



## Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 06:35 pm GMT

PDB ID : 9GHA  
EMDB ID : EMD-51350  
Title : Fusidic acid-locked Escherichia coli 70S ribosome with Staphylococcus aureus EF-G and a tRNA in pe/E chimeric state (CHI)  
Authors : Gonzalez-Lopez, A.; Selmer, M.  
Deposited on : 2024-08-15  
Resolution : 2.24 Å (reported)  
Based on initial models : 9GHE, 7N2C, 8P2H

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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  
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

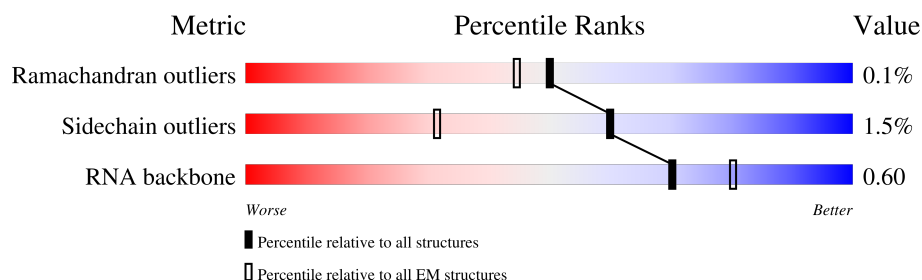
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.24 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.




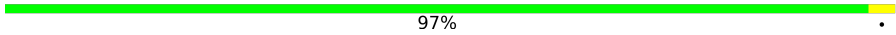



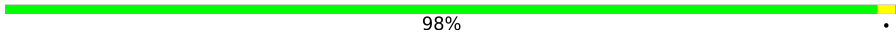



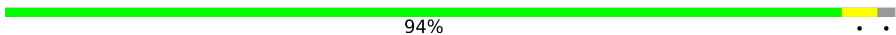
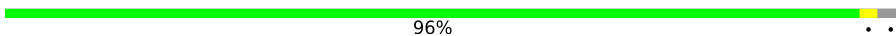
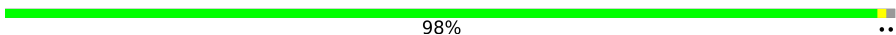
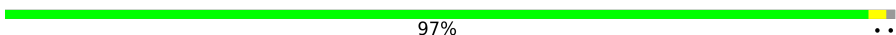
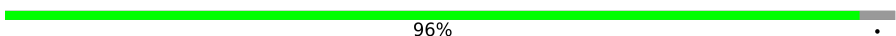



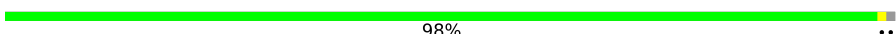

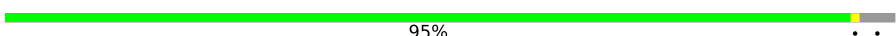

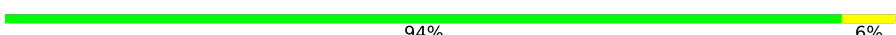
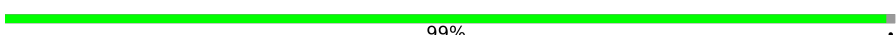
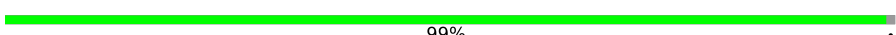
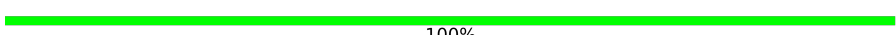
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	0	55	87% 9%
2	1	46	98% .
3	2	65	95% ..
4	3	38	97% .
5	4	70	69% 31%
6	8	77	81% 19%
7	9	24	21% 79%
8	A	1554	82% 16% .
9	B	241	88% . 8%

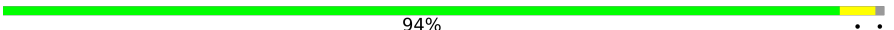
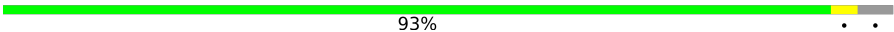

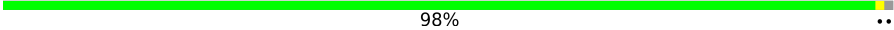
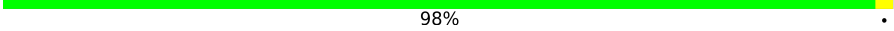
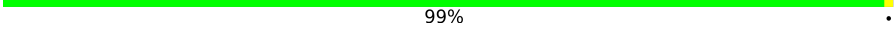
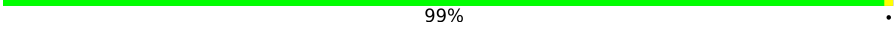
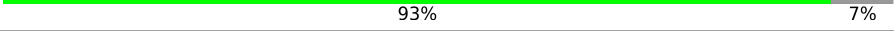
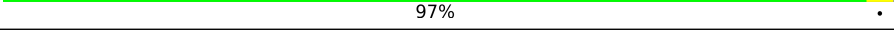
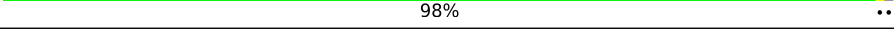
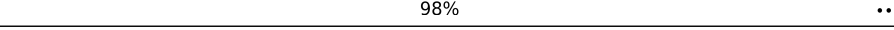
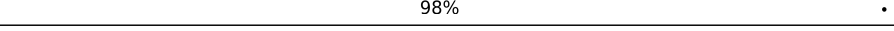
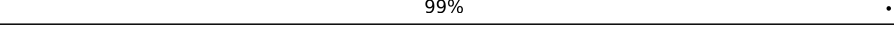
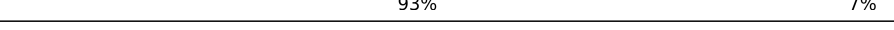

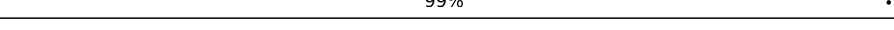

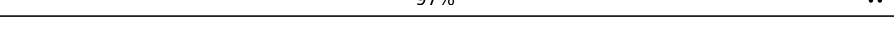
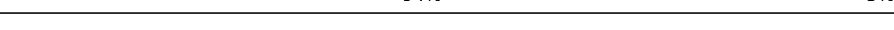


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Mol	Chain	Length	Quality of chain
10	C	233	
11	D	206	
12	E	167	
13	F	135	
14	G	179	
15	H	130	
16	I	130	
17	J	103	
18	K	129	
19	L	124	
20	M	118	
21	N	101	
22	O	89	
23	P	82	
24	Q	84	
25	R	75	
26	S	92	
27	T	87	
28	U	71	
29	W	693	
30	a	2930	
31	b	119	
32	c	273	
33	d	209	
34	e	201	

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Mol	Chain	Length	Quality of chain
35	f	179	 94% . .
36	g	177	 93% . .
37	h	149	 28% 72%
38	i	142	 98% ..
39	j	123	 98% .
40	k	144	 99% .
41	l	136	 99% .
42	m	127	 93% 7%
43	n	117	 97% . .
44	o	115	 98% ..
45	p	118	 98% ..
46	q	103	 98% .
47	r	110	 99% .
48	s	100	 93% 7%
49	t	104	 88% . 11%
50	u	94	 99% .
51	v	85	 88% 12%
52	w	78	 97% ..
53	x	63	 94% . 5%
54	y	59	 98% .
55	z	57	 95% 5%

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 145564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 6 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	5	Total	C	N	O	P	0	0
			110	49	22	34	5		

- Molecule 8 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1526	Total	C	N	O	P	0	0
			32757	14617	6009	10605	1526		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 10 is a protein called 30S ribosomal protein S3.

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

- Molecule 11 is a protein called 30S ribosomal protein S4.

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

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 15 is a protein called 30S ribosomal protein S8.

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

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 21 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 22 is a protein called 30S ribosomal protein S15.

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

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	666	Total	C	N	O	S	0	0
			5154	3232	865	1028	29		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	170	Total	C	N	O	S	0	0
			1273	803	232	236	2		

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	93	Total	C	N	O	S	0	0
			717	452	135	130			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	14	Total	K	0
			14	14	
57	F	1	Total	K	0
			1	1	
57	a	74	Total	K	0
			74	74	
57	c	3	Total	K	0
			3	3	
57	e	1	Total	K	0
			1	1	
57	t	1	Total	K	0
			1	1	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

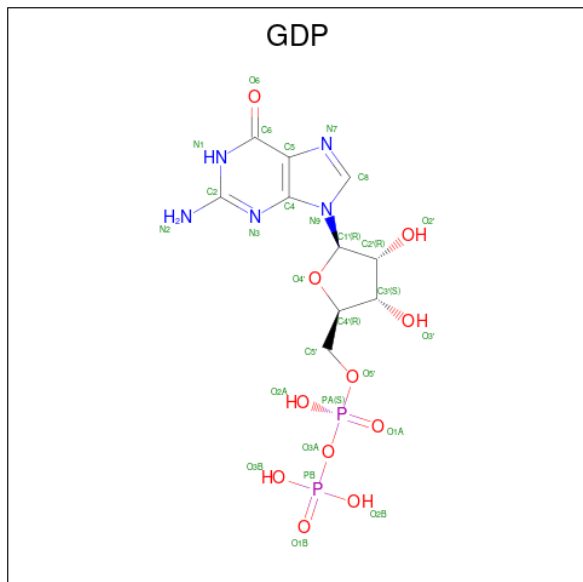
Mol	Chain	Residues	Atoms		AltConf
58	A	27	Total	Mg	0
			27	27	
58	W	1	Total	Mg	0
			1	1	
58	a	233	Total	Mg	0
			233	233	

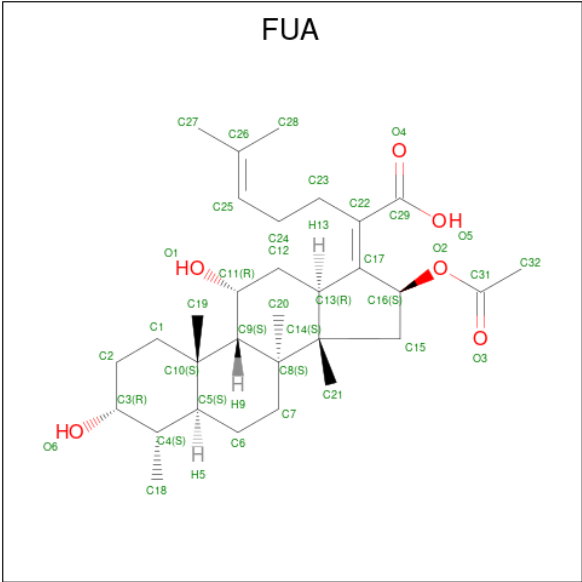
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Mol	Chain	Residues	Atoms		AltConf
58	b	3	Total	Mg	0
			3	3	
58	c	3	Total	Mg	0
			3	3	
58	d	2	Total	Mg	0
			2	2	
58	k	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





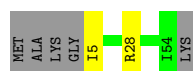
Mol	Chain	Residues	Atoms			AltConf
60	W	1	Total	C	O	0
			37	31	6	

### 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 L33

Chain 0:  87% 9%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  98%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  95%



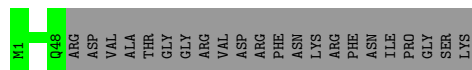
- Molecule 4: 50S ribosomal protein L36

Chain 3:  97%




- Molecule 5: 50S ribosomal protein L31

Chain 4:  69% 31%

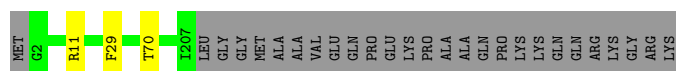


- Molecule 6: tRNA

Chain 8:  81% 19%







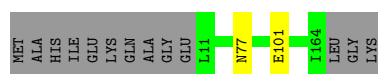
- Molecule 11: 30S ribosomal protein S4

Chain D: 97% .



- Molecule 12: 30S ribosomal protein S5

Chain E: 91% . 8%



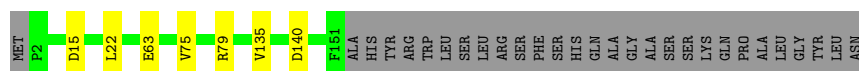
- Molecule 13: 30S ribosomal protein S6

Chain F: 75% 25%



- Molecule 14: 30S ribosomal protein S7

Chain G: 80% . 16%



- Molecule 15: 30S ribosomal protein S8

Chain H: 98% ..



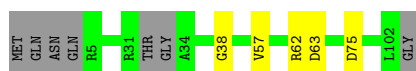
- Molecule 16: 30S ribosomal protein S9

Chain I: 92% 5% .



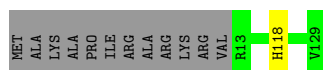
- Molecule 17: 30S ribosomal protein S10

Chain J: 88% 5% 7%



- Molecule 18: Small ribosomal subunit protein uS11

Chain K: 90% 9%



- Molecule 19: 30S ribosomal protein S12

Chain L: 94% . .



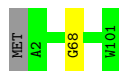
- Molecule 20: 30S ribosomal protein S13

Chain M: 96% . .



- Molecule 21: 30S ribosomal protein S14

Chain N: 98% . .



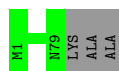
- Molecule 22: 30S ribosomal protein S15

Chain O: 97% . .



- Molecule 23: 30S ribosomal protein S16

Chain P: 96% .



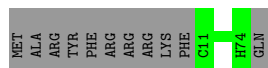
- Molecule 24: 30S ribosomal protein S17

Chain Q: 89% 5% 6%



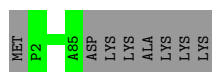
- Molecule 25: 30S ribosomal protein S18

Chain R: 85% 15%



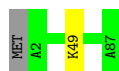
- Molecule 26: 30S ribosomal protein S19

Chain S: 91% 9%



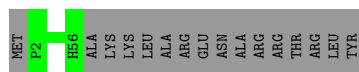
- Molecule 27: 30S ribosomal protein S20

Chain T: 98% ..



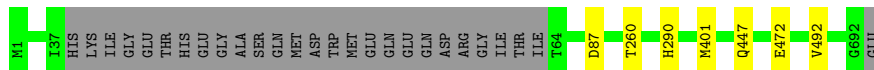
- Molecule 28: 30S ribosomal protein S21

Chain U: 77% 23%



- Molecule 29: Elongation factor G

Chain W: 95% ..



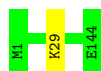
- Molecule 30: 23S rRNA

Chain a: 84% 11% 5%



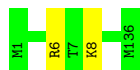






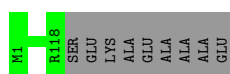
- Molecule 41: 50S ribosomal protein L16

Chain l: 99%



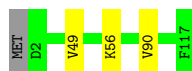
- Molecule 42: 50S ribosomal protein L17

Chain m: 93%



- Molecule 43: 50S ribosomal protein L18

Chain n: 97%



- Molecule 44: 50S ribosomal protein L19

Chain o: 98%



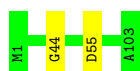
- Molecule 45: 50S ribosomal protein L20

Chain p: 98%



- Molecule 46: 50S ribosomal protein L21

Chain q: 98%



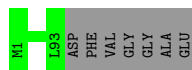
- Molecule 47: 50S ribosomal protein L22

Chain r: 99%



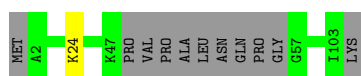
- Molecule 48: 50S ribosomal protein L23

Chain s: 93% 7%



- Molecule 49: 50S ribosomal protein L24

Chain t: 88% 11%



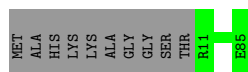
- Molecule 50: 50S ribosomal protein L25

Chain u: 99%



- Molecule 51: 50S ribosomal protein L27

Chain v: 88% 12%



- Molecule 52: 50S ribosomal protein L28

Chain w: 97%



- Molecule 53: 50S ribosomal protein L29

Chain x: 94% 5%



- Molecule 54: 50S ribosomal protein L30

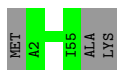
Chain y: 98%





- Molecule 55: 50S ribosomal protein L32

Chain z:  95% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88568	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: K, 4OC, OMC, PSU, 2MA, OMG, 1MG, 5MC, IAS, G7M, 6MZ, H2U, OMU, ZN, MS6, FUA, 4D4, 2MG, 3TD, D2T, GDP, UR3, MG, MEQ, 5MU, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.31	0/420	0.52	0/560
2	1	0.29	0/370	0.61	0/487
3	2	0.32	0/513	0.55	0/676
4	3	0.30	0/303	0.57	0/397
5	4	0.31	0/380	0.53	0/508
6	8	0.46	0/1832	0.89	0/2855
7	9	0.55	0/123	0.86	0/190
8	A	0.44	0/36398	0.88	0/56774
9	B	0.29	0/1768	0.53	0/2381
10	C	0.28	0/1651	0.51	0/2225
11	D	0.29	0/1665	0.52	0/2227
12	E	0.29	0/1148	0.52	0/1545
13	F	0.28	0/843	0.49	0/1140
14	G	0.29	0/1190	0.53	0/1595
15	H	0.29	0/989	0.55	0/1326
16	I	0.29	0/1013	0.53	0/1350
17	J	0.28	0/784	0.59	0/1059
18	K	0.31	0/884	0.53	0/1191
19	L	0.29	0/945	0.58	0/1268
20	M	0.29	0/900	0.53	0/1204
21	N	0.30	0/817	0.51	0/1088
22	O	0.28	0/722	0.50	0/964
23	P	0.28	0/639	0.54	0/859
24	Q	0.28	0/650	0.53	0/871
25	R	0.29	0/532	0.52	0/715
26	S	0.32	0/685	0.52	0/922
27	T	0.28	0/676	0.50	0/895
28	U	0.31	0/467	0.58	0/620
29	W	0.29	0/5244	0.49	0/7091
30	a	0.42	0/66355	0.90	8/103511 (0.0%)
31	b	0.44	0/2850	0.90	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	c	0.29	0/2121	0.56	0/2852
33	d	0.29	0/1562	0.54	0/2102
34	e	0.28	0/1571	0.51	0/2113
35	f	0.29	0/1434	0.52	0/1926
36	g	0.29	0/1291	0.54	0/1747
37	h	0.30	0/306	0.53	0/413
38	i	0.28	0/1144	0.54	0/1541
39	j	0.28	0/955	0.57	0/1279
40	k	0.31	0/1062	0.54	0/1413
41	l	0.29	0/1073	0.55	0/1433
42	m	0.28	0/958	0.55	0/1281
43	n	0.29	0/902	0.54	0/1209
44	o	0.29	0/929	0.55	0/1242
45	p	0.29	0/960	0.56	0/1278
46	q	0.29	0/829	0.54	0/1107
47	r	0.28	0/852	0.56	0/1142
48	s	0.27	0/744	0.51	0/994
49	t	0.30	0/721	0.54	0/956
50	u	0.29	0/758	0.54	0/1015
51	v	0.32	0/576	0.56	0/762
52	w	0.30	0/635	0.57	0/848
53	x	0.27	0/492	0.49	0/655
54	y	0.29	0/453	0.52	0/605
55	z	0.30	0/435	0.56	0/581
All	All	0.39	0/156519	0.81	8/233432 (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
3	2	0	1
4	3	0	1
10	C	0	1
11	D	0	1
14	G	0	1
16	I	0	2
17	J	0	2
18	K	0	1
19	L	0	1
36	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	i	0	1
45	p	0	1
52	w	0	1
53	x	0	1
All	All	0	16

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	512	G	O4'-C1'-N9	7.53	114.23	108.20
30	a	2447	G	C3'-C2'-C1'	-5.94	96.75	101.50
30	a	2546	U	O3'-P-O5'	-5.94	92.71	104.00
30	a	512	G	C1'-O4'-C4'	-5.93	105.16	109.90
30	a	1936	A	C1'-O4'-C4'	-5.50	105.50	109.90
30	a	1936	A	O4'-C1'-N9	5.34	112.47	108.20
30	a	1905	C	O3'-P-O5'	-5.10	94.32	104.00
30	a	242	G	C3'-C2'-C1'	-5.01	97.50	101.50

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
4	3	36	ARG	Sidechain
10	C	11	ARG	Sidechain
11	D	184	ARG	Sidechain
14	G	79	ARG	Sidechain
16	I	41	ARG	Sidechain
16	I	95	ARG	Sidechain
17	J	38	GLY	Peptide
17	J	62	ARG	Sidechain
18	K	118	HIS	Peptide
19	L	9	ARG	Sidechain
36	g	35	ARG	Sidechain
38	i	96	ARG	Sidechain
45	p	51	ARG	Sidechain
52	w	74	ARG	Sidechain
53	x	52	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	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
9	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	24
10	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
11	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
12	E	152/167 (91%)	148 (97%)	4 (3%)	0	100	100
13	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
14	G	148/179 (83%)	145 (98%)	3 (2%)	0	100	100
15	H	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	13
16	I	123/130 (95%)	118 (96%)	5 (4%)	0	100	100
17	J	92/103 (89%)	88 (96%)	3 (3%)	1 (1%)	12	8
18	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
19	L	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
20	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
21	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	13	9
22	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
23	P	77/82 (94%)	74 (96%)	3 (4%)	0	100	100
24	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	R	62/75 (83%)	62 (100%)	0	0	100	100
26	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
27	T	84/87 (97%)	84 (100%)	0	0	100	100
28	U	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
29	W	662/693 (96%)	647 (98%)	15 (2%)	0	100	100
32	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
33	d	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
34	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
35	f	175/179 (98%)	170 (97%)	4 (2%)	1 (1%)	22	20
36	g	166/177 (94%)	164 (99%)	2 (1%)	0	100	100
37	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
38	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
39	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
40	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19	17
41	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
42	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
43	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
46	q	101/103 (98%)	100 (99%)	0	1 (1%)	13	9
47	r	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
48	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
49	t	89/104 (86%)	88 (99%)	1 (1%)	0	100	100
50	u	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
51	v	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	58/63 (92%)	58 (100%)	0	0	100	100
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
55	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
All	All	6064/6606 (92%)	5915 (98%)	142 (2%)	7 (0%)	50	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	57	VAL
35	f	42	GLU
9	B	165	ASP
40	k	29	LYS
15	H	75	ILE
46	q	44	GLY
21	N	68	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	44 (96%)	2 (4%)	25	26
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	57
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	44/62 (71%)	44 (100%)	0	100	100
9	B	184/199 (92%)	176 (96%)	8 (4%)	25	26
10	C	170/190 (90%)	168 (99%)	2 (1%)	67	75
11	D	172/173 (99%)	167 (97%)	5 (3%)	37	43
12	E	117/126 (93%)	115 (98%)	2 (2%)	56	64
13	F	88/116 (76%)	88 (100%)	0	100	100
14	G	124/147 (84%)	118 (95%)	6 (5%)	21	21
15	H	104/105 (99%)	103 (99%)	1 (1%)	73	79
16	I	103/107 (96%)	99 (96%)	4 (4%)	27	30
17	J	85/90 (94%)	83 (98%)	2 (2%)	44	50
18	K	89/98 (91%)	89 (100%)	0	100	100
19	L	101/103 (98%)	98 (97%)	3 (3%)	36	42
20	M	93/96 (97%)	91 (98%)	2 (2%)	47	54
21	N	83/84 (99%)	83 (100%)	0	100	100
22	O	76/77 (99%)	74 (97%)	2 (3%)	41	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	64/65 (98%)	64 (100%)	0	100	100
24	Q	73/78 (94%)	69 (94%)	4 (6%)	18	16
25	R	55/65 (85%)	55 (100%)	0	100	100
26	S	72/79 (91%)	72 (100%)	0	100	100
27	T	65/66 (98%)	64 (98%)	1 (2%)	60	69
28	U	48/61 (79%)	48 (100%)	0	100	100
29	W	556/579 (96%)	549 (99%)	7 (1%)	65	73
32	c	216/218 (99%)	215 (100%)	1 (0%)	86	90
33	d	162/163 (99%)	162 (100%)	0	100	100
34	e	165/165 (100%)	165 (100%)	0	100	100
35	f	148/150 (99%)	141 (95%)	7 (5%)	22	23
36	g	132/138 (96%)	128 (97%)	4 (3%)	36	42
37	h	32/114 (28%)	32 (100%)	0	100	100
38	i	115/116 (99%)	114 (99%)	1 (1%)	75	82
39	j	104/104 (100%)	102 (98%)	2 (2%)	52	60
40	k	103/103 (100%)	103 (100%)	0	100	100
41	l	107/107 (100%)	105 (98%)	2 (2%)	52	60
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	83 (96%)	3 (4%)	31	35
44	o	99/100 (99%)	98 (99%)	1 (1%)	73	79
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	83 (99%)	1 (1%)	67	75
47	r	92/93 (99%)	92 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	76/85 (89%)	75 (99%)	1 (1%)	65	73
50	u	77/78 (99%)	77 (100%)	0	100	100
51	v	56/63 (89%)	56 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	46/48 (96%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5070/5404 (94%)	4995 (98%)	75 (2%)	60 69

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

Mol	Chain	Res	Type
1	0	5	ILE
1	0	28	ARG
3	2	31	HIS
9	B	23	TRP
9	B	78	GLU
9	B	103	ASN
9	B	133	GLU
9	B	143	LYS
9	B	192	ASP
9	B	196	VAL
9	B	204	ASP
10	C	29	PHE
10	C	70	THR
11	D	44	ARG
11	D	45	LYS
11	D	58	LYS
11	D	145	ILE
11	D	147	GLU
12	E	77	ASN
12	E	101	GLU
14	G	15	ASP
14	G	22	LEU
14	G	63	GLU
14	G	75	VAL
14	G	135	VAL
14	G	140	ASP
15	H	89	LYS
16	I	63	LEU
16	I	66	THR
16	I	72	ILE
16	I	123	ARG
17	J	63	ASP
17	J	75	ASP
19	L	52	VAL
19	L	112	GLN
19	L	120	LYS
20	M	14	HIS

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Mol	Chain	Res	Type
20	M	93	ARG
22	O	17	ARG
22	O	89	ARG
24	Q	28	PHE
24	Q	42	THR
24	Q	52	GLU
24	Q	74	THR
27	T	49	LYS
29	W	87	ASP
29	W	260	THR
29	W	290	HIS
29	W	401	MET
29	W	447	GLN
29	W	472	GLU
29	W	492	VAL
32	c	37	ASN
35	f	30	ARG
35	f	40	VAL
35	f	47	LYS
35	f	125	ARG
35	f	143	TYR
35	f	150	ARG
35	f	152	LEU
36	g	25	THR
36	g	104	ASN
36	g	155	GLU
36	g	173	GLU
38	i	95	ARG
39	j	49	ARG
39	j	58	LEU
41	l	6	ARG
41	l	8	LYS
43	n	49	VAL
43	n	56	LYS
43	n	90	VAL
44	o	53	ARG
46	q	55	ASP
49	t	24	LYS

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

Mol	Chain	Res	Type
5	4	41	HIS
9	B	42	ASN
9	B	103	ASN
9	B	146	ASN
10	C	100	GLN
10	C	139	GLN
10	C	140	ASN
11	D	71	GLN
11	D	152	GLN
12	E	77	ASN
12	E	82	GLN
14	G	148	ASN
17	J	58	ASN
19	L	112	GLN
21	N	66	GLN
22	O	35	GLN
25	R	31	ASN
26	S	52	HIS
27	T	61	GLN
27	T	68	HIS
27	T	84	ASN
29	W	447	GLN
32	c	37	ASN
35	f	23	ASN
35	f	27	GLN
37	h	18	GLN
43	n	116	GLN
45	p	44	GLN
46	q	12	HIS
46	q	43	ASN
49	t	40	ASN
50	u	5	ASN
50	u	49	ASN
53	x	45	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2774/2930 (94%)	298 (10%)	0
31	b	118/119 (99%)	7 (5%)	0
6	8	76/77 (98%)	15 (19%)	3 (3%)
7	9	4/24 (16%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	1521/1554 (97%)	233 (15%)	47 (3%)
All	All	4493/4704 (95%)	553 (12%)	50 (1%)

All (553) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	8	U
6	8	9	G
6	8	16	C
6	8	17(A)	U
6	8	19	G
6	8	20	U
6	8	21	A
6	8	22	G
6	8	43	A
6	8	46	G
6	8	47	U
6	8	55	U
6	8	58	A
6	8	76	A
8	A	3	A
8	A	4	U
8	A	5	U
8	A	6	G
8	A	7	A
8	A	8	A
8	A	9	G
8	A	32	A
8	A	39	G
8	A	47	C
8	A	48	C
8	A	49	U
8	A	50	A
8	A	51	A
8	A	66	A
8	A	72	A
8	A	76	G
8	A	77	A
8	A	78	A
8	A	80	A
8	A	81	A

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Mol	Chain	Res	Type
8	A	82	G
8	A	83	C
8	A	84	U
8	A	85	U
8	A	86	G
8	A	87	C
8	A	90	C
8	A	94	G
8	A	95	C
8	A	96	U
8	A	97	G
8	A	120	A
8	A	122	G
8	A	130	A
8	A	131	A
8	A	137	U
8	A	143	A
8	A	144	G
8	A	159	G
8	A	163	C
8	A	164	G
8	A	170	U
8	A	182	A
8	A	196	A
8	A	197	A
8	A	207	C
8	A	208	U
8	A	209	U
8	A	210	C
8	A	226	G
8	A	240	G
8	A	245	U
8	A	247	G
8	A	250	A
8	A	251	G
8	A	253	A
8	A	266	G
8	A	267	C
8	A	289	G
8	A	305	G
8	A	306	A
8	A	321	A

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Mol	Chain	Res	Type
8	A	328	C
8	A	329	A
8	A	330	C
8	A	332	G
8	A	352	C
8	A	354	G
8	A	367	U
8	A	372	C
8	A	398	U
8	A	406	G
8	A	411	A
8	A	412	A
8	A	413	G
8	A	414	A
8	A	421	U
8	A	422	C
8	A	429	U
8	A	455	G
8	A	457	G
8	A	458	U
8	A	463	U
8	A	467	U
8	A	468	A
8	A	482	A
8	A	484	G
8	A	486	U
8	A	495	A
8	A	499	A
8	A	500	G
8	A	511	C
8	A	518	C
8	A	524	G
8	A	527	G7M
8	A	530	G
8	A	532	A
8	A	547	A
8	A	559	A
8	A	562	U
8	A	572	A
8	A	573	A
8	A	576	C
8	A	589	U

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Mol	Chain	Res	Type
8	A	596	A
8	A	607	A
8	A	615	G
8	A	619	U
8	A	635	A
8	A	642	A
8	A	650	G
8	A	665	A
8	A	687	A
8	A	695	A
8	A	702	A
8	A	703	G
8	A	721	G
8	A	723	U
8	A	724	G
8	A	755	G
8	A	777	A
8	A	793	U
8	A	794	A
8	A	815	A
8	A	817	C
8	A	829	G
8	A	849	G
8	A	874	G
8	A	884	U
8	A	885	G
8	A	890	G
8	A	902	G
8	A	914	A
8	A	926	G
8	A	927	G
8	A	934	C
8	A	935	A
8	A	942	G
8	A	958	A
8	A	960	U
8	A	965	U
8	A	969	A
8	A	975	A
8	A	976	G
8	A	977	A
8	A	989	U

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Mol	Chain	Res	Type
8	A	991	U
8	A	992	U
8	A	993	G
8	A	994	A
8	A	1004	A
8	A	1013	G
8	A	1014	A
8	A	1015	G
8	A	1016	A
8	A	1017	U
8	A	1020	G
8	A	1021	A
8	A	1030	U
8	A	1031	C
8	A	1032	G
8	A	1056	U
8	A	1065	U
8	A	1085	U
8	A	1092	A
8	A	1094	G
8	A	1095	U
8	A	1101	A
8	A	1104	G
8	A	1108	G
8	A	1109	C
8	A	1124	G
8	A	1130	A
8	A	1135	U
8	A	1139	G
8	A	1141	C
8	A	1146	A
8	A	1150	A
8	A	1152	A
8	A	1157	A
8	A	1158	C
8	A	1159	U
8	A	1160	G
8	A	1183	U
8	A	1196	A
8	A	1197	A
8	A	1213	A
8	A	1226	C

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Mol	Chain	Res	Type
8	A	1227	A
8	A	1238	A
8	A	1240	U
8	A	1250	A
8	A	1256	A
8	A	1257	A
8	A	1260	G
8	A	1268	G
8	A	1279	G
8	A	1280	A
8	A	1286	U
8	A	1287	A
8	A	1297	G
8	A	1298	U
8	A	1300	G
8	A	1305	G
8	A	1311	A
8	A	1312	G
8	A	1320	C
8	A	1331	G
8	A	1332	A
8	A	1336	C
8	A	1338	G
8	A	1346	A
8	A	1363	A
8	A	1364	U
8	A	1379	G
8	A	1398	A
8	A	1419	G
8	A	1429	A
8	A	1441	A
8	A	1453	G
8	A	1494	G
8	A	1497	G
8	A	1499	A
8	A	1503	A
8	A	1505	G
8	A	1506	U
8	A	1507	A
8	A	1517	G
8	A	1529	G
8	A	1530	G

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Mol	Chain	Res	Type
8	A	1533	C
8	A	1534	A
30	a	10	A
30	a	12	U
30	a	15	G
30	a	34	U
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	118	A
30	a	119	A
30	a	120	U
30	a	131	A
30	a	139	U
30	a	142	A
30	a	162	U
30	a	181	A
30	a	196	A
30	a	199	A
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	272	A
30	a	278	A
30	a	279	A
30	a	281	C
30	a	285	G
30	a	289	G
30	a	311	A
30	a	330	A
30	a	346	A
30	a	354	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	411	G
30	a	448	U
30	a	451	U
30	a	481	G

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Mol	Chain	Res	Type
30	a	491	G
30	a	505	A
30	a	509	C
30	a	531	C
30	a	532	A
30	a	533	G
30	a	544	C
30	a	545	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	556	A
30	a	563	A
30	a	573	U
30	a	574	A
30	a	575	A
30	a	586	A
30	a	603	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	716	A
30	a	717	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	792	A
30	a	805	G
30	a	812	C
30	a	827	U

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Mol	Chain	Res	Type
30	a	828	U
30	a	845	A
30	a	846	U
30	a	858	G
30	a	869	G
30	a	910	A
30	a	914	G
30	a	915	C
30	a	931	U
30	a	934	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1026	G
30	a	1033	U
30	a	1041	G
30	a	1047	G
30	a	1059	G
30	a	1060	U
30	a	1070	A
30	a	1077	A
30	a	1080	A
30	a	1083	U
30	a	1087	G
30	a	1088	A
30	a	1097	U
30	a	1101	U
30	a	1112	G
30	a	1116	G
30	a	1128	G
30	a	1129	A
30	a	1130	U
30	a	1132	U
30	a	1133	A
30	a	1134	A

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Mol	Chain	Res	Type
30	a	1135	C
30	a	1142	A
30	a	1144	A
30	a	1151	A
30	a	1169	A
30	a	1170	C
30	a	1179	G
30	a	1188	U
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1300	G
30	a	1301	A
30	a	1321	A
30	a	1352	U
30	a	1365	A
30	a	1378	A
30	a	1379	U
30	a	1383	A
30	a	1386	C
30	a	1409	U
30	a	1416	G
30	a	1419	A
30	a	1428	C
30	a	1451	C
30	a	1452	G
30	a	1453	A
30	a	1455	G
30	a	1458	U
30	a	1460	U
30	a	1482	G
30	a	1490	A
30	a	1493	C
30	a	1508	A
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G

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Mol	Chain	Res	Type
30	a	1538	G
30	a	1569	A
30	a	1578	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1698	A
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1734	G
30	a	1737	G
30	a	1738	G
30	a	1744	A
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1872	A
30	a	1906	G
30	a	1907	G
30	a	1913	A
30	a	1914	C
30	a	1929	G
30	a	1930	G
30	a	1931	U
30	a	1937	A
30	a	1955	U
30	a	1967	C

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Mol	Chain	Res	Type
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2093	G
30	a	2096	C
30	a	2193	G
30	a	2198	A
30	a	2204	G
30	a	2211	A
30	a	2225	A
30	a	2238	G
30	a	2268	A
30	a	2273	A
30	a	2278	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2312	U
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2366	A
30	a	2383	G
30	a	2385	C
30	a	2402	U

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Mol	Chain	Res	Type
30	a	2406	A
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2459	A
30	a	2469	A
30	a	2476	A
30	a	2478	A
30	a	2491	U
30	a	2502	G
30	a	2504	PSU
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2547	A
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2661	G
30	a	2663	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2798	U
30	a	2799	A
30	a	2803	G

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Mol	Chain	Res	Type
30	a	2809	A
30	a	2818	U
30	a	2820	A
30	a	2821	A
30	a	2883	A
30	a	2884	U
31	b	35	C
31	b	36	C
31	b	37	C
31	b	44	G
31	b	45	A
31	b	89	U
31	b	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	17(A)	U
6	8	20	U
8	A	7	A
8	A	30	U
8	A	84	U
8	A	86	G
8	A	182	A
8	A	199	A
8	A	305	G
8	A	329	A
8	A	345	C
8	A	411	A
8	A	428	G
8	A	434	U
8	A	446	G
8	A	499	A
8	A	575	G
8	A	595	A
8	A	702	A
8	A	776	G
8	A	827	U
8	A	884	U
8	A	958	A
8	A	974	A

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Mol	Chain	Res	Type
8	A	991	U
8	A	993	G
8	A	1013	G
8	A	1031	C
8	A	1092	A
8	A	1101	A
8	A	1108	G
8	A	1124	G
8	A	1129	C
8	A	1145	A
8	A	1157	A
8	A	1159	U
8	A	1160	G
8	A	1187	G
8	A	1256	A
8	A	1297	G
8	A	1320	C
8	A	1331	G
8	A	1364	U
8	A	1380	U
8	A	1397	C
8	A	1447	A
8	A	1452	C
8	A	1459	G
8	A	1505	G

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

39 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
30	5MC	a	1962	30	18,22,23	0.34	0	26,32,35	0.50	0
8	2MG	A	1516	8	18,26,27	1.02	2 (11%)	16,38,41	0.82	0
30	6MZ	a	2030	30	18,25,26	0.70	0	16,36,39	0.75	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	PSU	a	2457	30	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
30	OMC	a	2498	58,30	19,22,23	0.28	0	26,31,34	0.53	0
30	5MU	a	1939	30,57	19,22,23	0.30	0	28,32,35	0.37	0
8	2MG	A	966	8	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
30	PSU	a	1917	30	18,21,22	0.89	1 (5%)	22,30,33	0.52	0
30	5MU	a	747	30	19,22,23	0.26	0	28,32,35	0.42	0
8	5MC	A	1407	8	18,22,23	0.32	0	26,32,35	0.54	0
19	D2T	L	89	19	7,9,10	0.94	0	6,11,13	1.85	4 (66%)
8	4OC	A	1402	8	20,23,24	0.39	0	26,32,35	0.42	0
30	2MG	a	2445	30	18,26,27	1.01	2 (11%)	16,38,41	0.75	0
30	3TD	a	1915	30	18,22,23	0.98	1 (5%)	22,32,35	0.62	0
30	OMU	a	2552	30	19,22,23	0.21	0	26,31,34	0.40	0
30	2MG	a	1835	30	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
30	G7M	a	2069	30	20,26,27	1.11	3 (15%)	17,39,42	0.55	0
30	PSU	a	955	30	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
41	4D4	l	81	41	9,11,12	0.55	0	8,13,15	0.70	0
30	PSU	a	2604	30	18,21,22	0.91	1 (5%)	22,30,33	0.75	1 (4%)
18	IAS	K	119	18	6,7,8	0.91	0	6,8,10	0.99	0
30	6MZ	a	1618	30	18,25,26	0.66	0	16,36,39	0.74	1 (6%)
8	5MC	A	967	8	18,22,23	0.33	0	26,32,35	0.49	0
30	PSU	a	2580	30,57	18,21,22	0.90	1 (5%)	22,30,33	0.85	1 (4%)
8	PSU	A	516	8	18,21,22	0.91	1 (5%)	22,30,33	0.59	0
30	1MG	a	745	30	18,26,27	0.97	1 (5%)	19,39,42	0.52	0
8	G7M	A	527	8	20,26,27	1.13	2 (10%)	17,39,42	0.30	0
8	MA6	A	1518	8	18,26,27	0.75	0	19,38,41	0.45	0
30	PSU	a	1911	30	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
8	UR3	A	1498	8	19,22,23	0.28	0	26,32,35	0.64	0
30	PSU	a	2504	30,57	18,21,22	0.85	1 (5%)	22,30,33	0.76	0
8	MA6	A	1519	8	18,26,27	0.73	0	19,38,41	0.58	0
8	2MG	A	1207	8	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
30	PSU	a	746	58,30	18,21,22	0.95	1 (5%)	22,30,33	0.60	0
30	H2U	a	2449	30	18,21,22	0.60	0	21,30,33	0.88	2 (9%)
30	PSU	a	2605	30	18,21,22	0.90	1 (5%)	22,30,33	0.75	0
30	OMG	a	2251	30,57	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
30	2MA	a	2503	58,30,57	19,25,26	0.99	1 (5%)	21,37,40	1.78	5 (23%)
33	MEQ	d	150	33	8,9,10	0.43	0	5,10,12	0.54	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
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
8	2MG	A	1516	8	-	0/5/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	58,30	-	0/9/27/28	0/2/2/2
30	5MU	a	1939	30,57	-	0/7/25/26	0/2/2/2
8	2MG	A	966	8	-	2/5/27/28	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
8	5MC	A	1407	8	-	0/7/25/26	0/2/2/2
19	D2T	L	89	19	-	4/7/12/14	-
8	4OC	A	1402	8	-	0/9/29/30	0/2/2/2
30	2MG	a	2445	30	-	1/5/27/28	0/3/3/3
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	1/11/12/14	-
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
18	IAS	K	119	18	-	2/7/7/8	-
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
8	5MC	A	967	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2580	30,57	-	0/7/25/26	0/2/2/2
8	PSU	A	516	8	-	0/7/25/26	0/2/2/2
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
8	G7M	A	527	8	-	2/3/25/26	0/3/3/3
8	MA6	A	1518	8	-	0/7/29/30	0/3/3/3
30	PSU	a	1911	30	-	2/7/25/26	0/2/2/2
8	UR3	A	1498	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2504	30,57	-	2/7/25/26	0/2/2/2
8	MA6	A	1519	8	-	0/7/29/30	0/3/3/3
8	2MG	A	1207	8	-	0/5/27/28	0/3/3/3
30	PSU	a	746	58,30	-	2/7/25/26	0/2/2/2
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2251	30,57	-	1/5/27/28	0/3/3/3
30	2MA	a	2503	58,30,57	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	MEQ	d	150	33	-	2/8/9/11	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	746	PSU	C6-C5	3.77	1.39	1.35
30	a	1915	3TD	C6-C5	3.71	1.39	1.35
30	a	1911	PSU	C6-C5	3.65	1.39	1.35
8	A	516	PSU	C6-C5	3.58	1.39	1.35
30	a	2580	PSU	C6-C5	3.58	1.39	1.35
30	a	2604	PSU	C6-C5	3.53	1.39	1.35
30	a	1917	PSU	C6-C5	3.52	1.39	1.35
8	A	527	G7M	C8-N9	3.50	1.39	1.33
30	a	2605	PSU	C6-C5	3.49	1.39	1.35
30	a	2457	PSU	C6-C5	3.47	1.39	1.35
30	a	955	PSU	C6-C5	3.41	1.39	1.35
30	a	2504	PSU	C6-C5	3.36	1.39	1.35
30	a	2069	G7M	C8-N9	3.35	1.39	1.33
30	a	2251	OMG	C5-C6	-2.55	1.42	1.47
8	A	1207	2MG	C5-C6	-2.50	1.42	1.47
30	a	1835	2MG	C5-C6	-2.49	1.42	1.47
8	A	527	G7M	C8-N7	2.46	1.37	1.33
8	A	966	2MG	C5-C6	-2.45	1.42	1.47
8	A	1516	2MG	C5-C6	-2.43	1.42	1.47
30	a	2445	2MG	C5-C6	-2.37	1.42	1.47
30	a	2069	G7M	C8-N7	2.36	1.37	1.33
30	a	745	1MG	C5-C4	-2.22	1.37	1.43
30	a	2445	2MG	C8-N7	-2.14	1.31	1.35
8	A	1207	2MG	C8-N7	-2.10	1.31	1.35
30	a	2069	G7M	C5-C6	-2.08	1.40	1.45
30	a	1835	2MG	C8-N7	-2.06	1.31	1.35
8	A	966	2MG	C8-N7	-2.05	1.31	1.35
30	a	2251	OMG	C8-N7	-2.05	1.31	1.35
8	A	1516	2MG	C8-N7	-2.03	1.31	1.35
30	a	2503	2MA	C6-N1	2.02	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2503	2MA	C5-C6-N1	-5.42	117.45	121.01
30	a	2503	2MA	C5-C6-N6	4.25	126.81	120.35
30	a	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	89	D2T	OD1-CG-CB	-2.58	117.03	122.44
30	a	2503	2MA	CM2-C2-N1	2.37	120.85	117.15
30	a	2449	H2U	O2-C2-N1	-2.36	120.15	123.11
30	a	2449	H2U	N3-C2-N1	2.28	119.06	116.65
30	a	2503	2MA	C2-N1-C6	2.27	121.62	118.08
19	L	89	D2T	CB-CA-N	2.24	113.87	109.10
30	a	2503	2MA	N3-C2-N1	-2.23	121.65	125.73
30	a	1618	6MZ	C2-N1-C6	2.23	118.50	116.59
30	a	2030	6MZ	C2-N1-C6	2.22	118.49	116.59
19	L	89	D2T	OD2-CG-CB	2.07	117.62	113.15
19	L	89	D2T	O-C-CA	-2.03	119.46	124.78
30	a	2604	PSU	C2'-C3'-C4'	-2.01	98.74	102.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	L	89	D2T	CA-CB-CG-OD1
19	L	89	D2T	CA-CB-CG-OD2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
8	A	527	G7M	O4'-C4'-C5'-O5'
8	A	527	G7M	C3'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
19	L	89	D2T	CG-CB-SB-CB1
30	a	2445	2MG	C3'-C4'-C5'-O5'
30	a	2504	PSU	O4'-C4'-C5'-O5'
8	A	966	2MG	O4'-C4'-C5'-O5'
18	K	119	IAS	CA-CB-CG-OD1
18	K	119	IAS	O-C-CA-N
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	1962	5MC	C2'-C1'-N1-C6
8	A	966	2MG	C3'-C4'-C5'-O5'
19	L	89	D2T	SB-CB-CG-OD2
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	747	5MU	C3'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
30	a	2504	PSU	C3'-C4'-C5'-O5'
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
41	l	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 369 ligands modelled in this entry, 367 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
59	GDP	W	701	58	24,30,30	0.95	2 (8%)	30,47,47	0.63	0
60	FUA	W	703	-	39,40,40	1.48	2 (5%)	49,64,64	0.91	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	W	701	58	-	1/12/32/32	0/3/3/3
60	FUA	W	703	-	-	7/15/92/92	0/4/4/4

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	W	703	FUA	C29-C22	-8.49	1.35	1.47
59	W	701	GDP	C5-C6	-2.61	1.42	1.47
60	W	703	FUA	O5-C29	-2.32	1.23	1.30
59	W	701	GDP	C8-N7	-2.09	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	W	703	FUA	C14-C8-C9	-2.20	105.10	109.40
60	W	703	FUA	C16-O2-C31	2.16	120.34	117.06

There are no chirality outliers.

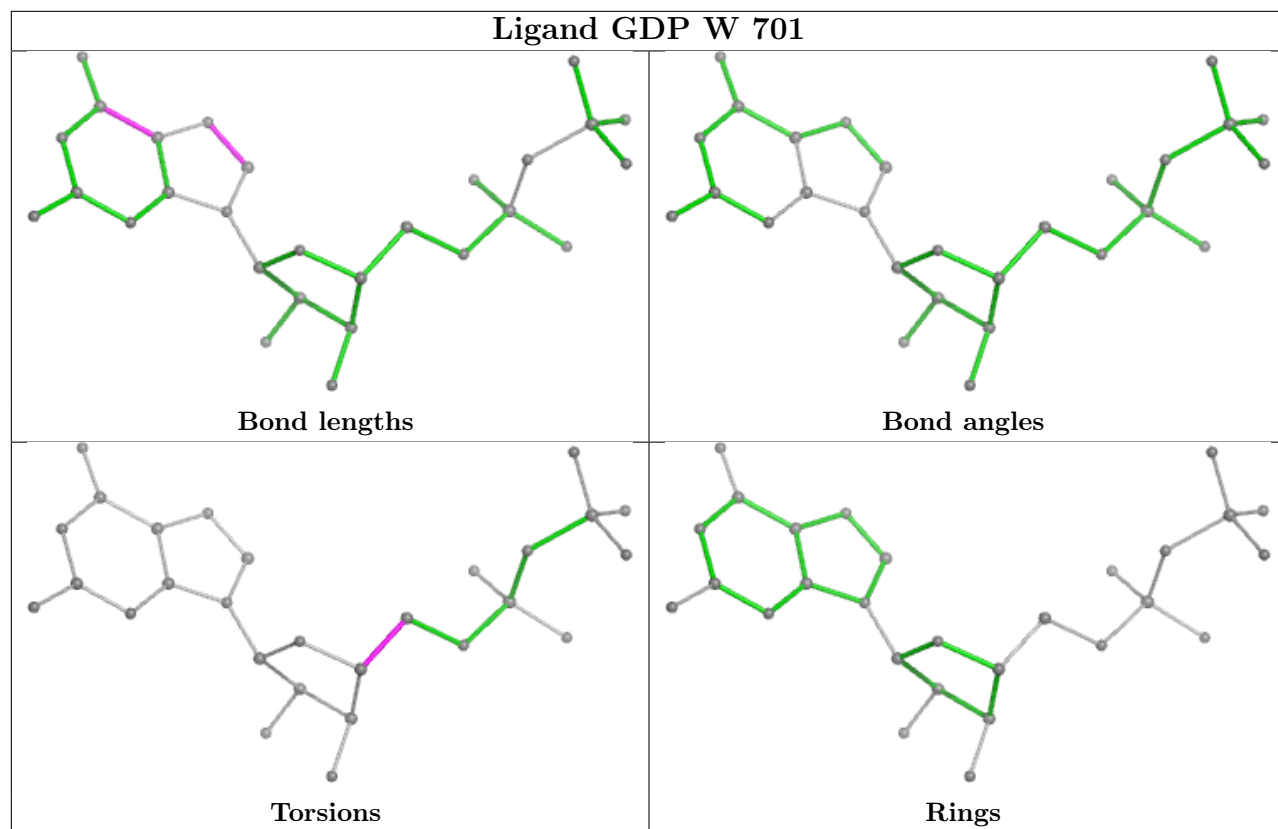
All (8) torsion outliers are listed below:

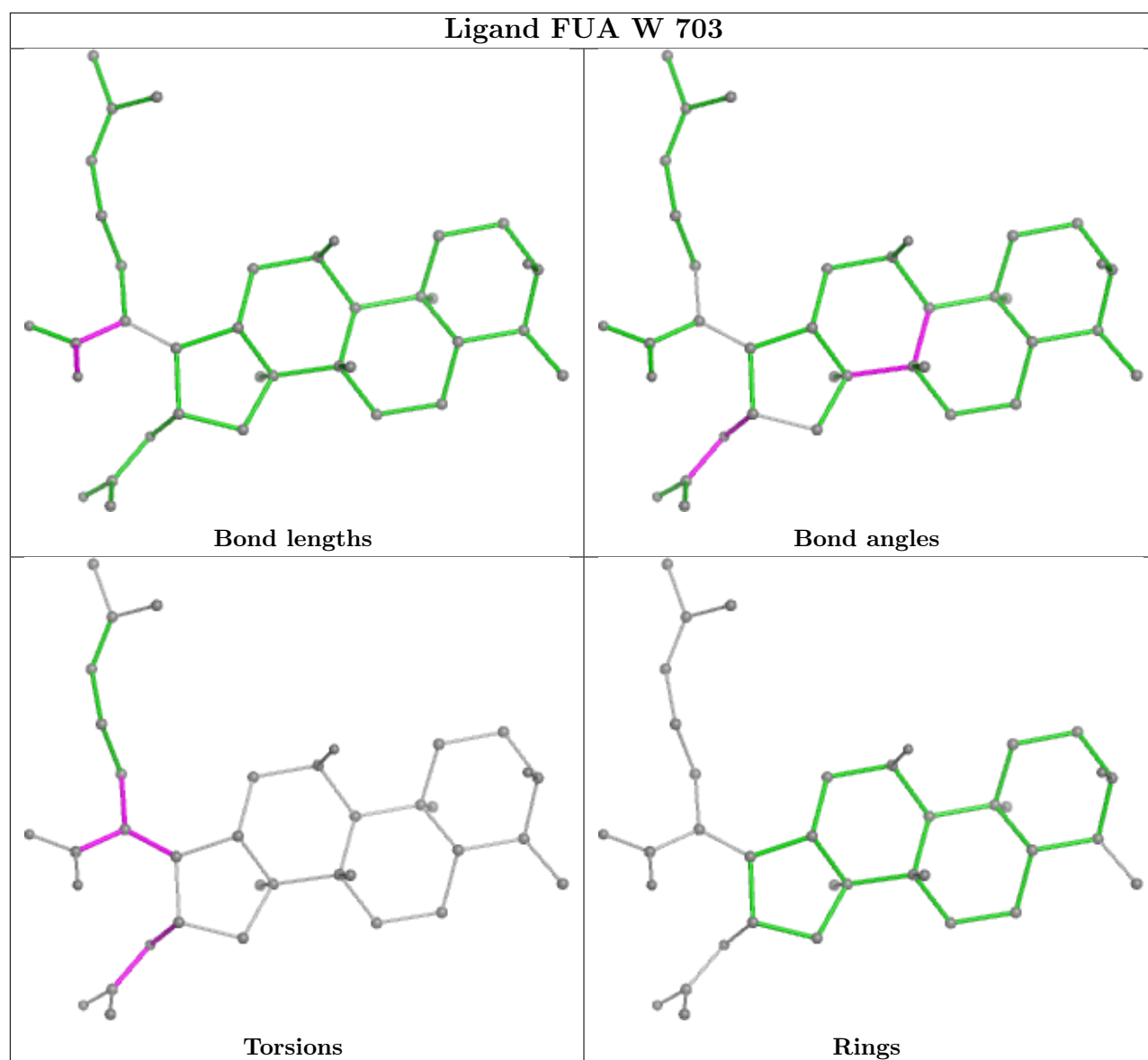
Mol	Chain	Res	Type	Atoms
60	W	703	FUA	C13-C17-C22-C29
60	W	703	FUA	C32-C31-O2-C16
60	W	703	FUA	O3-C31-O2-C16
60	W	703	FUA	C29-C22-C23-C24
60	W	703	FUA	C17-C22-C29-O4
60	W	703	FUA	C17-C22-C29-O5
59	W	701	GDP	O4'-C4'-C5'-O5'
60	W	703	FUA	C17-C16-O2-C31

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.