



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 10, 2016 – 11:45 AM EST

PDB ID : 3JCJ
EMDB ID: : EMD-6559
Title : Structures of ribosome-bound initiation factor 2 reveal the mechanism of sub-unit association
Authors : Sprink, T.; Ramrath, D.J.F.; Yamamoto, H.; Yamamoto, K.; Loerke, J.; Ismer, J.; Hildebrand, P.W.; Scheerer, P.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2015-12-18
Resolution : 3.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

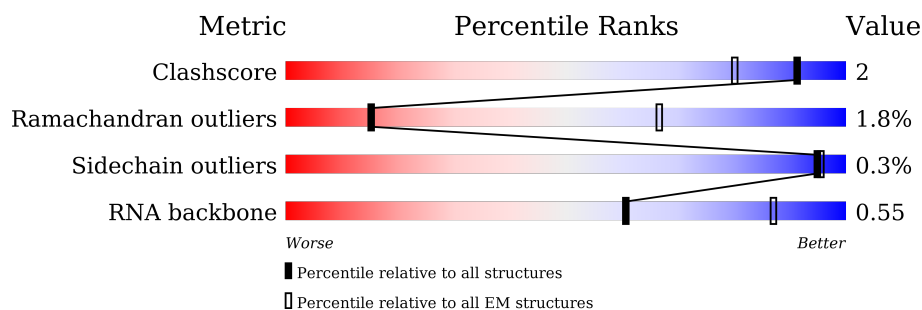
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	118	91% 9%
2	1	75	69% 27%
3	2	71	69% 28%
4	3	87	93% 5%
5	4	52	6% 6% 88%
6	A	2904	86% 12%
7	B	273	94% 5%
8	C	209	91% 9%

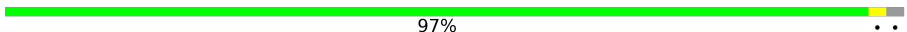
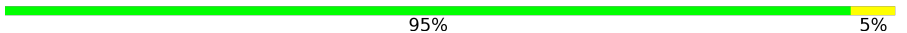






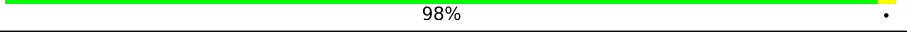


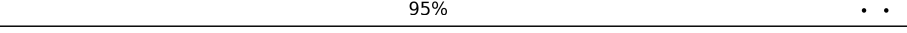
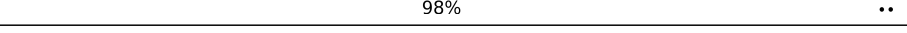
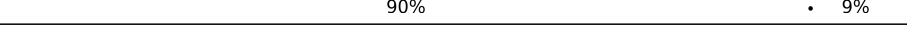
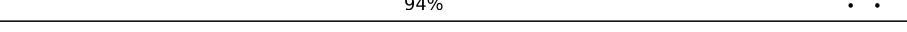
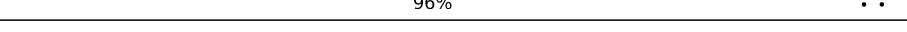
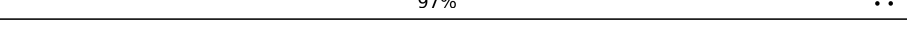
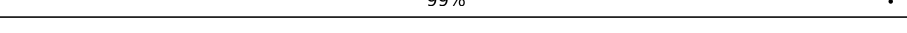

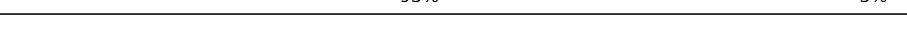
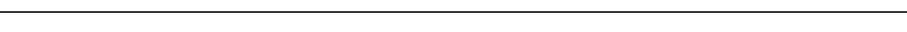

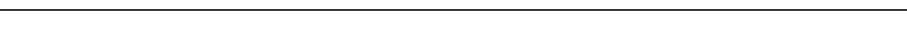
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Mol	Chain	Length	Quality of chain
9	D	201	
10	E	179	
11	F	177	
12	G	149	
13	H	142	
14	I	142	
15	J	123	
16	K	144	
17	L	136	
18	M	127	
19	N	117	
20	O	115	
21	P	118	
22	Q	103	
23	R	110	
24	S	100	
25	T	104	
26	U	94	
27	V	85	
28	W	78	
29	X	63	
30	Y	59	
31	Z	57	
32	a	55	
33	b	46	

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Mol	Chain	Length	Quality of chain
34	c	65	 97% ..
35	d	38	 95% 5%
36	e	165	 68% .. 29%
37	f	890	 57% . 43%
38	g	1542	 88% 12%
39	h	233	 87% . 12%
40	j	241	 88% . 10%
41	k	167	 86% . 10%
42	l	206	 98% .
43	m	179	 84% 16%
44	n	135	 72% . 26%
45	o	130	 95% ..
46	p	130	 98% ..
47	q	129	 90% . 9%
48	r	102	 94% . .
49	s	118	 96% ..
50	t	124	 97% ..
51	u	89	 99% .
52	v	77	 73% 25% .
53	w	101	 93% . 5%
54	x	84	 94% . 5%
55	y	82	 98% .
56	z	92	 86% 14%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148348 atoms, of which 1 is hydrogen and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 2 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 4 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 5 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 6 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	a	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	117	Total	C	N	O	S	0	0
			884	559	157	163	5		

- Molecule 37 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	509	Total	C	N	O	S	0	0
			3847	2409	675	748	15		

- Molecule 38 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 39 is a protein called 30S ribosomal protein S3.

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

- Molecule 40 is a protein called 30S ribosomal protein S2.

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

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 42 is a protein called 30S ribosomal protein S4.

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

- Molecule 43 is a protein called 30S ribosomal protein S7.

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

- Molecule 44 is a protein called 30S ribosomal protein S6.

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

- Molecule 45 is a protein called 30S ribosomal protein S9.

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

- Molecule 46 is a protein called 30S ribosomal protein S8.

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

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 48 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 50 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 51 is a protein called 30S ribosomal protein S15.

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

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	v	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 53 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S16.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

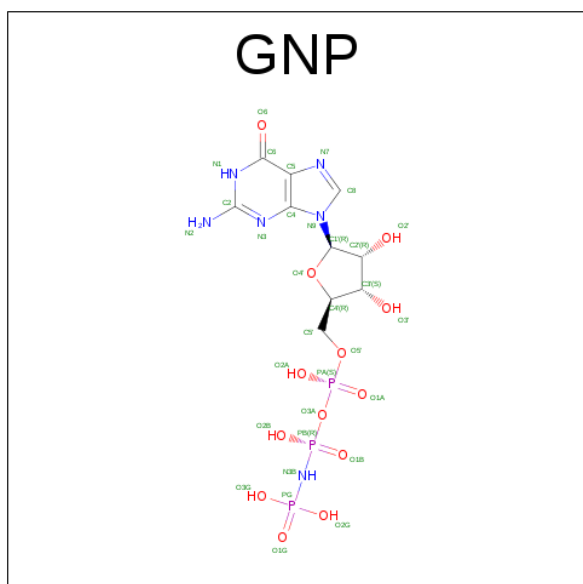
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	g	54	Total	Mg	0
			54	54	
57	d	1	Total	Mg	0
			1	1	
57	B	1	Total	Mg	0
			1	1	
57	w	1	Total	Mg	0
			1	1	
57	A	137	Total	Mg	0
			137	137	
57	3	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

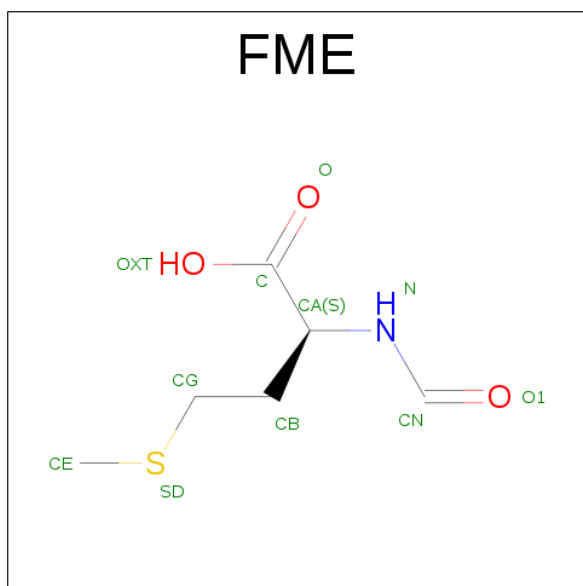
Mol	Chain	Residues	Atoms		AltConf
58	d	1	Total	Zn	0
			1	1	

- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
59	f	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms						AltConf
60	v	1	Total	C	H	N	O	S	0
			10	6	1	1	1	1	

- Molecule 61 is water.

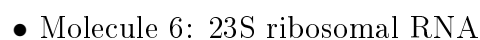
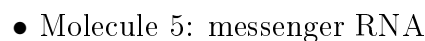
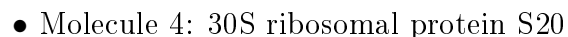
Mol	Chain	Residues	Atoms		AltConf
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			4	4	
61	A	599	Total	O	0
			599	599	
61	B	7	Total	O	0
			7	7	
61	C	2	Total	O	0
			2	2	
61	D	2	Total	O	0
			2	2	
61	I	1	Total	O	0
			1	1	
61	K	8	Total	O	0
			8	8	
61	M	5	Total	O	0
			5	5	

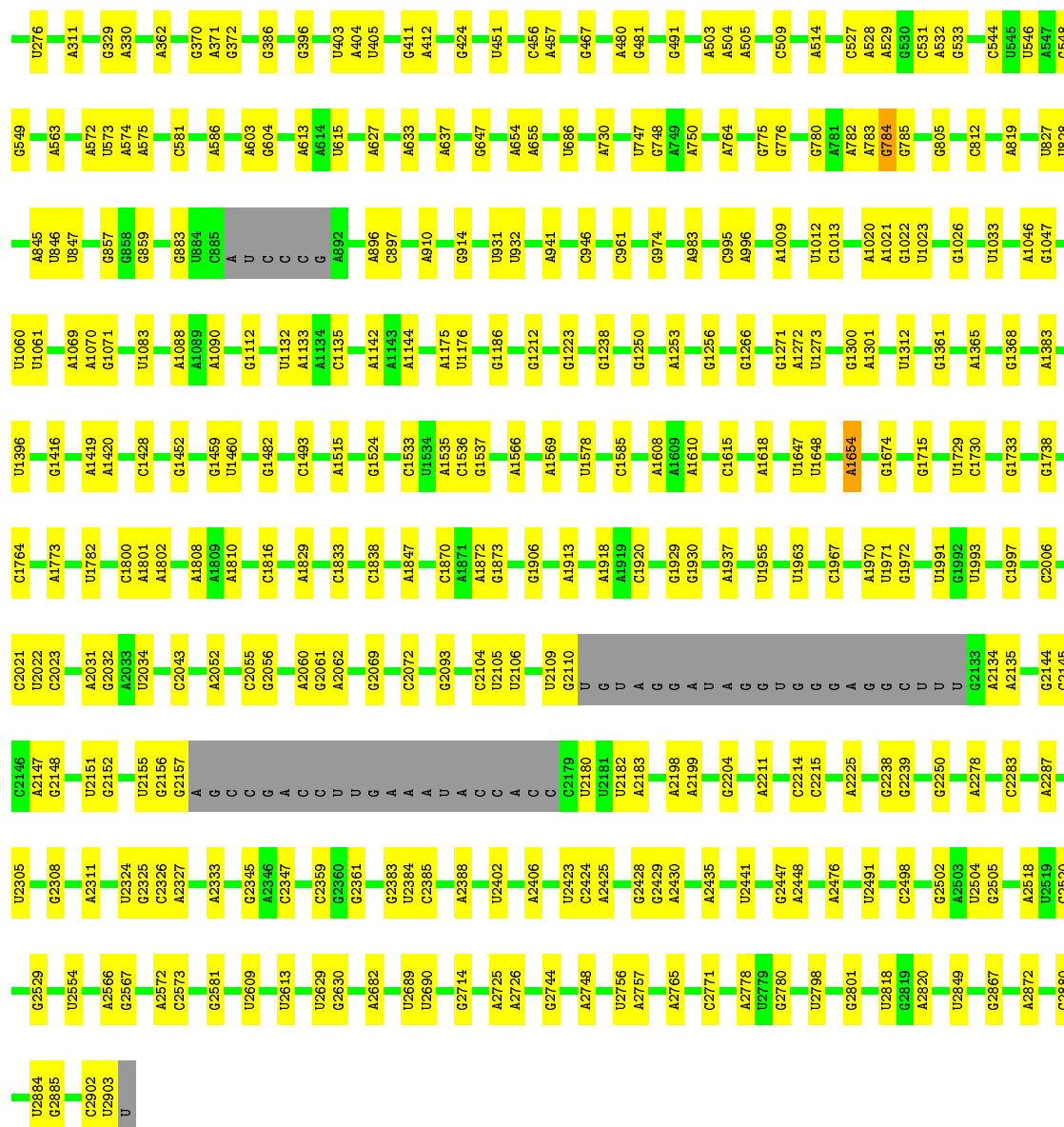
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Mol	Chain	Residues	Atoms		AltConf
61	P	3	Total 3	O 3	0
61	Q	3	Total 3	O 3	0
61	R	3	Total 3	O 3	0
61	S	2	Total 2	O 2	0
61	b	1	Total 1	O 1	0
61	d	3	Total 3	O 3	0
61	g	189	Total 189	O 189	0
61	q	1	Total 1	O 1	0
61	t	2	Total 2	O 2	0
61	w	2	Total 2	O 2	0

- Molecule 1: 5S ribosomal RNA





- Molecule 7: 50S ribosomal protein L2

Chain B: 94% 5% .



- Molecule 8: 50S ribosomal protein L3

Chain C: 91% 9%



- Molecule 9: 50S ribosomal protein L4

Chain D:  97% .



- Molecule 10: 50S ribosomal protein L5

Chain E:  97% ..



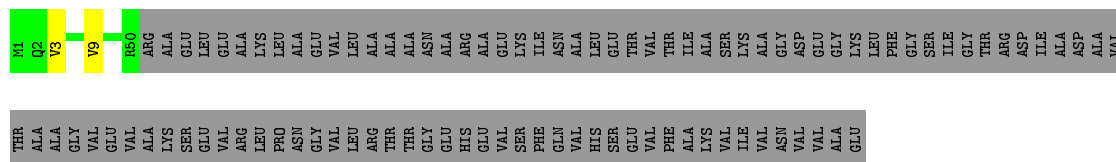
- Molecule 11: 50S ribosomal protein L6

Chain F:  97% ..



- Molecule 12: 50S ribosomal protein L9

Chain G:  32% . 66%



- Molecule 13: 50S ribosomal protein L11

Chain H:  97% ..




- Molecule 14: 50S ribosomal protein L13

Chain I:  95% 5%



- Molecule 15: 50S ribosomal protein L14

Chain J:  89% 11% .



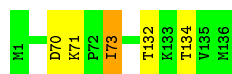
- Molecule 16: 50S ribosomal protein L15

Chain K:  96% ..



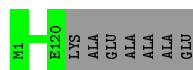
- Molecule 17: 50S ribosomal protein L16

Chain L:  96% ..



- Molecule 18: 50S ribosomal protein L17

Chain M:  94% 6%



- Molecule 19: 50S ribosomal protein L18

Chain N:  94% 5% .



- Molecule 20: 50S ribosomal protein L19

Chain O:  95% ..



- Molecule 21: 50S ribosomal protein L20

Chain P:  97% ..



- Molecule 22: 50S ribosomal protein L21

Chain Q:  97% .



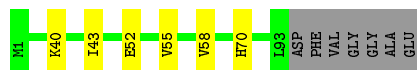
- Molecule 23: 50S ribosomal protein L22

Chain R:  96% .



- Molecule 24: 50S ribosomal protein L23

Chain S: 87% 6% 7%



- Molecule 25: 50S ribosomal protein L24

Chain T: 93% 5%



- Molecule 26: 50S ribosomal protein L25

Chain U: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L27

Chain V: 82% 9% 7%



- Molecule 28: 50S ribosomal protein L28

Chain W: 96%



- Molecule 29: 50S ribosomal protein L29

Chain X: 98%



- Molecule 30: 50S ribosomal protein L30

Chain Y: 98%



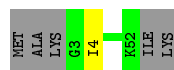
- Molecule 31: 50S ribosomal protein L32

Chain Z: 95%



- Molecule 32: 50S ribosomal protein L33

Chain a: 89% • 9%



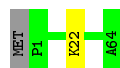
- Molecule 33: 50S ribosomal protein L34

Chain b: 100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L35

Chain c: 97% ..



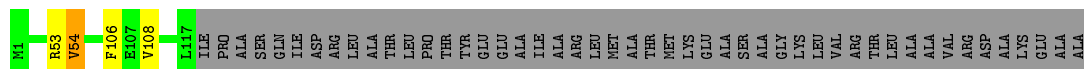
- Molecule 35: 50S ribosomal protein L36

Chain d:  95% 5%



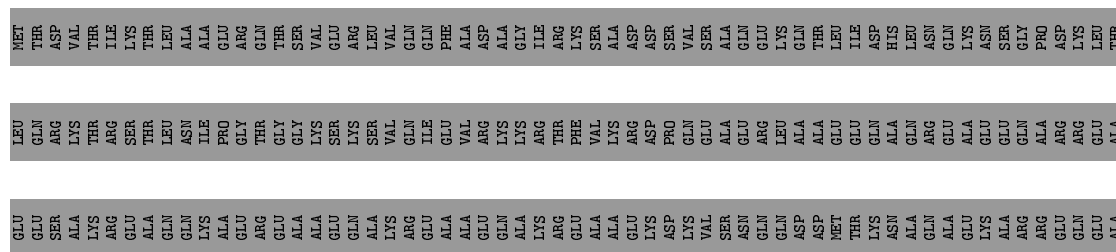
- Molecule 36: 50S ribosomal protein L10

Chain e: 68% .. 29%



- Molecule 37: Translation initiation factor IF-2

Chain f: 57% . 43%





- Molecule 42: 30S ribosomal protein S4

Chain l: 98%



- Molecule 43: 30S ribosomal protein S7

Chain m: 84%



- Molecule 44: 30S ribosomal protein S6

Chain n: 72%



- Molecule 45: 30S ribosomal protein S9

Chain o: 95%



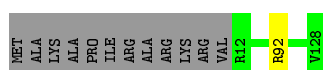
- Molecule 46: 30S ribosomal protein S8

Chain p: 98%



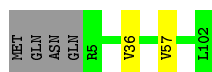
- Molecule 47: 30S ribosomal protein S11

Chain q: 90%



- Molecule 48: 30S ribosomal protein S10

Chain r: 94%



- Molecule 49: 30S ribosomal protein S13

Chain s:  96% ..



- Molecule 50: 30S ribosomal protein S12

Chain t:  97% ..



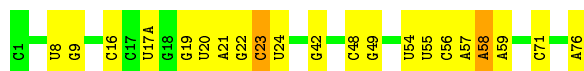
- Molecule 51: 30S ribosomal protein S15

Chain u:  99% .



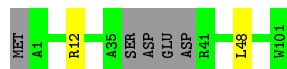
- Molecule 52: tRNA

Chain v:  73% 25% .



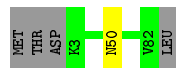
- Molecule 53: 30S ribosomal protein S14

Chain w:  93% . 5%



- Molecule 54: 30S ribosomal protein S17

Chain x:  94% . 5%

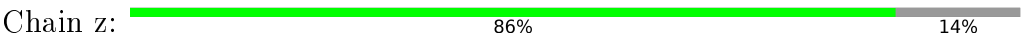


- Molecule 55: 30S ribosomal protein S16

Chain y:  98% .



- Molecule 56: 30S ribosomal protein S19



MET	PRO	ARG	GLY	HIS	ALA	ASP	LYS	LYS	ALA	LYS	LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	54585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300, FEI POLARA 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20, 20	Depositor
Minimum defocus (nm)	640, 190	Depositor
Maximum defocus (nm)	7180, 7570	Depositor
Magnification	39000, 39000	Depositor
Image detector	GATAN K2 Summit (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, FME, H2U, ZN, GNP, 4SU, PSU

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 > 2$	RMSZ	# $ Z > 2$
1	0	0.21	0/2828	0.66	0/4410
10	E	0.49	0/1434	0.65	0/1926
11	F	0.46	0/1343	0.61	0/1816
12	G	0.50	0/389	0.61	0/523
13	H	0.48	0/1046	0.57	0/1410
14	I	0.48	0/1152	0.65	0/1551
15	J	0.47	0/947	0.73	0/1268
16	K	0.48	0/1054	0.72	0/1403
17	L	0.45	0/1093	0.64	0/1460
18	M	0.49	0/973	0.69	0/1301
19	N	0.46	0/902	0.64	0/1209
2	1	0.51	0/462	0.71	0/621
20	O	0.49	0/929	0.72	0/1242
21	P	0.48	0/960	0.71	0/1278
22	Q	0.44	0/829	0.62	0/1107
23	R	0.44	0/864	0.68	0/1156
24	S	0.48	0/744	0.70	0/994
25	T	0.47	0/787	0.66	0/1051
26	U	0.45	0/766	0.60	0/1025
27	V	0.49	0/603	0.72	0/797
28	W	0.46	0/635	0.69	0/848
29	X	0.47	0/510	0.67	0/677
3	2	0.54	0/430	0.80	0/570
30	Y	0.48	0/453	0.69	0/605
31	Z	0.44	0/450	0.67	0/599
32	a	0.46	0/416	0.63	0/554
33	b	0.46	0/380	0.77	0/498
34	c	0.44	0/513	0.69	0/676
35	d	0.45	0/303	0.72	0/397
36	e	0.52	0/895	0.69	0/1203
37	f	0.25	0/3895	0.46	1/5264 (0.0%)
38	g	0.21	0/36966	0.66	0/57666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	h	0.47	0/1651	0.63	0/2225
4	3	0.46	0/671	0.63	0/888
40	j	0.50	0/1735	0.66	0/2338
41	k	0.48	0/1118	0.68	0/1504
42	l	0.48	0/1665	0.69	0/2227
43	m	0.47	0/1195	0.66	0/1602
44	n	0.50	0/835	0.69	0/1128
45	o	0.50	0/1034	0.78	0/1375
46	p	0.45	0/989	0.60	0/1326
47	q	0.47	0/893	0.63	0/1205
48	r	0.47	0/797	0.70	0/1077
49	s	0.47	0/892	0.72	0/1193
5	4	0.39	0/144	1.37	4/222 (1.8%)
50	t	0.46	0/969	0.72	0/1300
51	u	0.47	0/722	0.65	0/964
52	v	0.21	0/1746	0.77	3/2721 (0.1%)
53	w	0.50	0/785	0.78	1/1043 (0.1%)
54	x	0.49	0/657	0.69	0/881
55	y	0.47	0/659	0.69	0/884
56	z	0.48	0/652	0.66	0/877
6	A	0.21	0/68626	0.65	1/107056 (0.0%)
7	B	0.46	0/2121	0.72	0/2852
8	C	0.47	0/1586	0.65	0/2134
9	D	0.46	0/1571	0.63	0/2113
All	All	0.31	0/159664	0.66	10/238240 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
36	e	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	f	787	SER	C-N-CD	5.40	139.74	128.40
5	4	17	U	N1-C1'-C2'	-5.37	106.09	112.00
5	4	15	U	C4'-C3'-O3'	5.33	123.67	113.00
5	4	16	A	N9-C1'-C2'	-5.33	106.14	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	v	23	C	C2'-C3'-O3'	-5.32	97.80	109.50
52	v	23	C	N1-C1'-C2'	-5.31	106.16	112.00
6	A	784	G	C2'-C3'-O3'	5.19	122.01	113.70
52	v	58	A	C2'-C3'-O3'	-5.19	98.08	109.50
5	4	15	U	C3'-C2'-C1'	5.15	105.62	101.50
53	w	12	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	e	53	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2529	0	1281	0	0
2	1	455	0	478	1	0
3	2	425	0	449	0	0
4	3	665	0	714	1	0
5	4	129	0	65	31	0
6	A	61274	0	30819	12	0
7	B	2082	0	2157	5	0
8	C	1565	0	1616	8	0
9	D	1552	0	1619	0	0
10	E	1410	0	1447	1	0
11	F	1323	0	1374	0	0
12	G	384	0	405	0	0
13	H	1032	0	1088	1	0
14	I	1129	0	1162	3	0
15	J	938	0	1012	5	0
16	K	1045	0	1117	1	0
17	L	1074	0	1157	1	0
18	M	960	0	1000	0	0
19	N	892	0	923	3	0
20	O	917	0	965	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	P	947	0	1022	1	0
22	Q	816	0	839	1	0
23	R	857	0	922	2	0
24	S	738	0	807	1	0
25	T	779	0	834	1	0
26	U	753	0	780	0	0
27	V	596	0	610	4	0
28	W	625	0	655	1	0
29	X	509	0	543	0	0
30	Y	449	0	491	0	0
31	Z	444	0	461	0	0
32	a	409	0	440	0	0
33	b	377	0	418	0	0
34	c	504	0	574	0	0
35	d	302	0	342	0	0
36	e	884	0	913	0	0
37	f	3847	0	3909	0	0
38	g	33015	0	16616	0	0
39	h	1624	0	1699	0	0
40	j	1704	0	1732	0	0
41	k	1105	0	1148	0	0
42	l	1643	0	1710	0	0
43	m	1181	0	1240	0	0
44	n	817	0	808	0	0
45	o	1022	0	1070	0	0
46	p	979	0	1034	0	0
47	q	877	0	887	0	0
48	r	787	0	828	0	0
49	s	883	0	944	0	0
50	t	955	0	1019	0	0
51	u	714	0	737	0	0
52	v	1643	0	836	0	0
53	w	774	0	827	0	0
54	x	648	0	691	0	0
55	y	649	0	666	0	0
56	z	637	0	665	0	0
57	3	1	0	0	0	0
57	A	137	0	0	0	0
57	B	1	0	0	0	0
57	d	1	0	0	0	0
57	g	54	0	0	0	0
57	w	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	d	1	0	0	0	0
59	f	32	0	13	0	0
60	v	9	1	10	0	0
61	3	4	0	0	0	0
61	A	599	0	0	1	0
61	B	7	0	0	0	0
61	C	2	0	0	0	0
61	D	2	0	0	0	0
61	I	1	0	0	0	0
61	K	8	0	0	0	0
61	M	5	0	0	0	0
61	P	3	0	0	0	0
61	Q	3	0	0	0	0
61	R	3	0	0	0	0
61	S	2	0	0	0	0
61	b	1	0	0	0	0
61	d	3	0	0	0	0
61	g	189	0	0	0	0
61	q	1	0	0	0	0
61	t	2	0	0	0	0
61	w	2	0	0	0	0
All	All	148347	1	100588	79	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 2.

All (79) 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)
5:4:16:A:C2	5:4:17:U:C4	2.49	1.00
5:4:13:A:O2'	5:4:14:A:O4'	1.85	0.94
5:4:13:A:H2'	5:4:14:A:C8	2.04	0.91
5:4:16:A:C2	5:4:17:U:N3	2.47	0.82
5:4:14:A:O2'	5:4:15:U:H5''	1.86	0.76
5:4:15:U:O2'	5:4:16:A:OP2	2.07	0.73
5:4:16:A:N1	5:4:17:U:C4	2.57	0.72
5:4:17:U:O2'	5:4:18:G:H5'	1.94	0.68
5:4:16:A:C2	5:4:17:U:C5	2.83	0.65
8:C:110:THR:HG23	8:C:171:THR:HG22	1.78	0.65
19:N:27:VAL:HG21	19:N:40:ILE:HD12	1.79	0.63
5:4:16:A:N3	5:4:17:U:C5	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:16:A:C2	5:4:17:U:C2	2.89	0.60
6:A:2771:C:H5''	8:C:207:VAL:HG21	1.83	0.59
13:H:82:ALA:HB1	13:H:108:ILE:HD13	1.85	0.59
15:J:61:VAL:HG23	15:J:87:LEU:HD11	1.86	0.58
8:C:121:THR:HG21	8:C:143:PRO:HG3	1.86	0.57
5:4:15:U:O3'	5:4:16:A:H8	1.86	0.57
5:4:14:A:C2'	5:4:15:U:C5'	2.84	0.56
5:4:16:A:N3	5:4:17:U:C6	2.75	0.55
4:3:66:ILE:HD11	4:3:70:LYS:HE3	1.88	0.54
19:N:20:GLU:HG3	27:V:50:VAL:HG11	1.89	0.54
8:C:46:ARG:HG2	8:C:84:LEU:HD12	1.91	0.53
6:A:1918:A:O2'	6:A:1920:C:N4	2.41	0.53
5:4:14:A:C2'	5:4:15:U:H5''	2.38	0.52
5:4:16:A:C4	5:4:17:U:C5	2.98	0.52
2:1:25:ILE:HD13	2:1:66:LEU:HB3	1.92	0.52
10:E:59:ILE:HD11	10:E:140:ILE:HD11	1.93	0.51
5:4:16:A:H2	5:4:17:U:C2	2.28	0.51
6:A:1654:A:N6	6:A:2006:C:O4'	2.44	0.50
6:A:514:A:N3	6:A:581:C:O2'	2.43	0.50
19:N:75:GLY:HA2	19:N:106:LEU:HD12	1.94	0.49
5:4:13:A:OP2	5:4:13:A:H8	1.96	0.49
6:A:574:A:N6	6:A:2034:U:OP1	2.45	0.49
5:4:15:U:HO2'	5:4:16:A:P	2.33	0.49
6:A:750:A:OP1	6:A:1615:C:N4	2.42	0.49
24:S:43:ILE:HD11	24:S:58:VAL:HG21	1.93	0.49
5:4:14:A:C2'	5:4:15:U:H5'	2.43	0.48
23:R:17:VAL:HG11	23:R:76:VAL:HG11	1.96	0.48
16:K:110:VAL:HG21	16:K:127:VAL:HG23	1.95	0.48
5:4:14:A:C3'	5:4:15:U:H5'	2.45	0.47
23:R:76:VAL:HG12	23:R:103:ILE:HA	1.96	0.47
5:4:15:U:O3'	5:4:16:A:C8	2.67	0.47
15:J:94:PRO:CG	15:J:115:ILE:HD11	2.45	0.47
7:B:171:VAL:HG23	7:B:185:ALA:HB2	1.96	0.47
15:J:94:PRO:HG2	15:J:115:ILE:HD11	1.97	0.47
6:A:1223:G:OP2	22:Q:90:ARG:NH1	2.48	0.46
17:L:71:LYS:HE3	17:L:73:ILE:HD11	1.97	0.46
7:B:52:HIS:CE1	7:B:218:THR:HG23	2.50	0.46
7:B:261:ARG:HG3	7:B:262:THR:HG23	1.98	0.46
6:A:195:A:N6	61:A:3731:HOH:O	2.49	0.45
14:I:18:VAL:HG11	14:I:28:LEU:HD11	1.99	0.45
27:V:49:ASN:HB3	27:V:81:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:16:A:H2'	5:4:17:U:C6	2.52	0.45
6:A:857:G:N3	27:V:19:ARG:NH1	2.64	0.45
15:J:19:VAL:HG21	15:J:41:ILE:HD13	1.99	0.45
14:I:23:LYS:HD3	14:I:28:LEU:HD13	1.99	0.44
5:4:13:A:OP2	5:4:13:A:C8	2.70	0.44
28:W:36:ARG:HG2	28:W:47:THR:HG22	1.99	0.44
8:C:151:THR:HG23	8:C:152:PRO:HD3	1.97	0.44
7:B:161:VAL:HG11	7:B:173:LEU:HD23	1.99	0.44
5:4:16:A:C6	5:4:17:U:O4	2.71	0.43
25:T:27:VAL:HG23	25:T:33:VAL:HG12	2.01	0.43
6:A:780:G:O2'	6:A:783:A:N6	2.50	0.43
8:C:48:ILE:HG23	8:C:84:LEU:HD11	1.99	0.43
8:C:37:VAL:HG22	8:C:48:ILE:HG22	2.01	0.43
5:4:16:A:HO2'	5:4:17:U:H6	1.66	0.43
6:A:996:A:OP2	21:P:91:ARG:NH2	2.52	0.43
5:4:14:A:C3'	5:4:15:U:C5'	2.97	0.43
5:4:14:A:H2'	5:4:15:U:H5'	2.00	0.43
7:B:173:LEU:HD22	7:B:183:VAL:HG21	2.00	0.43
14:I:47:HIS:CD2	14:I:48:VAL:HG23	2.53	0.43
15:J:63:VAL:HG21	15:J:103:VAL:HG12	2.02	0.42
8:C:121:THR:HG23	8:C:162:ALA:HB2	2.00	0.42
5:4:16:A:C6	5:4:17:U:C4	3.08	0.41
6:A:1361:G:HO2'	6:A:2215:C:HO2'	1.69	0.41
5:4:15:U:O2'	5:4:16:A:P	2.79	0.41
5:4:13:A:HO2'	5:4:14:A:C4'	2.17	0.41
27:V:50:VAL:HG12	27:V:51:GLY:H	1.87	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	
2	1	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	10	55
3	2	49/71 (69%)	37 (76%)	10 (20%)	2 (4%)	3	37
4	3	83/87 (95%)	80 (96%)	1 (1%)	2 (2%)	7	51
7	B	269/273 (98%)	239 (89%)	25 (9%)	5 (2%)	10	55
8	C	207/209 (99%)	179 (86%)	22 (11%)	6 (3%)	6	46
9	D	199/201 (99%)	169 (85%)	24 (12%)	6 (3%)	5	46
10	E	175/179 (98%)	154 (88%)	19 (11%)	2 (1%)	17	65
11	F	174/177 (98%)	153 (88%)	17 (10%)	4 (2%)	8	52
12	G	48/149 (32%)	42 (88%)	4 (8%)	2 (4%)	3	36
13	H	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	26	72
14	I	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	26	72
15	J	120/123 (98%)	101 (84%)	15 (12%)	4 (3%)	5	44
16	K	141/144 (98%)	124 (88%)	14 (10%)	3 (2%)	9	53
17	L	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	8	52
18	M	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
19	N	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	21	68
20	O	112/115 (97%)	99 (88%)	8 (7%)	5 (4%)	3	34
21	P	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	21	68
22	Q	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	9	55
23	R	108/110 (98%)	104 (96%)	3 (3%)	1 (1%)	21	68
24	S	91/100 (91%)	68 (75%)	19 (21%)	4 (4%)	3	35
25	T	100/104 (96%)	82 (82%)	15 (15%)	3 (3%)	5	46
26	U	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
27	V	77/85 (91%)	51 (66%)	22 (29%)	4 (5%)	2	30
28	W	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
29	X	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	12	58
30	Y	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
31	Z	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	4	40
32	a	48/55 (87%)	46 (96%)	1 (2%)	1 (2%)	9	53
33	b	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
34	c	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	12	58
35	d	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	e	115/165 (70%)	99 (86%)	13 (11%)	3 (3%)	7	48
37	f	507/890 (57%)	488 (96%)	17 (3%)	2 (0%)	39	80
39	h	204/233 (88%)	185 (91%)	16 (8%)	3 (2%)	13	59
40	j	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	8	52
41	k	148/167 (89%)	128 (86%)	15 (10%)	5 (3%)	5	43
42	l	203/206 (98%)	184 (91%)	15 (7%)	4 (2%)	9	55
43	m	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
44	n	98/135 (73%)	84 (86%)	11 (11%)	3 (3%)	5	45
45	o	125/130 (96%)	106 (85%)	15 (12%)	4 (3%)	5	44
46	p	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
47	q	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	21	68
48	r	96/102 (94%)	80 (83%)	14 (15%)	2 (2%)	9	53
49	s	112/118 (95%)	105 (94%)	6 (5%)	1 (1%)	21	68
50	t	121/124 (98%)	108 (89%)	10 (8%)	3 (2%)	7	49
51	u	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
53	w	92/101 (91%)	76 (83%)	16 (17%)	0	100	100
54	x	78/84 (93%)	65 (83%)	12 (15%)	1 (1%)	15	62
55	y	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	7	49
56	z	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
All	All	6144/7039 (87%)	5468 (89%)	567 (9%)	109 (2%)	15	56

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	121	ALA
12	G	3	VAL
27	V	14	ASP
39	h	16	PRO
42	l	28	ASP
2	1	46	THR
3	2	12	ASP
7	B	77	VAL
8	C	73	VAL
8	C	107	VAL
8	C	170	VAL

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Mol	Chain	Res	Type
9	D	79	ARG
20	O	103	THR
21	P	87	VAL
24	S	40	LYS
25	T	92	VAL
25	T	98	ASN
36	e	54	VAL
36	e	106	PHE
40	j	19	THR
40	j	21	TYR
41	k	110	MET
42	l	192	ALA
44	n	85	ILE
45	o	57	VAL
48	r	57	VAL
54	x	50	ASN
4	3	5	SER
4	3	68	LYS
8	C	122	VAL
8	C	192	ALA
10	E	11	VAL
15	J	46	ALA
27	V	29	SER
35	d	8	LYS
40	j	22	TRP
40	j	72	LYS
49	s	4	ALA
50	t	75	GLU
7	B	94	LEU
9	D	6	LYS
10	E	149	ARG
11	F	61	TRP
13	H	64	ARG
15	J	14	SER
16	K	69	ARG
17	L	70	ASP
20	O	5	LYS
20	O	81	ASP
24	S	52	GLU
25	T	16	LYS
27	V	23	LYS
27	V	76	ARG

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Mol	Chain	Res	Type
29	X	9	LYS
36	e	108	VAL
37	f	886	GLN
41	k	102	THR
42	l	173	ASP
44	n	53	LYS
44	n	94	HIS
45	o	38	PHE
45	o	122	ARG
47	q	92	ARG
3	2	24	LYS
9	D	96	VAL
11	F	164	ALA
14	I	65	THR
15	J	35	VAL
16	K	41	ARG
16	K	111	ILE
17	L	134	THR
20	O	34	GLY
22	Q	91	GLN
24	S	55	VAL
24	S	70	HIS
37	f	788	PRO
41	k	77	ASN
41	k	109	ALA
41	k	124	ALA
42	l	191	SER
45	o	9	GLY
48	r	36	VAL
50	t	43	LYS
50	t	101	LEU
7	B	255	LYS
9	D	83	VAL
15	J	71	ARG
17	L	73	ILE
31	Z	34	GLY
34	c	22	LYS
39	h	145	ALA
40	j	73	ARG
7	B	64	VAL
9	D	148	ILE
11	F	168	VAL

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Mol	Chain	Res	Type
12	G	9	VAL
31	Z	54	ILE
32	a	4	ILE
39	h	65	VAL
11	F	97	VAL
19	N	58	ILE
20	O	63	ILE
23	R	96	ILE
35	d	16	ILE
8	C	109	VAL
22	Q	98	ILE
55	y	10	GLY
55	y	42	ILE
9	D	175	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	
2	1	48/65 (74%)	48 (100%)	0	100	100
3	2	44/61 (72%)	44 (100%)	0	100	100
4	3	65/66 (98%)	65 (100%)	0	100	100
7	B	216/218 (99%)	216 (100%)	0	100	100
8	C	164/164 (100%)	164 (100%)	0	100	100
9	D	165/165 (100%)	165 (100%)	0	100	100
10	E	148/150 (99%)	148 (100%)	0	100	100
11	F	137/138 (99%)	136 (99%)	1 (1%)	88	95
12	G	40/114 (35%)	40 (100%)	0	100	100
13	H	109/110 (99%)	109 (100%)	0	100	100
14	I	116/116 (100%)	115 (99%)	1 (1%)	84	93
15	J	103/104 (99%)	102 (99%)	1 (1%)	82	92
16	K	102/103 (99%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L	109/109 (100%)	108 (99%)	1 (1%)	84	93
18	M	100/103 (97%)	100 (100%)	0	100	100
19	N	86/87 (99%)	86 (100%)	0	100	100
20	O	99/100 (99%)	99 (100%)	0	100	100
21	P	89/90 (99%)	88 (99%)	1 (1%)	80	92
22	Q	84/84 (100%)	84 (100%)	0	100	100
23	R	93/93 (100%)	93 (100%)	0	100	100
24	S	80/84 (95%)	80 (100%)	0	100	100
25	T	83/85 (98%)	83 (100%)	0	100	100
26	U	78/78 (100%)	78 (100%)	0	100	100
27	V	59/63 (94%)	58 (98%)	1 (2%)	68	89
28	W	67/68 (98%)	67 (100%)	0	100	100
29	X	55/55 (100%)	55 (100%)	0	100	100
30	Y	48/49 (98%)	48 (100%)	0	100	100
31	Z	47/48 (98%)	47 (100%)	0	100	100
32	a	45/49 (92%)	45 (100%)	0	100	100
33	b	38/38 (100%)	38 (100%)	0	100	100
34	c	51/52 (98%)	51 (100%)	0	100	100
35	d	34/34 (100%)	34 (100%)	0	100	100
36	e	88/123 (72%)	87 (99%)	1 (1%)	80	92
37	f	409/713 (57%)	406 (99%)	3 (1%)	88	95
39	h	170/190 (90%)	170 (100%)	0	100	100
40	j	180/199 (90%)	177 (98%)	3 (2%)	68	89
41	k	113/126 (90%)	111 (98%)	2 (2%)	66	89
42	l	172/173 (99%)	172 (100%)	0	100	100
43	m	124/147 (84%)	124 (100%)	0	100	100
44	n	87/116 (75%)	87 (100%)	0	100	100
45	o	105/107 (98%)	105 (100%)	0	100	100
46	p	104/105 (99%)	103 (99%)	1 (1%)	82	92
47	q	90/99 (91%)	90 (100%)	0	100	100
48	r	86/90 (96%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	s	92/96 (96%)	92 (100%)	0	100	100
50	t	103/104 (99%)	103 (100%)	0	100	100
51	u	76/77 (99%)	76 (100%)	0	100	100
53	w	79/84 (94%)	78 (99%)	1 (1%)	76	91
54	x	74/78 (95%)	74 (100%)	0	100	100
55	y	65/65 (100%)	65 (100%)	0	100	100
56	z	70/79 (89%)	70 (100%)	0	100	100
All	All	5089/5714 (89%)	5072 (100%)	17 (0%)	95	98

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	F	10	VAL
14	I	43	GLU
15	J	73	ASP
17	L	132	THR
21	P	5	ARG
27	V	50	VAL
36	e	54	VAL
37	f	541	ILE
37	f	790	LEU
37	f	861	CYS
40	j	19	THR
40	j	71	THR
40	j	219	THR
41	k	100	GLU
41	k	130	THR
46	p	53	ASP
53	w	48	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	60	GLN
4	3	77	ASN
7	B	89	ASN
7	B	196	ASN
8	C	150	GLN

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Mol	Chain	Res	Type
16	K	99	ASN
17	L	22	GLN
20	O	65	ASN
21	P	65	ASN
23	R	15	GLN
27	V	45	HIS
28	W	16	ASN
33	b	29	GLN
37	f	402	HIS
37	f	426	GLN
37	f	437	ASN
37	f	448	HIS
37	f	484	GLN
37	f	498	ASN
37	f	886	GLN
39	h	7	ASN
40	j	14	HIS
41	k	76	ASN
43	m	85	GLN
44	n	46	GLN
44	n	63	ASN
48	r	15	HIS
49	s	51	GLN
49	s	104	ASN
51	u	34	GLN
55	y	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	117/118 (99%)	11 (9%)	0
38	g	1538/1542 (99%)	187 (12%)	0
5	4	6/52 (11%)	5 (83%)	4 (66%)
52	v	76/77 (98%)	21 (27%)	0
6	A	2850/2904 (98%)	332 (11%)	14 (0%)
All	All	4587/4693 (97%)	556 (12%)	18 (0%)

All (556) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	A

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Mol	Chain	Res	Type
1	0	24	G
1	0	35	C
1	0	42	C
1	0	44	G
1	0	87	U
1	0	88	C
1	0	89	U
1	0	90	C
1	0	99	A
1	0	109	A
5	4	14	A
5	4	15	U
5	4	16	A
5	4	17	U
5	4	18	G
6	A	10	A
6	A	34	U
6	A	46	G
6	A	61	C
6	A	63	A
6	A	71	A
6	A	74	A
6	A	75	G
6	A	84	A
6	A	101	A
6	A	118	A
6	A	119	A
6	A	120	U
6	A	136	G
6	A	138	U
6	A	139	U
6	A	140	C
6	A	141	G
6	A	142	A
6	A	162	U
6	A	164	C
6	A	181	A
6	A	196	A
6	A	199	A
6	A	215	G
6	A	216	A
6	A	221	A

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Mol	Chain	Res	Type
6	A	222	A
6	A	230	G
6	A	248	G
6	A	255	A
6	A	266	G
6	A	272	A
6	A	273	G
6	A	276	U
6	A	311	A
6	A	329	G
6	A	330	A
6	A	362	A
6	A	370	G
6	A	371	A
6	A	372	G
6	A	386	G
6	A	396	G
6	A	403	U
6	A	404	A
6	A	405	U
6	A	411	G
6	A	412	A
6	A	424	G
6	A	451	U
6	A	456	C
6	A	457	A
6	A	467	G
6	A	480	A
6	A	481	G
6	A	491	G
6	A	504	A
6	A	505	A
6	A	509	C
6	A	528	A
6	A	529	A
6	A	531	C
6	A	532	A
6	A	533	G
6	A	544	C
6	A	546	U
6	A	548	G
6	A	549	G

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Mol	Chain	Res	Type
6	A	563	A
6	A	572	A
6	A	573	U
6	A	575	A
6	A	586	A
6	A	603	A
6	A	604	G
6	A	613	A
6	A	615	U
6	A	627	A
6	A	633	A
6	A	637	A
6	A	647	G
6	A	654	A
6	A	655	A
6	A	686	U
6	A	730	A
6	A	747	U
6	A	748	G
6	A	764	A
6	A	775	G
6	A	776	G
6	A	782	A
6	A	784	G
6	A	785	G
6	A	805	G
6	A	812	C
6	A	819	A
6	A	827	U
6	A	828	U
6	A	845	A
6	A	846	U
6	A	847	U
6	A	859	G
6	A	883	G
6	A	896	A
6	A	897	C
6	A	910	A
6	A	914	G
6	A	931	U
6	A	932	U
6	A	941	A

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Mol	Chain	Res	Type
6	A	946	C
6	A	961	C
6	A	974	G
6	A	983	A
6	A	995	C
6	A	1009	A
6	A	1012	U
6	A	1013	C
6	A	1021	A
6	A	1022	G
6	A	1023	U
6	A	1026	G
6	A	1033	U
6	A	1046	A
6	A	1047	G
6	A	1060	U
6	A	1061	U
6	A	1069	A
6	A	1070	A
6	A	1071	G
6	A	1083	U
6	A	1088	A
6	A	1090	A
6	A	1112	G
6	A	1132	U
6	A	1133	A
6	A	1135	C
6	A	1142	A
6	A	1144	A
6	A	1175	A
6	A	1176	U
6	A	1186	G
6	A	1212	G
6	A	1238	G
6	A	1250	G
6	A	1253	A
6	A	1256	G
6	A	1266	G
6	A	1271	G
6	A	1272	A
6	A	1273	U
6	A	1300	G

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Mol	Chain	Res	Type
6	A	1301	A
6	A	1312	U
6	A	1365	A
6	A	1368	G
6	A	1383	A
6	A	1396	U
6	A	1416	G
6	A	1419	A
6	A	1420	A
6	A	1428	C
6	A	1452	G
6	A	1459	G
6	A	1460	U
6	A	1482	G
6	A	1493	C
6	A	1515	A
6	A	1524	G
6	A	1533	C
6	A	1535	A
6	A	1536	C
6	A	1537	G
6	A	1566	A
6	A	1569	A
6	A	1578	U
6	A	1585	C
6	A	1608	A
6	A	1610	A
6	A	1618	A
6	A	1647	U
6	A	1648	U
6	A	1654	A
6	A	1674	G
6	A	1715	G
6	A	1729	U
6	A	1730	C
6	A	1733	G
6	A	1738	G
6	A	1764	C
6	A	1773	A
6	A	1782	U
6	A	1800	C
6	A	1801	A

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Mol	Chain	Res	Type
6	A	1802	A
6	A	1808	A
6	A	1810	A
6	A	1816	C
6	A	1829	A
6	A	1833	C
6	A	1847	A
6	A	1870	C
6	A	1872	A
6	A	1873	G
6	A	1906	G
6	A	1913	A
6	A	1929	G
6	A	1930	G
6	A	1937	A
6	A	1955	U
6	A	1963	U
6	A	1967	C
6	A	1970	A
6	A	1971	U
6	A	1972	G
6	A	1991	U
6	A	1993	U
6	A	1997	C
6	A	2021	C
6	A	2022	U
6	A	2023	C
6	A	2031	A
6	A	2032	G
6	A	2043	C
6	A	2052	A
6	A	2055	C
6	A	2056	G
6	A	2060	A
6	A	2061	G
6	A	2062	A
6	A	2069	G
6	A	2072	C
6	A	2093	G
6	A	2104	C
6	A	2105	U
6	A	2106	U

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Mol	Chain	Res	Type
6	A	2109	U
6	A	2110	G
6	A	2134	A
6	A	2135	A
6	A	2144	G
6	A	2145	C
6	A	2147	A
6	A	2148	G
6	A	2151	U
6	A	2152	G
6	A	2155	U
6	A	2156	G
6	A	2157	G
6	A	2180	U
6	A	2182	U
6	A	2183	A
6	A	2198	A
6	A	2199	A
6	A	2204	G
6	A	2211	A
6	A	2214	C
6	A	2225	A
6	A	2238	G
6	A	2239	G
6	A	2250	G
6	A	2278	A
6	A	2283	C
6	A	2287	A
6	A	2305	U
6	A	2308	G
6	A	2311	A
6	A	2325	G
6	A	2327	A
6	A	2333	A
6	A	2345	G
6	A	2347	C
6	A	2359	C
6	A	2361	G
6	A	2383	G
6	A	2384	U
6	A	2385	C
6	A	2388	A

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Mol	Chain	Res	Type
6	A	2402	U
6	A	2406	A
6	A	2423	U
6	A	2424	C
6	A	2425	A
6	A	2428	G
6	A	2429	G
6	A	2430	A
6	A	2435	A
6	A	2441	U
6	A	2447	G
6	A	2448	A
6	A	2476	A
6	A	2491	U
6	A	2498	C
6	A	2502	G
6	A	2504	U
6	A	2505	G
6	A	2518	A
6	A	2520	C
6	A	2529	G
6	A	2554	U
6	A	2566	A
6	A	2567	G
6	A	2572	A
6	A	2573	C
6	A	2609	U
6	A	2613	U
6	A	2629	U
6	A	2630	G
6	A	2682	A
6	A	2689	U
6	A	2690	U
6	A	2714	G
6	A	2725	A
6	A	2726	A
6	A	2744	G
6	A	2748	A
6	A	2757	A
6	A	2765	A
6	A	2778	A
6	A	2780	G

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Mol	Chain	Res	Type
6	A	2798	U
6	A	2801	G
6	A	2818	U
6	A	2820	A
6	A	2849	U
6	A	2867	G
6	A	2872	A
6	A	2880	C
6	A	2884	U
6	A	2885	G
6	A	2903	U
38	g	4	U
38	g	9	G
38	g	31	G
38	g	32	A
38	g	39	G
38	g	47	C
38	g	48	C
38	g	51	A
38	g	52	C
38	g	61	G
38	g	70	U
38	g	71	A
38	g	74	A
38	g	83	C
38	g	85	U
38	g	87	C
38	g	88	U
38	g	97	G
38	g	108	G
38	g	116	A
38	g	120	A
38	g	121	U
38	g	130	A
38	g	131	A
38	g	144	G
38	g	155	A
38	g	159	G
38	g	182	A
38	g	183	C
38	g	204	G
38	g	207	C

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Mol	Chain	Res	Type
38	g	209	U
38	g	210	C
38	g	211	G
38	g	212	G
38	g	247	G
38	g	251	G
38	g	266	G
38	g	267	C
38	g	280	C
38	g	289	G
38	g	328	C
38	g	329	A
38	g	330	C
38	g	332	G
38	g	346	G
38	g	347	G
38	g	352	C
38	g	354	G
38	g	367	U
38	g	372	C
38	g	406	G
38	g	411	A
38	g	412	A
38	g	413	G
38	g	414	A
38	g	421	U
38	g	424	G
38	g	429	U
38	g	451	A
38	g	467	U
38	g	468	A
38	g	469	C
38	g	479	U
38	g	485	U
38	g	497	G
38	g	511	C
38	g	518	C
38	g	524	G
38	g	527	G
38	g	532	A
38	g	547	A
38	g	563	A

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Mol	Chain	Res	Type
38	g	572	A
38	g	573	A
38	g	576	C
38	g	577	G
38	g	596	A
38	g	633	G
38	g	650	G
38	g	665	A
38	g	721	G
38	g	723	U
38	g	724	G
38	g	731	G
38	g	734	G
38	g	747	A
38	g	755	G
38	g	777	A
38	g	793	U
38	g	794	A
38	g	815	A
38	g	817	C
38	g	828	U
38	g	829	G
38	g	832	G
38	g	841	C
38	g	843	U
38	g	844	G
38	g	845	A
38	g	846	G
38	g	914	A
38	g	926	G
38	g	927	G
38	g	934	C
38	g	960	U
38	g	969	A
38	g	975	A
38	g	976	G
38	g	977	A
38	g	983	A
38	g	993	G
38	g	1004	A
38	g	1008	U
38	g	1018	G

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Mol	Chain	Res	Type
38	g	1022	A
38	g	1026	G
38	g	1027	C
38	g	1028	C
38	g	1030	U
38	g	1032	G
38	g	1033	G
38	g	1034	G
38	g	1043	G
38	g	1054	C
38	g	1065	U
38	g	1073	U
38	g	1080	A
38	g	1086	U
38	g	1094	G
38	g	1095	U
38	g	1101	A
38	g	1102	A
38	g	1125	U
38	g	1132	C
38	g	1133	G
38	g	1134	G
38	g	1136	C
38	g	1137	C
38	g	1139	G
38	g	1140	C
38	g	1141	C
38	g	1142	G
38	g	1159	U
38	g	1160	G
38	g	1161	C
38	g	1167	A
38	g	1168	U
38	g	1196	A
38	g	1197	A
38	g	1202	U
38	g	1212	U
38	g	1213	A
38	g	1226	C
38	g	1227	A
38	g	1238	A
38	g	1240	U

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Mol	Chain	Res	Type
38	g	1241	G
38	g	1253	G
38	g	1275	A
38	g	1280	A
38	g	1286	U
38	g	1287	A
38	g	1299	A
38	g	1302	C
38	g	1304	G
38	g	1305	G
38	g	1317	C
38	g	1318	A
38	g	1362	A
38	g	1363	A
38	g	1364	U
38	g	1370	G
38	g	1379	G
38	g	1398	A
38	g	1419	G
38	g	1441	A
38	g	1446	A
38	g	1497	G
38	g	1503	A
38	g	1505	G
38	g	1506	U
38	g	1517	G
38	g	1529	G
38	g	1530	G
38	g	1535	C
38	g	1536	C
52	v	8	4SU
52	v	9	G
52	v	16	C
52	v	17(A)	U
52	v	19	G
52	v	20	H2U
52	v	21	A
52	v	22	G
52	v	23	C
52	v	24	U
52	v	42	G
52	v	48	C

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Mol	Chain	Res	Type
52	v	49	G
52	v	54	5MU
52	v	55	PSU
52	v	56	C
52	v	57	A
52	v	58	A
52	v	59	A
52	v	71	C
52	v	76	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	4	13	A
5	4	14	A
5	4	16	A
5	4	17	U
6	A	119	A
6	A	404	A
6	A	503	A
6	A	527	C
6	A	784	G
6	A	1020	A
6	A	1838	C
6	A	2324	U
6	A	2326	C
6	A	2384	U
6	A	2423	U
6	A	2581	G
6	A	2756	U
6	A	2902	C

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

4 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
52	H2U	v	20	52	17,21,22	0.81	0	23,30,33	1.33	5 (21%)
52	5MU	v	54	52	13,22,23	0.77	0	16,32,35	2.62	2 (12%)
52	PSU	v	55	52	15,21,22	1.39	1 (6%)	16,30,33	2.39	5 (31%)
52	4SU	v	8	52	12,21,22	1.14	2 (16%)	15,30,33	1.88	6 (40%)

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
52	H2U	v	20	52	-	0/7/38/39	0/2/2/2
52	5MU	v	54	52	-	0/3/25/26	0/2/2/2
52	PSU	v	55	52	-	0/7/25/26	0/2/2/2
52	4SU	v	8	52	-	0/3/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	55	PSU	C5-C1'	-4.42	1.48	1.52
52	v	8	4SU	C2-N3	-2.18	1.33	1.38
52	v	8	4SU	O4'-C1'	2.58	1.44	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	v	54	5MU	C5-C4-N3	-7.44	119.11	125.35
52	v	55	PSU	C5-C6-N1	-3.75	119.15	124.38
52	v	8	4SU	C5-C4-N3	-3.40	119.96	123.56
52	v	55	PSU	C5-C1'-C2'	-3.18	110.03	115.44
52	v	20	H2U	C4-N3-C2	-2.65	123.37	125.77
52	v	8	4SU	O4'-C4'-C3'	-2.64	99.81	105.16
52	v	20	H2U	C5-C6-N1	-2.27	108.28	110.76
52	v	8	4SU	C2'-C1'-N1	-2.13	107.75	113.46
52	v	20	H2U	C6-N1-C2	2.22	125.58	122.16
52	v	20	H2U	C3'-C2'-C1'	2.22	105.89	101.44
52	v	55	PSU	O4'-C1'-C2'	2.26	107.13	104.69
52	v	20	H2U	C1'-N1-C2	2.55	121.76	118.19
52	v	8	4SU	O4'-C1'-N1	2.57	112.98	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	v	8	4SU	O3'-C3'-C2'	2.71	120.62	111.86
52	v	8	4SU	O3'-C3'-C4'	3.16	120.45	111.01
52	v	55	PSU	C3'-C2'-C1'	3.48	105.84	101.71
52	v	55	PSU	C4-N3-C2	6.60	120.66	115.16
52	v	54	5MU	C4-N3-C2	6.62	120.68	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 198 ligands modelled in this entry, 196 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GNP	f	901	-	29,34,34	4.62	11 (37%)	28,54,54	1.37	4 (14%)
60	FME	v	101	52	8,8,10	0.40	0	8,8,11	1.42	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GNP	f	901	-	-	0/16/38/38	0/3/3/3
60	FME	v	101	52	-	0/7/7/11	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	f	901	GNP	C4-N9	-10.33	1.34	1.47
59	f	901	GNP	C8-N9	-3.77	1.35	1.47
59	f	901	GNP	PB-O2B	-3.10	1.48	1.56
59	f	901	GNP	PG-O3G	-3.09	1.48	1.56
59	f	901	GNP	C5-C6	-2.39	1.48	1.53
59	f	901	GNP	C2-N1	-2.15	1.35	1.44
59	f	901	GNP	C1'-N9	3.53	1.48	1.42
59	f	901	GNP	PB-N3B	4.39	1.75	1.63
59	f	901	GNP	PG-N3B	4.42	1.75	1.63
59	f	901	GNP	PB-O1B	14.22	1.61	1.46
59	f	901	GNP	PG-O1G	14.23	1.61	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	f	901	GNP	PA-O3A-PB	-3.41	120.33	132.71
60	v	101	FME	O1-CN-N	-2.79	120.53	124.80
60	v	101	FME	CA-N-CN	-2.35	121.08	124.12
59	f	901	GNP	C3'-C2'-C1'	2.23	105.92	101.44
59	f	901	GNP	C4-C5-N7	2.48	106.55	102.67
59	f	901	GNP	C8-N9-C4	3.18	108.40	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.