



Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 06:22 pm GMT

PDB ID : 9GHG
EMDB ID : EMD-51356
Title : Staphylococcus aureus FusB bound to the small subunit of the S. aureus 70S ribosome (FusB-Sa70S:SSU)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.22 Å (reported)
Based on initial models : 4ADN, ., 8P2F

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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
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

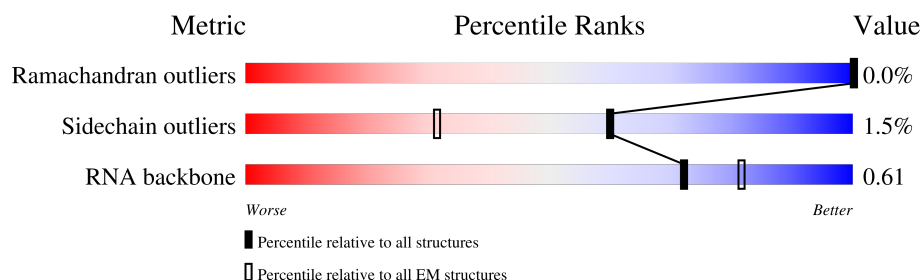
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.22 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.
















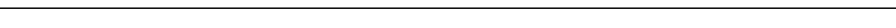

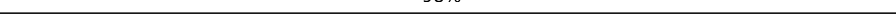
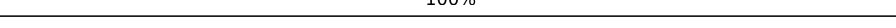
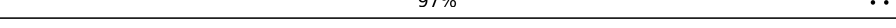
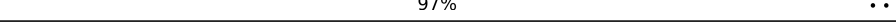
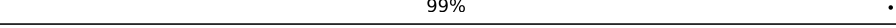
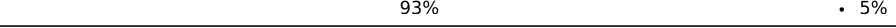
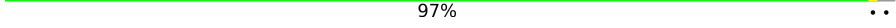
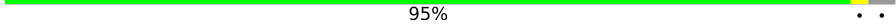


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	62	
2	2	69	
3	3	59	
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	

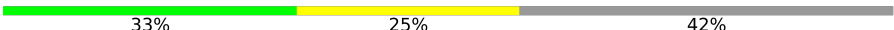


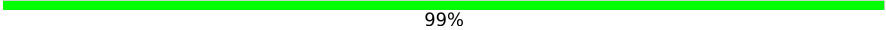



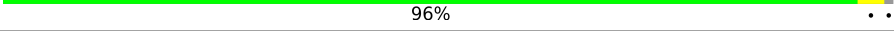
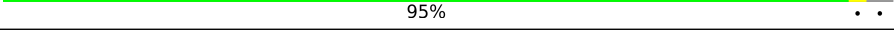
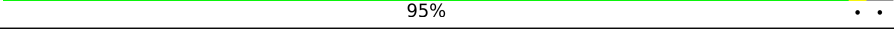

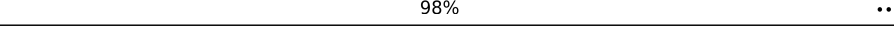
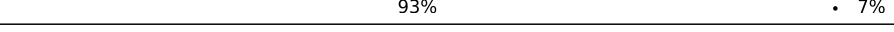
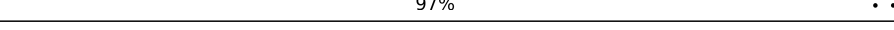
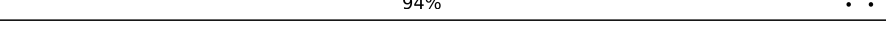
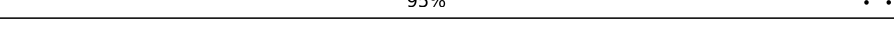





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Mol	Chain	Length	Quality of chain
10	A	2923	 85% 12% .
11	B	115	 84% 14% .
12	C	213	 92% . 5%
13	D	77	 75% 25%
13	F	77	 84% 14% .
14	G	277	 97% ..
15	H	220	 97% ..
16	I	207	 97% ..
17	J	179	 97% ..
18	K	178	 95% . .
19	M	145	 99% .
20	N	122	 98% .
21	O	146	 99% ..
22	P	144	 93% . 6%
23	Q	122	 98% ..
24	R	119	 100%
25	S	116	 97% ..
26	T	118	 97% ..
27	U	102	 99% .
28	V	117	 93% . 5%
29	W	91	 97% ..
30	X	105	 95% . .
31	Y	217	 43% 57%
32	Z	94	 87% 13%
33	a	1555	 86% 12% .

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Mol	Chain	Length	Quality of chain
34	b	24	 33% 25% 42%
35	c	255	 86% 13%
36	d	217	 92% 6%
37	e	200	 99%
38	f	166	 93% 6%
39	g	98	 91% 5%
40	h	156	 89% 6%
41	i	132	 96% ..
42	j	132	 95% ..
43	k	102	 95% ..
44	l	129	 87% .. 9%
45	m	137	 98% ..
46	n	121	 93% 7%
47	o	61	 97% ..
48	p	89	 94% ..
49	q	91	 95% ..
50	r	87	 89% 8%
51	s	80	 74% 5% 21%
52	t	92	 85% 13%
53	u	83	 95% ..
54	v	58	 84% 7% 9%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 150404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			481	298	104	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	80	Total	C	N	O	S	0	0
			654	417	111	123	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2848	Total	C	N	O	P	0	0
			61064	27267	11166	19783	2848		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	G	A	conflict	GB CP000253
A	1584	U	A	conflict	GB CP000253
A	2261	G	A	conflict	GB CP000253

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	203	Total	C	N	O	S	1	0
			1703	1102	278	315	8		

- Molecule 13 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
13	F	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	178	Total	C	N	O	S	0	0
			1412	897	244	264	7		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	174	Total	C	N	O	S	0	0
			1361	846	249	263	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	144	Total	C	N	O	S	0	0
			1146	715	210	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	114	Total	C	N	O		0	0
			922	580	185	157			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	82	Total	C	N	O	0	0
			626	386	122	118		

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1526	Total	C	N	O	P	0	0
			32707	14608	5975	10598	1526		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	14	Total	C	N	O	P	0	0
			306	137	62	93	14		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1612	1015	302	293	2		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	146	Total	C	N	O	S	0	0
			1165	727	222	212	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	128	Total	C	N	O	S	0	0
			1016	629	203	183	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	99	Total	C	N	O	S	0	0
			792	499	145	147	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			662	419	120	122	1		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	80	Total	C	N	O	S	0	0
			651	419	117	113	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	53	Total	C	N	O	0	0
			446	275	93	78		

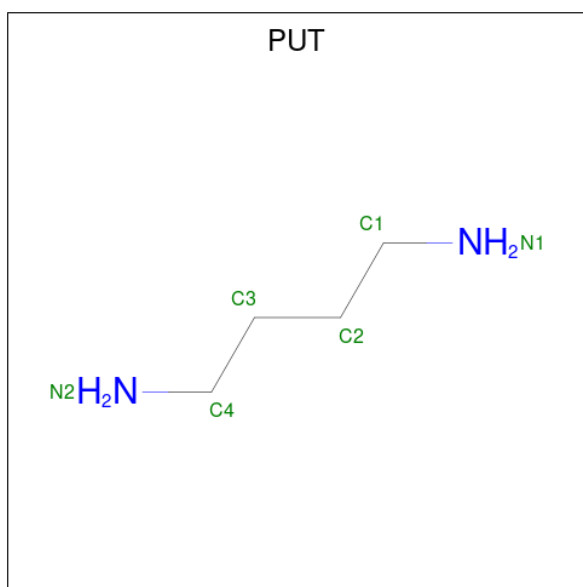
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	
55	C	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	117	Total	Mg	0
			117	117	
56	F	2	Total	Mg	0
			2	2	
56	G	1	Total	Mg	0
			1	1	
56	O	1	Total	Mg	0
			1	1	
56	a	24	Total	Mg	0
			24	24	

- Molecule 57 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
57	A	1	Total	C	N	0
			6	4	2	
57	A	1	Total	C	N	0
			6	4	2	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	1	8	Total	O	0
			8	8	
58	2	2	Total	O	0
			2	2	
58	3	4	Total	O	0
			4	4	
58	5	18	Total	O	0
			18	18	
58	6	1	Total	O	0
			1	1	
58	7	31	Total	O	0
			31	31	
58	8	32	Total	O	0
			32	32	
58	9	2	Total	O	0
			2	2	
58	A	4272	Total	O	0
			4272	4272	
58	B	24	Total	O	0
			24	24	

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Mol	Chain	Residues	Atoms		AltConf
58	D	5	Total 5	O 5	0
58	F	5	Total 5	O 5	0
58	G	109	Total 109	O 109	0
58	H	63	Total 63	O 63	0
58	I	68	Total 68	O 68	0
58	J	1	Total 1	O 1	0
58	M	29	Total 29	O 29	0
58	N	21	Total 21	O 21	0
58	O	62	Total 62	O 62	0
58	P	24	Total 24	O 24	0
58	Q	26	Total 26	O 26	0
58	S	10	Total 10	O 10	0
58	T	60	Total 60	O 60	0
58	U	34	Total 34	O 34	0
58	V	33	Total 33	O 33	0
58	W	13	Total 13	O 13	0
58	X	1	Total 1	O 1	0
58	Y	1	Total 1	O 1	0
58	Z	13	Total 13	O 13	0
58	a	522	Total 522	O 522	0
58	b	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
58	c	1	Total 1	O 1	0
58	d	2	Total 2	O 2	0
58	e	1	Total 1	O 1	0
58	f	2	Total 2	O 2	0
58	h	1	Total 1	O 1	0
58	i	2	Total 2	O 2	0
58	k	2	Total 2	O 2	0
58	l	1	Total 1	O 1	0
58	m	1	Total 1	O 1	0
58	o	1	Total 1	O 1	0
58	r	2	Total 2	O 2	0
58	s	1	Total 1	O 1	0
58	u	1	Total 1	O 1	0
58	v	1	Total 1	O 1	0

3 Residue-property plots [i](#)

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

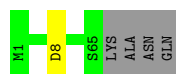
- Molecule 1: 50S ribosomal protein L28

Chain 1:  98% .



- Molecule 2: 50S ribosomal protein L29

Chain 2:  93% • 6%



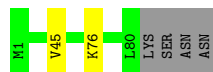
- Molecule 3: 50S ribosomal protein L30

Chain 3:  95% 5%



- Molecule 4: 50S ribosomal protein L31 type B

Chain 4:  93% • 5%



- Molecule 5: Large ribosomal subunit protein bL32

Chain 5:  91% • 7%



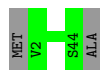
- Molecule 6: Large ribosomal subunit protein bL33A

Chain 6:  96% ..



- Molecule 7: 50S ribosomal protein L34

Chain 7: 96% .



- Molecule 8: 50S ribosomal protein L35

Chain 8: 92% 5% .



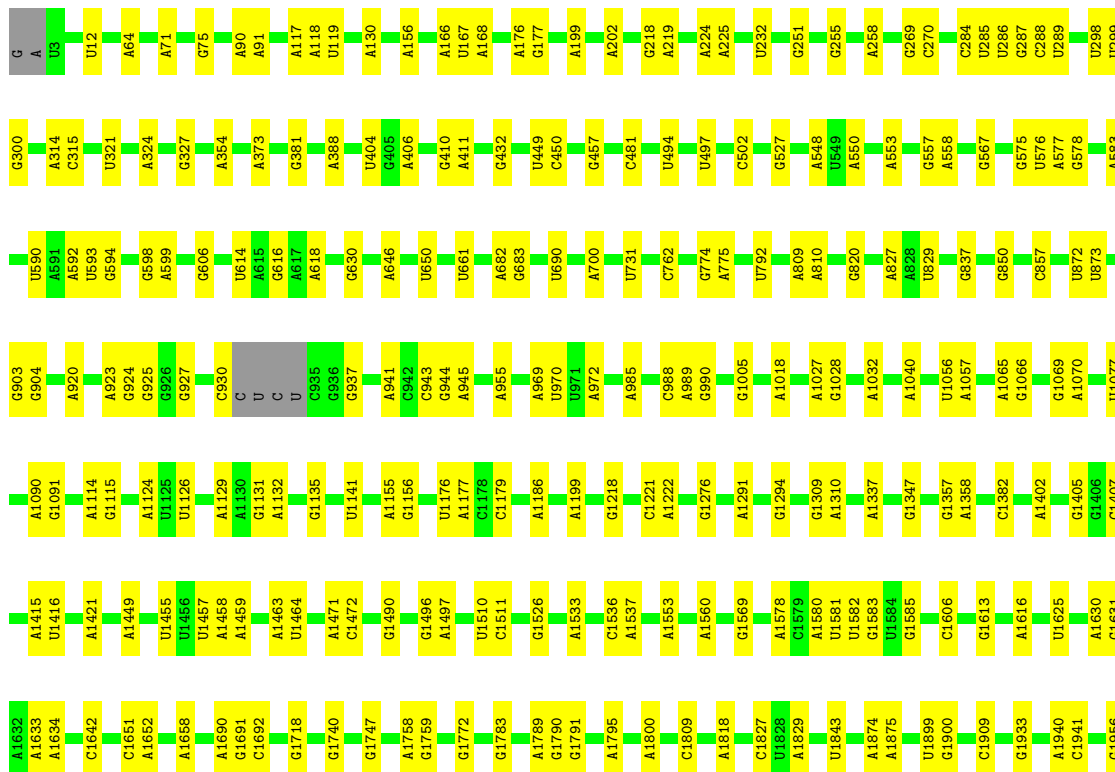
- Molecule 9: 50S ribosomal protein L36

Chain 9: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: 23S rRNA

Chain A: 85% 12% .





- Molecule 15: 50S ribosomal protein L3

Chain H: 97% ..



- Molecule 16: 50S ribosomal protein L4

Chain I: 97% ..



- Molecule 17: 50S ribosomal protein L5

Chain J: 97% ..



- Molecule 18: 50S ribosomal protein L6

Chain K: 95% ..



- Molecule 19: 50S ribosomal protein L13

Chain M: 99% .



- Molecule 20: 50S ribosomal protein L14

Chain N: 98% .



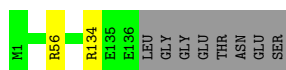
- Molecule 21: 50S ribosomal protein L15

Chain O: 99% ..



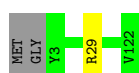
- Molecule 22: 50S ribosomal protein L16

Chain P: 93% • 6%



- Molecule 23: 50S ribosomal protein L17

Chain Q: 98% ..



- Molecule 24: 50S ribosomal protein L18

Chain R: 100%

There are no outlier residues recorded for this chain.

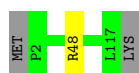
- Molecule 25: 50S ribosomal protein L19

Chain S: 97% ..



- Molecule 26: 50S ribosomal protein L20

Chain T: 97% ..



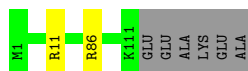
- Molecule 27: 50S ribosomal protein L21

Chain U: 99% .



- Molecule 28: 50S ribosomal protein L22

Chain V: 93% • 5%



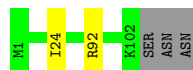
- Molecule 29: 50S ribosomal protein L23

Chain W:  97% ..



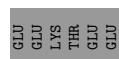
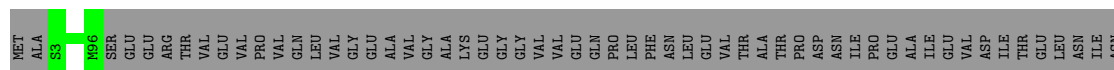
- Molecule 30: 50S ribosomal protein L24

Chain X:  95% . .




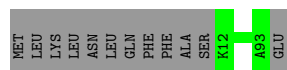
- Molecule 31: 50S ribosomal protein L25

Chain Y:  43% 57%




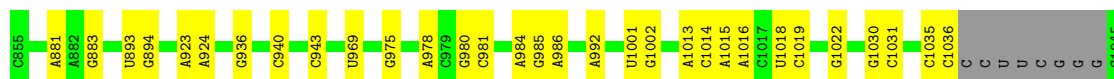
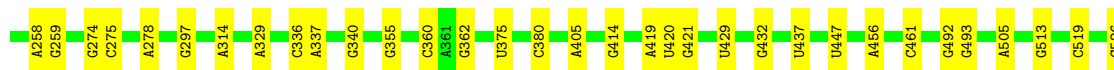
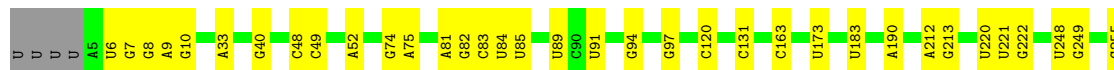
- Molecule 32: 50S ribosomal protein L27

Chain Z:  87% 13%




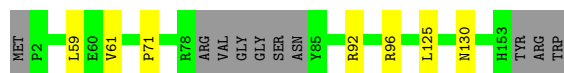
- Molecule 33: 23S rRNA

Chain a:  86% 12% .



WORLDWIDE
PDB
PROTEIN DATA BANK

Chain h:  89% • 6%



- Molecule 41: 30S ribosomal protein S8

Chain i:  96% • •



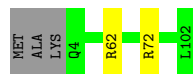
- Molecule 42: 30S ribosomal protein S9

Chain j:  95% • •




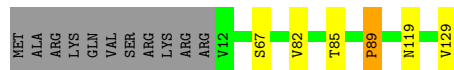
- Molecule 43: Small ribosomal subunit protein uS10

Chain k:  95% • •



- Molecule 44: 30S ribosomal protein S11

Chain l:  87% • • 9%



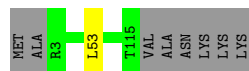
- Molecule 45: 30S ribosomal protein S12

Chain m:  98% • •



- Molecule 46: 30S ribosomal protein S13

Chain n:  93% • 7%



- Molecule 47: 30S ribosomal protein S14 type Z

Chain o:  97% ..



- Molecule 48: 30S ribosomal protein S15

Chain p:  94% ..




- Molecule 49: 30S ribosomal protein S16

Chain q:  95% ..



- Molecule 50: 30S ribosomal protein S17

Chain r:  89% . 8%




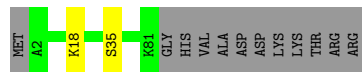
- Molecule 51: 30S ribosomal protein S18

Chain s:  74% 5% 21%



- Molecule 52: 30S ribosomal protein S19

Chain t:  85% . 13%

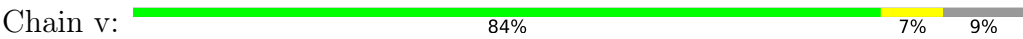


- Molecule 53: 30S ribosomal protein S20

Chain u:  95% ..



- Molecule 54: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67441	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.14	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (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, 3TD, H2U, UR3, MA6, 2MA, MG, PUT, 4OC, 2MG, OMG, G7M, 5MC, ZN

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	0.29	0/487	0.58	0/649
2	2	0.27	0/536	0.47	0/713
3	3	0.27	0/438	0.52	0/590
4	4	0.31	0/671	0.52	0/900
5	5	0.30	0/429	0.56	0/571
6	6	0.26	0/407	0.56	0/545
7	7	0.32	0/371	0.68	0/484
8	8	0.30	0/526	0.59	0/690
9	9	0.29	0/299	0.55	0/393
10	A	0.42	0/68213	0.88	3/106380 (0.0%)
11	B	0.43	0/2692	0.88	0/4193
12	C	0.28	0/1737	0.48	0/2331
13	D	0.46	0/1832	0.90	0/2855
13	F	0.47	0/1813	0.89	0/2825
14	G	0.29	0/2120	0.57	0/2847
15	H	0.29	0/1661	0.56	0/2227
16	I	0.28	0/1587	0.52	0/2143
17	J	0.28	0/1430	0.52	0/1918
18	K	0.29	0/1379	0.54	0/1855
19	M	0.29	0/1168	0.51	0/1573
20	N	0.28	0/927	0.58	0/1243
21	O	0.30	0/1104	0.53	0/1471
22	P	0.29	0/1113	0.56	0/1493
23	Q	0.27	0/956	0.53	0/1277
24	R	0.29	0/931	0.53	0/1244
25	S	0.28	0/934	0.55	0/1249
26	T	0.29	0/955	0.58	0/1265
27	U	0.29	0/803	0.56	0/1073
28	V	0.27	0/861	0.57	0/1159
29	W	0.28	0/733	0.57	0/978
30	X	0.29	0/796	0.53	0/1063
31	Y	0.29	0/746	0.51	0/1000

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.32	0/632	0.57	0/838
33	a	0.43	0/36440	0.88	0/56820
34	b	0.47	0/344	0.89	0/535
35	c	0.28	0/1808	0.52	0/2426
36	d	0.28	0/1634	0.54	0/2195
37	e	0.29	0/1647	0.53	0/2211
38	f	0.28	0/1174	0.56	0/1583
39	g	0.27	0/784	0.55	0/1052
40	h	0.28	0/1181	0.57	0/1587
41	i	0.28	0/1044	0.57	0/1401
42	j	0.29	0/1032	0.57	0/1386
43	k	0.29	0/804	0.56	0/1083
44	l	0.31	0/891	0.60	1/1203 (0.1%)
45	m	0.30	0/1075	0.61	0/1439
46	n	0.28	0/909	0.56	0/1218
47	o	0.30	0/511	0.57	0/678
48	p	0.28	0/730	0.60	0/975
49	q	0.29	0/723	0.62	0/971
50	r	0.29	0/670	0.61	0/895
51	s	0.29	0/525	0.67	0/704
52	t	0.31	0/668	0.56	0/896
53	u	0.27	0/606	0.53	0/810
54	v	0.31	0/449	0.60	0/589
All	All	0.39	0/156936	0.81	4/234692 (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
5	5	0	1
8	8	0	1
12	C	0	1
14	G	0	3
15	H	0	1
16	I	0	1
20	N	0	1
21	O	0	1
22	P	0	2
26	T	0	1
29	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	X	0	1
38	f	0	1
39	g	0	1
40	h	0	1
42	j	0	1
43	k	0	2
48	p	0	1
49	q	0	1
50	r	0	2
54	v	0	1
All	All	0	26

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	l	89	PRO	N-CA-CB	-6.32	95.65	102.60
10	A	2474	G	C3'-C2'-C1'	-5.86	96.81	101.50
10	A	557	G	O4'-C1'-N9	5.53	112.63	108.20
10	A	1065	A	O3'-P-O5'	-5.21	94.11	104.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	5	6	ARG	Sidechain
8	8	16	ARG	Sidechain
12	C	190	ARG	Sidechain
14	G	13	ARG	Sidechain
14	G	189	ARG	Sidechain
14	G	261	ARG	Sidechain
15	H	159	ASP	Peptide
16	I	168	ARG	Sidechain
20	N	104	ARG	Sidechain
21	O	59	ARG	Sidechain
22	P	134	ARG	Sidechain
22	P	56	ARG	Sidechain
26	T	48	ARG	Sidechain
29	W	9	ARG	Sidechain
30	X	92	ARG	Sidechain
38	f	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
39	g	88	ARG	Sidechain
40	h	92	ARG	Sidechain
42	j	14	ARG	Sidechain
43	k	62	ARG	Sidechain
43	k	72	ARG	Sidechain
48	p	77	ARG	Sidechain
49	q	14	ARG	Sidechain
50	r	67	ARG	Sidechain
50	r	7	ARG	Sidechain
54	v	35	ARG	Sidechain

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	59/62 (95%)	59 (100%)	0	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
4	4	78/84 (93%)	78 (100%)	0	0	100	100
5	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
6	6	46/49 (94%)	46 (100%)	0	0	100	100
7	7	41/45 (91%)	41 (100%)	0	0	100	100
8	8	62/66 (94%)	62 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	200/213 (94%)	199 (100%)	1 (0%)	0	100	100
14	G	271/277 (98%)	266 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	214/220 (97%)	205 (96%)	9 (4%)	0	100	100
16	I	202/207 (98%)	202 (100%)	0	0	100	100
17	J	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
18	K	172/178 (97%)	171 (99%)	1 (1%)	0	100	100
19	M	142/145 (98%)	140 (99%)	2 (1%)	0	100	100
20	N	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
21	O	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
22	P	134/144 (93%)	134 (100%)	0	0	100	100
23	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	R	117/119 (98%)	117 (100%)	0	0	100	100
25	S	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
26	T	114/118 (97%)	114 (100%)	0	0	100	100
27	U	99/102 (97%)	99 (100%)	0	0	100	100
28	V	109/117 (93%)	109 (100%)	0	0	100	100
29	W	87/91 (96%)	87 (100%)	0	0	100	100
30	X	100/105 (95%)	100 (100%)	0	0	100	100
31	Y	92/217 (42%)	92 (100%)	0	0	100	100
32	Z	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
35	c	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
36	d	202/217 (93%)	197 (98%)	5 (2%)	0	100	100
37	e	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
38	f	154/166 (93%)	152 (99%)	2 (1%)	0	100	100
39	g	91/98 (93%)	91 (100%)	0	0	100	100
40	h	142/156 (91%)	141 (99%)	0	1 (1%)	19	19
41	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
42	j	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
43	k	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
44	l	116/129 (90%)	113 (97%)	3 (3%)	0	100	100
45	m	133/137 (97%)	130 (98%)	3 (2%)	0	100	100
46	n	111/121 (92%)	109 (98%)	2 (2%)	0	100	100
47	o	58/61 (95%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	p	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
49	q	88/91 (97%)	87 (99%)	1 (1%)	0	100	100
50	r	78/87 (90%)	78 (100%)	0	0	100	100
51	s	61/80 (76%)	61 (100%)	0	0	100	100
52	t	78/92 (85%)	77 (99%)	1 (1%)	0	100	100
53	u	78/83 (94%)	78 (100%)	0	0	100	100
54	v	51/58 (88%)	51 (100%)	0	0	100	100
All	All	5584/6046 (92%)	5510 (99%)	73 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	h	71	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	51/52 (98%)	51 (100%)	0	100	100
2	2	59/62 (95%)	58 (98%)	1 (2%)	56	69
3	3	51/53 (96%)	51 (100%)	0	100	100
4	4	71/75 (95%)	69 (97%)	2 (3%)	38	49
5	5	48/50 (96%)	48 (100%)	0	100	100
6	6	46/47 (98%)	45 (98%)	1 (2%)	47	59
7	7	39/40 (98%)	39 (100%)	0	100	100
8	8	55/57 (96%)	53 (96%)	2 (4%)	30	38
9	9	35/35 (100%)	35 (100%)	0	100	100
12	C	196/204 (96%)	191 (97%)	5 (3%)	41	52
14	G	220/224 (98%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	H	174/177 (98%)	173 (99%)	1 (1%)	84	91
16	I	168/169 (99%)	166 (99%)	2 (1%)	67	79
17	J	157/158 (99%)	152 (97%)	5 (3%)	34	43
18	K	152/155 (98%)	147 (97%)	5 (3%)	33	42
19	M	123/123 (100%)	123 (100%)	0	100	100
20	N	100/100 (100%)	99 (99%)	1 (1%)	73	83
21	O	111/112 (99%)	111 (100%)	0	100	100
22	P	113/119 (95%)	113 (100%)	0	100	100
23	Q	101/102 (99%)	100 (99%)	1 (1%)	73	83
24	R	95/95 (100%)	95 (100%)	0	100	100
25	S	100/102 (98%)	99 (99%)	1 (1%)	73	83
26	T	96/98 (98%)	96 (100%)	0	100	100
27	U	86/86 (100%)	86 (100%)	0	100	100
28	V	90/94 (96%)	88 (98%)	2 (2%)	47	59
29	W	80/82 (98%)	80 (100%)	0	100	100
30	X	87/90 (97%)	86 (99%)	1 (1%)	70	81
31	Y	83/190 (44%)	83 (100%)	0	100	100
32	Z	64/75 (85%)	64 (100%)	0	100	100
35	c	192/221 (87%)	191 (100%)	1 (0%)	86	93
36	d	166/175 (95%)	162 (98%)	4 (2%)	44	56
37	e	174/175 (99%)	173 (99%)	1 (1%)	84	91
38	f	122/131 (93%)	122 (100%)	0	100	100
39	g	81/86 (94%)	77 (95%)	4 (5%)	21	25
40	h	124/132 (94%)	119 (96%)	5 (4%)	27	34
41	i	112/113 (99%)	108 (96%)	4 (4%)	30	38
42	j	106/109 (97%)	104 (98%)	2 (2%)	52	65
43	k	89/91 (98%)	89 (100%)	0	100	100
44	l	94/104 (90%)	88 (94%)	6 (6%)	14	16
45	m	117/119 (98%)	116 (99%)	1 (1%)	75	85
46	n	98/104 (94%)	97 (99%)	1 (1%)	73	83
47	o	52/53 (98%)	51 (98%)	1 (2%)	52	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	p	79/81 (98%)	78 (99%)	1 (1%)	65	77
49	q	76/77 (99%)	73 (96%)	3 (4%)	27	35
50	r	75/82 (92%)	74 (99%)	1 (1%)	65	77
51	s	56/68 (82%)	52 (93%)	4 (7%)	12	12
52	t	70/80 (88%)	68 (97%)	2 (3%)	37	48
53	u	67/69 (97%)	66 (98%)	1 (2%)	60	73
54	v	49/54 (91%)	46 (94%)	3 (6%)	15	17
All	All	4850/5150 (94%)	4775 (98%)	75 (2%)	60	73

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	8	ASP
4	4	45	VAL
4	4	76	LYS
6	6	28	GLU
8	8	31	HIS
8	8	55	MET
12	C	54	ASP
12	C	99	LYS
12	C	104	ILE
12	C	144	LEU
12	C	157	CYS
15	H	127	PHE
16	I	49	HIS
16	I	58	SER
17	J	42	ASP
17	J	80	ARG
17	J	101	ASP
17	J	132	VAL
17	J	135	GLN
18	K	16	THR
18	K	43	PHE
18	K	73	ASN
18	K	80	SER
18	K	107	VAL
20	N	47	THR
23	Q	29	ARG
25	S	2	THR
28	V	11	ARG

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Mol	Chain	Res	Type
28	V	86	ARG
30	X	24	ILE
35	c	23	TRP
36	d	75	VAL
36	d	86	LEU
36	d	90	LEU
36	d	102	VAL
37	e	64	THR
39	g	43	TRP
39	g	65	VAL
39	g	84	ASP
39	g	88	ARG
40	h	59	LEU
40	h	61	VAL
40	h	96	ARG
40	h	125	LEU
40	h	130	ASN
41	i	25	LEU
41	i	27	LEU
41	i	77	LEU
41	i	101	LEU
42	j	50	LEU
42	j	125	ARG
44	l	67	SER
44	l	82	VAL
44	l	85	THR
44	l	89	PRO
44	l	119	ASN
44	l	129	VAL
45	m	58	PRO
46	n	53	LEU
47	o	57	ARG
48	p	12	ILE
49	q	27	SER
49	q	54	GLU
49	q	87	GLN
50	r	44	LYS
51	s	14	LYS
51	s	23	ILE
51	s	32	GLU
51	s	40	GLU
52	t	18	LYS

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Mol	Chain	Res	Type
52	t	35	SER
53	u	28	MET
54	v	17	ARG
54	v	28	THR
54	v	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	27	ASN
12	C	11	ASN
12	C	77	ASN
12	C	198	GLN
12	C	207	ASN
14	G	86	ASN
16	I	119	GLN
16	I	179	GLN
19	M	48	HIS
19	M	137	GLN
22	P	13	HIS
22	P	35	GLN
23	Q	61	ASN
30	X	39	ASN
36	d	91	ASN
36	d	101	ASN
38	f	146	ASN
40	h	67	ASN
42	j	70	HIS
44	l	18	ASN
46	n	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2843/2923 (97%)	339 (11%)	47 (1%)
11	B	112/115 (97%)	12 (10%)	5 (4%)
13	D	76/77 (98%)	19 (25%)	2 (2%)
13	F	75/77 (97%)	10 (13%)	2 (2%)
33	a	1520/1555 (97%)	190 (12%)	0
34	b	13/24 (54%)	6 (46%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4639/4771 (97%)	576 (12%)	56 (1%)

All (576) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	12	U
10	A	64	A
10	A	71	A
10	A	75	G
10	A	90	A
10	A	91	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	130	A
10	A	156	A
10	A	166	A
10	A	167	U
10	A	168	A
10	A	177	G
10	A	199	A
10	A	202	A
10	A	218	G
10	A	219	A
10	A	224	A
10	A	225	A
10	A	251	G
10	A	255	G
10	A	269	G
10	A	270	C
10	A	284	C
10	A	285	U
10	A	286	U
10	A	287	G
10	A	288	C
10	A	289	U
10	A	299	U
10	A	300	G
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A

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Mol	Chain	Res	Type
10	A	327	G
10	A	354	A
10	A	373	A
10	A	381	G
10	A	404	U
10	A	406	A
10	A	410	G
10	A	411	A
10	A	432	G
10	A	449	U
10	A	450	C
10	A	457	G
10	A	481	C
10	A	494	U
10	A	497	U
10	A	502	C
10	A	527	G
10	A	550	A
10	A	553	A
10	A	558	A
10	A	567	G
10	A	575	G
10	A	576	U
10	A	577	A
10	A	578	G
10	A	583	A
10	A	590	U
10	A	592	A
10	A	593	U
10	A	594	G
10	A	598	G
10	A	599	A
10	A	606	G
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	682	A
10	A	683	G
10	A	690	U
10	A	700	A

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Mol	Chain	Res	Type
10	A	731	U
10	A	762	C
10	A	774	G
10	A	775	A
10	A	792	5MU
10	A	809	A
10	A	810	A
10	A	820	G
10	A	827	A
10	A	829	U
10	A	837	G
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	904	G
10	A	920	A
10	A	923	A
10	A	924	G
10	A	925	G
10	A	927	G
10	A	930	C
10	A	937	G
10	A	941	A
10	A	943	C
10	A	944	G
10	A	945	A
10	A	955	A
10	A	970	U
10	A	972	A
10	A	985	A
10	A	989	A
10	A	990	G
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1032	A
10	A	1040	A
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A

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Mol	Chain	Res	Type
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1114	A
10	A	1115	G
10	A	1124	A
10	A	1126	U
10	A	1129	A
10	A	1131	G
10	A	1132	A
10	A	1141	U
10	A	1155	A
10	A	1156	G
10	A	1176	U
10	A	1177	A
10	A	1179	C
10	A	1186	A
10	A	1199	A
10	A	1218	G
10	A	1222	A
10	A	1276	G
10	A	1291	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1337	A
10	A	1358	A
10	A	1382	C
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1421	A
10	A	1449	A
10	A	1455	U
10	A	1457	U
10	A	1458	A
10	A	1459	A
10	A	1463	A
10	A	1464	U
10	A	1471	A
10	A	1472	C

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Mol	Chain	Res	Type
10	A	1490	G
10	A	1496	G
10	A	1497	A
10	A	1510	U
10	A	1511	C
10	A	1526	G
10	A	1533	A
10	A	1536	C
10	A	1537	A
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1578	A
10	A	1580	A
10	A	1581	U
10	A	1582	U
10	A	1583	G
10	A	1585	G
10	A	1606	C
10	A	1613	G
10	A	1616	A
10	A	1625	U
10	A	1630	A
10	A	1631	G
10	A	1633	A
10	A	1634	A
10	A	1642	C
10	A	1651	C
10	A	1652	A
10	A	1658	A
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1718	G
10	A	1740	G
10	A	1747	G
10	A	1758	A
10	A	1759	G
10	A	1772	G
10	A	1783	G
10	A	1789	A
10	A	1790	G

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Mol	Chain	Res	Type
10	A	1791	G
10	A	1795	A
10	A	1800	A
10	A	1809	C
10	A	1818	A
10	A	1827	C
10	A	1829	A
10	A	1843	U
10	A	1874	A
10	A	1875	A
10	A	1899	U
10	A	1900	G
10	A	1909	C
10	A	1933	G
10	A	1940	A
10	A	1941	C
10	A	1956	G
10	A	1957	G
10	A	1958	U
10	A	1963	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G
10	A	2018	U
10	A	2020	U
10	A	2040	A
10	A	2045	A
10	A	2047	A
10	A	2050	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2070	C
10	A	2076	A
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A

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Mol	Chain	Res	Type
10	A	2096	G
10	A	2120	G
10	A	2136	U
10	A	2137	G
10	A	2205	C
10	A	2208	A
10	A	2209	G
10	A	2215	U
10	A	2217	G
10	A	2225	A
10	A	2230	G
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2266	G
10	A	2295	A
10	A	2305	A
10	A	2306	G
10	A	2310	C
10	A	2314	A
10	A	2316	G
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2339	U
10	A	2347	A
10	A	2348	G
10	A	2349	A
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2410	G
10	A	2412	C
10	A	2429	U
10	A	2430	C
10	A	2433	C
10	A	2452	A
10	A	2456	G
10	A	2457	A
10	A	2462	A

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Mol	Chain	Res	Type
10	A	2468	C
10	A	2474	G
10	A	2475	A
10	A	2476	H2U
10	A	2496	A
10	A	2502	C
10	A	2505	A
10	A	2529	G
10	A	2531	U
10	A	2532	G
10	A	2545	A
10	A	2556	G
10	A	2557	U
10	A	2561	C
10	A	2581	U
10	A	2593	A
10	A	2594	G
10	A	2600	C
10	A	2605	G
10	A	2629	A
10	A	2637	C
10	A	2640	U
10	A	2657	G
10	A	2666	A
10	A	2690	G
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2769	G
10	A	2771	G
10	A	2775	A
10	A	2784	A
10	A	2791	A
10	A	2792	A
10	A	2793	G
10	A	2805	A
10	A	2807	G
10	A	2824	G
10	A	2825	U

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Mol	Chain	Res	Type
10	A	2827	A
10	A	2828	U
10	A	2852	U
10	A	2887	G
10	A	2888	A
10	A	2892	G
10	A	2903	A
10	A	2913	G
11	B	10	U
11	B	11	A
11	B	23	U
11	B	33	U
11	B	43	A
11	B	51	A
11	B	54	U
11	B	55	A
11	B	64	A
11	B	87	C
11	B	88	G
11	B	106	G
13	D	2	G
13	D	7	G
13	D	9	G
13	D	16	C
13	D	17	C
13	D	17(A)	U
13	D	18	G
13	D	19	G
13	D	21	A
13	D	22	G
13	D	27	U
13	D	28	C
13	D	30	G
13	D	34	C
13	D	48	C
13	D	59	A
13	D	63	G
13	D	74	C
13	D	76	A
13	F	9	G
13	F	17(A)	U
13	F	18	G

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Mol	Chain	Res	Type
13	F	19	G
13	F	21	A
13	F	47	U
13	F	48	C
13	F	52	G
13	F	58	A
13	F	76	A
33	a	6	U
33	a	7	G
33	a	8	G
33	a	9	A
33	a	10	G
33	a	33	A
33	a	40	G
33	a	48	C
33	a	49	C
33	a	52	A
33	a	74	G
33	a	75	A
33	a	81	A
33	a	82	G
33	a	83	C
33	a	84	U
33	a	85	U
33	a	89	U
33	a	91	U
33	a	94	G
33	a	97	G
33	a	120	C
33	a	131	C
33	a	163	C
33	a	173	U
33	a	183	U
33	a	190	A
33	a	212	A
33	a	213	G
33	a	220	U
33	a	221	U
33	a	222	G
33	a	248	U
33	a	249	G
33	a	255	G

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Mol	Chain	Res	Type
33	a	258	A
33	a	259	G
33	a	274	G
33	a	275	C
33	a	278	A
33	a	297	G
33	a	314	A
33	a	329	A
33	a	336	C
33	a	337	A
33	a	340	G
33	a	355	G
33	a	360	C
33	a	362	G
33	a	375	U
33	a	380	C
33	a	405	A
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G
33	a	429	U
33	a	432	G
33	a	437	U
33	a	447	U
33	a	456	A
33	a	461	C
33	a	492	G
33	a	493	G
33	a	505	A
33	a	513	G
33	a	519	C
33	a	526	C
33	a	529	G
33	a	534	C
33	a	535	G7M
33	a	540	A
33	a	541	A
33	a	544	C
33	a	555	A
33	a	567	A
33	a	580	A

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Mol	Chain	Res	Type
33	a	581	A
33	a	584	C
33	a	626	C
33	a	649	A
33	a	650	A
33	a	661	U
33	a	673	A
33	a	695	A
33	a	696	G
33	a	710	A
33	a	711	G
33	a	731	U
33	a	732	G
33	a	757	A
33	a	763	G
33	a	785	A
33	a	801	U
33	a	802	A
33	a	823	A
33	a	825	C
33	a	836	A
33	a	881	A
33	a	883	G
33	a	893	U
33	a	894	G
33	a	923	A
33	a	924	A
33	a	936	G
33	a	940	C
33	a	943	C
33	a	969	U
33	a	978	A
33	a	980	G
33	a	981	C
33	a	984	A
33	a	985	G
33	a	986	A
33	a	992	A
33	a	1001	U
33	a	1002	G
33	a	1013	A
33	a	1014	C

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Mol	Chain	Res	Type
33	a	1015	A
33	a	1016	A
33	a	1018	U
33	a	1019	C
33	a	1022	G
33	a	1030	G
33	a	1031	C
33	a	1035	C
33	a	1036	C
33	a	1046	G
33	a	1047	A
33	a	1048	C
33	a	1056	C
33	a	1066	A
33	a	1076	U
33	a	1081	U
33	a	1096	U
33	a	1105	G
33	a	1106	U
33	a	1111	C
33	a	1112	A
33	a	1135	G
33	a	1141	A
33	a	1149	G
33	a	1151	U
33	a	1152	G
33	a	1155	C
33	a	1156	A
33	a	1169	U
33	a	1170	G
33	a	1174	G
33	a	1175	U
33	a	1177	A
33	a	1178	C
33	a	1194	G
33	a	1206	A
33	a	1207	A
33	a	1221	U
33	a	1222	U
33	a	1223	A
33	a	1235	A
33	a	1236	C

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Mol	Chain	Res	Type
33	a	1237	A
33	a	1267	A
33	a	1270	G
33	a	1289	A
33	a	1290	A
33	a	1296	U
33	a	1297	A
33	a	1310	G
33	a	1312	U
33	a	1330	C
33	a	1348	G
33	a	1356	A
33	a	1363	G
33	a	1374	U
33	a	1388	C
33	a	1408	A
33	a	1429	G
33	a	1452	G
33	a	1456	A
33	a	1464	A
33	a	1503	A
33	a	1513	A
33	a	1514	A
33	a	1516	G
33	a	1517	U
33	a	1528	G
33	a	1540	G
33	a	1541	G
33	a	1544	C
34	b	10	G
34	b	12	A
34	b	19	G
34	b	20	C
34	b	21	A
34	b	22	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	90	A
10	A	130	A
10	A	176	A

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Mol	Chain	Res	Type
10	A	202	A
10	A	232	U
10	A	258	A
10	A	298	U
10	A	299	U
10	A	388	A
10	A	449	U
10	A	548	A
10	A	598	G
10	A	614	U
10	A	661	U
10	A	809	A
10	A	903	G
10	A	923	A
10	A	969	A
10	A	988	C
10	A	1028	G
10	A	1069	G
10	A	1135	G
10	A	1176	U
10	A	1177	A
10	A	1186	A
10	A	1221	C
10	A	1291	A
10	A	1347	G
10	A	1357	G
10	A	1407	C
10	A	1496	G
10	A	1510	U
10	A	1633	A
10	A	1691	G
10	A	1789	A
10	A	1874	A
10	A	1940	A
10	A	2062	G
10	A	2313	A
10	A	2347	A
10	A	2457	A
10	A	2501	U
10	A	2508	G
10	A	2783	U
10	A	2791	A

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Mol	Chain	Res	Type
10	A	2805	A
10	A	2887	G
11	B	19	G
11	B	32	U
11	B	63	U
11	B	64	A
11	B	105	C
13	D	7	G
13	D	27	U
13	F	7	G
13	F	17(A)	U

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

14 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	3TD	A	1942	10	18,22,23	0.19	0	22,32,35	0.35	0
33	MA6	a	1530	33	18,26,27	0.73	0	19,38,41	0.66	0
10	H2U	A	2476	10	18,21,22	0.19	0	21,30,33	0.49	0
10	5MU	A	792	10	19,22,23	0.15	0	28,32,35	0.33	0
33	4OC	a	1412	56,33	20,23,24	0.23	0	26,32,35	0.42	0
10	2MG	A	2472	10	18,26,27	0.85	0	16,38,41	0.56	0
10	2MA	A	2530	56,10	19,25,26	0.97	1 (5%)	21,37,40	2.96	5 (23%)
10	OMG	A	2278	13,10	18,26,27	0.89	2 (11%)	19,38,41	0.54	0
33	5MC	a	976	33	18,22,23	0.14	0	26,32,35	0.35	0
33	UR3	a	1509	33	19,22,23	0.15	0	26,32,35	0.21	0
33	G7M	a	535	33	20,26,27	0.49	0	17,39,42	0.29	0
33	2MG	a	975	33	18,26,27	0.87	1 (5%)	16,38,41	0.59	0
10	5MU	A	1966	10	19,22,23	0.17	0	28,32,35	0.33	0
33	MA6	a	1529	33	18,26,27	0.73	0	19,38,41	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3TD	A	1942	10	-	0/7/25/26	0/2/2/2
33	MA6	a	1530	33	-	2/7/29/30	0/3/3/3
10	H2U	A	2476	10	-	1/7/38/39	0/2/2/2
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
33	4OC	a	1412	56,33	-	0/9/29/30	0/2/2/2
10	2MG	A	2472	10	-	0/5/27/28	0/3/3/3
10	2MA	A	2530	56,10	-	1/3/25/26	0/3/3/3
10	OMG	A	2278	13,10	-	1/5/27/28	0/3/3/3
33	5MC	a	976	33	-	0/7/25/26	0/2/2/2
33	UR3	a	1509	33	-	0/7/25/26	0/2/2/2
33	G7M	a	535	33	-	3/3/25/26	0/3/3/3
33	2MG	a	975	33	-	0/5/27/28	0/3/3/3
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
33	MA6	a	1529	33	-	0/7/29/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2530	2MA	C6-N1	2.26	1.37	1.33
33	a	975	2MG	C5-C6	-2.21	1.42	1.47
10	A	2278	OMG	C5-C6	-2.16	1.43	1.47
10	A	2278	OMG	C8-N7	-2.06	1.31	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2530	2MA	C5-C6-N1	-12.07	113.09	121.01
10	A	2530	2MA	C2-N1-C6	3.64	123.75	118.08
10	A	2530	2MA	C2-N3-C4	-3.50	112.68	115.52
10	A	2530	2MA	N6-C6-N1	2.24	123.17	117.07
10	A	2530	2MA	C5-C6-N6	2.23	123.74	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2278	OMG	C1'-C2'-O2'-CM2
33	a	535	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	a	1530	MA6	O4'-C4'-C5'-O5'
33	a	1530	MA6	C3'-C4'-C5'-O5'
33	a	535	G7M	O4'-C4'-C5'-O5'
33	a	535	G7M	C4'-C5'-O5'-P
10	A	2476	H2U	C4'-C5'-O5'-P
10	A	2530	2MA	O4'-C4'-C5'-O5'

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 151 ligands modelled in this entry, 149 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	$\# Z > 2$
57	PUT	A	3101	-	5,5,5	0.10	0	4,4,4	0.21	0
57	PUT	A	3102	-	5,5,5	0.15	0	4,4,4	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PUT	A	3101	-	-	0/3/3/3	-
57	PUT	A	3102	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	3102	PUT	C2-C3-C4-N2

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.