



Full wwPDB EM Validation Report ⓘ

Sep 17, 2026 – 03:04 AM EDT

PDB ID : 7RYG / pdb_00007ryg
EMDB ID : EMD-24739
Title : A. baumannii Ribosome-TP-6076 complex: E-site tRNA 70S
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2021-08-25
Resolution : 2.38 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

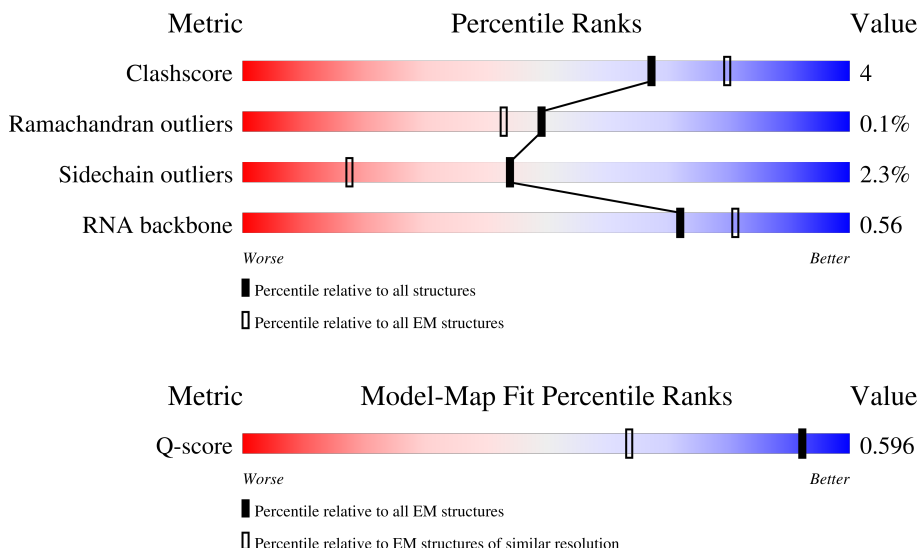
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.38 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.



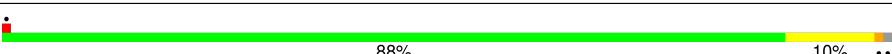
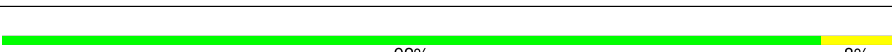
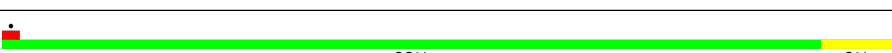
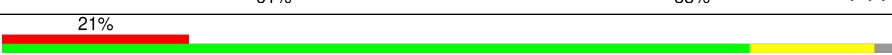
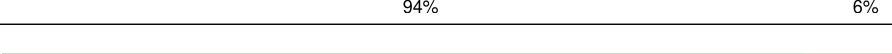
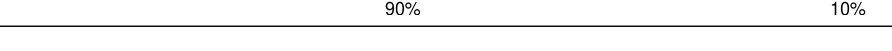
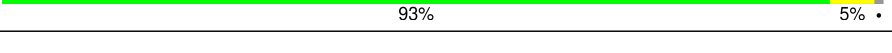
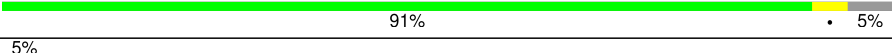
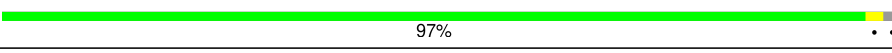
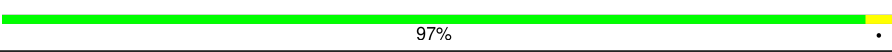
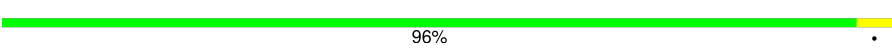
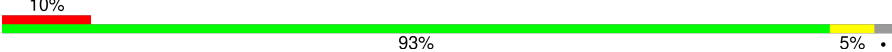
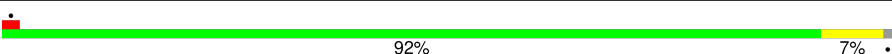
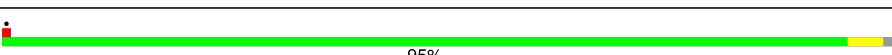
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4811 (1.88 - 2.88)

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	0	51	
2	1	44	
3	2	64	

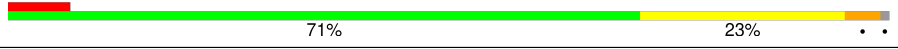
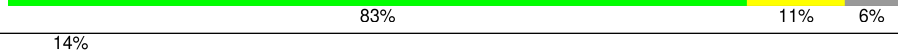
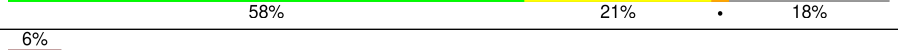
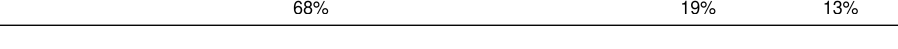
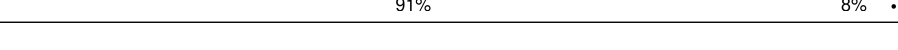
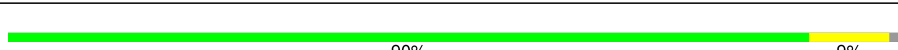
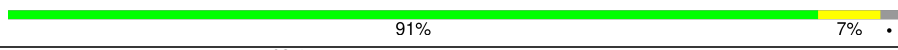
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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26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

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Mol	Chain	Length	Quality of chain
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	
52	v	77	
53	w	3	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 137579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

- Molecule 55 is (4S,4aS,5aR,12aS)-4-(diethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-8-[(2S)-pyrrolidin-2-yl]-7-(trifluoromethyl)-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide (CCD ID: 80P) (formula: C₂₈H₃₂F₃N₃O₇) (labeled as "Ligand of Interest" by depositor).



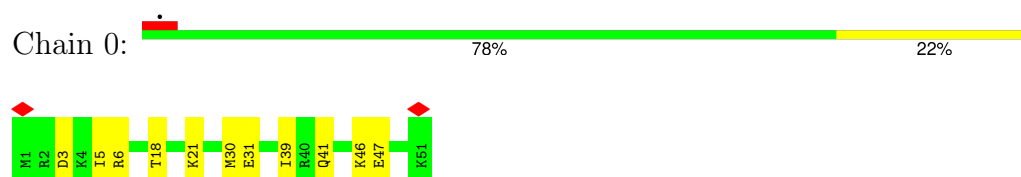
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).



3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L33

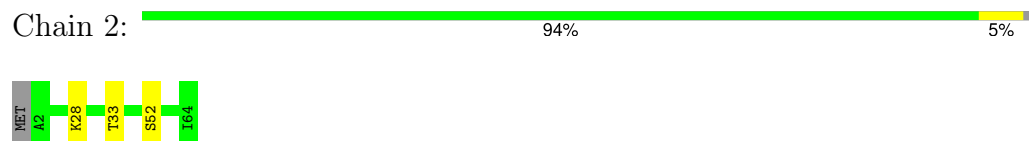


- Molecule 2: 50S ribosomal protein L34

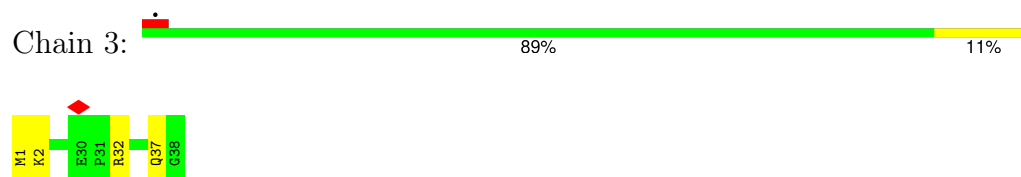


There are no outlier residues recorded for this chain.

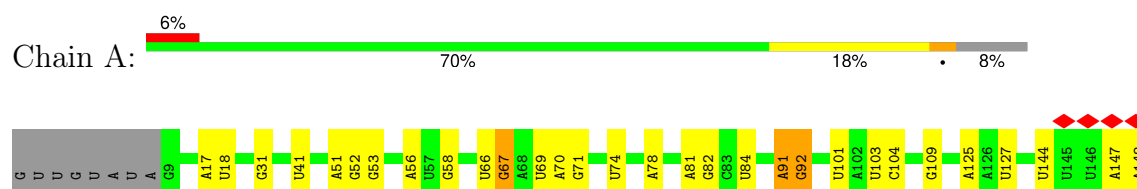
- Molecule 3: 50S ribosomal protein L35



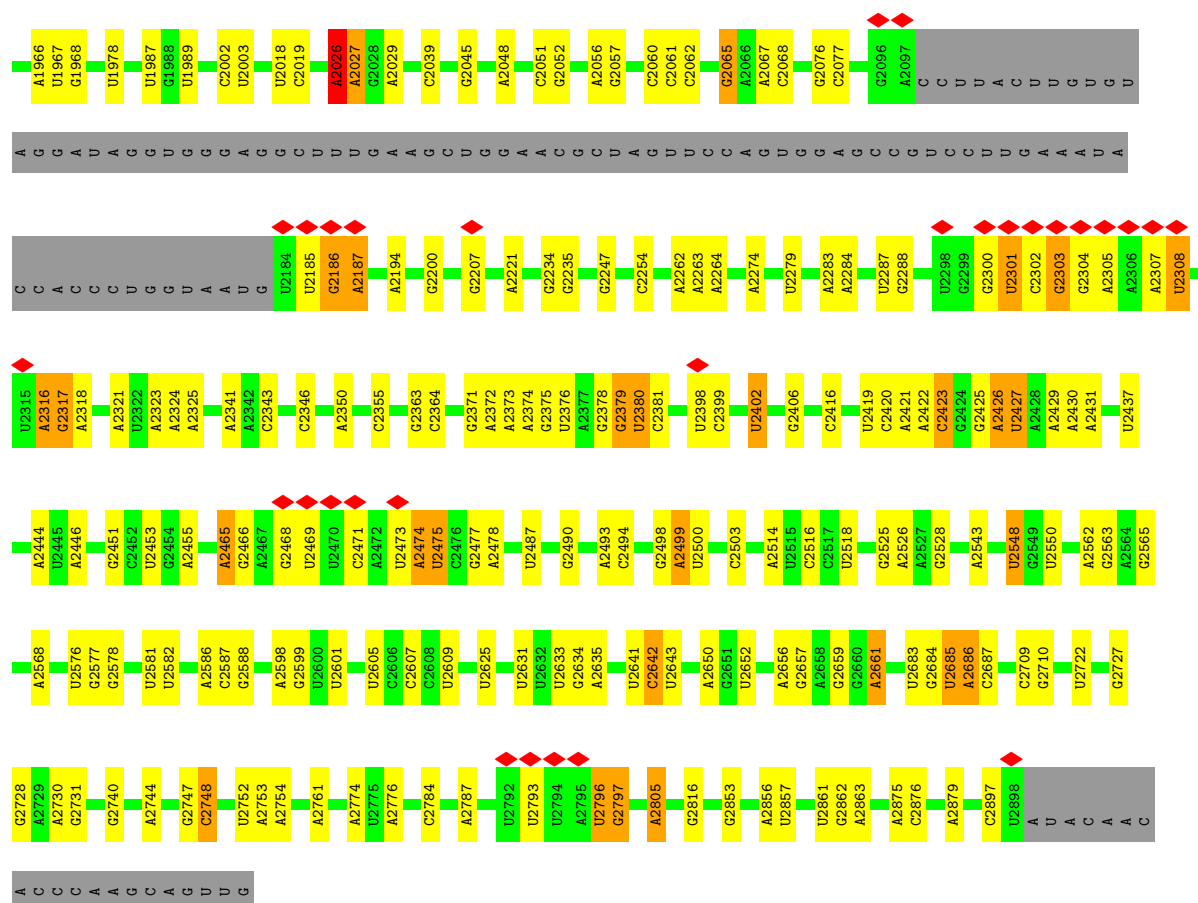
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 23S ribosomal RNA



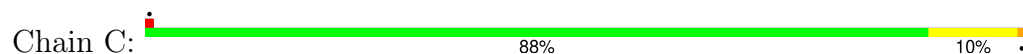




• Molecule 6: 5S ribosomal RNA



• Molecule 7: 50S ribosomal protein L2



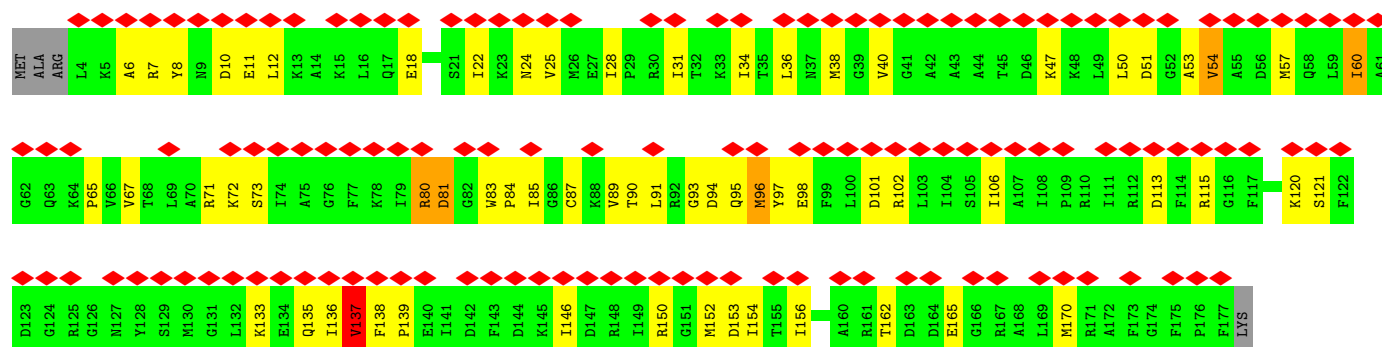
• Molecule 8: 50S ribosomal protein L3



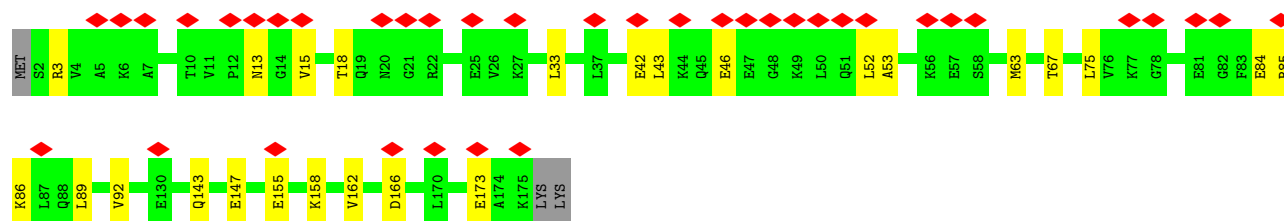
• Molecule 9: 50S ribosomal protein L4

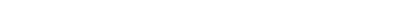
	M1	N2	L3	L13	S14	E15	G19	H45	S74	R87	E122	F123	D170	A171	D175	S178	E196	L199	G200
--	----	----	----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

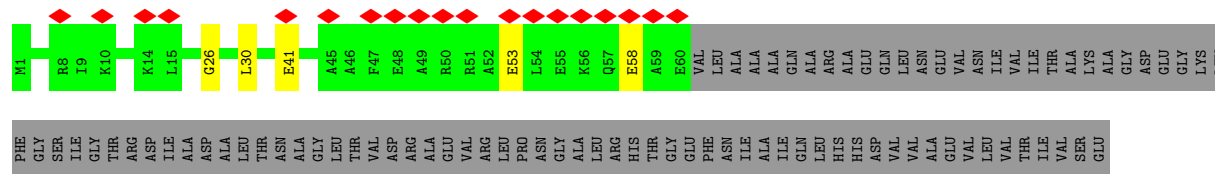
- Chain F: 76% 61% 33%

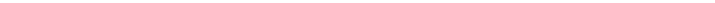


- Chain G: 



- Chain H:  13% 37% 59%



- Chain I:  94% 6%



- 

Chain J:  90% 10%



- Molecule 15: 50S ribosomal protein L15

Chain K:  93% 5%

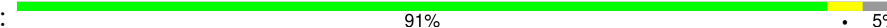


- Molecule 16: 50S ribosomal protein L16

Chain L:  87% 12%



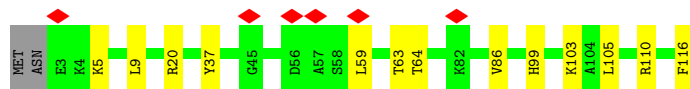
- Molecule 17: 50S ribosomal protein L17

Chain M:  91% 5%



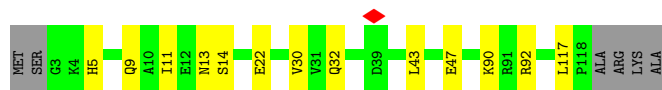
- Molecule 18: 50S ribosomal protein L18

Chain N:  5% 87% 11%

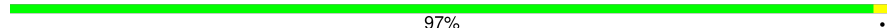


- Molecule 19: 50S ribosomal protein L19

Chain O:  5% 84% 11% 5%

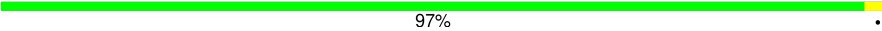


- Molecule 20: 50S ribosomal protein L20

Chain P:  97% 2% 1%

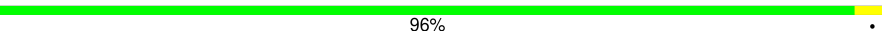


- Molecule 21: 50S ribosomal protein L21

Chain Q:  97%



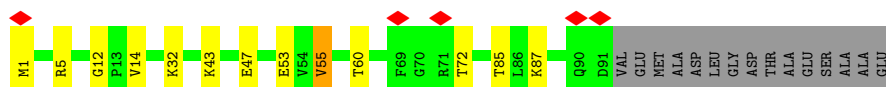
- Molecule 22: 50S ribosomal protein L22

Chain R:  96%



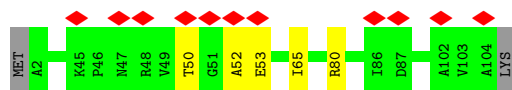
- Molecule 23: 50S ribosomal protein L23

Chain S:  5% 74% 11% 14%

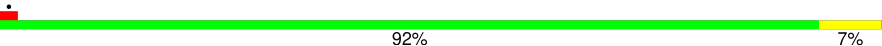


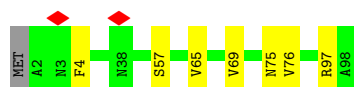
- Molecule 24: 50S ribosomal protein L24

Chain T:  10% 93% 5%



- Molecule 25: 50S ribosomal protein L25

Chain U:  92% 7%

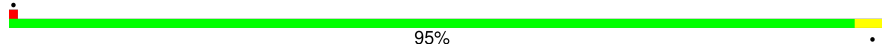


- Molecule 26: 50S ribosomal protein L27

Chain V:  85% 6% 9%

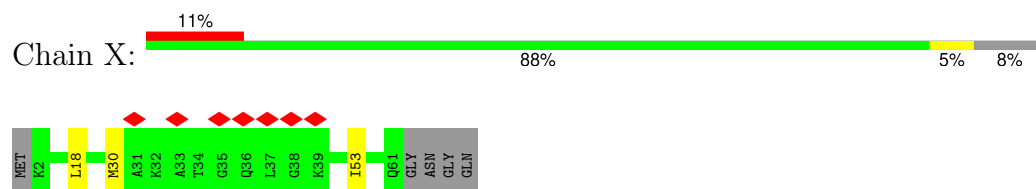


- Molecule 27: 50S ribosomal protein L28

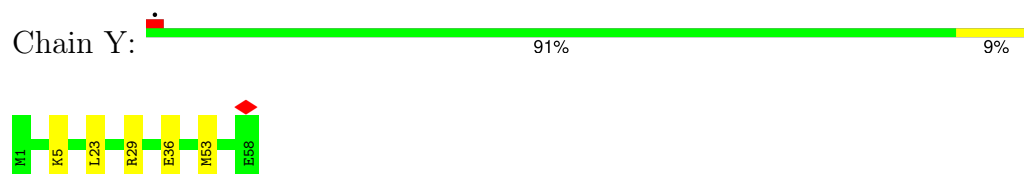
Chain W:  95%



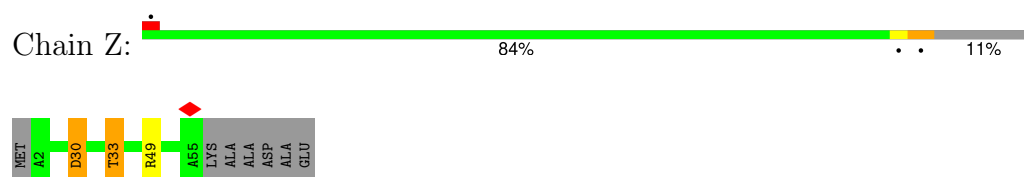
- Molecule 28: 50S ribosomal protein L29



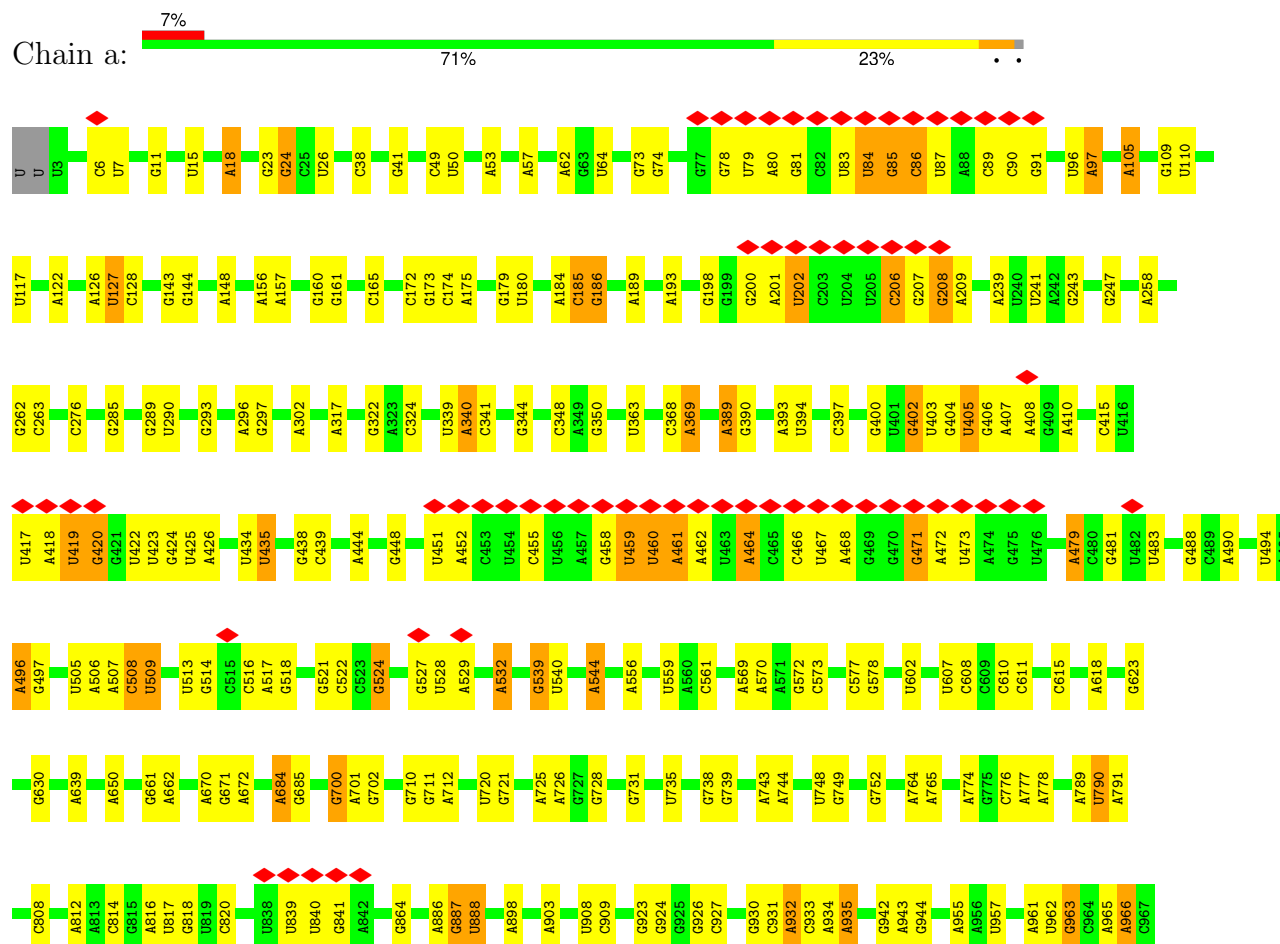
- Molecule 29: 50S ribosomal protein L30

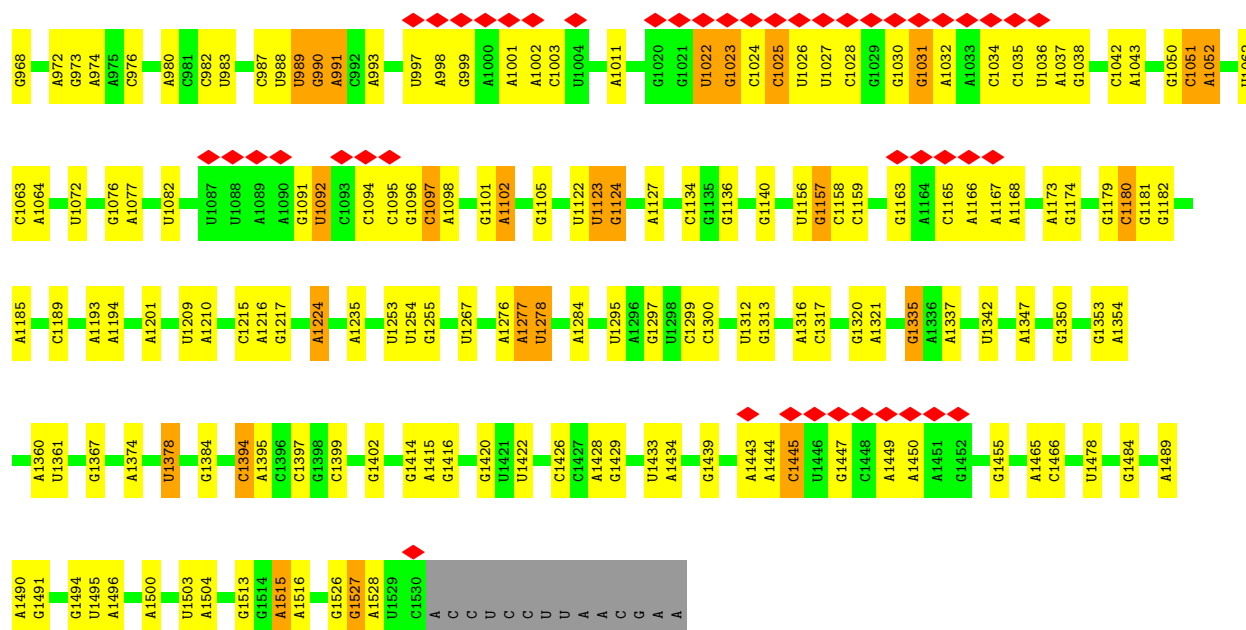


- Molecule 30: 50S ribosomal protein L32

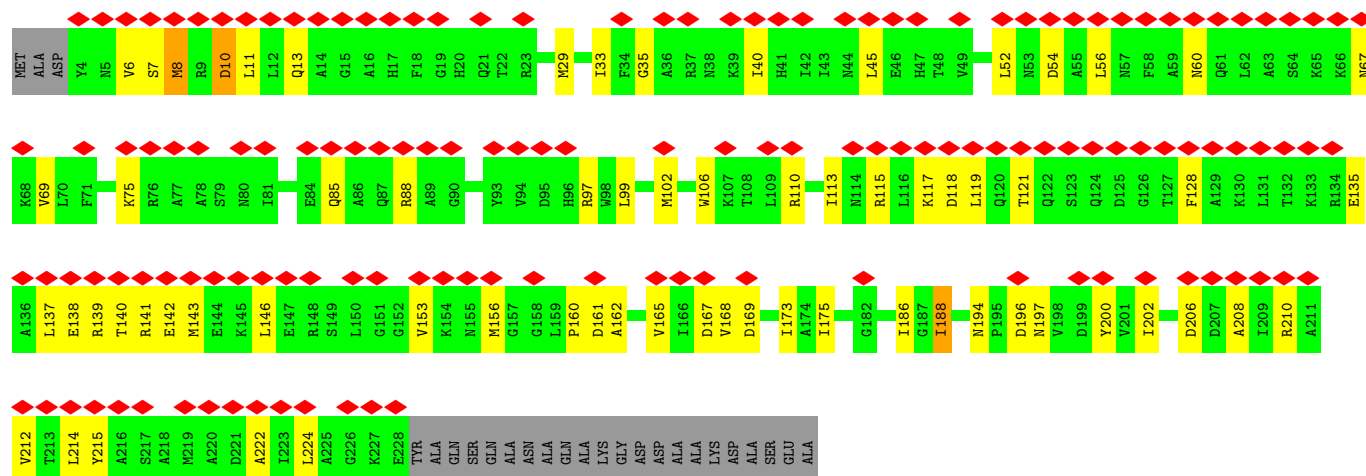


- Molecule 31: 16S Ribosomal RNA

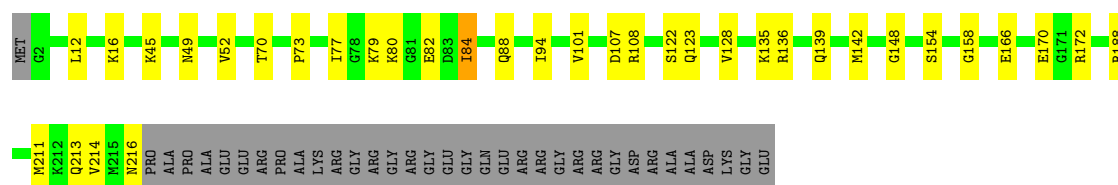




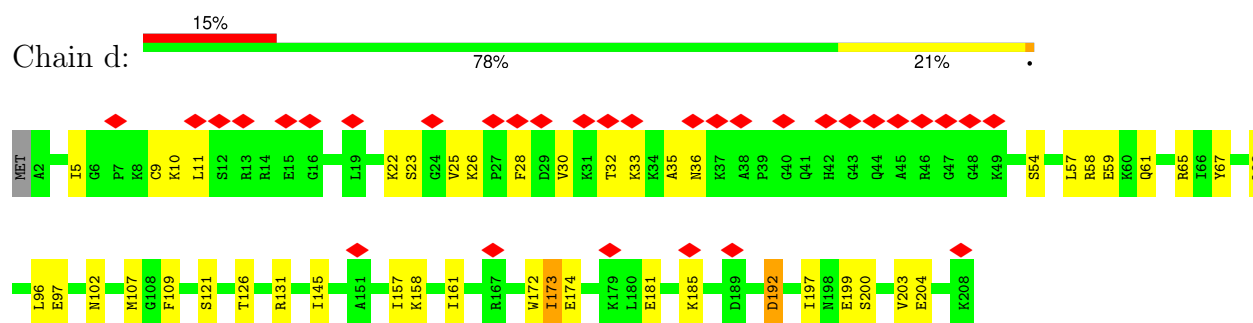
• Molecule 32: 30S ribosomal protein S2



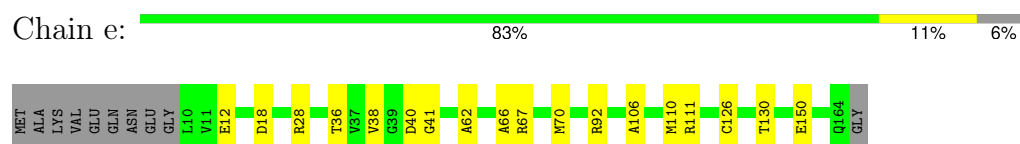
• Molecule 33: 30S ribosomal protein S3



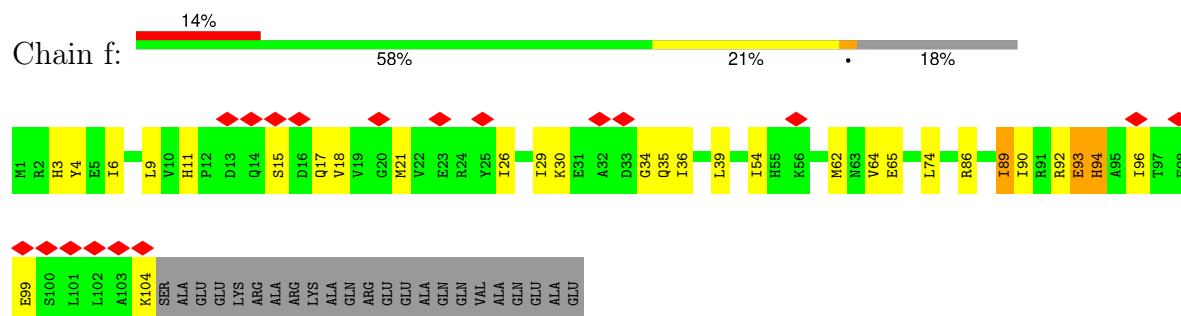
• Molecule 34: 30S ribosomal protein S4



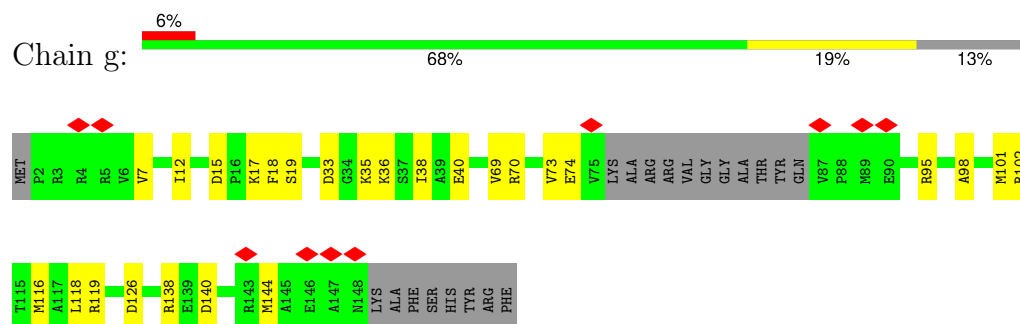
- Molecule 35: 30S ribosomal protein S5



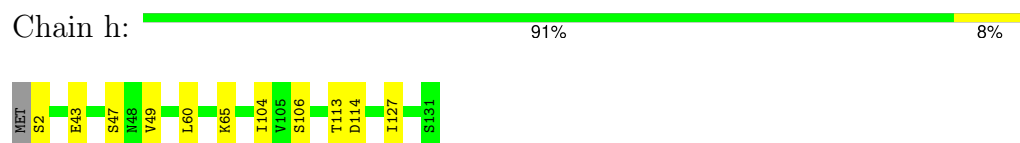
- Molecule 36: 30S ribosomal protein S6



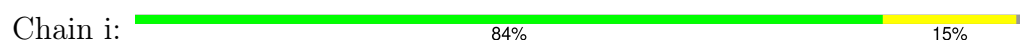
- Molecule 37: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S9





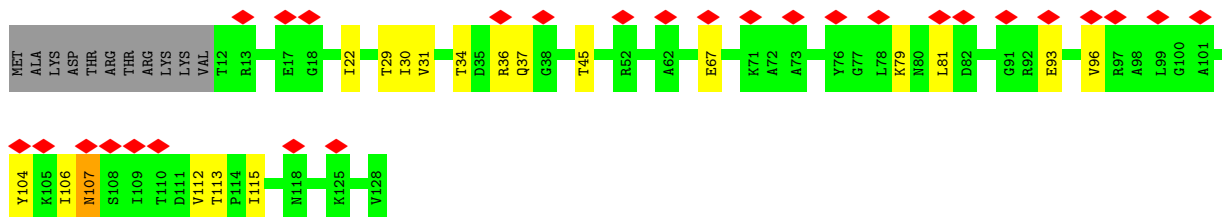
- Molecule 40: 30S ribosomal protein S10

Chain j: 85% 11% ..



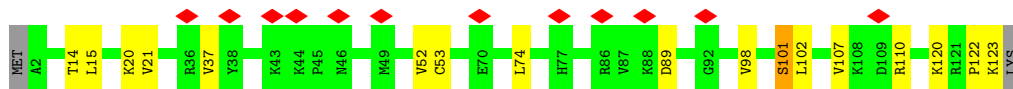
- Molecule 41: 30S ribosomal protein S11

Chain k: 22% 77% 14% 9% .



- Molecule 42: 30S ribosomal protein S12

Chain l: 10% 85% 13% ..



- Molecule 43: 30S ribosomal protein S13

Chain m: 85% 13% .



- Molecule 44: 30S ribosomal protein S14

Chain n: 90% 9% .



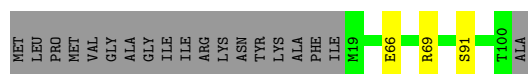
- Molecule 45: 30S ribosomal protein S15

Chain o: 91% 8% .



- Molecule 46: 30S ribosomal protein S16

Chain p:  78% 19%



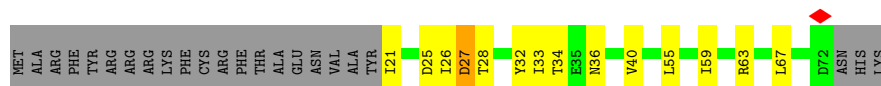
- Molecule 47: 30S ribosomal protein S17

Chain q:  75% 16% 7%



- Molecule 48: 30S ribosomal protein S18

Chain r:  51% 17% 31%



- Molecule 49: 30S ribosomal protein S19

Chain s:  82% 7% 10%



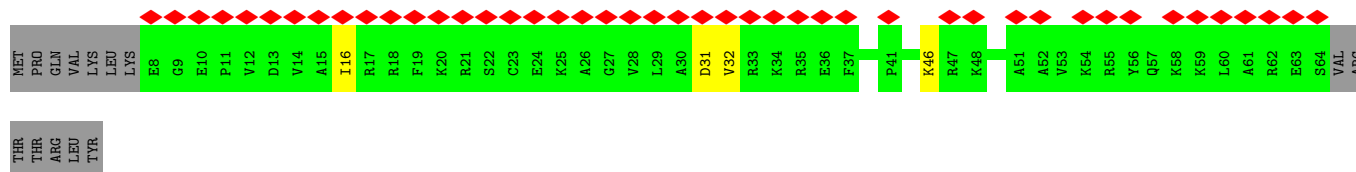
- Molecule 50: 30S ribosomal protein S20

Chain t:  91% 7%



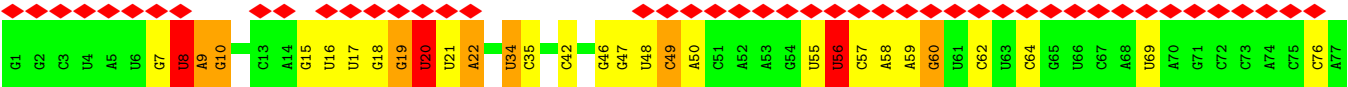
- Molecule 51: 30S ribosomal protein S21

Chain u:  63% 75% 6% 20%



- Molecule 52: tRNA-met

Chain v:  60% 61% 26% 9%



● Molecule 53: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.067	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.568, 557.568, 557.568	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.089, 1.089, 1.089	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 7MG, 4OC, OMU, PSU, MG, OMG, 5MC, MA6, 6MZ, 2MG, 5MU, 4SU, H2U, 2MA, UR3, 80P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.21	0/434	0.43	0/573
2	1	0.14	0/367	0.28	0/481
3	2	0.14	0/515	0.33	0/678
4	3	0.16	0/296	0.37	0/389
5	A	0.10	1/64227 (0.0%)	0.27	0/100172
6	B	0.09	0/2739	0.25	0/4266
7	C	0.13	0/2152	0.33	0/2891
8	D	0.12	0/1590	0.28	0/2142
9	E	0.12	0/1537	0.27	0/2073
10	F	0.20	0/1390	0.51	0/1863
11	G	0.13	0/1337	0.35	0/1807
12	H	0.16	0/461	0.38	0/616
13	I	0.13	0/1151	0.31	0/1551
14	J	0.14	0/956	0.35	0/1286
15	K	0.13	0/1079	0.30	0/1439
16	L	0.14	0/1104	0.34	0/1475
17	M	0.15	0/956	0.33	0/1282
18	N	0.11	0/865	0.30	0/1156
19	O	0.12	0/925	0.29	0/1241
20	P	0.14	0/947	0.31	0/1262
21	Q	0.14	0/818	0.32	0/1094
22	R	0.14	0/831	0.30	0/1113
23	S	0.13	0/716	0.28	0/957
24	T	0.09	0/770	0.26	0/1034
25	U	0.12	0/770	0.30	0/1036
26	V	0.11	0/589	0.31	0/788
27	W	0.12	0/642	0.27	0/856
28	X	0.10	0/487	0.23	0/646
29	Y	0.14	0/468	0.26	0/624
30	Z	0.12	0/453	0.30	0/604
31	a	0.14	0/36476	0.29	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.16	0/1799	0.41	0/2429
33	c	0.18	0/1714	0.41	0/2304
34	d	0.15	0/1653	0.40	0/2213
35	e	0.13	0/1141	0.33	0/1537
36	f	0.16	0/882	0.40	0/1189
37	g	0.14	0/1087	0.38	0/1456
38	h	0.14	0/993	0.33	0/1331
39	i	0.16	0/1002	0.37	0/1339
40	j	0.17	0/811	0.37	0/1096
41	k	0.12	0/878	0.29	0/1189
42	l	0.13	0/958	0.36	0/1284
43	m	0.16	0/913	0.41	0/1226
44	n	0.17	0/803	0.41	0/1071
45	o	0.14	0/715	0.32	0/958
46	p	0.13	0/655	0.35	0/879
47	q	0.14	0/628	0.35	0/847
48	r	0.13	0/432	0.37	0/583
49	s	0.15	0/664	0.34	0/897
50	t	0.18	0/669	0.33	0/892
51	u	0.10	0/478	0.21	0/631
52	v	0.16	1/1739 (0.1%)	0.29	0/2709
53	w	0.09	0/72	0.31	0/110
All	All	0.13	2/148734 (0.0%)	0.30	0/222460

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	O3'-P	5.27	1.61	1.56
5	A	2548	OMU	O3'-P	5.14	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	427	0	462	8	0
2	1	363	0	401	0	0
3	2	509	0	566	2	0
4	3	295	0	326	2	0
5	A	57610	0	28970	217	0
6	B	2450	0	1241	19	0
7	C	2111	0	2176	19	0
8	D	1572	0	1610	7	0
9	E	1516	0	1569	7	0
10	F	1370	0	1420	64	0
11	G	1318	0	1373	19	0
12	H	458	0	480	1	0
13	I	1125	0	1148	4	0
14	J	946	0	1007	12	0
15	K	1071	0	1141	6	0
16	L	1087	0	1162	10	0
17	M	942	0	987	4	0
18	N	857	0	899	10	0
19	O	913	0	968	9	0
20	P	934	0	997	2	0
21	Q	807	0	842	4	0
22	R	826	0	894	2	0
23	S	710	0	768	8	0
24	T	766	0	816	3	0
25	U	760	0	783	3	0
26	V	581	0	583	1	0
27	W	632	0	667	3	0
28	X	486	0	528	3	0
29	Y	463	0	488	5	0
30	Z	447	0	435	2	0
31	a	32782	0	16508	166	0
32	b	1769	0	1787	60	0
33	c	1690	0	1774	24	0
34	d	1631	0	1691	38	0
35	e	1129	0	1174	9	0
36	f	867	0	868	20	0
37	g	1073	0	1118	25	0
38	h	985	0	1047	8	0
39	i	991	0	1048	10	0
40	j	801	0	832	7	0
41	k	862	0	877	11	0
42	l	945	0	998	10	0
43	m	903	0	962	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	792	0	833	8	0
45	o	705	0	712	5	0
46	p	644	0	655	1	0
47	q	621	0	665	8	0
48	r	426	0	447	13	0
49	s	646	0	663	3	0
50	t	663	0	715	4	0
51	u	473	0	503	5	0
52	v	1636	0	835	13	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	a	123	0	0	2	0
56	a	4	0	0	0	0
All	All	137579	0	92452	851	0

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

All (851) 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)
32:b:13:GLN:O	32:b:210:ARG:NH2	1.94	1.00
5:A:799:G:O2'	5:A:800:A:OP1	1.80	0.99
31:a:406:G:OP2	34:d:26:LYS:NZ	2.01	0.93
16:L:107:GLU:OE1	16:L:108:GLY:N	2.02	0.92
5:A:1923:A:O2'	5:A:1924:A:O5'	1.89	0.90
39:i:53:LEU:HD21	39:i:92:LEU:HD13	1.52	0.90
39:i:128:ARG:NH2	52:v:34:U:OP2	2.05	0.88
31:a:423:U:OP2	31:a:424:G:O2'	1.92	0.86
5:A:1880:G:O2'	5:A:1881:A:OP1	1.93	0.86
5:A:533:U:O2'	20:P:49:ASP:OD2	1.92	0.85
10:F:94:ASP:OD1	10:F:95:GLN:N	2.11	0.84
5:A:1335:U:O2'	5:A:1336:G:OP1	1.94	0.84
37:g:111:ARG:NH1	37:g:126:ASP:OD2	2.11	0.83
31:a:572:G:O2'	31:a:818:G:OP2	1.94	0.83
5:A:1172:U:O2'	5:A:1173:G:OP1	1.96	0.82
52:v:15:G:OP2	52:v:15:G:N2	2.12	0.81
5:A:1519:U:O2'	5:A:1520:A:OP2	1.97	0.80
37:g:40:GLU:OE2	39:i:41:THR:HG21	1.82	0.80
5:A:1749:G:N2	5:A:1752:G:OP2	2.14	0.80
32:b:56:LEU:HD12	32:b:222:ALA:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:997:U:O4	31:a:998:A:N6	2.14	0.79
31:a:189:A:O2'	50:t:59:ASP:OD1	1.99	0.79
5:A:2301:U:O5'	10:F:133:LYS:NZ	2.14	0.79
6:B:11:A:N1	6:B:67:G:O2'	2.15	0.79
32:b:106:TRP:O	32:b:110:ARG:NH1	2.16	0.79
31:a:1429:G:O2'	31:a:1465:A:N6	2.15	0.78
31:a:1124:G:OP1	31:a:1277:A:O2'	1.99	0.78
43:m:3:ARG:NH2	43:m:8:ASN:OD1	2.16	0.78
10:F:22:ILE:HD12	10:F:22:ILE:O	1.83	0.78
5:A:2853:G:N2	5:A:2856:A:OP2	2.17	0.77
37:g:70:ARG:O	37:g:138:ARG:NH1	2.17	0.77
5:A:67:G:O2'	5:A:69:U:OP2	2.03	0.77
5:A:2373:A:O2'	18:N:116:PHE:OXT	2.02	0.77
14:J:103:THR:OG1	14:J:105:GLU:OE1	2.01	0.76
31:a:1402:G:HO2'	31:a:1515:MA6:HO2'	1.26	0.76
34:d:174:GLU:OE2	34:d:185:LYS:NZ	2.16	0.76
6:B:11:A:O2'	6:B:13:A:OP2	2.01	0.76
5:A:2861:U:OP2	5:A:2862:G:O2'	2.03	0.76
33:c:107:ASP:OD2	33:c:108:ARG:NE	2.16	0.76
32:b:115:ARG:NH1	32:b:142:GLU:OE2	2.18	0.76
5:A:184:G:N2	5:A:184:G:OP2	2.18	0.75
31:a:206:C:OP2	31:a:208:G:O2'	2.04	0.75
5:A:1938:C:OP2	5:A:1939:U:O2'	2.04	0.74
10:F:101:ASP:OD2	10:F:102:ARG:N	2.20	0.74
31:a:529:A:N6	33:c:158:GLY:O	2.21	0.74
10:F:136:ILE:O	10:F:137:VAL:HG22	1.87	0.74
32:b:196:ASP:OD1	32:b:197:ASN:N	2.20	0.73
46:p:66:GLU:OE1	46:p:69:ARG:NH1	2.22	0.73
36:f:3:HIS:NE2	36:f:65:GLU:OE1	2.20	0.73
9:E:175:ASP:OD2	9:E:178:SER:OG	2.04	0.73
14:J:47:ILE:HD12	14:J:48:PRO:HD2	1.70	0.72
31:a:1163:G:O2'	31:a:1167:A:N6	2.22	0.72
40:j:57:VAL:O	40:j:58:ASN:ND2	2.22	0.72
9:E:170:ASP:OD1	9:E:171:ALA:N	2.23	0.72
5:A:2301:U:N3	5:A:2303:G:O6	2.23	0.71
5:A:1733:U:O2'	5:A:1734:G:OP1	2.08	0.71
32:b:208:ALA:O	32:b:212:VAL:HG23	1.89	0.71
37:g:101:MET:O	37:g:105:VAL:HG23	1.90	0.71
5:A:2254:C:O2'	5:A:2423:C:OP2	2.08	0.71
32:b:188:ILE:HD13	32:b:202:ILE:HD11	1.73	0.71
5:A:1605:G:OP2	5:A:1605:G:N2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:86:LYS:NZ	11:G:166:ASP:OD1	2.24	0.70
34:d:28:PHE:O	34:d:32:THR:HG22	1.91	0.70
32:b:75:LYS:NZ	32:b:206:ASP:OD2	2.23	0.70
37:g:98:ALA:HB1	37:g:102:ARG:NH1	2.05	0.70
23:S:12:GLY:HA2	28:X:30:MET:HE1	1.73	0.70
31:a:1201:A:O2'	33:c:188:ARG:NH2	2.24	0.70
47:q:40:ARG:O	47:q:41:ARG:NH1	2.24	0.70
23:S:53:GLU:OE1	23:S:87:LYS:NZ	2.23	0.70
31:a:1444:A:OP1	31:a:1445:C:N4	2.25	0.70
10:F:50:LEU:O	10:F:54:VAL:HG12	1.91	0.69
31:a:927:C:O2	31:a:1384:G:N2	2.15	0.69
31:a:1347:A:O2'	37:g:33:ASP:OD1	2.10	0.69
31:a:1097:C:OP2	32:b:97:ARG:NH2	2.25	0.69
5:A:2186:G:O2'	5:A:2187:A:OP2	2.10	0.69
6:B:50:A:O2'	6:B:51:A:O5'	2.10	0.69
16:L:79:LEU:HD12	16:L:80:GLU:H	1.57	0.69
31:a:935:A:O2'	37:g:95:ARG:NH2	2.26	0.69
49:s:12:ASP:OD2	49:s:35:SER:OG	2.11	0.69
34:d:172:TRP:CD1	34:d:173:ILE:HD12	2.28	0.68
10:F:115:ARG:O	10:F:115:ARG:NH1	2.26	0.68
19:O:47:GLU:OE2	19:O:90:LYS:NZ	2.22	0.68
1:O:46:LYS:HA	1:O:46:LYS:HE3	1.75	0.68
6:B:63:U:O2'	6:B:64:A:O4'	2.12	0.68
32:b:135:GLU:N	32:b:135:GLU:OE1	2.27	0.68
5:A:1310:C:O2'	5:A:1387:A:N3	2.22	0.68
5:A:1933:A:H1'	5:A:1935:5MU:H72	1.75	0.67
3:2:33:THR:OG1	5:A:2416:C:OP1	2.09	0.67
31:a:684:A:N6	31:a:700:G:O2'	2.27	0.67
10:F:47:LYS:HA	10:F:47:LYS:HE2	1.77	0.67
37:g:69:VAL:HG12	37:g:69:VAL:O	1.95	0.67
34:d:97:GLU:O	34:d:102:ASN:ND2	2.27	0.67
5:A:2577:G:N2	5:A:2577:G:OP2	2.27	0.66
10:F:72:LYS:N	10:F:81:ASP:OD1	2.28	0.66
41:k:81:LEU:HD22	41:k:104:TYR:HB3	1.78	0.66
13:I:61:GLN:O	13:I:63:GLN:NE2	2.29	0.66
5:A:1962:A:N3	5:A:2588:G:O2'	2.26	0.65
10:F:36:LEU:CD2	10:F:89:VAL:HG23	2.27	0.65
10:F:38:MET:HE1	10:F:150:ARG:CD	2.26	0.65
32:b:69:VAL:HG22	32:b:162:ALA:HB3	1.78	0.65
5:A:545:C:O2'	5:A:546:G:N2	2.29	0.65
28:X:30:MET:HE2	28:X:30:MET:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2379:G:O2'	5:A:2380:U:OP1	2.13	0.64
31:a:290:U:OP1	31:a:607:U:O2'	2.13	0.64
29:Y:23:LEU:HD11	29:Y:53:MET:HE2	1.79	0.64
31:a:1374:A:C6	37:g:7:VAL:HG21	2.32	0.64
5:A:2469:U:O4	5:A:2474:A:N6	2.31	0.64
17:M:49:GLU:HG3	17:M:95:LEU:HD13	1.80	0.64
29:Y:23:LEU:HD11	29:Y:53:MET:CE	2.28	0.64
5:A:1924:A:O2'	5:A:1925:G:O5'	2.10	0.64
5:A:1306:G:OP2	5:A:1306:G:N2	2.24	0.63
33:c:211:MET:HE3	33:c:216:ASN:C	2.24	0.63
5:A:1937:C:N4	5:A:1961:C:O4'	2.31	0.62
5:A:499:G:N1	5:A:502:A:OP2	2.32	0.62
39:i:53:LEU:HD22	39:i:85:LEU:HD13	1.81	0.62
34:d:107:MET:HE1	34:d:109:PHE:CD2	2.34	0.62
40:j:88:MET:HE3	40:j:88:MET:HA	1.81	0.62
31:a:198:G:O2'	31:a:464:A:N3	2.33	0.62
5:A:1462:G:H1	5:A:1521:G:HO2'	1.46	0.62
31:a:423:U:O3'	34:d:10:LYS:NZ	2.33	0.62
38:h:43:GLU:OE1	38:h:113:THR:HG21	2.00	0.62
32:b:137:LEU:HD12	32:b:138:GLU:N	2.15	0.61
37:g:98:ALA:HB1	37:g:102:ARG:HH11	1.65	0.61
31:a:1092:U:OP2	31:a:1105:G:N1	2.32	0.61
45:o:40:GLN:O	45:o:44:LYS:NZ	2.26	0.61
5:A:2308:U:C4'	10:F:85:ILE:HD11	2.31	0.61
5:A:148:A:N6	5:A:1594:G:O4'	2.34	0.61
31:a:820:C:HO2'	38:h:2:SER:N	1.99	0.61
5:A:843:G:O2'	5:A:845:A:N6	2.33	0.61
31:a:1447:G:N2	31:a:1450:A:OP2	2.33	0.60
36:f:90:ILE:HG22	36:f:92:ARG:HD3	1.81	0.60
31:a:38:C:OP1	42:l:120:LYS:NZ	2.26	0.60
14:J:47:ILE:HD12	14:J:48:PRO:CD	2.30	0.60
31:a:148:A:N6	31:a:165:C:O2	2.35	0.60
31:a:808:C:O2'	31:a:898:A:N1	2.33	0.60
31:a:1011:A:OP2	49:s:18:LYS:NZ	2.34	0.60
48:r:27:ASP:OD1	48:r:27:ASP:N	2.26	0.60
36:f:93:GLU:O	36:f:94:HIS:CG	2.55	0.60
25:U:76:VAL:HG12	25:U:97:ARG:HA	1.83	0.60
32:b:67:ASN:ND2	32:b:161:ASP:OD2	2.34	0.60
31:a:1394:C:OP2	35:e:28:ARG:NH2	2.35	0.59
40:j:28:THR:O	40:j:32:THR:HG22	2.02	0.59
32:b:173:ILE:HD12	32:b:173:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:150:GLU:OE1	35:e:150:GLU:N	2.33	0.59
55:a:1603:80P:F24	55:a:1603:80P:N27	2.24	0.59
31:a:976:C:O2	44:n:59:ARG:NH1	2.35	0.59
31:a:156:A:N1	31:a:340:A:O2'	2.31	0.59
33:c:142:MET:HE1	33:c:148:GLY:HA2	1.84	0.59
29:Y:5:LYS:NZ	29:Y:36:GLU:OE1	2.36	0.59
33:c:82:GLU:OE1	33:c:82:GLU:N	2.35	0.58
31:a:96:U:O2'	31:a:97:A:N7	2.34	0.58
23:S:1:MET:HE3	23:S:5:ARG:HG2	1.85	0.58
52:v:8:4SU:O2'	52:v:9:A:OP1	2.15	0.58
10:F:38:MET:HE1	10:F:150:ARG:HD3	1.86	0.58
33:c:135:LYS:O	33:c:139:GLN:HG3	2.02	0.58
31:a:1051:C:O2'	31:a:1052:A:OP2	2.20	0.58
10:F:57:MET:HA	10:F:60:ILE:HG22	1.85	0.58
8:D:6:VAL:HG11	8:D:79:LEU:HD11	1.85	0.57
52:v:22:A:N6	52:v:49:C:O4'	2.36	0.57
5:A:1411:G:O2'	5:A:1585:G:N2	2.37	0.57
7:C:123:PRO:O	7:C:128:ASN:ND2	2.35	0.57
10:F:106:ILE:HD11	10:F:139:PRO:HD3	1.86	0.57
31:a:962:U:O2'	31:a:963:2MG:OP2	2.13	0.57
5:A:2300:G:N2	10:F:153:ASP:OD2	2.35	0.57
11:G:155:GLU:OE2	11:G:158:LYS:N	2.31	0.57
31:a:508:C:O2'	31:a:509:U:OP2	2.21	0.57
5:A:2518:U:O2'	5:A:2643:U:OP1	2.21	0.57
32:b:117:LYS:O	32:b:121:THR:HG23	2.05	0.57
5:A:1866:U:O2'	5:A:1867:A:O4'	2.23	0.57
37:g:144:MET:N	37:g:144:MET:HE2	2.20	0.57
5:A:1359:G:OP1	27:W:3:LYS:NZ	2.37	0.56
5:A:1853:G:N2	5:A:1880:G:N3	2.53	0.56
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.19	0.56
31:a:524:7MG:O2'	31:a:532:A:N1	2.31	0.56
38:h:49:VAL:HG13	38:h:60:LEU:HD11	1.86	0.56
6:B:5:G:OP1	18:N:5:LYS:NZ	2.32	0.56
23:S:1:MET:HE3	23:S:5:ARG:CG	2.36	0.56
10:F:57:MET:HE1	10:F:87:CYS:HB3	1.87	0.56
40:j:57:VAL:O	40:j:57:VAL:HG23	2.06	0.56
39:i:32:THR:HG23	39:i:35:GLN:OE1	2.06	0.56
32:b:7:SER:O	32:b:8:MET:HB3	2.05	0.56
36:f:99:GLU:OE1	36:f:104:LYS:NZ	2.25	0.56
15:K:80:ARG:N	15:K:83:GLU:OE2	2.36	0.56
48:r:32:TYR:O	48:r:40:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2631:U:O2'	8:D:82:GLU:OE2	2.18	0.56
31:a:1527:G:N7	51:u:46:LYS:NZ	2.54	0.55
35:e:110:MET:HE2	35:e:126:CYS:SG	2.46	0.55
37:g:113:GLU:OE1	37:g:113:GLU:HA	2.05	0.55
47:q:76:LEU:HD23	47:q:77:VAL:N	2.21	0.55
35:e:36:THR:HG22	35:e:62:ALA:HB1	1.87	0.55
19:O:30:VAL:HG22	19:O:47:GLU:HG3	1.88	0.55
32:b:10:ASP:OD1	32:b:10:ASP:N	2.37	0.55
19:O:117:LEU:O	19:O:117:LEU:HD12	2.05	0.55
10:F:6:ALA:O	10:F:10:ASP:OD2	2.25	0.55
31:a:397:C:O2'	31:a:618:A:N3	2.38	0.55
5:A:1960:G:O2'	5:A:1963:C:OP2	2.23	0.55
5:A:2371:G:N2	5:A:2374:A:OP2	2.38	0.55
36:f:9:LEU:HD12	36:f:9:LEU:N	2.22	0.55
47:q:29:ARG:NE	47:q:38:SER:OG	2.39	0.55
31:a:1094:C:O3'	32:b:141:ARG:NH2	2.37	0.55
42:l:21:VAL:HG23	42:l:21:VAL:O	2.06	0.55
5:A:1717:G:O2'	5:A:1735:A:N6	2.40	0.54
10:F:85:ILE:HD12	10:F:85:ILE:C	2.32	0.54
31:a:1374:A:C5	37:g:7:VAL:HG21	2.42	0.54
41:k:107:ASN:OD1	41:k:107:ASN:N	2.40	0.54
5:A:308:U:H2'	5:A:309:G:O4'	2.06	0.54
36:f:93:GLU:O	36:f:94:HIS:CD2	2.60	0.54
32:b:156:MET:HE2	32:b:160:PRO:HD3	1.89	0.54
31:a:122:A:OP1	31:a:602:U:O2'	2.24	0.54
32:b:110:ARG:HA	32:b:110:ARG:NE	2.22	0.54
36:f:6:ILE:HD13	36:f:89:ILE:HD13	1.88	0.54
36:f:36:ILE:N	36:f:36:ILE:HD12	2.22	0.54
31:a:955:A:N3	31:a:982:C:O2'	2.38	0.54
33:c:49:ASN:O	33:c:49:ASN:ND2	2.39	0.54
42:l:15:LEU:H	42:l:15:LEU:HD23	1.72	0.54
5:A:410:G:OP2	5:A:2402:U:O2'	2.25	0.54
11:G:85:ARG:O	11:G:86:LYS:HD2	2.07	0.54
15:K:138:GLU:HA	15:K:138:GLU:OE1	2.08	0.54
34:d:192:ASP:OD1	34:d:192:ASP:N	2.41	0.54
36:f:15:SER:HA	36:f:18:VAL:HG13	1.89	0.54
45:o:3:LEU:O	45:o:8:ARG:NH2	2.41	0.54
37:g:114:LYS:O	37:g:119:ARG:NH2	2.42	0.54
43:m:50:ASP:OD1	43:m:51:ALA:N	2.40	0.54
5:A:1733:U:HO2'	5:A:1734:G:P	2.31	0.53
9:E:3:LEU:HD12	9:E:13:LEU:HD12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:25:VAL:HG22	10:F:25:VAL:O	2.08	0.53
31:a:1064:A:N1	31:a:1105:G:O2'	2.30	0.53
31:a:1489:A:H2'	31:a:1490:A:O4'	2.07	0.53
18:N:105:LEU:C	18:N:105:LEU:HD23	2.33	0.53
31:a:439:C:N4	31:a:488:G:O6	2.42	0.53
5:A:2048:A:H4'	8:D:151:GLN:O	2.08	0.53
31:a:661:G:H22	31:a:738:G:H1	1.56	0.53
5:A:545:C:HO2'	5:A:546:G:N2	2.06	0.53
19:O:11:ILE:O	19:O:14:SER:OG	2.24	0.53
31:a:1025:C:O2	31:a:1031:G:N2	2.41	0.53
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.91	0.53
31:a:888:U:OP2	31:a:903:A:N6	2.32	0.53
5:A:1036:A:H2	5:A:1113:G:H22	1.57	0.53
5:A:1178:C:O3'	29:Y:29:ARG:NH1	2.42	0.53
32:b:60:ASN:ND2	32:b:222:ALA:O	2.42	0.53
34:d:54:SER:O	34:d:58:ARG:HG2	2.09	0.53
5:A:363:G:OP2	5:A:364:A:O2'	2.23	0.53
7:C:3:ILE:O	7:C:3:ILE:HG22	2.09	0.53
13:I:60:GLU:OE1	13:I:60:GLU:N	2.40	0.53
5:A:1411:G:N2	5:A:1583:C:H42	2.07	0.53
5:A:2747:G:O2'	5:A:2748:C:P	2.67	0.53
31:a:1002:A:N3	31:a:1034:C:O2'	2.40	0.53
31:a:735:U:OP1	36:f:4:TYR:OH	2.25	0.53
31:a:930:G:N2	31:a:932:A:O4'	2.42	0.53
31:a:989:U:H4'	31:a:990:G:O5'	2.08	0.53
52:v:20:H2U:O2'	52:v:60:G:O6	2.17	0.53
1:0:31:GLU:HG2	1:0:46:LYS:HZ2	1.74	0.52
5:A:2784:C:O2'	5:A:2805:A:N3	2.40	0.52
15:K:87:VAL:HG13	15:K:96:THR:CG2	2.39	0.52
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.91	0.52
32:b:52:LEU:O	32:b:56:LEU:HD23	2.09	0.52
5:A:782:G:H5'	5:A:783:G:OP1	2.09	0.52
5:A:1923:A:HO2'	5:A:1924:A:P	2.27	0.52
34:d:67:TYR:CG	34:d:96:LEU:HD23	2.44	0.52
5:A:1810:G:OP2	5:A:1811:A:O2'	2.20	0.52
10:F:170:MET:HE3	10:F:170:MET:HA	1.91	0.52
33:c:166:GLU:HA	33:c:166:GLU:OE1	2.08	0.52
34:d:11:LEU:HD11	34:d:65:ARG:HH21	1.75	0.52
10:F:135:GLN:CD	10:F:146:ILE:HD11	2.34	0.52
31:a:84:U:H4'	31:a:85:G:O5'	2.09	0.52
5:A:633:C:O2'	5:A:637:U:OP1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:799:G:HO2'	5:A:800:A:P	2.20	0.52
7:C:135:MET:HE2	7:C:141:LEU:HD21	1.92	0.52
9:E:45:HIS:O	9:E:87:ARG:NH2	2.42	0.52
14:J:112:MET:HA	14:J:112:MET:HE2	1.90	0.52
18:N:63:THR:O	18:N:64:THR:OG1	2.20	0.52
45:o:7:ASP:O	45:o:11:ILE:HG13	2.09	0.52
31:a:460:U:H1'	31:a:461:A:OP2	2.10	0.52
32:b:88:ARG:CD	32:b:224:LEU:HD11	2.40	0.52
5:A:31:G:O2'	22:R:78:GLU:O	2.27	0.52
34:d:197:ILE:N	34:d:197:ILE:HD12	2.24	0.52
8:D:58:GLU:OE1	8:D:66:LYS:NZ	2.23	0.51
19:O:32:GLN:HB3	19:O:43:LEU:HD22	1.92	0.51
11:G:46:GLU:N	11:G:46:GLU:OE1	2.43	0.51
31:a:887:G:H1'	31:a:888:U:OP2	2.10	0.51
31:a:1335:G:N3	52:v:42:C:O2'	2.44	0.51
48:r:55:LEU:HD23	48:r:59:ILE:HD12	1.93	0.51
5:A:226:A:N3	5:A:241:U:O2'	2.31	0.51
10:F:31:ILE:HD13	10:F:96:MET:HE1	1.93	0.51
31:a:670:A:H2'	31:a:671:G:C8	2.45	0.51
31:a:963:2MG:HM22	52:v:35:C:H5'	1.91	0.51
31:a:400:G:OP1	34:d:121:SER:OG	2.28	0.51
31:a:1050:G:H4'	31:a:1051:C:H3'	1.92	0.51
34:d:59:GLU:OE1	34:d:59:GLU:HA	2.11	0.51
35:e:12:GLU:OE2	35:e:67:ARG:NH2	2.44	0.51
41:k:115:ILE:HD12	51:u:31:ASP:HB2	1.91	0.51
5:A:1794:U:OP2	7:C:271:ARG:NH2	2.43	0.51
10:F:71:ARG:H	10:F:71:ARG:HD3	1.75	0.51
45:o:88:ARG:HB2	45:o:88:ARG:NH1	2.26	0.51
14:J:109:GLU:OE1	14:J:109:GLU:N	2.42	0.51
33:c:45:LYS:HE3	33:c:45:LYS:HA	1.93	0.51
5:A:198:A:H3'	5:A:199:G:H21	1.76	0.50
5:A:2379:G:O2'	5:A:2380:U:P	2.69	0.50
31:a:1024:C:O2'	31:a:1025:C:O5'	2.24	0.50
44:n:39:GLU:N	44:n:39:GLU:OE1	2.42	0.50
31:a:156:A:N6	31:a:339:U:O2'	2.44	0.50
34:d:199:GLU:N	34:d:199:GLU:OE1	2.45	0.50
10:F:57:MET:HA	10:F:60:ILE:CG2	2.41	0.50
31:a:1353:G:H2'	31:a:1354:A:C8	2.46	0.50
9:E:14:SER:N	9:E:196:GLU:OE2	2.45	0.50
5:A:2303:G:N2	5:A:2307:A:O2'	2.44	0.50
19:O:22:GLU:O	19:O:92:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1335:U:O2'	23:S:60:THR:OG1	2.28	0.50
32:b:110:ARG:HA	32:b:110:ARG:CZ	2.41	0.50
33:c:135:LYS:HE2	33:c:135:LYS:HA	1.93	0.50
6:B:61:C:C2	6:B:62:U:C5	3.00	0.50
13:I:98:GLU:CD	13:I:98:GLU:H	2.20	0.50
31:a:18:A:H8	31:a:1077:A:HO2'	1.58	0.50
33:c:211:MET:HE3	33:c:216:ASN:O	2.11	0.50
32:b:135:GLU:O	32:b:139:ARG:HD2	2.11	0.50
8:D:43:THR:HG23	8:D:44:ASP:OD2	2.12	0.50
10:F:38:MET:HE2	10:F:40:VAL:HG13	1.94	0.50
10:F:152:MET:HE3	10:F:154:ILE:HB	1.93	0.50
34:d:32:THR:O	34:d:33:LYS:HD3	2.11	0.50
48:r:55:LEU:CD2	48:r:59:ILE:HD12	2.42	0.50
37:g:15:ASP:OD1	37:g:18:PHE:N	2.38	0.49
5:A:666:A:H2'	5:A:668:A:H62	1.76	0.49
11:G:42:GLU:OE1	11:G:53:ALA:HB3	2.12	0.49
14:J:53:LYS:HD2	14:J:53:LYS:N	2.27	0.49
47:q:71:THR:O	47:q:71:THR:HG22	2.12	0.49
5:A:854:G:H2'	5:A:855:G:C8	2.46	0.49
5:A:1775:U:OP2	5:A:1780:A:N6	2.36	0.49
10:F:91:LEU:HD12	10:F:91:LEU:N	2.26	0.49
31:a:424:G:P	34:d:10:LYS:HZ1	2.35	0.49
32:b:142:GLU:O	32:b:146:LEU:HD22	2.12	0.49
48:r:33:ILE:HD11	48:r:59:ILE:HG12	1.93	0.49
49:s:11:VAL:HG21	49:s:41:LEU:HD11	1.94	0.49
5:A:1373:A:O2'	5:A:1374:U:OP2	2.25	0.49
10:F:67:VAL:HG12	10:F:84:PRO:HB3	1.93	0.49
7:C:69:ARG:O	7:C:189:ARG:NH2	2.46	0.49
31:a:459:U:H4'	31:a:460:U:OP1	2.13	0.49
31:a:999:G:N2	31:a:1036:U:O2	2.46	0.49
31:a:1313:G:N1	31:a:1316:A:OP2	2.43	0.49
48:r:32:TYR:CG	48:r:55:LEU:HD11	2.48	0.49
5:A:2747:G:OP2	11:G:3:ARG:NH1	2.45	0.49
18:N:99:HIS:HA	18:N:103:LYS:HD3	1.94	0.49
31:a:202:U:H2'	31:a:202:U:O2	2.13	0.49
34:d:126:THR:HG22	34:d:131:ARG:HA	1.93	0.49
36:f:29:ILE:HD11	36:f:74:LEU:HD21	1.94	0.49
5:A:1172:U:HO2'	5:A:1173:G:P	2.28	0.49
5:A:1924:A:HO2'	5:A:1925:G:P	2.34	0.49
32:b:56:LEU:HD12	32:b:222:ALA:CB	2.38	0.49
32:b:214:LEU:C	32:b:214:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:60:U:C2	6:B:61:C:C5	3.00	0.49
21:Q:37:ASP:OD2	21:Q:37:ASP:N	2.46	0.49
32:b:29:MET:O	32:b:33:ILE:HG13	2.13	0.49
5:A:1506:U:C2	5:A:1507:G:C8	3.01	0.49
31:a:1123:U:O2'	31:a:1124:G:OP1	2.31	0.48
42:l:37:VAL:HG22	42:l:53:CYS:SG	2.53	0.48
32:b:99:LEU:HB3	32:b:102:MET:HE1	1.95	0.48
31:a:1490:A:HO2'	31:a:1491:G:C5'	2.26	0.48
5:A:1317:A:C5	5:A:1318:C:C5	3.02	0.48
5:A:2796:U:O2'	5:A:2797:G:OP1	2.27	0.48
7:C:66:ASP:OD2	7:C:102:ARG:NH1	2.45	0.48
10:F:57:MET:HE3	10:F:65:PRO:HB3	1.96	0.48
31:a:507:A:O2'	31:a:539:G:O2'	2.27	0.48
31:a:1320:G:H2'	31:a:1321:A:C8	2.49	0.48
32:b:119:LEU:HD13	32:b:119:LEU:C	2.37	0.48
31:a:1123:U:H1'	31:a:1124:G:OP1	2.14	0.48
31:a:1180:C:O2'	31:a:1182:G:OP2	2.32	0.48
10:F:136:ILE:HD12	10:F:137:VAL:CG1	2.44	0.48
36:f:6:ILE:HD13	36:f:89:ILE:CD1	2.44	0.48
5:A:394:U:O2'	5:A:395:G:N7	2.34	0.48
13:I:31:GLU:OE1	13:I:35:ARG:NE	2.41	0.48
16:L:57:ARG:NH1	16:L:116:GLU:HG2	2.29	0.48
31:a:1277:A:O2'	31:a:1278:U:OP1	2.31	0.48
44:n:43:GLU:HA	44:n:43:GLU:OE1	2.14	0.48
52:v:55:5MU:H2'	52:v:56:PSU:C6	2.49	0.48
5:A:1797:A:OP2	7:C:150:LYS:NZ	2.45	0.48
5:A:1923:A:HO2'	5:A:1924:A:C5'	2.15	0.48
5:A:2379:G:HO2'	5:A:2380:U:P	2.35	0.48
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.43	0.48
32:b:6:VAL:HG21	32:b:11:LEU:HG	1.95	0.48
32:b:40:ILE:HD12	32:b:40:ILE:O	2.13	0.48
11:G:143:GLN:O	11:G:147:GLU:HG3	2.14	0.47
31:a:1455:G:OP1	50:t:26:SER:OG	2.32	0.47
32:b:167:ASP:OD1	32:b:169:ASP:OD1	2.31	0.47
34:d:200:SER:O	34:d:204:GLU:OE1	2.31	0.47
40:j:8:ILE:HG23	40:j:100:ILE:HG12	1.95	0.47
42:l:74:LEU:HD12	42:l:74:LEU:H	1.79	0.47
47:q:41:ARG:HH11	47:q:41:ARG:HG2	1.79	0.47
5:A:1044:G:O2'	5:A:1108:A:N6	2.44	0.47
34:d:58:ARG:HE	34:d:58:ARG:HA	1.79	0.47
5:A:91:A:H1'	5:A:92:G:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:711:G:H21	5:A:716:A:H62	1.61	0.47
5:A:1268:C:H4'	5:A:1269:A:OP2	2.13	0.47
5:A:2363:G:C2	5:A:2364:C:C5	3.02	0.47
10:F:101:ASP:OD2	10:F:101:ASP:C	2.56	0.47
31:a:172:C:H3'	31:a:173:G:H21	1.79	0.47
31:a:1002:A:O2'	31:a:1035:C:O4'	2.31	0.47
5:A:254:G:OP2	5:A:256:C:N4	2.43	0.47
32:b:186:ILE:HG22	32:b:200:TYR:HB2	1.96	0.47
5:A:1531:C:O2	5:A:1532:U:N3	2.41	0.47
32:b:75:LYS:NZ	32:b:167:ASP:OD2	2.43	0.47
38:h:104:ILE:HG22	38:h:127:ILE:HD12	1.97	0.47
1:0:30:MET:H	1:0:47:GLU:HB2	1.80	0.47
5:A:302:A:OP2	24:T:80:ARG:NH2	2.47	0.47
5:A:1844:A:O2'	5:A:1845:G:P	2.71	0.47
5:A:2324:A:H2'	5:A:2325:A:C8	2.50	0.47
10:F:136:ILE:HD12	10:F:137:VAL:HG13	1.97	0.47
31:a:927:C:N3	31:a:1384:G:N1	2.41	0.47
31:a:993:A:N1	31:a:1042:C:O2'	2.47	0.47
32:b:113:ILE:HD11	32:b:153:VAL:HG23	1.97	0.47
5:A:799:G:C2'	5:A:800:A:OP1	2.63	0.47
31:a:23:G:H2'	31:a:24:G:C8	2.50	0.47
7:C:256:LYS:HE2	7:C:273:VAL:HG13	1.96	0.47
10:F:36:LEU:HD21	10:F:89:VAL:HG23	1.96	0.47
10:F:57:MET:HE3	10:F:65:PRO:CB	2.45	0.47
48:r:26:ILE:HD11	48:r:67:LEU:HD22	1.96	0.47
10:F:25:VAL:O	10:F:28:ILE:HD12	2.15	0.47
52:v:10:G:O6	52:v:46:G:N2	2.48	0.47
5:A:277:A:N6	5:A:367:A:OP2	2.48	0.46
5:A:1173:G:H4'	5:A:1174:U:OP1	2.14	0.46
19:O:9:GLN:O	19:O:13:ASN:ND2	2.48	0.46
31:a:467:U:C2	31:a:468:A:C8	3.03	0.46
32:b:128:PHE:CE1	32:b:140:THR:HG23	2.51	0.46
48:r:34:THR:CG2	48:r:40:VAL:HG22	2.45	0.46
5:A:546:G:N3	5:A:546:G:H2'	2.29	0.46
6:B:30:U:C2	6:B:49:G:N2	2.83	0.46
32:b:106:TRP:CD2	32:b:110:ARG:NH1	2.83	0.46
43:m:3:ARG:HB2	43:m:3:ARG:NH1	2.30	0.46
52:v:20:H2U:O3'	52:v:22:A:OP1	2.32	0.46
5:A:2753:A:N1	11:G:67:THR:HG21	2.30	0.46
25:U:4:PHE:HB2	25:U:65:VAL:HG23	1.97	0.46
31:a:710:G:H2'	31:a:711:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:113:GLU:HB3	37:g:119:ARG:HB3	1.98	0.46
44:n:73:TYR:O	44:n:79:LEU:O	2.34	0.46
5:A:1922:U:O2	5:A:1925:G:N1	2.49	0.46
5:A:2490:G:H4'	16:L:80:GLU:OE2	2.16	0.46
18:N:5:LYS:O	18:N:9:LEU:HD23	2.15	0.46
31:a:471:G:H2'	31:a:472:A:C8	2.50	0.46
41:k:112:VAL:HG12	41:k:112:VAL:O	2.16	0.46
52:v:19:G:O5'	52:v:20:H2U:H5''	2.15	0.46
5:A:605:U:C5	5:A:618:G:C5	3.04	0.46
5:A:1588:A:H2'	5:A:1589:C:O4'	2.15	0.46
10:F:60:ILE:HD12	10:F:138:PHE:CG	2.51	0.46
31:a:84:U:H1'	31:a:85:G:OP2	2.15	0.46
31:a:789:A:H1'	31:a:790:U:OP2	2.16	0.46
31:a:1051:C:H1'	31:a:1052:A:OP2	2.16	0.46
31:a:1277:A:H1'	31:a:1278:U:OP1	2.15	0.46
34:d:92:LEU:HD12	34:d:96:LEU:CD1	2.46	0.46
48:r:25:ASP:OD2	48:r:28:THR:OG1	2.27	0.46
5:A:1719:U:O4	5:A:1734:G:N2	2.48	0.46
14:J:49:ARG:NH2	31:a:1420:G:OP1	2.49	0.46
31:a:404:G:H2'	31:a:405:U:O4'	2.16	0.46
32:b:7:SER:O	32:b:8:MET:CB	2.63	0.46
34:d:25:VAL:HG23	34:d:26:LYS:HD2	1.97	0.46
38:h:106:SER:HB2	38:h:127:ILE:HD11	1.96	0.46
48:r:34:THR:HG22	48:r:40:VAL:HG22	1.98	0.46
14:J:12:ASP:OD2	14:J:12:ASP:C	2.58	0.46
31:a:143:G:H2'	31:a:144:G:C8	2.51	0.46
32:b:8:MET:HE2	32:b:45:LEU:HB2	1.97	0.46
36:f:26:ILE:HD11	36:f:39:LEU:HD22	1.97	0.46
5:A:309:G:N1	5:A:312:A:OP2	2.43	0.46
5:A:2426:A:C3'	5:A:2427:U:H5'	2.44	0.46
10:F:137:VAL:HG23	10:F:137:VAL:O	2.14	0.46
31:a:419:U:H2'	31:a:420:G:O4'	2.15	0.46
31:a:776:C:H2'	31:a:777:A:O4'	2.16	0.46
33:c:107:ASP:OD2	33:c:108:ARG:N	2.49	0.46
35:e:38:VAL:HG22	35:e:66:ALA:HB1	1.98	0.46
37:g:69:VAL:O	37:g:69:VAL:CG1	2.64	0.46
41:k:22:ILE:HG13	41:k:31:VAL:HG13	1.98	0.46
5:A:2262:A:H4'	5:A:2263:A:N3	2.31	0.46
5:A:2287:U:OP1	5:A:2376:U:O2'	2.29	0.46
7:C:240:LYS:O	7:C:242:ILE:HG22	2.16	0.46
10:F:133:LYS:N	10:F:133:LYS:HD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:12:ASP:OD2	14:J:14:SER:OG	2.31	0.46
5:A:395:G:OP2	27:W:10:LYS:NZ	2.47	0.46
5:A:1507:G:C2	5:A:1508:C:C5	3.04	0.46
31:a:458:G:C6	31:a:459:U:O4	2.68	0.46
31:a:943:A:H2'	31:a:944:G:C8	2.51	0.46
33:c:52:VAL:HG22	33:c:70:THR:HB	1.96	0.46
34:d:158:LYS:O	34:d:161:ILE:HG12	2.16	0.46
5:A:434:C:O4'	5:A:434:C:O2	2.34	0.45
32:b:165:VAL:HG21	32:b:175:ILE:HD11	1.98	0.45
1:O:18:THR:HG21	3:2:33:THR:OG1	2.16	0.45
5:A:391:C:C2	5:A:392:C:C5	3.04	0.45
5:A:1922:U:H2'	5:A:1923:A:H3'	1.98	0.45
10:F:57:MET:HE1	10:F:87:CYS:CB	2.46	0.45
31:a:982:C:H2'	31:a:983:U:C6	2.51	0.45
31:a:1157:G:C2	31:a:1158:C:C6	3.04	0.45
34:d:157:ILE:O	34:d:161:ILE:HG23	2.17	0.45
36:f:11:HIS:CD2	36:f:54:ILE:HD13	2.52	0.45
5:A:701:U:H2'	5:A:702:G:O4'	2.17	0.45
5:A:2027:A:N3	5:A:2451:G:O2'	2.41	0.45
6:B:13:A:OP1	6:B:104:U:O2'	2.28	0.45
6:B:22:G:O6	6:B:54:G:O2'	2.29	0.45
30:Z:30:ASP:OD2	30:Z:33:THR:OG1	2.35	0.45
31:a:711:G:H2'	31:a:712:A:C8	2.50	0.45
39:i:33:LEU:CD2	39:i:47:ARG:HE	2.30	0.45
52:v:55:5MU:H71	52:v:56:PSU:H2'	1.98	0.45
5:A:2308:U:H4'	10:F:85:ILE:HD11	1.98	0.45
5:A:2317:G:N2	5:A:2318:A:O4'	2.50	0.45
5:A:1862:A:N6	5:A:1871:G:O2'	2.44	0.45
5:A:2426:A:H2'	5:A:2426:A:N3	2.31	0.45
10:F:115:ARG:O	10:F:115:ARG:HG2	2.16	0.45
31:a:1097:C:OP2	32:b:97:ARG:CZ	2.64	0.45
32:b:118:ASP:C	32:b:118:ASP:OD1	2.59	0.45
34:d:9:CYS:HG	34:d:22:LYS:HZ1	1.60	0.45
5:A:2262:A:H4'	5:A:2263:A:O5'	2.16	0.45
7:C:3:ILE:HD12	7:C:3:ILE:N	2.30	0.45
31:a:701:A:C4	31:a:702:G:C8	3.05	0.45
31:a:1527:G:O6	51:u:46:LYS:NZ	2.50	0.45
44:n:37:SER:HG	44:n:39:GLU:CD	2.23	0.45
5:A:427:A:C2'	5:A:428:A:O5'	2.65	0.45
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.67	0.45
6:B:50:A:O2'	6:B:51:A:C8	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:42:MET:HE3	16:L:125:LEU:HD22	1.98	0.45
32:b:52:LEU:HD13	32:b:202:ILE:HD12	1.99	0.45
37:g:35:LYS:HE2	37:g:38:ILE:HD12	1.99	0.45
6:B:50:A:O2'	6:B:51:A:P	2.74	0.45
10:F:98:GLU:HA	10:F:101:ASP:OD1	2.17	0.45
26:V:20:MET:SD	26:V:20:MET:N	2.90	0.45
31:a:73:G:H2'	31:a:74:G:C8	2.52	0.45
31:a:1173:A:H2'	31:a:1174:G:C8	2.52	0.45
55:a:1603:80P:N27	55:a:1603:80P:C22	2.79	0.45
32:b:99:LEU:C	32:b:99:LEU:HD23	2.41	0.45
33:c:214:VAL:HG12	33:c:214:VAL:O	2.17	0.45
41:k:36:ARG:O	41:k:37:GLN:HB2	2.17	0.45
5:A:2879:A:OP2	30:Z:49:ARG:NH1	2.48	0.45
10:F:93:GLY:O	10:F:96:MET:HG3	2.17	0.45
31:a:1096:G:H2'	31:a:1096:G:N3	2.32	0.45
32:b:88:ARG:HD3	32:b:224:LEU:HD11	1.99	0.45
34:d:32:THR:O	34:d:33:LYS:CD	2.65	0.45
34:d:199:GLU:O	34:d:203:VAL:HG23	2.17	0.45
5:A:862:G:H2'	5:A:863:C:C6	2.51	0.45
5:A:1199:A:O4'	5:A:1201:G:C8	2.70	0.45
9:E:15:GLU:O	9:E:19:GLY:N	2.49	0.45
10:F:90:THR:C	10:F:91:LEU:HD12	2.41	0.45
10:F:162:THR:HG23	10:F:165:GLU:H	1.81	0.45
31:a:293:G:N2	31:a:296:A:OP2	2.39	0.45
39:i:11:LYS:O	39:i:12:THR:OG1	2.24	0.45
50:t:39:ILE:HD11	50:t:83:VAL:HG23	1.97	0.45
5:A:2287:U:H2'	5:A:2288:G:C8	2.51	0.44
15:K:16:ARG:HG2	15:K:16:ARG:HH11	1.82	0.44
31:a:127:U:O2'	31:a:258:A:N3	2.45	0.44
5:A:1848:U:O2	5:A:1885:A:N6	2.47	0.44
15:K:16:ARG:HG2	15:K:16:ARG:NH1	2.31	0.44
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.99	0.44
17:M:106:ASP:OD1	17:M:106:ASP:N	2.51	0.44
31:a:185:C:H1'	31:a:186:G:OP2	2.17	0.44
31:a:369:A:C2	31:a:479:A:C6	3.06	0.44
31:a:1023:G:N3	31:a:1023:G:H2'	2.32	0.44
31:a:1433:U:C2	31:a:1434:A:C8	3.05	0.44
31:a:1444:A:P	31:a:1445:C:H41	2.38	0.44
34:d:36:ASN:OD1	34:d:36:ASN:C	2.59	0.44
40:j:80:THR:HG22	40:j:81:ASP:N	2.33	0.44
5:A:591:U:H2'	5:A:592:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:715:C:O4'	5:A:715:C:O2	2.34	0.44
5:A:1413:G:H1'	5:A:1578:A:H61	1.82	0.44
5:A:2465:A:N6	5:A:2477:G:O2'	2.50	0.44
10:F:152:MET:HG2	10:F:153:ASP:N	2.31	0.44
31:a:789:A:O2'	31:a:790:U:OP2	2.25	0.44
31:a:989:U:H1'	31:a:990:G:OP2	2.17	0.44
31:a:1428:A:H2	31:a:1466:C:H42	1.66	0.44
34:d:5:ILE:N	34:d:5:ILE:HD12	2.31	0.44
37:g:15:ASP:OD1	37:g:19:SER:N	2.47	0.44
41:k:113:THR:HG21	51:u:32:VAL:HG21	1.99	0.44
5:A:392:C:C2	5:A:393:U:C5	3.05	0.44
5:A:606:A:H2'	5:A:607:A:C8	2.52	0.44
5:A:1389:U:H2'	5:A:1390:A:O4'	2.17	0.44
5:A:1428:A:H2'	5:A:1429:A:H8	1.82	0.44
5:A:1718:A:N6	5:A:1734:G:O2'	2.50	0.44
5:A:2067:A:H2'	5:A:2068:C:C6	2.52	0.44
7:C:17:GLU:OE1	7:C:204:SER:N	2.50	0.44
10:F:22:ILE:HD13	10:F:24:ASN:O	2.17	0.44
18:N:103:LYS:NZ	18:N:103:LYS:HB3	2.33	0.44
19:O:5:HIS:O	19:O:9:GLN:HG3	2.17	0.44
37:g:113:GLU:HG3	37:g:118:LEU:HB3	2.00	0.44
48:r:59:ILE:O	48:r:63:ARG:HG2	2.17	0.44
1:0:5:ILE:HD13	1:0:21:LYS:HD2	2.00	0.44
5:A:1193:U:C2	5:A:1194:U:C5	3.05	0.44
5:A:1315:C:H2'	5:A:1324:U:OP1	2.18	0.44
5:A:1786:U:H2'	5:A:1787:A:C8	2.53	0.44
32:b:175:ILE:HD12	32:b:175:ILE:H	1.83	0.44
32:b:202:ILE:HG13	32:b:202:ILE:O	2.18	0.44
34:d:92:LEU:HD12	34:d:96:LEU:HD13	2.00	0.44
18:N:20:ARG:HG2	18:N:20:ARG:HH11	1.81	0.44
5:A:1316:A:C4	5:A:1317:A:C8	3.05	0.44
11:G:86:LYS:O	11:G:86:LYS:CD	2.65	0.44
32:b:214:LEU:HD23	32:b:215:TYR:N	2.33	0.44
5:A:579:C:H2'	5:A:580:A:H8	1.83	0.44
5:A:1355:G:N7	5:A:1356:G:C8	2.86	0.44
5:A:1634:G:H2'	5:A:1635:A:C8	2.53	0.44
7:C:203:ARG:NH2	7:C:214:ARG:HH22	2.16	0.44
14:J:47:ILE:CD1	14:J:48:PRO:HD2	2.44	0.44
31:a:908:U:H2'	31:a:909:C:C6	2.53	0.44
32:b:45:LEU:N	32:b:45:LEU:HD22	2.33	0.44
5:A:1147:G:H2'	5:A:1148:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1317:A:C6	5:A:1318:C:C5	3.06	0.44
10:F:93:GLY:N	10:F:96:MET:HG2	2.33	0.44
10:F:94:ASP:OD1	10:F:94:ASP:C	2.60	0.44
15:K:12:GLU:OE1	15:K:12:GLU:HA	2.16	0.44
31:a:105:A:O2'	31:a:322:G:N2	2.51	0.44
31:a:1215:C:H2'	31:a:1216:A:C8	2.53	0.44
5:A:386:U:O2	5:A:386:U:O4'	2.36	0.43
7:C:94:LEU:HD13	7:C:116:VAL:HG21	1.99	0.43
31:a:172:C:H2'	31:a:173:G:N3	2.33	0.43
41:k:81:LEU:HD23	41:k:81:LEU:O	2.17	0.43
11:G:43:LEU:HD13	11:G:52:LEU:CD2	2.48	0.43
50:t:28:VAL:CG2	50:t:61:MET:HG3	2.47	0.43
5:A:1860:U:OP1	5:A:2406:G:O2'	2.35	0.43
10:F:81:ASP:OD2	10:F:81:ASP:N	2.52	0.43
32:b:10:ASP:O	32:b:13:GLN:HG3	2.19	0.43
32:b:202:ILE:O	32:b:202:ILE:CG1	2.66	0.43
43:m:87:ARG:HG2	43:m:97:VAL:HG13	2.00	0.43
1:0:39:ILE:HD12	1:0:41:GLN:HB2	2.00	0.43
4:3:2:LYS:NZ	4:3:32:ARG:O	2.50	0.43
5:A:1923:A:C2'	5:A:1924:A:O5'	2.65	0.43
6:B:44:A:C5	6:B:45:C:C5	3.05	0.43
11:G:173:GLU:OE1	11:G:173:GLU:N	2.44	0.43
31:a:748:U:H2'	31:a:749:G:O4'	2.18	0.43
32:b:128:PHE:CZ	32:b:140:THR:HG23	2.54	0.43
32:b:175:ILE:HD12	32:b:175:ILE:N	2.33	0.43
36:f:35:GLN:HB2	36:f:65:GLU:HB3	2.01	0.43
42:l:89:ASP:C	42:l:89:ASP:OD1	2.60	0.43
5:A:1412:C:H2'	5:A:1413:G:O4'	2.17	0.43
31:a:404:G:C2	31:a:405:U:H1'	2.54	0.43
31:a:1428:A:H2'	31:a:1429:G:O4'	2.18	0.43
39:i:82:THR:HG23	39:i:96:LEU:HD13	2.01	0.43
1:0:3:ASP:OD2	1:0:3:ASP:N	2.52	0.43
5:A:1335:U:C2'	5:A:1336:G:OP1	2.65	0.43
8:D:136:THR:O	8:D:137:HIS:HB2	2.18	0.43
16:L:89:ASN:O	16:L:91:GLU:OE1	2.36	0.43
20:P:111:GLU:OE1	20:P:111:GLU:HA	2.18	0.43
31:a:1063:C:O2	31:a:1063:C:H2'	2.19	0.43
36:f:30:LYS:HA	36:f:34:GLY:HA3	2.01	0.43
5:A:2060:C:H2'	5:A:2061:C:C6	2.54	0.43
5:A:2185:U:O2'	5:A:2186:G:H5'	2.19	0.43
11:G:33:LEU:HD13	11:G:75:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:20:ARG:HG2	18:N:20:ARG:NH1	2.34	0.43
31:a:961:A:N3	31:a:966:A:O2'	2.47	0.43
36:f:6:ILE:HG21	36:f:62:MET:SD	2.58	0.43
36:f:17:GLN:O	36:f:21:MET:HE2	2.19	0.43
5:A:390:A:C5	5:A:391:C:C5	3.07	0.43
10:F:6:ALA:O	10:F:7:ARG:C	2.60	0.43
16:L:78:PRO:O	16:L:79:LEU:HB2	2.19	0.43
18:N:110:ARG:NH1	18:N:116:PHE:O	2.52	0.43
19:O:117:LEU:HD12	19:O:117:LEU:C	2.44	0.43
31:a:1158:C:C2	31:a:1159:C:C5	3.07	0.43
5:A:2685:U:H4'	5:A:2686:A:OP2	2.18	0.43
23:S:14:VAL:HG22	23:S:32:LYS:HD2	2.01	0.43
35:e:106:ALA:O	35:e:111:ARG:NH1	2.49	0.43
1:O:46:LYS:HE3	1:O:46:LYS:CA	2.46	0.43
5:A:301:A:N3	5:A:321:C:O2'	2.44	0.43
5:A:368:C:C4'	5:A:369:G:OP2	2.67	0.43
31:a:577:C:H2'	31:a:578:G:O4'	2.18	0.43
38:h:114:ASP:OD2	38:h:114:ASP:N	2.50	0.43
44:n:37:SER:OG	44:n:39:GLU:OE1	2.30	0.43
5:A:1192:G:C2	5:A:1193:U:C5	3.07	0.42
12:H:26:GLY:HA2	12:H:30:LEU:HD12	2.01	0.42
17:M:49:GLU:CG	17:M:95:LEU:HD13	2.48	0.42
31:a:434:U:HO2'	31:a:435:U:P	2.41	0.42
5:A:1519:U:HO2'	5:A:1520:A:P	2.29	0.42
10:F:34:ILE:HG23	10:F:156:ILE:HG13	2.01	0.42
23:S:43:LYS:HG2	23:S:47:GLU:OE1	2.19	0.42
31:a:991:A:N3	44:n:8:ASN:ND2	2.66	0.42
42:l:101:SER:O	42:l:102:LEU:C	2.61	0.42
47:q:8:THR:O	47:q:9:LEU:HD12	2.19	0.42
5:A:2186:G:O2'	5:A:2187:A:P	2.78	0.42
7:C:140:THR:HG22	7:C:163:GLN:OE1	2.20	0.42
14:J:58:MET:HE2	14:J:58:MET:HB3	1.98	0.42
31:a:174:C:C2	31:a:175:A:C8	3.07	0.42
31:a:1224:A:O3'	43:m:114:LYS:HE2	2.19	0.42
32:b:88:ARG:NE	32:b:224:LEU:HD11	2.35	0.42
34:d:58:ARG:HA	34:d:58:ARG:NE	2.34	0.42
5:A:542:C:H2'	5:A:543:U:O4'	2.19	0.42
5:A:665:U:H2'	5:A:666:A:O4'	2.20	0.42
5:A:1314:C:O2'	5:A:1315:C:H5'	2.20	0.42
5:A:2641:U:H3'	5:A:2642:C:H5'	2.01	0.42
23:S:55:VAL:HG12	23:S:85:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:23:LEU:HD11	29:Y:53:MET:HE1	2.01	0.42
31:a:764:A:H2'	31:a:765:A:O4'	2.20	0.42
31:a:1101:G:O2'	31:a:1102:A:P	2.77	0.42
33:c:77:ILE:HG23	33:c:84:ILE:HG21	2.01	0.42
34:d:57:LEU:O	34:d:61:GLN:HG2	2.20	0.42
38:h:43:GLU:OE2	38:h:43:GLU:HA	2.19	0.42
7:C:135:MET:HE2	7:C:141:LEU:CD2	2.49	0.42
33:c:123:GLN:HG2	33:c:128:VAL:HG21	2.01	0.42
35:e:40:ASP:OD1	35:e:41:GLY:N	2.52	0.42
5:A:1731:C:C2	5:A:1732:C:C5	3.07	0.42
10:F:72:LYS:NZ	10:F:73:SER:H	2.18	0.42
24:T:50:THR:O	24:T:50:THR:HG22	2.19	0.42
31:a:451:U:C2	31:a:452:A:C8	3.08	0.42
33:c:88:GLN:HG2	33:c:101:VAL:HG23	2.01	0.42
5:A:17:A:H2'	5:A:18:U:O4'	2.20	0.42
5:A:2587:C:C2	5:A:2588:G:C8	3.08	0.42
6:B:34:C:N4	6:B:35:C:H41	2.18	0.42
10:F:53:ALA:O	10:F:57:MET:HG2	2.20	0.42
31:a:743:A:H2'	31:a:744:A:C8	2.55	0.42
7:C:168:ASP:OD1	7:C:168:ASP:N	2.53	0.42
10:F:136:ILE:C	10:F:137:VAL:HG13	2.45	0.42
21:Q:51:ALA:CB	21:Q:52:PRO:HD3	2.48	0.42
31:a:933:C:C4	31:a:934:A:N7	2.88	0.42
34:d:145:ILE:HD13	34:d:145:ILE:N	2.34	0.42
5:A:637:U:H2'	5:A:638:C:C6	2.54	0.42
6:B:7:G:C2	6:B:8:A:C8	3.08	0.42
11:G:92:VAL:O	11:G:92:VAL:HG13	2.19	0.42
31:a:438:G:N1	31:a:490:A:C6	2.88	0.42
31:a:607:U:N3	31:a:608:C:C5	2.88	0.42
44:n:72:GLY:O	44:n:80:SER:HA	2.20	0.42
5:A:51:A:H2'	5:A:52:G:O4'	2.19	0.41
5:A:984:C:O2'	5:A:997:A:N3	2.51	0.41
5:A:2641:U:H3'	5:A:2642:C:C5'	2.50	0.41
11:G:63:MET:O	11:G:67:THR:HG23	2.20	0.41
5:A:605:U:H5	5:A:618:G:C5	2.39	0.41
5:A:2422:A:H3'	5:A:2423:C:H5'	2.02	0.41
5:A:2753:A:N3	11:G:63:MET:HE2	2.34	0.41
8:D:152:ASN:O	8:D:153:GLN:C	2.64	0.41
31:a:472:A:H2'	31:a:473:U:O4'	2.20	0.41
31:a:942:G:C2	31:a:943:A:C8	3.08	0.41
31:a:1031:G:H2'	31:a:1032:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1378:U:O2	31:a:1378:U:O4'	2.38	0.41
33:c:12:LEU:O	33:c:16:LYS:O	2.38	0.41
47:q:77:VAL:HG12	47:q:78:GLU:OE1	2.20	0.41
5:A:1109:G:H2'	5:A:1110:U:O4'	2.20	0.41
5:A:2633:U:H2'	5:A:2634:G:O4'	2.20	0.41
6:B:28:C:H2'	6:B:29:C:O4'	2.19	0.41
10:F:113:ASP:OD2	10:F:113:ASP:C	2.64	0.41
41:k:106:ILE:HG13	41:k:106:ILE:O	2.21	0.41
48:r:36:ASN:O	48:r:36:ASN:ND2	2.52	0.41
5:A:1169:C:H3'	5:A:1170:U:H4'	2.02	0.41
5:A:1862:A:H61	5:A:1871:G:C2'	2.32	0.41
31:a:459:U:H2'	31:a:460:U:C4	2.56	0.41
31:a:1494:G:H1'	31:a:1515:MA6:H2	2.03	0.41
41:k:93:GLU:HG2	51:u:16:ILE:HG21	2.02	0.41
43:m:75:MET:N	43:m:75:MET:HE3	2.35	0.41
5:A:303:C:H5''	5:A:336:U:H2'	2.03	0.41
5:A:507:U:C4'	5:A:508:C:OP2	2.69	0.41
5:A:1844:A:C2'	5:A:1845:G:OP2	2.69	0.41
5:A:2683:U:H2'	5:A:2684:G:O4'	2.19	0.41
10:F:38:MET:CE	10:F:40:VAL:HG13	2.49	0.41
10:F:51:ASP:OD2	10:F:51:ASP:N	2.53	0.41
31:a:160:G:C2	31:a:161:G:C8	3.08	0.41
40:j:57:VAL:O	40:j:58:ASN:CG	2.63	0.41
41:k:30:ILE:HG12	41:k:45:THR:HG22	2.02	0.41
5:A:1296:A:C4'	5:A:1297:A:OP1	2.69	0.41
5:A:1577:A:C4	5:A:1578:A:C8	3.09	0.41
5:A:1730:U:C2	5:A:1731:C:C5	3.09	0.41
5:A:2316:A:C2'	5:A:2317:G:OP2	2.69	0.41
5:A:2468:G:N2	5:A:2475:U:O4	2.53	0.41
11:G:89:LEU:HD23	11:G:162:VAL:HG13	2.03	0.41
11:G:143:GLN:OE1	11:G:143:GLN:HA	2.21	0.41
31:a:466:C:C2	31:a:467:U:C5	3.08	0.41
5:A:579:C:H2'	5:A:580:A:C8	2.55	0.41
5:A:2747:G:O2'	5:A:2748:C:OP1	2.38	0.41
25:U:75:ASN:OD1	25:U:75:ASN:N	2.53	0.41
31:a:109:G:H2'	31:a:110:U:C6	2.56	0.41
31:a:402:G:H2'	31:a:403:U:C6	2.55	0.41
31:a:671:G:H2'	31:a:672:A:H8	1.86	0.41
32:b:168:VAL:HG23	32:b:169:ASP:N	2.35	0.41
47:q:49:ASP:OD2	47:q:53:VAL:N	2.54	0.41
5:A:299:G:H2'	5:A:300:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:872:G:OP1	16:L:63:LYS:NZ	2.49	0.41
5:A:2002:C:C2	5:A:2003:U:C5	3.08	0.41
5:A:2061:C:N3	5:A:2062:C:C5	2.89	0.41
5:A:2528:G:N2	5:A:2659:G:O2'	2.54	0.41
5:A:2652:U:O2	5:A:2661:A:N7	2.54	0.41
10:F:80:ARG:NH1	10:F:83:TRP:HB2	2.36	0.41
10:F:120:LYS:HG2	10:F:121:SER:H	1.86	0.41
31:a:1002:A:O3'	31:a:1035:C:O2'	2.33	0.41
31:a:1312:U:H2'	31:a:1313:G:O4'	2.21	0.41
33:c:73:PRO:O	33:c:77:ILE:HG13	2.21	0.41
35:e:70:MET:HE3	35:e:70:MET:HB3	1.95	0.41
36:f:94:HIS:CD2	36:f:94:HIS:C	2.99	0.41
37:g:36:LYS:O	37:g:40:GLU:HG3	2.21	0.41
37:g:116:MET:HA	37:g:119:ARG:HG2	2.03	0.41
38:h:47:SER:OG	38:h:65:LYS:HG2	2.21	0.41
5:A:314:G:C2	5:A:315:U:C6	3.09	0.41
5:A:831:A:H2'	5:A:832:G:C8	2.56	0.41
5:A:1168:A:H2'	5:A:1169:C:C6	2.56	0.41
6:B:43:A:C4	6:B:44:A:C8	3.09	0.41
6:B:45:C:C4	6:B:46:U:C5	3.09	0.41
7:C:270:ASP:OD2	7:C:273:VAL:HG12	2.21	0.41
10:F:170:MET:N	10:F:170:MET:SD	2.94	0.41
11:G:84:GLU:OE1	11:G:84:GLU:C	2.63	0.41
16:L:58:ILE:HD13	16:L:64:ILE:HD11	2.01	0.41
31:a:26:U:OP1	42:l:20:LYS:NZ	2.54	0.41
31:a:85:G:H1'	31:a:86:C:OP2	2.21	0.41
31:a:496:A:O4'	31:a:544:A:N6	2.53	0.41
31:a:725:A:H2'	31:a:726:A:C8	2.56	0.41
33:c:136:ARG:CZ	33:c:136:ARG:HB3	2.50	0.41
34:d:67:TYR:CD2	34:d:96:LEU:HD23	2.56	0.41
42:l:122:PRO:O	42:l:123:LYS:C	2.64	0.41
43:m:43:THR:HG21	43:m:48:LEU:HD21	2.01	0.41
5:A:847:A:H2'	5:A:848:C:C6	2.56	0.41
5:A:1006:A:N3	5:A:1151:C:O2'	2.50	0.41
5:A:1404:G:H2'	5:A:1405:U:C6	2.56	0.41
5:A:1411:G:N2	5:A:1584:A:C6	2.85	0.41
9:E:122:GLU:OE1	9:E:123:PHE:N	2.54	0.41
24:T:52:ALA:O	24:T:53:GLU:C	2.64	0.41
31:a:610:C:H2'	31:a:611:C:C6	2.55	0.41
34:d:9:CYS:SG	34:d:22:LYS:NZ	2.81	0.41
34:d:61:GLN:O	34:d:65:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:144:MET:HE2	37:g:144:MET:H	1.85	0.41
31:a:516:C:H2'	31:a:517:A:O4'	2.21	0.40
31:a:943:A:OP1	43:m:113:ARG:NH1	2.54	0.40
31:a:1037:A:C2	31:a:1038:G:C5	3.09	0.40
32:b:45:LEU:HD22	32:b:45:LEU:H	1.85	0.40
33:c:142:MET:HE2	33:c:170:GLU:HB3	2.03	0.40
33:c:213:GLN:OE1	33:c:213:GLN:C	2.64	0.40
34:d:35:ALA:O	34:d:36:ASN:CG	2.64	0.40
39:i:40:GLU:N	39:i:40:GLU:OE2	2.54	0.40
45:o:40:GLN:O	45:o:44:LYS:HG2	2.21	0.40
48:r:21:ILE:N	48:r:21:ILE:HD12	2.36	0.40
52:v:20:H2U:O2	52:v:20:H2U:C2'	2.69	0.40
5:A:1267:A:C4'	5:A:1268:C:OP1	2.70	0.40
5:A:1590:A:H2'	5:A:1591:C:O4'	2.21	0.40
10:F:96:MET:HG3	10:F:97:TYR:N	2.37	0.40
31:a:127:U:H2'	31:a:128:C:C6	2.56	0.40
37:g:17:LYS:HG2	37:g:18:PHE:CD1	2.56	0.40
39:i:110:GLU:OE2	39:i:113:LYS:NZ	2.52	0.40
5:A:1016:U:O2'	5:A:1018:A:N7	2.50	0.40
5:A:2076:G:H5''	27:W:19:SER:CB	2.51	0.40
31:a:1022:U:H4'	31:a:1023:G:O5'	2.22	0.40
36:f:36:ILE:N	36:f:36:ILE:CD1	2.84	0.40
42:l:107:VAL:HG21	42:l:110:ARG:HD3	2.03	0.40
4:3:1:MET:HE3	4:3:1:MET:HB2	1.95	0.40
5:A:372:U:OP2	5:A:372:U:C6	2.75	0.40
5:A:1256:C:OP2	22:R:83:LYS:NZ	2.53	0.40
5:A:1324:U:OP2	5:A:1325:C:N4	2.52	0.40
5:A:1352:C:H2'	5:A:1353:G:O4'	2.21	0.40
5:A:1589:C:H2'	5:A:1590:A:H8	1.86	0.40
5:A:2026:6MZ:O2'	5:A:2027:A:P	2.79	0.40
5:A:2468:G:H21	5:A:2474:A:H62	1.67	0.40
5:A:2586:A:H2'	5:A:2587:C:H6	1.87	0.40
7:C:183:LYS:HB3	7:C:268:ILE:HD11	2.02	0.40
10:F:8:TYR:HA	10:F:12:LEU:HB2	2.04	0.40
17:M:94:TYR:C	17:M:95:LEU:HD12	2.47	0.40
31:a:78:G:H2'	31:a:79:U:C6	2.56	0.40
31:a:886:A:H4'	31:a:887:G:OP1	2.20	0.40
31:a:987:C:O2'	31:a:988:U:H5'	2.22	0.40
34:d:22:LYS:O	34:d:23:SER:HB3	2.22	0.40
37:g:140:ASP:O	37:g:144:MET:CE	2.69	0.40
5:A:324:A:H1'	5:A:325:G:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2727:G:H2'	5:A:2728:G:C8	2.57	0.40
5:A:2752:U:H4'	5:A:2753:A:OP1	2.21	0.40
6:B:36:C:H2'	6:B:37:U:C6	2.56	0.40
7:C:93:LEU:HD12	7:C:102:ARG:O	2.22	0.40
11:G:89:LEU:HD22	11:G:162:VAL:HG22	2.04	0.40
14:J:17:ARG:HG3	14:J:17:ARG:NH1	2.36	0.40
31:a:179:G:C5	31:a:180:U:C6	3.09	0.40
31:a:389:A:C2	31:a:390:G:C8	3.10	0.40
32:b:33:ILE:O	32:b:35:GLY:N	2.51	0.40
32:b:137:LEU:HA	32:b:140:THR:OG1	2.20	0.40
33:c:79:LYS:HG2	33:c:80:LYS:HD3	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	
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	C	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	157 (91%)	14 (8%)	1 (1%)	21	30
11	G	172/177 (97%)	166 (96%)	5 (3%)	1 (1%)	21	30
12	H	58/148 (39%)	56 (97%)	2 (3%)	0	100	100
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18	26
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	112/116 (97%)	109 (97%)	3 (3%)	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
21	Q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	56/58 (97%)	56 (100%)	0	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	216 (97%)	6 (3%)	1 (0%)	30	40
33	c	213/250 (85%)	203 (95%)	10 (5%)	0	100	100
34	d	205/208 (99%)	199 (97%)	6 (3%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
36	f	102/127 (80%)	95 (93%)	5 (5%)	2 (2%)	6	6
37	g	132/156 (85%)	130 (98%)	2 (2%)	0	100	100
38	h	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
39	i	124/128 (97%)	118 (95%)	6 (5%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
45	o	86/89 (97%)	86 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	77 (100%)	0	0	100	100
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	55/71 (78%)	55 (100%)	0	0	100	100
All	All	5407/5872 (92%)	5258 (97%)	143 (3%)	6 (0%)	49	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	b	8	MET
10	F	137	VAL
11	G	13	ASN
36	f	86	ARG
36	f	94	HIS
16	L	78	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	
1	0	47/47 (100%)	46 (98%)	1 (2%)	47	67
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	50 (96%)	2 (4%)	29	46
4	3	33/33 (100%)	32 (97%)	1 (3%)	36	56
7	C	218/220 (99%)	213 (98%)	5 (2%)	44	64
8	D	166/167 (99%)	162 (98%)	4 (2%)	43	63
9	E	155/155 (100%)	154 (99%)	1 (1%)	78	88
10	F	144/147 (98%)	136 (94%)	8 (6%)	19	30
11	G	139/142 (98%)	137 (99%)	2 (1%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	H	45/112 (40%)	42 (93%)	3 (7%)	15	23
13	I	118/118 (100%)	115 (98%)	3 (2%)	42	61
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	105 (99%)	1 (1%)	70	84
16	L	113/113 (100%)	111 (98%)	2 (2%)	51	71
17	M	96/101 (95%)	95 (99%)	1 (1%)	68	82
18	N	83/85 (98%)	80 (96%)	3 (4%)	31	49
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	86 (98%)	2 (2%)	44	64
23	S	77/87 (88%)	75 (97%)	2 (3%)	40	60
24	T	83/85 (98%)	82 (99%)	1 (1%)	63	79
25	U	79/80 (99%)	77 (98%)	2 (2%)	42	61
26	V	59/64 (92%)	55 (93%)	4 (7%)	14	23
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	46/50 (92%)	44 (96%)	2 (4%)	26	41
32	b	185/200 (92%)	179 (97%)	6 (3%)	34	53
33	c	175/198 (88%)	170 (97%)	5 (3%)	37	57
34	d	170/171 (99%)	166 (98%)	4 (2%)	43	63
35	e	113/120 (94%)	110 (97%)	3 (3%)	39	59
36	f	94/111 (85%)	90 (96%)	4 (4%)	26	41
37	g	113/128 (88%)	110 (97%)	3 (3%)	39	59
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	96 (97%)	3 (3%)	36	56
40	j	89/91 (98%)	85 (96%)	4 (4%)	24	39
41	k	88/98 (90%)	82 (93%)	6 (7%)	14	23
42	l	104/106 (98%)	100 (96%)	4 (4%)	29	46
43	m	95/98 (97%)	91 (96%)	4 (4%)	26	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	62 (98%)	1 (2%)	55	74
47	q	71/76 (93%)	67 (94%)	4 (6%)	19	30
48	r	46/66 (70%)	45 (98%)	1 (2%)	45	65
49	s	70/78 (90%)	67 (96%)	3 (4%)	26	41
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	48/62 (77%)	48 (100%)	0	100	100
All	All	4477/4756 (94%)	4372 (98%)	105 (2%)	44	64

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	6	ARG
3	2	28	LYS
3	2	52	SER
4	3	37	GLN
7	C	72	ASP
7	C	124	ILE
7	C	140	THR
7	C	268	ILE
7	C	273	VAL
8	D	18	ASP
8	D	52	THR
8	D	91	GLU
8	D	98	THR
9	E	74	SER
10	F	11	GLU
10	F	18	GLU
10	F	54	VAL
10	F	60	ILE
10	F	80	ARG
10	F	81	ASP
10	F	96	MET
10	F	137	VAL
11	G	15	VAL
11	G	18	THR
12	H	41	GLU
12	H	53	GLU

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Mol	Chain	Res	Type
12	H	58	GLU
13	I	87	THR
13	I	93	VAL
13	I	119	ILE
15	K	29	VAL
16	L	28	SER
16	L	109	VAL
17	M	116	VAL
18	N	37	TYR
18	N	59	LEU
18	N	86	VAL
22	R	13	SER
22	R	105	VAL
23	S	55	VAL
23	S	72	THR
24	T	65	ILE
25	U	57	SER
25	U	69	VAL
26	V	10	THR
26	V	31	VAL
26	V	67	VAL
26	V	74	GLN
30	Z	30	ASP
30	Z	33	THR
32	b	10	ASP
32	b	54	ASP
32	b	85	GLN
32	b	143	MET
32	b	188	ILE
32	b	194	ASN
33	c	84	ILE
33	c	94	ILE
33	c	122	SER
33	c	154	SER
33	c	172	ARG
34	d	30	VAL
34	d	173	ILE
34	d	181	GLU
34	d	192	ASP
35	e	18	ASP
35	e	92	ARG
35	e	130	THR

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Mol	Chain	Res	Type
36	f	64	VAL
36	f	89	ILE
36	f	93	GLU
36	f	96	ILE
37	g	12	ILE
37	g	73	VAL
37	g	74	GLU
39	i	64	THR
39	i	70	ILE
39	i	126	SER
40	j	18	ILE
40	j	28	THR
40	j	47	GLU
40	j	48	ARG
41	k	29	THR
41	k	34	THR
41	k	67	GLU
41	k	79	LYS
41	k	96	VAL
41	k	107	ASN
42	l	14	THR
42	l	52	VAL
42	l	98	VAL
42	l	101	SER
43	m	11	ASP
43	m	29	THR
43	m	47	GLU
43	m	89	LEU
46	p	91	SER
47	q	24	VAL
47	q	75	THR
47	q	78	GLU
47	q	81	GLU
48	r	27	ASP
49	s	35	SER
49	s	55	ARG
49	s	71	LEU

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

Mol	Chain	Res	Type
3	2	19	ASN

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Mol	Chain	Res	Type
7	C	70	ASN
7	C	185	HIS
7	C	239	ASN
8	D	63	ASN
8	D	65	GLN
8	D	133	GLN
9	E	96	ASN
10	F	135	GLN
13	I	61	GLN
13	I	136	GLN
14	J	29	HIS
14	J	110	GLN
15	K	18	HIS
15	K	101	ASN
15	K	125	GLN
21	Q	82	HIS
23	S	90	GLN
29	Y	8	GLN
29	Y	14	HIS
30	Z	4	GLN
30	Z	19	HIS
32	b	120	GLN
33	c	3	GLN
33	c	28	GLN
34	d	102	ASN
35	e	88	HIS
35	e	96	GLN
36	f	94	HIS
43	m	32	ASN
46	p	81	GLN
49	s	57	HIS
50	t	3	ASN
50	t	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	250 (16%)	0
5	A	2679/2918 (91%)	392 (14%)	30 (1%)
52	v	76/77 (98%)	25 (32%)	0
53	w	2/3 (66%)	1 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	B	114/115 (99%)	16 (14%)	2 (1%)
All	All	4398/4657 (94%)	684 (15%)	32 (0%)

All (684) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	41	U
5	A	53	G
5	A	56	A
5	A	58	G
5	A	66	U
5	A	67	G
5	A	70	A
5	A	71	G
5	A	74	U
5	A	78	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	101	U
5	A	103	U
5	A	104	C
5	A	109	G
5	A	125	A
5	A	127	U
5	A	144	U
5	A	147	A
5	A	170	A
5	A	171	C
5	A	172	A
5	A	188	A
5	A	203	A
5	A	206	A
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	237	G
5	A	240	A
5	A	255	G
5	A	257	G
5	A	259	G

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Mol	Chain	Res	Type
5	A	262	A
5	A	278	U
5	A	279	U
5	A	303	C
5	A	313	A
5	A	318	G
5	A	325	G
5	A	331	G
5	A	332	A
5	A	333	U
5	A	336	U
5	A	340	G
5	A	347	A
5	A	348	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	395	G
5	A	403	A
5	A	410	G
5	A	423	G
5	A	428	A
5	A	455	C
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	495	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	530	C
5	A	531	A
5	A	532	G
5	A	535	G
5	A	544	U
5	A	545	C

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Mol	Chain	Res	Type
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	613	U
5	A	625	A
5	A	635	A
5	A	636	G
5	A	643	U
5	A	644	A
5	A	651	U
5	A	666	A
5	A	675	A
5	A	684	U
5	A	724	G
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	845	A
5	A	857	G
5	A	864	A
5	A	874	C
5	A	908	A
5	A	912	C
5	A	929	C
5	A	930	U

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Mol	Chain	Res	Type
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1002	C
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1031	G
5	A	1042	U
5	A	1043	A
5	A	1105	U
5	A	1106	C
5	A	1107	G
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1140	A
5	A	1170	U
5	A	1173	G
5	A	1201	G
5	A	1242	A
5	A	1243	G
5	A	1244	U
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1269	A
5	A	1295	A

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Mol	Chain	Res	Type
5	A	1296	A
5	A	1297	A
5	A	1327	G
5	A	1328	G
5	A	1332	G
5	A	1336	G
5	A	1338	G
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1411	G
5	A	1414	A
5	A	1422	A
5	A	1423	C
5	A	1424	G
5	A	1443	U
5	A	1447	G
5	A	1448	U
5	A	1453	U
5	A	1462	G
5	A	1511	A
5	A	1519	U
5	A	1520	A
5	A	1522	C
5	A	1523	A
5	A	1528	G
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1539	G
5	A	1541	G
5	A	1542	A
5	A	1543	A
5	A	1553	G
5	A	1557	U
5	A	1564	A
5	A	1567	A

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Mol	Chain	Res	Type
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1583	C
5	A	1606	A
5	A	1645	U
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1691	U
5	A	1697	G
5	A	1725	U
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1734	G
5	A	1742	G
5	A	1760	G
5	A	1769	A
5	A	1772	G
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1845	G
5	A	1847	U
5	A	1849	A
5	A	1866	U
5	A	1868	A
5	A	1869	G
5	A	1872	A
5	A	1874	G
5	A	1881	A
5	A	1885	A
5	A	1886	A
5	A	1895	A
5	A	1897	A
5	A	1902	G

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Mol	Chain	Res	Type
5	A	1923	A
5	A	1924	A
5	A	1925	G
5	A	1932	A
5	A	1934	A
5	A	1936	U
5	A	1939	U
5	A	1951	U
5	A	1959	U
5	A	1960	G
5	A	1962	A
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2045	G
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2065	7MG
5	A	2077	C
5	A	2186	G
5	A	2187	A
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2264	A
5	A	2274	A
5	A	2279	U

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Mol	Chain	Res	Type
5	A	2283	A
5	A	2284	A
5	A	2301	U
5	A	2302	C
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2316	A
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2350	A
5	A	2355	C
5	A	2372	A
5	A	2375	G
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2398	U
5	A	2399	C
5	A	2402	U
5	A	2420	C
5	A	2421	A
5	A	2423	C
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2429	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2446	A
5	A	2455	A
5	A	2465	A
5	A	2466	G
5	A	2471	C

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Mol	Chain	Res	Type
5	A	2473	U
5	A	2474	A
5	A	2475	U
5	A	2478	A
5	A	2487	U
5	A	2493	A
5	A	2494	C
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2526	A
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2565	G
5	A	2568	A
5	A	2578	G
5	A	2581	U
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2607	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2642	C
5	A	2650	A
5	A	2656	A
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C
5	A	2710	G
5	A	2722	U

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Mol	Chain	Res	Type
5	A	2730	A
5	A	2731	G
5	A	2740	G
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2774	A
5	A	2776	A
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2805	A
5	A	2816	G
5	A	2857	U
5	A	2863	A
5	A	2875	A
5	A	2876	C
5	A	2897	C
6	B	9	C
6	B	11	A
6	B	13	A
6	B	22	G
6	B	23	A
6	B	38	U
6	B	40	C
6	B	43	A
6	B	44	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	106	A
31	a	6	C
31	a	7	U
31	a	11	G
31	a	15	U
31	a	18	A
31	a	24	G

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Mol	Chain	Res	Type
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	64	U
31	a	80	A
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	87	U
31	a	89	C
31	a	90	C
31	a	91	G
31	a	97	A
31	a	105	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	157	A
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A
31	a	200	G
31	a	201	A
31	a	202	U
31	a	206	C
31	a	207	G
31	a	208	G
31	a	209	A
31	a	239	A
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G

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Mol	Chain	Res	Type
31	a	289	G
31	a	297	G
31	a	302	A
31	a	317	A
31	a	324	C
31	a	340	A
31	a	341	C
31	a	344	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	369	A
31	a	389	A
31	a	393	A
31	a	394	U
31	a	402	G
31	a	405	U
31	a	407	A
31	a	408	A
31	a	410	A
31	a	415	C
31	a	417	U
31	a	418	A
31	a	419	U
31	a	420	G
31	a	422	U
31	a	425	U
31	a	426	A
31	a	435	U
31	a	444	A
31	a	448	G
31	a	455	C
31	a	459	U
31	a	460	U
31	a	461	A
31	a	462	A
31	a	464	A
31	a	471	G
31	a	479	A
31	a	481	G
31	a	483	U

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Mol	Chain	Res	Type
31	a	494	U
31	a	496	A
31	a	497	G
31	a	505	U
31	a	506	A
31	a	508	C
31	a	509	U
31	a	514	G
31	a	518	G
31	a	521	G
31	a	522	C
31	a	527	G
31	a	528	U
31	a	532	A
31	a	539	G
31	a	540	U
31	a	544	A
31	a	556	A
31	a	559	U
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	615	C
31	a	623	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	685	G
31	a	700	G
31	a	720	U
31	a	721	G
31	a	728	G
31	a	731	G
31	a	739	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	790	U
31	a	791	A

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Mol	Chain	Res	Type
31	a	812	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	839	U
31	a	840	U
31	a	841	G
31	a	864	G
31	a	887	G
31	a	888	U
31	a	923	G
31	a	924	G
31	a	926	G
31	a	931	C
31	a	932	A
31	a	935	A
31	a	957	U
31	a	963	2MG
31	a	965	A
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	980	A
31	a	989	U
31	a	990	G
31	a	991	A
31	a	1001	A
31	a	1003	C
31	a	1022	U
31	a	1023	G
31	a	1025	C
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1030	G
31	a	1031	G
31	a	1043	A
31	a	1051	C
31	a	1052	A
31	a	1062	U

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Mol	Chain	Res	Type
31	a	1072	U
31	a	1076	G
31	a	1082	U
31	a	1091	G
31	a	1092	U
31	a	1095	C
31	a	1097	C
31	a	1098	A
31	a	1102	A
31	a	1122	U
31	a	1123	U
31	a	1124	G
31	a	1127	A
31	a	1134	C
31	a	1136	G
31	a	1140	G
31	a	1156	U
31	a	1157	G
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1181	G
31	a	1185	A
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1209	U
31	a	1210	A
31	a	1217	G
31	a	1224	A
31	a	1235	A
31	a	1253	U
31	a	1254	U
31	a	1255	G
31	a	1267	U
31	a	1276	A
31	a	1277	A
31	a	1278	U
31	a	1284	A
31	a	1295	U

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Mol	Chain	Res	Type
31	a	1297	G
31	a	1299	C
31	a	1300	C
31	a	1317	C
31	a	1335	G
31	a	1337	A
31	a	1342	U
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1397	C
31	a	1414	G
31	a	1415	A
31	a	1416	G
31	a	1422	U
31	a	1426	C
31	a	1439	G
31	a	1443	A
31	a	1445	C
31	a	1449	A
31	a	1478	U
31	a	1484	G
31	a	1496	A
31	a	1500	A
31	a	1503	U
31	a	1504	A
31	a	1513	G
31	a	1526	G
31	a	1527	G
31	a	1528	A
52	v	7	G
52	v	8	4SU
52	v	9	A
52	v	10	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G

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Mol	Chain	Res	Type
52	v	20	H2U
52	v	21	U
52	v	22	A
52	v	34	U
52	v	47	G
52	v	48	U
52	v	49	C
52	v	50	A
52	v	56	PSU
52	v	57	C
52	v	58	A
52	v	59	A
52	v	60	G
52	v	62	C
52	v	64	C
52	v	69	U
52	v	76	C
53	w	2	U

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	84	U
5	A	91	A
5	A	256	C
5	A	324	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	424	G
5	A	478	A
5	A	507	U
5	A	782	G
5	A	799	G
5	A	1106	C
5	A	1127	U
5	A	1172	U
5	A	1179	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1335	U

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Mol	Chain	Res	Type
5	A	1337	A
5	A	1519	U
5	A	1733	U
5	A	1844	A
5	A	1880	G
5	A	1923	A
5	A	1924	A
5	A	2379	G
5	A	2419	U
5	A	2525	G
6	B	50	A
6	B	86	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6MZ	A	2026	5	22,25,26	2.47	4 (18%)	29,36,39	3.32	10 (34%)
5	7MG	A	2065	5	23,26,27	1.07	1 (4%)	27,39,42	0.87	1 (3%)
31	5MC	a	964	31	19,22,23	0.53	0	26,32,35	0.56	0
5	PSU	A	2576	5	18,21,22	1.15	1 (5%)	21,30,33	1.92	5 (23%)
5	2MA	A	2499	5	22,25,26	3.96	9 (40%)	32,37,40	2.69	11 (34%)
52	H2U	v	20	52	18,21,22	0.56	0	19,30,33	1.36	3 (15%)
5	OMU	A	2548	5	19,22,23	3.13	8 (42%)	25,31,34	1.81	5 (20%)
5	2MG	A	2441	5	23,26,27	0.46	0	33,38,41	0.52	0
5	PSU	A	2601	5	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
52	5MU	v	55	52	19,22,23	0.38	0	27,32,35	0.44	0
5	OMG	A	2247	5	23,26,27	0.45	0	32,38,41	0.50	0
52	4SU	v	8	52	18,21,22	4.47	8 (44%)	25,30,33	2.28	5 (20%)
31	4OC	a	1399	31	20,23,24	3.20	8 (40%)	25,32,35	0.91	1 (4%)
31	MA6	a	1516	31	23,26,27	1.38	4 (17%)	33,38,41	3.28	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	A	2500	5	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
5	PSU	A	2453	5	18,21,22	1.11	1 (5%)	21,30,33	1.97	6 (28%)
31	UR3	a	1495	31	19,22,23	2.95	6 (31%)	26,32,35	1.60	3 (11%)
31	PSU	a	513	31	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
31	MA6	a	1515	31	23,26,27	1.37	4 (17%)	33,38,41	3.18	12 (36%)
5	PSU	A	952	5	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
31	2MG	a	963	31	23,26,27	0.47	0	33,38,41	0.53	0
31	7MG	a	524	31	23,26,27	1.09	1 (4%)	27,39,42	0.88	2 (7%)
5	5MU	A	1935	5	19,22,23	0.38	0	27,32,35	0.53	0
31	2MG	a	1204	31	23,26,27	0.47	0	33,38,41	0.54	0
52	PSU	v	56	52	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	7MG	a	524	31	-	1/7/37/38	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
52	PSU	v	56	52	-	4/7/25/26	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C4-N3	12.16	1.50	1.34
5	A	2026	6MZ	C6-N6	10.16	1.45	1.34
52	v	8	4SU	C2-N1	9.55	1.53	1.38
52	v	8	4SU	C4-N3	8.96	1.46	1.37
5	A	2499	2MA	C2-N3	7.48	1.46	1.34
5	A	2548	OMU	C2-N1	7.44	1.50	1.38
52	v	8	4SU	C5-C4	7.36	1.51	1.42
31	a	1495	UR3	C2-N1	7.34	1.48	1.38
52	v	8	4SU	C2-N3	7.18	1.50	1.38
31	a	1399	4OC	C4-N3	7.14	1.44	1.32
5	A	2499	2MA	C6-N1	6.96	1.44	1.35
5	A	2548	OMU	C2-N3	6.87	1.49	1.38
31	a	1495	UR3	C6-C5	6.81	1.50	1.35
52	v	8	4SU	C6-C5	6.50	1.50	1.35
31	a	1399	4OC	C6-C5	6.28	1.49	1.35
31	a	1399	4OC	C2-N3	6.26	1.48	1.36
5	A	2499	2MA	C2-N1	5.96	1.44	1.34
5	A	2548	OMU	C6-C5	5.81	1.48	1.35
31	a	1495	UR3	C2-N3	5.68	1.50	1.39
31	a	1399	4OC	C4-N4	4.87	1.46	1.36
52	v	8	4SU	C4-S4	-4.87	1.60	1.68
5	A	2499	2MA	C5-C6	4.73	1.54	1.41
5	A	2065	7MG	C5-N7	4.50	1.41	1.35
31	a	524	7MG	C5-N7	4.50	1.41	1.35
5	A	2548	OMU	C4-N3	4.39	1.46	1.38
31	a	1399	4OC	C2-N1	4.34	1.49	1.40
31	a	1515	MA6	C6-N6	4.00	1.47	1.36
31	a	1516	MA6	C6-N6	3.90	1.47	1.36
5	A	2500	PSU	C6-C5	3.80	1.39	1.35
52	v	56	PSU	C6-C5	3.79	1.39	1.35
5	A	2601	PSU	C6-C5	3.78	1.39	1.35
5	A	2576	PSU	C6-C5	3.78	1.39	1.35
31	a	513	PSU	C6-C5	3.75	1.39	1.35
5	A	952	PSU	C6-C5	3.72	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1399	4OC	C5-C4	3.68	1.49	1.41
5	A	2453	PSU	C6-C5	3.65	1.39	1.35
5	A	2499	2MA	C6-N6	-3.42	1.25	1.34
31	a	1495	UR3	C6-N1	3.41	1.46	1.38
31	a	1399	4OC	C6-N1	3.35	1.46	1.38
5	A	2026	6MZ	C5-N7	-2.98	1.33	1.39
5	A	2548	OMU	C6-N1	2.96	1.45	1.38
5	A	2548	OMU	O4-C4	-2.86	1.18	1.24
31	a	1516	MA6	C5-C4	-2.84	1.34	1.39
31	a	1515	MA6	C5-C4	-2.77	1.34	1.39
31	a	1495	UR3	C4-N3	2.71	1.46	1.40
52	v	8	4SU	C6-N1	2.71	1.44	1.38
52	v	8	4SU	O2-C2	-2.64	1.18	1.23
31	a	1399	4OC	O2-C2	-2.63	1.18	1.23
5	A	2548	OMU	C5-C4	2.57	1.49	1.43
5	A	2026	6MZ	C5-C4	-2.52	1.34	1.39
5	A	2548	OMU	O2-C2	-2.41	1.18	1.23
31	a	1515	MA6	C5-N7	-2.38	1.34	1.39
5	A	2499	2MA	C5-N7	-2.35	1.34	1.39
31	a	1516	MA6	C5-N7	-2.35	1.34	1.39
31	a	1495	UR3	C5-C4	2.33	1.49	1.43
5	A	2026	6MZ	C8-N9	-2.19	1.33	1.37
5	A	2499	2MA	C4-N9	-2.17	1.33	1.37
31	a	1516	MA6	C8-N9	-2.15	1.33	1.37
5	A	2499	2MA	C8-N7	2.12	1.35	1.31
31	a	1515	MA6	C8-N9	-2.04	1.34	1.37

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	N1-C6-N6	-11.91	102.35	116.86
31	a	1515	MA6	N1-C6-N6	-11.39	102.98	116.86
5	A	2026	6MZ	C4-N9-C1'	-8.57	106.59	126.63
5	A	2026	6MZ	C1'-N9-C8	8.51	145.99	127.09
31	a	1516	MA6	C5-C6-N6	7.90	137.84	125.33
52	v	8	4SU	C4-N3-C2	-7.76	119.88	127.31
31	a	1515	MA6	C5-C6-N6	7.64	137.42	125.33
5	A	2499	2MA	C1'-N9-C8	-7.39	110.69	127.09
5	A	2026	6MZ	C5-C4-N3	-6.27	118.08	126.72
5	A	2026	6MZ	N1-C2-N3	-5.76	119.87	128.58
31	a	1516	MA6	N1-C2-N3	-5.65	120.03	128.58
5	A	2499	2MA	C5-C4-N3	-5.61	121.28	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2499	2MA	N9-C8-N7	-5.59	106.00	113.94
31	a	1515	MA6	N1-C2-N3	-5.57	120.16	128.58
31	a	1495	UR3	C4-N3-C2	-5.56	120.10	124.58
5	A	2548	OMU	C4-N3-C2	-5.54	119.73	126.61
52	v	8	4SU	C5-C4-N3	5.26	119.64	114.75
5	A	2499	2MA	C4-N9-C1'	5.06	138.47	126.63
31	a	513	PSU	C4-N3-C2	-4.95	119.56	126.37
5	A	2453	PSU	N1-C2-N3	4.90	120.34	115.17
31	a	1516	MA6	C5-C4-N3	-4.90	119.97	126.72
5	A	952	PSU	C4-N3-C2	-4.90	119.62	126.37
5	A	2601	PSU	C4-N3-C2	-4.89	119.63	126.37
5	A	2499	2MA	C4-N9-C8	4.85	110.83	105.74
5	A	2453	PSU	C4-N3-C2	-4.85	119.69	126.37
5	A	2601	PSU	N1-C2-N3	4.83	120.26	115.17
5	A	2500	PSU	C4-N3-C2	-4.82	119.73	126.37
31	a	1515	MA6	C5-C4-N3	-4.80	120.10	126.72
5	A	952	PSU	N1-C2-N3	4.80	120.23	115.17
52	v	56	PSU	N1-C2-N3	4.79	120.22	115.17
52	v	56	PSU	C4-N3-C2	-4.78	119.78	126.37
31	a	513	PSU	N1-C2-N3	4.78	120.21	115.17
5	A	2500	PSU	N1-C2-N3	4.77	120.20	115.17
5	A	2576	PSU	N1-C2-N3	4.67	120.10	115.17
5	A	2576	PSU	C4-N3-C2	-4.62	120.01	126.37
5	A	2026	6MZ	C4-C5-C6	4.52	120.54	116.78
5	A	2026	6MZ	N3-C4-N9	4.39	134.64	127.17
31	a	1516	MA6	N9-C8-N7	-4.25	107.90	113.94
5	A	2499	2MA	N3-C4-N9	4.22	132.35	126.99
31	a	1515	MA6	N9-C8-N7	-4.14	108.06	113.94
31	a	1515	MA6	C4-C5-C6	4.02	120.06	115.91
52	v	20	H2U	C5-C4-N3	-3.92	112.51	116.69
5	A	2548	OMU	N3-C2-N1	3.92	120.00	114.89
31	a	1516	MA6	C4-C5-C6	3.92	119.96	115.91
5	A	2026	6MZ	C2-N3-C4	3.90	121.35	111.83
52	v	8	4SU	N3-C2-N1	3.88	119.94	114.89
52	v	8	4SU	C5-C4-S4	-3.62	120.17	124.31
31	a	1495	UR3	C5-C4-N3	3.61	119.79	115.04
5	A	2026	6MZ	N9-C8-N7	-3.58	108.86	113.94
5	A	2548	OMU	C5-C4-N3	3.56	119.78	114.80
31	a	1515	MA6	C2-N1-C6	3.44	120.23	111.83
31	a	1516	MA6	C2-N1-C6	3.41	120.16	111.83
31	a	1516	MA6	C2-N3-C4	3.37	120.07	111.83
5	A	2499	2MA	N3-C2-N1	-3.32	119.91	125.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1515	MA6	C2-N3-C4	3.28	119.85	111.83
5	A	2499	2MA	C5-N7-C8	3.26	108.57	103.45
5	A	2500	PSU	O2-C2-N1	-3.03	119.67	122.79
31	a	1516	MA6	N3-C4-N9	3.00	132.28	127.17
52	v	20	H2U	O2-C2-N1	2.93	126.63	123.10
5	A	2576	PSU	O2-C2-N1	-2.93	119.77	122.79
31	a	1515	MA6	N3-C4-N9	2.92	132.14	127.17
5	A	2026	6MZ	C5-N7-C8	2.92	108.03	103.45
31	a	1516	MA6	C5-N7-C8	2.90	108.02	103.45
31	a	1515	MA6	C5-N7-C8	2.86	107.94	103.45
5	A	2548	OMU	O4-C4-C5	-2.82	120.31	125.16
31	a	513	PSU	O2-C2-N1	-2.77	119.94	122.79
5	A	952	PSU	O2-C2-N1	-2.76	119.94	122.79
52	v	56	PSU	O2-C2-N1	-2.73	119.97	122.79
5	A	2453	PSU	O2-C2-N1	-2.69	120.01	122.79
5	A	2065	7MG	C4-C5-N7	2.63	108.49	105.38
5	A	2601	PSU	O2-C2-N1	-2.54	120.17	122.79
5	A	2576	PSU	O4'-C1'-C2'	2.50	108.60	105.15
52	v	56	PSU	C6-N1-C2	-2.46	120.41	122.69
5	A	2576	PSU	C6-N1-C2	-2.45	120.42	122.69
31	a	1399	4OC	C6-C5-C4	2.44	119.94	117.00
31	a	524	7MG	C4-C5-N7	2.42	108.24	105.38
31	a	1516	MA6	C4-N9-C8	2.41	108.27	105.74
5	A	2453	PSU	C6-C5-C4	2.40	119.79	118.17
5	A	2453	PSU	C6-N1-C2	-2.39	120.47	122.69
5	A	2026	6MZ	C5-C6-N1	2.35	120.67	118.15
5	A	2601	PSU	C6-N1-C2	-2.29	120.56	122.69
31	a	1495	UR3	C6-N1-C2	-2.27	119.94	121.80
31	a	1515	MA6	C4-N9-C8	2.26	108.11	105.74
5	A	952	PSU	C6-N1-C2	-2.25	120.60	122.69
31	a	524	7MG	C5-C4-N9	2.25	109.21	106.33
52	v	56	PSU	O4'-C1'-C2'	2.24	108.26	105.15
5	A	2500	PSU	C6-N1-C2	-2.24	120.61	122.69
5	A	2548	OMU	O2-C2-N1	-2.22	119.90	122.80
31	a	1516	MA6	C4-C5-N7	-2.21	108.05	110.58
5	A	2601	PSU	C6-C5-C4	2.21	119.66	118.17
52	v	20	H2U	O2-C2-N3	-2.20	117.44	121.49
5	A	2500	PSU	C6-C5-C4	2.18	119.65	118.17
31	a	513	PSU	C6-N1-C2	-2.16	120.68	122.69
31	a	1515	MA6	C4-C5-N7	-2.15	108.13	110.58
5	A	2499	2MA	N6-C6-N1	2.13	119.90	117.03
31	a	513	PSU	C6-C5-C4	2.13	119.61	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2453	PSU	O4'-C1'-C2'	2.12	108.09	105.15
5	A	2499	2MA	CM2-C2-N1	2.10	120.27	117.13
5	A	2499	2MA	C4-C5-N7	-2.07	108.22	110.58
52	v	8	4SU	O2-C2-N1	-2.06	120.11	122.80

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	55	5MU	C2'-C1'-N1-C2
52	v	55	5MU	C2'-C1'-N1-C6
52	v	56	PSU	C2'-C1'-C5-C4
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2499	2MA	O4'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C2
31	a	1399	4OC	O4'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
5	A	2548	OMU	C3'-C4'-C5'-O5'
5	A	2548	OMU	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
52	v	56	PSU	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
52	v	56	PSU	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	8	4SU	O4'-C1'-N1-C6
31	a	524	7MG	C3'-C4'-C5'-O5'
31	a	963	2MG	C4'-C5'-O5'-P
52	v	20	H2U	C4'-C5'-O5'-P
52	v	8	4SU	C4'-C5'-O5'-P
5	A	2499	2MA	C4'-C5'-O5'-P
52	v	8	4SU	O4'-C1'-N1-C2
52	v	55	5MU	O4'-C1'-N1-C6
5	A	2065	7MG	O4'-C4'-C5'-O5'
52	v	55	5MU	O4'-C1'-N1-C2
5	A	2499	2MA	O4'-C1'-N9-C8
5	A	2065	7MG	C4'-C5'-O5'-P
52	v	56	PSU	C2'-C1'-C5-C6
5	A	2548	OMU	C3'-C2'-O2'-CM2
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2026	6MZ	2	0
52	v	20	H2U	4	0
52	v	55	5MU	2	0
5	A	2247	OMG	1	0
52	v	8	4SU	1	0
31	a	1515	MA6	2	0
31	a	963	2MG	2	0
31	a	524	7MG	1	0
5	A	1935	5MU	1	0
52	v	56	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	80P	a	1603	56	45,45,45	3.83	23 (51%)	51,72,72	2.51	19 (37%)
55	80P	a	1602	56	45,45,45	3.95	21 (46%)	51,72,72	2.60	18 (35%)
55	80P	a	1601	56	45,45,45	3.40	21 (46%)	51,72,72	2.46	19 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	80P	a	1603	56	-	10/22/87/87	0/5/5/5
55	80P	a	1602	56	-	5/22/87/87	0/5/5/5
55	80P	a	1601	56	-	14/22/87/87	0/5/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	C08-C09	13.05	1.63	1.52
55	a	1603	80P	C08-C09	12.24	1.62	1.52
55	a	1602	80P	C21-C04	10.43	1.64	1.54
55	a	1601	80P	C08-C09	10.38	1.61	1.52
55	a	1602	80P	C08-C21	9.37	1.61	1.53
55	a	1603	80P	C08-C21	9.00	1.61	1.53
55	a	1601	80P	C21-C04	8.71	1.62	1.54
55	a	1603	80P	C21-C04	8.28	1.62	1.54
55	a	1603	80P	C04-N03	7.89	1.55	1.47
55	a	1602	80P	C04-N03	7.23	1.54	1.47
55	a	1601	80P	C08-C21	7.12	1.59	1.53
55	a	1601	80P	C04-N03	6.48	1.53	1.47
55	a	1603	80P	C06-C36	6.46	1.60	1.47
55	a	1602	80P	C06-C36	6.40	1.60	1.47
55	a	1603	80P	C06-C07	6.20	1.63	1.46
55	a	1601	80P	C04-C05	6.13	1.63	1.51
55	a	1602	80P	C06-C07	6.08	1.62	1.46
55	a	1601	80P	C06-C36	5.44	1.58	1.47
55	a	1603	80P	C04-C05	5.43	1.62	1.51
55	a	1602	80P	C08-C07	5.26	1.61	1.55
55	a	1602	80P	C04-C05	5.25	1.62	1.51
55	a	1601	80P	C06-C07	5.17	1.60	1.46
55	a	1603	80P	C08-C07	4.76	1.61	1.55
55	a	1601	80P	C18-C19	4.12	1.63	1.52
55	a	1603	80P	C18-C17	4.12	1.57	1.51
55	a	1602	80P	C18-C19	4.07	1.63	1.52
55	a	1603	80P	C18-C19	3.98	1.63	1.52
55	a	1602	80P	C10-C11	3.90	1.55	1.46
55	a	1603	80P	C15-C26	3.89	1.57	1.52
55	a	1601	80P	C18-C17	3.89	1.57	1.51
55	a	1602	80P	C12-C11	3.63	1.55	1.46
55	a	1602	80P	C18-C17	3.62	1.56	1.51
55	a	1603	80P	C10-C11	3.57	1.54	1.46
55	a	1601	80P	C16-C17	3.49	1.46	1.40
55	a	1601	80P	C08-C07	3.42	1.59	1.55
55	a	1602	80P	C16-C17	3.41	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	C22-C16	3.33	1.59	1.51
55	a	1603	80P	C12-C11	3.31	1.55	1.46
55	a	1603	80P	C16-C17	3.24	1.45	1.40
55	a	1603	80P	C22-C16	3.23	1.59	1.51
55	a	1601	80P	C22-C16	3.15	1.58	1.51
55	a	1602	80P	C12-C13	3.09	1.46	1.41
55	a	1603	80P	C19-C10	2.99	1.54	1.51
55	a	1601	80P	C12-C11	2.97	1.54	1.46
55	a	1603	80P	C30-C26	2.88	1.57	1.54
55	a	1602	80P	C15-C26	2.86	1.56	1.52
55	a	1601	80P	C19-C10	2.75	1.54	1.51
55	a	1603	80P	C12-C13	2.74	1.45	1.41
55	a	1601	80P	C12-C13	2.72	1.45	1.41
55	a	1601	80P	C10-C11	2.71	1.52	1.46
55	a	1603	80P	C16-C15	2.65	1.44	1.40
55	a	1601	80P	C15-C26	2.63	1.55	1.52
55	a	1603	80P	C40-N03	2.52	1.54	1.47
55	a	1602	80P	C36-N38	2.49	1.40	1.33
55	a	1601	80P	C36-N38	2.48	1.40	1.33
55	a	1603	80P	C36-N38	2.43	1.40	1.33
55	a	1603	80P	C14-C15	2.43	1.43	1.39
55	a	1602	80P	C19-C10	2.32	1.54	1.51
55	a	1602	80P	C14-C15	2.22	1.43	1.39
55	a	1601	80P	C40-N03	2.21	1.53	1.47
55	a	1603	80P	C20-C19	2.17	1.58	1.53
55	a	1602	80P	C40-N03	2.09	1.53	1.47
55	a	1602	80P	C16-C15	2.09	1.43	1.40
55	a	1601	80P	C30-C26	2.03	1.56	1.54
55	a	1601	80P	C20-C19	2.02	1.57	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1602	80P	C11-C10-C09	9.40	126.24	118.80
55	a	1603	80P	C11-C10-C09	8.53	125.55	118.80
55	a	1601	80P	C11-C10-C09	8.02	125.14	118.80
55	a	1602	80P	C08-C21-C04	5.71	119.44	111.64
55	a	1603	80P	C36-C06-C07	-5.48	114.49	120.97
55	a	1603	80P	C08-C21-C04	4.87	118.30	111.64
55	a	1601	80P	C36-C06-C07	-4.78	115.31	120.97
55	a	1603	80P	C12-C11-C10	4.73	127.14	118.28
55	a	1602	80P	C12-C11-C10	4.61	126.92	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1601	80P	C12-C11-C10	4.57	126.85	118.28
55	a	1602	80P	O33-C09-C08	-4.54	106.80	113.37
55	a	1601	80P	C08-C21-C04	4.52	117.82	111.64
55	a	1601	80P	C18-C17-C16	4.50	126.92	119.75
55	a	1602	80P	C36-C06-C07	-4.44	115.71	120.97
55	a	1603	80P	O33-C09-C08	-4.39	107.02	113.37
55	a	1601	80P	C13-C12-C17	4.29	123.63	119.03
55	a	1601	80P	O33-C09-C08	-4.14	107.37	113.37
55	a	1602	80P	C20-C21-C04	-4.06	107.86	113.73
55	a	1603	80P	C17-C18-C19	3.96	118.36	113.12
55	a	1603	80P	C13-C12-C17	3.87	123.19	119.03
55	a	1602	80P	C18-C17-C16	3.83	125.85	119.75
55	a	1602	80P	C13-C12-C17	3.81	123.13	119.03
55	a	1602	80P	C17-C18-C19	3.56	117.83	113.12
55	a	1602	80P	O33-C09-C10	3.55	130.41	123.52
55	a	1603	80P	O33-C09-C10	3.44	130.20	123.52
55	a	1601	80P	O33-C09-C10	3.43	130.17	123.52
55	a	1603	80P	C18-C17-C16	3.34	125.07	119.75
55	a	1601	80P	C13-C12-C11	-3.21	116.69	121.45
55	a	1603	80P	C20-C21-C04	-3.17	109.15	113.73
55	a	1602	80P	F25-C22-C16	3.10	119.54	112.32
55	a	1601	80P	O32-C11-C10	-3.05	115.84	121.14
55	a	1603	80P	O32-C11-C10	-3.03	115.87	121.14
55	a	1601	80P	F23-C22-C16	3.03	119.38	112.32
55	a	1603	80P	C13-C12-C11	-3.02	116.97	121.45
55	a	1602	80P	O32-C11-C10	-2.95	116.01	121.14
55	a	1601	80P	C14-C13-C12	-2.87	117.71	120.92
55	a	1601	80P	C21-C04-N03	-2.86	104.45	111.30
55	a	1602	80P	C13-C12-C11	-2.84	117.24	121.45
55	a	1603	80P	F25-C22-C16	2.82	118.89	112.32
55	a	1603	80P	O32-C11-C12	-2.81	116.98	122.06
55	a	1603	80P	C14-C13-C12	-2.78	117.81	120.92
55	a	1602	80P	O32-C11-C12	-2.76	117.07	122.06
55	a	1602	80P	O37-C36-N38	-2.73	116.78	122.89
55	a	1603	80P	O37-C36-N38	-2.68	116.88	122.89
55	a	1602	80P	C14-C13-C12	-2.67	117.92	120.92
55	a	1601	80P	O37-C36-N38	-2.65	116.95	122.89
55	a	1601	80P	O32-C11-C12	-2.62	117.31	122.06
55	a	1601	80P	C20-C21-C04	-2.49	110.14	113.73
55	a	1601	80P	C21-C08-C07	-2.42	108.27	111.05
55	a	1603	80P	C08-C07-C06	2.32	119.44	115.75
55	a	1601	80P	C17-C18-C19	2.23	116.07	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1603	80P	C15-C26-N27	2.22	116.16	112.59
55	a	1601	80P	F25-C22-C16	2.22	117.48	112.32
55	a	1603	80P	F23-C22-C16	2.20	117.44	112.32
55	a	1602	80P	C08-C07-C06	2.17	119.21	115.75
55	a	1602	80P	F23-C22-C16	2.15	117.34	112.32

There are no chirality outliers.

All (29) torsion outliers are listed below:

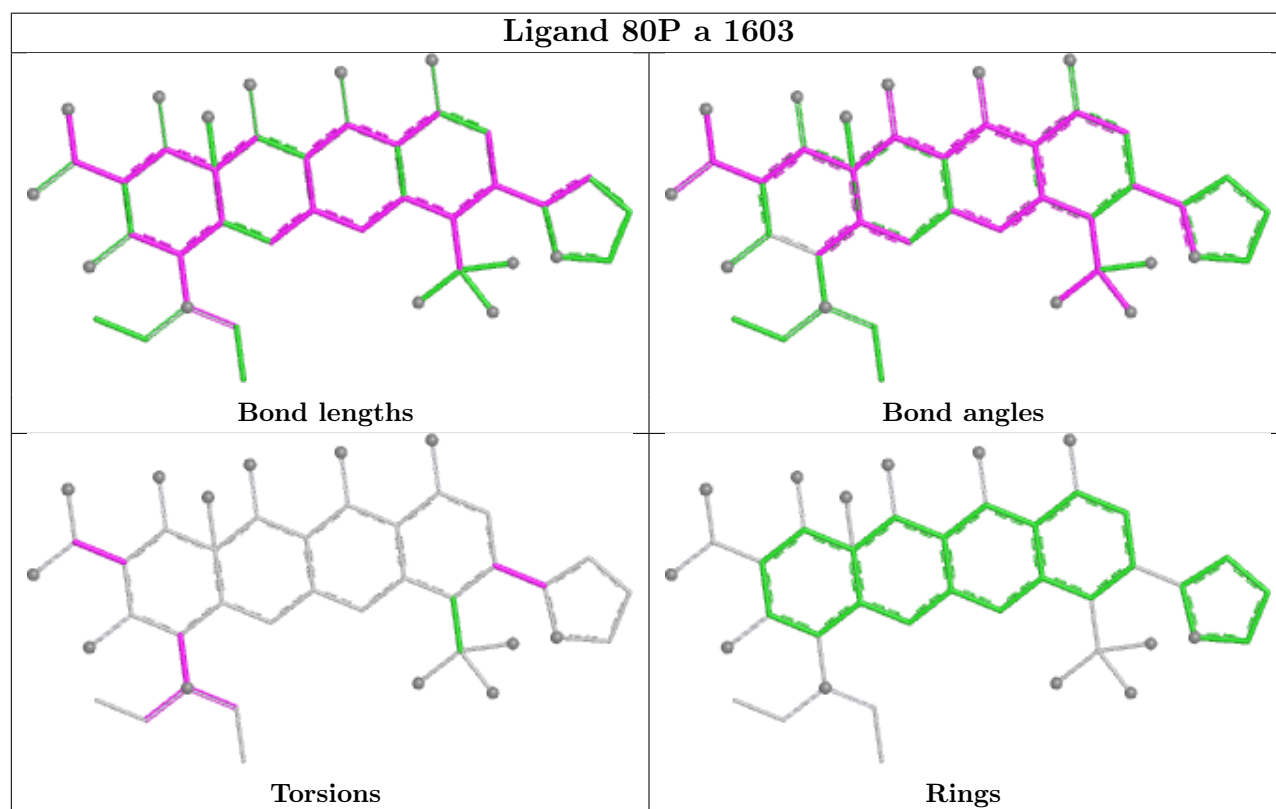
Mol	Chain	Res	Type	Atoms
55	a	1601	80P	C05-C04-N03-C01
55	a	1601	80P	C14-C15-C26-N27
55	a	1601	80P	C16-C15-C26-C30
55	a	1601	80P	C16-C15-C26-N27
55	a	1603	80P	C05-C04-N03-C01
55	a	1603	80P	C05-C04-N03-C40
55	a	1603	80P	C16-C15-C26-C30
55	a	1603	80P	C41-C40-N03-C01
55	a	1603	80P	C41-C40-N03-C04
55	a	1602	80P	C41-C40-N03-C01
55	a	1601	80P	C21-C04-N03-C40
55	a	1603	80P	C21-C04-N03-C01
55	a	1603	80P	C21-C04-N03-C40
55	a	1601	80P	C41-C40-N03-C04
55	a	1602	80P	C41-C40-N03-C04
55	a	1603	80P	C02-C01-N03-C04
55	a	1603	80P	C16-C15-C26-N27
55	a	1603	80P	C07-C06-C36-O37
55	a	1601	80P	C07-C06-C36-N38
55	a	1601	80P	C14-C15-C26-C30
55	a	1601	80P	C15-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F25
55	a	1601	80P	C15-C16-C22-F24
55	a	1602	80P	C15-C16-C22-F24
55	a	1601	80P	C15-C16-C22-F25
55	a	1602	80P	C15-C16-C22-F23
55	a	1601	80P	C41-C40-N03-C01
55	a	1601	80P	C21-C04-N03-C01
55	a	1601	80P	C17-C16-C22-F23

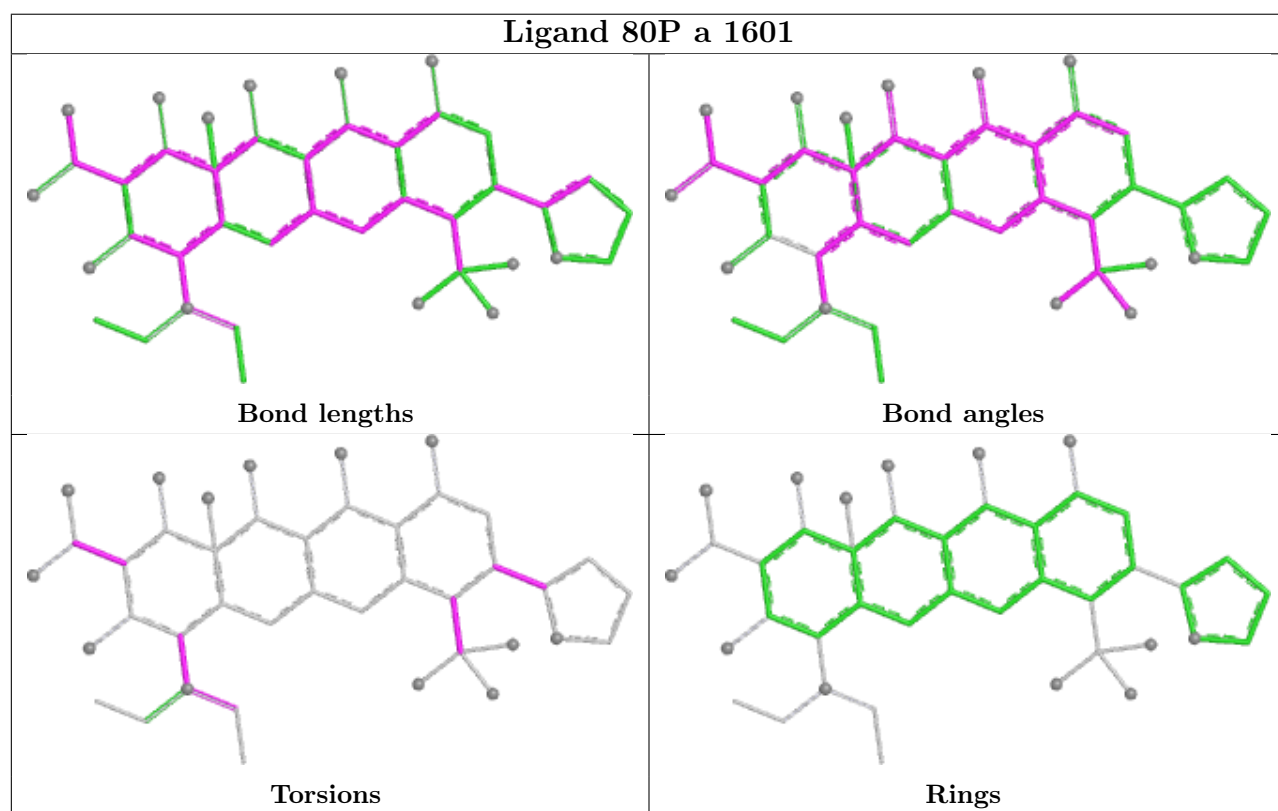
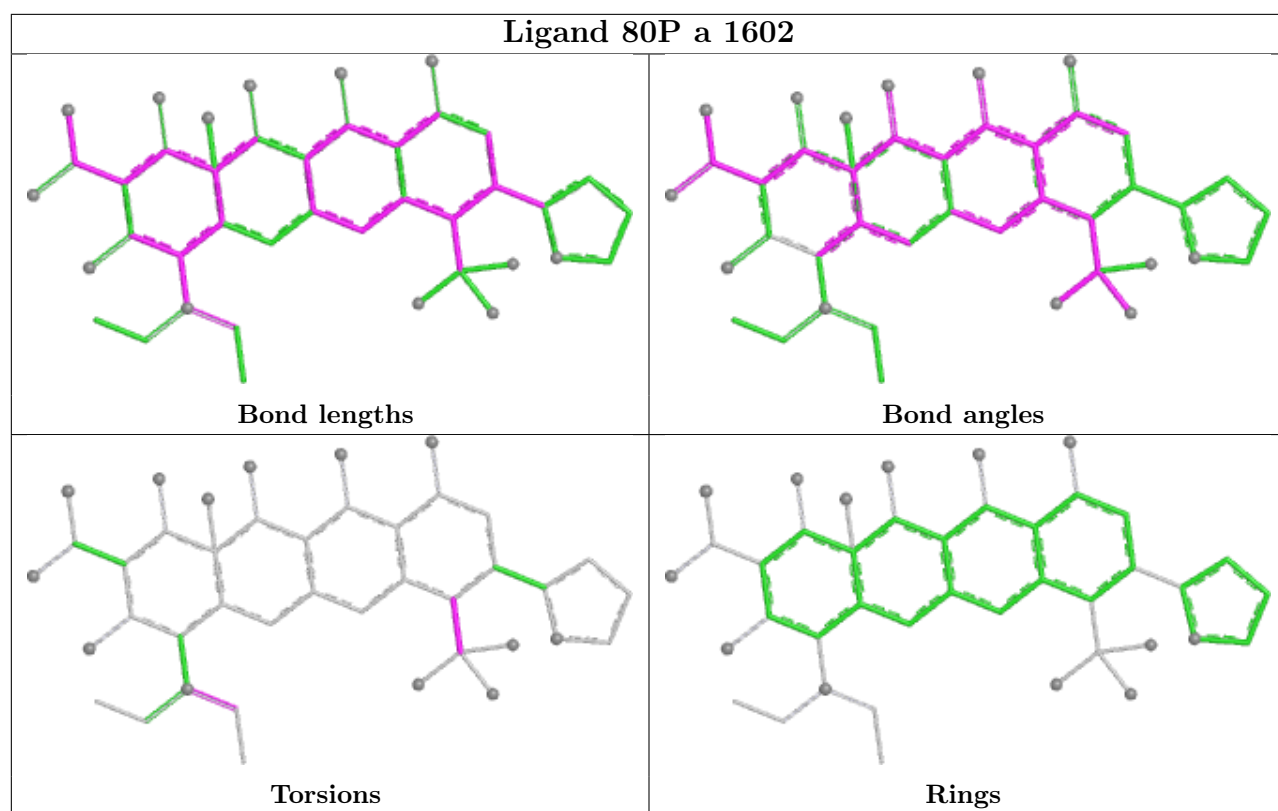
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	a	1603	80P	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

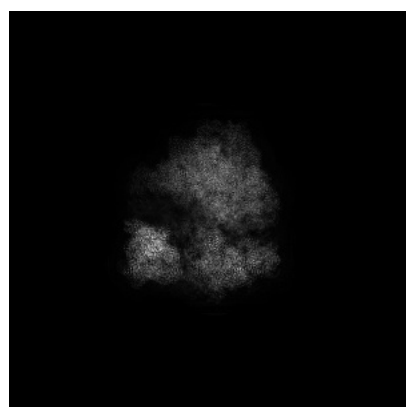
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24739. These allow visual inspection of the internal detail of the map and identification of artifacts.

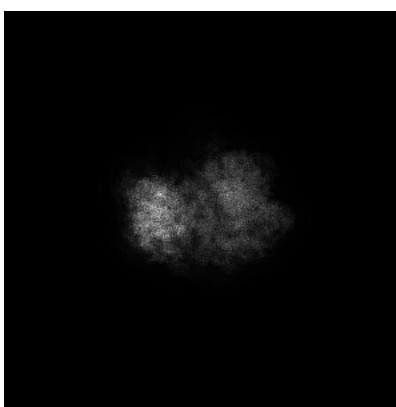
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

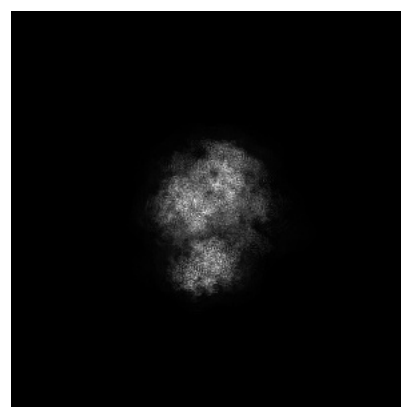
6.1.1 Primary map



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

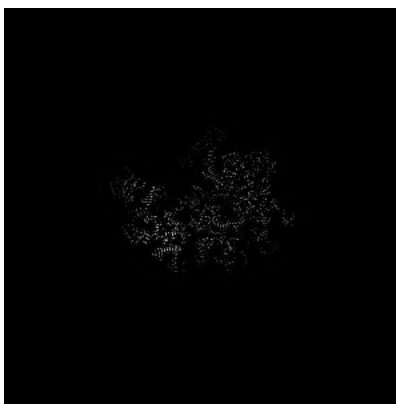
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 248



Y Index: 267

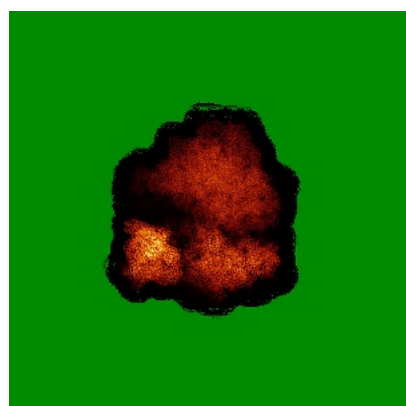


Z Index: 200

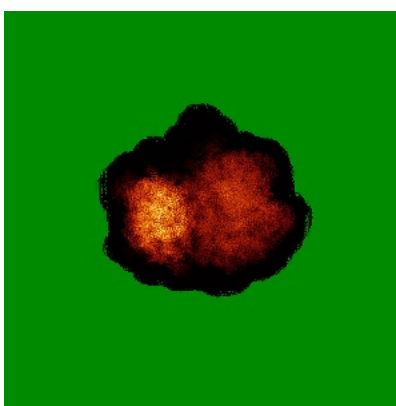
The images above show the largest variance slices of the map in three orthogonal directions.

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

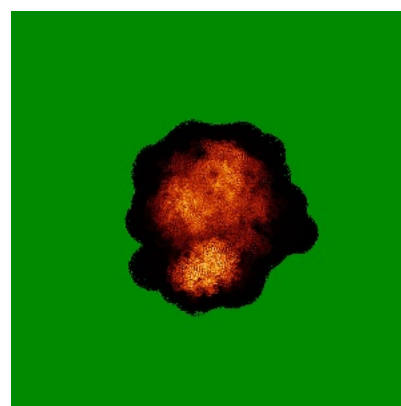
6.4.1 Primary map



X



Y

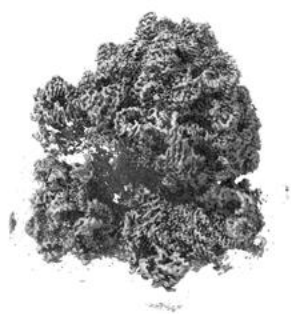


Z

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



X



Y



Z

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

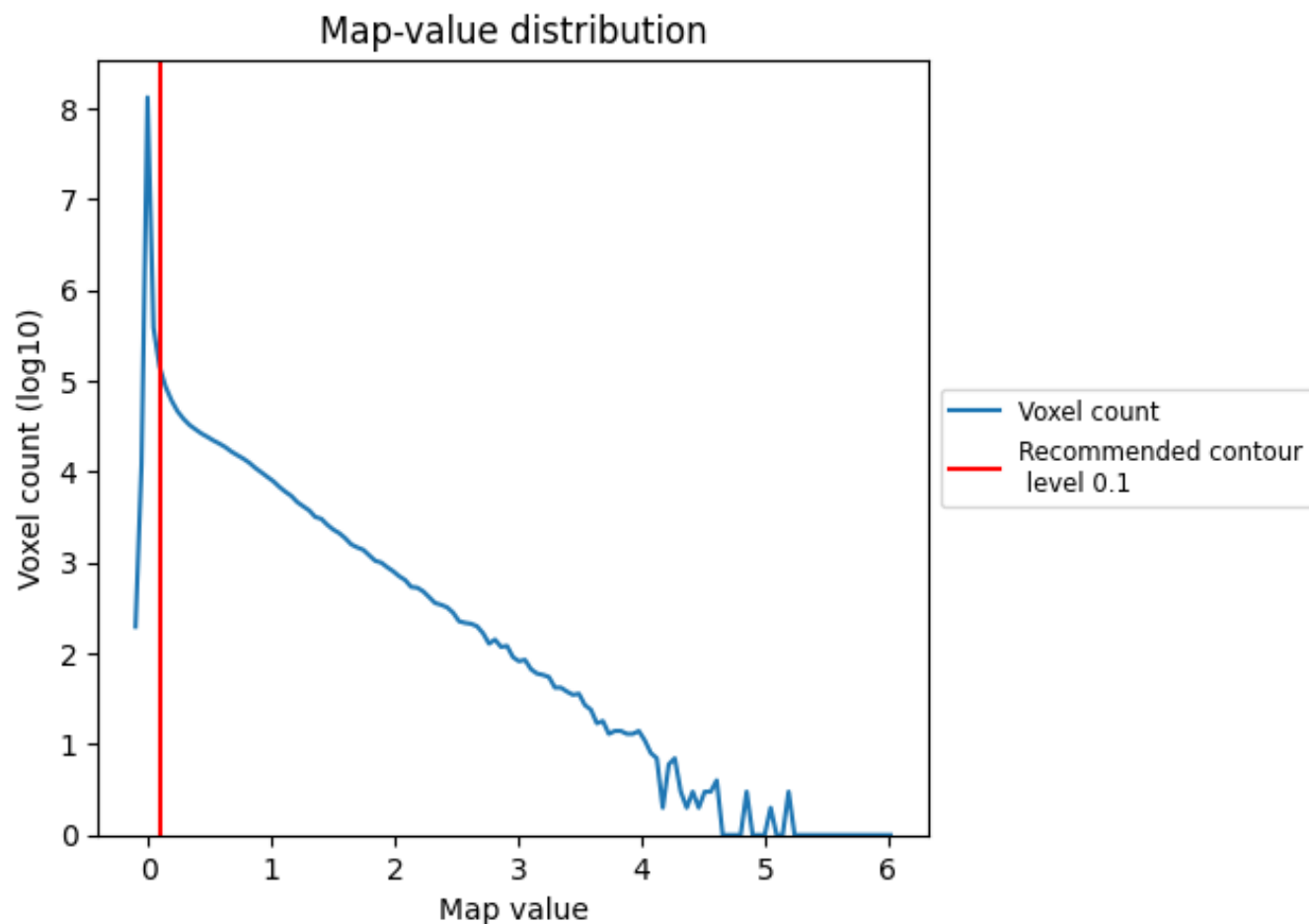
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

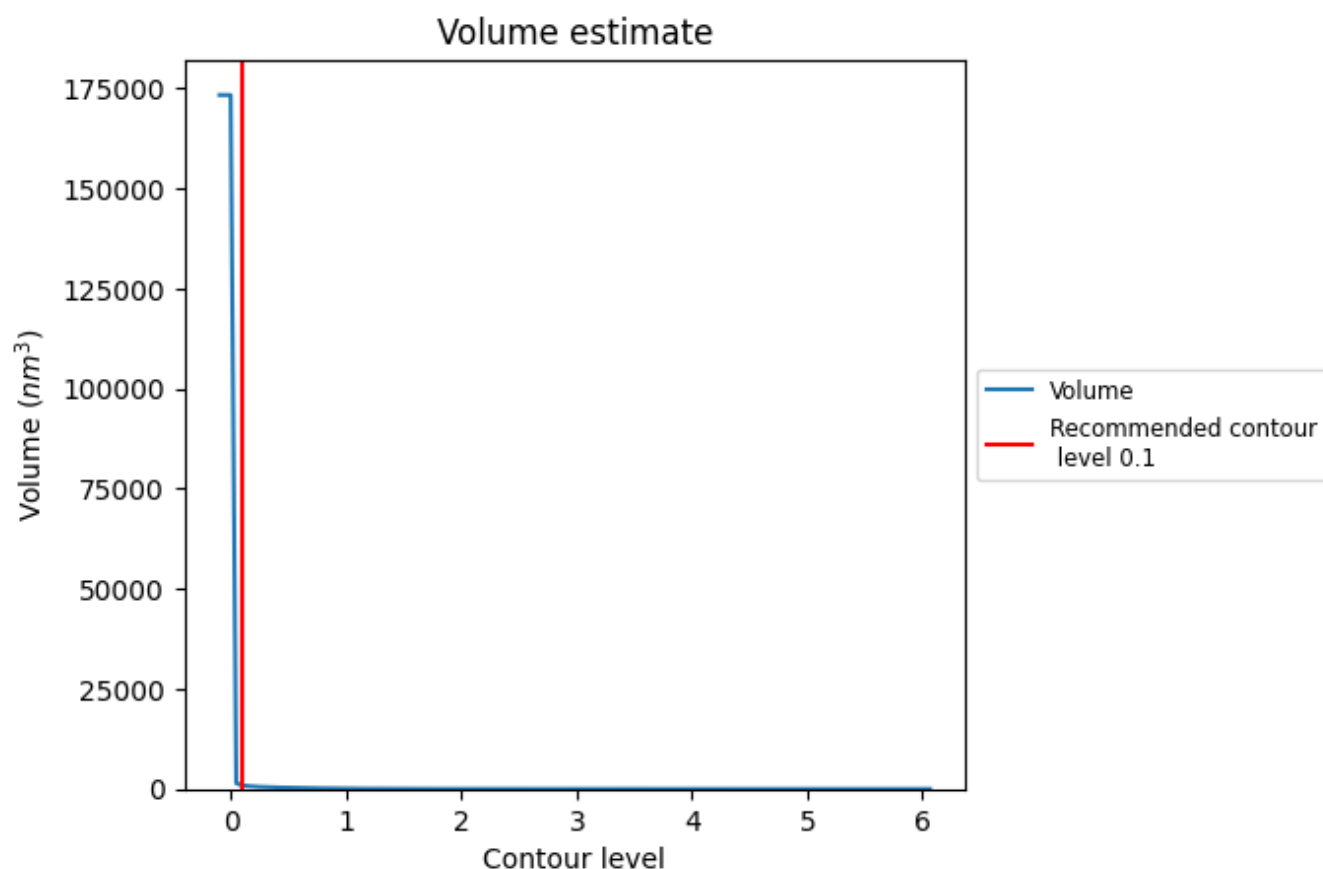
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

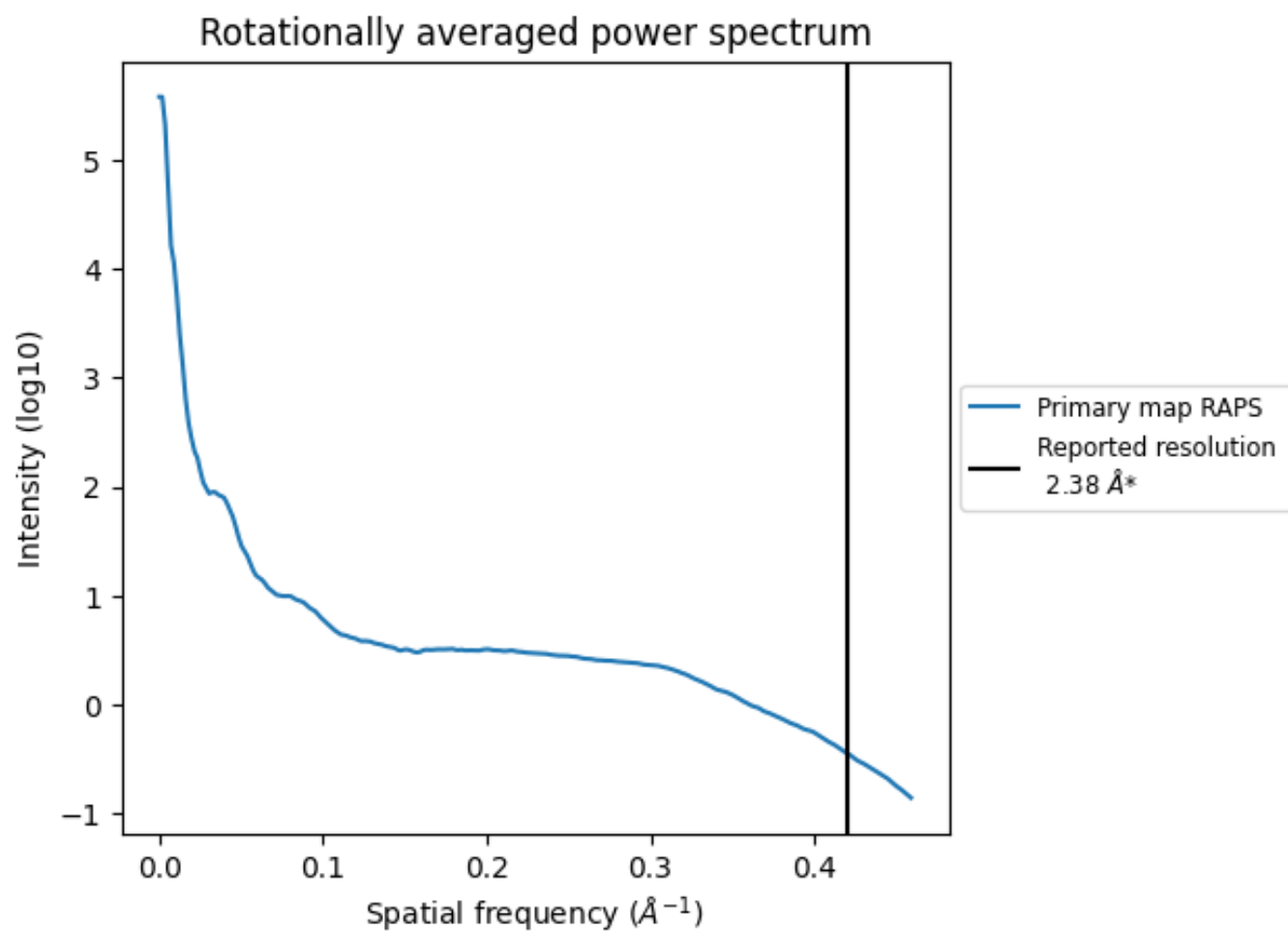
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 894 nm^3 ; this corresponds to an approximate mass of 807 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 0.420 $\text{\AA}^{-1}$

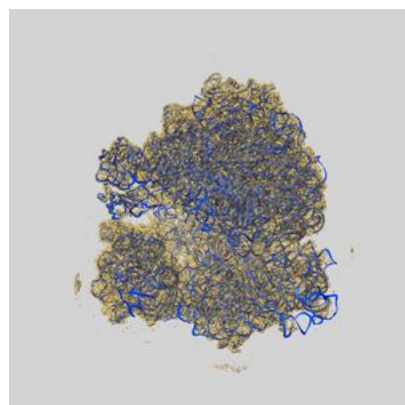
8 Fourier-Shell correlation ⓘ

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

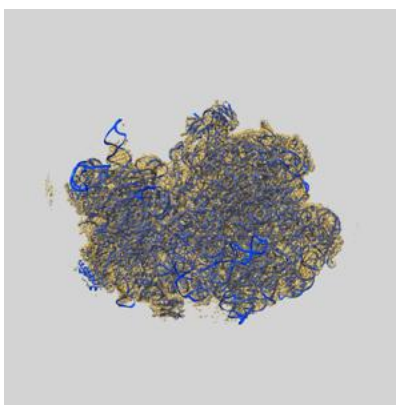
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24739 and PDB model 7RYG. Per-residue inclusion information can be found in section [3](#) on page [14](#).

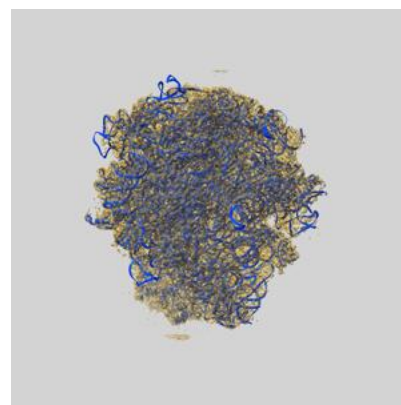
9.1 Map-model overlay [i](#)



X



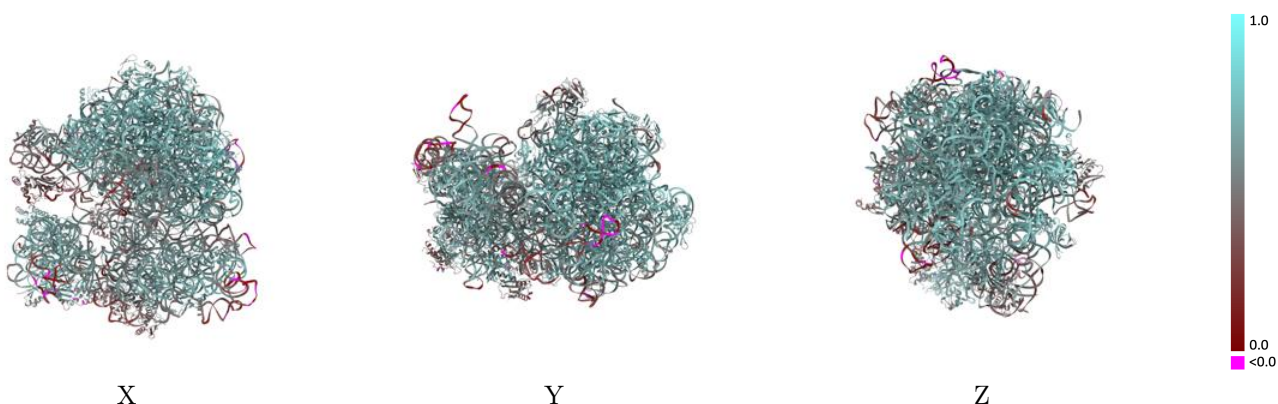
Y



Z

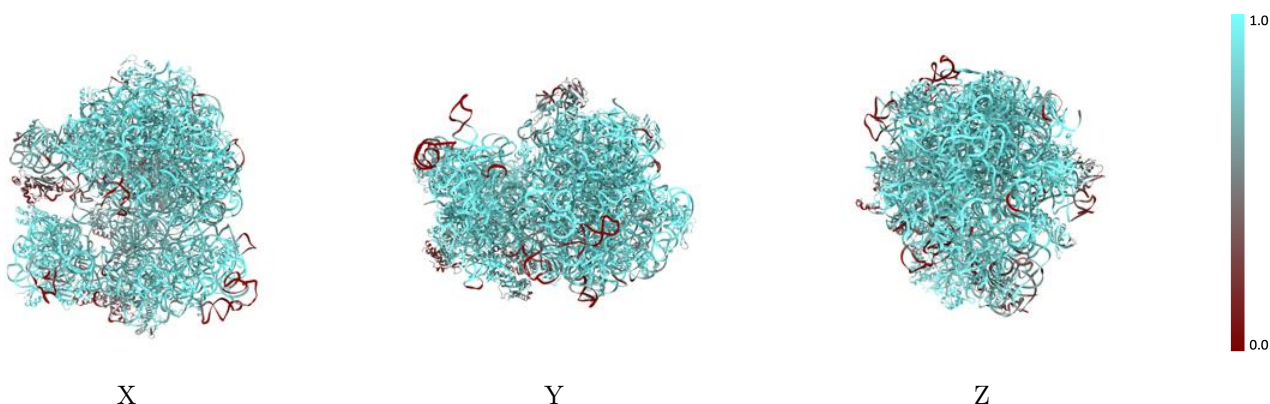
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



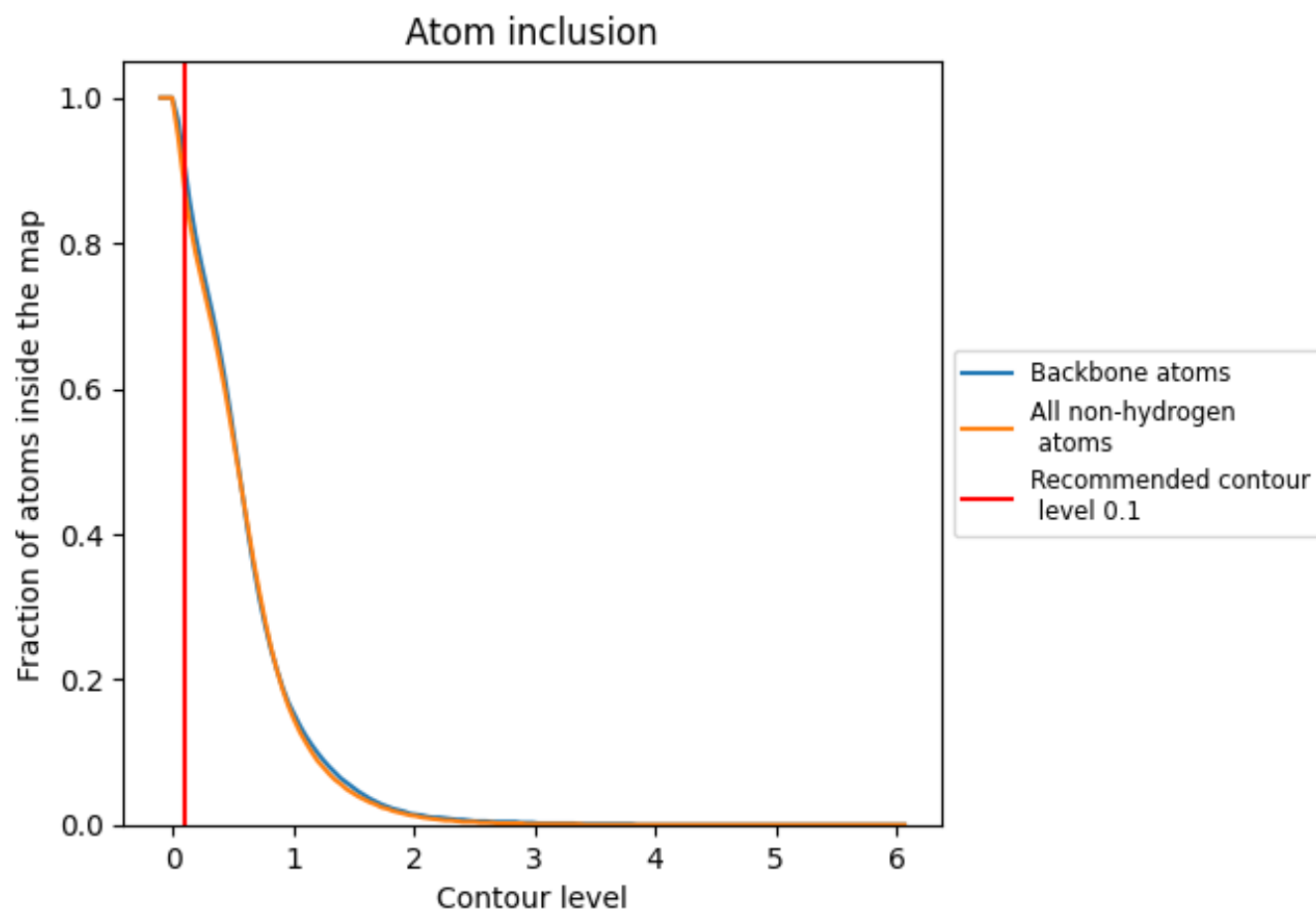
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5960
0	 0.8750	 0.6340
1	 0.9800	 0.7360
2	 0.9840	 0.7180
3	 0.8250	 0.5900
A	 0.9090	 0.6260
B	 0.7270	 0.4930
C	 0.9620	 0.6900
D	 0.9660	 0.7220
E	 0.9270	 0.6880
F	 0.2510	 0.3340
G	 0.5580	 0.4820
H	 0.5590	 0.4720
I	 0.9720	 0.7180
J	 0.9620	 0.6810
K	 0.9620	 0.7100
L	 0.9290	 0.6660
M	 0.9900	 0.7330
N	 0.7760	 0.5340
O	 0.9320	 0.6700
P	 0.9930	 0.7300
Q	 0.9540	 0.7020
R	 0.9630	 0.7150
S	 0.8810	 0.6560
T	 0.8310	 0.6180
U	 0.8690	 0.6280
V	 0.9420	 0.7080
W	 0.9310	 0.6860
X	 0.7540	 0.5610
Y	 0.9400	 0.6990
Z	 0.9300	 0.6850
a	 0.8850	 0.5580
b	 0.3370	 0.3450
c	 0.9650	 0.6220
d	 0.6890	 0.4320



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Chain	Atom inclusion	Q-score
e	 0.9530	 0.6220
f	 0.6590	 0.4130
g	 0.8270	 0.4880
h	 0.9660	 0.6680
i	 0.9860	 0.6630
j	 0.9510	 0.6200
k	 0.5700	 0.3900
l	 0.7560	 0.5290
m	 0.9860	 0.6370
n	 0.9690	 0.6610
o	 0.9680	 0.6290
p	 0.9580	 0.6670
q	 0.9310	 0.6120
r	 0.8350	 0.5090
s	 0.9860	 0.6560
t	 0.9640	 0.6410
u	 0.2100	 0.3140
v	 0.4330	 0.2890
w	 0.8310	 0.3420