



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 12:37 PM EDT

PDB ID : 5MDV  
EMDB ID: : EMD-3489  
Title : Structure of ArfA and RF2 bound to the 70S ribosome (accommodated state)  
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : unknown  
Resolution : 2.97 Å(reported)

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

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

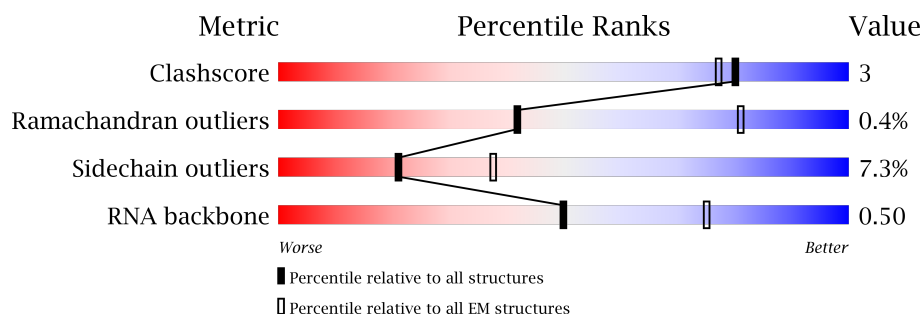
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 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.














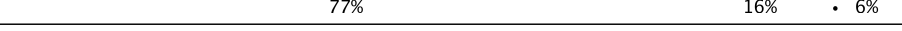







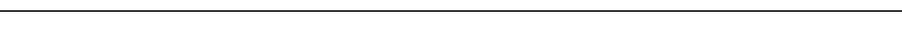

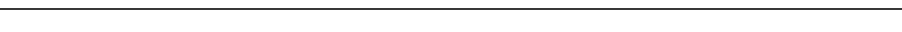
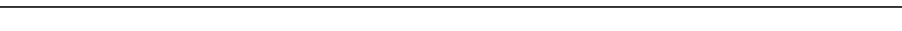


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1	2904	73% 24% .
2	2	1534	72% 25% .
3	3	120	87% 13% .
4	4	18	22% 6% 72%
5	5	78	62% 31% 5% .
6	6	61	57% 18% 25%
7	7	365	83% 14% ..
8	B	273	86% 12% ..








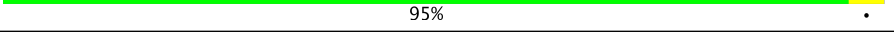



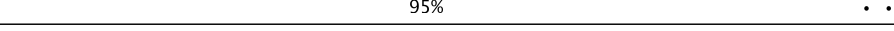





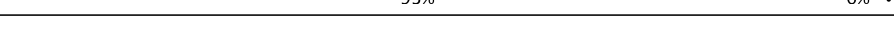

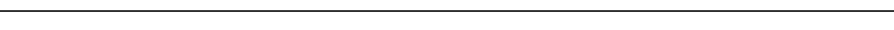

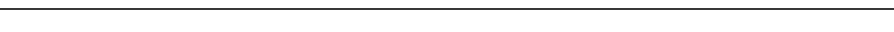
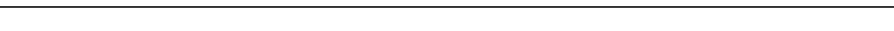


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Mol	Chain	Length	Quality of chain
9	C	209	 89% 11% .
10	D	201	 87% 12%
11	E	179	 84% 14% ..
12	F	177	 89% 9% ..
13	G	149	 85% 13% .
14	H	165	 61% 16% . 21%
15	I	142	 79% 15% . 5%
16	J	142	 88% 10% .
17	K	123	 86% 13% .
18	L	144	 83% 15% .
19	M	136	 89% 9% .
20	N	127	 77% 16% . 6%
21	O	117	 81% 17% ..
22	P	115	 84% 15% .
23	Q	118	 84% 14% ..
24	R	103	 92% 8%
25	S	110	 79% 20% .
26	T	100	 81% 13% 6%
27	U	104	 87% 12% ..
28	V	94	 93% 7%
29	W	85	 82% 7% 11%
30	X	78	 81% 18% .
31	Y	63	 86% 13% .
32	Z	59	 92% 7% .
33	a	70	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
34	b	57	 93% 5% .
35	c	55	 91% . 5%
36	d	46	 93% 7%
37	e	65	 94% 5% .
38	f	38	 92% 8%
39	g	241	 91% . 7%
40	h	233	 84% 5% 11%
41	i	206	 95% .
42	j	167	 84% 9% 7%
43	k	135	 71% 5% . 23%
44	l	179	 78% 6% . 15%
45	m	130	 95% . .
46	n	130	 91% 6% . .
47	o	103	 87% 8% . .
48	p	129	 85% 5% 9%
49	q	124	 92% 7% .
50	r	118	 90% 8% .
51	s	101	 93% 6% .
52	t	89	 87% 12% .
53	u	82	 93% 7%
54	v	84	 90% 5% 5%
55	w	75	 85% . 12%
56	x	92	 86% . 10%
57	y	87	 91% 8% .
58	z	71	 96% . .

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149892 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	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	234	77	64	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	362	Total	C	N	O	S	0	0
			2863	1762	501	590	10		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 14 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	103	Total	C	N	O	S	0	0
			788	498	148	142			

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

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

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

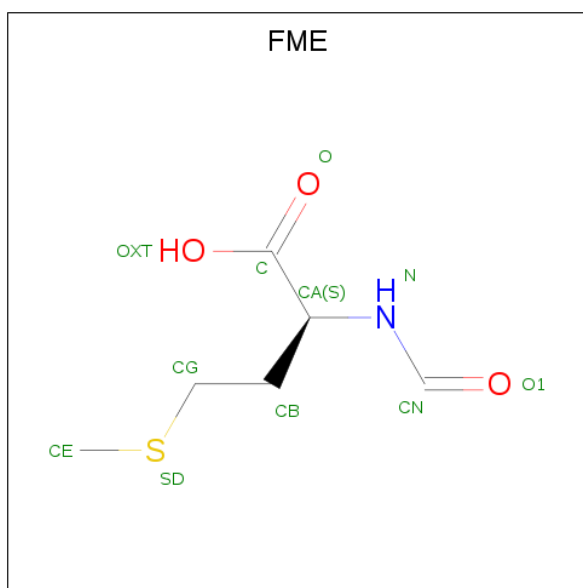
- Molecule 58 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	296	Total	Mg	0
			296	296	
59	b	1	Total	Mg	0
			1	1	
59	i	1	Total	Mg	0
			1	1	
59	5	4	Total	Mg	0
			4	4	
59	2	129	Total	Mg	0
			129	129	
59	3	9	Total	Mg	0
			9	9	

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



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
61	a	1	Total	Zn	0
			1	1	
61	f	1	Total	Zn	0
			1	1	

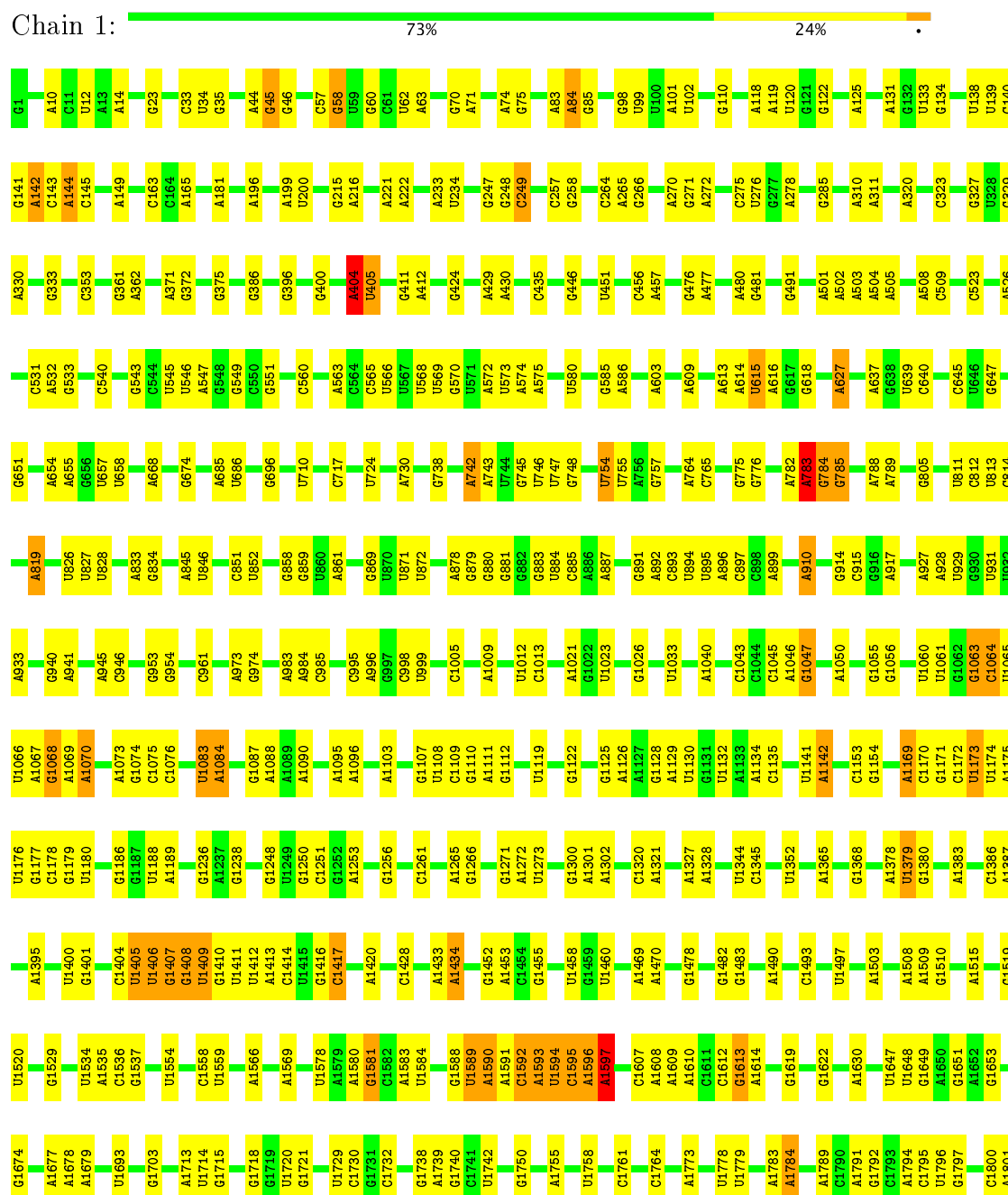
- Molecule 62 is water.

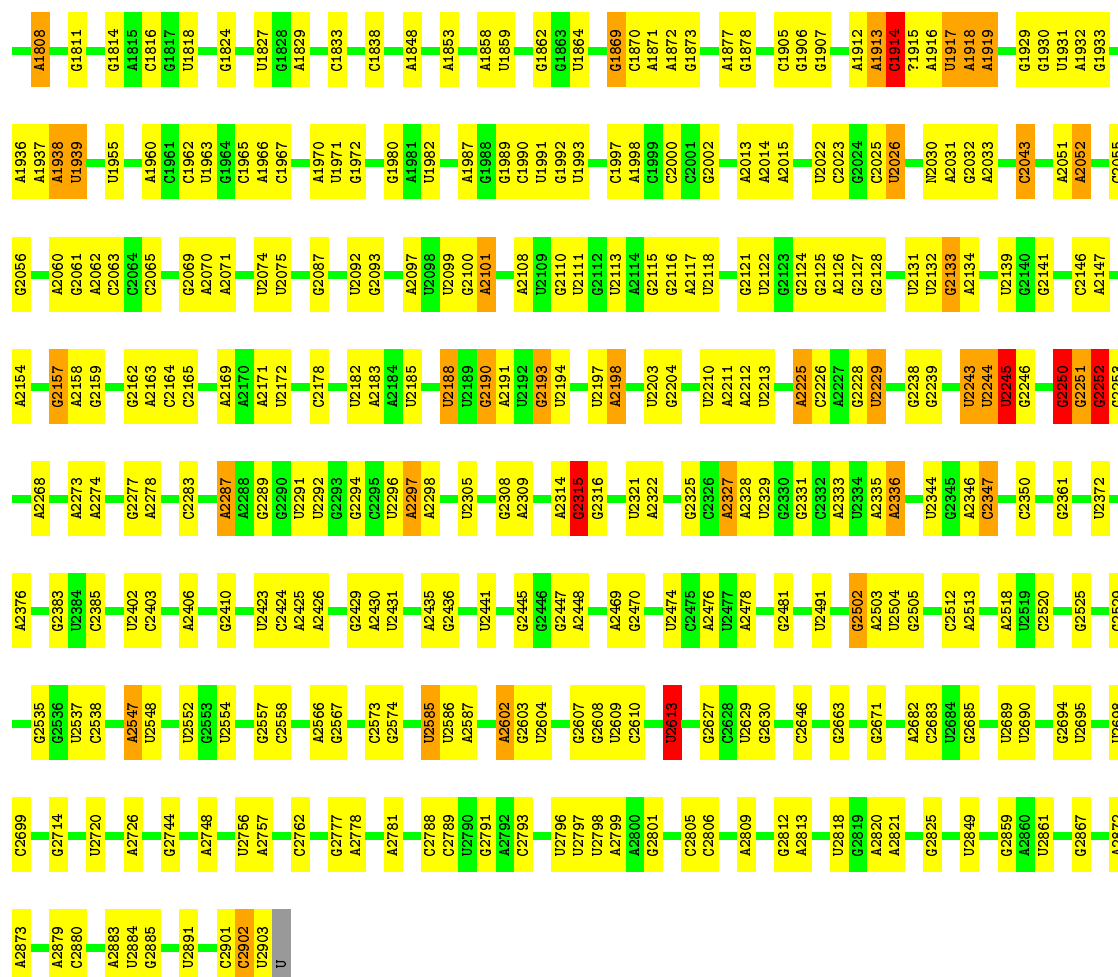
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	

### 3 Residue-property plots

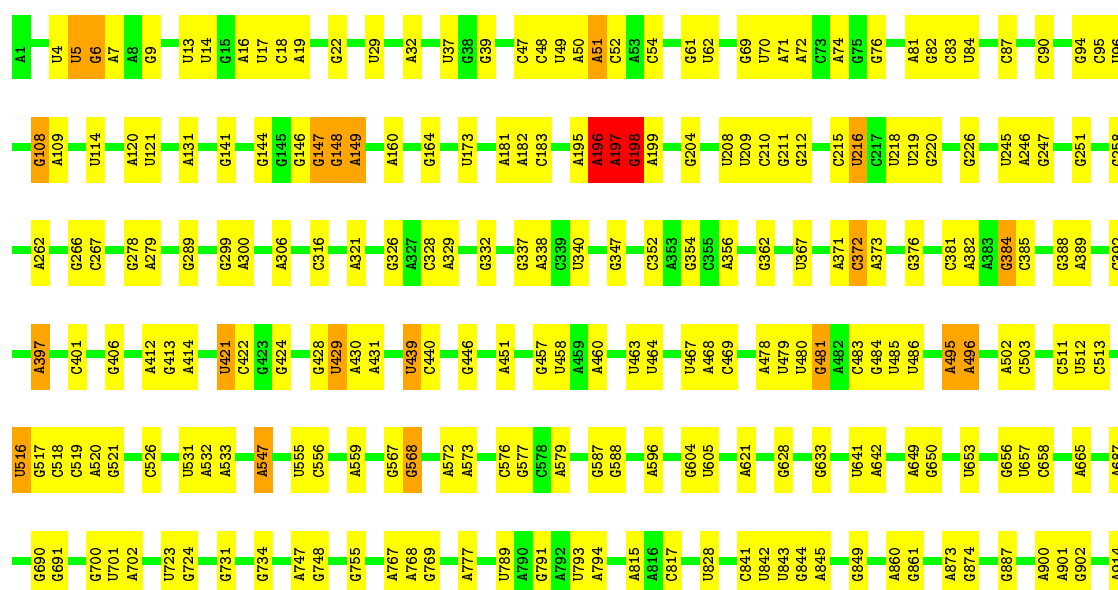
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

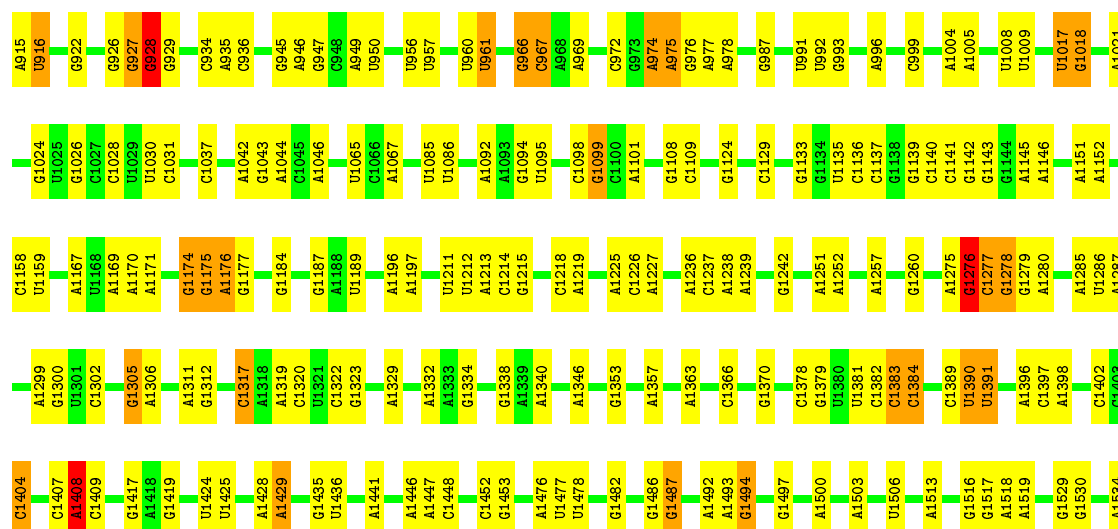
#### • Molecule 1: 23S ribosomal RNA



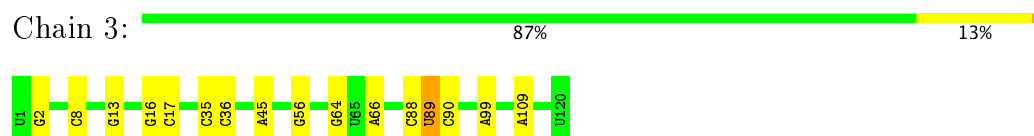


- Molecule 2: 16S ribosomal RNA





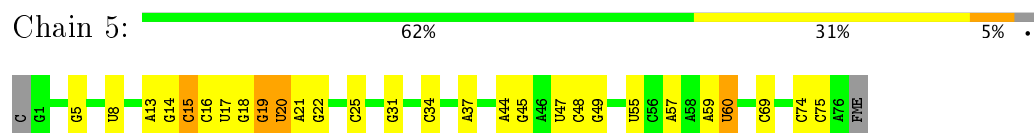
• Molecule 3: 5S ribosomal RNA



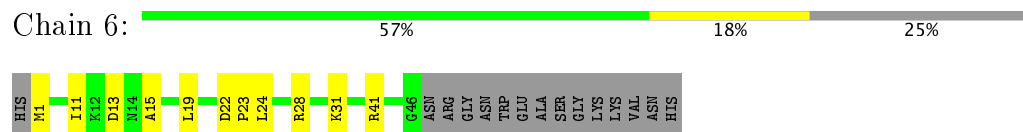
• Molecule 4: mRNA



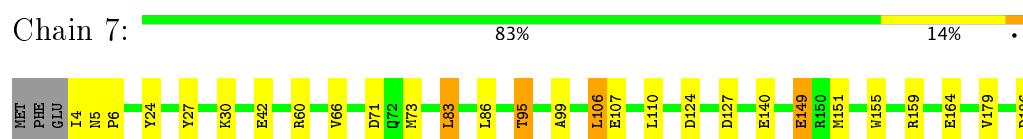
• Molecule 5: fMet-NH-tRNA(fMet)



• Molecule 6: Alternative ribosome-rescue factor A



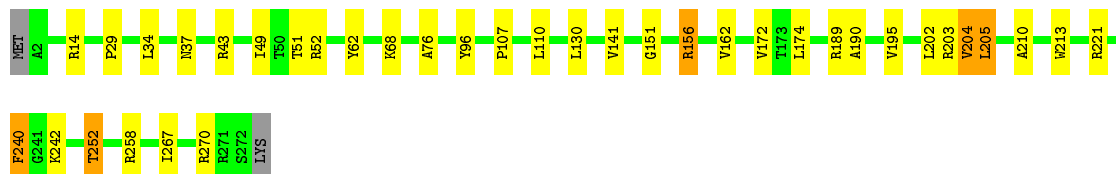
• Molecule 7: Peptide chain release factor 2





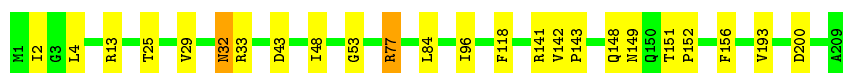
• Molecule 8: 50S ribosomal protein L2

Chain B: 86% 12% ..



• Molecule 9: 50S ribosomal protein L3

Chain C: 89% 11% .



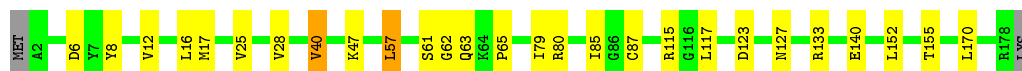
• Molecule 10: 50S ribosomal protein L4

Chain D: 87% 12%



• Molecule 11: 50S ribosomal protein L5

Chain E: 84% 14% ..



• Molecule 12: 50S ribosomal protein L6

Chain F: 89% 9% ..



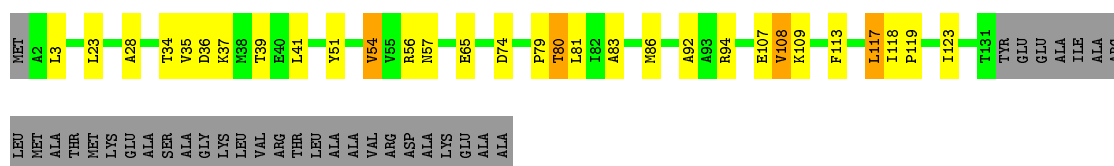
• Molecule 13: 50S ribosomal protein L9

Chain G: 85% 13% .



• Molecule 14: 50S ribosomal protein L10

Chain H: 61% 16% . 21%



- Molecule 15: 50S ribosomal protein L11

Chain I: 79% 15% 5%



- Molecule 16: 50S ribosomal protein L13

Chain J: 88% 10% 2%



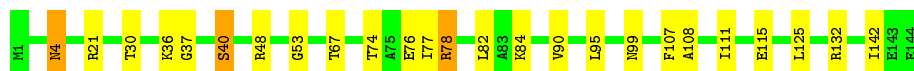
- Molecule 17: 50S ribosomal protein L14

Chain K: 86% 13% 1%



- Molecule 18: 50S ribosomal protein L15

Chain L: 83% 15% 2%



- Molecule 19: 50S ribosomal protein L16

Chain M: 89% 9% 2%



- Molecule 20: 50S ribosomal protein L17

Chain N: 77% 16% 6%



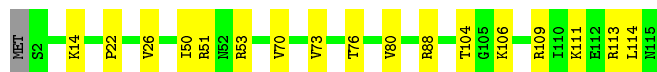
- Molecule 21: 50S ribosomal protein L18

Chain O: 81% 17% 2%



- Molecule 22: 50S ribosomal protein L19

Chain P: 84% 15%



- Molecule 23: 50S ribosomal protein L20

Chain Q: 84% 14%



- Molecule 24: 50S ribosomal protein L21

Chain R: 92% 8%



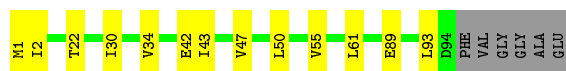
- Molecule 25: 50S ribosomal protein L22

Chain S: 79% 20%



- Molecule 26: 50S ribosomal protein L23

Chain T: 81% 13% 6%



- Molecule 27: 50S ribosomal protein L24

Chain U: 87% 12%




- Molecule 28: 50S ribosomal protein L25

Chain V: 93% 7%




- Molecule 29: 50S ribosomal protein L27

Chain W:  82% 7% 11%




- Molecule 30: 50S ribosomal protein L28

Chain X:  81% 18% .



- Molecule 31: 50S ribosomal protein L29

Chain Y:  86% 13% .




- Molecule 32: 50S ribosomal protein L30

Chain Z:  92% 7% .



- Molecule 33: 50S ribosomal protein L31

Chain a:  87% 7% 6%




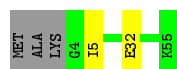
- Molecule 34: 50S ribosomal protein L32

Chain b:  93% 5% .



- Molecule 35: 50S ribosomal protein L33

Chain c:  91% . 5%



- Molecule 36: 50S ribosomal protein L34

Chain d:  93% 7%



- Molecule 37: 50S ribosomal protein L35

Chain e: 94% 5%



- Molecule 38: 50S ribosomal protein L36

Chain f: 92% 8%



- Molecule 39: 30S ribosomal protein S2

Chain g: 91% 7%



- Molecule 40: 30S ribosomal protein S3

Chain h: 84% 5% 11%



- Molecule 41: 30S ribosomal protein S4

Chain i: 95% 5%



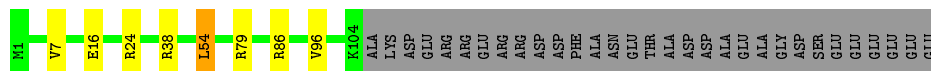
- Molecule 42: 30S ribosomal protein S5

Chain j: 84% 9% 7%

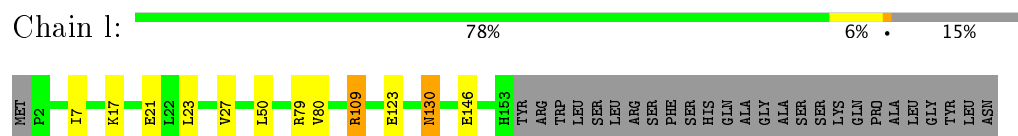


- Molecule 43: 30S ribosomal protein S6

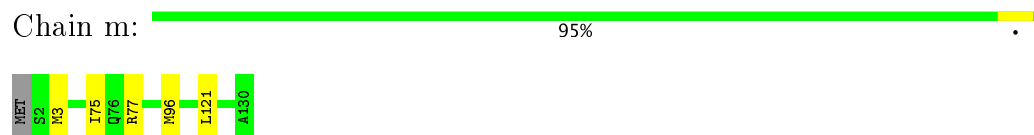
Chain k: 71% 5% 23%



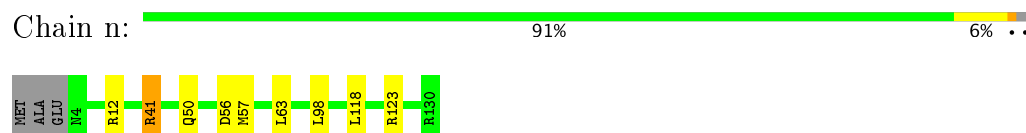
- Molecule 44: 30S ribosomal protein S7



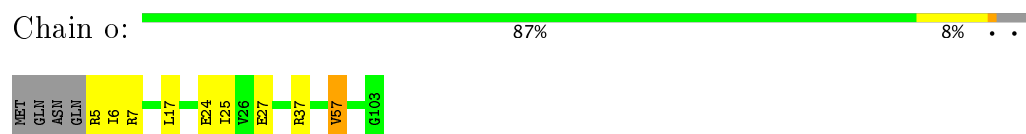
- Molecule 45: 30S ribosomal protein S8



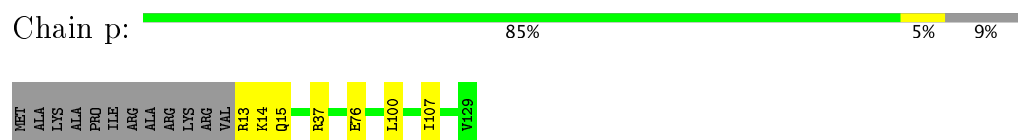
- Molecule 46: 30S ribosomal protein S9



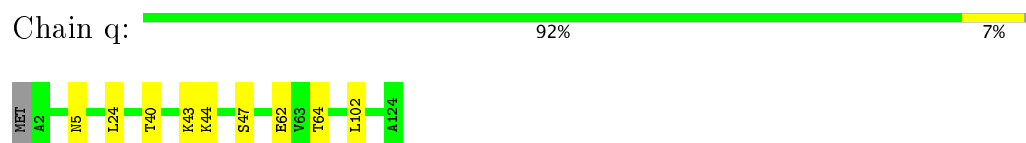
- Molecule 47: 30S ribosomal protein S10



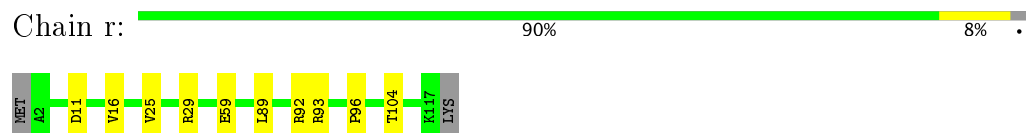
- Molecule 48: 30S ribosomal protein S11



- Molecule 49: 30S ribosomal protein S12

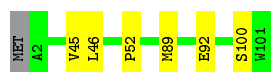


- Molecule 50: 30S ribosomal protein S13




- Molecule 51: 30S ribosomal protein S14

Chain s:  93% 6%



- Molecule 52: 30S ribosomal protein S15

Chain t:  87% 12%




- Molecule 53: 30S ribosomal protein S16

Chain u:  93% 7%




- Molecule 54: 30S ribosomal protein S17

Chain v:  90% 5% 5%



- Molecule 55: 30S ribosomal protein S18

Chain w:  85% 12%



- Molecule 56: 30S ribosomal protein S19

Chain x:  86% 10%



- Molecule 57: 30S ribosomal protein S20

Chain y:  91% 8%



- Molecule 58: 30S ribosomal protein S21

Chain z:  96%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139792	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 0TD, 2MA, 2MG, 1MG, 3TD, G7M, 8AN, UR3, 7MG, 5MU, ZN, OMU, 6MZ, FME, OMC, MG, OMG, H2U, MEQ, 5MC, 4OC, 4SU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	1	0.35	0/69286	0.72	22/108087 (0.0%)
10	D	0.45	0/1571	0.77	1/2113 (0.0%)
11	E	0.46	0/1434	0.78	0/1926
12	F	0.39	0/1333	0.67	0/1805
13	G	0.43	0/1122	0.67	0/1515
14	H	0.50	0/993	0.74	0/1340
15	I	0.46	0/998	0.68	0/1348
16	J	0.44	0/1152	0.72	0/1551
17	K	0.39	0/955	0.75	0/1279
18	L	0.43	0/1062	0.78	0/1413
19	M	0.44	0/1093	0.78	0/1460
2	2	0.35	0/36590	0.73	19/57074 (0.0%)
20	N	0.49	0/964	0.87	0/1289
21	O	0.47	0/902	0.80	0/1209
22	P	0.41	0/929	0.77	0/1242
23	Q	0.57	0/960	0.89	0/1278
24	R	0.34	0/829	0.64	0/1107
25	S	0.47	0/864	0.82	0/1156
26	T	0.41	0/752	0.72	0/1005
27	U	0.34	0/796	0.61	0/1062
28	V	0.40	0/766	0.67	0/1025
29	W	0.42	0/589	0.75	0/779
3	3	0.26	0/2872	0.69	0/4478
30	X	0.46	0/635	0.80	0/848
31	Y	0.53	0/502	0.86	0/667
32	Z	0.43	0/452	0.76	0/605
33	a	0.39	0/531	0.73	0/709
34	b	0.43	0/450	0.78	0/599
35	c	0.37	0/433	0.69	0/576
36	d	0.51	0/380	0.96	0/498
37	e	0.45	0/513	0.82	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	f	0.38	0/303	0.79	0/397
39	g	0.46	0/1791	0.70	0/2413
4	4	0.34	0/122	0.60	0/188
40	h	0.47	0/1663	0.74	0/2241
41	i	0.47	0/1665	0.78	0/2227
42	j	0.50	0/1165	0.79	0/1568
43	k	0.43	0/867	0.75	1/1171 (0.1%)
44	l	0.51	0/1206	0.85	1/1617 (0.1%)
45	m	0.42	0/989	0.69	0/1326
46	n	0.44	0/1034	0.81	1/1375 (0.1%)
47	o	0.41	0/800	0.76	0/1082
48	p	0.41	0/893	0.74	0/1205
49	q	0.46	0/960	0.81	0/1286
5	5	0.29	0/1672	0.73	0/2603
50	r	0.48	0/909	0.85	0/1215
51	s	0.50	0/817	0.80	0/1088
52	t	0.56	0/722	0.86	0/964
53	u	0.46	0/659	0.78	0/884
54	v	0.34	0/657	0.66	0/881
55	w	0.46	0/553	0.79	0/743
56	x	0.39	0/680	0.68	0/915
57	y	0.59	0/675	0.86	0/895
58	z	0.55	0/597	0.88	0/792
6	6	0.41	0/383	0.68	0/504
7	7	0.49	0/2892	0.76	0/3897
8	B	0.39	0/2121	0.78	0/2852
9	C	0.40	0/1586	0.68	0/2134
All	All	0.38	0/161089	0.73	45/240182 (0.0%)

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	198	G	N9-C1'-C2'	-10.10	100.87	114.00
2	2	1408	A	N9-C1'-C2'	-9.66	101.38	112.00
2	2	1404	C	N1-C1'-C2'	-9.40	101.66	112.00
2	2	928	G	N9-C1'-C2'	-9.08	102.01	112.00
2	2	927	G	N9-C1'-C2'	-8.22	102.96	112.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31369	269	0
2	2	32929	0	16587	148	0
3	3	2569	0	1301	2	0
4	4	109	0	55	0	0
5	5	1622	0	830	5	0
6	6	377	0	393	10	0
7	7	2863	0	2760	26	0
8	B	2082	0	2154	24	0
9	C	1565	0	1616	16	0
10	D	1552	0	1619	9	0
11	E	1410	0	1444	12	0
12	F	1313	0	1358	9	0
13	G	1111	0	1148	8	0
14	H	980	0	1013	13	0
15	I	984	0	1035	7	0
16	J	1129	0	1162	9	0
17	K	946	0	1023	8	0
18	L	1053	0	1129	13	0
19	M	1074	0	1157	8	0
20	N	951	0	994	11	0
21	O	892	0	923	10	0
22	P	917	0	962	7	0
23	Q	947	0	1019	11	0
24	R	816	0	839	2	0
25	S	857	0	922	13	0
26	T	746	0	811	9	0
27	U	788	0	843	6	0
28	V	753	0	780	1	0
29	W	582	0	599	3	0
30	X	625	0	652	8	0
31	Y	501	0	531	3	0
32	Z	448	0	488	1	0
33	a	522	0	522	0	0
34	b	444	0	458	0	0
35	c	426	0	464	0	0
36	d	377	0	418	0	0
37	e	504	0	572	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	302	0	341	0	0
39	g	1760	0	1787	0	0
40	h	1636	0	1710	0	0
41	i	1643	0	1707	0	0
42	j	1152	0	1196	0	0
43	k	848	0	846	0	0
44	l	1191	0	1245	0	0
45	m	979	0	1031	0	0
46	n	1022	0	1070	0	0
47	o	790	0	831	0	0
48	p	877	0	887	0	0
49	q	957	0	1017	0	0
50	r	900	0	965	0	0
51	s	805	0	844	0	0
52	t	714	0	734	0	0
53	u	649	0	666	0	0
54	v	648	0	691	0	0
55	w	544	0	560	0	0
56	x	663	0	688	0	0
57	y	669	0	719	0	0
58	z	589	0	629	0	0
59	1	296	0	0	0	0
59	2	129	0	0	0	0
59	3	9	0	0	0	0
59	5	4	0	0	0	0
59	b	1	0	0	0	0
59	i	1	0	0	0	0
60	5	10	0	10	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	B	2	0	0	0	0
All	All	149892	0	102124	604	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 3.

The worst 5 of 604 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)
2:2:37:U:O4	2:2:397:A:N1	1.57	1.33
1:1:2287:A:N1	1:1:2344:U:O4	1.70	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1590:A:C2	1:1:1591:A:C6	2.29	1.19
1:1:234:U:O4	1:1:429:A:N1	1.75	1.19
2:2:148:G:O2'	2:2:149:A:C5'	1.95	1.15

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	
6	6	44/61 (72%)	39 (89%)	5 (11%)	0	100	100
7	7	359/365 (98%)	344 (96%)	14 (4%)	1 (0%)	44	80
8	B	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	38	76
9	C	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	32	72
10	D	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
11	E	175/179 (98%)	166 (95%)	8 (5%)	1 (1%)	28	68
12	F	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
13	G	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
14	H	128/165 (78%)	104 (81%)	20 (16%)	4 (3%)	5	24
15	I	133/142 (94%)	114 (86%)	17 (13%)	2 (2%)	12	46
16	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
17	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
18	L	142/144 (99%)	133 (94%)	7 (5%)	2 (1%)	13	47
19	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
20	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
21	O	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	20	60
22	P	112/115 (97%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Q	115/118 (98%)	112 (97%)	2 (2%)	1 (1%)	20	60
24	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
25	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
26	T	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
27	U	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	18	57
28	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
29	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
32	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
33	a	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
34	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
35	c	50/55 (91%)	50 (100%)	0	0	100	100
36	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
37	e	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
38	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
39	g	223/241 (92%)	213 (96%)	10 (4%)	0	100	100
40	h	206/233 (88%)	197 (96%)	6 (3%)	3 (2%)	12	46
41	i	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
42	j	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	28	68
43	k	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	18	57
44	l	150/179 (84%)	143 (95%)	6 (4%)	1 (1%)	25	65
45	m	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	22	62
46	n	125/130 (96%)	116 (93%)	7 (6%)	2 (2%)	11	44
47	o	97/103 (94%)	90 (93%)	6 (6%)	1 (1%)	18	57
48	p	115/129 (89%)	104 (90%)	11 (10%)	0	100	100
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
51	s	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
52	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
53	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	v	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
55	w	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
56	x	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
57	y	84/87 (97%)	84 (100%)	0	0	100	100
58	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	6273/6646 (94%)	5943 (95%)	305 (5%)	25 (0%)	42	76

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	L	36	LYS
27	U	7	ARG
46	n	56	ASP
47	o	57	VAL
8	B	240	PHE

### 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	
6	6	39/51 (76%)	37 (95%)	2 (5%)	28	65
7	7	306/310 (99%)	275 (90%)	31 (10%)	9	31
8	B	216/218 (99%)	204 (94%)	12 (6%)	25	61
9	C	164/164 (100%)	159 (97%)	5 (3%)	46	80
10	D	165/165 (100%)	150 (91%)	15 (9%)	11	37
11	E	148/150 (99%)	136 (92%)	12 (8%)	14	43
12	F	136/138 (99%)	128 (94%)	8 (6%)	23	59
13	G	114/114 (100%)	103 (90%)	11 (10%)	10	34
14	H	99/123 (80%)	86 (87%)	13 (13%)	5	19
15	I	104/110 (94%)	91 (88%)	13 (12%)	5	21
16	J	116/116 (100%)	108 (93%)	8 (7%)	18	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	K	104/104 (100%)	97 (93%)	7 (7%)	19	53
18	L	103/103 (100%)	95 (92%)	8 (8%)	15	45
19	M	109/109 (100%)	101 (93%)	8 (7%)	16	48
20	N	99/103 (96%)	93 (94%)	6 (6%)	22	57
21	O	86/87 (99%)	81 (94%)	5 (6%)	23	60
22	P	99/100 (99%)	92 (93%)	7 (7%)	17	50
23	Q	89/90 (99%)	81 (91%)	8 (9%)	11	38
24	R	84/84 (100%)	79 (94%)	5 (6%)	22	58
25	S	93/93 (100%)	85 (91%)	8 (9%)	12	40
26	T	81/84 (96%)	79 (98%)	2 (2%)	53	83
27	U	84/85 (99%)	79 (94%)	5 (6%)	22	58
28	V	78/78 (100%)	73 (94%)	5 (6%)	20	55
29	W	58/63 (92%)	56 (97%)	2 (3%)	42	77
30	X	67/68 (98%)	64 (96%)	3 (4%)	32	69
31	Y	54/55 (98%)	51 (94%)	3 (6%)	25	61
32	Z	48/49 (98%)	45 (94%)	3 (6%)	21	56
33	a	59/62 (95%)	54 (92%)	5 (8%)	12	41
34	b	47/48 (98%)	44 (94%)	3 (6%)	20	55
35	c	47/49 (96%)	45 (96%)	2 (4%)	33	71
36	d	38/38 (100%)	35 (92%)	3 (8%)	14	44
37	e	51/52 (98%)	48 (94%)	3 (6%)	23	59
38	f	34/34 (100%)	31 (91%)	3 (9%)	12	39
39	g	187/199 (94%)	182 (97%)	5 (3%)	50	81
40	h	171/190 (90%)	160 (94%)	11 (6%)	20	55
41	i	172/173 (99%)	163 (95%)	9 (5%)	27	64
42	j	119/126 (94%)	105 (88%)	14 (12%)	6	24
43	k	91/116 (78%)	84 (92%)	7 (8%)	15	46
44	l	125/147 (85%)	113 (90%)	12 (10%)	10	34
45	m	104/105 (99%)	100 (96%)	4 (4%)	38	74
46	n	105/107 (98%)	98 (93%)	7 (7%)	19	53
47	o	86/90 (96%)	77 (90%)	9 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	p	90/99 (91%)	83 (92%)	7 (8%)	15	45
49	q	102/103 (99%)	93 (91%)	9 (9%)	12	39
50	r	94/96 (98%)	84 (89%)	10 (11%)	8	28
51	s	83/84 (99%)	77 (93%)	6 (7%)	17	49
52	t	76/77 (99%)	65 (86%)	11 (14%)	4	16
53	u	65/65 (100%)	59 (91%)	6 (9%)	11	37
54	v	74/78 (95%)	70 (95%)	4 (5%)	26	62
55	w	57/65 (88%)	55 (96%)	2 (4%)	41	76
56	x	72/79 (91%)	68 (94%)	4 (6%)	25	61
57	y	65/66 (98%)	58 (89%)	7 (11%)	7	28
58	z	60/61 (98%)	58 (97%)	2 (3%)	43	78
All	All	5217/5423 (96%)	4837 (93%)	380 (7%)	21	48

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Q	11	ARG
32	Z	10	THR
52	t	70	LEU
23	Q	59	GLN
26	T	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2904 (99%)	556 (19%)	81 (2%)
2	2	1528/1534 (99%)	295 (19%)	37 (2%)
3	3	119/120 (99%)	15 (12%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	23 (31%)	9 (12%)
All	All	4622/4654 (99%)	890 (19%)	127 (2%)

5 of 890 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	14	A
1	1	23	G
1	1	34	U
1	1	35	G

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1962	5MC
1	1	2425	A
2	2	1516	2MG
1	1	2146	C
1	1	2210	U

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

41 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	1	1618	1	18,25,26	0.90	1 (5%)	16,36,39	1.84	3 (18%)
1	2MG	1	1835	1	19,26,27	1.26	1 (5%)	20,38,41	2.72	6 (30%)
1	PSU	1	1911	1	16,21,22	1.89	4 (25%)	20,30,33	3.41	9 (45%)
1	3TD	1	1915	1	16,22,23	1.19	2 (12%)	19,32,35	2.51	8 (42%)
1	PSU	1	1917	1	16,21,22	1.94	4 (25%)	20,30,33	3.51	7 (35%)
1	5MU	1	1939	1	14,22,23	1.21	2 (14%)	16,32,35	2.11	3 (18%)
1	5MC	1	1962	1	15,22,23	1.52	1 (6%)	17,32,35	1.09	1 (5%)
1	6MZ	1	2030	1	18,25,26	0.98	1 (5%)	16,36,39	2.16	4 (25%)
1	G7M	1	2069	1	19,26,27	1.65	2 (10%)	19,39,42	3.62	7 (36%)
1	OMG	1	2251	1,5	18,26,27	1.05	2 (11%)	22,38,41	2.21	7 (31%)
1	2MG	1	2445	1	19,26,27	1.38	1 (5%)	20,38,41	2.64	6 (30%)
1	PSU	1	2457	1,59	16,21,22	2.75	4 (25%)	20,30,33	5.63	11 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	1	2498	1,59	15,22,23	1.09	1 (6%)	19,31,34	2.06	3 (15%)
1	2MA	1	2503	1,59	18,25,26	1.44	3 (16%)	17,37,40	2.96	5 (29%)
1	PSU	1	2504	1	16,21,22	2.83	4 (25%)	20,30,33	5.64	11 (55%)
1	OMU	1	2552	1,59	14,22,23	1.12	1 (7%)	18,31,34	2.89	2 (11%)
1	PSU	1	2580	1	16,21,22	2.52	4 (25%)	20,30,33	5.68	9 (45%)
1	PSU	1	2605	1	16,21,22	2.90	4 (25%)	20,30,33	5.71	12 (60%)
1	1MG	1	745	1	18,26,27	1.47	2 (11%)	18,39,42	1.94	4 (22%)
1	PSU	1	746	1,59	16,21,22	2.84	3 (18%)	20,30,33	5.82	10 (50%)
1	5MU	1	747	1	14,22,23	1.60	2 (14%)	16,32,35	3.47	3 (18%)
1	PSU	1	955	1	16,21,22	2.74	4 (25%)	20,30,33	5.67	12 (60%)
2	2MG	2	1207	2	19,26,27	1.49	3 (15%)	20,38,41	2.73	10 (50%)
2	4OC	2	1402	2	16,23,24	1.38	2 (12%)	19,32,35	1.40	3 (15%)
2	5MC	2	1407	2	15,22,23	0.64	0	17,32,35	0.90	0
2	UR3	2	1498	2	14,22,23	1.65	3 (21%)	16,32,35	1.17	1 (6%)
2	2MG	2	1516	2	19,26,27	1.30	1 (5%)	20,38,41	2.65	6 (30%)
2	MA6	2	1518	2	16,26,27	0.56	0	18,38,41	1.35	2 (11%)
2	MA6	2	1519	2	16,26,27	0.59	0	18,38,41	1.36	3 (16%)
2	PSU	2	516	2,59	16,21,22	2.34	4 (25%)	20,30,33	5.68	9 (45%)
2	7MG	2	527	2	20,26,27	1.39	4 (20%)	22,39,42	2.96	6 (27%)
2	2MG	2	966	2	19,26,27	1.30	1 (5%)	20,38,41	3.09	8 (40%)
2	5MC	2	967	2	15,22,23	1.42	1 (6%)	17,32,35	1.56	2 (11%)
5	H2U	5	20	5	17,21,22	0.69	0	21,30,33	1.91	4 (19%)
5	4OC	5	32	5	16,23,24	0.73	0	19,32,35	1.58	3 (15%)
5	5MU	5	54	5	14,22,23	1.37	2 (14%)	16,32,35	3.57	4 (25%)
5	PSU	5	55	5	16,21,22	2.54	4 (25%)	20,30,33	5.60	9 (45%)
5	8AN	5	76	60,5	17,24,25	0.66	0	14,35,38	0.89	1 (7%)
5	4SU	5	8	5	14,21,22	1.37	1 (7%)	15,30,33	1.48	2 (13%)
7	MEQ	7	252	7	9,9,10	0.58	0	7,10,12	2.01	3 (42%)
49	0TD	q	89	49	5,9,10	4.67	4 (80%)	3,11,13	4.37	3 (100%)

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	1	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2457	1,59	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	1,59	-	0/5/27/28	0/2/2/2
1	2MA	1	2503	1,59	-	0/3/25/26	0/3/3/3
1	PSU	1	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1,59	-	0/5/27/28	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1	746	1,59	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/7/29/30	0/2/2/2
2	5MC	2	1407	2	-	0/3/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/3/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
2	MA6	2	1519	2	-	0/7/29/30	0/3/3/3
2	PSU	2	516	2,59	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2	-	0/7/37/38	0/3/3/3
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
2	5MC	2	967	2	-	0/3/25/26	0/2/2/2
5	H2U	5	20	5	-	0/7/38/39	0/2/2/2
5	4OC	5	32	5	-	0/7/29/30	0/2/2/2
5	5MU	5	54	5	-	0/3/25/26	0/2/2/2
5	PSU	5	55	5	-	0/7/25/26	0/2/2/2
5	8AN	5	76	60,5	-	0/3/25/26	0/3/3/3
5	4SU	5	8	5	-	0/3/25/26	0/2/2/2
7	MEQ	7	252	7	-	1/7/9/11	0/0/0/0
49	0TD	q	89	49	-	0/2/12/14	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	746	PSU	C2'-C1'	-10.14	1.42	1.53
1	1	2605	PSU	C2'-C1'	-9.87	1.42	1.53
1	1	2504	PSU	C2'-C1'	-9.72	1.42	1.53
1	1	2457	PSU	C2'-C1'	-9.23	1.43	1.53
1	1	955	PSU	C2'-C1'	-8.89	1.43	1.53

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2504	PSU	N1-C2-N3	-16.93	116.22	128.40
1	1	2605	PSU	N1-C2-N3	-16.92	116.23	128.40
2	2	516	PSU	N1-C2-N3	-16.89	116.25	128.40
1	1	955	PSU	N1-C2-N3	-16.87	116.27	128.40
1	1	2580	PSU	N1-C2-N3	-16.86	116.27	128.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	7	252	MEQ	CG-CD-NE2-CE

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1915	3TD	4	0
1	1	1917	PSU	2	0
1	1	1939	5MU	3	0
1	1	2030	6MZ	2	0
1	1	2251	OMG	3	0
1	1	2503	2MA	1	0
1	1	745	1MG	1	0
2	2	1402	4OC	1	0
2	2	1407	5MC	1	0
2	2	1518	MA6	2	0
2	2	1519	MA6	2	0
2	2	516	PSU	1	0
2	2	966	2MG	4	0
2	2	967	5MC	1	0
5	5	20	H2U	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 443 ligands modelled in this entry, 442 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	FME	5	103	5	9,9,10	1.20	1 (11%)	7,9,11	1.36	1 (14%)

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
60	FME	5	103	5	-	0/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	5	103	FME	CA-C	3.30	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	5	103	FME	O-C-CA	-3.53	116.91	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.