



## wwPDB EM Map/Model Validation Report ⓘ

Aug 10, 2016 – 09:11 PM EDT

PDB ID : 5KCR  
EMDB ID: : EMD-8237  
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Avilamycin C, mRNA and P-site tRNA at 3.6Å resolution  
Authors : Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.  
Deposited on : 2016-06-06  
Resolution : 3.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

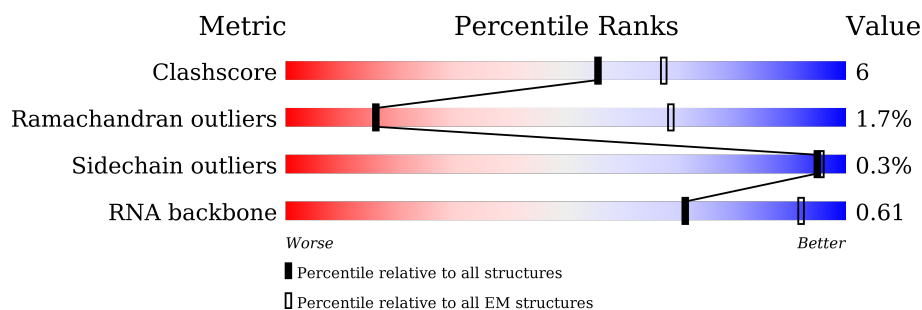
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1A	2904	75% 22% .
2	1B	120	83% 16% .
3	1D	273	71% 28% .
4	1E	209	78% 22%
5	1F	201	79% 21%
6	1G	179	73% 25% ..
7	1H	177	77% 22% ..
8	1I	149	78% 22%



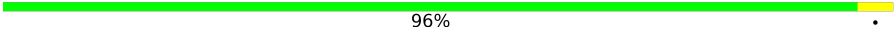



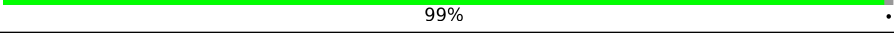
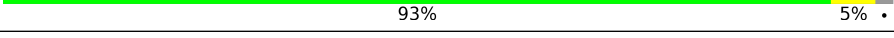
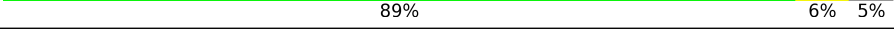

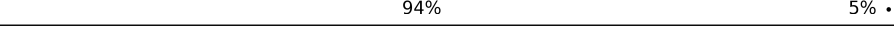
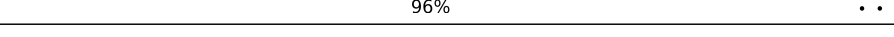

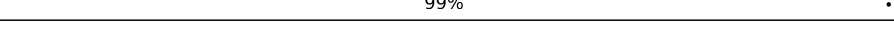
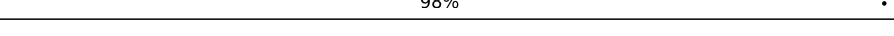

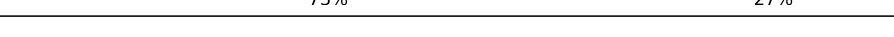

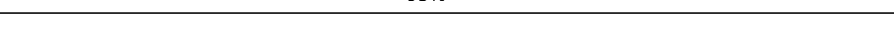



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Mol	Chain	Length	Quality of chain
9	1J	165	
10	1K	142	
11	1N	142	
12	1O	123	
13	1P	144	
14	1Q	136	
15	1R	127	
16	1S	117	
17	1T	115	
18	1U	118	
19	1V	103	
20	1W	110	
21	1X	100	
22	1Y	104	
23	1Z	94	
24	10	85	
25	11	78	
26	12	63	
27	13	59	
28	15	57	
29	16	55	
30	17	46	
31	18	65	
32	19	38	
33	1a	1539	

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Mol	Chain	Length	Quality of chain
34	1b	241	
35	1c	233	
36	1d	206	
37	1e	167	
38	1f	135	
39	1g	179	
40	1h	130	
41	1i	130	
42	1j	103	
43	1k	129	
44	1l	124	
45	1m	118	
46	1n	101	
47	1o	89	
48	1p	82	
49	1q	84	
50	1r	75	
51	1s	92	
52	1t	87	
53	1u	71	
54	1v	9	
55	1x	87	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145689 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 RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2897	Total	C	N	O	P	8	0
			62361	27826	11476	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	1	0
			1576	986	290	296	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1404	896	246	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1J	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1K	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1O	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1P	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Q	136	Total	C	N	O	S	2	0
			1090	696	211	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1R	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1S	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1Y	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	10	76	Total	C	N	O	S	1	0
			591	365	121	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	12	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	58	Total	C	N	O	S	2	0
			463	290	90	81	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1o	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	1r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

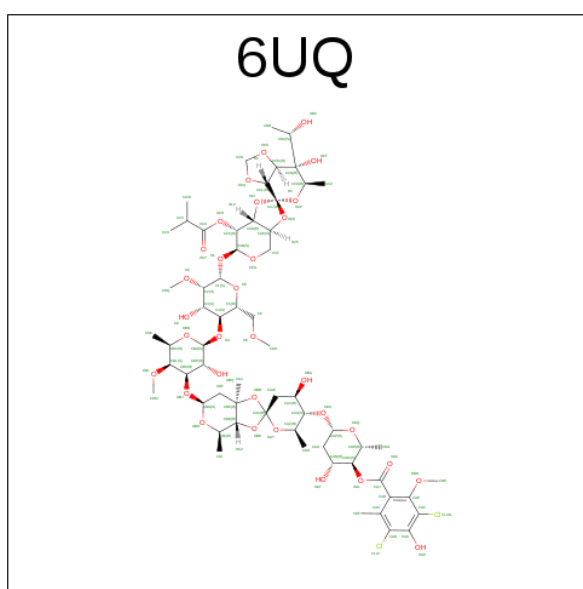
- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1v	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1x	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 56 is (2R,3S,4R,6S)-4-hydroxy-6-{{[(2R,3aR,4R,4'R,5'S,6S,6'R,7aR)-4'-hydroxy-6-{{[(2S,3R,4R,5S,6R)-3-hydroxy-2-{{[(2R,3S,4S,5S,6S)-4-hydroxy-6-{{(2R,3aS,3a'R,6S,6'R,7R,7'R,7aR,7a'R)-7'-hydroxy-7'-[(1S)-1-hydroxyethyl]-6'-methyl-7-[(2-methylpropanoyl)oxy]octahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: 6UQ) (formula: C<sub>61</sub>H<sub>90</sub>Cl<sub>2</sub>O<sub>32</sub>).



Mol	Chain	Residues	Atoms				AltConf
56	1A	1	Total	C	Cl	O	0
			95	61	2	32	

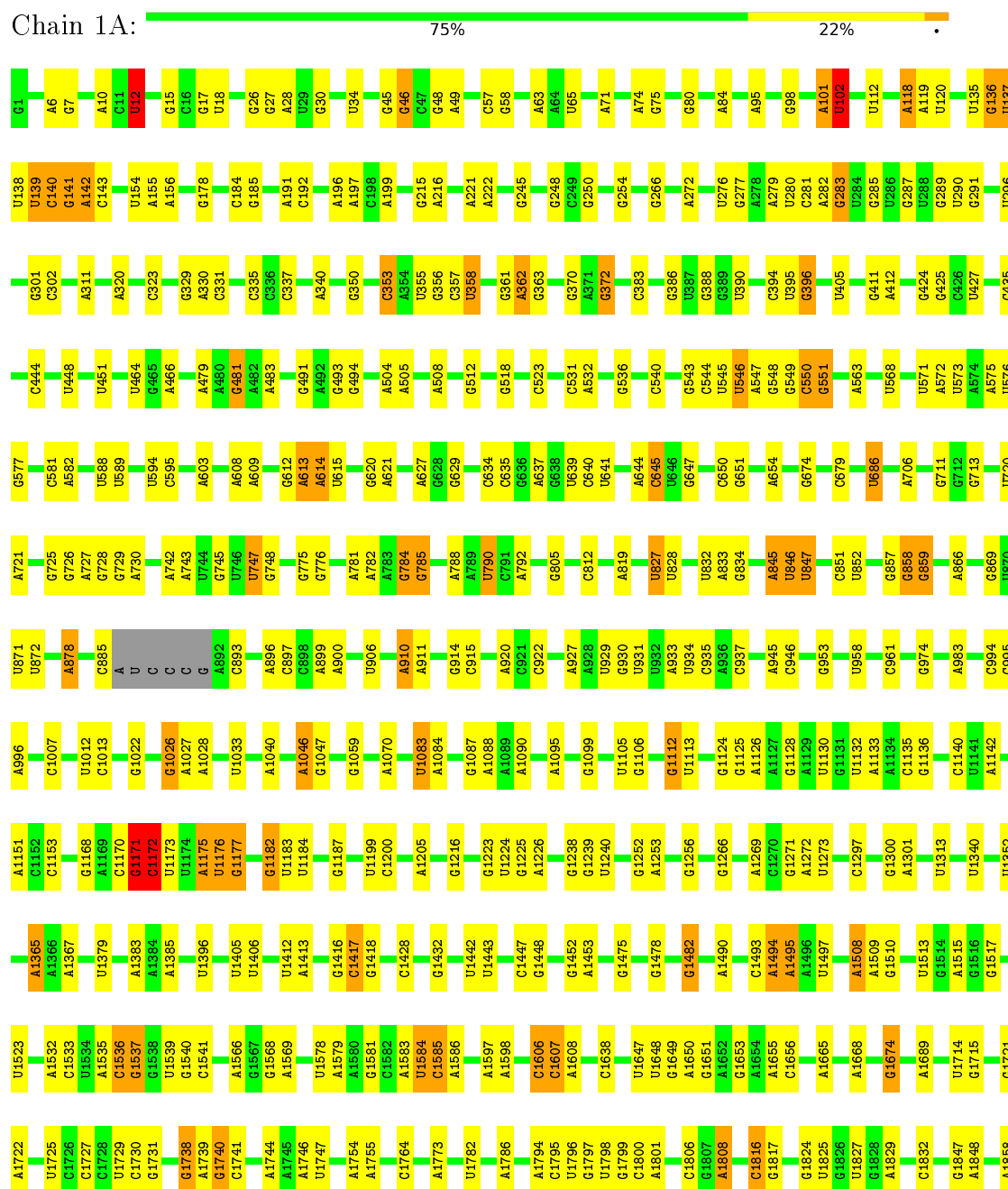
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	19	1	Total	Zn	0
			1	1	

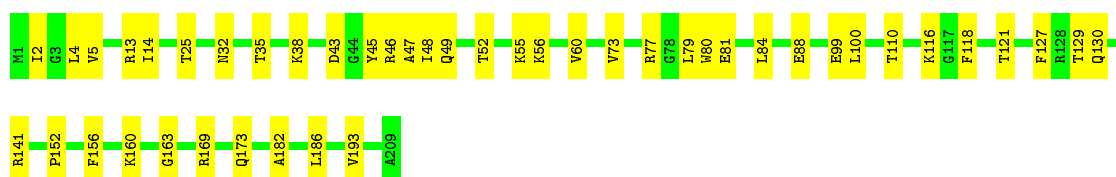
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

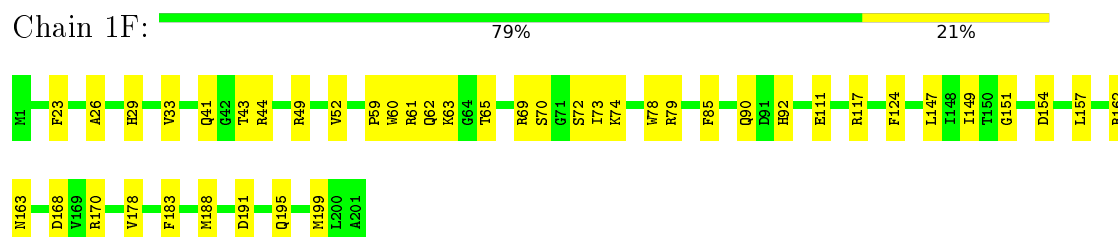
- Molecule 1: 23S Ribosomal RNA



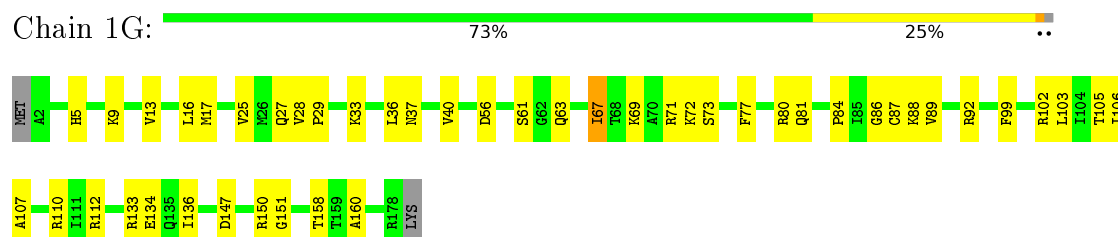




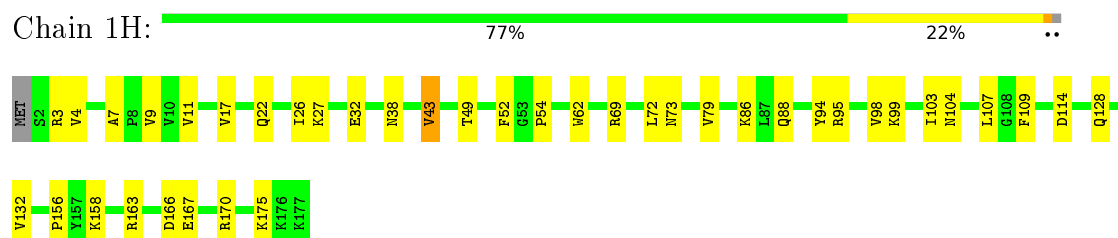
- Molecule 5: 50S ribosomal protein L4



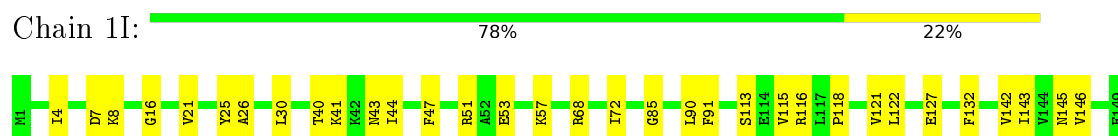
- Molecule 6: 50S ribosomal protein L5



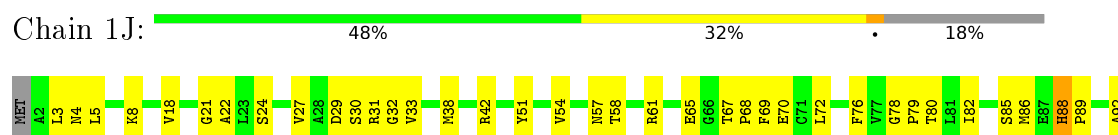
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L10







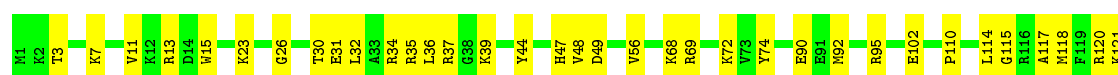
- Molecule 10: 50S ribosomal protein L11

Chain 1K: 63% 30% 6%



- Molecule 11: 50S ribosomal protein L13

Chain 1N: 71% 27%



- Molecule 12: 50S ribosomal protein L14

Chain 1O: 84% 16%



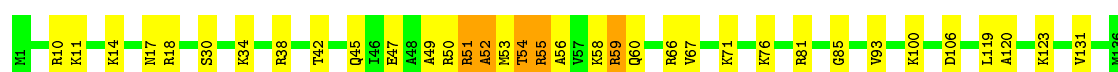
- Molecule 13: 50S ribosomal protein L15

Chain 1P: 81% 19%



- Molecule 14: 50S ribosomal protein L16

Chain 1Q: 74% 22%



- Molecule 15: 50S ribosomal protein L17

Chain 1R: 72% 26%





- Molecule 16: 50S ribosomal protein L18

Chain 1S: 78% 22%



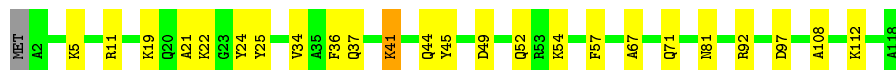
- Molecule 17: 50S ribosomal protein L19

Chain 1T: 70% 29% .



- Molecule 18: 50S ribosomal protein L20

Chain 1U: 79% 19% ..



- Molecule 19: 50S ribosomal protein L21

Chain 1V: 83% 16% .



- Molecule 20: 50S ribosomal protein L22

Chain 1W: 81% 19%



- Molecule 21: 50S ribosomal protein L23

Chain 1X: 73% 20% 7%

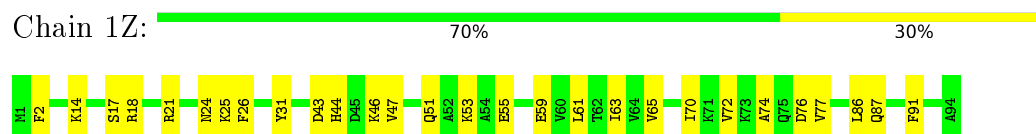


- Molecule 22: 50S ribosomal protein L24

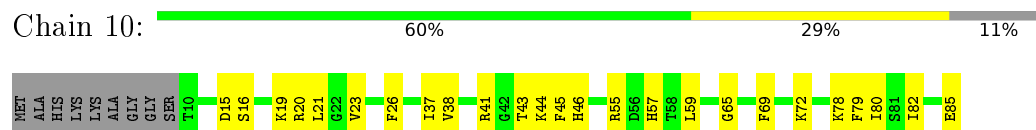
Chain 1Y: 79% 19% .



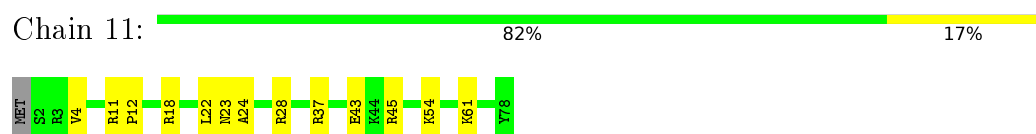
- Molecule 23: 50S ribosomal protein L25



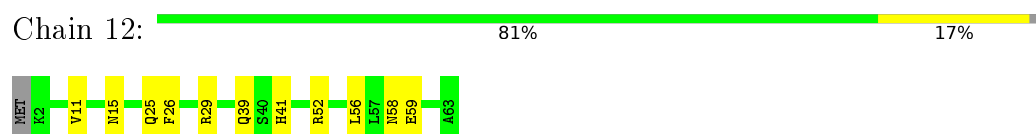
- Molecule 24: 50S ribosomal protein L27



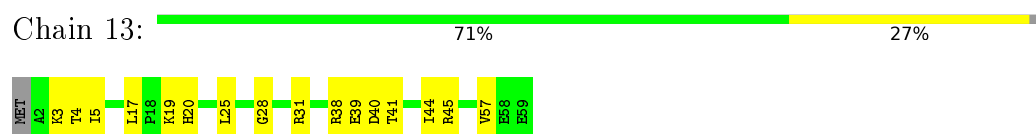
- Molecule 25: 50S ribosomal protein L28



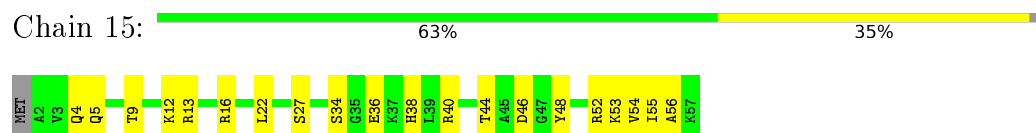
- Molecule 26: 50S ribosomal protein L29



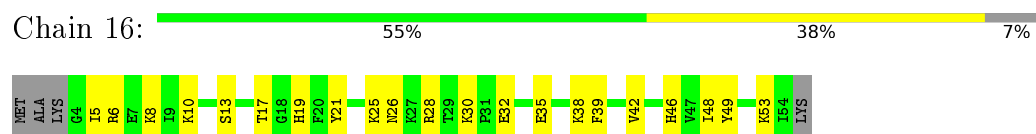
- Molecule 27: 50S ribosomal protein L30



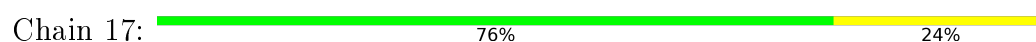
- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L35

Chain 18: 65% 34%



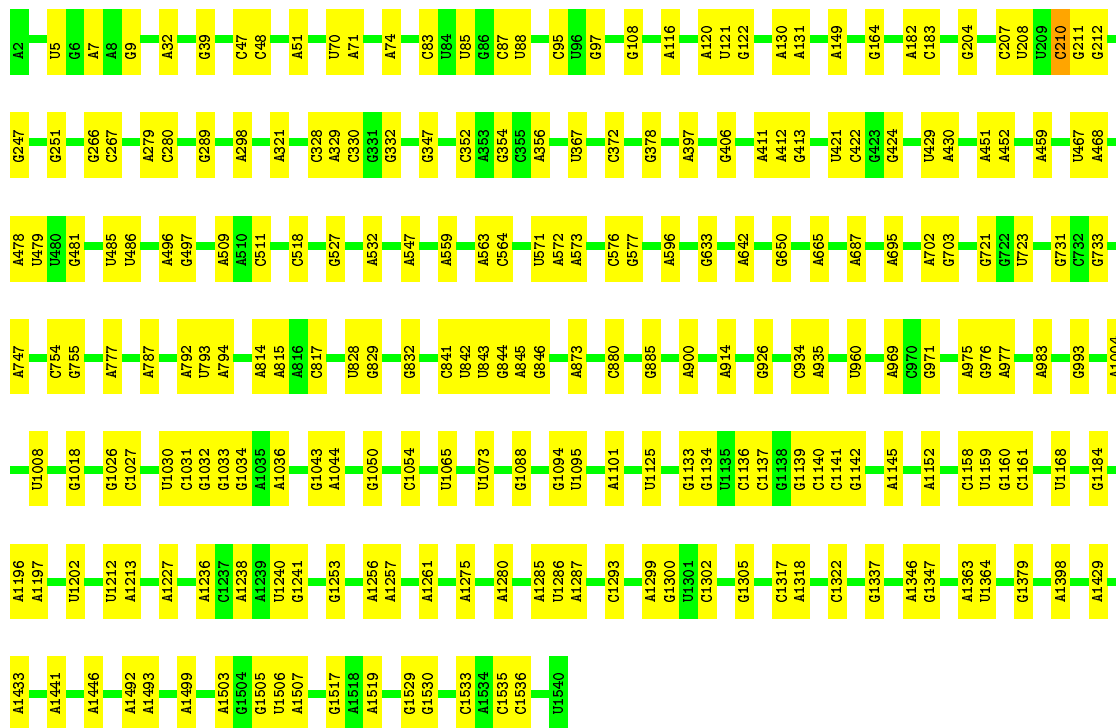
- Molecule 32: 50S ribosomal protein L36

Chain 19: 84% 16%



- Molecule 33: 16S Ribosomal RNA

Chain 1a: 85% 15%




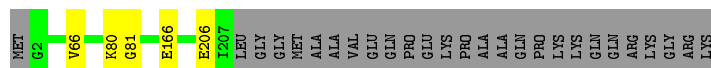
- Molecule 34: 30S ribosomal protein S2

Chain 1b: 87% 10%



- Molecule 35: 30S ribosomal protein S3

Chain 1c:  86% 12%




- Molecule 36: 30S ribosomal protein S4

Chain 1d:  96%



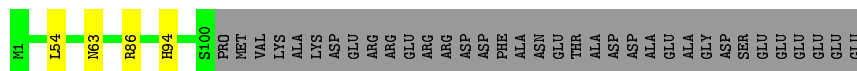
- Molecule 37: 30S ribosomal protein S5

Chain 1e:  86% 10%




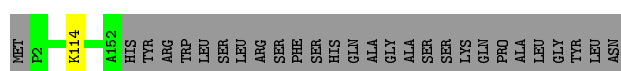
- Molecule 38: 30S ribosomal protein S6

Chain 1f:  71% 26%



- Molecule 39: 30S ribosomal protein S7

Chain 1g:  84% 16%



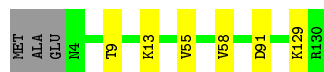
- Molecule 40: 30S ribosomal protein S8

Chain 1h:  99%




- Molecule 41: 30S ribosomal protein S9

Chain 1i:  93% 5%

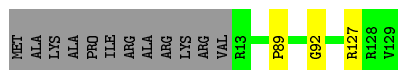


- Molecule 42: 30S ribosomal protein S10

Chain 1j:  89% 6% 5%



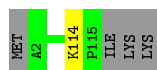
- Molecule 43: 30S ribosomal protein S11



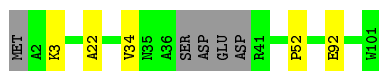
- Molecule 44: 30S ribosomal protein S12



- Molecule 45: 30S ribosomal protein S13



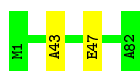
- Molecule 46: 30S ribosomal protein S14



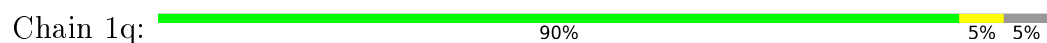
- Molecule 47: 30S ribosomal protein S15



- Molecule 48: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S17




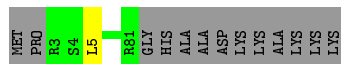
- Molecule 50: 30S ribosomal protein S18

Chain 1r:  73% 27%



- Molecule 51: 30S ribosomal protein S19

Chain 1s:  85% 14%



- Molecule 52: 30S ribosomal protein S20

Chain 1t:  95% ..



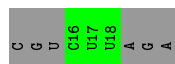
- Molecule 53: 30S ribosomal protein S21

Chain 1u:  65% 7% 28%




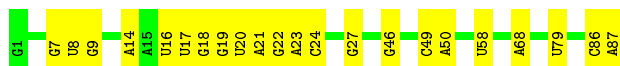
- Molecule 54: mRNA

Chain 1v:  33% 67%



- Molecule 55: P-site tRNA

Chain 1x:  75% 25%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	61651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, OMC, ZN, OMG, OMU, G7M, H2U, 2MA, MEQ, 2MG, 5MC, 6UQ, 6MZ, 1MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	1A	0.27	0/69297	0.81	26/108106 (0.0%)
10	1K	0.29	0/993	0.53	0/1341
11	1N	0.38	0/1152	0.54	0/1551
12	1O	0.30	0/955	0.51	0/1279
13	1P	0.28	0/1062	0.52	0/1413
14	1Q	0.29	0/1115	0.50	0/1488
15	1R	0.27	0/1006	0.49	0/1345
16	1S	0.28	0/910	0.48	0/1219
17	1T	0.29	0/929	0.53	0/1242
18	1U	0.29	0/960	0.43	0/1278
19	1V	0.27	0/829	0.51	0/1107
2	1B	0.23	0/2872	0.77	0/4478
20	1W	0.25	0/864	0.47	0/1156
21	1X	0.27	0/744	0.50	0/994
22	1Y	0.30	0/787	0.52	0/1051
23	1Z	0.28	0/766	0.48	0/1025
24	10	0.29	0/598	0.49	0/790
25	11	0.26	0/635	0.47	0/848
26	12	0.24	0/502	0.41	0/667
27	13	0.27	0/467	0.42	0/623
28	15	0.30	0/450	0.51	0/599
29	16	0.38	0/421	0.55	0/561
3	1D	0.29	0/2121	0.54	0/2852
30	17	0.32	0/380	0.59	0/498
31	18	0.27	0/513	0.49	0/676
32	19	0.26	0/303	0.48	0/397
33	1a	0.25	0/36966	0.73	12/57666 (0.0%)
34	1b	0.25	0/1735	0.42	0/2338
35	1c	0.24	0/1651	0.40	0/2225
36	1d	0.25	0/1665	0.43	0/2227
37	1e	0.26	0/1118	0.46	0/1504
38	1f	0.25	0/835	0.43	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	1g	0.24	0/1195	0.39	0/1602
4	1E	0.28	0/1576	0.50	0/2119
40	1h	0.26	0/989	0.45	0/1326
41	1i	0.25	0/1034	0.47	0/1375
42	1j	0.25	0/796	0.49	0/1077
43	1k	0.25	0/893	0.43	0/1205
44	1l	0.27	0/969	0.48	0/1300
45	1m	0.23	0/892	0.43	0/1193
46	1n	0.23	0/785	0.41	0/1043
47	1o	0.24	0/718	0.41	0/959
48	1p	0.24	0/659	0.43	0/884
49	1q	0.26	0/657	0.47	0/881
5	1F	0.27	0/1571	0.47	0/2113
50	1r	0.24	0/462	0.40	0/621
51	1s	0.25	0/652	0.41	0/877
52	1t	0.23	0/671	0.38	0/888
53	1u	0.26	0/430	0.48	0/570
54	1v	0.33	0/65	0.91	0/98
55	1x	0.25	0/2080	0.76	0/3242
6	1G	0.30	0/1428	0.51	0/1919
7	1H	0.28	0/1343	0.49	0/1816
8	1I	0.29	0/1121	0.51	0/1515
9	1J	0.31	0/1037	0.59	0/1400
All	All	0.27	0/157624	0.72	38/235695 (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
11	1N	0	1
27	13	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	N1-C2-O2	8.80	124.18	118.90
1	1A	1584	U	C2-N1-C1'	8.32	127.68	117.70
1	1A	1584	U	N1-C2-O2	8.29	128.61	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	C2-N1-C1'	8.29	127.91	118.80
33	1a	210	C	N1-C2-O2	8.01	123.70	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	13	3[B]	LYS	Peptide
11	1N	135	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	62361	0	31379	418	0
2	1B	2569	0	1301	18	0
3	1D	2082	0	2154	63	0
4	1E	1576	0	1627	44	0
5	1F	1552	0	1619	40	0
6	1G	1404	0	1433	34	0
7	1H	1323	0	1371	32	0
8	1I	1110	0	1148	20	0
9	1J	1023	0	1050	51	0
10	1K	979	0	1028	32	0
11	1N	1129	0	1162	41	0
12	1O	946	0	1023	12	0
13	1P	1053	0	1129	24	0
14	1Q	1090	0	1183	31	0
15	1R	993	0	1034	28	0
16	1S	900	0	935	24	0
17	1T	917	0	962	39	0
18	1U	947	0	1019	24	0
19	1V	816	0	839	21	0
20	1W	857	0	922	15	0
21	1X	738	0	807	15	0
22	1Y	779	0	831	18	0
23	1Z	753	0	780	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	10	591	0	606	25	0
25	11	625	0	652	13	0
26	12	501	0	531	10	0
27	13	463	0	504	12	0
28	15	444	0	458	23	0
29	16	414	0	442	21	0
30	17	377	0	418	15	0
31	18	504	0	572	22	0
32	19	302	0	340	5	0
33	1a	33015	0	16617	0	0
34	1b	1704	0	1732	0	0
35	1c	1624	0	1696	0	0
36	1d	1643	0	1707	0	0
37	1e	1105	0	1148	0	0
38	1f	817	0	808	0	0
39	1g	1181	0	1238	0	0
40	1h	979	0	1031	0	0
41	1i	1022	0	1070	0	0
42	1j	786	0	828	0	0
43	1k	877	0	887	0	0
44	1l	955	0	1016	0	0
45	1m	883	0	941	0	0
46	1n	774	0	824	0	0
47	1o	710	0	728	0	0
48	1p	649	0	666	0	0
49	1q	648	0	691	0	0
50	1r	455	0	478	0	0
51	1s	637	0	665	0	0
52	1t	665	0	714	0	0
53	1u	425	0	449	0	0
54	1v	60	0	32	0	0
55	1x	1861	0	938	0	0
56	1A	95	0	0	2	0
57	19	1	0	0	0	0
All	All	145689	0	98163	965	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 965 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1J:22:ALA:HB2	9:1J:86:MET:SD	1.64	1.35
1:1A:1847:G:N2	1:1A:1848:A:H62	1.52	1.07
9:1J:22:ALA:CB	9:1J:86:MET:SD	2.48	1.02
1:1A:1847:G:H21	1:1A:1848:A:N6	1.63	0.97
1:1A:1799:G:OP1	3:1D:258:ARG:NH1	2.03	0.91

There are no symmetry-related clashes.

## 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	
3	1D	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	39	80
4	1E	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
5	1F	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	1G	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
7	1H	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
8	1I	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	14	59
9	1J	133/165 (81%)	114 (86%)	13 (10%)	6 (4%)	3	31
10	1K	132/142 (93%)	122 (92%)	6 (4%)	4 (3%)	5	44
11	1N	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	1O	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	24	69
13	1P	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	1Q	136/136 (100%)	126 (93%)	8 (6%)	2 (2%)	13	57
15	1R	123/127 (97%)	117 (95%)	5 (4%)	1 (1%)	24	69
16	1S	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	1T	112/115 (97%)	108 (96%)	3 (3%)	1 (1%)	21	67
18	1U	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1V	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	19	66
20	1W	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
21	1X	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	17	64
22	1Y	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	19	66
23	1Z	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	10	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	11	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	12	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	13	57/59 (97%)	55 (96%)	1 (2%)	1 (2%)	11	54
28	15	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	16	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	17	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
31	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	19	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	1b	216/241 (90%)	189 (88%)	19 (9%)	8 (4%)	4	38
35	1c	204/233 (88%)	180 (88%)	19 (9%)	5 (2%)	7	48
36	1d	203/206 (98%)	187 (92%)	8 (4%)	8 (4%)	4	36
37	1e	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	3	30
38	1f	98/135 (73%)	84 (86%)	10 (10%)	4 (4%)	3	34
39	1g	149/179 (83%)	141 (95%)	7 (5%)	1 (1%)	26	72
40	1h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
41	1i	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	3	30
42	1j	96/103 (93%)	83 (86%)	7 (7%)	6 (6%)	2	23
43	1k	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	7	46
44	1l	121/124 (98%)	106 (88%)	9 (7%)	6 (5%)	3	29
45	1m	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	21	67
46	1n	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	2	27
47	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
48	1p	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	7	48
49	1q	78/84 (93%)	62 (80%)	12 (15%)	4 (5%)	2	28
50	1r	53/75 (71%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1s	77/92 (84%)	72 (94%)	4 (5%)	1 (1%)	15	60
52	1t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	49
53	1u	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	1	11
All	All	5755/6150 (94%)	5333 (93%)	326 (6%)	96 (2%)	16	55

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1K	15	ALA
10	1K	19	ASN
14	1Q	51	ARG
22	1Y	52	LEU
36	1d	30	THR

### 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	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	163/163 (100%)	163 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	147/150 (98%)	146 (99%)	1 (1%)	88	96
7	1H	137/138 (99%)	136 (99%)	1 (1%)	88	96
8	1I	114/114 (100%)	114 (100%)	0	100	100
9	1J	103/123 (84%)	102 (99%)	1 (1%)	82	93
10	1K	104/110 (94%)	104 (100%)	0	100	100
11	1N	116/116 (100%)	114 (98%)	2 (2%)	68	89
12	1O	104/104 (100%)	104 (100%)	0	100	100
13	1P	103/103 (100%)	103 (100%)	0	100	100
14	1Q	111/109 (102%)	106 (96%)	5 (4%)	34	74
15	1R	102/103 (99%)	101 (99%)	1 (1%)	82	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1S	87/87 (100%)	87 (100%)	0	100	100
17	1T	99/100 (99%)	99 (100%)	0	100	100
18	1U	89/90 (99%)	88 (99%)	1 (1%)	80	92
19	1V	84/84 (100%)	84 (100%)	0	100	100
20	1W	93/93 (100%)	93 (100%)	0	100	100
21	1X	80/84 (95%)	80 (100%)	0	100	100
22	1Y	83/85 (98%)	83 (100%)	0	100	100
23	1Z	78/78 (100%)	78 (100%)	0	100	100
24	10	58/63 (92%)	58 (100%)	0	100	100
25	11	67/68 (98%)	67 (100%)	0	100	100
26	12	54/55 (98%)	54 (100%)	0	100	100
27	13	49/49 (100%)	49 (100%)	0	100	100
28	15	47/48 (98%)	47 (100%)	0	100	100
29	16	45/49 (92%)	45 (100%)	0	100	100
30	17	38/38 (100%)	38 (100%)	0	100	100
31	18	51/52 (98%)	51 (100%)	0	100	100
32	19	34/34 (100%)	34 (100%)	0	100	100
34	1b	180/199 (90%)	180 (100%)	0	100	100
35	1c	170/190 (90%)	170 (100%)	0	100	100
36	1d	172/173 (99%)	172 (100%)	0	100	100
37	1e	113/126 (90%)	113 (100%)	0	100	100
38	1f	87/116 (75%)	87 (100%)	0	100	100
39	1g	124/147 (84%)	124 (100%)	0	100	100
40	1h	104/105 (99%)	104 (100%)	0	100	100
41	1i	105/107 (98%)	105 (100%)	0	100	100
42	1j	86/90 (96%)	86 (100%)	0	100	100
43	1k	90/99 (91%)	90 (100%)	0	100	100
44	1l	103/104 (99%)	103 (100%)	0	100	100
45	1m	92/96 (96%)	92 (100%)	0	100	100
46	1n	79/84 (94%)	79 (100%)	0	100	100
47	1o	75/77 (97%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1p	65/65 (100%)	65 (100%)	0	100	100
49	1q	74/78 (95%)	74 (100%)	0	100	100
50	1r	48/65 (74%)	48 (100%)	0	100	100
51	1s	70/79 (89%)	70 (100%)	0	100	100
52	1t	65/66 (98%)	65 (100%)	0	100	100
53	1u	44/61 (72%)	44 (100%)	0	100	100
All	All	4767/5000 (95%)	4755 (100%)	12 (0%)	95	99

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	1Q	54	THR
14	1Q	55	ARG
14	1Q	60	GLN
11	1N	142	ILE
14	1Q	59	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
21	1X	92	ASN
26	12	58	ASN
48	1p	63	GLN
24	10	57	HIS
27	13	20	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2884/2904 (99%)	360 (12%)	10 (0%)
2	1B	119/120 (99%)	8 (6%)	0
33	1a	1538/1539 (99%)	226 (14%)	0
54	1v	2/9 (22%)	0	0
55	1x	86/87 (98%)	22 (25%)	0
All	All	4629/4659 (99%)	616 (13%)	10 (0%)

5 of 616 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	15	G
1	1A	34	U
1	1A	46	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2127	G
1	1A	2158	A
1	1A	2406	A
1	1A	2118	U
1	1A	2324	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

26 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	$\# Z  > 2$
1	6MZ	1A	1618	1	17,25,26	1.00	1 (5%)	15,36,39	2.49	2 (13%)
1	2MG	1A	1835	1	18,26,27	1.16	2 (11%)	21,38,41	2.19	6 (28%)
1	PSU	1A	1911	1	15,21,22	1.36	1 (6%)	16,30,33	2.22	4 (25%)
1	PSU	1A	1915	1	15,21,22	1.37	1 (6%)	16,30,33	2.21	4 (25%)
1	PSU	1A	1917	1	15,21,22	1.34	1 (6%)	16,30,33	2.21	4 (25%)
1	5MU	1A	1939	1	13,22,23	0.59	0	16,32,35	2.47	2 (12%)
1	5MC	1A	1962	1	14,22,23	1.33	1 (7%)	17,32,35	0.82	1 (5%)
1	6MZ	1A	2030	1	17,25,26	0.92	1 (5%)	15,36,39	2.82	3 (20%)
1	G7M	1A	2069	1	18,26,27	0.99	1 (5%)	21,39,42	2.67	8 (38%)
1	OMG	1A	2251	1,55	18,26,27	1.18	2 (11%)	21,38,41	1.92	4 (19%)
1	2MG	1A	2445	1	18,26,27	1.14	2 (11%)	21,38,41	2.30	7 (33%)
1	H2U	1A	2449	1	17,21,22	1.04	2 (11%)	23,30,33	1.95	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	2457	1	15,21,22	1.35	1 (6%)	16,30,33	2.06	3 (18%)
1	OMC	1A	2498	1	15,22,23	0.62	0	20,31,34	2.07	1 (5%)
1	2MA	1A	2503	1	17,25,26	1.55	3 (17%)	18,37,40	2.67	1 (5%)
1	PSU	1A	2504	1	15,21,22	1.30	1 (6%)	16,30,33	2.32	4 (25%)
1	OMU	1A	2552	1	14,22,23	0.67	0	19,31,34	1.52	1 (5%)
1	PSU	1A	2580	1	15,21,22	1.46	2 (13%)	16,30,33	2.15	3 (18%)
1	PSU	1A	2604	1	15,21,22	1.33	1 (6%)	16,30,33	2.39	4 (25%)
1	PSU	1A	2605	1	15,21,22	1.42	1 (6%)	16,30,33	2.29	4 (25%)
1	1MG	1A	745	1	17,26,27	1.34	2 (11%)	19,39,42	0.71	0
1	PSU	1A	746	1	15,21,22	1.51	2 (13%)	16,30,33	2.19	3 (18%)
1	5MU	1A	747	1	13,22,23	0.55	0	16,32,35	2.56	2 (12%)
1	PSU	1A	955	1	15,21,22	1.37	1 (6%)	16,30,33	2.09	4 (25%)
4	MEQ	1E	150[A]	4	7,9,10	0.51	0	8,10,12	1.08	1 (12%)
4	MEQ	1E	150[B]	4	7,9,10	0.56	0	8,10,12	1.14	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	1A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1A	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1,55	-	0/5/27/28	0/3/3/3
1	2MG	1A	2445	1	-	0/5/27/28	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/5/27/28	0/2/2/2
1	2MA	1A	2503	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	746	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
4	MEQ	1E	150[A]	4	-	0/7/9/11	0/0/0/0
4	MEQ	1E	150[B]	4	-	1/7/9/11	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	746	PSU	C5-C1'	-4.55	1.48	1.52
1	1A	2580	PSU	C5-C1'	-4.49	1.48	1.52
1	1A	2605	PSU	C5-C1'	-4.45	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.21	1.48	1.52
1	1A	1915	PSU	C5-C1'	-4.20	1.48	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	747	5MU	C5-C4-N3	-7.70	118.88	125.35
1	1A	1939	5MU	C5-C4-N3	-7.47	119.07	125.35
1	1A	2030	6MZ	N3-C2-N1	-7.03	123.35	128.87
1	1A	2069	G7M	C2'-C1'-N9	-6.32	96.53	113.47
1	1A	1618	6MZ	N3-C2-N1	-6.09	124.09	128.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1E	150[B]	MEQ	CG-CD-NE2-CE

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	5MU	1	0
1	1A	2030	6MZ	1	0
1	1A	2069	G7M	4	0
1	1A	2251	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2498	OMC	1	0
1	1A	2604	PSU	1	0
1	1A	745	1MG	1	0
1	1A	747	5MU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	6UQ	1A	3001	1	101,105,105	1.59	13 (12%)	125,164,164	2.09	38 (30%)

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
56	6UQ	1A	3001	1	-	0/47/211/211	0/11/11/11

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	CDF-CAC	-5.41	1.40	1.51
56	1A	3001	6UQ	CAD-CAJ	-4.02	1.40	1.50
56	1A	3001	6UQ	CCL-CCM	-3.35	1.48	1.54
56	1A	3001	6UQ	O1-C1	2.21	1.47	1.41
56	1A	3001	6UQ	OAL-CAM	2.21	1.48	1.44

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	CCC-OCH-CCU	-7.83	105.14	118.06
56	1A	3001	6UQ	CCZ-CCO-CCN	-6.58	104.75	114.68
56	1A	3001	6UQ	CBC-CBF-CBG	-6.25	104.14	115.04
56	1A	3001	6UQ	OCI-CCD-CCE	-5.08	97.02	103.51
56	1A	3001	6UQ	CAP-OAQ-CAR	-4.05	104.69	114.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1A	3001	6UQ	2	0

## 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.