



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:39 AM EDT

PDB ID : 7S1J
EMDB ID : EMD-24803
Title : Wild-type Escherichia coli ribosome with antibiotic radezolid
Authors : Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on : 2021-09-02
Resolution : 2.47 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

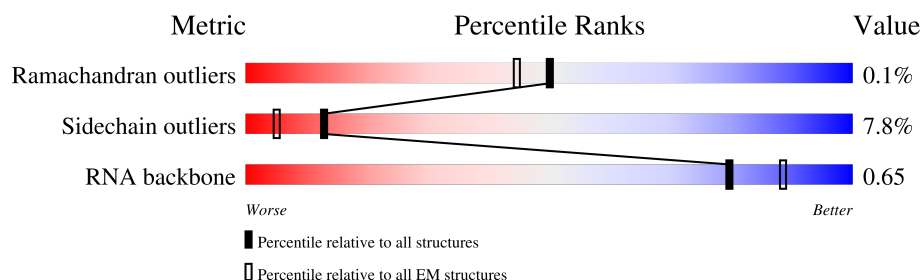
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 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.





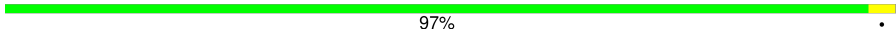
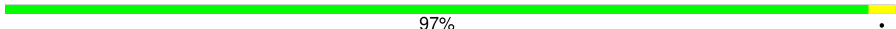



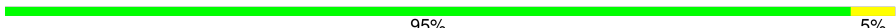

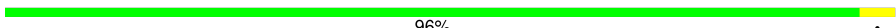


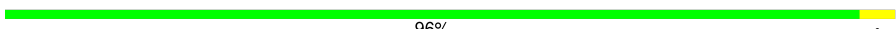

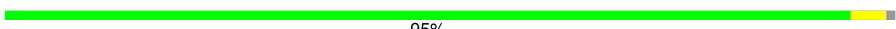

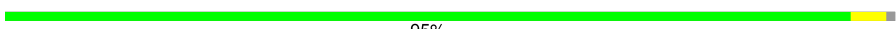

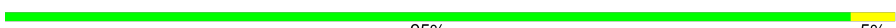






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	92	
2	2	87	
3	3	71	
4	C	1540	
5	D	241	
6	E	233	
7	F	206	
8	G	167	
9	H	135	

















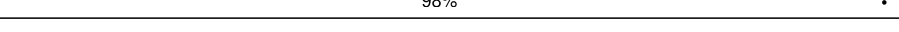
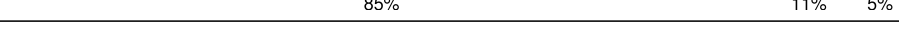
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Mol	Chain	Length	Quality of chain
10	I	2904	 87% 13%
11	J	120	 89% 9% .
12	K	273	 97% . .
13	L	209	 97% .
14	M	201	 95% 5%
15	N	179	 90% 9% .
16	O	177	 91% 8% .
17	P	149	 95% 5%
18	Q	70	 79% 7% 14%
19	R	142	 96% .
20	S	123	 91% 8% .
21	T	144	 97% .
22	U	136	 96% .
23	V	127	 94% . 6%
24	W	117	 95% . .
25	X	115	 93% 6% .
26	Y	118	 95% . .
27	Z	103	 93% 7%
28	a	110	 95% 5%
29	b	100	 83% 10% 7%
30	c	104	 89% 9% .
31	d	94	 94% 6%
32	e	85	 85% . 12%
33	f	78	 90% 9% .
34	g	63	 89% 10% .

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Mol	Chain	Length	Quality of chain
35	h	59	 88% 10% .
36	i	57	 89% 9% .
37	j	55	 89% . 9%
38	k	46	 91% 9%
39	l	65	 92% 6% .
40	m	38	 97% .
41	n	179	 78% 7% 16%
42	o	130	 92% 7% .
43	p	130	 85% 12% .
44	q	103	 87% 8% 5%
45	r	129	 84% 6% 9%
46	t	124	 94% 6% .
47	u	118	 90% 8% .
48	v	101	 87% 8% 5%
49	w	89	 90% 9% .
50	x	82	 98% .
51	y	84	 85% 11% 5%
52	z	75	 67% 7% 27%

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 238134 atoms, of which 95754 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 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	79	Total	C	H	N	O	S	0	0
			1303	408	666	120	107	2		

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	85	Total	C	H	N	O	S	0	0
			1380	411	715	137	114	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	1540	Total	C	H	N	O	P	0	0
			49665	14735	16628	6057	10705	1540		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	218	Total	C	H	N	O	S	0	0
			3437	1081	1733	305	311	7		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	206	Total	C	H	N	O	S	0	0
			3321	1028	1697	305	288	3		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	205	Total	C	H	N	O	S	0	0
			3351	1026	1708	315	298	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	150	Total	C	H	N	O	S	0	0
			2254	687	1149	211	201	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	100	Total	C	H	N	O	S	0	0
			1625	515	808	148	148	6		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	2898	Total	C	H	N	O	P	2	0
			93612	27787	31341	11455	20129	2900		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	118	Total	C	H	N	O	P	0	0
			3809	1126	1280	464	821	118		

- Molecule 12 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	271	Total	C	H	N	O	S	2	0
			4237	1288	2155	423	364	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	209	Total	C	H	N	O	S	0	0
			3183	979	1618	288	294	4		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 15 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	N	177	Total	C	H	N	O	S	0	0
			2855	899	1445	249	256	6		

- Molecule 16 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	O	176	Total	C	H	N	O	S	0	0
			2695	832	1372	243	246	2		

- Molecule 17 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 18 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Q	60	Total	C	H	N	O	S	0	0
			963	299	483	90	85	6		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	U	136	Total	C	H	N	O	S	0	0
			2230	686	1155	205	178	6		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	116	Total	C	H	N	O	0	0
			1816	552	924	178	162		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	X	114	Total	C	H	N	O	S	0	0
			1880	574	963	179	163	1		

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	117	Total	C	H	N	O	0	0
			1968	604	1021	192	151		

- Molecule 27 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	a	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	b	93	Total	C	H	N	O	S	0	0
			1545	466	807	139	131	2		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	c	102	Total	C	H	N	O	S	0	0
			1611	492	832	146	141			

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	e	75	Total	C	H	N	O	S	0	0
			1168	356	593	116	102	1		

- Molecule 33 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	f	77	Total	C	H	N	O	S	0	0
			1278	388	653	129	106	2		

- Molecule 34 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	g	62	Total	C	H	N	O	S	0	0
			1034	308	533	98	94	1		

- Molecule 35 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	h	58	Total	C	H	N	O	S	0	0
			938	281	489	87	79	2		

- Molecule 36 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	j	50	Total	C	H	N	O		0	0
			850	263	441	75	71			

- Molecule 38 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 39 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	l	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

- Molecule 40 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	n	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	129	Total	C	H	N	O	S	0	0
			2011	616	1032	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	127	Total	C	H	N	O	S	0	0
			2093	634	1071	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	98	Total	C	H	N	O	S	0	0
			1615	493	829	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	117	Total	C	H	N	O	S	0	0
			1765	540	888	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	t	123	Total	C	H	N	O	S	0	0
			1972	590	1017	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	115	Total	C	H	N	O	S	0	0
			1844	552	953	179	157	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	96	Total	C	H	N	O	S	0	0
			1600	483	826	160	128	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	88	Total	C	H	N	O	S	0	0
			1439	437	729	143	129	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	x	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	y	80	Total	C	H	N	O	S	0	0
			1340	411	692	121	113	3		

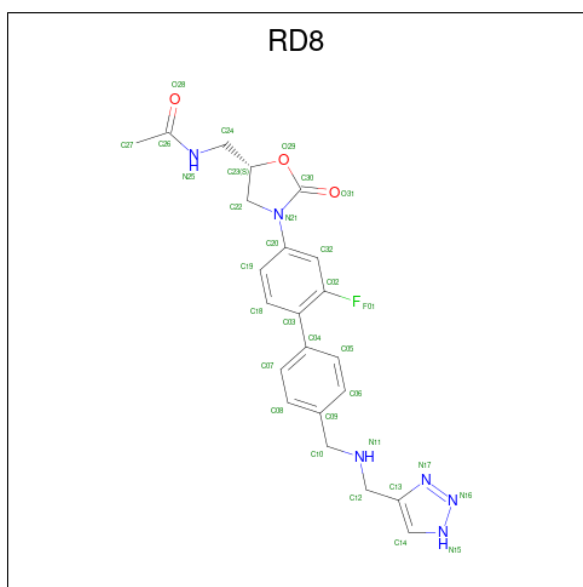
- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	55	Total	C	H	N	O	0	0
			934	288	479	86	81		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	C	84	Total	Mg	0
			84	84	
53	I	111	Total	Mg	0
			111	111	
53	K	1	Total	Mg	0
			1	1	
53	L	1	Total	Mg	0
			1	1	
53	T	1	Total	Mg	0
			1	1	
53	v	1	Total	Mg	0
			1	1	

- Molecule 54 is Radezolid (three-letter code: RD8) (formula: C₂₂H₂₃FN₆O₃) (labeled as "Ligand of Interest" by depositor).

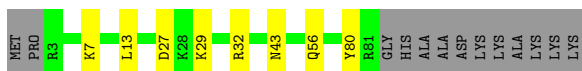


3 Residue-property plots [i](#)


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. 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. 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: 30S ribosomal protein S19

Chain 1: 



- Molecule 2: 30S ribosomal protein S20

Chain 2: 




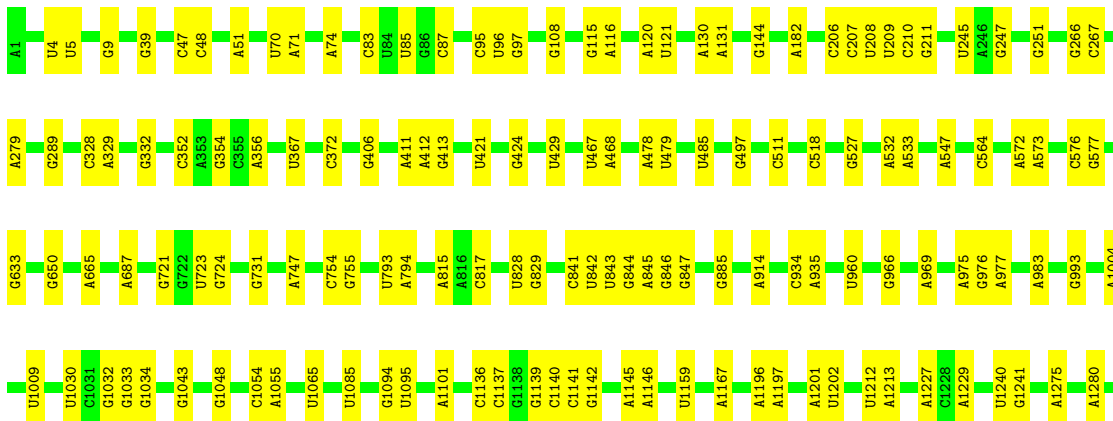
- Molecule 3: 30S ribosomal protein S21

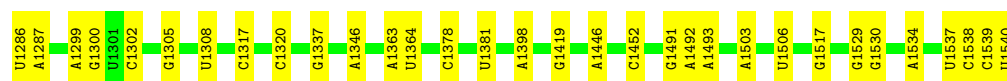
Chain 3: 



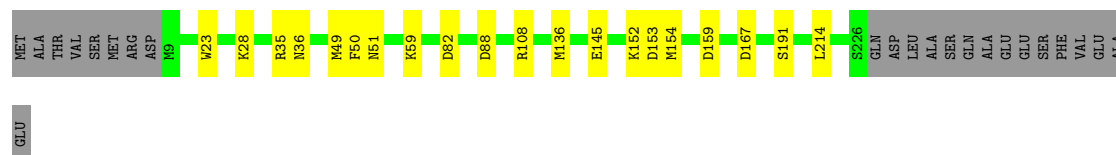
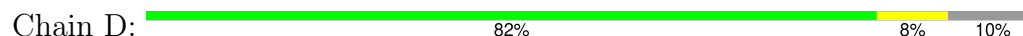
- Molecule 4: 16S rRNA

Chain C: 

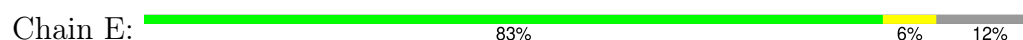




- Molecule 5: 30S ribosomal protein S2



- Molecule 6: 30S ribosomal protein S3



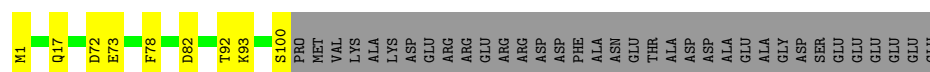
- Molecule 7: 30S ribosomal protein S4



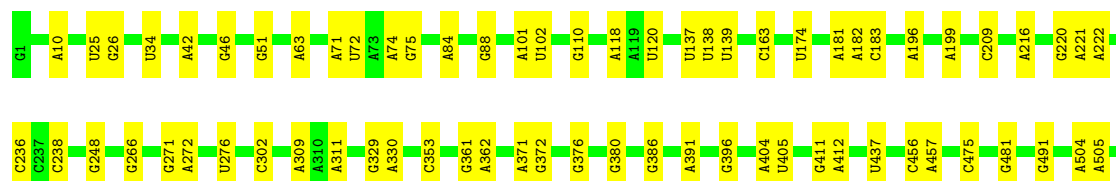
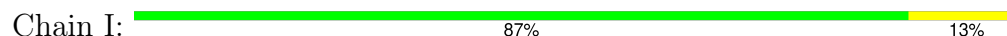
- Molecule 8: 30S ribosomal protein S5

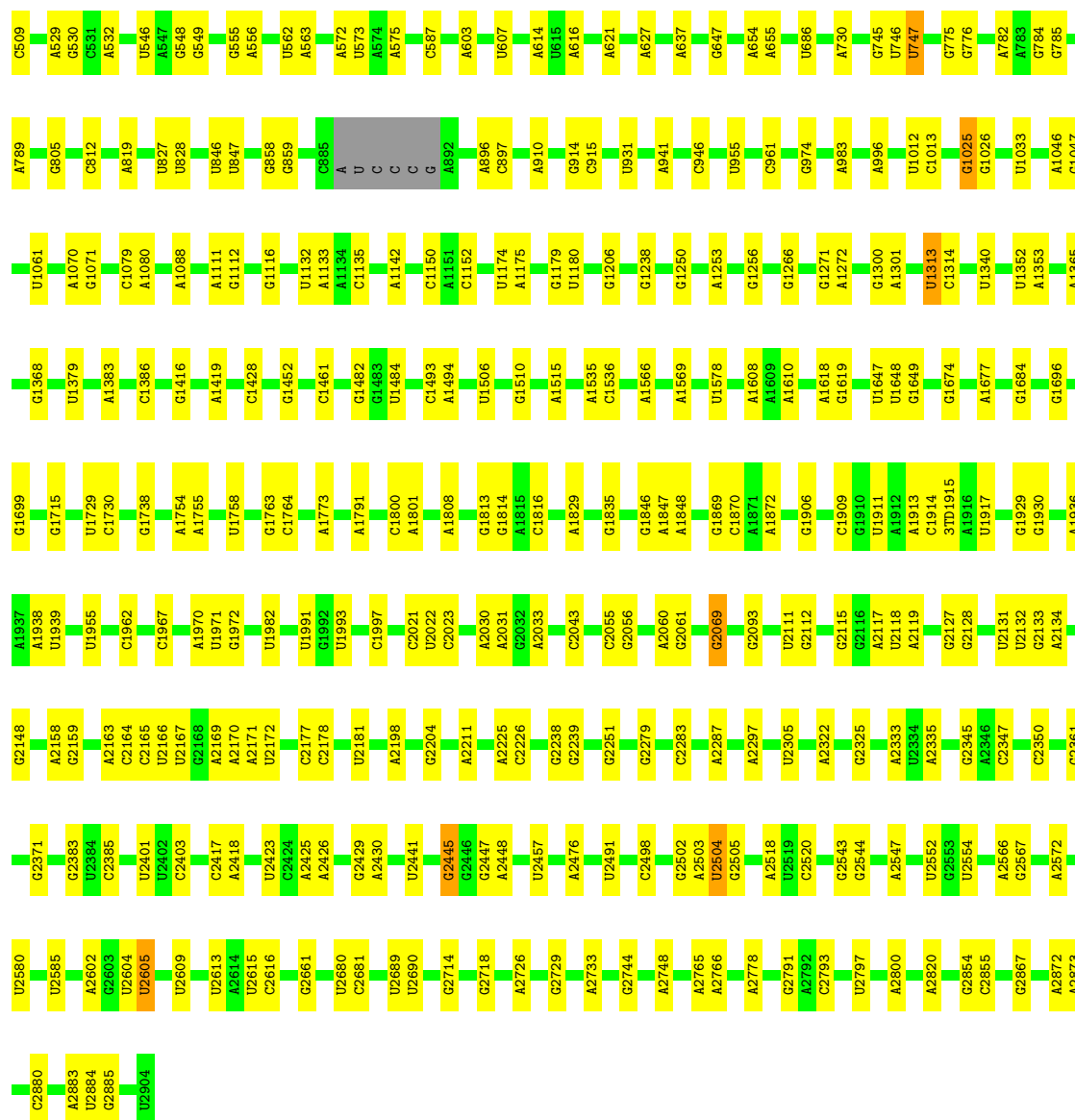


- Molecule 9: 30S ribosomal protein S6



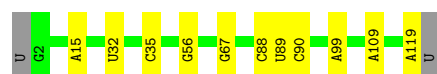
- Molecule 10: 23S rRNA





• Molecule 11: 5S rRNA

Chain J: 89% 9%



• Molecule 12: 50S ribosomal protein L2

Chain K: 97%



• Molecule 13: 50S ribosomal protein L3

Chain L:  97% .



- Molecule 14: 50S ribosomal protein L4

Chain M:  95% 5%



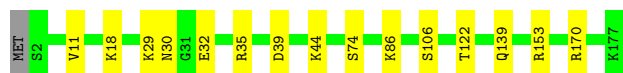
- Molecule 15: 50S ribosomal protein L5

Chain N:  90% 9% .



- Molecule 16: 50S ribosomal protein L6

Chain O:  91% 8% .




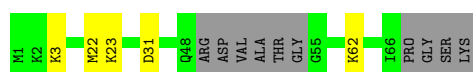
- Molecule 17: 50S ribosomal protein L9

Chain P:  95% 5%



- Molecule 18: 50S ribosomal protein L31

Chain Q:  79% 7% 14%




- Molecule 19: 50S ribosomal protein L13

Chain R:  96% .



- Molecule 20: 50S ribosomal protein L14

Chain S:  91% 8% .



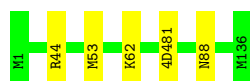
- Molecule 21: 50S ribosomal protein L15

Chain T:  97% .



- Molecule 22: 50S ribosomal protein L16

Chain U:  96% .



- Molecule 23: 50S ribosomal protein L17

Chain V:  94% 6% .



- Molecule 24: 50S ribosomal protein L18

Chain W:  95% . .



- Molecule 25: 50S ribosomal protein L19

Chain X:  93% 6% .



- Molecule 26: 50S ribosomal protein L20

Chain Y:  95% . .



- Molecule 27: Ribosomal protein L21

Chain Z:  93% 7%




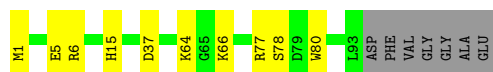
- Molecule 28: 50S ribosomal protein L22

Chain a:  95% 5%




- Molecule 29: 50S ribosomal protein L23

Chain b:  83% 10% 7%



- Molecule 30: 50S ribosomal protein L24

Chain c:  89% 9% .




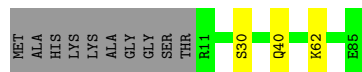
- Molecule 31: 50S ribosomal protein L25

Chain d:  94% 6%



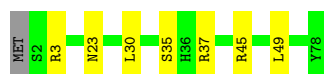
- Molecule 32: 50S ribosomal protein L27

Chain e:  85% . 12%




- Molecule 33: 50S ribosomal protein L28

Chain f:  90% 9% .




- Molecule 34: 50S ribosomal protein L29

Chain g:  89% 10%




- Molecule 35: 50S ribosomal protein L30

Chain h:  88% 10%




- Molecule 36: 50S ribosomal protein L32

Chain i:  89% 9%




- Molecule 37: 50S ribosomal protein L33

Chain j:  89% 9%




- Molecule 38: 50S ribosomal protein L34

Chain k:  91% 9%



- Molecule 39: 50S ribosomal protein L35

Chain l:  92% 6%




- Molecule 40: 50S ribosomal protein L36

Chain m:  97%



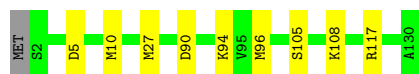
- Molecule 41: 30S ribosomal protein S7

Chain n:  78% 7% 16%




- Molecule 42: 30S ribosomal protein S8

Chain o:  92% 7% .




- Molecule 43: 30S ribosomal protein S9

Chain p:  85% 12% .




- Molecule 44: 30S ribosomal protein S10

Chain q:  87% 8% 5%



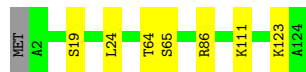
- Molecule 45: 30S ribosomal protein S11

Chain r:  84% 6% 9%




- Molecule 46: 30S ribosomal protein S12

Chain t:  94% 6% .




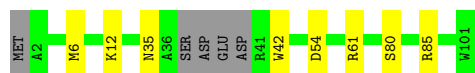
- Molecule 47: 30S ribosomal protein S13

Chain u:  90% 8% .



- Molecule 48: 30S ribosomal protein S14

Chain v:  87% 8% 5%



- Molecule 49: 30S ribosomal protein S15

Chain w:  90% 9% .




- Molecule 50: 30S ribosomal protein S16

Chain x:  98% .



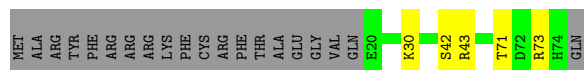
- Molecule 51: 30S ribosomal protein S17

Chain y:  85% 11% 5%



- Molecule 52: 30S ribosomal protein S18

Chain z:  67% 7% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146245	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 ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
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: 3TD, OMG, 2MA, 1MG, MG, OMU, OMC, 4D4, ZN, H2U, 5MU, PSU, 6MZ, 2MG, 5MC, G7M, RD8

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	1	0.27	0/652	0.60	0/877
2	2	0.27	0/671	0.55	0/888
3	3	0.24	0/598	0.61	0/792
4	C	0.17	0/36991	0.66	1/57705 (0.0%)
5	D	0.26	0/1735	0.53	0/2338
6	E	0.25	0/1651	0.57	0/2225
7	F	0.26	0/1665	0.57	0/2227
8	G	0.26	0/1118	0.55	0/1504
9	H	0.26	0/835	0.58	0/1128
10	I	0.20	0/69168	0.66	7/107901 (0.0%)
11	J	0.16	0/2828	0.64	0/4410
12	K	0.26	0/2121	0.58	0/2852
13	L	0.26	0/1586	0.54	0/2134
14	M	0.26	0/1571	0.55	0/2113
15	N	0.26	0/1434	0.56	0/1926
16	O	0.26	0/1343	0.52	0/1816
17	P	0.25	0/1122	0.53	0/1515
18	Q	0.27	0/488	0.53	0/649
19	R	0.25	0/1152	0.52	0/1551
20	S	0.27	0/947	0.63	0/1268
21	T	0.25	0/1062	0.58	0/1413
22	U	0.26	0/1081	0.60	0/1443
23	V	0.24	0/973	0.57	0/1301
24	W	0.27	0/902	0.61	0/1209
25	X	0.26	0/929	0.58	0/1242
26	Y	0.25	0/960	0.55	0/1278
27	Z	0.28	0/829	0.60	0/1107
28	a	0.24	0/864	0.54	0/1156
29	b	0.26	0/744	0.55	0/994
30	c	0.26	0/787	0.52	0/1051
31	d	0.27	0/766	0.53	0/1025

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.26	0/582	0.55	0/769
33	f	0.25	0/635	0.60	0/848
34	g	0.27	0/502	0.57	0/667
35	h	0.25	0/453	0.56	0/605
36	i	0.24	0/450	0.58	0/599
37	j	0.29	0/416	0.52	0/554
38	k	0.24	0/380	0.68	0/498
39	l	0.25	0/513	0.57	0/676
40	m	0.26	0/303	0.60	0/397
41	n	0.25	0/1195	0.56	0/1602
42	o	0.25	0/989	0.54	0/1326
43	p	0.28	0/1034	0.68	0/1375
44	q	0.25	0/796	0.60	0/1077
45	r	0.26	0/893	0.61	0/1205
46	t	0.26	0/969	0.60	0/1300
47	u	0.26	0/900	0.64	0/1204
48	v	0.26	0/785	0.63	0/1043
49	w	0.24	0/718	0.56	0/959
50	x	0.25	0/659	0.59	0/884
51	y	0.28	0/657	0.59	0/881
52	z	0.27	0/462	0.64	0/621
All	All	0.21	0/153864	0.64	8/230128 (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
27	Z	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	2418	A	OP1-P-OP2	-6.98	109.13	119.60
10	I	2401	U	OP1-P-OP2	-6.77	109.44	119.60
10	I	2616	C	OP1-P-OP2	-6.63	109.65	119.60
10	I	1025	G	OP1-P-OP2	-6.57	109.74	119.60
10	I	1313	U	C2-N1-C1'	5.89	124.77	117.70
4	C	754	C	C2-N1-C1'	5.62	124.98	118.80
10	I	2417	C	OP1-P-O3'	5.17	116.58	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	2401	U	O4'-C1'-N1	5.16	112.33	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Z	51	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
5	D	216/241 (90%)	208 (96%)	8 (4%)	0	100	100
6	E	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
7	F	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	25	41
8	G	148/167 (89%)	142 (96%)	6 (4%)	0	100	100
9	H	98/135 (73%)	97 (99%)	1 (1%)	0	100	100
12	K	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
13	L	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
14	M	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
15	N	175/179 (98%)	170 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
17	P	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
18	Q	56/70 (80%)	56 (100%)	0	0	100	100
19	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
20	S	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
21	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
22	U	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
23	V	118/127 (93%)	117 (99%)	1 (1%)	0	100	100
24	W	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
25	X	112/115 (97%)	112 (100%)	0	0	100	100
26	Y	115/118 (98%)	115 (100%)	0	0	100	100
27	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
28	a	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
29	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
30	c	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
31	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
32	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
33	f	75/78 (96%)	75 (100%)	0	0	100	100
34	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
35	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
36	i	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
37	j	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
38	k	44/46 (96%)	44 (100%)	0	0	100	100
39	l	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
40	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
41	n	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
42	o	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
43	p	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	29
44	q	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	13	23
45	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	t	121/124 (98%)	114 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	u	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
48	v	92/101 (91%)	88 (96%)	4 (4%)	0	100	100
49	w	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
50	x	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
51	y	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
52	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
All	All	5553/5913 (94%)	5405 (97%)	145 (3%)	3 (0%)	50	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	28	ILE
43	p	55	VAL
44	q	57	VAL

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	1	70/79 (89%)	62 (89%)	8 (11%)	4	8
2	2	65/66 (98%)	57 (88%)	8 (12%)	4	7
3	3	60/61 (98%)	55 (92%)	5 (8%)	9	17
5	D	180/199 (90%)	160 (89%)	20 (11%)	5	9
6	E	170/190 (90%)	157 (92%)	13 (8%)	11	20
7	F	172/173 (99%)	162 (94%)	10 (6%)	17	32
8	G	113/126 (90%)	107 (95%)	6 (5%)	19	36
9	H	87/116 (75%)	78 (90%)	9 (10%)	6	10
12	K	216/218 (99%)	209 (97%)	7 (3%)	34	57
13	L	164/164 (100%)	158 (96%)	6 (4%)	29	52
14	M	165/165 (100%)	155 (94%)	10 (6%)	15	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	N	148/150 (99%)	132 (89%)	16 (11%)	5	9
16	O	137/138 (99%)	122 (89%)	15 (11%)	5	9
17	P	114/114 (100%)	106 (93%)	8 (7%)	12	23
18	Q	55/62 (89%)	50 (91%)	5 (9%)	7	14
19	R	116/116 (100%)	111 (96%)	5 (4%)	25	45
20	S	103/104 (99%)	93 (90%)	10 (10%)	6	12
21	T	103/103 (100%)	99 (96%)	4 (4%)	27	49
22	U	108/108 (100%)	104 (96%)	4 (4%)	29	52
23	V	100/103 (97%)	99 (99%)	1 (1%)	73	87
24	W	86/87 (99%)	81 (94%)	5 (6%)	17	32
25	X	99/100 (99%)	92 (93%)	7 (7%)	12	23
26	Y	89/90 (99%)	84 (94%)	5 (6%)	17	33
27	Z	84/84 (100%)	78 (93%)	6 (7%)	12	23
28	a	93/93 (100%)	87 (94%)	6 (6%)	14	27
29	b	80/84 (95%)	70 (88%)	10 (12%)	3	6
30	c	83/85 (98%)	74 (89%)	9 (11%)	5	9
31	d	78/78 (100%)	72 (92%)	6 (8%)	10	20
32	e	57/63 (90%)	54 (95%)	3 (5%)	19	36
33	f	67/68 (98%)	60 (90%)	7 (10%)	5	10
34	g	54/55 (98%)	48 (89%)	6 (11%)	5	9
35	h	48/49 (98%)	42 (88%)	6 (12%)	3	6
36	i	47/48 (98%)	42 (89%)	5 (11%)	5	10
37	j	45/49 (92%)	44 (98%)	1 (2%)	47	70
38	k	38/38 (100%)	34 (90%)	4 (10%)	5	10
39	l	51/52 (98%)	47 (92%)	4 (8%)	10	19
40	m	34/34 (100%)	33 (97%)	1 (3%)	37	61
41	n	124/147 (84%)	112 (90%)	12 (10%)	6	12
42	o	104/105 (99%)	95 (91%)	9 (9%)	8	15
43	p	105/107 (98%)	90 (86%)	15 (14%)	2	4
44	q	86/90 (96%)	79 (92%)	7 (8%)	9	18
45	r	90/99 (91%)	82 (91%)	8 (9%)	8	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	t	103/104 (99%)	96 (93%)	7 (7%)	13	25
47	u	93/96 (97%)	84 (90%)	9 (10%)	6	12
48	v	79/84 (94%)	71 (90%)	8 (10%)	6	11
49	w	75/77 (97%)	67 (89%)	8 (11%)	5	10
50	x	65/65 (100%)	63 (97%)	2 (3%)	35	59
51	y	74/78 (95%)	65 (88%)	9 (12%)	4	7
52	z	48/65 (74%)	43 (90%)	5 (10%)	5	10
All	All	4625/4829 (96%)	4265 (92%)	360 (8%)	13	19

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	LYS
1	1	13	LEU
1	1	27	ASP
1	1	29	LYS
1	1	32	ARG
1	1	43	ASN
1	1	56	GLN
1	1	80	TYR
2	2	5	LYS
2	2	23	SER
2	2	43	ASP
2	2	48	GLN
2	2	55	GLN
2	2	66	LEU
2	2	69	LYS
2	2	79	LEU
3	3	5	LYS
3	3	19	PHE
3	3	38	TYR
3	3	49	LYS
3	3	70	LEU
5	D	23	TRP
5	D	28	LYS
5	D	35	ARG
5	D	36	ASN
5	D	49	MET
5	D	50	PHE
5	D	51	ASN

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Mol	Chain	Res	Type
5	D	59	LYS
5	D	82	ASP
5	D	88	ASP
5	D	108	ARG
5	D	136	MET
5	D	145	GLU
5	D	152	LYS
5	D	153	ASP
5	D	154	MET
5	D	159	ASP
5	D	167	ASP
5	D	191	SER
5	D	214	LEU
6	E	29	PHE
6	E	35	SER
6	E	62	LYS
6	E	72	ARG
6	E	88	ARG
6	E	93	ASP
6	E	108	LYS
6	E	112	ASP
6	E	115	LEU
6	E	127	ARG
6	E	156	ARG
6	E	169	ARG
6	E	187	SER
7	F	44	ARG
7	F	57	GLU
7	F	82	LEU
7	F	134	SER
7	F	156	LYS
7	F	164	GLN
7	F	171	LEU
7	F	181	THR
7	F	184	ARG
7	F	190	ASP
8	G	55	GLU
8	G	69	ARG
8	G	92	SER
8	G	122	ASN
8	G	130	SER
8	G	148	ASN

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Mol	Chain	Res	Type
9	H	1	MET
9	H	17	GLN
9	H	72	ASP
9	H	73	GLU
9	H	78	PHE
9	H	82	ASP
9	H	92	THR
9	H	93	LYS
9	H	100	SER
12	K	38	SER
12	K	97	LYS
12	K	173	THR
12	K	214	ARG
12	K	259	SER
12	K	264	ASP
12	K	265	LYS
13	L	1	MET
13	L	18	ASP
13	L	58	ASN
13	L	59	ARG
13	L	103	ASP
13	L	110	THR
14	M	21	ARG
14	M	91	ASP
14	M	124	PHE
14	M	136	GLN
14	M	166	LYS
14	M	170	ARG
14	M	176	ASP
14	M	185	LYS
14	M	195	GLN
14	M	198	GLU
15	N	3	LYS
15	N	24	SER
15	N	26	MET
15	N	36	LEU
15	N	72	LYS
15	N	80	ARG
15	N	83	TYR
15	N	92	ARG
15	N	96	MET
15	N	114	PHE

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Mol	Chain	Res	Type
15	N	117	LEU
15	N	143	TYR
15	N	148	ARG
15	N	173	PHE
15	N	175	PHE
15	N	178	ARG
16	O	11	VAL
16	O	18	LYS
16	O	29	LYS
16	O	30	ASN
16	O	32	GLU
16	O	35	ARG
16	O	39	ASP
16	O	44	LYS
16	O	74	SER
16	O	86	LYS
16	O	106	SER
16	O	122	THR
16	O	139	GLN
16	O	153	ARG
16	O	170	ARG
17	P	43	ASN
17	P	46	PHE
17	P	47	PHE
17	P	71	LYS
17	P	87	GLU
17	P	97	ARG
17	P	112	LYS
17	P	136	SER
18	Q	3	LYS
18	Q	22	MET
18	Q	23	LYS
18	Q	31	ASP
18	Q	62	LYS
19	R	1	MET
19	R	61	LYS
19	R	71	ASP
19	R	99	ARG
19	R	129	GLU
20	S	17	ARG
20	S	51	LYS
20	S	53	LYS

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Mol	Chain	Res	Type
20	S	59	LYS
20	S	66	LYS
20	S	67	LYS
20	S	73	ASP
20	S	80	ASP
20	S	109	SER
20	S	111	LYS
21	T	2	ARG
21	T	42	SER
21	T	84	LYS
21	T	118	THR
22	U	44	ARG
22	U	53	MET
22	U	62	LYS
22	U	88	ASN
23	V	89	SER
24	W	33	ARG
24	W	63	LYS
24	W	69	ASP
24	W	95	SER
24	W	100	HIS
25	X	33	VAL
25	X	37	LYS
25	X	44	GLU
25	X	57	SER
25	X	65	SER
25	X	101	ARG
25	X	103	ARG
26	Y	33	ARG
26	Y	72	ASN
26	Y	78	LYS
26	Y	87	SER
26	Y	102	ASP
27	Z	1	MET
27	Z	12	HIS
27	Z	55	ASP
27	Z	79	ARG
27	Z	81	LYS
27	Z	102	SER
28	a	12	SER
28	a	13	SER
28	a	22	ASP

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Mol	Chain	Res	Type
28	a	53	SER
28	a	70	LYS
28	a	86	MET
29	b	1	MET
29	b	5	GLU
29	b	6	ARG
29	b	15	HIS
29	b	37	ASP
29	b	64	LYS
29	b	66	LYS
29	b	77	ARG
29	b	78	SER
29	b	80	TRP
30	c	18	ASP
30	c	24	LYS
30	c	26	LYS
30	c	30	SER
30	c	36	VAL
30	c	46	GLN
30	c	79	LYS
30	c	89	ASP
30	c	101	GLU
31	d	41	GLU
31	d	53	LYS
31	d	58	SER
31	d	66	ASP
31	d	68	LYS
31	d	71	LYS
32	e	30	SER
32	e	40	GLN
32	e	62	LYS
33	f	3	ARG
33	f	23	ASN
33	f	30	LEU
33	f	35	SER
33	f	37	ARG
33	f	45	ARG
33	f	49	LEU
34	g	4	LYS
34	g	13	GLU
34	g	23	ARG
34	g	34	SER

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Mol	Chain	Res	Type
34	g	37	LEU
34	g	54	LYS
35	h	3	LYS
35	h	6	LYS
35	h	12	SER
35	h	16	ARG
35	h	17	LEU
35	h	39	GLU
36	i	12	LYS
36	i	31	ASP
36	i	34	SER
36	i	42	HIS
36	i	52	ARG
37	j	13	SER
38	k	1	MET
38	k	8	SER
38	k	12	ARG
38	k	25	LYS
39	l	16	LYS
39	l	31	HIS
39	l	51	SER
39	l	52	LYS
40	m	1	MET
41	n	11	LYS
41	n	20	SER
41	n	52	GLN
41	n	58	GLU
41	n	59	LEU
41	n	62	PHE
41	n	68	ASN
41	n	69	VAL
41	n	92	ARG
41	n	120	LEU
41	n	123	GLU
41	n	136	LYS
42	o	5	ASP
42	o	10	MET
42	o	27	MET
42	o	90	ASP
42	o	94	LYS
42	o	96	MET
42	o	105	SER

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Mol	Chain	Res	Type
42	o	108	LYS
42	o	117	ARG
43	p	14	SER
43	p	15	SER
43	p	27	LYS
43	p	38	TYR
43	p	46	MET
43	p	50	GLN
43	p	56	ASP
43	p	62	ASP
43	p	85	ARG
43	p	95	ARG
43	p	105	THR
43	p	106	ARG
43	p	107	ASP
43	p	123	ARG
43	p	128	SER
44	q	20	GLN
44	q	35	GLN
44	q	37	ARG
44	q	78	GLU
44	q	81	GLU
44	q	89	ARG
44	q	90	LEU
45	r	37	ARG
45	r	58	SER
45	r	64	GLN
45	r	72	ASP
45	r	94	GLU
45	r	105	PHE
45	r	119	ASN
45	r	128	ARG
46	t	19	SER
46	t	24	LEU
46	t	64	THR
46	t	65	SER
46	t	86	ARG
46	t	111	LYS
46	t	123	LYS
47	u	31	LYS
47	u	41	GLU
47	u	57	ARG

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Mol	Chain	Res	Type
47	u	81	MET
47	u	93	ARG
47	u	98	ARG
47	u	107	ARG
47	u	113	ARG
47	u	114	LYS
48	v	6	MET
48	v	12	LYS
48	v	35	ASN
48	v	42	TRP
48	v	54	ASP
48	v	61	ARG
48	v	80	SER
48	v	85	ARG
49	w	4	SER
49	w	14	GLU
49	w	58	ARG
49	w	61	SER
49	w	71	LYS
49	w	72	ARG
49	w	73	LYS
49	w	74	ASP
50	x	3	THR
50	x	25	ARG
51	y	6	ARG
51	y	7	THR
51	y	11	ARG
51	y	48	ASP
51	y	49	GLU
51	y	60	GLU
51	y	72	SER
51	y	77	ARG
51	y	81	LYS
52	z	30	LYS
52	z	42	SER
52	z	43	ARG
52	z	71	THR
52	z	73	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	43	ASN
18	Q	30	HIS
50	x	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	I	2890/2904 (99%)	341 (11%)	25 (0%)
11	J	117/120 (97%)	11 (9%)	0
4	C	1539/1540 (99%)	169 (10%)	7 (0%)
All	All	4546/4564 (99%)	521 (11%)	32 (0%)

All (521) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	C	4	U
4	C	5	U
4	C	9	G
4	C	39	G
4	C	47	C
4	C	48	C
4	C	51	A
4	C	70	U
4	C	71	A
4	C	74	A
4	C	83	C
4	C	85	U
4	C	87	C
4	C	95	C
4	C	97	G
4	C	108	G
4	C	116	A
4	C	120	A
4	C	121	U
4	C	130	A
4	C	131	A
4	C	144	G
4	C	182	A
4	C	207	C
4	C	208	U
4	C	209	U
4	C	210	C

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Mol	Chain	Res	Type
4	C	211	G
4	C	245	U
4	C	247	G
4	C	251	G
4	C	266	G
4	C	267	C
4	C	279	A
4	C	289	G
4	C	328	C
4	C	329	A
4	C	332	G
4	C	352	C
4	C	354	G
4	C	356	A
4	C	367	U
4	C	372	C
4	C	406	G
4	C	411	A
4	C	412	A
4	C	413	G
4	C	421	U
4	C	424	G
4	C	429	U
4	C	467	U
4	C	468	A
4	C	478	A
4	C	479	U
4	C	485	U
4	C	497	G
4	C	511	C
4	C	518	C
4	C	527	G
4	C	532	A
4	C	533	A
4	C	547	A
4	C	564	C
4	C	572	A
4	C	573	A
4	C	576	C
4	C	577	G
4	C	633	G
4	C	650	G

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Mol	Chain	Res	Type
4	C	665	A
4	C	687	A
4	C	721	G
4	C	723	U
4	C	724	G
4	C	731	G
4	C	747	A
4	C	755	G
4	C	793	U
4	C	794	A
4	C	815	A
4	C	817	C
4	C	828	U
4	C	829	G
4	C	841	C
4	C	842	U
4	C	843	U
4	C	844	G
4	C	845	A
4	C	846	G
4	C	847	G
4	C	885	G
4	C	914	A
4	C	934	C
4	C	935	A
4	C	960	U
4	C	966	G
4	C	969	A
4	C	975	A
4	C	976	G
4	C	977	A
4	C	983	A
4	C	993	G
4	C	1004	A
4	C	1009	U
4	C	1030	U
4	C	1032	G
4	C	1033	G
4	C	1034	G
4	C	1043	G
4	C	1048	G
4	C	1054	C

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Mol	Chain	Res	Type
4	C	1055	A
4	C	1065	U
4	C	1085	U
4	C	1094	G
4	C	1095	U
4	C	1101	A
4	C	1136	C
4	C	1137	C
4	C	1139	G
4	C	1140	C
4	C	1141	C
4	C	1142	G
4	C	1145	A
4	C	1146	A
4	C	1159	U
4	C	1167	A
4	C	1196	A
4	C	1197	A
4	C	1202	U
4	C	1212	U
4	C	1213	A
4	C	1227	A
4	C	1229	A
4	C	1240	U
4	C	1241	G
4	C	1275	A
4	C	1280	A
4	C	1286	U
4	C	1287	A
4	C	1299	A
4	C	1300	G
4	C	1302	C
4	C	1305	G
4	C	1308	U
4	C	1317	C
4	C	1320	C
4	C	1337	G
4	C	1346	A
4	C	1363	A
4	C	1364	U
4	C	1378	C
4	C	1381	U

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Mol	Chain	Res	Type
4	C	1398	A
4	C	1419	G
4	C	1446	A
4	C	1452	C
4	C	1492	A
4	C	1493	A
4	C	1503	A
4	C	1506	U
4	C	1517	G
4	C	1529	G
4	C	1530	G
4	C	1534	A
4	C	1537	U
4	C	1538	C
4	C	1539	C
4	C	1540	U
10	I	10	A
10	I	26	G
10	I	34	U
10	I	42	A
10	I	46	G
10	I	51	G
10	I	63	A
10	I	71	A
10	I	72	U
10	I	74	A
10	I	75	G
10	I	84	A
10	I	88	G
10	I	101	A
10	I	102	U
10	I	110	G
10	I	118	A
10	I	120	U
10	I	137	U
10	I	139	U
10	I	163	C
10	I	174	U
10	I	181	A
10	I	183	C
10	I	196	A
10	I	199	A

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Mol	Chain	Res	Type
10	I	209	C
10	I	216	A
10	I	220	G
10	I	221	A
10	I	222	A
10	I	236	C
10	I	238	C
10	I	248	G
10	I	266	G
10	I	272	A
10	I	276	U
10	I	302	C
10	I	309	A
10	I	311	A
10	I	329	G
10	I	330	A
10	I	353	C
10	I	361	G
10	I	362	A
10	I	371	A
10	I	372	G
10	I	376	G
10	I	380	G
10	I	386	G
10	I	391	A
10	I	396	G
10	I	405	U
10	I	411	G
10	I	412	A
10	I	437	U
10	I	456	C
10	I	457	A
10	I	475	C
10	I	481	G
10	I	491	G
10	I	504	A
10	I	505	A
10	I	509	C
10	I	529	A
10	I	530	G
10	I	532	A
10	I	546	U

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Mol	Chain	Res	Type
10	I	549	G
10	I	556	A
10	I	562	U
10	I	563	A
10	I	572	A
10	I	573	U
10	I	575	A
10	I	587	C
10	I	603	A
10	I	607	U
10	I	614	A
10	I	616	A
10	I	621	A
10	I	627	A
10	I	637	A
10	I	647	G
10	I	654	A
10	I	655	A
10	I	686	U
10	I	730	A
10	I	747	5MU
10	I	775	G
10	I	776	G
10	I	782	A
10	I	784	G
10	I	785	G
10	I	789	A
10	I	805	G
10	I	812	C
10	I	819	A
10	I	827	U
10	I	828	U
10	I	846	U
10	I	847	U
10	I	858	G
10	I	859	G
10	I	896	A
10	I	897	C
10	I	910	A
10	I	914	G
10	I	915	C
10	I	931	U

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Mol	Chain	Res	Type
10	I	941	A
10	I	946	C
10	I	961	C
10	I	974	G
10	I	983	A
10	I	996	A
10	I	1012	U
10	I	1013	C
10	I	1025	G
10	I	1026	G
10	I	1033	U
10	I	1046	A
10	I	1047	G
10	I	1061	U
10	I	1070	A
10	I	1071	G
10	I	1080	A
10	I	1088	A
10	I	1111	A
10	I	1112	G
10	I	1116	G
10	I	1132	U
10	I	1133	A
10	I	1135	C
10	I	1142	A
10	I	1150	C
10	I	1152	C
10	I	1174	U
10	I	1175	A
10	I	1179	G
10	I	1180	U
10	I	1206	G
10	I	1238	G
10	I	1250	G
10	I	1253	A
10	I	1256	G
10	I	1266	G
10	I	1271	G
10	I	1272	A
10	I	1300	G
10	I	1301	A
10	I	1314	C

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Mol	Chain	Res	Type
10	I	1340	U
10	I	1352	U
10	I	1353	A
10	I	1365	A
10	I	1368	G
10	I	1379	U
10	I	1383	A
10	I	1386	C
10	I	1416	G
10	I	1419	A
10	I	1428	C
10	I	1452	G
10	I	1461	C
10	I	1482	G
10	I	1484	U
10	I	1493	C
10	I	1494	A
10	I	1506	U
10	I	1510	G
10	I	1515	A
10	I	1535	A
10	I	1536	C
10	I	1566	A
10	I	1569	A
10	I	1578	U
10	I	1608	A
10	I	1610	A
10	I	1619	G
10	I	1647	U
10	I	1648	U
10	I	1649	G
10	I	1674	G
10	I	1677	A
10	I	1684	G
10	I	1696	G
10	I	1699	G
10	I	1715	G
10	I	1729	U
10	I	1730	C
10	I	1738	G
10	I	1755	A
10	I	1758	U

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Mol	Chain	Res	Type
10	I	1763	G
10	I	1764	C
10	I	1773	A
10	I	1791	A
10	I	1800	C
10	I	1801	A
10	I	1808	A
10	I	1814	G
10	I	1816	C
10	I	1829	A
10	I	1847	A
10	I	1848	A
10	I	1869	G
10	I	1870	C
10	I	1872	A
10	I	1906	G
10	I	1909	C
10	I	1913	A
10	I	1914	C
10	I	1929	G
10	I	1930	G
10	I	1936	A
10	I	1938	A
10	I	1955	U
10	I	1967	C
10	I	1970	A
10	I	1971	U
10	I	1972	G
10	I	1982	U
10	I	1991	U
10	I	1993	U
10	I	1997	C
10	I	2021	C
10	I	2022	U
10	I	2023	C
10	I	2031	A
10	I	2033	A
10	I	2043	C
10	I	2055	C
10	I	2056	G
10	I	2060	A
10	I	2061	G

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Mol	Chain	Res	Type
10	I	2069	G7M
10	I	2093	G
10	I	2111	U
10	I	2112	G
10	I	2115	G
10	I	2117	A
10	I	2118	U
10	I	2119	A
10	I	2128	G
10	I	2131	U
10	I	2132	U
10	I	2133	G
10	I	2134	A
10	I	2148	G
10	I	2159	G
10	I	2163	A
10	I	2164	C
10	I	2165	C
10	I	2166	U
10	I	2167	U
10	I	2169	A
10	I	2170	A
10	I	2171	A
10	I	2172	U
10	I	2177	C
10	I	2178	C
10	I	2181	U
10	I	2198	A
10	I	2204	G
10	I	2211	A
10	I	2225	A
10	I	2226	C
10	I	2238	G
10	I	2239	G
10	I	2279	G
10	I	2283	C
10	I	2287	A
10	I	2297	A
10	I	2305	U
10	I	2322	A
10	I	2325	G
10	I	2333	A

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Mol	Chain	Res	Type
10	I	2335	A
10	I	2345	G
10	I	2347	C
10	I	2350	C
10	I	2361	G
10	I	2371	G
10	I	2383	G
10	I	2385	C
10	I	2403	C
10	I	2423	U
10	I	2425	A
10	I	2426	A
10	I	2429	G
10	I	2430	A
10	I	2441	U
10	I	2445	2MG
10	I	2448	A
10	I	2476	A
10	I	2491	U
10	I	2502	G
10	I	2504	PSU
10	I	2505	G
10	I	2518	A
10	I	2520	C
10	I	2544	G
10	I	2547	A
10	I	2554	U
10	I	2566	A
10	I	2567	G
10	I	2572	A
10	I	2585	U
10	I	2602	A
10	I	2605	PSU
10	I	2609	U
10	I	2613	U
10	I	2615	U
10	I	2661	G
10	I	2681	C
10	I	2689	U
10	I	2690	U
10	I	2714	G
10	I	2718	G

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Mol	Chain	Res	Type
10	I	2726	A
10	I	2729	G
10	I	2733	A
10	I	2744	G
10	I	2748	A
10	I	2765	A
10	I	2766	A
10	I	2778	A
10	I	2791	G
10	I	2793	C
10	I	2797	U
10	I	2800	A
10	I	2820	A
10	I	2855	C
10	I	2867	G
10	I	2872	A
10	I	2873	A
10	I	2880	C
10	I	2883	A
10	I	2884	U
10	I	2885	G
11	J	15	A
11	J	32	U
11	J	35	C
11	J	56	G
11	J	67	G
11	J	88	C
11	J	89	U
11	J	90	C
11	J	99	A
11	J	109	A
11	J	119	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	C	96	U
4	C	115	G
4	C	206	C
4	C	846	G
4	C	1145	A
4	C	1201	A

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Mol	Chain	Res	Type
4	C	1491	G
10	I	25	U
10	I	138	U
10	I	182	A
10	I	271	G
10	I	404	A
10	I	504	A
10	I	548	G
10	I	555	G
10	I	784	G
10	I	1025	G
10	I	1079	C
10	I	1313	U
10	I	1352	U
10	I	1754	A
10	I	1813	G
10	I	1846	G
10	I	1913	A
10	I	2127	G
10	I	2158	A
10	I	2225	A
10	I	2425	A
10	I	2447	G
10	I	2543	G
10	I	2680	U
10	I	2854	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	PSU	I	2504	53,10	18,21,22	0.88	0	21,30,33	1.97	4 (19%)
10	PSU	I	1917	10	18,21,22	0.88	0	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PSU	I	746	53,10	18,21,22	0.99	1 (5%)	21,30,33	1.88	4 (19%)
10	1MG	I	745	10	19,26,27	1.24	4 (21%)	18,39,42	1.50	3 (16%)
10	2MA	I	2503	53,10	18,25,26	1.29	2 (11%)	20,37,40	1.92	3 (15%)
10	3TD	I	1915	10	19,22,23	1.09	2 (10%)	23,32,35	1.88	2 (8%)
10	PSU	I	2457	10	18,21,22	0.93	1 (5%)	21,30,33	2.01	4 (19%)
10	OMU	I	2552	10	19,22,23	0.95	2 (10%)	25,31,34	1.94	6 (24%)
10	2MG	I	1835	10	18,26,27	1.26	2 (11%)	16,38,41	1.48	3 (18%)
10	PSU	I	2604	10	18,21,22	0.91	0	21,30,33	1.99	4 (19%)
10	5MU	I	747	10	19,22,23	1.02	2 (10%)	27,32,35	2.13	6 (22%)
10	H2U	I	2449	10	18,21,22	0.42	0	19,30,33	0.71	0
10	OMG	I	2251	10	19,26,27	1.20	2 (10%)	21,38,41	1.38	4 (19%)
10	6MZ	I	2030	10	17,25,26	1.15	2 (11%)	15,36,39	2.24	4 (26%)
10	G7M	I	2069	10	20,26,27	0.94	1 (5%)	16,39,42	0.51	0
10	PSU	I	2605	10	18,21,22	0.92	1 (5%)	21,30,33	1.97	4 (19%)
10	5MU	I	1939	10	19,22,23	1.02	2 (10%)	27,32,35	2.12	6 (22%)
10	5MC	I	1962	10	19,22,23	1.22	2 (10%)	26,32,35	1.11	3 (11%)
10	PSU	I	955	10	18,21,22	0.91	0	21,30,33	1.99	4 (19%)
10	6MZ	I	1618	10	17,25,26	1.16	2 (11%)	15,36,39	2.21	4 (26%)
22	4D4	U	81	22	9,11,12	2.14	2 (22%)	7,13,15	1.96	3 (42%)
10	2MG	I	2445	10	18,26,27	1.27	2 (11%)	16,38,41	1.59	4 (25%)
10	OMC	I	2498	53,10	19,22,23	0.89	1 (5%)	25,31,34	0.97	1 (4%)
10	PSU	I	2580	53,10	18,21,22	0.95	0	21,30,33	1.97	5 (23%)
10	PSU	I	1911	10	18,21,22	0.88	0	21,30,33	1.98	4 (19%)

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
10	PSU	I	2504	53,10	-	2/7/25/26	0/2/2/2
10	PSU	I	1917	10	-	0/7/25/26	0/2/2/2
10	PSU	I	746	53,10	-	1/7/25/26	0/2/2/2
10	1MG	I	745	10	-	0/3/25/26	0/3/3/3
10	2MA	I	2503	53,10	-	2/3/25/26	0/3/3/3
10	3TD	I	1915	10	-	2/7/25/26	0/2/2/2
10	PSU	I	2457	10	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	OMU	I	2552	10	-	0/9/27/28	0/2/2/2
10	2MG	I	1835	10	-	0/5/27/28	0/3/3/3
10	PSU	I	2604	10	-	0/7/25/26	0/2/2/2
10	5MU	I	747	10	-	0/7/25/26	0/2/2/2
10	H2U	I	2449	10	-	0/7/38/39	0/2/2/2
10	OMG	I	2251	10	-	0/5/27/28	0/3/3/3
10	6MZ	I	2030	10	-	2/5/27/28	0/3/3/3
10	G7M	I	2069	10	-	0/3/25/26	0/3/3/3
10	PSU	I	2605	10	-	2/7/25/26	0/2/2/2
10	5MU	I	1939	10	-	0/7/25/26	0/2/2/2
10	5MC	I	1962	10	-	0/7/25/26	0/2/2/2
10	PSU	I	955	10	-	0/7/25/26	0/2/2/2
10	6MZ	I	1618	10	-	2/5/27/28	0/3/3/3
22	4D4	U	81	22	-	1/11/12/14	-
10	2MG	I	2445	10	-	2/5/27/28	0/3/3/3
10	OMC	I	2498	53,10	-	0/9/27/28	0/2/2/2
10	PSU	I	2580	53,10	-	0/7/25/26	0/2/2/2
10	PSU	I	1911	10	-	0/7/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	81	4D4	CZ-NE	5.38	1.43	1.33
10	I	1962	5MC	C5-C4	-3.87	1.41	1.44
10	I	2503	2MA	C6-N1	3.54	1.40	1.33
10	I	1835	2MG	C5-C6	-2.98	1.41	1.47
10	I	2069	G7M	C8-N9	2.93	1.38	1.33
10	I	2445	2MG	C5-C6	-2.90	1.41	1.47
10	I	2251	OMG	C5-C6	-2.88	1.41	1.47
10	I	745	1MG	C8-N7	-2.86	1.30	1.34
10	I	2251	OMG	C8-N7	-2.81	1.30	1.34
10	I	2445	2MG	C8-N7	-2.81	1.30	1.34
22	U	81	4D4	CZ-NH1	2.81	1.44	1.34
10	I	1835	2MG	C8-N7	-2.77	1.30	1.34
10	I	1618	6MZ	C6-C5	-2.73	1.40	1.44
10	I	2030	6MZ	C6-C5	-2.66	1.40	1.44
10	I	2498	OMC	C2-N1	-2.56	1.34	1.40
10	I	1915	3TD	C4-N3	-2.52	1.35	1.40
10	I	747	5MU	C2-N1	-2.50	1.34	1.38
10	I	1962	5MC	C2-N1	-2.48	1.34	1.40
10	I	1915	3TD	C4-C5	-2.44	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	1939	5MU	C2-N1	-2.37	1.34	1.38
10	I	2552	OMU	C2-N1	-2.36	1.34	1.38
10	I	1618	6MZ	C8-N7	-2.35	1.30	1.34
10	I	2030	6MZ	C8-N7	-2.33	1.30	1.34
10	I	745	1MG	C6-N1	-2.23	1.35	1.39
10	I	746	PSU	O4'-C1'	-2.13	1.40	1.43
10	I	1939	5MU	C4-N3	-2.12	1.34	1.38
10	I	745	1MG	C5-C6	-2.08	1.41	1.47
10	I	747	5MU	C4-N3	-2.06	1.35	1.38
10	I	2552	OMU	C4-N3	-2.05	1.35	1.38
10	I	745	1MG	C2-N2	2.04	1.37	1.34
10	I	2503	2MA	C8-N7	-2.02	1.31	1.34
10	I	2605	PSU	C4-N3	-2.01	1.35	1.38
10	I	2457	PSU	C4-N3	-2.00	1.35	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	1915	3TD	N1-C2-N3	6.59	120.92	116.13
10	I	1618	6MZ	C2-N1-C6	5.87	121.16	116.60
10	I	2030	6MZ	C2-N1-C6	5.75	121.06	116.60
10	I	2503	2MA	C2-N3-C4	5.69	120.06	115.46
10	I	2457	PSU	N1-C2-N3	5.63	121.11	115.17
10	I	2504	PSU	N1-C2-N3	5.60	121.07	115.17
10	I	2604	PSU	N1-C2-N3	5.56	121.03	115.17
10	I	955	PSU	N1-C2-N3	5.55	121.02	115.17
10	I	2605	PSU	N1-C2-N3	5.53	121.00	115.17
10	I	1911	PSU	N1-C2-N3	5.52	120.99	115.17
10	I	2580	PSU	N1-C2-N3	5.45	120.92	115.17
10	I	746	PSU	N1-C2-N3	5.44	120.90	115.17
10	I	1917	PSU	N1-C2-N3	5.42	120.89	115.17
10	I	1939	5MU	C4-N3-C2	-5.42	120.23	127.34
10	I	747	5MU	C4-N3-C2	-5.40	120.26	127.34
10	I	2552	OMU	C4-N3-C2	-5.21	120.14	126.61
10	I	2503	2MA	C5-C6-N1	-5.06	114.86	120.84
10	I	747	5MU	N3-C2-N1	4.81	121.15	114.89
10	I	1939	5MU	N3-C2-N1	4.80	121.14	114.89
10	I	2552	OMU	N3-C2-N1	4.79	121.13	114.89
10	I	1939	5MU	C5-C4-N3	4.65	119.36	115.32
10	I	747	5MU	C5-C4-N3	4.62	119.33	115.32
10	I	1618	6MZ	N3-C2-N1	-4.58	122.45	128.67
10	I	2030	6MZ	N3-C2-N1	-4.57	122.47	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	2457	PSU	C4-N3-C2	-4.54	120.12	126.37
10	I	1917	PSU	C4-N3-C2	-4.53	120.13	126.37
10	I	2605	PSU	C4-N3-C2	-4.52	120.15	126.37
10	I	1911	PSU	C4-N3-C2	-4.51	120.15	126.37
10	I	955	PSU	C4-N3-C2	-4.51	120.16	126.37
10	I	2604	PSU	C4-N3-C2	-4.51	120.16	126.37
10	I	2580	PSU	C4-N3-C2	-4.42	120.28	126.37
10	I	2504	PSU	C4-N3-C2	-4.41	120.30	126.37
10	I	746	PSU	C4-N3-C2	-4.39	120.33	126.37
10	I	1915	3TD	C4-N3-C2	-4.23	120.13	124.61
10	I	747	5MU	O4-C4-C5	-4.02	120.32	124.92
22	U	81	4D4	NE-CZ-NH2	4.02	127.57	120.67
10	I	2445	2MG	C8-N7-C5	3.97	109.31	102.55
10	I	745	1MG	C8-N7-C5	3.96	109.28	102.55
10	I	2251	OMG	C8-N7-C5	3.95	109.27	102.55
10	I	1835	2MG	C8-N7-C5	3.92	109.23	102.55
10	I	1939	5MU	O4-C4-C5	-3.92	120.43	124.92
10	I	2030	6MZ	C9-N6-C6	-3.58	119.53	122.85
10	I	1939	5MU	C5-C6-N1	-3.40	119.62	123.31
10	I	747	5MU	C5-C6-N1	-3.40	119.62	123.31
10	I	2552	OMU	C5-C4-N3	3.28	119.39	114.80
10	I	1618	6MZ	C9-N6-C6	-3.27	119.82	122.85
10	I	1962	5MC	C5-C6-N1	-3.22	119.82	123.31
10	I	2580	PSU	O2-C2-N1	-3.19	119.50	122.79
10	I	2552	OMU	CM2-O2'-C2'	-3.18	106.30	114.47
10	I	2604	PSU	O2-C2-N1	-3.17	119.52	122.79
10	I	745	1MG	C5-C6-N1	3.15	118.51	113.96
10	I	2504	PSU	O2-C2-N1	-3.14	119.55	122.79
10	I	955	PSU	O2-C2-N1	-3.09	119.60	122.79
10	I	2457	PSU	O2-C2-N1	-3.09	119.60	122.79
10	I	2605	PSU	O2-C2-N1	-3.08	119.61	122.79
10	I	1911	PSU	O2-C2-N1	-3.08	119.62	122.79
10	I	1917	PSU	O2-C2-N1	-3.02	119.68	122.79
10	I	746	PSU	O2-C2-N1	-3.01	119.69	122.79
10	I	2445	2MG	N1-C2-N2	2.95	119.57	116.56
10	I	2552	OMU	O4-C4-C5	-2.76	120.40	125.16
10	I	747	5MU	O2-C2-N1	-2.70	119.28	122.80
10	I	2251	OMG	C2-N1-C6	-2.68	120.20	125.11
10	I	2552	OMU	O2-C2-N1	-2.54	119.49	122.80
10	I	2498	OMC	CM2-O2'-C2'	-2.52	108.01	114.47
10	I	1835	2MG	N1-C2-N2	2.37	118.98	116.56
10	I	2504	PSU	C6-N1-C2	-2.33	120.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	2030	6MZ	C4-C5-N7	-2.33	106.88	109.34
10	I	745	1MG	O6-C6-C5	-2.32	120.36	124.18
10	I	1835	2MG	C5-C6-N1	2.30	118.46	114.07
10	I	1939	5MU	O2-C2-N1	-2.30	119.81	122.80
10	I	1962	5MC	C5-C4-N3	-2.29	119.41	121.75
10	I	2457	PSU	C6-N1-C2	-2.28	120.57	122.69
10	I	2251	OMG	C5-C6-N1	2.28	118.41	114.07
10	I	2445	2MG	C5-C6-N1	2.27	118.39	114.07
10	I	2604	PSU	C6-N1-C2	-2.26	120.59	122.69
10	I	2580	PSU	C6-N1-C2	-2.26	120.60	122.69
10	I	1962	5MC	O2-C2-N3	-2.25	118.78	122.33
10	I	746	PSU	C6-N1-C2	-2.24	120.61	122.69
10	I	1911	PSU	C6-N1-C2	-2.24	120.61	122.69
10	I	2605	PSU	C6-N1-C2	-2.24	120.61	122.69
10	I	955	PSU	C6-N1-C2	-2.23	120.62	122.69
22	U	81	4D4	NH1-CZ-NE	-2.19	114.28	119.27
10	I	2251	OMG	CM2-O2'-C2'	-2.15	108.95	114.47
10	I	1618	6MZ	C4-C5-N7	-2.15	107.06	109.34
22	U	81	4D4	O-C-CA	-2.15	119.24	124.77
10	I	1917	PSU	C6-N1-C2	-2.14	120.71	122.69
10	I	2503	2MA	N6-C6-N1	2.10	122.75	117.11
10	I	2580	PSU	O4'-C1'-C2'	2.08	108.03	105.15
10	I	2445	2MG	CM2-N2-C2	-2.00	119.35	123.65

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	I	1618	6MZ	O4'-C4'-C5'-O5'
10	I	1915	3TD	O4'-C4'-C5'-O5'
10	I	2605	PSU	O4'-C4'-C5'-O5'
10	I	1618	6MZ	C3'-C4'-C5'-O5'
10	I	1915	3TD	C3'-C4'-C5'-O5'
10	I	2445	2MG	C3'-C4'-C5'-O5'
10	I	2605	PSU	C3'-C4'-C5'-O5'
10	I	2030	6MZ	O4'-C4'-C5'-O5'
10	I	2504	PSU	O4'-C4'-C5'-O5'
10	I	2030	6MZ	C3'-C4'-C5'-O5'
10	I	2503	2MA	C3'-C4'-C5'-O5'
10	I	2445	2MG	O4'-C4'-C5'-O5'
10	I	2503	2MA	O4'-C4'-C5'-O5'
10	I	2504	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	I	746	PSU	O4'-C1'-C5-C6
22	U	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 201 are monoatomic - leaving 1 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
54	RD8	I	3112	53	34,35,35	1.20	3 (8%)	45,48,48	1.76	10 (22%)

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
54	RD8	I	3112	53	-	0/17/31/31	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	I	3112	RD8	C30-N21	3.70	1.40	1.36
54	I	3112	RD8	C24-C23	3.27	1.55	1.51
54	I	3112	RD8	O29-C23	-3.12	1.41	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	I	3112	RD8	C23-O29-C30	4.50	113.70	110.10
54	I	3112	RD8	C22-N21-C30	-4.07	108.16	111.17
54	I	3112	RD8	N17-N16-N15	3.98	116.19	111.24
54	I	3112	RD8	O29-C23-C22	-2.91	101.68	104.50
54	I	3112	RD8	O29-C30-N21	-2.91	107.47	109.92
54	I	3112	RD8	C23-C22-N21	2.89	104.57	101.85
54	I	3112	RD8	C14-N15-N16	-2.79	101.96	107.97
54	I	3112	RD8	O31-C30-N21	2.63	131.23	128.80
54	I	3112	RD8	C22-C23-C24	2.39	116.09	113.38
54	I	3112	RD8	C13-C12-N11	-2.03	109.50	113.29

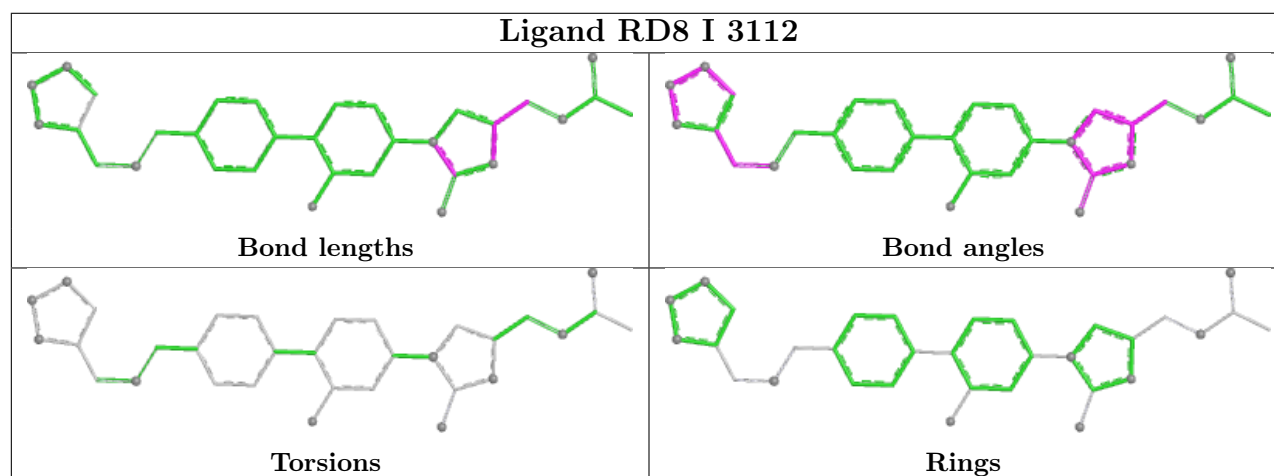
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24803. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section was not generated.