



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 10:22 am BST

PDB ID : 5MDY
EMDB ID : EMD-3492
Title : Structure of ArfA and TtRF2 bound to the 70S ribosome (pre-accommodated state)
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-11-13
Resolution : 3.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

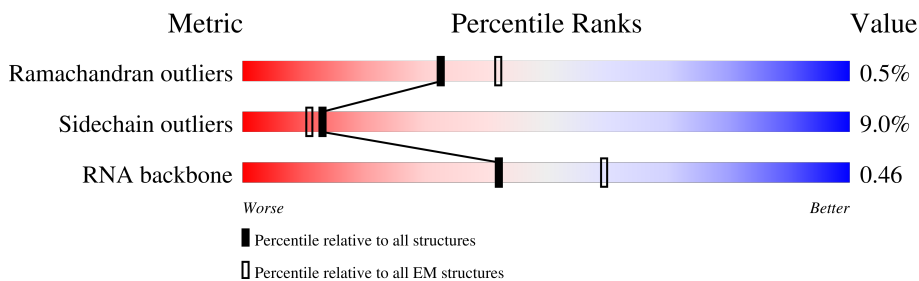
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	2904	
2	2	1534	
3	3	120	
4	4	18	
5	5	78	
6	6	61	
7	7	378	
8	B	273	
9	C	209	

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Mol	Chain	Length	Quality of chain
10	D	201	94% 6%
11	E	179	88% 10% ..
12	F	177	94% 5% .
13	G	149	86% 12% .
14	H	165	71% 7% . 21%
15	I	142	89% 6% 5%
16	J	142	94% 6%
17	K	123	90% 10%
18	L	144	94% 6%
19	M	136	93% 7%
20	N	127	87% 6% 6%
21	O	117	93% 6% .
22	P	115	89% 10% ..
23	Q	118	91% 8% .
24	R	103	94% 5% .
25	S	110	93% 7%
26	T	100	87% 7% 6%
27	U	104	91% 8% .
28	V	94	97% .
29	W	85	87% . 11%
30	X	78	90% 8% ..
31	Y	63	90% 6% ..
32	Z	59	81% 17% .
33	a	70	86% .. 10%
34	b	57	84% 14% .

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Mol	Chain	Length	Quality of chain
35	c	55	87% 7% 5%
36	d	46	85% 15%
37	e	65	89% 9% .
38	f	38	87% 13%
39	g	241	89% 5% 7%
40	h	233	83% 6% 11%
41	i	206	96% .
42	j	167	84% 9% 7%
43	k	135	70% 6% . 23%
44	l	179	74% 10% . 16%
45	m	130	94% 5% .
46	n	130	88% 8% . .
47	o	103	87% 8% . .
48	p	129	84% 6% 9%
49	q	124	91% 8% .
50	r	118	92% 7% .
51	s	101	95% . .
52	t	89	88% 11% .
53	u	82	93% 7%
54	v	84	90% 5% 5%
55	w	75	83% 5% 12%
56	x	92	85% 5% 10%
57	y	87	95% . .
58	z	71	92% 7% .

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149460 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
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

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
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

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

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

- Molecule 4 is a RNA chain called mRNA.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	32	Total	C	N	O	S	0	0
			259	163	53	42	1		

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	324	Total	C	N	O	S	0	0
			2597	1630	471	488	8		

- 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
			Total	C	N	O	S		
12	F	175	1313	826	241	244	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	146	1089	686	194	208	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	63	Total	C	N	O	S	0	0
			495	304	95	90	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	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	151	Total	C	N	O	S	0	0
			1181	735	227	215	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).

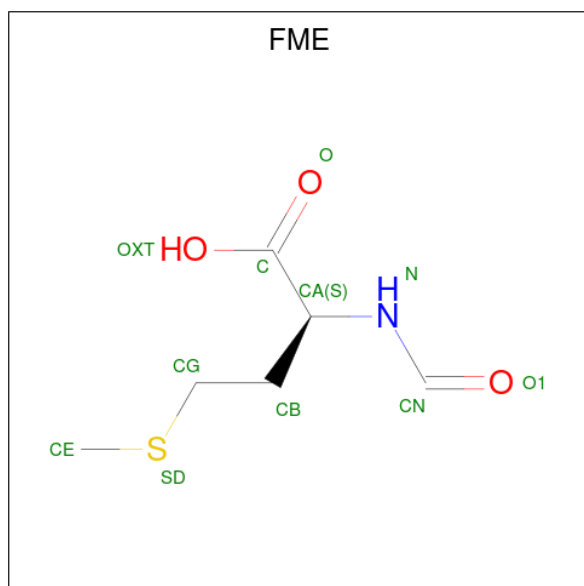
Mol	Chain	Residues	Atoms		AltConf
59	1	293	Total	Mg	0
			293	293	
59	2	143	Total	Mg	0
			143	143	
59	3	7	Total	Mg	0
			7	7	
59	5	4	Total	Mg	0
			4	4	
59	b	1	Total	Mg	0
			1	1	
59	f	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
59	i	1	1	1	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



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

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

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

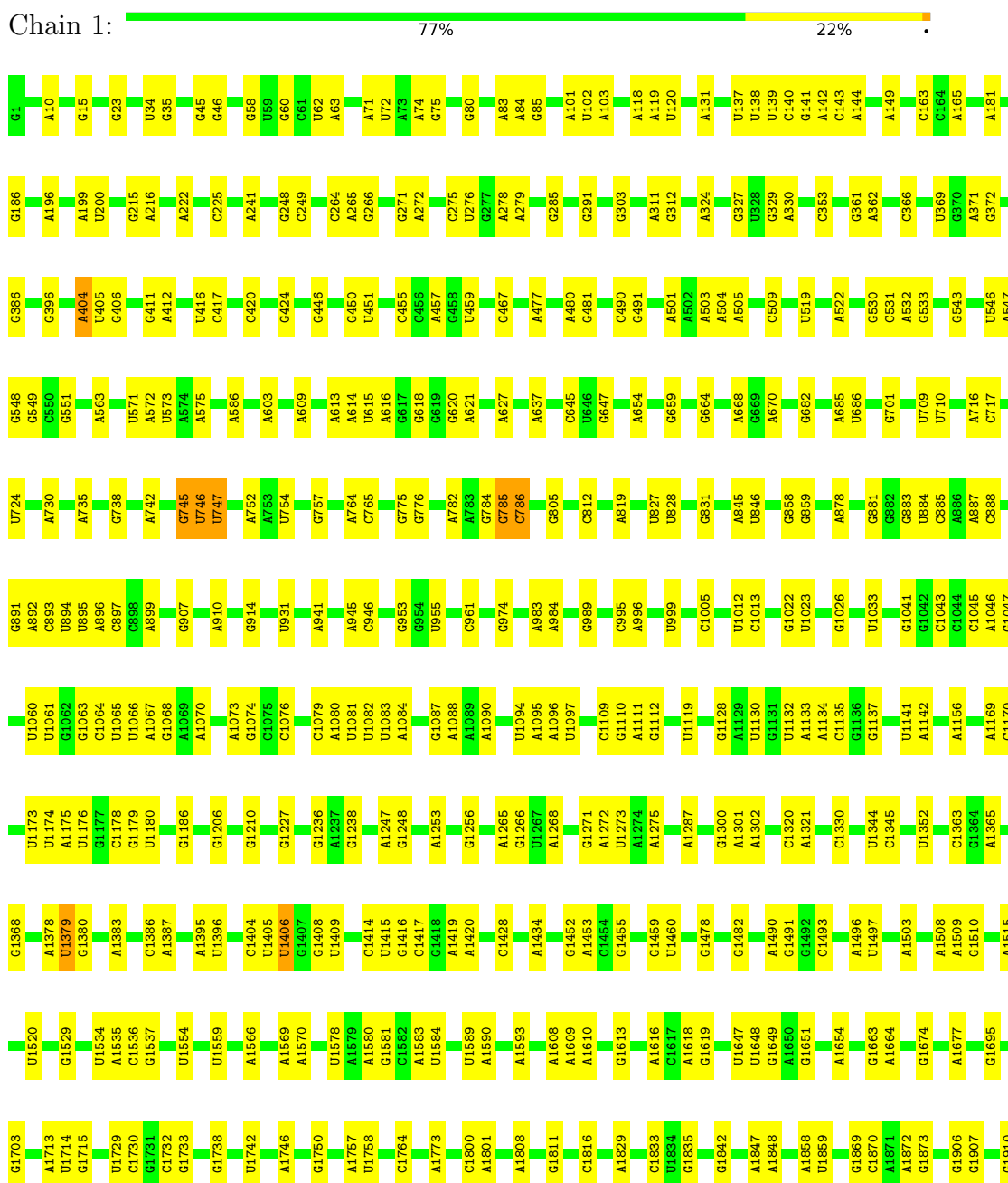
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	B	2	2	2	0
62	O	1	1	1	0

3 Residue-property plots [i](#)

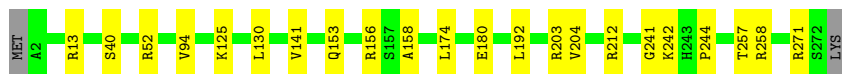
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA



- Molecule 8: 50S ribosomal protein L2

Chain B:  91% 8%



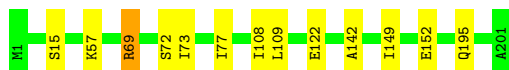
- Molecule 9: 50S ribosomal protein L3

Chain C:  97%




- Molecule 10: 50S ribosomal protein L4

Chain D:  94% 6%



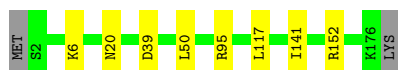
- Molecule 11: 50S ribosomal protein L5

Chain E:  88% 10%




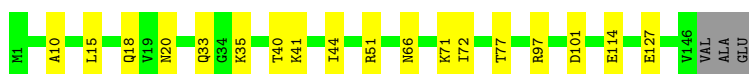
- Molecule 12: 50S ribosomal protein L6

Chain F:  94% 5%



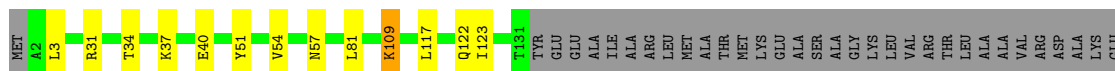
- Molecule 13: 50S ribosomal protein L9

Chain G:  86% 12%




- Molecule 14: 50S ribosomal protein L10

Chain H:  71% 7% 21%



ALA
ALA

- Molecule 15: 50S ribosomal protein L11

Chain I:  89% 6% 5%

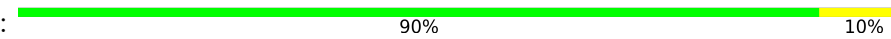
MET
ALA
LYS
LYS
VAL
Q5
L10
Q11
C38
E41
M42
D63
L78
G136
V139
GLU
ASP

- Molecule 16: 50S ribosomal protein L13

Chain J:  94% 6%

H1
F4
K12
D19
H40
V100
V124
M28
L140
D141
I142

- Molecule 17: 50S ribosomal protein L14

Chain K:  90% 10%

H1
N7
L8
R17
R18
R49
K53
L58
R70
D80
T97
T104
R105
L123

- Molecule 18: 50S ribosomal protein L15

Chain L:  94% 6%


H1
M4
S7
V46
R47
R48
R59
R78
K84
D91
E144

- Molecule 19: 50S ribosomal protein L16

Chain M:  93% 7%

H1
L2
Q3
D25
E47
R84
K100
E110
L119
T132
K133
M136

- Molecule 20: 50S ribosomal protein L17

Chain N:  87% 6% 6%

H1
R17
M20
M24
E43
L51
S59
R63
R69
S119
GLU
LYS
ALA
GLU
ALA
ALA
ALA
GLU

- Molecule 21: 50S ribosomal protein L18

Chain O:  93% 6%



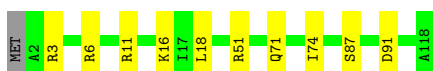
- Molecule 22: 50S ribosomal protein L19

Chain P: 89% 10% ..



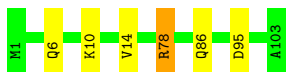
- Molecule 23: 50S ribosomal protein L20

Chain Q: 91% 8% .



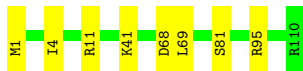
- Molecule 24: 50S ribosomal protein L21

Chain R: 94% 5% .



- Molecule 25: 50S ribosomal protein L22

Chain S: 93% 7%



- Molecule 26: 50S ribosomal protein L23

Chain T: 87% 7% 6%



- Molecule 27: 50S ribosomal protein L24

Chain U: 91% 8% .

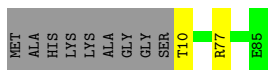
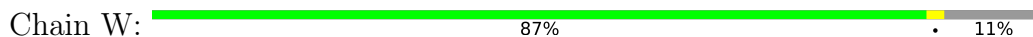


- Molecule 28: 50S ribosomal protein L25

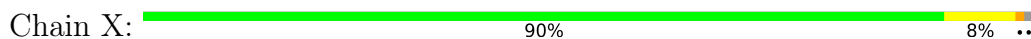
Chain V: 97% .



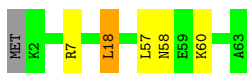
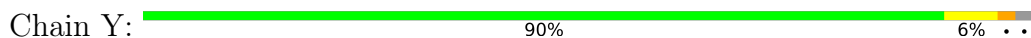
- Molecule 29: 50S ribosomal protein L27



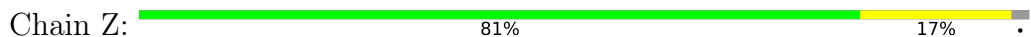
- Molecule 30: 50S ribosomal protein L28



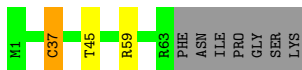
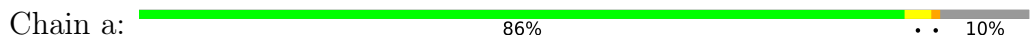
- Molecule 31: 50S ribosomal protein L29



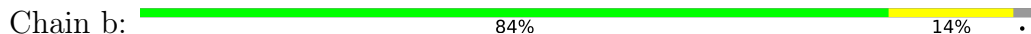
- Molecule 32: 50S ribosomal protein L30



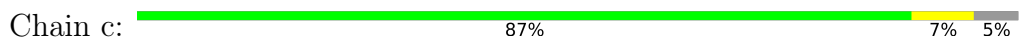
- Molecule 33: 50S ribosomal protein L31



- Molecule 34: 50S ribosomal protein L32

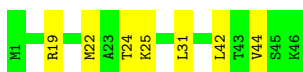
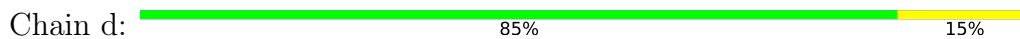


- Molecule 35: 50S ribosomal protein L33

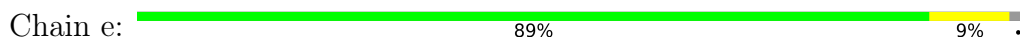




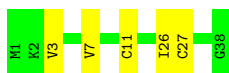
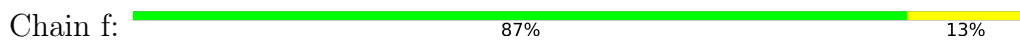
- Molecule 36: 50S ribosomal protein L34



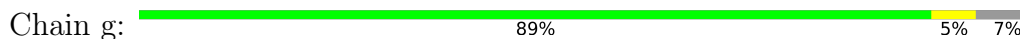
- Molecule 37: 50S ribosomal protein L35



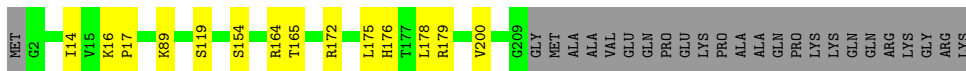
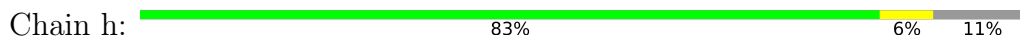
- Molecule 38: 50S ribosomal protein L36



- Molecule 39: 30S ribosomal protein S2



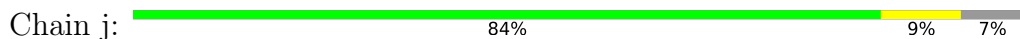
- Molecule 40: 30S ribosomal protein S3



- Molecule 41: 30S ribosomal protein S4

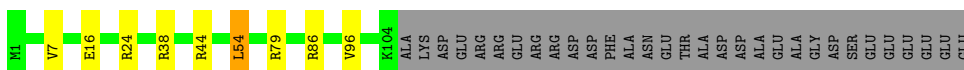


- Molecule 42: 30S ribosomal protein S5

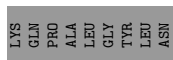




• Molecule 43: 30S ribosomal protein S6



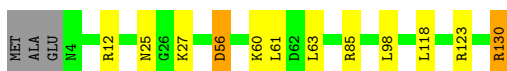
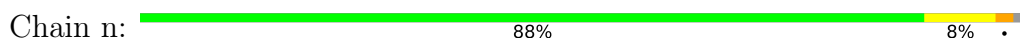
• Molecule 44: 30S ribosomal protein S7



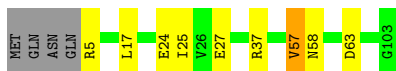
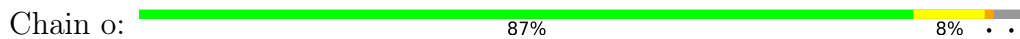
• Molecule 45: 30S ribosomal protein S8



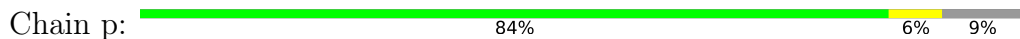
• Molecule 46: 30S ribosomal protein S9



• Molecule 47: 30S ribosomal protein S10



• Molecule 48: 30S ribosomal protein S11




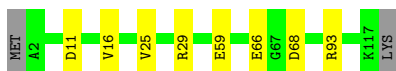
• Molecule 49: 30S ribosomal protein S12

Chain q:  91% 8%



- Molecule 50: 30S ribosomal protein S13

Chain r:  92% 7%




- Molecule 51: 30S ribosomal protein S14

Chain s:  95%



- Molecule 52: 30S ribosomal protein S15

Chain t:  88% 11%




- Molecule 53: 30S ribosomal protein S16

Chain u:  93% 7%




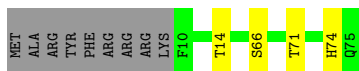
- Molecule 54: 30S ribosomal protein S17

Chain v:  90% 5% 5%




- Molecule 55: 30S ribosomal protein S18

Chain w:  83% 5% 12%



- Molecule 56: 30S ribosomal protein S19

Chain x:  85% 5% 10%



- Molecule 57: 30S ribosomal protein S20

Chain y:  95% ..



- Molecule 58: 30S ribosomal protein S21

Chain z:  92% 7% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54465	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.39	0/69285	0.75	25/108083 (0.0%)
2	2	0.33	0/36590	0.76	35/57074 (0.1%)
3	3	0.29	0/2872	0.71	0/4478
4	4	0.39	0/122	0.70	0/188
5	5	0.28	0/1672	0.72	0/2603
6	6	0.41	0/263	0.78	0/345
7	7	0.55	0/2642	0.85	1/3563 (0.0%)
8	B	0.52	0/2121	0.85	2/2852 (0.1%)
9	C	0.52	0/1586	0.76	0/2134
10	D	0.52	0/1571	0.83	2/2113 (0.1%)
11	E	0.48	0/1434	0.80	0/1926
12	F	0.41	0/1333	0.72	0/1805
13	G	0.45	0/1100	0.72	0/1486
14	H	0.50	0/993	0.75	1/1340 (0.1%)
15	I	0.45	0/998	0.71	0/1348
16	J	0.52	0/1152	0.82	0/1551
17	K	0.50	0/955	0.87	1/1279 (0.1%)
18	L	0.49	0/1062	0.83	0/1413
19	M	0.53	0/1093	0.86	0/1460
20	N	0.57	0/964	0.90	0/1289
21	O	0.54	0/902	0.86	0/1209
22	P	0.49	0/929	0.84	1/1242 (0.1%)
23	Q	0.69	0/960	0.99	1/1278 (0.1%)
24	R	0.46	0/829	0.74	1/1107 (0.1%)
25	S	0.56	0/864	0.87	0/1156
26	T	0.49	0/752	0.78	0/1005
27	U	0.40	0/796	0.69	0/1062
28	V	0.43	0/766	0.68	0/1025
29	W	0.52	0/589	0.84	0/779
30	X	0.53	0/635	0.92	1/848 (0.1%)
31	Y	0.56	0/502	0.90	1/667 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.45	0/452	0.78	0/605
33	a	0.42	0/503	0.78	1/671 (0.1%)
34	b	0.49	0/450	0.83	0/599
35	c	0.44	0/433	0.70	0/576
36	d	0.60	0/380	0.99	0/498
37	e	0.52	0/513	0.86	0/676
38	f	0.45	0/303	0.89	0/397
39	g	0.47	0/1791	0.73	0/2413
40	h	0.48	0/1663	0.76	0/2241
41	i	0.50	0/1665	0.79	0/2227
42	j	0.52	0/1165	0.84	0/1568
43	k	0.47	0/867	0.78	1/1171 (0.1%)
44	l	0.52	0/1195	0.89	1/1602 (0.1%)
45	m	0.47	0/989	0.75	0/1326
46	n	0.46	0/1034	0.84	1/1375 (0.1%)
47	o	0.43	0/800	0.83	1/1082 (0.1%)
48	p	0.44	0/893	0.75	0/1205
49	q	0.46	0/960	0.83	0/1286
50	r	0.50	0/909	0.89	0/1215
51	s	0.51	0/817	0.80	0/1088
52	t	0.56	0/722	0.88	1/964 (0.1%)
53	u	0.50	0/659	0.82	0/884
54	v	0.41	0/657	0.70	0/881
55	w	0.50	0/553	0.84	0/743
56	x	0.41	0/680	0.70	0/915
57	y	0.59	0/675	0.87	0/895
58	z	0.55	0/597	0.91	0/792
All	All	0.42	0/160657	0.77	78/239603 (0.0%)

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	786	C	N1-C1'-C2'	-13.18	96.86	114.00
2	2	1277	C	N1-C1'-C2'	-12.59	97.64	114.00
2	2	928	G	N9-C1'-C2'	-12.13	98.23	114.00
2	2	198	G	N9-C1'-C2'	-10.73	100.05	114.00
2	2	1401	G	N9-C1'-C2'	-10.71	100.08	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	30/61 (49%)	27 (90%)	3 (10%)	0	100	100
7	7	316/378 (84%)	287 (91%)	26 (8%)	3 (1%)	17	51
8	B	269/273 (98%)	252 (94%)	15 (6%)	2 (1%)	22	56
9	C	207/209 (99%)	191 (92%)	15 (7%)	1 (0%)	29	63
10	D	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	29	63
11	E	175/179 (98%)	160 (91%)	12 (7%)	3 (2%)	9	36
12	F	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
13	G	144/149 (97%)	133 (92%)	10 (7%)	1 (1%)	22	56
14	H	128/165 (78%)	107 (84%)	18 (14%)	3 (2%)	6	31
15	I	133/142 (94%)	116 (87%)	16 (12%)	1 (1%)	19	53
16	J	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	56
17	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
18	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
19	M	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
20	N	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
21	O	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	17	51
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	Q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	9	36
24	R	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
25	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
26	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	U	101/104 (97%)	91 (90%)	9 (9%)	1 (1%)	15	49
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
32	Z	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	35
33	a	61/70 (87%)	56 (92%)	5 (8%)	0	100	100
34	b	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
35	c	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
36	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
37	e	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	24
38	f	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
39	g	223/241 (92%)	207 (93%)	15 (7%)	1 (0%)	34	68
40	h	206/233 (88%)	191 (93%)	14 (7%)	1 (0%)	29	63
41	i	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
42	j	154/167 (92%)	148 (96%)	5 (3%)	1 (1%)	25	59
43	k	102/135 (76%)	94 (92%)	7 (7%)	1 (1%)	15	49
44	l	149/179 (83%)	143 (96%)	3 (2%)	3 (2%)	7	33
45	m	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
46	n	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	19	53
47	o	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
48	p	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	17	51
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	106 (93%)	7 (6%)	1 (1%)	17	51
51	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
52	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
53	u	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
54	v	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
57	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6209/6659 (93%)	5804 (94%)	371 (6%)	34 (0%)	32	63

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	7	128	ASN
9	C	150	GLN
14	H	117	LEU
46	n	56	ASP
7	7	93	PRO

5.3.2 Protein sidechains [i](#)

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	26/51 (51%)	21 (81%)	5 (19%)	1	5
7	7	275/319 (86%)	223 (81%)	52 (19%)	1	6
8	B	216/218 (99%)	197 (91%)	19 (9%)	10	34
9	C	164/164 (100%)	158 (96%)	6 (4%)	34	63
10	D	165/165 (100%)	153 (93%)	12 (7%)	14	43
11	E	148/150 (99%)	131 (88%)	17 (12%)	5	22
12	F	136/138 (99%)	128 (94%)	8 (6%)	19	51
13	G	112/114 (98%)	95 (85%)	17 (15%)	3	12
14	H	99/123 (80%)	89 (90%)	10 (10%)	7	28
15	I	104/110 (94%)	97 (93%)	7 (7%)	16	47
16	J	116/116 (100%)	109 (94%)	7 (6%)	19	50
17	K	104/104 (100%)	93 (89%)	11 (11%)	6	26
18	L	103/103 (100%)	95 (92%)	8 (8%)	12	40
19	M	109/109 (100%)	99 (91%)	10 (9%)	9	32
20	N	99/103 (96%)	91 (92%)	8 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	O	86/87 (99%)	80 (93%)	6 (7%)	15	45
22	P	99/100 (99%)	87 (88%)	12 (12%)	5	20
23	Q	89/90 (99%)	82 (92%)	7 (8%)	12	40
24	R	84/84 (100%)	78 (93%)	6 (7%)	14	45
25	S	93/93 (100%)	85 (91%)	8 (9%)	10	36
26	T	81/84 (96%)	74 (91%)	7 (9%)	10	36
27	U	84/85 (99%)	77 (92%)	7 (8%)	11	37
28	V	78/78 (100%)	75 (96%)	3 (4%)	33	63
29	W	58/63 (92%)	56 (97%)	2 (3%)	37	66
30	X	67/68 (98%)	60 (90%)	7 (10%)	7	27
31	Y	54/55 (98%)	49 (91%)	5 (9%)	9	32
32	Z	48/49 (98%)	39 (81%)	9 (19%)	1	6
33	a	56/62 (90%)	53 (95%)	3 (5%)	22	54
34	b	47/48 (98%)	39 (83%)	8 (17%)	2	9
35	c	47/49 (96%)	43 (92%)	4 (8%)	10	36
36	d	38/38 (100%)	31 (82%)	7 (18%)	1	6
37	e	51/52 (98%)	47 (92%)	4 (8%)	12	40
38	f	34/34 (100%)	29 (85%)	5 (15%)	3	13
39	g	187/199 (94%)	177 (95%)	10 (5%)	22	54
40	h	171/190 (90%)	158 (92%)	13 (8%)	13	41
41	i	172/173 (99%)	165 (96%)	7 (4%)	30	61
42	j	119/126 (94%)	105 (88%)	14 (12%)	5	21
43	k	91/116 (78%)	83 (91%)	8 (9%)	10	34
44	l	124/147 (84%)	108 (87%)	16 (13%)	4	17
45	m	104/105 (99%)	98 (94%)	6 (6%)	20	52
46	n	105/107 (98%)	93 (89%)	12 (11%)	5	22
47	o	86/90 (96%)	77 (90%)	9 (10%)	7	26
48	p	90/99 (91%)	83 (92%)	7 (8%)	12	40
49	q	102/103 (99%)	93 (91%)	9 (9%)	10	34
50	r	94/96 (98%)	87 (93%)	7 (7%)	13	42
51	s	83/84 (99%)	79 (95%)	4 (5%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	t	76/77 (99%)	67 (88%)	9 (12%)	5	21
53	u	65/65 (100%)	59 (91%)	6 (9%)	9	32
54	v	74/78 (95%)	70 (95%)	4 (5%)	22	54
55	w	57/65 (88%)	53 (93%)	4 (7%)	15	45
56	x	72/79 (91%)	67 (93%)	5 (7%)	15	46
57	y	65/66 (98%)	62 (95%)	3 (5%)	27	59
58	z	60/61 (98%)	55 (92%)	5 (8%)	11	37
All	All	5167/5432 (95%)	4702 (91%)	465 (9%)	13	33

5 of 465 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	S	41	LYS
53	u	35	ARG
34	b	52	ARG
53	u	2	VAL
47	o	57	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
12	F	22	GLN
30	X	36	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2904 (99%)	619 (21%)	91 (3%)
2	2	1528/1534 (99%)	332 (21%)	39 (2%)
3	3	119/120 (99%)	20 (16%)	1 (0%)
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	24 (32%)	7 (9%)
All	All	4621/4654 (99%)	996 (21%)	138 (2%)

5 of 996 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	992	U
2	2	1213	A
3	3	48	U
1	1	1395	A
1	1	1379	U

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

40 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$
2	4OC	2	1402	2	20,23,24	0.68	0	26,32,35	1.59	3 (11%)
2	7MG	2	527	2	22,26,27	1.46	4 (18%)	29,39,42	2.99	10 (34%)
2	2MG	2	966	2	18,26,27	1.17	3 (16%)	16,38,41	2.07	3 (18%)
1	PSU	1	746	59,1	18,21,22	2.01	1 (5%)	22,30,33	2.10	3 (13%)
2	MA6	2	1519	2	18,26,27	0.65	0	19,38,41	0.85	1 (5%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.08	4 (14%)
1	PSU	1	1911	1	18,21,22	0.83	1 (5%)	22,30,33	1.11	2 (9%)
1	2MG	1	2445	1	18,26,27	1.31	3 (16%)	16,38,41	1.50	3 (18%)
1	PSU	1	1917	1	18,21,22	1.23	2 (11%)	22,30,33	1.34	4 (18%)
1	OMC	1	2498	59,1	19,22,23	1.17	2 (10%)	26,31,34	1.61	3 (11%)
1	2MA	1	2503	59,1	17,25,26	1.14	3 (17%)	17,37,40	3.15	6 (35%)
1	PSU	1	2605	1	18,21,22	1.90	1 (5%)	22,30,33	1.69	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5MU	5	54	5	19,22,23	0.67	0	28,32,35	0.97	2 (7%)
1	OMG	1	2251	1,5	18,26,27	1.29	4 (22%)	19,38,41	3.06	4 (21%)
2	PSU	2	516	59,2	18,21,22	1.55	1 (5%)	22,30,33	1.62	2 (9%)
1	PSU	1	2457	1	18,21,22	2.22	1 (5%)	22,30,33	1.42	4 (18%)
1	6MZ	1	1618	1	18,25,26	0.83	1 (5%)	16,36,39	1.72	2 (12%)
1	PSU	1	2504	1	18,21,22	1.86	1 (5%)	22,30,33	1.64	3 (13%)
2	MA6	2	1518	2	18,26,27	0.59	0	19,38,41	0.83	1 (5%)
5	H2U	5	20	5	18,21,22	0.65	0	21,30,33	1.92	4 (19%)
1	2MG	1	1835	1	18,26,27	1.20	3 (16%)	16,38,41	1.74	3 (18%)
2	UR3	2	1498	2	19,22,23	0.81	0	26,32,35	1.02	1 (3%)
2	2MG	2	1516	2	18,26,27	1.20	3 (16%)	16,38,41	1.73	2 (12%)
1	3TD	1	1915	1	18,22,23	2.41	6 (33%)	22,32,35	1.85	4 (18%)
1	6MZ	1	2030	1	18,25,26	0.87	0	16,36,39	2.24	4 (25%)
5	4SU	5	8	5	18,21,22	1.55	3 (16%)	26,30,33	2.78	12 (46%)
2	5MC	2	1407	2	18,22,23	0.84	1 (5%)	26,32,35	1.29	3 (11%)
5	PSU	5	55	5	18,21,22	1.79	1 (5%)	22,30,33	1.60	3 (13%)
1	1MG	1	745	1	18,26,27	1.83	3 (16%)	19,39,42	2.19	4 (21%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	OMU	1	2552	1	19,22,23	0.53	0	26,31,34	0.81	1 (3%)
5	8AN	5	76	59,60,1,5	19,24,25	0.67	0	13,35,38	0.88	1 (7%)
2	2MG	2	1207	2	18,26,27	1.64	4 (22%)	16,38,41	1.11	1 (6%)
1	G7M	1	2069	1	20,26,27	1.82	2 (10%)	17,39,42	2.08	4 (23%)
1	PSU	1	955	1	18,21,22	1.87	1 (5%)	22,30,33	1.66	3 (13%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	3 (11%)
5	4OC	5	32	5	20,23,24	0.58	0	26,32,35	1.23	2 (7%)
1	PSU	1	2580	1	18,21,22	1.88	1 (5%)	22,30,33	1.37	3 (13%)
1	5MU	1	1939	1	19,22,23	0.79	1 (5%)	28,32,35	1.05	3 (10%)
2	5MC	2	967	2	18,22,23	0.76	1 (5%)	26,32,35	1.30	3 (11%)

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
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	2457	PSU	C2'-C1'	-9.03	1.42	1.53
1	1	746	PSU	C2'-C1'	-8.32	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.74	1.43	1.53
1	1	2504	PSU	C2'-C1'	-7.60	1.43	1.53

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	O2'-C2'-C1'	10.15	129.21	109.09
2	2	527	7MG	N9-C4-N3	9.24	139.29	125.47
1	1	2503	2MA	C3'-C2'-C1'	-8.61	88.01	100.98
1	1	746	PSU	C3'-C2'-C1'	7.62	110.52	101.64
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	N1-C2-N2-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 453 ligands modelled in this entry, 452 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	8,9,10	0.55	0	7,9,11	1.31	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	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	5	103	FME	O-C-CA	-3.24	116.30	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	103	FME	O1-CN-N-CA
60	5	103	FME	N-CA-CB-CG

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.71

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3492. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.