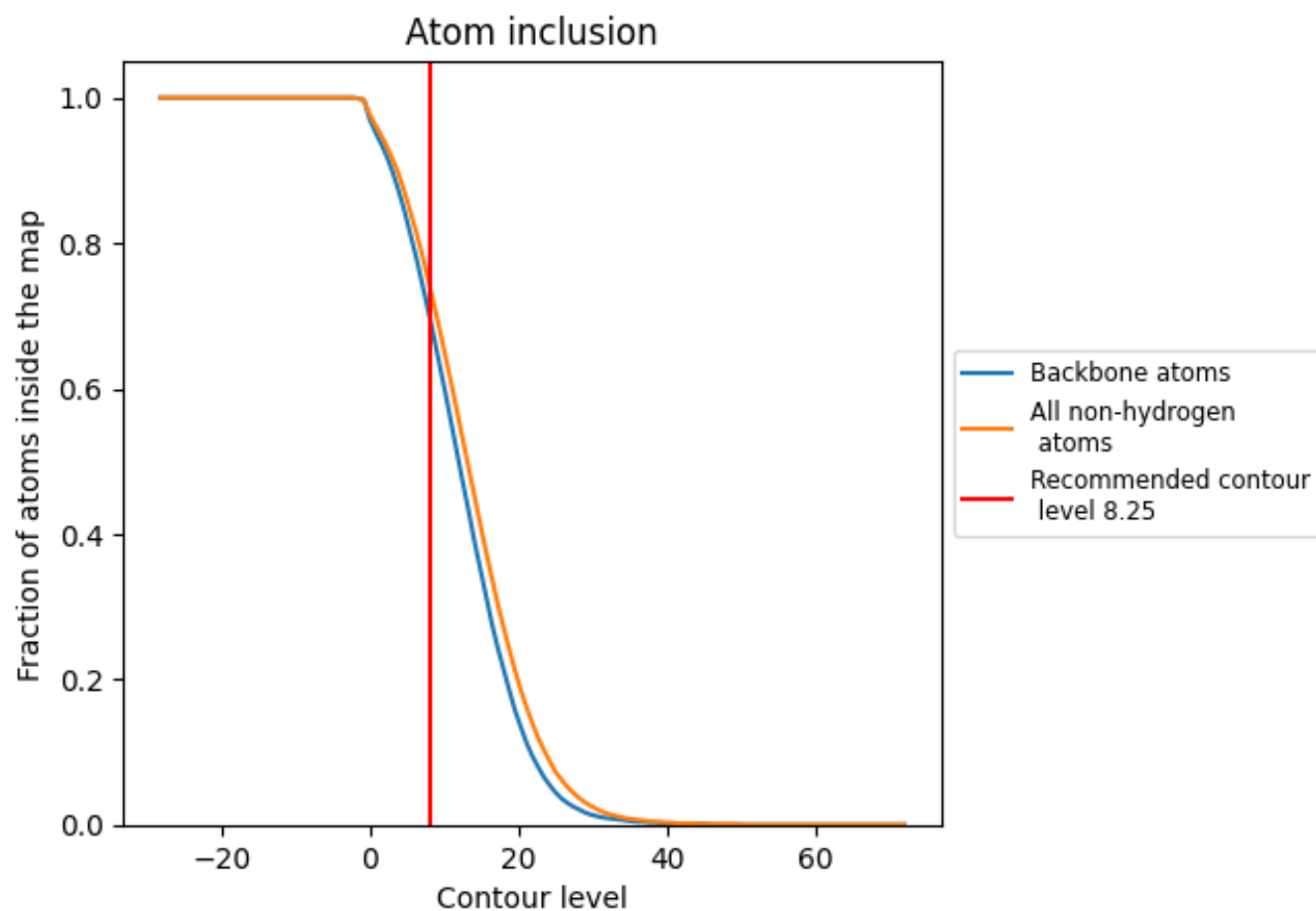
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.25).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 74% 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 (8.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.6100
0	 0.6500	 0.6540
1	 0.8000	 0.6990
2	 0.7430	 0.6950
3	 0.5840	 0.6000
4	 0.1500	 0.4090
A	 0.7860	 0.5870
B	 0.1070	 0.2800
C	 0.5240	 0.5120
D	 0.3070	 0.4210
E	 0.6550	 0.5850
F	 0.4790	 0.5230
G	 0.3760	 0.4760
H	 0.6820	 0.5910
I	 0.4370	 0.4720
J	 0.2930	 0.4110
K	 0.5540	 0.5530
L	 0.6090	 0.5850
M	 0.4880	 0.5020
N	 0.5970	 0.5230
O	 0.6420	 0.5970
P	 0.5910	 0.5100
Q	 0.5800	 0.5380
R	 0.4440	 0.4310
S	 0.4530	 0.4640
T	 0.6370	 0.5620
U	 0.1040	 0.2930
X	 0.4750	 0.4680
Y	 0.3300	 0.3870
Z	 0.5330	 0.4970
a	 0.8650	 0.6690
b	 0.7640	 0.6190
c	 0.7840	 0.6840
d	 0.7700	 0.6870
e	 0.5180	 0.5860



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Chain	Atom inclusion	Q-score
f	 0.3210	 0.4610
g	 0.2850	 0.4530
h	 0.1330	 0.2180
i	 0.7040	 0.6660
j	 0.6580	 0.6350
k	 0.6630	 0.6610
l	 0.6680	 0.6570
m	 0.8520	 0.7020
n	 0.5770	 0.6120
o	 0.6400	 0.6220
p	 0.8180	 0.7000
q	 0.6060	 0.6270
r	 0.6580	 0.6640
s	 0.5110	 0.5970
t	 0.4990	 0.5890
u	 0.4850	 0.5980
v	 0.7430	 0.6840
w	 0.7750	 0.6810
x	 0.4780	 0.5780
y	 0.7070	 0.6790
z	 0.7270	 0.6550