



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 04:43 AM EDT

PDB ID : 7M4X / pdb_00007m4x
EMDB ID : EMD-23669
Title : A. baumannii Ribosome-Eravacycline complex: P-site tRNA 70S
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2021-03-22
Resolution : 2.66 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

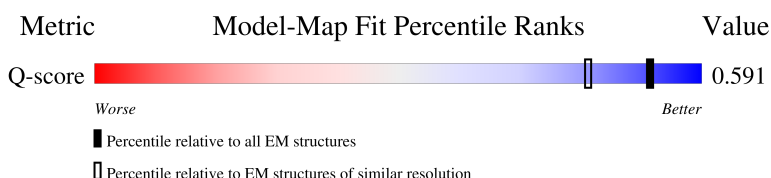
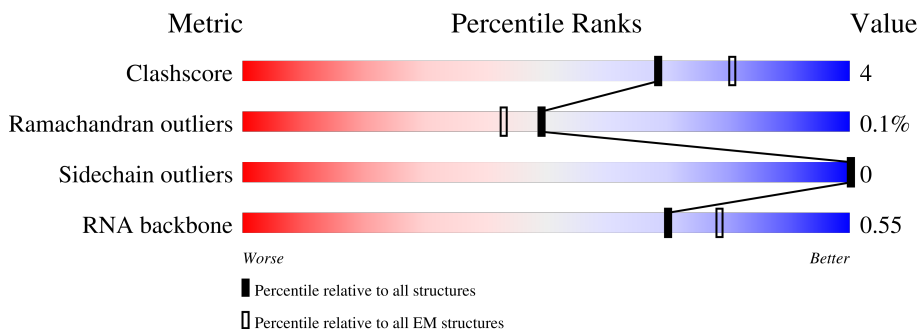
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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 57 unique types of molecules in this entry. The entry contains 139446 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	49	Total	C	N	O	S	0	0
			409	263	74	70	2		

- 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	2730	Total	C	N	O	P	0	0
			58566	26143	10721	18972	2730		

- 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	210	Total	C	N	O	S	0	0
			1566	969	296	298	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	82	Total	C	N	O	S	0	0
			616	382	119	113	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	55	Total	C	N	O	S	0	0
			456	271	102	82	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	151	Total	C	N	O	S	0	0
			1188	743	225	213	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	99	Total	C	N	O	S	0	0
			793	496	148	146	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	63	Total	C	N	O	S	0	0
			522	327	105	89	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		

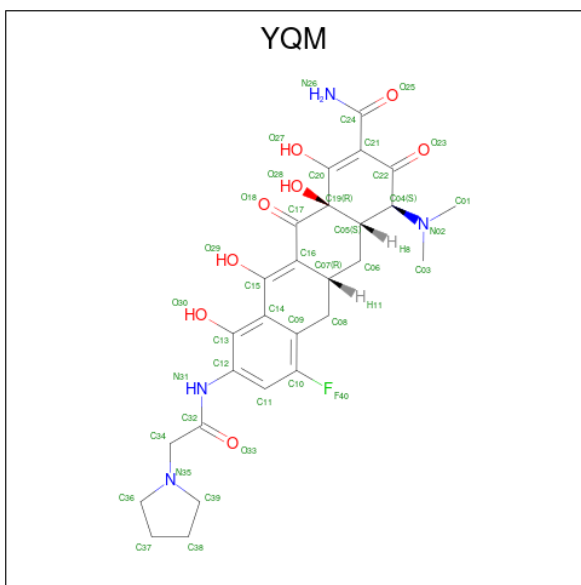
- Molecule 53 is a RNA chain called mRNA.

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 Eravacycline (CCD ID: YQM) (formula: C₂₇H₃₁FN₄O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total 40	C 27	F 1	N 4	O 8	0
55	A	1	Total 40	C 27	F 1	N 4	O 8	0
55	a	1	Total 40	C 27	F 1	N 4	O 8	0

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

Mol	Chain	Residues	Atoms	AltConf
56	A	134	Total Mg 134 134	0
56	B	1	Total Mg 1 1	0
56	C	1	Total Mg 1 1	0
56	D	1	Total Mg 1 1	0
56	K	1	Total Mg 1 1	0
56	a	51	Total Mg 51 51	0
56	t	1	Total Mg 1 1	0

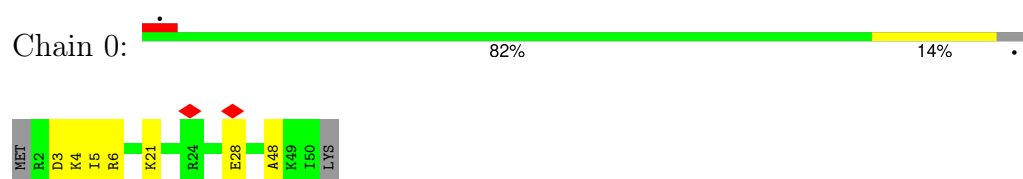
- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	2	1	Total 1	O 1	0
57	A	392	Total 392	O 392	0
57	B	3	Total 3	O 3	0
57	C	7	Total 7	O 7	0
57	D	3	Total 3	O 3	0
57	E	2	Total 2	O 2	0
57	I	1	Total 1	O 1	0
57	K	5	Total 5	O 5	0
57	R	2	Total 2	O 2	0
57	Z	1	Total 1	O 1	0
57	a	131	Total 131	O 131	0
57	n	4	Total 4	O 4	0

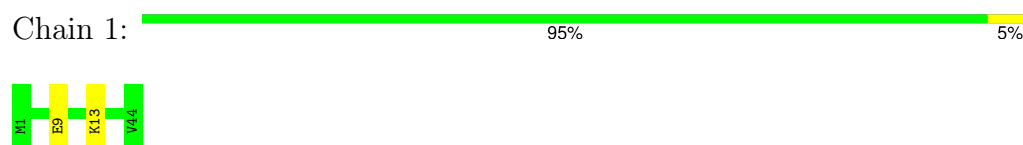
3 Residue-property plots [i](#)

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

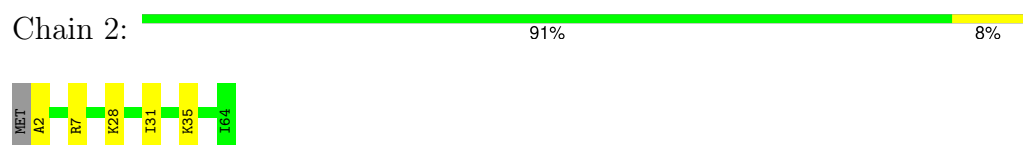
- Molecule 1: 50S ribosomal protein L33



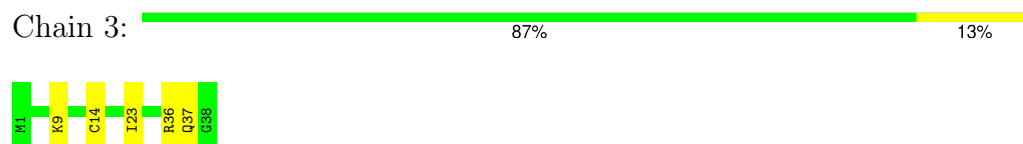
- Molecule 2: 50S ribosomal protein L34



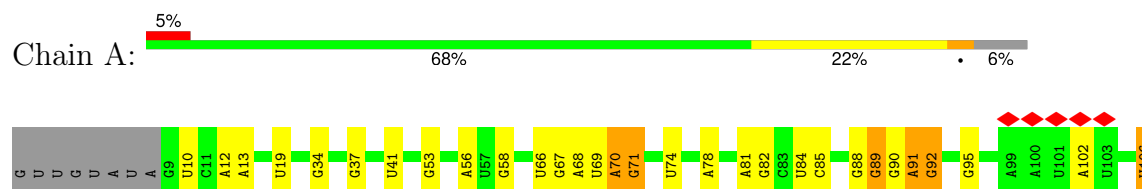
- Molecule 3: 50S ribosomal protein L35

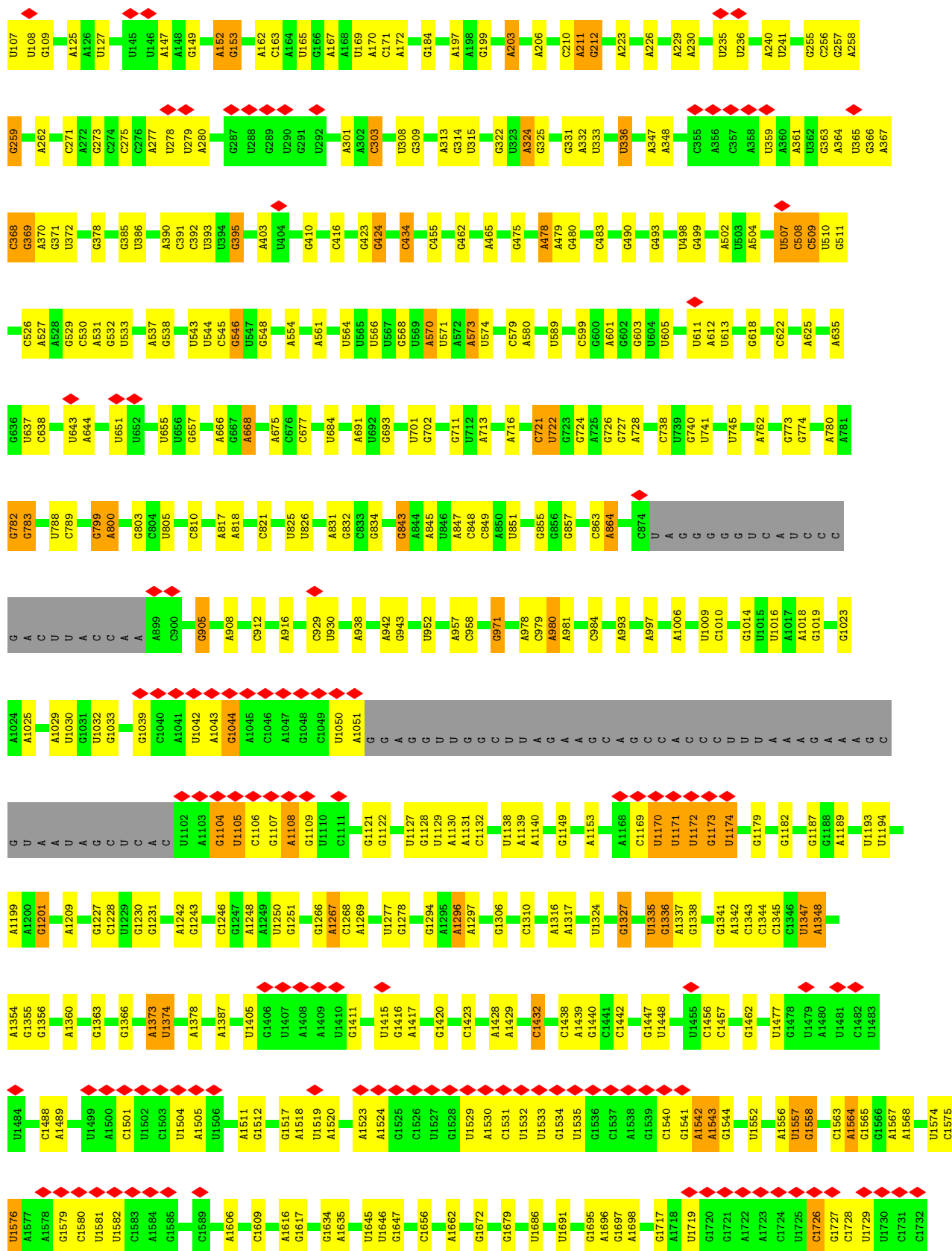


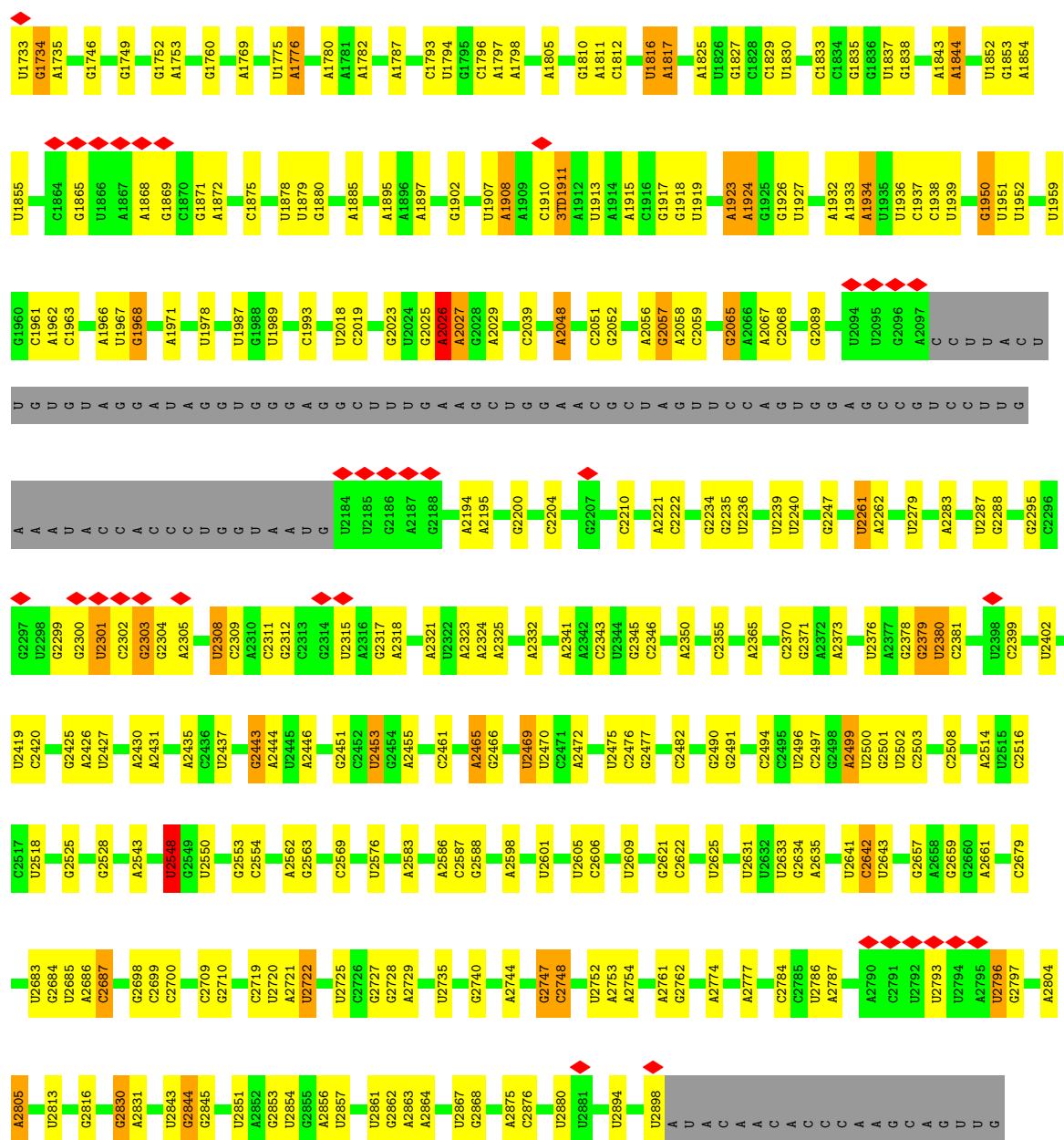
- Molecule 4: 50S ribosomal protein L36



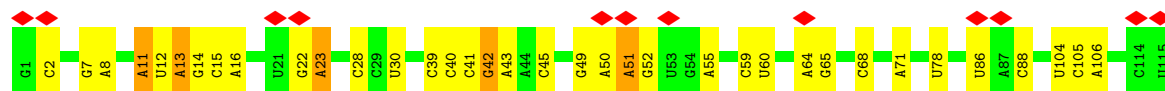
- Molecule 5: 23s ribosomal RNA



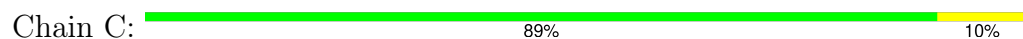




• Molecule 6: 5s ribosomal RNA



• Molecule 7: 50S ribosomal protein L2



LEU	ASN	GLU	VAL	ASN	ILE	VAL	THR	ALA	LYS	ALA	GLY	ASP	GLU	GLY	LYS	LEU	PRO	GLY	GLY	THR	ARG	ASP	ILE	ASP	ASP	ALA	LEU	THR	ASN	ASN	GLY	LEU	THR	VAL	ASP	ARG	ARG	GLU	VAL	ARG	LEU	PRO	ASN	GLY	ALA	LEU	ARG	THR	THR	GLY	GLU	PRO	ILE	ALA	ALA	ILE
M1	D2	V3	I4	L5	L6	Q7	R8	I9	K10	M11	L12	G13	K14	L15	G16	D17	K18	V19	S20	V21	Q33	G34	V37	A38	A39	T40	E41	A42	M43	T44	A45	A46	F47	E48	A49	R50	R51	A52	E53	L54	E55	K56	Q57	E58	A59	E60	VAL	LEU	ALA	ALA	GLN	ALA	ARG	ALA	GLU	

GLN
LEU
HIS
HIS
ASP
VAL
VAL
ALA
GLU
VAL
LEU
VAL
THR
THR
TLE
VAL
SER
GLU

- Molecule 13: 50S ribosomal protein L13

Chain I:  98%



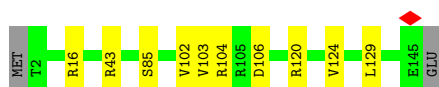
- Molecule 14: 50S ribosomal protein L14

Chain J:  95%



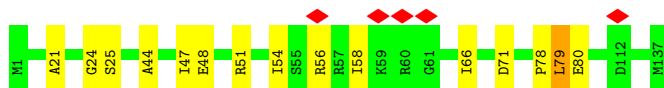
- Molecule 15: 50S ribosomal protein L15

Chain K:  92%



- Molecule 16: 50S ribosomal protein L16

Chain L:  89%



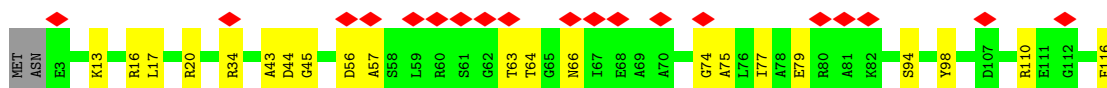
- Molecule 17: 50S ribosomal protein L17

Chain M:  84%



- Molecule 18: 50S ribosomal protein L18

Chain N:  16%



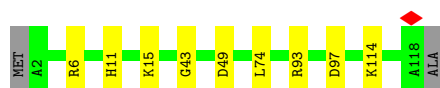
- Molecule 19: 50S ribosomal protein L19

Chain O:  79% 16% 5%



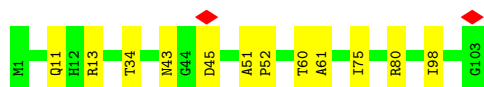
- Molecule 20: 50S ribosomal protein L20

Chain P:  91% 8%

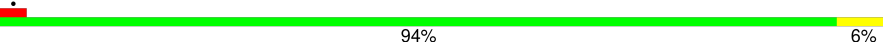


- Molecule 21: 50S ribosomal protein L21

Chain Q:  88% 12%



- Molecule 22: 50S ribosomal protein L22

Chain R:  94% 6%

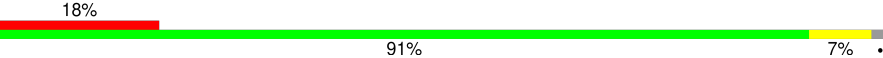


- Molecule 23: 50S ribosomal protein L23

Chain S:  10% 80% 6% 14%

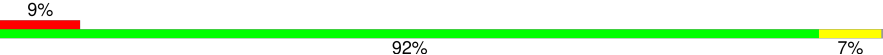


- Molecule 24: 50S ribosomal protein L24

Chain T:  18% 91% 7%

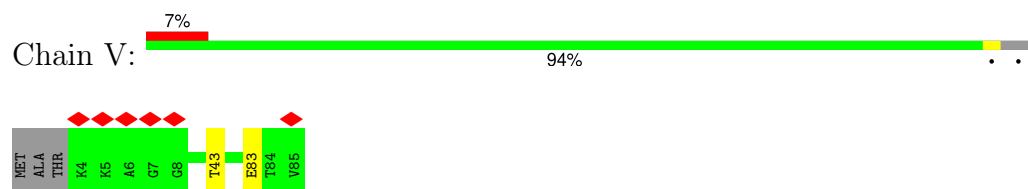


- Molecule 25: 50S ribosomal protein L25

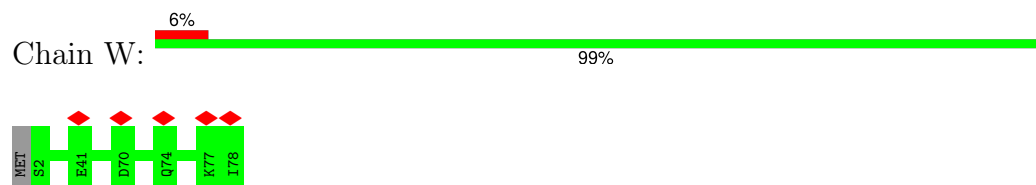
Chain U:  9% 92% 7%



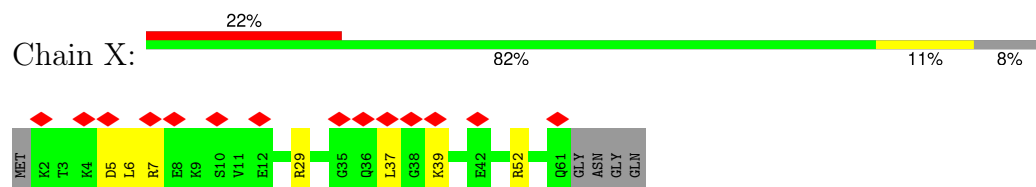
- Molecule 26: 50S ribosomal protein L27



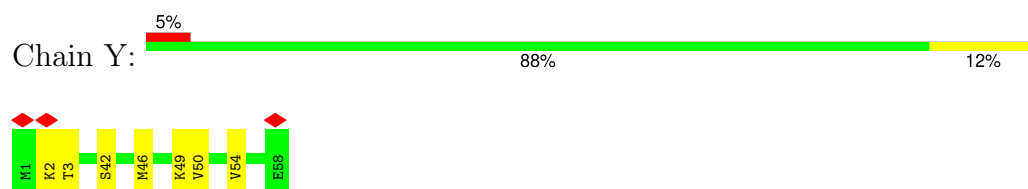
- Molecule 27: 50S ribosomal protein L28



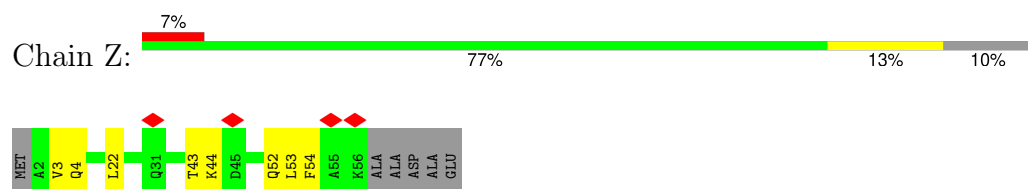
- Molecule 28: 50S ribosomal protein L29



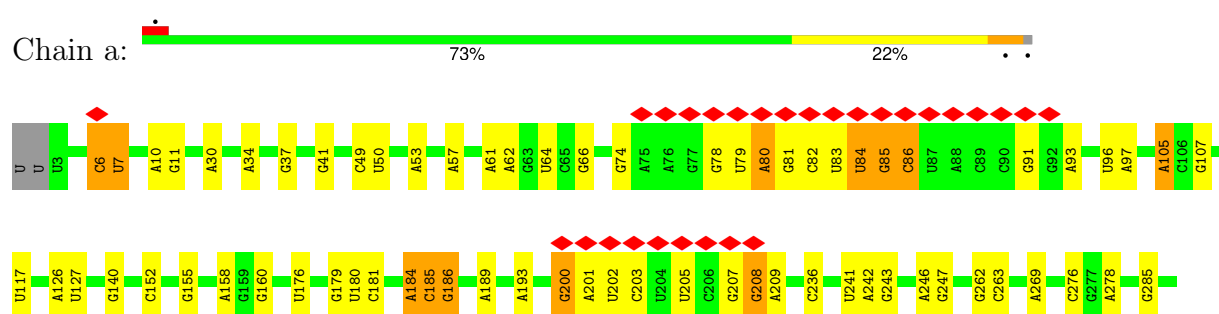
- Molecule 29: 50S ribosomal protein L30



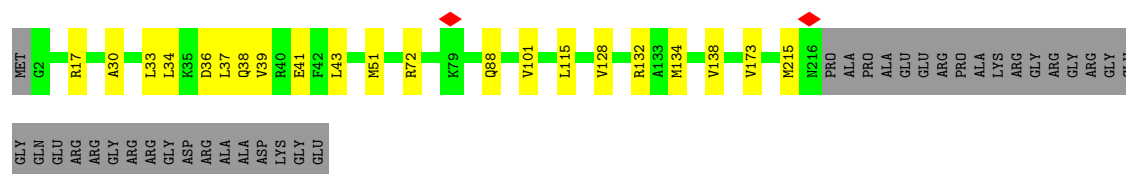
- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 16s Ribosomal RNA

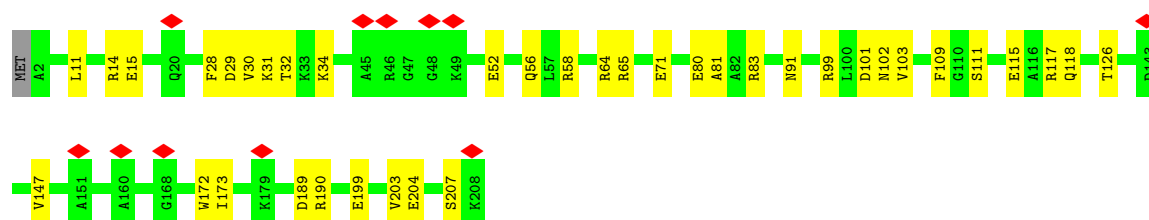


Chain c: 



- Molecule 34: 30S ribosomal protein S4

Chain d: 



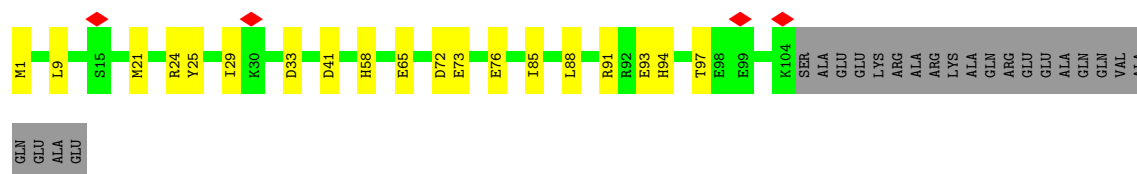
- Molecule 35: 30S ribosomal protein S5

Chain e: 



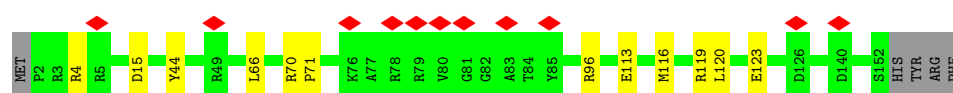
- Molecule 36: 30S ribosomal protein S6

Chain f: 



- Molecule 37: 30S ribosomal protein S7

Chain g: 



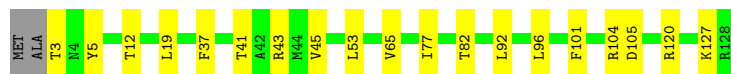
- Molecule 38: 30S ribosomal protein S8

Chain h: 



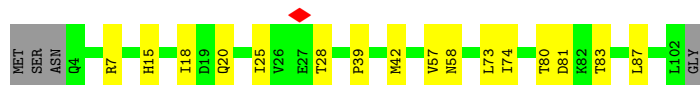
- Molecule 39: 30S ribosomal protein S9

Chain i:  84% 15% .



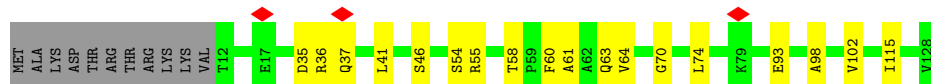
- Molecule 40: 30S ribosomal protein S10

Chain j:  81% 16% .



- Molecule 41: 30S ribosomal protein S11

Chain k:  77% 14% 9% .



- Molecule 42: 30S ribosomal protein S12

Chain l:  85% 13% ..



- Molecule 43: 30S ribosomal protein S13

Chain m:  86% 11% .



- Molecule 44: 30S ribosomal protein S14

Chain n:  84% 15% .



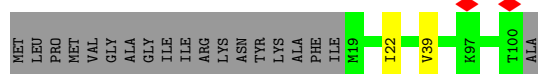
- Molecule 45: 30S ribosomal protein S15

Chain o:  92% 7% .



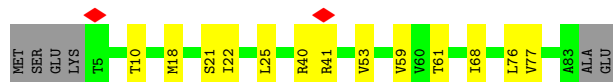
- Molecule 46: 30S ribosomal protein S16

Chain p:  79% 19%



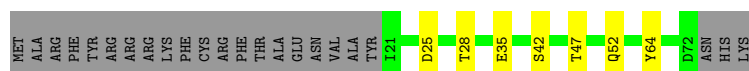
- Molecule 47: 30S ribosomal protein S17

Chain q:  78% 15% 7%



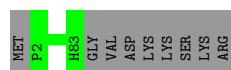
- Molecule 48: 30S ribosomal protein S18

Chain r:  60% 9% 31%



- Molecule 49: 30S ribosomal protein S19

Chain s:  90% 10%



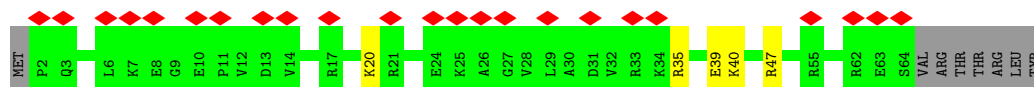
- Molecule 50: 30S ribosomal protein S20

Chain t:  81% 17%



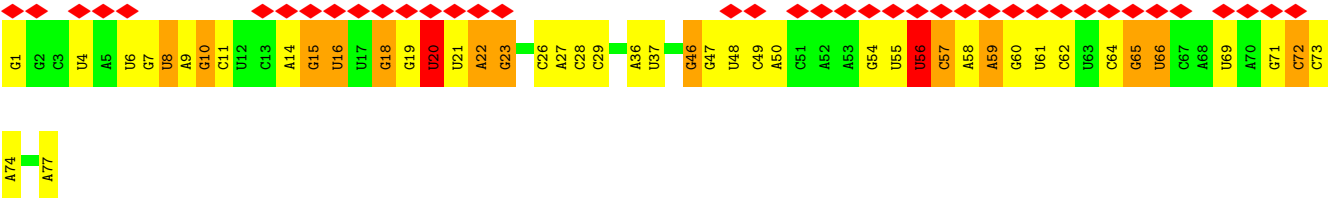
- Molecule 51: 30S ribosomal protein S21

Chain u:  32% 82% 7% 11%



- Molecule 52: tRNA-met

Chain v:  51% 40% 40% 17%



- Molecule 53: mRNA

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40679	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.097	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, YQM, OMG, H2U, MG, PSU, 5MU, MA6, 5MC, OMU, 2MA, 2MG, G7M, 4SU, 4OC, ZN, 3TD, UR3

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	0.11	0/416	0.30	0/552
2	1	0.14	0/367	0.29	0/481
3	2	0.12	0/515	0.34	0/678
4	3	0.16	0/296	0.36	0/389
5	A	0.10	0/65229	0.26	0/101736
6	B	0.08	0/2739	0.26	0/4266
7	C	0.11	0/2152	0.31	0/2891
8	D	0.12	0/1584	0.30	0/2135
9	E	0.11	0/1537	0.26	0/2073
10	F	0.17	0/1390	0.46	0/1863
11	G	0.12	0/1337	0.31	0/1807
12	H	0.13	0/461	0.34	0/616
13	I	0.12	0/1151	0.29	0/1551
14	J	0.13	0/956	0.30	0/1286
15	K	0.10	0/1079	0.27	0/1439
16	L	0.14	0/1104	0.33	0/1475
17	M	0.14	0/956	0.34	0/1282
18	N	0.10	0/865	0.29	0/1156
19	O	0.17	0/925	0.36	0/1241
20	P	0.12	0/947	0.29	0/1262
21	Q	0.12	0/818	0.30	0/1094
22	R	0.12	0/831	0.25	0/1113
23	S	0.13	0/716	0.27	0/957
24	T	0.09	0/770	0.24	0/1034
25	U	0.11	0/770	0.30	0/1036
26	V	0.11	0/624	0.33	0/832
27	W	0.10	0/642	0.29	0/856
28	X	0.10	0/487	0.23	0/646
29	Y	0.13	0/468	0.28	0/624
30	Z	0.10	0/462	0.27	0/615
31	a	0.12	0/36476	0.27	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.15	0/1799	0.35	0/2429
33	c	0.16	0/1714	0.36	0/2304
34	d	0.11	0/1653	0.29	0/2213
35	e	0.12	0/1141	0.30	0/1537
36	f	0.17	0/882	0.44	0/1189
37	g	0.14	0/1205	0.33	0/1614
38	h	0.12	0/993	0.30	0/1331
39	i	0.13	0/1002	0.31	0/1339
40	j	0.13	0/803	0.35	0/1085
41	k	0.12	0/878	0.33	0/1189
42	l	0.12	0/958	0.34	0/1284
43	m	0.15	0/913	0.38	0/1226
44	n	0.14	0/803	0.33	0/1071
45	o	0.12	0/715	0.27	0/958
46	p	0.10	0/655	0.32	0/879
47	q	0.12	0/628	0.33	0/847
48	r	0.12	0/432	0.30	0/583
49	s	0.14	0/664	0.32	0/897
50	t	0.15	0/669	0.31	0/892
51	u	0.11	0/528	0.31	0/697
52	v	0.16	1/1739 (0.1%)	0.28	0/2709
53	w	0.13	0/72	0.23	0/110
All	All	0.11	1/149916 (0.0%)	0.28	0/224264

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	O3'-P	5.12	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	409	0	437	4	0
2	1	363	0	401	1	0
3	2	509	0	566	5	0
4	3	295	0	326	5	0
5	A	58566	0	29450	256	0
6	B	2450	0	1241	21	0
7	C	2111	0	2176	20	0
8	D	1566	0	1605	12	0
9	E	1516	0	1569	8	0
10	F	1370	0	1420	52	0
11	G	1318	0	1373	16	0
12	H	458	0	480	6	0
13	I	1125	0	1148	2	0
14	J	946	0	1007	6	0
15	K	1071	0	1141	6	0
16	L	1087	0	1162	10	0
17	M	942	0	987	9	0
18	N	857	0	899	14	0
19	O	913	0	968	13	0
20	P	934	0	997	7	0
21	Q	807	0	842	11	0
22	R	826	0	894	5	0
23	S	710	0	768	4	0
24	T	766	0	816	5	0
25	U	760	0	783	5	0
26	V	616	0	626	2	0
27	W	632	0	667	0	0
28	X	486	0	528	6	0
29	Y	463	0	488	5	0
30	Z	456	0	448	5	0
31	a	32782	0	16507	169	0
32	b	1769	0	1787	32	0
33	c	1690	0	1774	16	0
34	d	1631	0	1691	25	0
35	e	1129	0	1174	8	0
36	f	867	0	868	15	0
37	g	1188	0	1239	7	0
38	h	985	0	1047	11	0
39	i	991	0	1048	12	0
40	j	793	0	826	13	0
41	k	862	0	877	12	0
42	l	945	0	998	13	0
43	m	903	0	962	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	792	0	833	10	0
45	o	705	0	712	4	0
46	p	644	0	655	1	0
47	q	621	0	665	11	0
48	r	426	0	447	5	0
49	s	646	0	663	0	0
50	t	663	0	715	9	0
51	u	522	0	565	5	0
52	v	1636	0	835	25	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	A	80	0	0	1	0
55	a	40	0	0	0	0
56	A	134	0	0	0	0
56	B	1	0	0	0	0
56	C	1	0	0	0	0
56	D	1	0	0	0	0
56	K	1	0	0	0	0
56	a	51	0	0	0	0
56	t	1	0	0	0	0
57	2	1	0	0	0	0
57	A	392	0	0	14	0
57	B	3	0	0	0	0
57	C	7	0	0	0	0
57	D	3	0	0	2	0
57	E	2	0	0	0	0
57	I	1	0	0	0	0
57	K	5	0	0	0	0
57	R	2	0	0	0	0
57	Z	1	0	0	0	0
57	a	131	0	0	10	0
57	n	4	0	0	0	0
All	All	139446	0	93134	833	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 (833) 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)
52:v:55:5MU:O2'	52:v:56:PSU:O4'	1.79	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:424:G:O2'	34:d:34:LYS:NZ	2.02	0.93
17:M:37:THR:HG22	17:M:39:PRO:HD2	1.50	0.91
31:a:85:G:O2'	31:a:86:C:OP2	1.87	0.90
5:A:799:G:O2'	5:A:800:A:OP1	1.89	0.89
5:A:363:G:OP2	5:A:364:A:O2'	1.92	0.88
5:A:1923:A:O2'	5:A:1924:A:O5'	1.92	0.87
6:B:55:A:O2'	10:F:27:GLU:OE2	1.90	0.87
5:A:1306:G:OP2	5:A:1306:G:N2	2.08	0.86
48:r:25:ASP:OD2	48:r:28:THR:OG1	1.92	0.86
31:a:423:U:OP2	31:a:424:G:O2'	1.93	0.86
5:A:1865:G:N2	5:A:1868:A:OP2	2.08	0.86
52:v:16:U:O2'	52:v:61:U:O2	1.94	0.86
31:a:739:G:OP1	45:o:58:ARG:NH2	2.09	0.85
5:A:849:C:OP1	29:Y:49:LYS:NZ	2.09	0.85
5:A:533:U:O2'	20:P:49:ASP:OD2	1.97	0.82
31:a:504:C:OP2	31:a:505:U:O2'	1.98	0.82
31:a:572:G:O2'	31:a:818:G:OP2	1.96	0.82
5:A:210:C:OP2	5:A:211:A:O2'	1.98	0.81
31:a:728:G:OP2	57:a:1701:HOH:O	1.96	0.81
52:v:22:A:O2'	52:v:23:G:O4'	1.98	0.81
9:E:86:ALA:O	9:E:87:ARG:NH1	2.14	0.81
5:A:1843:A:O2'	5:A:1844:A:N7	2.14	0.80
31:a:407:A:O2'	31:a:409:G:OP2	1.99	0.80
31:a:1195:G:OP2	57:a:1702:HOH:O	1.99	0.80
31:a:1394:C:OP2	35:e:28:ARG:NH2	2.15	0.80
10:F:118:SER:O	10:F:128:TYR:OH	1.98	0.79
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.00	0.79
5:A:1246:C:OP2	20:P:6:ARG:NH2	2.16	0.79
6:B:50:A:O2'	6:B:51:A:N7	2.15	0.79
5:A:2465:A:N6	5:A:2477:G:O2'	2.15	0.79
5:A:1816:U:HO2'	7:C:157:SER:HG	1.30	0.79
31:a:691:A:OP1	41:k:54:SER:OG	2.01	0.78
31:a:200:G:O4'	31:a:461:A:N6	2.17	0.78
5:A:1563:C:O2	5:A:1564:A:O2'	2.00	0.78
31:a:409:G:N2	31:a:425:U:OP2	2.16	0.78
39:i:104:ARG:NH1	39:i:105:ASP:O	2.17	0.77
8:D:140:SER:O	57:D:401:HOH:O	2.01	0.77
5:A:2023:G:O6	57:A:3401:HOH:O	2.01	0.77
5:A:184:G:OP2	5:A:184:G:N2	2.13	0.77
5:A:1923:A:HO2'	5:A:1924:A:C5'	1.98	0.77
52:v:10:G:O6	52:v:46:G:N2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:689:U:OP1	57:a:1703:HOH:O	2.03	0.76
5:A:1327:G:OP2	57:A:3403:HOH:O	2.02	0.76
5:A:1230:G:O2'	5:A:1231:G:O4'	2.03	0.76
5:A:1749:G:N2	5:A:1752:G:OP2	2.19	0.76
5:A:2057:G:OP2	57:A:3406:HOH:O	2.04	0.75
52:v:20:H2U:O2'	52:v:22:A:OP1	2.03	0.75
31:a:207:G:O2'	31:a:208:G:O4'	2.03	0.75
5:A:2311:C:O2	10:F:125:ARG:NH2	2.20	0.75
5:A:2853:G:N2	5:A:2856:A:OP2	2.18	0.75
31:a:813:A:OP2	57:a:1704:HOH:O	2.03	0.75
31:a:1193:A:O2'	31:a:1194:A:OP1	2.05	0.75
10:F:54:VAL:HG23	10:F:65:PRO:HG2	1.68	0.75
31:a:1446:U:O2'	31:a:1447:G:O5'	2.03	0.75
5:A:1025:A:N3	5:A:2482:C:O2'	2.18	0.74
5:A:821:C:OP2	57:A:3407:HOH:O	2.04	0.74
5:A:789:C:OP2	57:A:3405:HOH:O	2.04	0.74
5:A:2301:U:O2'	10:F:133:LYS:NZ	2.19	0.73
41:k:55:ARG:O	41:k:58:THR:HG22	1.88	0.73
5:A:1908:A:HO2'	31:a:1491:G:HO2'	1.32	0.73
5:A:1517:G:OP2	5:A:1518:A:O2'	2.04	0.72
11:G:89:LEU:CD2	11:G:162:VAL:HG22	2.19	0.72
5:A:1776:A:OP1	57:A:3408:HOH:O	2.06	0.72
44:n:6:MET:SD	44:n:9:ARG:NH2	2.63	0.72
46:p:22:ILE:HG12	46:p:39:VAL:HG22	1.69	0.72
34:d:80:GLU:OE2	34:d:83:ARG:NH2	2.23	0.72
39:i:41:THR:O	39:i:45:VAL:HG23	1.90	0.72
5:A:167:A:N3	5:A:2204:C:O2'	2.21	0.72
5:A:1937:C:N4	5:A:1961:C:O4'	2.23	0.71
5:A:2747:G:O2'	5:A:2748:C:OP1	2.08	0.71
5:A:1542:A:O2'	5:A:1543:A:O5'	2.09	0.71
31:a:889:A:OP2	57:a:1705:HOH:O	2.07	0.71
5:A:322:G:O2'	5:A:324:A:OP2	2.08	0.71
32:b:13:GLN:O	32:b:210:ARG:NH2	2.23	0.71
5:A:1656:C:OP1	57:D:401:HOH:O	2.07	0.71
31:a:571:A:OP2	57:a:1707:HOH:O	2.09	0.70
31:a:649:U:O4	31:a:749:G:O2'	2.09	0.70
5:A:1348:A:O3'	7:C:38:LYS:NZ	2.23	0.70
5:A:2518:U:O2'	5:A:2643:U:OP1	2.04	0.70
5:A:85:C:OP1	28:X:7:ARG:NH2	2.25	0.70
5:A:2373:A:O2'	18:N:116:PHE:OXT	2.08	0.69
31:a:1123:U:OP1	40:j:7:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:97:ASP:OD2	21:Q:13:ARG:NE	2.25	0.69
12:H:5:LEU:HD13	12:H:9:ILE:HD13	1.74	0.69
31:a:908:U:OP2	42:l:94:ARG:NH2	2.26	0.69
5:A:2309:C:O4'	10:F:37:ASN:ND2	2.25	0.69
5:A:2435:A:N3	57:A:3421:HOH:O	2.25	0.69
52:v:19:G:H5''	52:v:20:H2U:H52	1.74	0.69
33:c:134:MET:O	33:c:138:VAL:HG23	1.93	0.68
31:a:977:C:O2	57:a:1708:HOH:O	2.10	0.68
31:a:84:U:O4'	31:a:85:G:N2	2.26	0.68
36:f:72:ASP:O	36:f:76:GLU:OE1	2.11	0.68
31:a:907:C:OP2	42:l:18:LYS:NZ	2.27	0.68
39:i:3:THR:N	39:i:19:LEU:O	2.27	0.68
52:v:55:5MU:H2'	52:v:56:PSU:C4	2.29	0.68
31:a:61:A:N1	57:a:1714:HOH:O	2.27	0.67
22:R:37:ASN:OD1	22:R:48:LYS:NZ	2.24	0.67
5:A:1938:C:OP2	5:A:1939:U:O2'	2.06	0.67
31:a:189:A:O2'	50:t:59:ASP:OD2	2.12	0.67
5:A:1335:U:O2'	23:S:60:THR:OG1	2.10	0.66
5:A:2496:U:O2	57:A:3410:HOH:O	2.09	0.66
5:A:1717:G:O2'	5:A:1735:A:N6	2.28	0.66
31:a:637:A:O2'	38:h:108:SER:OG	2.14	0.66
32:b:219:MET:O	32:b:223:ILE:HD12	1.95	0.66
5:A:2631:U:O2'	8:D:82:GLU:OE2	2.11	0.66
18:N:63:THR:O	18:N:64:THR:OG1	2.12	0.66
31:a:1433:U:OP1	50:t:18:ARG:NH2	2.29	0.66
5:A:2894:U:O2'	13:I:134:ALA:O	2.13	0.65
5:A:2379:G:O2'	5:A:2380:U:OP1	2.14	0.65
5:A:570:A:OP2	21:Q:80:ARG:NH1	2.30	0.65
31:a:10:A:N6	34:d:204:GLU:O	2.30	0.65
5:A:2308:U:O2	10:F:37:ASN:ND2	2.29	0.65
31:a:96:U:O2'	31:a:97:A:N7	2.28	0.65
37:g:15:ASP:OD1	37:g:44:TYR:OH	2.14	0.65
12:H:1:MET:N	12:H:21:VAL:O	2.24	0.64
5:A:691:A:OP2	7:C:39:ARG:NH2	2.30	0.64
10:F:54:VAL:HA	10:F:57:MET:HE3	1.77	0.64
10:F:57:MET:HE1	10:F:87:CYS:CB	2.26	0.64
31:a:656:U:OP1	45:o:8:ARG:NH1	2.29	0.64
31:a:1224:A:OP1	43:m:93:ARG:NH2	2.31	0.64
5:A:1968:G:OP2	57:A:3413:HOH:O	2.15	0.64
3:2:31:ILE:O	3:2:35:LYS:NZ	2.27	0.64
5:A:1810:G:OP2	5:A:1811:A:O2'	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:200:G:O2'	31:a:201:A:O4'	2.16	0.63
5:A:277:A:N6	5:A:367:A:OP2	2.32	0.63
33:c:37:LEU:O	33:c:41:GLU:OE1	2.16	0.63
8:D:86:THR:HG22	8:D:89:GLU:OE1	1.99	0.63
10:F:48:LYS:NZ	10:F:147:ASP:OD2	2.20	0.63
15:K:124:VAL:HG11	15:K:129:LEU:HD21	1.81	0.63
6:B:55:A:O4'	10:F:24:ASN:ND2	2.30	0.63
10:F:162:THR:HG22	10:F:163:ASP:H	1.64	0.63
41:k:93:GLU:OE2	51:u:20:LYS:NZ	2.22	0.63
5:A:1432:C:O2'	5:A:1512:G:O2'	2.14	0.62
6:B:41:C:O2	10:F:92:ARG:NH1	2.32	0.62
31:a:176:U:O4	57:a:1710:HOH:O	2.12	0.62
5:A:1962:A:N3	5:A:2588:G:O2'	2.31	0.62
28:X:5:ASP:OD1	28:X:6:LEU:N	2.33	0.62
5:A:89:G:O2'	5:A:90:G:O4'	2.17	0.62
3:2:2:ALA:N	5:A:589:U:O2	2.33	0.62
11:G:13:ASN:OD1	11:G:14:GLY:N	2.30	0.62
20:P:93:ARG:NH2	21:Q:11:GLN:O	2.32	0.62
31:a:406:G:OP2	34:d:31:LYS:NZ	2.33	0.61
5:A:2687:C:HO2'	5:A:2867:U:HO2'	1.47	0.61
18:N:75:ALA:O	18:N:79:GLU:OE1	2.18	0.61
31:a:973:G:OP2	31:a:1355:U:O2'	2.18	0.61
5:A:462:G:N2	5:A:465:A:OP2	2.27	0.61
5:A:483:C:OP2	24:T:45:LYS:NZ	2.23	0.61
31:a:888:U:OP2	31:a:903:A:N6	2.31	0.61
5:A:1267:A:O2'	5:A:1269:A:OP1	2.19	0.61
43:m:52:GLN:O	43:m:56:ILE:HD12	2.01	0.61
5:A:364:A:OP2	5:A:424:G:O2'	2.20	0.60
5:A:2721:A:O2'	5:A:2722:U:OP2	2.15	0.60
34:d:101:ASP:OD1	34:d:102:ASN:N	2.34	0.60
8:D:139:ASN:ND2	8:D:142:SER:O	2.32	0.60
5:A:527:A:OP1	57:A:3416:HOH:O	2.16	0.60
5:A:1442:C:O2'	5:A:1542:A:N3	2.29	0.60
38:h:106:SER:HB2	38:h:127:ILE:HD11	1.84	0.60
6:B:11:A:O2'	6:B:13:A:OP2	2.20	0.60
32:b:11:LEU:HD13	32:b:45:LEU:HD12	1.83	0.59
39:i:37:PHE:O	39:i:43:ARG:NH1	2.36	0.59
5:A:2453:PSU:O2	57:A:3414:HOH:O	2.16	0.59
47:q:76:LEU:HD23	47:q:77:VAL:N	2.18	0.59
15:K:104:ARG:NE	15:K:106:ASP:OD1	2.34	0.59
31:a:562:U:OP2	31:a:563:G:O2'	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:98:ALA:O	41:k:102:VAL:HG23	2.03	0.59
1:0:3:ASP:OD1	1:0:4:LYS:N	2.36	0.59
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.33	0.59
31:a:496:A:N1	31:a:543:G:O2'	2.35	0.59
31:a:922:G:O2'	31:a:924:G:OP1	2.15	0.59
31:a:976:C:O2	44:n:59:ARG:NH1	2.36	0.59
31:a:808:C:O2'	31:a:898:A:N1	2.35	0.58
8:D:30:VAL:O	8:D:188:SER:OG	2.16	0.58
18:N:20:ARG:NH1	18:N:43:ALA:O	2.36	0.58
38:h:87:TYR:O	38:h:88:ARG:NH1	2.33	0.58
5:A:843:G:O2'	5:A:845:A:N7	2.36	0.58
30:Z:52:GLN:NE2	30:Z:53:LEU:O	2.37	0.58
5:A:721:C:O2'	5:A:722:U:OP1	2.14	0.58
47:q:18:MET:HE3	47:q:21:SER:HB2	1.84	0.58
51:u:39:GLU:OE1	51:u:47:ARG:NH2	2.37	0.58
5:A:2784:C:O2'	5:A:2805:A:N3	2.34	0.57
36:f:21:MET:SD	36:f:24:ARG:NH2	2.77	0.57
18:N:98:TYR:OH	18:N:110:ARG:NH2	2.37	0.57
22:R:22:ASP:OD1	22:R:25:ARG:NH1	2.36	0.57
5:A:1373:A:O2'	5:A:1374:U:OP2	2.19	0.57
10:F:31:ILE:HD12	10:F:158:THR:HG22	1.85	0.57
10:F:148:ARG:O	10:F:150:ARG:NH1	2.38	0.57
31:a:496:A:O4'	31:a:544:A:N6	2.38	0.57
5:A:2861:U:OP2	5:A:2862:G:O2'	2.07	0.57
52:v:54:G:C5	52:v:55:5MU:H71	2.40	0.57
2:1:9:GLU:OE2	2:1:13:LYS:NZ	2.26	0.56
47:q:40:ARG:O	47:q:41:ARG:NE	2.34	0.56
5:A:69:U:O4	5:A:70:A:N6	2.39	0.56
5:A:978:A:OP2	5:A:979:C:N4	2.34	0.56
6:B:13:A:P	6:B:104:U:HO2'	2.29	0.56
34:d:199:GLU:O	34:d:203:VAL:HG23	2.05	0.56
19:O:93:GLY:HA2	19:O:115:GLU:HA	1.87	0.56
1:0:6:ARG:O	1:0:48:ALA:N	2.38	0.56
43:m:88:GLY:O	43:m:92:ARG:HG3	2.06	0.56
6:B:28:C:H1'	6:B:55:A:H61	1.70	0.56
31:a:397:C:O2'	31:a:618:A:N3	2.34	0.56
31:a:809:G:H1'	31:a:810:U:OP2	2.05	0.56
5:A:197:A:N3	5:A:677:C:O2'	2.37	0.56
31:a:400:G:OP2	34:d:117:ARG:NH2	2.39	0.56
31:a:560:A:HO2'	31:a:563:G:HO2'	1.47	0.56
31:a:1522:G:OP2	51:u:40:LYS:NZ	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:293:G:N2	31:a:296:A:OP2	2.38	0.56
51:u:39:GLU:OE2	51:u:47:ARG:NE	2.34	0.56
10:F:17:GLN:NE2	10:F:22:ILE:O	2.39	0.55
7:C:171:TYR:HB3	7:C:183:LYS:HE2	1.89	0.55
37:g:116:MET:O	37:g:120:LEU:HD23	2.06	0.55
7:C:135:MET:O	7:C:167:ARG:NH2	2.39	0.55
10:F:31:ILE:CD1	10:F:158:THR:HG22	2.36	0.55
12:H:5:LEU:HD11	12:H:12:LEU:HB3	1.88	0.55
31:a:1314:C:OP1	44:n:56:SER:OG	2.13	0.55
6:B:50:A:H62	18:N:34:ARG:HG2	1.72	0.55
10:F:15:LYS:O	10:F:19:GLU:OE1	2.25	0.55
52:v:18:G:N2	52:v:59:A:OP1	2.40	0.55
5:A:1556:A:H4'	5:A:1557:U:H3'	1.89	0.55
23:S:5:ARG:O	23:S:9:VAL:HG13	2.07	0.55
33:c:30:ALA:O	33:c:34:LEU:HD23	2.06	0.55
5:A:2312:G:O4'	10:F:125:ARG:NH1	2.36	0.55
10:F:68:THR:HG22	10:F:86:GLY:C	2.32	0.55
10:F:135:GLN:NE2	10:F:146:ILE:HD11	2.22	0.55
14:J:97:ARG:NH1	31:a:335:C:OP2	2.39	0.55
31:a:683:U:O2'	31:a:700:G:N2	2.38	0.55
33:c:128:VAL:HG13	33:c:132:ARG:NH2	2.23	0.54
5:A:1016:U:OP1	5:A:1032:U:O2'	2.09	0.54
12:H:5:LEU:HD13	12:H:9:ILE:CD1	2.37	0.54
43:m:68:ASP:OD1	43:m:71:ARG:NH2	2.40	0.54
7:C:124:ILE:O	7:C:124:ILE:HG13	2.07	0.54
22:R:23:LEU:HD22	22:R:35:ILE:HG21	1.90	0.54
31:a:1091:G:N7	57:a:1716:HOH:O	2.33	0.54
41:k:63:GLN:NE2	41:k:64:VAL:HG23	2.22	0.54
6:B:13:A:OP1	6:B:104:U:O2'	2.22	0.54
10:F:57:MET:HA	10:F:60:ILE:HG22	1.90	0.54
23:S:10:LEU:O	28:X:29:ARG:NH2	2.41	0.54
31:a:541:G:OP1	34:d:58:ARG:NH2	2.34	0.54
47:q:53:VAL:HG22	47:q:53:VAL:O	2.08	0.54
13:I:17:VAL:HG12	13:I:138:GLN:O	2.08	0.54
16:L:78:PRO:O	16:L:79:LEU:CB	2.55	0.54
32:b:58:PHE:CZ	32:b:62:LEU:HD21	2.43	0.54
50:t:75:HIS:O	50:t:79:LEU:HD13	2.08	0.54
5:A:84:U:OP1	28:X:52:ARG:NH1	2.41	0.54
31:a:424:G:H1'	31:a:425:U:OP2	2.08	0.54
31:a:1277:A:H8	40:j:42:MET:HE1	1.73	0.54
32:b:218:ALA:O	32:b:221:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:43:ASP:HB3	50:t:46:VAL:HG12	1.89	0.53
52:v:64:C:N4	52:v:65:G:O6	2.41	0.53
5:A:1775:U:OP2	5:A:1780:A:N6	2.28	0.53
5:A:2747:G:O2'	5:A:2748:C:P	2.66	0.53
35:e:76:ALA:N	35:e:81:GLN:OE1	2.41	0.53
39:i:12:THR:HG22	39:i:12:THR:O	2.08	0.53
40:j:7:ARG:HH11	40:j:73:LEU:HD11	1.72	0.53
52:v:55:5MU:H2'	52:v:56:PSU:C5	2.43	0.53
18:N:16:ARG:NH2	18:N:94:SER:OG	2.41	0.53
33:c:51:MET:HB3	33:c:115:LEU:HD22	1.90	0.53
32:b:52:LEU:O	32:b:56:LEU:HD23	2.08	0.53
4:3:9:LYS:NZ	4:3:14:CYS:O	2.37	0.53
10:F:74:ILE:HG12	10:F:79:ILE:HD11	1.91	0.53
31:a:489:C:H2'	31:a:490:A:C8	2.44	0.53
5:A:782:G:H5'	5:A:783:G:OP1	2.09	0.53
5:A:1310:C:O2'	5:A:1387:A:N3	2.36	0.53
5:A:2309:C:H4'	10:F:88:LYS:HD3	1.91	0.53
35:e:74:ASP:OD2	35:e:151:LYS:NZ	2.42	0.53
5:A:2443:G:O2'	57:A:3404:HOH:O	2.03	0.53
31:a:887:G:H1'	31:a:888:U:OP2	2.09	0.53
31:a:1050:G:H4'	31:a:1051:C:H3'	1.91	0.52
47:q:10:THR:HG23	47:q:61:THR:HG22	1.91	0.52
4:3:36:ARG:HG2	4:3:37:GLN:N	2.24	0.52
16:L:44:ALA:HA	16:L:47:ILE:HD12	1.90	0.52
32:b:171:GLU:O	32:b:175:ILE:HD12	2.08	0.52
33:c:39:VAL:O	33:c:43:LEU:HD23	2.09	0.52
5:A:1294:G:HO2'	5:A:1296:A:N6	2.07	0.52
11:G:101:THR:O	11:G:101:THR:HG22	2.10	0.52
33:c:215:MET:SD	40:j:20:GLN:NE2	2.83	0.52
34:d:109:PHE:CE2	34:d:147:VAL:HG23	2.45	0.52
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.91	0.52
41:k:70:GLY:O	41:k:74:LEU:HD23	2.09	0.52
5:A:905:G:OP1	16:L:24:GLY:N	2.42	0.52
31:a:1357:A:OP2	44:n:75:ARG:NH2	2.42	0.52
5:A:1908:A:O2'	31:a:1491:G:O2'	2.10	0.52
55:A:3201:YQM:O30	55:A:3201:YQM:O33	2.27	0.52
5:A:2844:G:O2'	5:A:2864:A:N6	2.43	0.52
19:O:92:ARG:O	19:O:115:GLU:HG3	2.10	0.52
29:Y:2:LYS:O	29:Y:3:THR:HG23	2.10	0.52
33:c:51:MET:HE2	33:c:72:ARG:NH1	2.25	0.52
32:b:45:LEU:O	32:b:49:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:55:5MU:HO2'	52:v:56:PSU:C1'	2.10	0.51
25:U:69:VAL:HG13	25:U:69:VAL:O	2.10	0.51
5:A:622:C:O2'	5:A:655:U:OP1	2.28	0.51
31:a:684:A:N7	31:a:698:U:N3	2.57	0.51
31:a:670:A:H2'	31:a:671:G:C8	2.46	0.51
40:j:57:VAL:HG23	40:j:57:VAL:O	2.11	0.51
31:a:1001:A:C6	31:a:1023:G:H1'	2.46	0.51
52:v:1:G:C6	52:v:74:A:N1	2.79	0.51
7:C:163:GLN:OE1	7:C:164:LEU:N	2.43	0.51
36:f:88:LEU:HD13	48:r:64:TYR:CE2	2.46	0.51
38:h:48:ASN:OD1	38:h:49:VAL:N	2.43	0.51
52:v:55:5MU:O2'	52:v:56:PSU:O5'	2.29	0.51
31:a:603:G:N2	31:a:629:U:OP1	2.43	0.51
5:A:2379:G:O2'	5:A:2380:U:P	2.69	0.51
10:F:159:THR:O	10:F:159:THR:HG22	2.11	0.51
7:C:120:ASN:O	7:C:134:ASN:ND2	2.44	0.51
5:A:1044:G:H2'	5:A:1108:A:H61	1.74	0.50
6:B:50:A:N7	18:N:34:ARG:NH1	2.59	0.50
31:a:64:U:O2'	31:a:375:G:N3	2.44	0.50
31:a:367:A:H2'	31:a:368:C:O4'	2.10	0.50
5:A:1923:A:C2'	5:A:1924:A:O5'	2.58	0.50
36:f:76:GLU:OE1	36:f:76:GLU:N	2.40	0.50
42:l:87:VAL:O	42:l:88:LYS:HB3	2.11	0.50
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.93	0.50
45:o:25:PRO:O	45:o:29:VAL:HG23	2.12	0.50
52:v:20:H2U:H5''	52:v:21:U:OP1	2.12	0.50
5:A:1189:A:OP2	15:K:16:ARG:NH2	2.44	0.50
38:h:74:GLU:OE2	38:h:131:SER:OG	2.23	0.50
52:v:16:U:H2'	52:v:16:U:O2	2.11	0.50
31:a:78:G:H2'	31:a:79:U:C6	2.46	0.50
5:A:1679:G:P	5:A:1753:A:H61	2.35	0.50
5:A:2548:OMU:OP2	5:A:2548:OMU:H6	2.11	0.50
10:F:57:MET:HE1	10:F:87:CYS:HB2	1.93	0.50
10:F:159:THR:O	10:F:161:ARG:NH1	2.45	0.50
38:h:39:VAL:O	38:h:43:GLU:OE1	2.29	0.50
5:A:91:A:O5'	24:T:5:LYS:NZ	2.39	0.50
34:d:11:LEU:HD13	34:d:65:ARG:HD3	1.94	0.50
34:d:29:ASP:OD1	34:d:30:VAL:N	2.45	0.50
5:A:37:G:O2'	5:A:1209:A:N3	2.40	0.49
52:v:1:G:C2	52:v:74:A:C2	3.00	0.49
5:A:2465:A:O4'	16:L:56:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:130:LYS:C	32:b:131:LEU:HD22	2.37	0.49
5:A:1344:C:C2	5:A:1345:C:C5	3.01	0.49
10:F:35:THR:OG1	10:F:88:LYS:NZ	2.19	0.49
19:O:46:PHE:CE1	19:O:66:LYS:HE2	2.48	0.49
31:a:1122:U:O2'	31:a:1123:U:H2'	2.12	0.49
32:b:7:SER:O	32:b:10:ASP:OD1	2.29	0.49
43:m:44:LYS:HB2	43:m:47:GLU:OE1	2.13	0.49
36:f:93:GLU:O	36:f:94:HIS:HB2	2.13	0.49
5:A:70:A:O2'	5:A:71:G:P	2.70	0.49
5:A:152:A:O2'	5:A:153:G:OP1	2.27	0.49
5:A:1557:U:H4'	5:A:1558:G:OP2	2.13	0.49
32:b:22:THR:HG22	32:b:41:HIS:CE1	2.47	0.49
32:b:58:PHE:O	32:b:62:LEU:HD23	2.12	0.49
52:v:65:G:O2'	52:v:66:U:OP1	2.23	0.49
31:a:320:G:N1	31:a:323:A:OP2	2.45	0.49
31:a:1051:C:H1'	31:a:1052:A:OP2	2.13	0.49
5:A:1173:G:H4'	5:A:1174:U:OP1	2.13	0.49
10:F:164:ASP:OD1	10:F:165:GLU:OE1	2.30	0.49
31:a:184:A:H3'	31:a:185:C:H5'	1.95	0.49
31:a:242:A:C2	31:a:278:A:C5	3.01	0.49
35:e:31:SER:OG	35:e:52:ALA:O	2.16	0.49
5:A:308:U:H2'	5:A:309:G:O4'	2.13	0.49
5:A:1542:A:O2'	5:A:1543:A:O4'	2.30	0.49
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.95	0.49
5:A:92:G:C2	5:A:106:U:O2	2.65	0.49
5:A:2528:G:N2	5:A:2659:G:O2'	2.46	0.49
22:R:33:LEU:O	22:R:37:ASN:ND2	2.45	0.49
31:a:789:A:O2'	31:a:790:U:OP2	2.25	0.49
5:A:498:U:H2'	5:A:499:G:O4'	2.12	0.49
9:E:101:ARG:O	9:E:105:GLN:HG3	2.13	0.49
9:E:130:THR:HG22	9:E:134:LEU:HD23	1.95	0.49
31:a:30:A:O2'	31:a:292:U:OP1	2.30	0.49
5:A:1016:U:O2'	5:A:1018:A:N7	2.41	0.48
5:A:1457:C:O2'	5:A:2698:G:O2'	2.28	0.48
31:a:661:G:H22	31:a:738:G:H1	1.61	0.48
45:o:26:GLU:HG3	45:o:81:LEU:HD13	1.95	0.48
8:D:18:ASP:OD1	8:D:19:ALA:N	2.46	0.48
31:a:1320:G:H2'	31:a:1321:A:C8	2.48	0.48
38:h:114:ASP:OD1	38:h:115:ARG:N	2.46	0.48
16:L:71:ASP:OD2	16:L:71:ASP:N	2.46	0.48
47:q:25:LEU:C	47:q:25:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:864:A:OP1	5:A:864:A:C8	2.67	0.48
5:A:2583:A:OP1	57:A:3417:HOH:O	2.20	0.48
9:E:170:ASP:OD1	9:E:172:THR:HG22	2.12	0.48
31:a:105:A:O2'	31:a:322:G:N2	2.45	0.48
5:A:2027:A:N3	5:A:2451:G:O2'	2.38	0.48
10:F:94:ASP:OD1	10:F:95:GLN:N	2.46	0.48
5:A:1294:G:OP1	57:A:3418:HOH:O	2.20	0.48
5:A:1833:C:O2'	5:A:1923:A:N3	2.38	0.48
17:M:36:THR:OG1	17:M:37:THR:N	2.46	0.48
32:b:209:ILE:HD12	32:b:209:ILE:H	1.78	0.48
18:N:63:THR:OG1	18:N:66:ASN:ND2	2.47	0.48
26:V:83:GLU:HA	26:V:83:GLU:OE1	2.13	0.48
32:b:81:ILE:H	32:b:81:ILE:HD12	1.79	0.48
32:b:130:LYS:O	32:b:131:LEU:HD22	2.14	0.48
14:J:103:THR:HG22	14:J:104:ARG:N	2.29	0.48
16:L:80:GLU:CD	16:L:80:GLU:O	2.56	0.48
31:a:472:A:H2'	31:a:473:U:O4'	2.13	0.48
31:a:991:A:N3	44:n:8:ASN:ND2	2.61	0.48
10:F:162:THR:HG22	10:F:163:ASP:N	2.27	0.48
17:M:24:LEU:HD23	17:M:44:LEU:HD13	1.96	0.48
32:b:56:LEU:HD12	32:b:222:ALA:HB2	1.94	0.48
5:A:799:G:C2'	5:A:800:A:OP1	2.61	0.48
5:A:1104:G:O2'	5:A:1105:U:O4'	2.31	0.48
33:c:36:ASP:O	33:c:39:VAL:HG22	2.13	0.48
42:l:98:VAL:HG13	42:l:101:SER:HB2	1.95	0.48
31:a:1010:G:N2	31:a:1013:A:OP2	2.37	0.47
31:a:1483:G:H2'	31:a:1484:G:O4'	2.14	0.47
40:j:15:HIS:HA	40:j:18:ILE:HG22	1.96	0.47
5:A:2747:G:HO2'	5:A:2748:C:P	2.35	0.47
20:P:74:LEU:HD11	20:P:114:LYS:HE2	1.95	0.47
21:Q:43:ASN:O	21:Q:45:ASP:N	2.47	0.47
5:A:391:C:C2	5:A:392:C:C5	3.02	0.47
12:H:5:LEU:O	12:H:16:GLY:N	2.47	0.47
31:a:74:G:H1	31:a:93:A:H61	1.61	0.47
34:d:189:ASP:OD1	34:d:190:ARG:N	2.47	0.47
52:v:15:G:H22	52:v:49:C:H42	1.62	0.47
50:t:11:ALA:O	50:t:15:VAL:HG23	2.14	0.47
10:F:128:TYR:CG	10:F:170:MET:HE1	2.49	0.47
32:b:150:LEU:O	32:b:150:LEU:HG	2.14	0.47
39:i:65:VAL:HG21	39:i:77:ILE:HD11	1.96	0.47
25:U:60:PHE:CE1	25:U:65:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:76:VAL:O	38:h:76:VAL:HG13	2.13	0.47
4:3:36:ARG:HG2	4:3:37:GLN:H	1.79	0.47
5:A:2683:U:H2'	5:A:2684:G:O4'	2.15	0.47
10:F:31:ILE:HD11	10:F:156:ILE:HG23	1.96	0.47
41:k:115:ILE:HG13	41:k:115:ILE:O	2.15	0.47
5:A:368:C:O2	5:A:368:C:O4'	2.33	0.47
5:A:1542:A:HO2'	5:A:1543:A:C5'	2.24	0.47
29:Y:46:MET:O	29:Y:50:VAL:HG22	2.15	0.47
31:a:734:A:OP1	36:f:91:ARG:N	2.40	0.47
31:a:1007:U:H3	31:a:1016:G:H22	1.62	0.47
31:a:1493:C:H2'	31:a:1494:G:O4'	2.14	0.47
33:c:88:GLN:HG2	33:c:101:VAL:HG23	1.96	0.47
31:a:710:G:H2'	31:a:711:G:C8	2.50	0.46
9:E:134:LEU:HD21	9:E:163:LEU:HD21	1.98	0.46
32:b:199:ASP:OD1	32:b:200:TYR:N	2.48	0.46
5:A:499:G:N1	5:A:502:A:OP2	2.40	0.46
5:A:1044:G:O2'	5:A:1108:A:N6	2.48	0.46
5:A:2067:A:H2'	5:A:2068:C:C6	2.50	0.46
10:F:34:ILE:HD12	10:F:156:ILE:HG13	1.97	0.46
19:O:37:GLU:OE2	19:O:42:ARG:NH2	2.48	0.46
42:l:15:LEU:HD23	42:l:16:VAL:O	2.14	0.46
42:l:21:VAL:HG23	42:l:21:VAL:O	2.15	0.46
5:A:2804:A:O2'	5:A:2805:A:N7	2.49	0.46
10:F:120:LYS:HG2	10:F:121:SER:H	1.79	0.46
17:M:114:GLU:OE2	17:M:118:ARG:NH1	2.47	0.46
5:A:1428:A:H2'	5:A:1429:A:C8	2.51	0.46
5:A:1695:G:OP2	5:A:1696:A:O2'	2.24	0.46
18:N:13:LYS:O	18:N:17:LEU:HD13	2.15	0.46
31:a:942:G:C2	31:a:943:A:C8	3.03	0.46
37:g:113:GLU:HB3	37:g:119:ARG:HG2	1.97	0.46
8:D:86:THR:HG23	8:D:88:ALA:H	1.80	0.46
11:G:71:VAL:O	11:G:75:LEU:HD13	2.14	0.46
5:A:88:G:C2'	5:A:89:G:O5'	2.63	0.46
5:A:1794:U:O2'	5:A:1798:A:N3	2.45	0.46
5:A:2324:A:H2'	5:A:2325:A:C8	2.51	0.46
31:a:1001:A:H2'	31:a:1002:A:O4'	2.16	0.46
34:d:99:ARG:O	34:d:103:VAL:HG23	2.16	0.46
36:f:25:TYR:O	36:f:29:ILE:HG12	2.15	0.46
42:l:79:VAL:HG13	42:l:79:VAL:O	2.16	0.46
5:A:2843:U:H2'	5:A:2844:G:O4'	2.15	0.46
7:C:132:LEU:O	7:C:167:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:80:SER:O	11:G:81:GLU:HB2	2.16	0.46
31:a:155:G:N2	31:a:158:A:OP2	2.46	0.46
31:a:607:U:N3	31:a:608:C:C5	2.83	0.46
34:d:204:GLU:O	34:d:207:SER:OG	2.28	0.46
40:j:83:THR:O	40:j:87:LEU:HD23	2.16	0.46
5:A:271:C:O2	5:A:271:C:O4'	2.34	0.46
5:A:509:C:N3	5:A:510:U:C5	2.84	0.46
22:R:23:LEU:HD12	30:Z:22:LEU:HB2	1.98	0.46
32:b:196:ASP:OD2	32:b:196:ASP:N	2.47	0.46
32:b:202:ILE:HG13	32:b:202:ILE:O	2.16	0.46
42:l:81:LEU:O	42:l:98:VAL:HG12	2.16	0.46
47:q:22:ILE:HD13	47:q:76:LEU:HD12	1.98	0.46
5:A:226:A:N3	5:A:241:U:O2'	2.35	0.46
5:A:2813:U:OP1	17:M:99:LYS:NZ	2.47	0.46
7:C:133:ARG:HB2	7:C:186:VAL:HG12	1.98	0.46
16:L:21:ALA:O	16:L:25:SER:OG	2.25	0.45
25:U:38:ASN:C	25:U:38:ASN:OD1	2.59	0.45
3:2:28:LYS:HG2	3:2:28:LYS:O	2.16	0.45
5:A:19:U:O2	5:A:2622:C:H4'	2.17	0.45
5:A:2026:6MZ:O2'	5:A:2027:A:P	2.74	0.45
31:a:185:C:H4'	31:a:186:G:O5'	2.16	0.45
34:d:52:GLU:O	34:d:56:GLN:HG3	2.16	0.45
42:l:40:THR:HG22	42:l:41:THR:N	2.32	0.45
42:l:52:VAL:HG12	42:l:53:CYS:N	2.31	0.45
6:B:12:U:OP2	6:B:68:C:O2'	2.31	0.45
10:F:132:LEU:HD23	10:F:133:LYS:O	2.16	0.45
16:L:54:ILE:O	16:L:58:ILE:HG12	2.16	0.45
32:b:150:LEU:HD23	32:b:150:LEU:H	1.81	0.45
5:A:1524:A:N6	5:A:1541:G:O2'	2.45	0.45
31:a:1353:G:H2'	31:a:1354:A:C8	2.51	0.45
5:A:971:G:OP1	5:A:1182:G:O2'	2.19	0.45
5:A:1106:C:H2'	5:A:1107:G:N7	2.32	0.45
5:A:1793:C:OP1	7:C:273:VAL:HG12	2.17	0.45
5:A:2287:U:H2'	5:A:2288:G:C8	2.51	0.45
25:U:34:ILE:HD11	25:U:67:ILE:HD13	1.99	0.45
31:a:508:C:O2'	31:a:509:U:OP2	2.27	0.45
31:a:887:G:N2	31:a:888:U:O4	2.42	0.45
5:A:91:A:H1'	5:A:92:G:OP2	2.16	0.45
5:A:599:C:O2'	5:A:603:G:OP1	2.34	0.45
35:e:114:LEU:HD13	35:e:122:VAL:HG11	1.98	0.45
36:f:73:GLU:HA	36:f:76:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:46:SER:HB3	41:k:61:ALA:HB1	1.98	0.45
19:O:28:THR:HB	19:O:91:ARG:HB3	1.98	0.45
30:Z:52:GLN:NE2	30:Z:54:PHE:O	2.48	0.45
31:a:185:C:H1'	31:a:186:G:OP2	2.17	0.45
32:b:175:ILE:HD12	32:b:175:ILE:H	1.82	0.45
5:A:2332:A:H61	26:V:43:THR:HG21	1.82	0.45
7:C:108:LYS:HE3	7:C:198:GLN:OE1	2.16	0.45
8:D:40:THR:OG1	8:D:43:THR:HG22	2.17	0.45
21:Q:34:THR:HG22	21:Q:60:THR:HG22	1.99	0.45
31:a:1059:U:H2'	31:a:1060:C:C6	2.52	0.45
5:A:2287:U:O2'	5:A:2370:C:O2	2.35	0.45
5:A:2469:U:H2'	5:A:2469:U:O2	2.17	0.45
31:a:471:G:H2'	31:a:472:A:C8	2.52	0.45
31:a:1120:A:O2'	40:j:39:PRO:O	2.28	0.45
5:A:1950:G:O2'	5:A:1952:U:O4	2.19	0.45
10:F:51:ASP:O	10:F:54:VAL:HG12	2.17	0.45
31:a:539:G:O3'	34:d:14:ARG:NH2	2.50	0.45
34:d:126:THR:HG23	34:d:126:THR:O	2.17	0.45
34:d:64:ARG:NH1	34:d:71:GLU:OE1	2.49	0.44
36:f:21:MET:N	36:f:21:MET:HE2	2.32	0.44
44:n:72:GLY:O	44:n:80:SER:HA	2.18	0.44
5:A:434:C:O2	5:A:434:C:O4'	2.34	0.44
5:A:2699:C:C2	5:A:2700:C:C5	3.06	0.44
8:D:8:ARG:NH1	8:D:201:GLY:O	2.50	0.44
9:E:130:THR:O	9:E:134:LEU:HD23	2.17	0.44
5:A:546:G:N3	5:A:546:G:H2'	2.32	0.44
28:X:37:LEU:HD21	28:X:39:LYS:O	2.17	0.44
35:e:106:ALA:O	35:e:111:ARG:NH1	2.50	0.44
37:g:123:GLU:OE2	37:g:123:GLU:HA	2.17	0.44
39:i:53:LEU:HD21	39:i:92:LEU:HD13	2.00	0.44
5:A:1933:A:O2'	5:A:1934:A:O5'	2.30	0.44
10:F:15:LYS:O	10:F:18:GLU:HG2	2.17	0.44
18:N:56:ASP:OD1	18:N:57:ALA:N	2.51	0.44
31:a:180:U:C2	31:a:181:C:C5	3.06	0.44
31:a:424:G:H4'	31:a:425:U:O5'	2.17	0.44
31:a:766:G:H4'	31:a:1510:A:H4'	1.98	0.44
5:A:280:A:OP2	5:A:364:A:N6	2.47	0.44
5:A:1193:U:C2	5:A:1194:U:C5	3.06	0.44
5:A:1347:U:O2'	5:A:1568:A:N3	2.44	0.44
5:A:1719:U:O4	5:A:1734:G:N2	2.50	0.44
7:C:167:ARG:HA	7:C:172:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:141:ILE:HG22	10:F:142:ASP:N	2.33	0.44
37:g:66:LEU:O	37:g:70:ARG:HG3	2.18	0.44
10:F:79:ILE:HG22	10:F:83:TRP:CE3	2.52	0.44
5:A:2719:C:H2'	5:A:2720:U:O4'	2.18	0.44
10:F:24:ASN:OD1	10:F:25:VAL:N	2.49	0.44
31:a:358:G:N1	31:a:361:U:OP2	2.47	0.44
44:n:69:ARG:NH1	44:n:71:HIS:O	2.51	0.44
5:A:701:U:H2'	5:A:702:G:O4'	2.18	0.44
10:F:10:ASP:OD2	10:F:11:GLU:N	2.49	0.44
31:a:606:A:C5	31:a:607:U:C6	3.06	0.44
31:a:1166:A:H2'	31:a:1167:A:C8	2.53	0.44
5:A:2508:C:OP2	8:D:131:ARG:NH2	2.51	0.44
15:K:102:VAL:HG23	15:K:103:VAL:HG23	2.00	0.44
5:A:568:G:O4'	5:A:980:A:N6	2.51	0.43
5:A:1439:A:C4	5:A:1440:G:C8	3.06	0.43
6:B:42:G:H1'	6:B:45:C:H42	1.83	0.43
15:K:85:SER:O	15:K:120:ARG:NH1	2.51	0.43
17:M:61:ALA:O	17:M:65:LEU:HD13	2.18	0.43
31:a:10:A:H62	34:d:207:SER:HG	1.65	0.43
32:b:71:PHE:CZ	32:b:219:MET:HE2	2.53	0.43
5:A:1793:C:HO2'	7:C:257:THR:HG1	1.65	0.43
5:A:1816:U:H4'	5:A:1817:A:OP2	2.19	0.43
5:A:2553:G:H2'	5:A:2554:C:C6	2.54	0.43
31:a:610:C:H2'	31:a:611:C:C6	2.53	0.43
31:a:1311:C:H2'	31:a:1312:U:C6	2.53	0.43
31:a:1428:A:H2	31:a:1466:C:H41	1.67	0.43
43:m:23:PHE:N	43:m:66:GLU:OE1	2.50	0.43
50:t:39:ILE:HD11	50:t:83:VAL:HG23	2.00	0.43
5:A:211:A:H4'	5:A:212:G:OP1	2.19	0.43
5:A:1634:G:H2'	5:A:1635:A:C8	2.53	0.43
6:B:7:G:C2	6:B:8:A:C8	3.06	0.43
10:F:128:TYR:CD1	10:F:170:MET:HE1	2.54	0.43
10:F:130:MET:HE1	10:F:156:ILE:HD13	2.00	0.43
32:b:6:VAL:HG12	32:b:7:SER:N	2.32	0.43
36:f:41:ASP:OD2	36:f:58:HIS:NE2	2.51	0.43
40:j:39:PRO:HA	40:j:74:ILE:HD13	2.01	0.43
47:q:18:MET:HE3	47:q:21:SER:CB	2.48	0.43
52:v:56:PSU:O2'	52:v:57:C:O2'	2.33	0.43
3:2:7:ARG:NH1	5:A:258:A:OP1	2.45	0.43
5:A:1782:A:H1'	5:A:1934:A:N6	2.33	0.43
10:F:121:SER:O	10:F:121:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:386:U:H2'	31:a:387:C:C6	2.53	0.43
31:a:402:G:O2'	34:d:118:GLN:NE2	2.52	0.43
31:a:1144:C:O2'	39:i:5:TYR:OH	2.33	0.43
31:a:1154:A:C2	31:a:1178:G:C4	3.06	0.43
5:A:726:G:H3'	5:A:727:G:C5'	2.48	0.43
6:B:59:C:C2	6:B:60:U:C5	3.06	0.43
11:G:43:LEU:HD11	11:G:50:LEU:HD22	2.00	0.43
14:J:77:ILE:HD11	19:O:75:ARG:NH1	2.34	0.43
38:h:78:ARG:NH1	38:h:80:SER:O	2.51	0.43
1:O:28:GLU:OE1	1:O:28:GLU:N	2.44	0.43
5:A:1428:A:H2'	5:A:1429:A:H8	1.83	0.43
5:A:1837:U:C2	5:A:1838:G:C8	3.06	0.43
36:f:1:MET:HB2	36:f:65:GLU:OE2	2.18	0.43
52:v:6:U:H2'	52:v:7:G:C8	2.54	0.43
4:3:37:GLN:O	4:3:37:GLN:HG3	2.18	0.43
5:A:2300:G:H22	5:A:2308:U:H3	1.65	0.43
9:E:1:MET:HE1	9:E:18:PHE:O	2.19	0.43
20:P:11:HIS:NE2	20:P:15:LYS:HD2	2.34	0.43
31:a:1179:G:C4'	31:a:1180:C:OP2	2.67	0.43
44:n:73:TYR:O	44:n:79:LEU:O	2.37	0.43
10:F:122:PHE:CG	10:F:163:ASP:OD1	2.72	0.43
10:F:130:MET:HE1	10:F:156:ILE:CD1	2.49	0.43
21:Q:61:ALA:HB2	21:Q:98:ILE:HD13	2.00	0.43
31:a:963:2MG:O2'	39:i:127:LYS:O	2.36	0.43
37:g:71:PRO:O	37:g:96:ARG:NE	2.52	0.43
50:t:49:GLU:OE2	50:t:53:LYS:HD2	2.18	0.43
5:A:637:U:H2'	5:A:638:C:C6	2.54	0.43
5:A:805:U:OP2	15:K:43:ARG:NH2	2.52	0.43
5:A:818:A:H4'	5:A:834:G:H22	1.82	0.43
5:A:1277:U:H2'	5:A:1278:G:O4'	2.17	0.43
5:A:1343:C:C5	5:A:1344:C:C5	3.06	0.43
5:A:2261:U:OP2	5:A:2262:A:O2'	2.27	0.43
7:C:132:LEU:HD22	7:C:164:LEU:HD12	2.00	0.43
33:c:215:MET:HG3	33:c:215:MET:O	2.18	0.43
38:h:98:GLN:HG2	38:h:98:GLN:O	2.18	0.43
5:A:368:C:C4'	5:A:369:G:OP2	2.67	0.43
5:A:507:U:C4'	5:A:508:C:OP2	2.67	0.43
5:A:1686:U:O2'	5:A:1698:A:N7	2.49	0.43
16:L:44:ALA:O	16:L:48:GLU:OE1	2.37	0.43
21:Q:51:ALA:CB	21:Q:52:PRO:CD	2.96	0.43
30:Z:3:VAL:HG22	30:Z:4:GLN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:37:G:O2'	42:l:115:SER:O	2.28	0.43
31:a:754:U:H2'	31:a:755:G:O4'	2.19	0.43
31:a:1128:G:C6	31:a:1129:C:C5	3.07	0.43
31:a:1423:G:H2'	31:a:1424:C:O4'	2.19	0.43
32:b:72:VAL:HG13	32:b:72:VAL:O	2.18	0.43
5:A:390:A:C5	5:A:391:C:C5	3.07	0.42
5:A:537:A:H2'	5:A:538:G:O4'	2.19	0.42
5:A:2302:C:H3'	5:A:2303:G:H5''	2.01	0.42
51:u:35:ARG:O	51:u:35:ARG:HG2	2.19	0.42
5:A:849:C:O2'	29:Y:42:SER:O	2.37	0.42
31:a:179:G:C5	31:a:180:U:C6	3.07	0.42
31:a:1233:A:H2'	31:a:1234:C:C6	2.55	0.42
5:A:916:A:N3	6:B:78:U:O2'	2.49	0.42
5:A:1879:U:H2'	5:A:1880:G:C1'	2.49	0.42
5:A:2287:U:OP1	5:A:2376:U:O2'	2.35	0.42
5:A:2621:G:H2'	5:A:2622:C:O4'	2.19	0.42
7:C:268:ILE:HG13	7:C:269:ARG:N	2.35	0.42
32:b:140:THR:O	32:b:143:MET:HG3	2.20	0.42
36:f:21:MET:HE2	36:f:21:MET:HA	2.01	0.42
5:A:1172:U:OP2	5:A:1173:G:N2	2.46	0.42
5:A:1575:C:H2'	5:A:1576:U:C1'	2.50	0.42
5:A:1827:G:C6	5:A:1971:A:C2	3.07	0.42
5:A:2048:A:H4'	8:D:151:GLN:O	2.18	0.42
5:A:2633:U:H2'	5:A:2634:G:O4'	2.20	0.42
5:A:2830:G:H2'	5:A:2875:A:H61	1.84	0.42
14:J:103:THR:HG22	14:J:105:GLU:OE1	2.20	0.42
31:a:716:C:OP2	31:a:717:C:N4	2.51	0.42
32:b:185:VAL:O	32:b:199:ASP:OD1	2.38	0.42
34:d:15:GLU:OE2	34:d:65:ARG:NH1	2.52	0.42
50:t:32:ILE:O	50:t:36:LEU:HG	2.19	0.42
5:A:579:C:H2'	5:A:580:A:H8	1.83	0.42
7:C:66:ASP:OD1	7:C:66:ASP:O	2.36	0.42
11:G:98:VAL:O	11:G:98:VAL:HG13	2.19	0.42
19:O:40:ARG:NH2	31:a:341:C:OP1	2.43	0.42
31:a:358:G:N2	31:a:361:U:OP2	2.52	0.42
31:a:1023:G:C2	31:a:1024:C:C6	3.07	0.42
33:c:17:ARG:NH1	33:c:17:ARG:HG3	2.34	0.42
36:f:21:MET:HE2	36:f:21:MET:CA	2.50	0.42
48:r:35:GLU:OE1	48:r:35:GLU:N	2.53	0.42
52:v:65:G:HO2'	52:v:66:U:P	2.38	0.42
5:A:1335:U:H4'	5:A:1336:G:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:42:G:O2'	6:B:45:C:N4	2.52	0.42
7:C:170:SER:C	7:C:186:VAL:HG23	2.45	0.42
31:a:1105:G:N3	31:a:1105:G:H2'	2.35	0.42
32:b:216:ALA:O	32:b:219:MET:HG2	2.20	0.42
48:r:42:SER:OG	48:r:47:THR:HG23	2.20	0.42
5:A:392:C:C2	5:A:393:U:C5	3.08	0.42
5:A:1852:U:H2'	5:A:1853:G:O4'	2.20	0.42
5:A:2587:C:OP1	7:C:238:ARG:NH1	2.52	0.42
5:A:2641:U:H3'	5:A:2642:C:H5'	2.02	0.42
17:M:94:TYR:O	17:M:116:VAL:HG23	2.19	0.42
34:d:111:SER:OG	34:d:115:GLU:OE1	2.36	0.42
35:e:152:VAL:O	35:e:155:LYS:HG2	2.19	0.42
39:i:82:THR:HG21	39:i:101:PHE:HB2	2.01	0.42
5:A:981:A:N3	5:A:981:A:H2'	2.34	0.42
11:G:12:PRO:O	11:G:13:ASN:HB3	2.20	0.42
14:J:104:ARG:NH2	19:O:35:VAL:HG21	2.35	0.42
28:X:5:ASP:OD1	28:X:5:ASP:C	2.63	0.42
31:a:943:A:H2'	31:a:944:G:C8	2.54	0.42
34:d:81:ALA:HB1	34:d:91:ASN:HB2	2.01	0.42
36:f:9:LEU:HB2	36:f:85:ILE:O	2.20	0.42
40:j:25:ILE:O	40:j:28:THR:HG22	2.20	0.42
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.88	0.42
5:A:2490:G:C2	5:A:2491:G:C8	3.07	0.42
6:B:23:A:N3	6:B:23:A:H2'	2.35	0.42
12:H:41:GLU:HG2	12:H:42:ALA:N	2.35	0.42
34:d:172:TRP:CD1	34:d:173:ILE:HG13	2.55	0.42
41:k:36:ARG:O	41:k:37:GLN:CB	2.68	0.42
3:2:7:ARG:NH1	5:A:259:G:OP2	2.52	0.42
9:E:116:ARG:HG2	9:E:183:ASP:O	2.20	0.42
30:Z:43:THR:HG22	30:Z:44:LYS:N	2.35	0.42
31:a:79:U:H2'	31:a:80:A:H8	1.84	0.42
31:a:1057:U:OP1	44:n:85:ARG:NH2	2.49	0.42
1:0:5:ILE:HD13	1:0:21:LYS:HD2	2.01	0.41
7:C:66:ASP:OD1	7:C:104:ILE:HG22	2.20	0.41
19:O:6:PRO:HA	19:O:9:GLN:HG2	2.02	0.41
19:O:94:ASP:HB2	19:O:116:LYS:HB2	2.02	0.41
31:a:552:U:H2'	31:a:553:C:C6	2.55	0.41
31:a:747:C:C2	31:a:748:U:C5	3.07	0.41
31:a:929:C:H5''	37:g:4:ARG:NH1	2.34	0.41
31:a:1342:U:OP1	39:i:120:ARG:NH1	2.52	0.41
5:A:303:C:H5''	5:A:336:U:H2'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:57:MET:HE1	10:F:87:CYS:SG	2.60	0.41
52:v:71:G:O2'	52:v:72:C:H5'	2.21	0.41
5:A:1726:C:C2'	5:A:1727:G:OP2	2.68	0.41
5:A:2345:G:O6	5:A:2365:A:N6	2.53	0.41
31:a:1122:U:O2'	31:a:1123:U:H3'	2.20	0.41
33:c:173:VAL:HG12	33:c:173:VAL:O	2.19	0.41
5:A:203:A:H2'	5:A:203:A:N3	2.36	0.41
5:A:1106:C:H2'	5:A:1107:G:C5	2.56	0.41
5:A:1354:A:OP2	5:A:1366:G:N1	2.45	0.41
31:a:425:U:H1'	31:a:426:A:OP2	2.19	0.41
31:a:560:A:O2'	31:a:563:G:O2'	2.23	0.41
31:a:711:G:H2'	31:a:712:A:C8	2.54	0.41
31:a:1277:A:C8	40:j:42:MET:HE1	2.52	0.41
33:c:17:ARG:HG3	33:c:17:ARG:HH11	1.85	0.41
33:c:34:LEU:O	33:c:38:GLN:HG3	2.21	0.41
5:A:199:G:O2'	5:A:675:A:N1	2.50	0.41
6:B:50:A:H62	18:N:34:ARG:CG	2.34	0.41
11:G:71:VAL:HG22	11:G:75:LEU:CD1	2.50	0.41
19:O:91:ARG:NH2	19:O:113:ILE:O	2.45	0.41
31:a:1388:U:H2'	31:a:1389:G:C8	2.56	0.41
31:a:1394:C:H2'	31:a:1394:C:O2	2.20	0.41
47:q:59:VAL:O	47:q:59:VAL:HG13	2.21	0.41
5:A:1355:G:N7	5:A:1356:G:C8	2.89	0.41
11:G:45:GLN:HG2	11:G:50:LEU:HD23	2.02	0.41
31:a:754:U:OP1	31:a:819:U:O2'	2.34	0.41
34:d:28:PHE:O	34:d:32:THR:HG22	2.21	0.41
36:f:97:THR:O	36:f:97:THR:HG22	2.20	0.41
5:A:378:G:N1	5:A:395:G:C6	2.88	0.41
11:G:77:LYS:O	11:G:81:GLU:HB3	2.20	0.41
19:O:94:ASP:N	19:O:114:ARG:O	2.43	0.41
31:a:680:G:C5	31:a:681:U:C5	3.08	0.41
41:k:36:ARG:O	41:k:37:GLN:HB3	2.20	0.41
4:3:23:ILE:HD13	5:A:1029:A:H1'	2.03	0.41
5:A:475:G:N1	5:A:478:A:OP2	2.53	0.41
5:A:984:C:O2'	5:A:997:A:N3	2.45	0.41
5:A:1025:A:N6	5:A:1122:G:H2'	2.35	0.41
5:A:2311:C:O2'	10:F:125:ARG:CZ	2.69	0.41
11:G:89:LEU:HD23	11:G:162:VAL:HG22	2.00	0.41
18:N:44:ASP:OD1	18:N:45:GLY:N	2.54	0.41
19:O:107:SER:O	19:O:111:ALA:N	2.52	0.41
24:T:49:VAL:HG23	24:T:50:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:684:A:C2	31:a:701:A:C5	3.09	0.41
31:a:1515:MA6:H102	31:a:1516:MA6:H103	2.02	0.41
42:l:74:LEU:HD12	42:l:74:LEU:N	2.36	0.41
47:q:68:ILE:O	47:q:68:ILE:HG22	2.21	0.41
5:A:12:A:H2'	5:A:13:A:C8	2.56	0.41
5:A:162:A:H2'	5:A:163:C:O4'	2.21	0.41
5:A:573:A:C2	5:A:574:U:C5	3.08	0.41
5:A:666:A:H2'	5:A:668:A:H62	1.86	0.41
5:A:1044:G:C2'	5:A:1108:A:H61	2.33	0.41
5:A:1199:A:O4'	5:A:1201:G:C8	2.73	0.41
5:A:1316:A:C4	5:A:1317:A:C8	3.07	0.41
5:A:1543:A:H5''	5:A:1544:G:OP2	2.21	0.41
5:A:1854:A:H2'	5:A:1855:U:O4'	2.21	0.41
5:A:2295:G:OP1	10:F:72:LYS:NZ	2.53	0.41
5:A:2752:U:H4'	5:A:2753:A:OP1	2.20	0.41
5:A:2796:U:H3'	5:A:2797:G:H5'	2.02	0.41
25:U:47:GLU:OE1	25:U:47:GLU:N	2.53	0.41
31:a:577:C:H2'	31:a:578:G:O4'	2.20	0.41
31:a:920:A:H2'	31:a:921:C:C6	2.56	0.41
31:a:1155:C:C4	31:a:1157:G:C8	3.09	0.41
31:a:1155:C:O2	31:a:1155:C:H3'	2.20	0.41
31:a:1410:A:H2	31:a:1484:G:H22	1.68	0.41
32:b:188:ILE:HG13	32:b:202:ILE:HD11	2.02	0.41
35:e:76:ALA:HB2	35:e:81:GLN:OE1	2.20	0.41
39:i:82:THR:HG23	39:i:96:LEU:HD13	2.02	0.41
41:k:35:ASP:OD2	41:k:41:LEU:HD11	2.21	0.41
44:n:42:PHE:CE2	44:n:46:LEU:HD21	2.56	0.41
5:A:70:A:O2'	5:A:71:G:O5'	2.39	0.41
5:A:314:G:C2	5:A:315:U:C6	3.09	0.41
5:A:605:U:C5	5:A:618:G:C5	3.09	0.41
5:A:2586:A:H2'	5:A:2587:C:H6	1.85	0.41
6:B:30:U:C2	6:B:49:G:N2	2.89	0.41
6:B:52:G:H21	10:F:26:MET:CE	2.34	0.41
11:G:87:LEU:HD12	11:G:133:LEU:HD13	2.02	0.41
11:G:89:LEU:HD22	11:G:162:VAL:HG22	1.97	0.41
29:Y:50:VAL:O	29:Y:54:VAL:HG22	2.21	0.41
31:a:1032:A:N3	31:a:1032:A:H2'	2.36	0.41
31:a:1409:C:H2'	31:a:1410:A:C8	2.56	0.41
32:b:81:ILE:O	32:b:85:GLN:HG2	2.21	0.41
33:c:33:LEU:O	33:c:37:LEU:HG	2.21	0.41
43:m:37:VAL:HG13	43:m:55:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:47:THR:HG21	48:r:52:GLN:OE1	2.21	0.41
5:A:1993:C:OP2	8:D:132:THR:OG1	2.27	0.40
5:A:2727:G:H2'	5:A:2728:G:C8	2.56	0.40
6:B:15:C:C2	6:B:16:A:C8	3.09	0.40
21:Q:51:ALA:CB	21:Q:52:PRO:HD3	2.52	0.40
31:a:6:C:C4'	31:a:7:U:OP1	2.69	0.40
31:a:1194:A:H2'	31:a:1195:G:H5'	2.02	0.40
41:k:60:PHE:O	41:k:63:GLN:HG3	2.21	0.40
5:A:34:G:N2	5:A:511:G:H1'	2.36	0.40
5:A:831:A:H2'	5:A:832:G:C8	2.56	0.40
5:A:847:A:H2'	5:A:848:C:C6	2.56	0.40
5:A:1227:G:C5	5:A:1228:C:C5	3.10	0.40
5:A:2679:C:O2	14:J:70:ARG:NH2	2.46	0.40
31:a:423:U:P	31:a:424:G:HO2'	2.35	0.40
31:a:1396:C:O2	31:a:1499:A:N6	2.53	0.40
47:q:61:THR:OG1	47:q:77:VAL:CG2	2.69	0.40
5:A:1341:G:H2'	5:A:1342:A:O4'	2.21	0.40
5:A:1355:G:C8	5:A:1356:G:C8	3.10	0.40
5:A:1835:G:N3	5:A:1835:G:H2'	2.37	0.40
31:a:333:G:H2'	31:a:334:A:C8	2.57	0.40
31:a:1001:A:N1	31:a:1023:G:H1'	2.35	0.40
31:a:1124:G:O5'	31:a:1277:A:O2'	2.39	0.40
32:b:10:ASP:O	32:b:13:GLN:HG3	2.21	0.40
40:j:57:VAL:O	40:j:58:ASN:CG	2.64	0.40
5:A:90:G:OP1	24:T:90:LYS:NZ	2.51	0.40
5:A:1438:C:C2	5:A:1439:A:C8	3.09	0.40
10:F:31:ILE:HD11	10:F:156:ILE:CG2	2.51	0.40
18:N:74:GLY:O	18:N:77:ILE:HG22	2.22	0.40
23:S:43:LYS:HG3	23:S:54:VAL:HB	2.04	0.40
31:a:85:G:C2'	31:a:86:C:OP2	2.66	0.40
31:a:377:G:H2'	31:a:378:A:O4'	2.22	0.40
31:a:447:A:H4'	31:a:448:G:O4'	2.22	0.40
31:a:499:A:OP1	42:l:115:SER:OG	2.32	0.40
40:j:80:THR:HG22	40:j:81:ASP:N	2.36	0.40
52:v:28:C:H2'	52:v:29:C:C6	2.56	0.40
5:A:70:A:C2'	5:A:71:G:OP2	2.69	0.40
5:A:509:C:C2	5:A:510:U:C5	3.09	0.40
5:A:566:U:H1'	5:A:2026:6MZ:H9C1	2.03	0.40
5:A:740:G:H2'	5:A:741:U:C6	2.56	0.40
5:A:1170:U:H5'	5:A:1171:U:H3'	2.04	0.40
5:A:2239:U:H2'	5:A:2240:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:57:GLU:O	11:G:57:GLU:HG3	2.21	0.40
11:G:71:VAL:O	11:G:75:LEU:CD1	2.70	0.40
17:M:79:LEU:HD23	17:M:83:LEU:HD12	2.03	0.40
17:M:94:TYR:C	17:M:116:VAL:HG23	2.47	0.40
24:T:52:ALA:O	24:T:53:GLU:C	2.65	0.40
31:a:673:A:H2'	31:a:674:U:H6	1.87	0.40
31:a:1123:U:O2	31:a:1277:A:H2'	2.22	0.40
31:a:1355:U:OP2	31:a:1356:C:N4	2.47	0.40
32:b:164:PHE:CE2	32:b:219:MET:SD	3.15	0.40
38:h:15:ARG:O	38:h:19:MET:HG3	2.22	0.40
50:t:35:THR:HG21	50:t:79:LEU:HD23	2.02	0.40
52:v:26:C:C2	52:v:27:A:C8	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	47/51 (92%)	47 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	270/274 (98%)	259 (96%)	10 (4%)	1 (0%)	30	45
8	D	208/212 (98%)	201 (97%)	7 (3%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	157 (91%)	15 (9%)	0	100	100
11	G	172/177 (97%)	166 (96%)	4 (2%)	2 (1%)	10	17
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
15	K	142/146 (97%)	140 (99%)	2 (1%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18	30
17	M	117/125 (94%)	113 (97%)	4 (3%)	0	100	100
18	N	112/116 (97%)	112 (100%)	0	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100
24	T	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	80/85 (94%)	80 (100%)	0	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	57 (98%)	1 (2%)	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	53/61 (87%)	50 (94%)	3 (6%)	0	100	100
32	b	223/250 (89%)	215 (96%)	8 (4%)	0	100	100
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%)	153 (100%)	0	0	100	100
36	f	102/127 (80%)	98 (96%)	3 (3%)	1 (1%)	12	20
37	g	149/156 (96%)	144 (97%)	5 (3%)	0	100	100
38	h	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
39	i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
40	j	97/103 (94%)	94 (97%)	3 (3%)	0	100	100
41	k	115/128 (90%)	109 (95%)	6 (5%)	0	100	100
42	l	120/124 (97%)	115 (96%)	4 (3%)	1 (1%)	16	27
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	o	86/89 (97%)	86 (100%)	0	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	61 (100%)	0	0	100	100
All	All	5432/5872 (92%)	5289 (97%)	137 (2%)	6 (0%)	49	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	G	81	GLU
16	L	79	LEU
36	f	33	ASP
11	G	13	ASN
42	l	88	LYS
7	C	3	ILE

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	45/47 (96%)	45 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	218 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	77 (100%)	0	100	100
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	62/64 (97%)	62 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	185 (100%)	0	100	100
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	94 (100%)	0	100	100
37	g	123/128 (96%)	123 (100%)	0	100	100
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	99 (100%)	0	100	100
40	j	88/91 (97%)	88 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	71 (100%)	0	100	100
48	r	46/66 (70%)	46 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	54/62 (87%)	54 (100%)	0	100	100
All	All	4494/4756 (94%)	4494 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
7	C	23	HIS
7	C	197	ASN
8	D	47	GLN
8	D	50	GLN
9	E	40	GLN
10	F	127	ASN
11	G	51	GLN
11	G	73	ASN
13	I	58	ASN
14	J	29	HIS
14	J	110	GLN
15	K	101	ASN
16	L	22	HIS
16	L	85	ASN
20	P	44	GLN
24	T	21	GLN
25	U	92	HIS
27	W	22	ASN
30	Z	4	GLN
30	Z	37	HIS
33	c	3	GLN
33	c	123	GLN
34	d	56	GLN

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Mol	Chain	Res	Type
34	d	148	HIS
34	d	177	HIS
36	f	94	HIS
40	j	99	GLN
41	k	27	ASN
41	k	107	ASN
42	l	111	ASN
43	m	28	HIS
43	m	105	ASN
45	o	48	HIS
50	t	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	229 (14%)	0
5	A	2726/2918 (93%)	444 (16%)	34 (1%)
52	v	76/77 (98%)	30 (39%)	0
53	w	2/3 (66%)	0	0
6	B	114/115 (99%)	18 (15%)	1 (0%)
All	All	4445/4657 (95%)	721 (16%)	35 (0%)

All (721) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
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	68	A
5	A	71	G
5	A	74	U
5	A	78	A
5	A	81	A
5	A	82	G
5	A	89	G
5	A	91	A
5	A	92	G

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Mol	Chain	Res	Type
5	A	95	G
5	A	102	A
5	A	106	U
5	A	107	U
5	A	108	U
5	A	109	G
5	A	125	A
5	A	127	U
5	A	147	A
5	A	149	G
5	A	153	G
5	A	165	U
5	A	169	U
5	A	170	A
5	A	171	C
5	A	172	A
5	A	203	A
5	A	206	A
5	A	212	G
5	A	223	A
5	A	229	A
5	A	230	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	273	G
5	A	275	C
5	A	278	U
5	A	279	U
5	A	301	A
5	A	303	C
5	A	313	A
5	A	324	A
5	A	325	G
5	A	331	G
5	A	332	A
5	A	333	U
5	A	336	U

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Mol	Chain	Res	Type
5	A	347	A
5	A	348	A
5	A	359	U
5	A	361	A
5	A	365	U
5	A	366	G
5	A	368	C
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	416	C
5	A	423	G
5	A	434	C
5	A	455	C
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	509	C
5	A	526	C
5	A	529	G
5	A	530	C
5	A	531	A
5	A	532	G
5	A	543	U
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	564	U
5	A	570	A

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Mol	Chain	Res	Type
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	643	U
5	A	644	A
5	A	651	U
5	A	657	G
5	A	668	A
5	A	684	U
5	A	693	G
5	A	711	G
5	A	713	A
5	A	716	A
5	A	721	C
5	A	722	U
5	A	724	G
5	A	728	A
5	A	738	C
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	788	U
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	843	G
5	A	851	U
5	A	855	G
5	A	857	G
5	A	864	A

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Mol	Chain	Res	Type
5	A	905	G
5	A	908	A
5	A	912	C
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1019	G
5	A	1023	G
5	A	1030	U
5	A	1033	G
5	A	1039	G
5	A	1042	U
5	A	1043	A
5	A	1044	G
5	A	1050	U
5	A	1051	A
5	A	1104	G
5	A	1105	U
5	A	1108	A
5	A	1109	G
5	A	1121	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1138	U
5	A	1139	A
5	A	1140	A
5	A	1149	G
5	A	1153	A
5	A	1169	C

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Mol	Chain	Res	Type
5	A	1170	U
5	A	1171	U
5	A	1173	G
5	A	1174	U
5	A	1201	G
5	A	1242	A
5	A	1243	G
5	A	1248	A
5	A	1250	U
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1297	A
5	A	1324	U
5	A	1327	G
5	A	1336	G
5	A	1338	G
5	A	1347	U
5	A	1348	A
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1405	U
5	A	1411	G
5	A	1415	U
5	A	1416	G
5	A	1417	A
5	A	1420	G
5	A	1423	C
5	A	1432	C
5	A	1447	G
5	A	1448	U
5	A	1456	C
5	A	1462	G
5	A	1477	U
5	A	1488	C
5	A	1489	A
5	A	1501	C

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Mol	Chain	Res	Type
5	A	1504	U
5	A	1505	A
5	A	1511	A
5	A	1520	A
5	A	1523	A
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1535	U
5	A	1540	C
5	A	1542	A
5	A	1543	A
5	A	1552	U
5	A	1557	U
5	A	1558	G
5	A	1564	A
5	A	1565	G
5	A	1567	A
5	A	1574	U
5	A	1576	U
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1606	A
5	A	1609	C
5	A	1617	G
5	A	1645	U
5	A	1646	U
5	A	1647	G
5	A	1662	A
5	A	1672	G
5	A	1691	U
5	A	1697	G
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1733	U
5	A	1734	G

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Mol	Chain	Res	Type
5	A	1746	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1787	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1829	C
5	A	1830	U
5	A	1844	A
5	A	1869	G
5	A	1871	G
5	A	1872	A
5	A	1875	C
5	A	1878	U
5	A	1885	A
5	A	1895	A
5	A	1897	A
5	A	1902	G
5	A	1908	A
5	A	1910	C
5	A	1911	3TD
5	A	1915	A
5	A	1917	G
5	A	1918	G
5	A	1919	U
5	A	1923	A
5	A	1924	A
5	A	1926	G
5	A	1927	U
5	A	1932	A
5	A	1934	A
5	A	1936	U
5	A	1950	G
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A

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Mol	Chain	Res	Type
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	2025	G
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2048	A
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2059	C
5	A	2065	G7M
5	A	2089	G
5	A	2194	A
5	A	2195	A
5	A	2200	G
5	A	2210	C
5	A	2221	A
5	A	2222	C
5	A	2234	G
5	A	2235	G
5	A	2236	U
5	A	2261	U
5	A	2279	U
5	A	2283	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2315	U
5	A	2317	G
5	A	2318	A

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Mol	Chain	Res	Type
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	2371	G
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2399	C
5	A	2402	U
5	A	2420	C
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2443	G
5	A	2444	A
5	A	2446	A
5	A	2455	A
5	A	2461	C
5	A	2465	A
5	A	2466	G
5	A	2469	U
5	A	2470	U
5	A	2472	A
5	A	2475	U
5	A	2476	C
5	A	2494	C
5	A	2497	C
5	A	2499	2MA
5	A	2501	G
5	A	2502	U
5	A	2503	C
5	A	2514	A
5	A	2516	C
5	A	2525	G

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Mol	Chain	Res	Type
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2569	C
5	A	2598	A
5	A	2605	U
5	A	2606	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2642	C
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
5	A	2725	U
5	A	2729	A
5	A	2735	U
5	A	2740	G
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2762	G
5	A	2774	A
5	A	2777	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2805	A
5	A	2816	G
5	A	2830	G
5	A	2831	A
5	A	2844	G
5	A	2845	G

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Mol	Chain	Res	Type
5	A	2851	U
5	A	2854	U
5	A	2857	U
5	A	2863	A
5	A	2868	G
5	A	2876	C
5	A	2880	U
5	A	2898	U
6	B	2	C
6	B	11	A
6	B	13	A
6	B	14	G
6	B	22	G
6	B	23	A
6	B	39	C
6	B	40	C
6	B	42	G
6	B	43	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	88	C
6	B	105	C
6	B	106	A
31	a	6	C
31	a	7	U
31	a	11	G
31	a	34	A
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	66	G
31	a	80	A
31	a	81	G
31	a	82	C
31	a	83	U
31	a	84	U

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Mol	Chain	Res	Type
31	a	85	G
31	a	86	C
31	a	91	G
31	a	105	A
31	a	107	G
31	a	117	U
31	a	126	A
31	a	127	U
31	a	140	G
31	a	152	C
31	a	160	G
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A
31	a	200	G
31	a	202	U
31	a	203	C
31	a	205	U
31	a	208	G
31	a	209	A
31	a	236	C
31	a	241	U
31	a	243	G
31	a	246	A
31	a	247	G
31	a	262	G
31	a	263	C
31	a	269	A
31	a	276	C
31	a	285	G
31	a	289	G
31	a	324	C
31	a	325	A
31	a	337	C
31	a	340	A
31	a	341	C
31	a	348	C
31	a	350	G
31	a	359	A
31	a	363	U
31	a	368	C

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Mol	Chain	Res	Type
31	a	369	A
31	a	393	A
31	a	402	G
31	a	407	A
31	a	408	A
31	a	409	G
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	461	A
31	a	462	A
31	a	463	U
31	a	479	A
31	a	482	U
31	a	483	U
31	a	492	A
31	a	494	U
31	a	496	A
31	a	508	C
31	a	509	U
31	a	512	G
31	a	515	C
31	a	518	G
31	a	521	G
31	a	522	C
31	a	524	G7M
31	a	527	G
31	a	528	U
31	a	529	A
31	a	532	A
31	a	544	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	574	G
31	a	593	A
31	a	630	G
31	a	639	A
31	a	650	A

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Mol	Chain	Res	Type
31	a	662	A
31	a	684	A
31	a	685	G
31	a	698	U
31	a	720	U
31	a	721	G
31	a	728	G
31	a	729	C
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	790	U
31	a	791	A
31	a	810	U
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	880	C
31	a	887	G
31	a	888	U
31	a	911	A
31	a	918	U
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	957	U
31	a	958	U
31	a	963	2MG
31	a	965	A
31	a	966	A
31	a	972	A
31	a	973	G
31	a	974	A
31	a	975	A
31	a	980	A
31	a	989	U

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Mol	Chain	Res	Type
31	a	990	G
31	a	1001	A
31	a	1007	U
31	a	1023	G
31	a	1027	U
31	a	1029	G
31	a	1030	G
31	a	1032	A
31	a	1033	A
31	a	1043	A
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1067	U
31	a	1068	C
31	a	1073	C
31	a	1076	G
31	a	1082	U
31	a	1085	G
31	a	1086	G
31	a	1091	G
31	a	1092	U
31	a	1098	A
31	a	1122	U
31	a	1124	G
31	a	1130	A
31	a	1136	G
31	a	1140	G
31	a	1141	G
31	a	1156	U
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1173	A
31	a	1179	G
31	a	1180	C
31	a	1181	G
31	a	1188	A
31	a	1193	A
31	a	1194	A
31	a	1195	G
31	a	1197	C

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Mol	Chain	Res	Type
31	a	1205	C
31	a	1209	U
31	a	1210	A
31	a	1223	C
31	a	1224	A
31	a	1235	A
31	a	1250	G
31	a	1255	G
31	a	1276	A
31	a	1277	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1317	C
31	a	1335	G
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1375	C
31	a	1398	G
31	a	1399	4OC
31	a	1416	G
31	a	1425	A
31	a	1426	C
31	a	1430	A
31	a	1438	A
31	a	1443	A
31	a	1445	C
31	a	1447	G
31	a	1449	A
31	a	1451	A
31	a	1462	A
31	a	1472	G
31	a	1484	G
31	a	1491	G
31	a	1494	G
31	a	1503	U
31	a	1514	G
31	a	1516	MA6
31	a	1517	C

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Mol	Chain	Res	Type
31	a	1526	G
31	a	1527	G
31	a	1529	U
52	v	4	U
52	v	8	4SU
52	v	9	A
52	v	10	G
52	v	11	C
52	v	14	A
52	v	15	G
52	v	16	U
52	v	18	G
52	v	20	H2U
52	v	22	A
52	v	23	G
52	v	36	A
52	v	37	U
52	v	46	G
52	v	47	G
52	v	48	U
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	65	G
52	v	66	U
52	v	69	U
52	v	72	C
52	v	73	C
52	v	77	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	70	A
5	A	91	A
5	A	152	A
5	A	211	A
5	A	256	C

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Mol	Chain	Res	Type
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	721	C
5	A	782	G
5	A	799	G
5	A	863	C
5	A	957	A
5	A	1127	U
5	A	1138	U
5	A	1172	U
5	A	1179	G
5	A	1187	G
5	A	1267	A
5	A	1296	A
5	A	1335	U
5	A	1337	A
5	A	1519	U
5	A	1542	A
5	A	1557	U
5	A	1616	A
5	A	1816	U
5	A	1923	A
5	A	2379	G
5	A	2419	U
5	A	2747	G
6	B	13	A

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

28 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	3TD	A	1911	5	19,22,23	4.46	6 (31%)	23,32,35	1.79	3 (13%)
31	PSU	a	513	31	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
31	5MC	a	964	31	19,22,23	0.54	0	26,32,35	0.59	0
5	PSU	A	2453	5	18,21,22	1.12	1 (5%)	21,30,33	1.93	6 (28%)
5	PSU	A	2576	5	18,21,22	1.15	1 (5%)	21,30,33	1.98	6 (28%)
5	2MA	A	2499	5,56	22,25,26	4.00	9 (40%)	32,37,40	2.78	11 (34%)
5	PSU	A	2601	5	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
52	4SU	v	8	52	18,21,22	4.43	8 (44%)	25,30,33	2.33	5 (20%)
5	5MU	A	1935	5	19,22,23	0.38	0	27,32,35	0.51	0
52	5MU	v	55	52	19,22,23	0.42	0	27,32,35	0.47	0
5	PSU	A	1913	5	18,21,22	1.14	1 (5%)	21,30,33	1.90	5 (23%)
5	6MZ	A	2026	5	22,25,26	2.47	4 (18%)	29,36,39	3.39	11 (37%)
31	UR3	a	1495	31	19,22,23	2.94	6 (31%)	26,32,35	1.61	3 (11%)
5	OMU	A	2548	5	19,22,23	3.13	8 (42%)	25,31,34	1.82	5 (20%)
31	MA6	a	1516	31	23,26,27	1.39	4 (17%)	33,38,41	3.20	12 (36%)
5	2MG	A	2441	5	23,26,27	0.45	0	33,38,41	0.50	0
31	4OC	a	1399	31	20,23,24	3.20	8 (40%)	25,32,35	0.83	1 (4%)
5	G7M	A	2065	5	23,26,27	1.88	2 (8%)	34,39,42	1.07	1 (2%)
31	MA6	a	1515	31	23,26,27	1.39	4 (17%)	33,38,41	3.22	12 (36%)
5	PSU	A	2500	5	18,21,22	1.16	1 (5%)	21,30,33	1.96	5 (23%)
52	PSU	v	56	52	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
31	2MG	a	1204	31	23,26,27	0.46	0	33,38,41	0.51	0
52	H2U	v	20	52	18,21,22	0.51	0	19,30,33	1.11	1 (5%)
5	PSU	A	1907	5	18,21,22	1.15	1 (5%)	21,30,33	1.95	5 (23%)
5	PSU	A	952	5	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
31	G7M	a	524	31	23,26,27	1.88	2 (8%)	34,39,42	1.06	1 (2%)
5	OMG	A	2247	5,52	23,26,27	0.45	0	32,38,41	0.50	0
31	2MG	a	963	31	23,26,27	0.46	0	33,38,41	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
31	PSU	a	513	31	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	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	5,56	-	4/7/25/26	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
52	4SU	v	8	52	-	2/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
52	5MU	v	55	52	-	2/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	2/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	1/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2
31	MA6	a	1516	31	-	1/11/29/30	0/3/3/3
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	G7M	A	2065	5	-	0/7/25/26	0/3/3/3
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
52	PSU	v	56	52	-	4/7/25/26	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
52	H2U	v	20	52	-	4/7/38/39	0/2/2/2
5	PSU	A	1907	5	-	1/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	G7M	a	524	31	-	3/7/25/26	0/3/3/3
5	OMG	A	2247	5,52	-	0/9/27/28	0/3/3/3
31	2MG	a	963	31	-	2/9/27/28	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.52	1.50	1.35
5	A	2499	2MA	C4-N3	12.21	1.50	1.34
5	A	1911	3TD	C2-N1	10.69	1.50	1.37
5	A	2026	6MZ	C6-N6	10.21	1.45	1.34
52	v	8	4SU	C2-N1	9.37	1.53	1.38
52	v	8	4SU	C4-N3	9.02	1.46	1.37
5	A	2499	2MA	C2-N3	7.64	1.47	1.34
5	A	2065	G7M	C8-N7	7.45	1.45	1.33
5	A	2548	OMU	C2-N1	7.43	1.50	1.38
31	a	524	G7M	C8-N7	7.41	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C5-C4	7.27	1.51	1.42
31	a	1495	UR3	C2-N1	7.23	1.48	1.38
52	v	8	4SU	C2-N3	7.16	1.50	1.38
31	a	1399	4OC	C4-N3	7.16	1.44	1.32
5	A	2499	2MA	C6-N1	7.06	1.44	1.35
5	A	2548	OMU	C2-N3	7.02	1.50	1.38
31	a	1495	UR3	C6-C5	6.76	1.50	1.35
52	v	8	4SU	C6-C5	6.40	1.49	1.35
31	a	1399	4OC	C6-C5	6.33	1.49	1.35
31	a	1399	4OC	C2-N3	6.25	1.48	1.36
5	A	2499	2MA	C2-N1	6.14	1.44	1.34
5	A	1911	3TD	C6-N1	5.76	1.45	1.36
5	A	2548	OMU	C6-C5	5.72	1.48	1.35
31	a	1495	UR3	C2-N3	5.71	1.50	1.39
5	A	1911	3TD	C2-N3	4.95	1.49	1.38
31	a	1399	4OC	C4-N4	4.91	1.46	1.36
52	v	8	4SU	C4-S4	-4.80	1.60	1.68
5	A	2499	2MA	C5-C6	4.72	1.54	1.41
5	A	2548	OMU	C4-N3	4.36	1.46	1.38
31	a	1399	4OC	C2-N1	4.30	1.49	1.40
31	a	524	G7M	C8-N9	4.10	1.46	1.35
5	A	2065	G7M	C8-N9	4.08	1.46	1.35
31	a	1515	MA6	C6-N6	4.01	1.47	1.36
31	a	1516	MA6	C6-N6	3.99	1.47	1.36
5	A	2500	PSU	C6-C5	3.87	1.39	1.35
5	A	1913	PSU	C6-C5	3.82	1.39	1.35
52	v	56	PSU	C6-C5	3.81	1.39	1.35
31	a	513	PSU	C6-C5	3.80	1.39	1.35
5	A	1907	PSU	C6-C5	3.79	1.39	1.35
5	A	952	PSU	C6-C5	3.77	1.39	1.35
5	A	2576	PSU	C6-C5	3.73	1.39	1.35
5	A	2601	PSU	C6-C5	3.71	1.39	1.35
5	A	2453	PSU	C6-C5	3.63	1.39	1.35
31	a	1399	4OC	C5-C4	3.62	1.49	1.41
31	a	1495	UR3	C6-N1	3.41	1.46	1.38
5	A	2499	2MA	C6-N6	-3.37	1.25	1.34
31	a	1399	4OC	C6-N1	3.33	1.46	1.38
5	A	1911	3TD	C4-N3	3.13	1.46	1.40
5	A	2548	OMU	O4-C4	-2.93	1.18	1.24
5	A	2026	6MZ	C5-N7	-2.87	1.33	1.39
31	a	1516	MA6	C5-C4	-2.85	1.34	1.39
5	A	2548	OMU	C6-N1	2.84	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1515	MA6	C5-C4	-2.82	1.34	1.39
5	A	2026	6MZ	C5-C4	-2.75	1.34	1.39
52	v	8	4SU	O2-C2	-2.72	1.18	1.23
31	a	1495	UR3	C4-N3	2.68	1.46	1.40
31	a	1399	4OC	O2-C2	-2.65	1.18	1.23
52	v	8	4SU	C6-N1	2.58	1.44	1.38
5	A	2548	OMU	C5-C4	2.47	1.49	1.43
5	A	2499	2MA	C5-N7	-2.45	1.34	1.39
5	A	2548	OMU	O2-C2	-2.41	1.18	1.23
31	a	1516	MA6	C5-N7	-2.40	1.34	1.39
31	a	1515	MA6	C5-N7	-2.37	1.34	1.39
31	a	1495	UR3	C5-C4	2.36	1.49	1.43
5	A	1911	3TD	O2-C2	-2.22	1.19	1.23
31	a	1516	MA6	C8-N9	-2.18	1.33	1.37
5	A	2026	6MZ	C8-N9	-2.17	1.33	1.37
31	a	1515	MA6	C8-N9	-2.12	1.33	1.37
5	A	2499	2MA	C8-N7	2.07	1.35	1.31
5	A	2499	2MA	C4-N9	-2.02	1.33	1.37

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1515	MA6	N1-C6-N6	-11.54	102.80	116.86
31	a	1516	MA6	N1-C6-N6	-11.36	103.01	116.86
5	A	2026	6MZ	C1'-N9-C8	8.90	146.85	127.09
5	A	2026	6MZ	C4-N9-C1'	-8.84	105.95	126.63
31	a	1515	MA6	C5-C6-N6	7.77	137.63	125.33
5	A	2499	2MA	C1'-N9-C8	-7.72	109.96	127.09
31	a	1516	MA6	C5-C6-N6	7.59	137.34	125.33
52	v	8	4SU	C4-N3-C2	-7.56	120.07	127.31
5	A	2026	6MZ	C5-C4-N3	-6.49	117.79	126.72
5	A	2499	2MA	C5-C4-N3	-5.95	120.91	127.18
5	A	2026	6MZ	N1-C2-N3	-5.63	120.06	128.58
31	a	1495	UR3	C4-N3-C2	-5.63	120.05	124.58
31	a	1516	MA6	N1-C2-N3	-5.63	120.07	128.58
5	A	2548	OMU	C4-N3-C2	-5.60	119.67	126.61
5	A	1911	3TD	N1-C2-N3	5.56	120.17	116.13
31	a	1515	MA6	N1-C2-N3	-5.54	120.20	128.58
5	A	2499	2MA	N9-C8-N7	-5.53	106.09	113.94
5	A	2499	2MA	C4-N9-C1'	5.44	139.36	126.63
52	v	8	4SU	C5-C4-N3	5.31	119.69	114.75
31	a	1516	MA6	C5-C4-N3	-4.95	119.90	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2601	PSU	C4-N3-C2	-4.94	119.56	126.37
5	A	2500	PSU	C4-N3-C2	-4.91	119.60	126.37
52	v	56	PSU	C4-N3-C2	-4.91	119.61	126.37
5	A	2500	PSU	N1-C2-N3	4.89	120.33	115.17
5	A	2601	PSU	N1-C2-N3	4.88	120.32	115.17
52	v	56	PSU	N1-C2-N3	4.88	120.31	115.17
5	A	1907	PSU	N1-C2-N3	4.85	120.28	115.17
5	A	952	PSU	C4-N3-C2	-4.83	119.72	126.37
5	A	1907	PSU	C4-N3-C2	-4.82	119.72	126.37
5	A	2453	PSU	C4-N3-C2	-4.82	119.73	126.37
31	a	1515	MA6	C5-C4-N3	-4.82	120.08	126.72
5	A	1913	PSU	N1-C2-N3	4.79	120.22	115.17
5	A	2453	PSU	N1-C2-N3	4.77	120.20	115.17
31	a	513	PSU	N1-C2-N3	4.76	120.19	115.17
5	A	1913	PSU	C4-N3-C2	-4.74	119.84	126.37
5	A	2576	PSU	N1-C2-N3	4.74	120.17	115.17
5	A	2499	2MA	C4-N9-C8	4.71	110.69	105.74
5	A	952	PSU	N1-C2-N3	4.69	120.11	115.17
5	A	2576	PSU	C4-N3-C2	-4.68	119.92	126.37
31	a	513	PSU	C4-N3-C2	-4.68	119.93	126.37
5	A	2499	2MA	N3-C4-N9	4.51	132.72	126.99
5	A	2026	6MZ	C4-C5-C6	4.32	120.38	116.78
31	a	1515	MA6	N9-C8-N7	-4.32	107.80	113.94
31	a	524	G7M	N9-C8-N7	-4.31	102.03	112.48
5	A	2026	6MZ	N3-C4-N9	4.30	134.49	127.17
5	A	1911	3TD	C4-N3-C2	-4.30	120.06	124.61
5	A	2065	G7M	N9-C8-N7	-4.30	102.05	112.48
31	a	1516	MA6	N9-C8-N7	-4.22	107.94	113.94
31	a	1516	MA6	C4-C5-C6	4.10	120.15	115.91
31	a	1515	MA6	C4-C5-C6	4.09	120.14	115.91
5	A	2026	6MZ	C2-N3-C4	4.04	121.69	111.83
52	v	8	4SU	C5-C4-S4	-3.98	119.76	124.31
5	A	2548	OMU	N3-C2-N1	3.89	119.95	114.89
5	A	2026	6MZ	N9-C8-N7	-3.64	108.77	113.94
31	a	1495	UR3	C5-C4-N3	3.57	119.74	115.04
5	A	2548	OMU	C5-C4-N3	3.56	119.78	114.80
52	v	8	4SU	N3-C2-N1	3.55	119.51	114.89
31	a	1515	MA6	C2-N1-C6	3.43	120.21	111.83
31	a	1516	MA6	C2-N1-C6	3.42	120.18	111.83
31	a	1516	MA6	C2-N3-C4	3.37	120.05	111.83
5	A	2499	2MA	C5-N7-C8	3.35	108.71	103.45
52	v	20	H2U	C5-C4-N3	-3.34	113.13	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2499	2MA	N3-C2-N1	-3.28	119.99	125.77
31	a	1515	MA6	C2-N3-C4	3.26	119.80	111.83
31	a	1516	MA6	N3-C4-N9	3.05	132.36	127.17
5	A	2576	PSU	O2-C2-N1	-3.02	119.67	122.79
31	a	513	PSU	O2-C2-N1	-3.02	119.67	122.79
5	A	2026	6MZ	C5-N7-C8	2.99	108.14	103.45
31	a	1515	MA6	C5-N7-C8	2.95	108.09	103.45
31	a	1515	MA6	N3-C4-N9	2.95	132.19	127.17
31	a	1516	MA6	C5-N7-C8	2.94	108.06	103.45
5	A	2500	PSU	O2-C2-N1	-2.90	119.80	122.79
52	v	56	PSU	O2-C2-N1	-2.89	119.81	122.79
5	A	1907	PSU	O2-C2-N1	-2.87	119.83	122.79
5	A	2601	PSU	O2-C2-N1	-2.84	119.86	122.79
5	A	2548	OMU	O4-C4-C5	-2.82	120.31	125.16
5	A	1913	PSU	O2-C2-N1	-2.79	119.91	122.79
5	A	2026	6MZ	C5-C6-N1	2.66	121.00	118.15
5	A	952	PSU	O2-C2-N1	-2.65	120.05	122.79
5	A	2453	PSU	O2-C2-N1	-2.59	120.11	122.79
5	A	2576	PSU	C6-C5-C4	2.55	119.90	118.17
5	A	1913	PSU	C6-N1-C2	-2.50	120.37	122.69
31	a	1515	MA6	C4-N9-C8	2.49	108.35	105.74
31	a	513	PSU	C6-N1-C2	-2.48	120.39	122.69
5	A	2576	PSU	O4'-C1'-C2'	2.48	108.58	105.15
52	v	56	PSU	C6-N1-C2	-2.43	120.44	122.69
5	A	1907	PSU	C6-N1-C2	-2.43	120.44	122.69
5	A	2453	PSU	C6-N1-C2	-2.42	120.45	122.69
5	A	2500	PSU	C6-C5-C4	2.41	119.80	118.17
52	v	8	4SU	C1'-N1-C2	2.41	121.92	117.59
5	A	2576	PSU	C6-N1-C2	-2.37	120.49	122.69
31	a	1516	MA6	C4-N9-C8	2.37	108.22	105.74
5	A	1907	PSU	C6-C5-C4	2.37	119.77	118.17
31	a	1495	UR3	C6-N1-C2	-2.35	119.88	121.80
31	a	513	PSU	O4'-C1'-C2'	2.35	108.40	105.15
5	A	2601	PSU	C6-C5-C4	2.35	119.76	118.17
5	A	2601	PSU	C6-N1-C2	-2.33	120.53	122.69
5	A	952	PSU	C6-N1-C2	-2.27	120.58	122.69
5	A	2499	2MA	N6-C6-N1	2.26	120.08	117.03
31	a	1515	MA6	C4-C5-N7	-2.24	108.02	110.58
31	a	1516	MA6	C4-C5-N7	-2.23	108.03	110.58
5	A	2500	PSU	C6-N1-C2	-2.22	120.63	122.69
5	A	1911	3TD	C1'-C5-C4	2.22	120.97	117.61
5	A	2453	PSU	O4'-C1'-C2'	2.19	108.19	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2453	PSU	C6-C5-C4	2.19	119.65	118.17
31	a	1399	4OC	C6-C5-C4	2.18	119.62	117.00
5	A	2548	OMU	O2-C2-N1	-2.15	120.00	122.80
5	A	2499	2MA	C4-C5-N7	-2.14	108.14	110.58
5	A	2026	6MZ	C4-C5-N7	-2.11	108.16	110.58
5	A	2499	2MA	CM2-C2-N1	2.09	120.25	117.13
5	A	1913	PSU	O4'-C1'-C2'	2.06	108.00	105.15
5	A	952	PSU	C6-C5-C4	2.04	119.55	118.17
52	v	56	PSU	O4'-C1'-C2'	2.01	107.94	105.15

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	C2'-C1'-C5-C4
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	56	PSU	O4'-C1'-C5-C4
52	v	56	PSU	O4'-C1'-C5-C6
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
31	a	524	G7M	C3'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	2548	OMU	C3'-C4'-C5'-O5'
5	A	2548	OMU	O4'-C4'-C5'-O5'
31	a	524	G7M	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	963	2MG	C3'-C4'-C5'-O5'
52	v	8	4SU	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
31	a	513	PSU	C3'-C4'-C5'-O5'
52	v	56	PSU	C3'-C4'-C5'-O5'
5	A	1913	PSU	C3'-C4'-C5'-O5'
52	v	56	PSU	O4'-C4'-C5'-O5'
5	A	1913	PSU	O4'-C4'-C5'-O5'
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	1516	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
52	v	20	H2U	C2'-C1'-N1-C6
5	A	2499	2MA	O4'-C1'-N9-C8
31	a	513	PSU	C2'-C1'-C5-C6
5	A	1907	PSU	C3'-C4'-C5'-O5'
31	a	524	G7M	C4'-C5'-O5'-P
52	v	20	H2U	C2'-C1'-N1-C2
5	A	2499	2MA	C2'-C1'-N9-C8
5	A	2026	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2453	PSU	1	0
52	v	55	5MU	6	0
5	A	2026	6MZ	3	0
5	A	2548	OMU	1	0
31	a	1516	MA6	1	0
31	a	1515	MA6	1	0
52	v	56	PSU	6	0
52	v	20	H2U	3	0
5	A	2247	OMG	1	0
31	a	963	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 194 ligands modelled in this entry, 191 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	YQM	A	3202	56	43,44,44	3.69	23 (53%)	53,69,69	2.85	24 (45%)
55	YQM	a	1601	56	43,44,44	3.40	23 (53%)	53,69,69	2.68	22 (41%)
55	YQM	A	3201	56	43,44,44	3.74	23 (53%)	53,69,69	2.92	25 (47%)

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	YQM	A	3202	56	-	3/16/81/81	0/5/5/5
55	YQM	a	1601	56	-	9/16/81/81	0/5/5/5
55	YQM	A	3201	56	-	3/16/81/81	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3202	YQM	C19-C20	13.94	1.64	1.52
55	A	3201	YQM	C19-C20	13.90	1.64	1.52
55	a	1601	YQM	C19-C20	12.98	1.63	1.52
55	A	3201	YQM	C19-C17	8.53	1.66	1.55
55	A	3202	YQM	C19-C17	8.37	1.66	1.55
55	A	3201	YQM	C05-C04	8.05	1.62	1.54
55	A	3202	YQM	C05-C04	7.80	1.61	1.54
55	a	1601	YQM	C19-C17	7.80	1.65	1.55
55	a	1601	YQM	C05-C04	7.36	1.61	1.54
55	A	3202	YQM	C21-C24	5.74	1.59	1.47
55	A	3201	YQM	C21-C24	5.71	1.59	1.47
55	a	1601	YQM	C21-C24	5.00	1.57	1.47
55	A	3202	YQM	C32-N31	4.49	1.45	1.35
55	A	3202	YQM	C09-C10	4.47	1.45	1.38
55	A	3201	YQM	C32-N31	4.42	1.45	1.35
55	A	3201	YQM	C09-C10	4.41	1.45	1.38
55	A	3201	YQM	C14-C15	4.40	1.58	1.45
55	A	3201	YQM	C14-C13	4.30	1.49	1.41
55	A	3202	YQM	C14-C15	4.22	1.58	1.45
55	A	3201	YQM	C19-C05	4.18	1.57	1.53
55	a	1601	YQM	C32-N31	4.15	1.44	1.35
55	a	1601	YQM	C09-C10	4.13	1.44	1.38
55	A	3202	YQM	C14-C13	4.05	1.49	1.41
55	A	3201	YQM	C12-N31	4.02	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3202	YQM	C12-N31	4.00	1.49	1.41
55	A	3201	YQM	C17-C16	3.89	1.54	1.46
55	A	3202	YQM	C17-C16	3.79	1.53	1.46
55	A	3201	YQM	C15-C16	3.71	1.42	1.36
55	a	1601	YQM	C12-N31	3.64	1.48	1.41
55	a	1601	YQM	C14-C15	3.61	1.56	1.45
55	a	1601	YQM	C17-C16	3.58	1.53	1.46
55	A	3202	YQM	C15-C16	3.43	1.42	1.36
55	A	3202	YQM	C19-C05	3.38	1.56	1.53
55	a	1601	YQM	C14-C13	3.33	1.47	1.41
55	A	3201	YQM	C24-N26	3.26	1.42	1.33
55	A	3202	YQM	C34-C32	3.25	1.58	1.52
55	A	3202	YQM	C24-N26	3.23	1.42	1.33
55	A	3201	YQM	C12-C13	3.23	1.44	1.40
55	A	3202	YQM	C21-C22	3.21	1.54	1.44
55	A	3201	YQM	C21-C22	3.19	1.54	1.44
55	a	1601	YQM	C15-C16	3.12	1.41	1.36
55	a	1601	YQM	C21-C22	3.06	1.53	1.44
55	a	1601	YQM	C24-N26	3.03	1.42	1.33
55	A	3201	YQM	C34-C32	3.02	1.57	1.52
55	A	3202	YQM	C12-C13	3.02	1.44	1.40
55	A	3201	YQM	C36-N35	2.89	1.53	1.47
55	a	1601	YQM	C34-C32	2.87	1.57	1.52
55	A	3202	YQM	C08-C09	2.84	1.55	1.51
55	a	1601	YQM	C19-C05	2.82	1.55	1.53
55	a	1601	YQM	C04-N02	2.78	1.53	1.47
55	A	3201	YQM	C04-N02	2.71	1.53	1.47
55	A	3201	YQM	C08-C09	2.69	1.55	1.51
55	a	1601	YQM	C08-C09	2.66	1.55	1.51
55	A	3202	YQM	C06-C07	2.60	1.59	1.53
55	A	3202	YQM	C08-C07	2.60	1.59	1.52
55	A	3202	YQM	C36-N35	2.55	1.52	1.47
55	A	3201	YQM	C08-C07	2.52	1.59	1.52
55	a	1601	YQM	C12-C13	2.47	1.43	1.40
55	a	1601	YQM	C11-C10	2.39	1.41	1.37
55	a	1601	YQM	C08-C07	2.35	1.58	1.52
55	A	3202	YQM	C11-C10	2.35	1.41	1.37
55	A	3201	YQM	C06-C07	2.34	1.58	1.53
55	A	3202	YQM	C04-N02	2.32	1.52	1.47
55	A	3201	YQM	C11-C10	2.27	1.41	1.37
55	a	1601	YQM	C36-N35	2.20	1.52	1.47
55	A	3201	YQM	C07-C16	2.08	1.53	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1601	YQM	C06-C07	2.08	1.58	1.53
55	A	3202	YQM	C07-C16	2.07	1.53	1.51
55	a	1601	YQM	C07-C16	2.03	1.53	1.51

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	3201	YQM	C34-N35-C39	-7.96	103.03	113.34
55	A	3202	YQM	C34-C32-N31	7.14	127.44	114.23
55	a	1601	YQM	C34-C32-N31	6.95	127.09	114.23
55	A	3201	YQM	C34-C32-N31	6.81	126.84	114.23
55	a	1601	YQM	C34-N35-C39	-6.69	104.67	113.34
55	A	3202	YQM	C34-N35-C39	-6.61	104.78	113.34
55	a	1601	YQM	C11-C12-C13	-5.91	114.80	120.53
55	A	3201	YQM	C11-C12-C13	-5.88	114.84	120.53
55	A	3202	YQM	C11-C12-C13	-5.83	114.89	120.53
55	A	3202	YQM	O27-C20-C21	5.78	127.76	121.90
55	A	3201	YQM	C39-N35-C36	5.33	110.33	104.04
55	a	1601	YQM	O27-C20-C21	4.96	126.93	121.90
55	A	3201	YQM	O18-C17-C16	4.88	128.46	121.47
55	a	1601	YQM	O18-C17-C19	-4.88	109.82	119.11
55	A	3201	YQM	C07-C06-C05	4.79	118.54	110.38
55	A	3202	YQM	O18-C17-C16	4.66	128.13	121.47
55	A	3201	YQM	O27-C20-C21	4.65	126.62	121.90
55	A	3202	YQM	O33-C32-C34	-4.64	112.89	121.02
55	A	3202	YQM	C07-C06-C05	4.62	118.25	110.38
55	A	3202	YQM	O18-C17-C19	-4.62	110.32	119.11
55	A	3201	YQM	O18-C17-C19	-4.61	110.34	119.11
55	a	1601	YQM	O33-C32-C34	-4.60	112.97	121.02
55	A	3201	YQM	O33-C32-C34	-4.49	113.16	121.02
55	a	1601	YQM	O18-C17-C16	4.12	127.37	121.47
55	A	3202	YQM	C21-C24-N26	4.10	127.00	118.64
55	A	3201	YQM	C21-C24-N26	4.09	126.98	118.64
55	a	1601	YQM	C07-C16-C15	-4.04	115.55	121.44
55	A	3202	YQM	C07-C16-C15	-4.04	115.56	121.44
55	A	3202	YQM	C24-C21-C22	-3.98	116.12	120.87
55	a	1601	YQM	C21-C24-N26	3.94	126.68	118.64
55	A	3202	YQM	O25-C24-N26	-3.67	114.66	122.89
55	A	3202	YQM	C17-C19-C20	3.65	114.16	109.88
55	A	3201	YQM	O25-C24-N26	-3.63	114.75	122.89
55	A	3201	YQM	C07-C16-C15	-3.61	116.18	121.44
55	A	3201	YQM	C24-C21-C22	-3.58	116.60	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1601	YQM	C07-C06-C05	3.51	116.37	110.38
55	A	3201	YQM	O27-C20-C19	-3.51	108.29	113.37
55	a	1601	YQM	O25-C24-N26	-3.46	115.14	122.89
55	a	1601	YQM	C24-C21-C22	-3.22	117.02	120.87
55	a	1601	YQM	C06-C07-C16	3.21	117.25	110.28
55	a	1601	YQM	C14-C13-C12	3.21	124.53	118.98
55	A	3201	YQM	C17-C19-C20	3.18	113.61	109.88
55	A	3201	YQM	C06-C05-C04	-3.15	109.19	113.73
55	A	3202	YQM	C14-C13-C12	3.14	124.41	118.98
55	A	3201	YQM	C14-C13-C12	3.11	124.36	118.98
55	A	3202	YQM	C39-N35-C36	3.08	107.68	104.04
55	A	3201	YQM	C19-C05-C04	3.06	115.83	111.64
55	a	1601	YQM	O27-C20-C19	-3.03	108.98	113.37
55	A	3202	YQM	C06-C07-C16	3.00	116.79	110.28
55	A	3202	YQM	C19-C20-C21	-2.98	118.62	122.89
55	A	3201	YQM	C19-C20-C21	-2.88	118.76	122.89
55	A	3202	YQM	O27-C20-C19	-2.83	109.27	113.37
55	A	3201	YQM	C06-C07-C16	2.80	116.36	110.28
55	a	1601	YQM	C19-C20-C21	-2.80	118.88	122.89
55	A	3202	YQM	C06-C05-C04	-2.79	109.70	113.73
55	A	3202	YQM	C19-C05-C04	2.75	115.40	111.64
55	a	1601	YQM	C17-C19-C20	2.74	113.10	109.88
55	A	3202	YQM	C22-C21-C20	-2.55	116.50	118.87
55	a	1601	YQM	C19-C05-C04	2.54	115.11	111.64
55	A	3202	YQM	O28-C19-C20	-2.41	106.29	110.14
55	A	3201	YQM	O28-C19-C20	-2.34	106.39	110.14
55	a	1601	YQM	O29-C15-C14	-2.29	113.41	118.45
55	A	3202	YQM	O33-C32-N31	-2.22	119.67	123.64
55	A	3201	YQM	O29-C15-C14	-2.21	113.58	118.45
55	a	1601	YQM	O28-C19-C20	-2.15	106.69	110.14
55	A	3201	YQM	C34-N35-C36	-2.14	110.56	113.34
55	A	3202	YQM	O29-C15-C14	-2.14	113.73	118.45
55	a	1601	YQM	C37-C36-N35	-2.11	101.42	103.90
55	a	1601	YQM	O33-C32-N31	-2.07	119.94	123.64
55	A	3201	YQM	C13-C12-N31	2.06	126.19	117.60
55	A	3201	YQM	O33-C32-N31	-2.03	120.00	123.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	a	1601	YQM	C20-C21-C24-N26

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Mol	Chain	Res	Type	Atoms
55	a	1601	YQM	C20-C21-C24-O25
55	a	1601	YQM	C22-C21-C24-N26
55	a	1601	YQM	C22-C21-C24-O25
55	A	3201	YQM	C11-C12-N31-C32
55	A	3201	YQM	C13-C12-N31-C32
55	A	3202	YQM	N31-C32-C34-N35
55	A	3202	YQM	O33-C32-C34-N35
55	a	1601	YQM	O33-C32-C34-N35
55	a	1601	YQM	N31-C32-C34-N35
55	A	3202	YQM	C13-C12-N31-C32
55	a	1601	YQM	C22-C04-N02-C01
55	a	1601	YQM	C22-C04-N02-C03
55	a	1601	YQM	C32-C34-N35-C36
55	A	3201	YQM	O33-C32-C34-N35

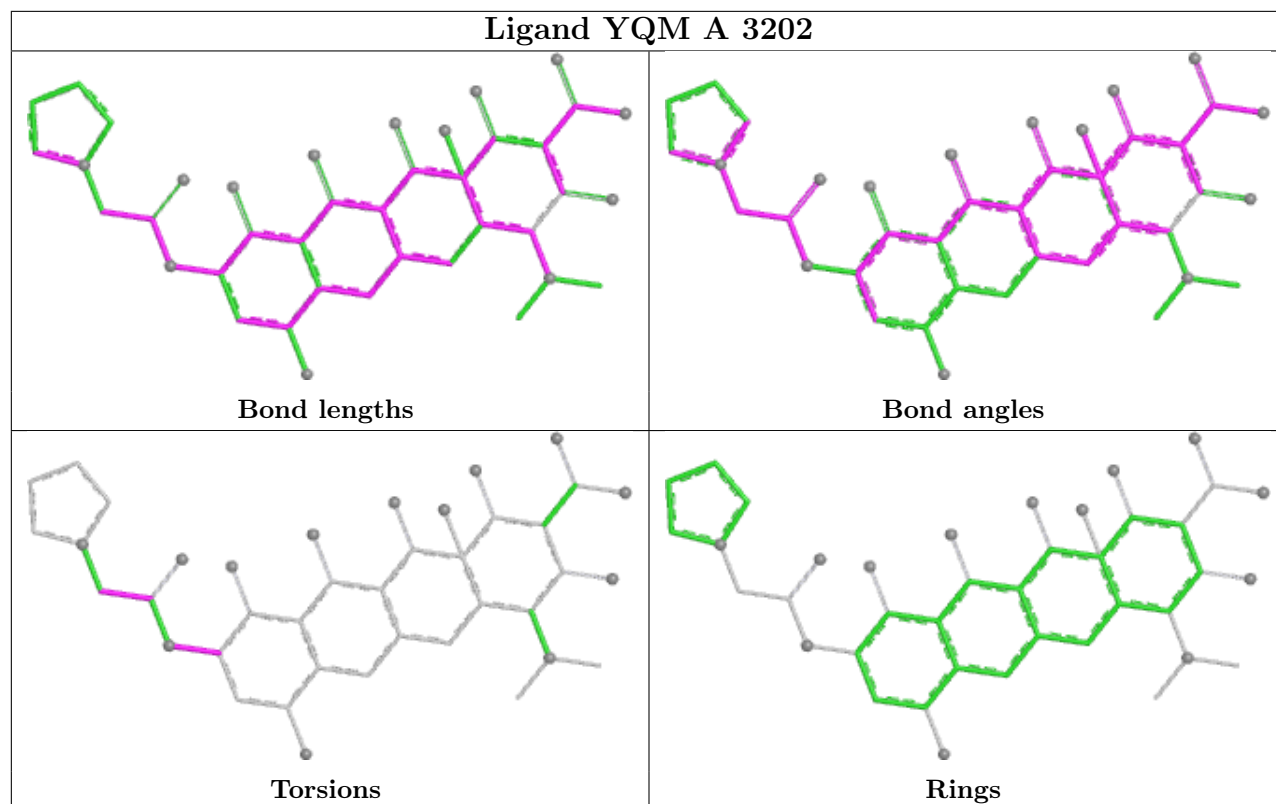
There are no ring outliers.

1 monomer is involved in 1 short contact:

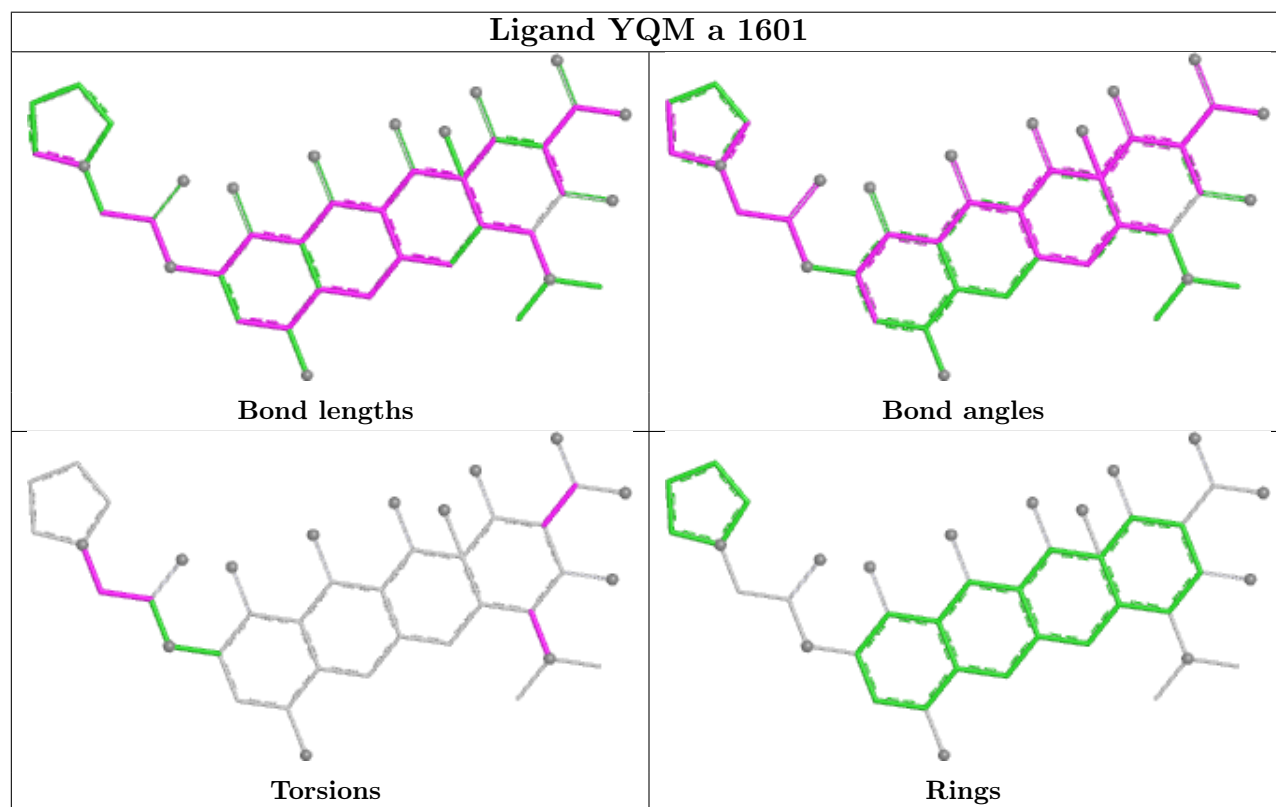
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A	3201	YQM	1	0

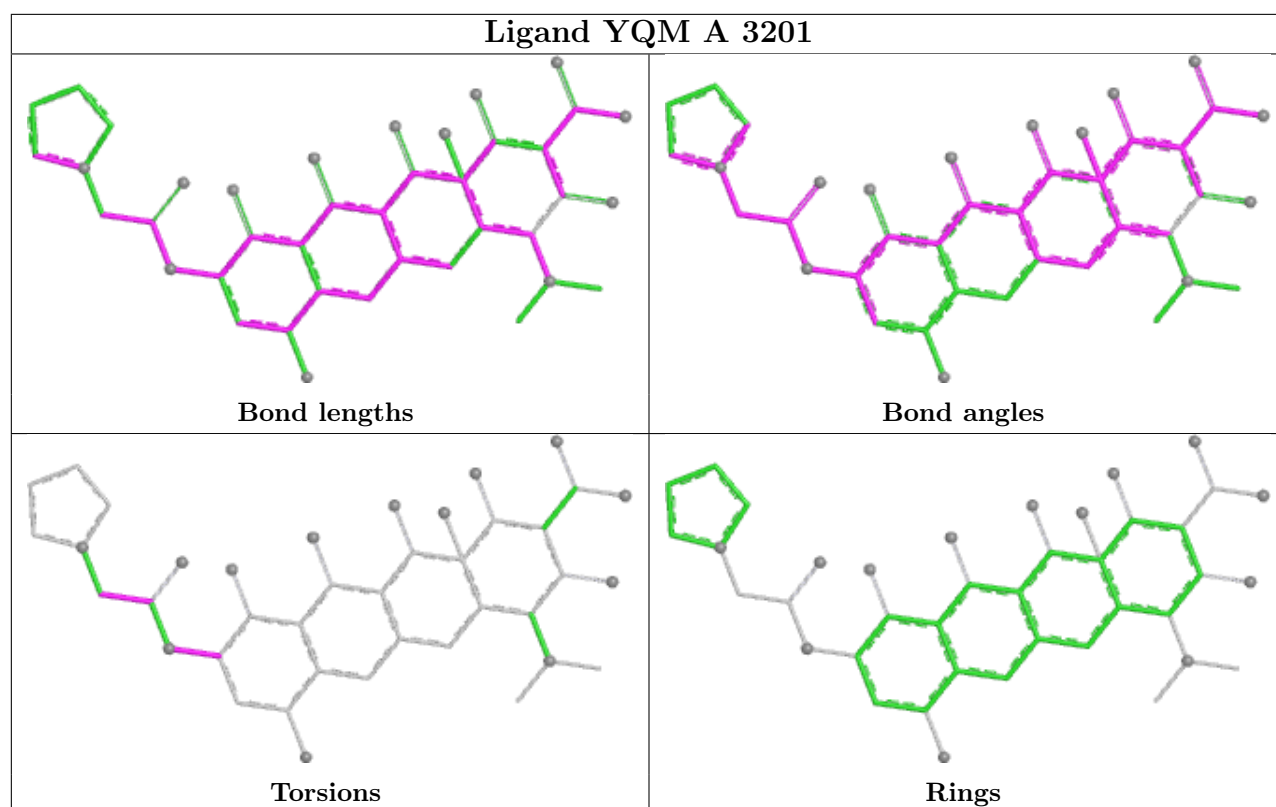
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand YQM A 3202



Ligand YQM a 1601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

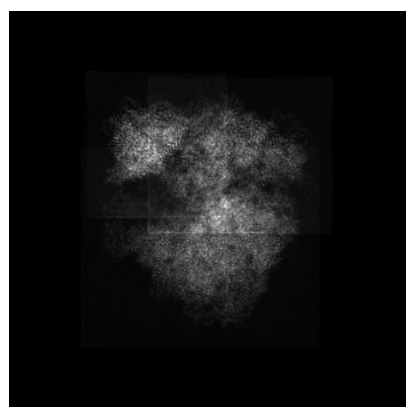
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23669. These allow visual inspection of the internal detail of the map and identification of artifacts.

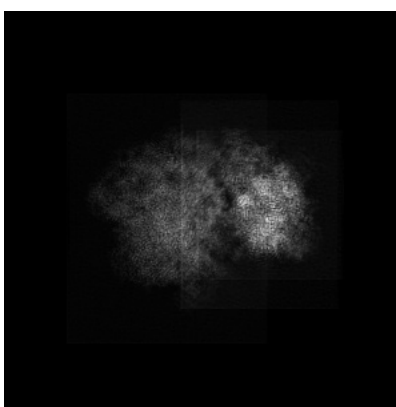
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

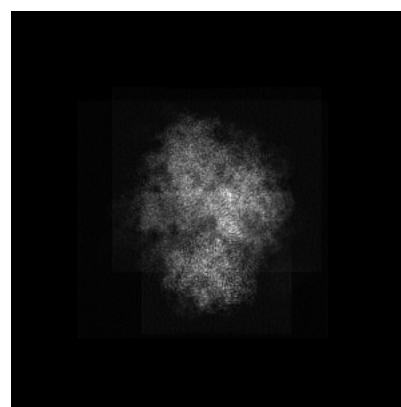
6.1.1 Primary map



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

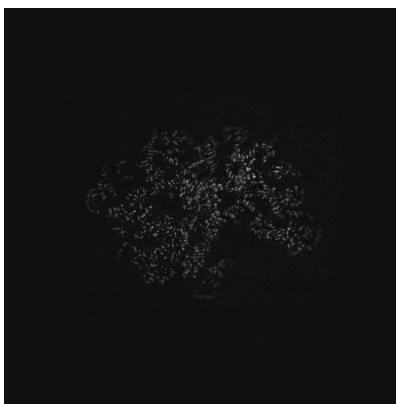
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

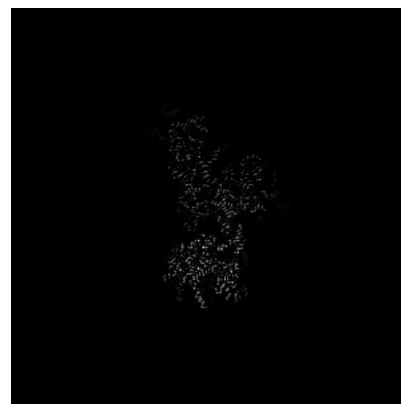
6.3.1 Primary map



X Index: 280



Y Index: 274

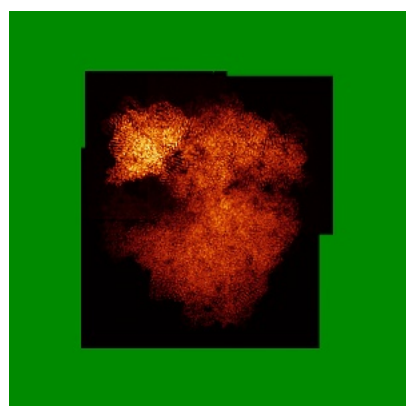


Z Index: 340

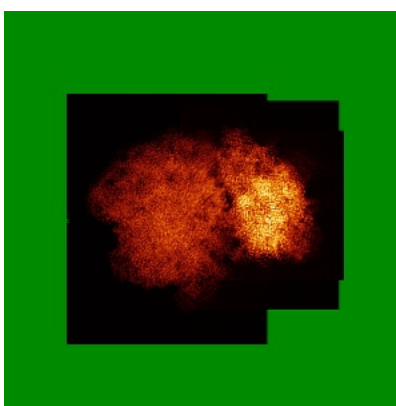
The images above show the largest variance slices of the map in three orthogonal directions.

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

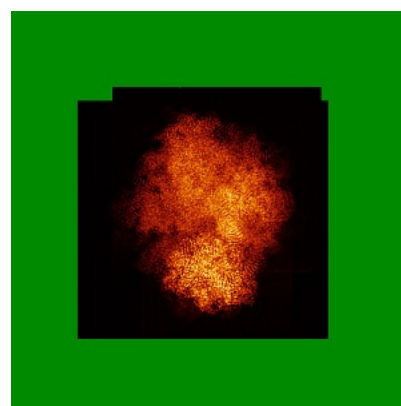
6.4.1 Primary map



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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

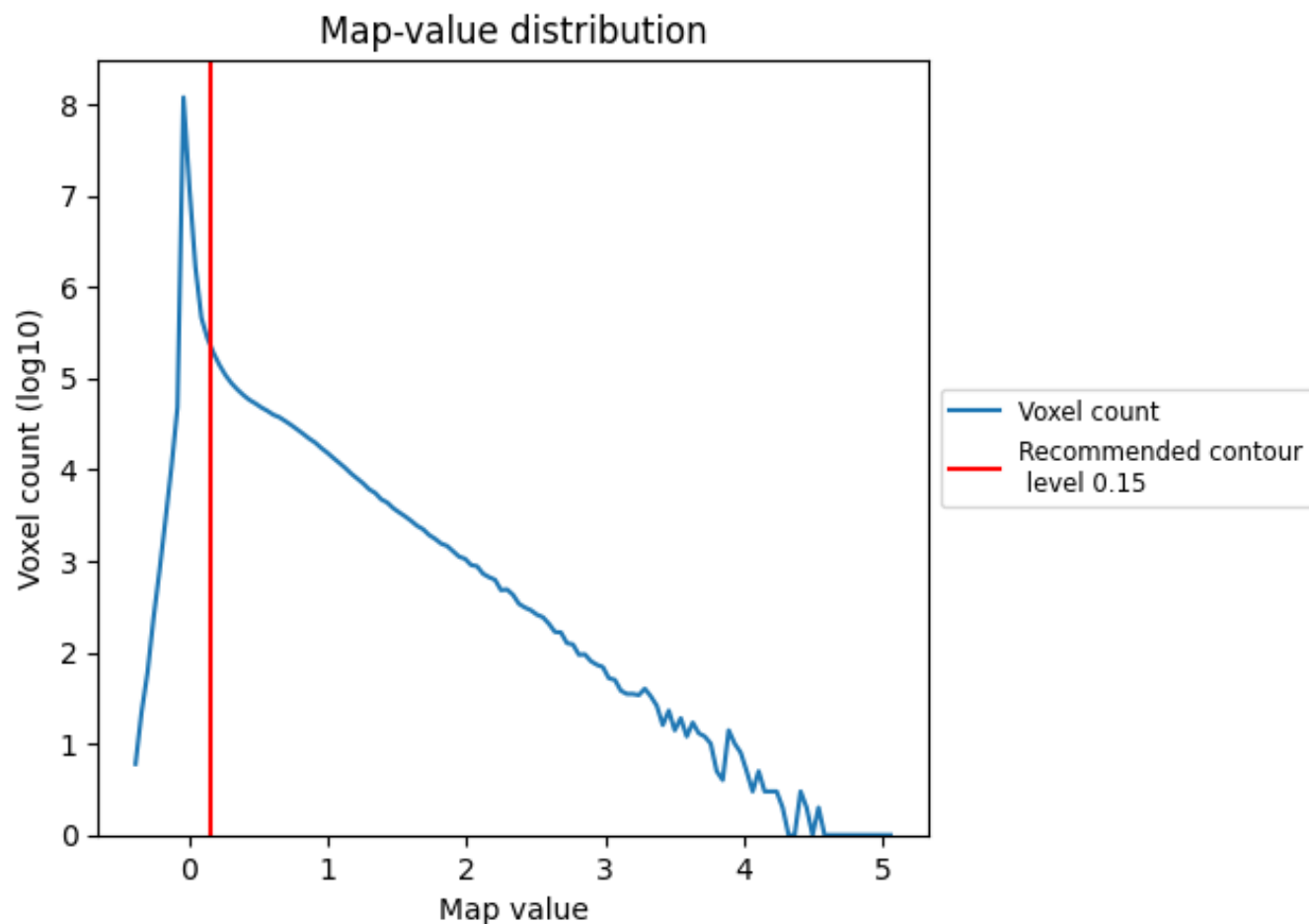
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

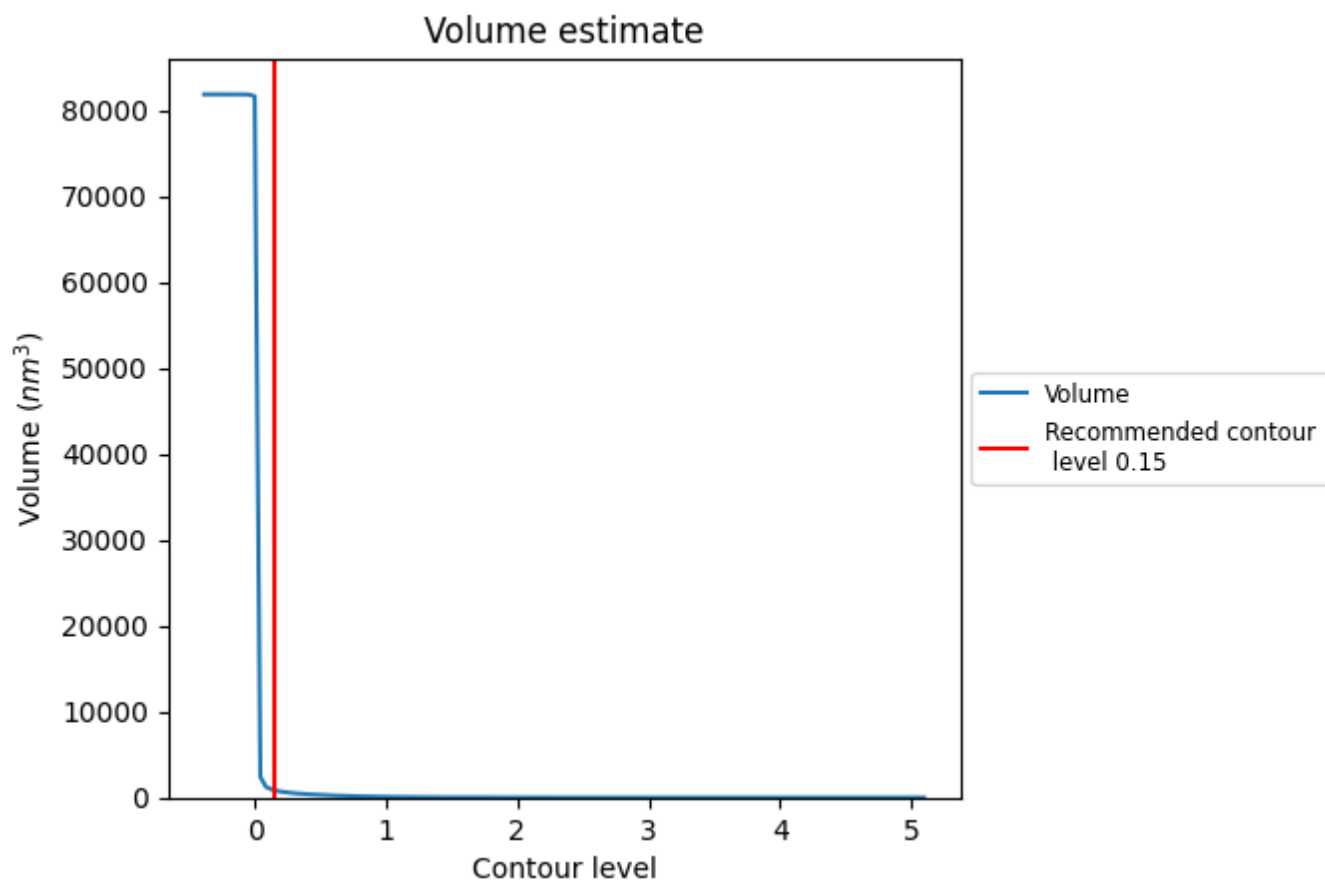
This section contains the results of statistical analysis of the map.

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.

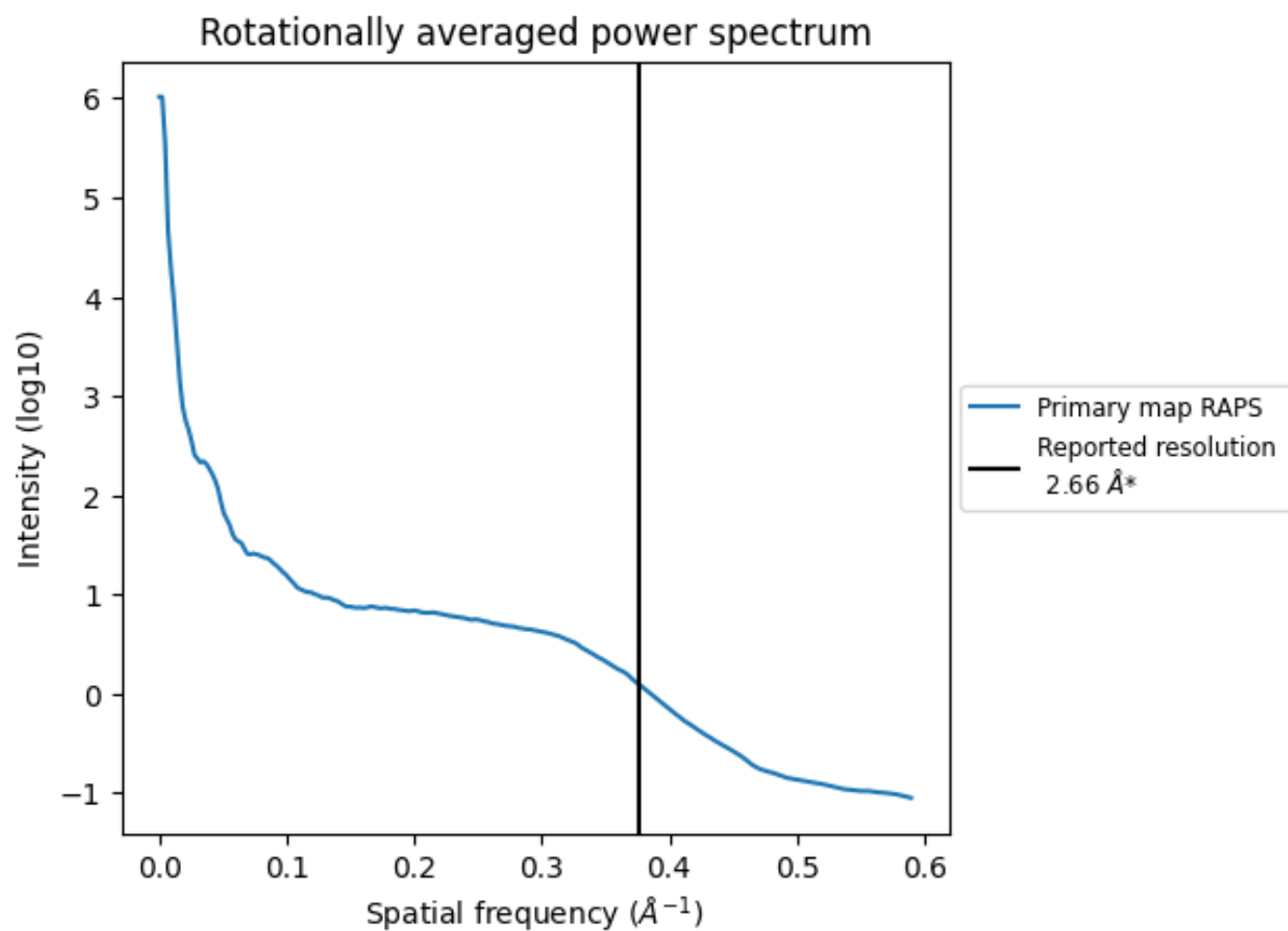
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860 nm^3 ; this corresponds to an approximate mass of 777 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 0.376 Å⁻¹

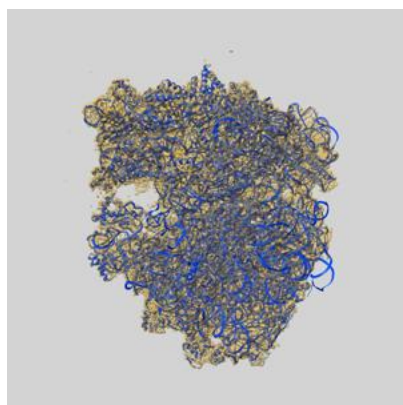
8 Fourier-Shell correlation

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

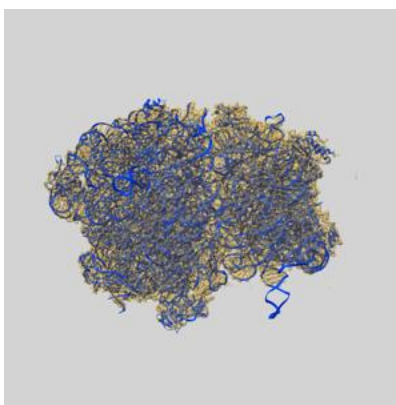
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23669 and PDB model 7M4X. Per-residue inclusion information can be found in section 3 on page 15.

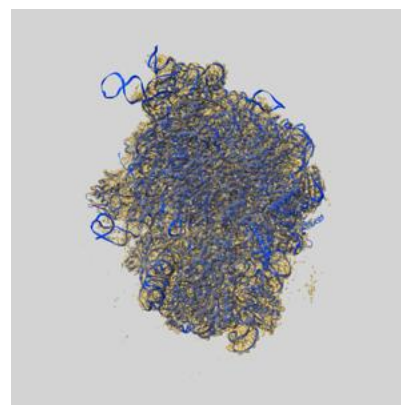
9.1 Map-model overlay [i](#)



X



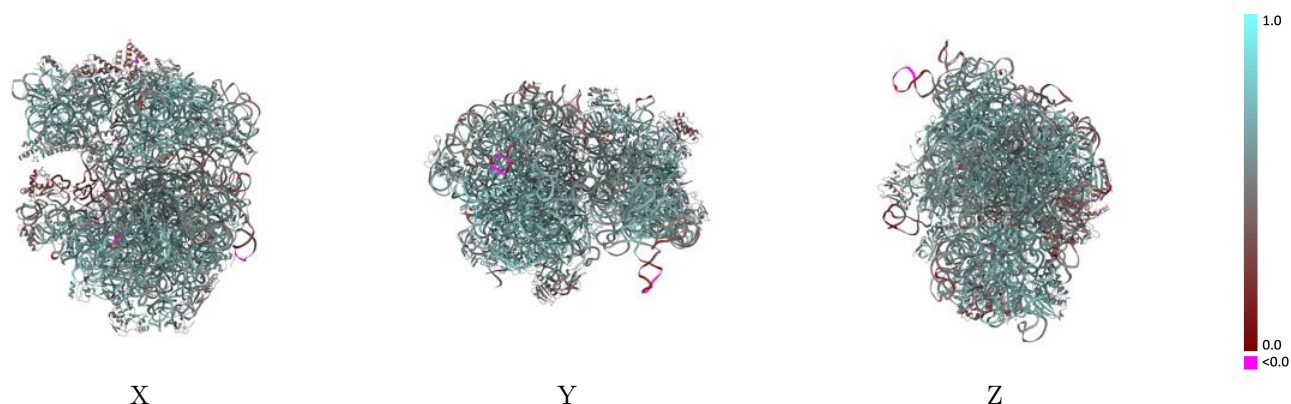
Y



Z

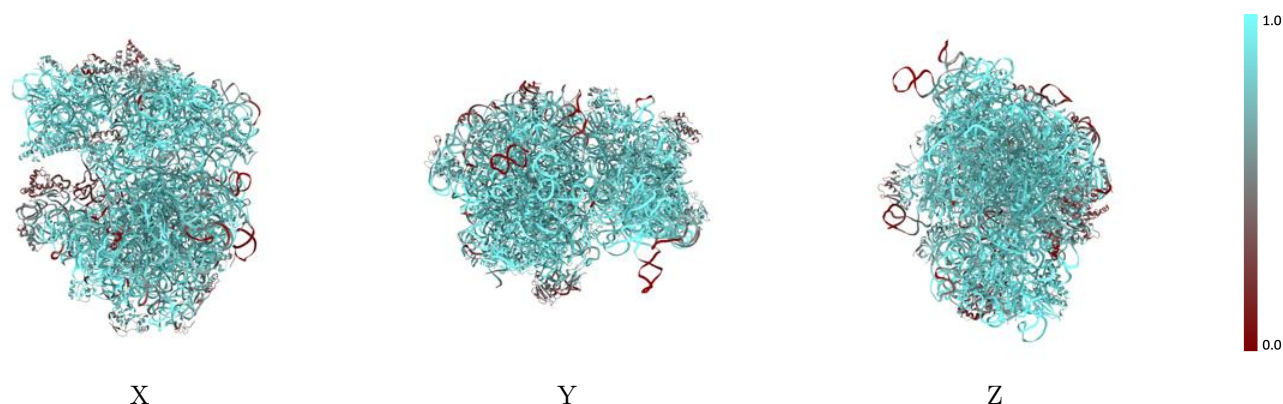
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



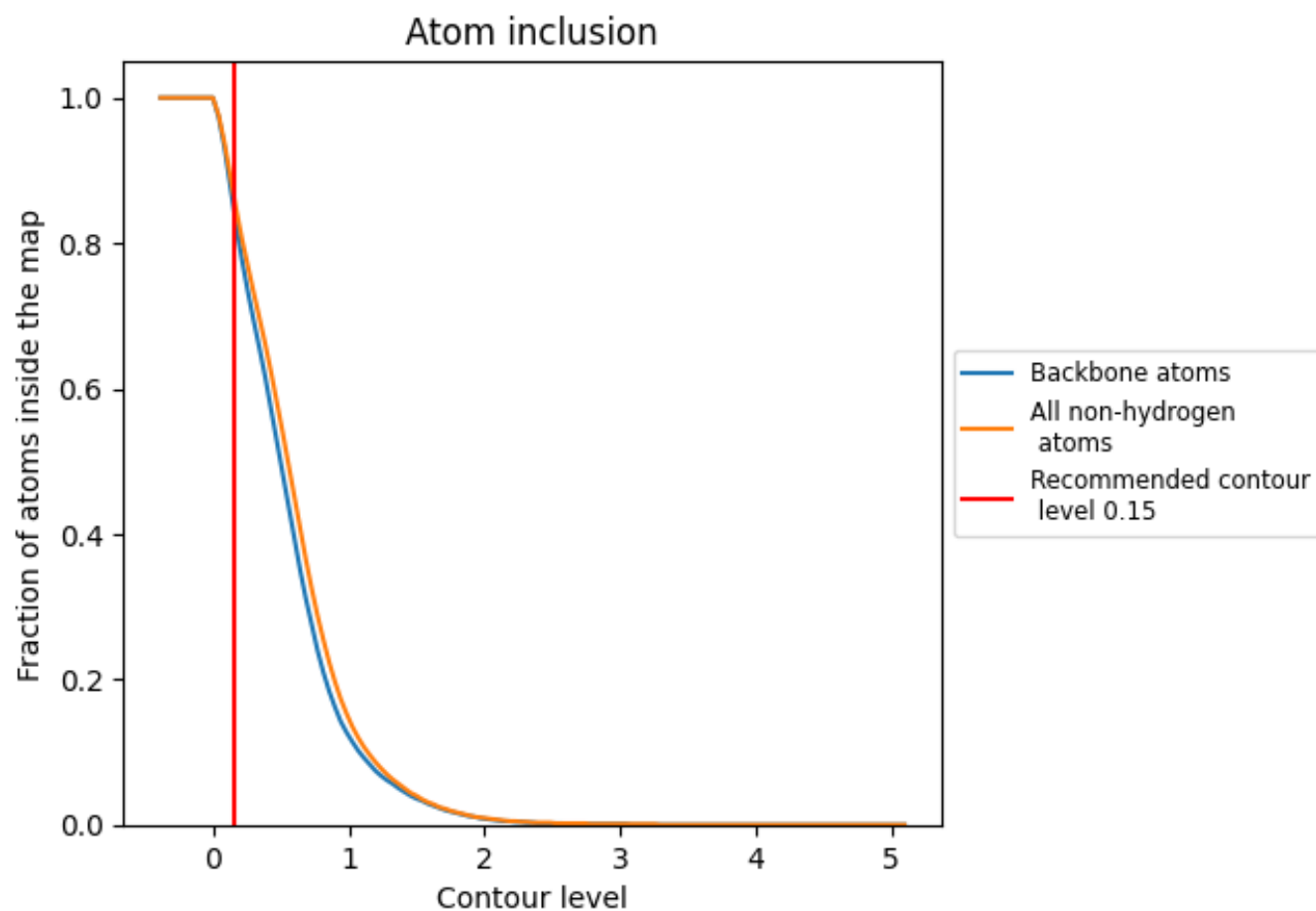
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5910
0	 0.8470	 0.6180
1	 0.9590	 0.6990
2	 0.9670	 0.6970
3	 0.8950	 0.6140
A	 0.8980	 0.6020
B	 0.6970	 0.5120
C	 0.9380	 0.5810
D	 0.9300	 0.6710
E	 0.8150	 0.6190
F	 0.2600	 0.2860
G	 0.5510	 0.4800
H	 0.2270	 0.3540
I	 0.9200	 0.6690
J	 0.9050	 0.6320
K	 0.9010	 0.6630
L	 0.8760	 0.6250
M	 0.9510	 0.6760
N	 0.6300	 0.5060
O	 0.8750	 0.6120
P	 0.9560	 0.6910
Q	 0.8490	 0.6430
R	 0.9160	 0.6670
S	 0.7450	 0.5840
T	 0.5910	 0.5150
U	 0.7480	 0.5800
V	 0.8650	 0.6580
W	 0.8710	 0.6460
X	 0.5800	 0.4930
Y	 0.8650	 0.6340
Z	 0.8390	 0.6470
a	 0.9290	 0.6020
b	 0.4850	 0.3610
c	 0.9040	 0.5990
d	 0.7570	 0.5340



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Chain	Atom inclusion	Q-score
e	 0.9140	 0.6100
f	 0.7820	 0.5130
g	 0.7690	 0.4880
h	 0.9270	 0.6520
i	 0.9400	 0.6340
j	 0.8690	 0.5970
k	 0.8150	 0.5150
l	 0.8790	 0.5910
m	 0.9230	 0.6080
n	 0.9540	 0.6530
o	 0.9280	 0.6180
p	 0.8910	 0.6410
q	 0.7870	 0.5270
r	 0.9130	 0.6100
s	 0.9520	 0.6560
t	 0.9050	 0.5890
u	 0.5300	 0.4580
v	 0.4890	 0.3630
w	 0.9540	 0.5810