wwPDB EM Map/Model Validation Report (i)

Sep 20, 2016 – 02:14 PM EDT

PDB ID	:	5JTE
EMDB ID:	:	EMD-8175
Title	:	Cryo-EM structure of an ErmBL-stalled ribosome in complex with A-, P-, and E-tRNA
Authors	:	Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.
Deposited on	:	2016-05-09
Resolution	:	3.60 Å(reported)
Based on PDB ID	:	5AFI

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

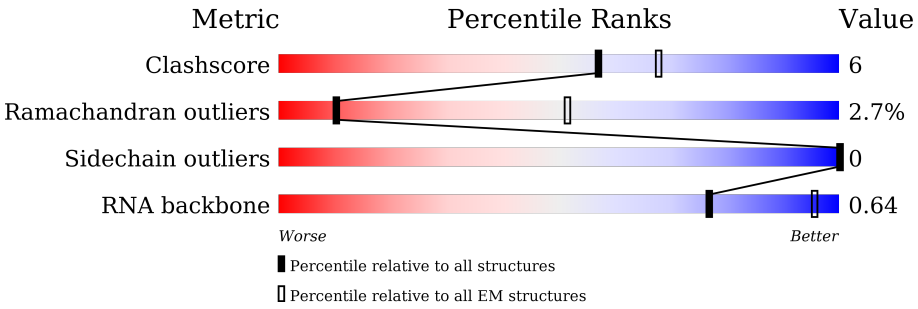
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	AA	1539	53% 35% 11% •
2	AB	240	65% 25% • 9%
3	AC	233	64% 24% 12%
4	AD	206	55% 43% •
5	AE	167	66% 22% • 10%
6	AF	135	56% 18% • 26%
7	AG	179	66% 18% 16%
8	AH	130	75% 24% •

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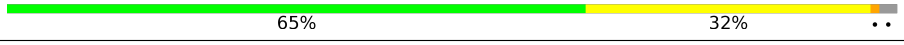
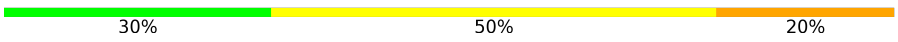
Mol	Chain	Length	Quality of chain
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AW	74	
24	AX	77	
25	AY	71	
26	BA	2897	
27	BB	120	
28	BC	273	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	149	

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Mol	Chain	Length	Quality of chain
34	BI	142	71% 27%
35	BJ	142	75% 25%
36	BK	123	66% 33%
37	BL	144	70% 28%
38	BM	136	75% 25%
39	BN	127	64% 29% 6%
40	BO	117	72% 26%
41	BP	115	70% 30%
42	BQ	118	87% 12%
43	BR	103	75% 25%
44	BS	110	83% 16%
45	BT	100	71% 21% 7%
46	BU	104	66% 30%
47	BV	94	83% 17%
48	BW	85	68% 20% 12%
49	BX	78	77% 22%
50	BY	63	86% 14%
51	BZ	59	71% 27%
52	B0	57	77% 21%
53	B1	55	62% 27% 9%
54	B2	46	80% 20%
55	B3	65	71% 28%
56	B4	38	82% 18%
57	B5	9	33% 67%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 146760 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 16S ribosomal RNA.

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	218	1704	1081	305	311	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	150	1105	687	211	201	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total 774	C 483	N 160	O 128	S 3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total 455	C 288	N 86	O 81	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total 637	C 408	N 120	O 107	S 2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called A-site Lysine tRNA Lysine.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0
			1593	716	280	522	73	2		

- Molecule 24 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 25 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BU	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

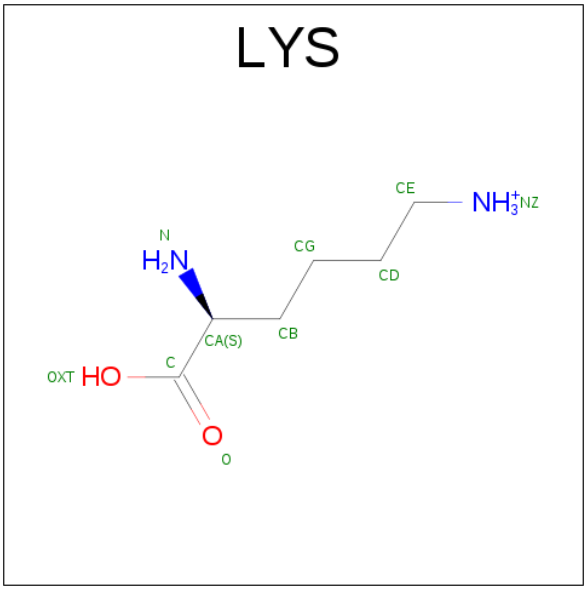
- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called ErmBL.

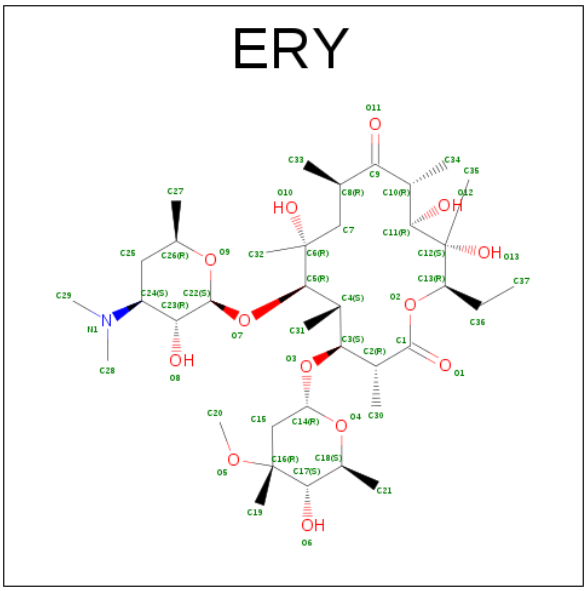
Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 58 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
58	AW	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 59 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



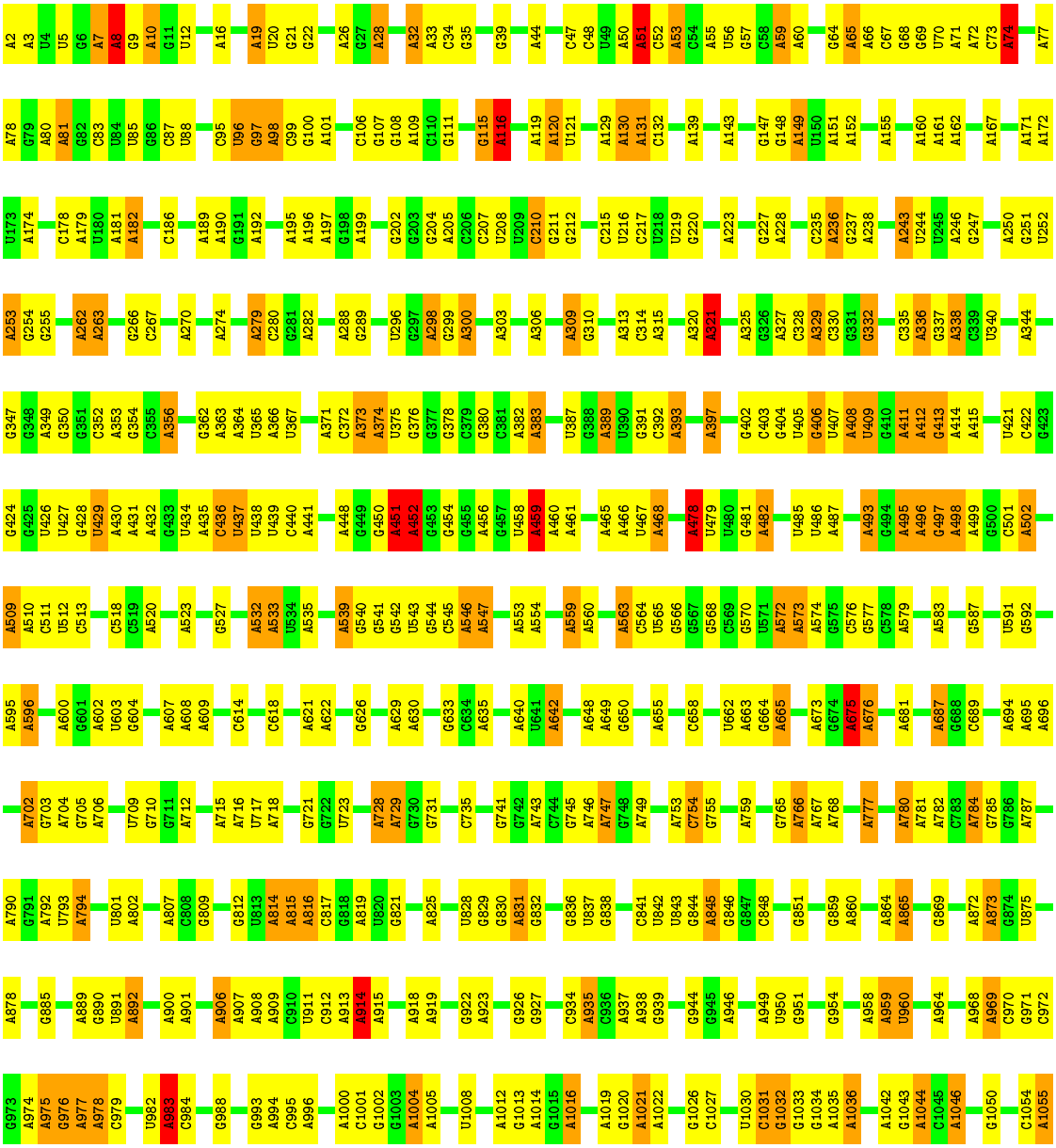
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	BA	1	51	37	1	13	0

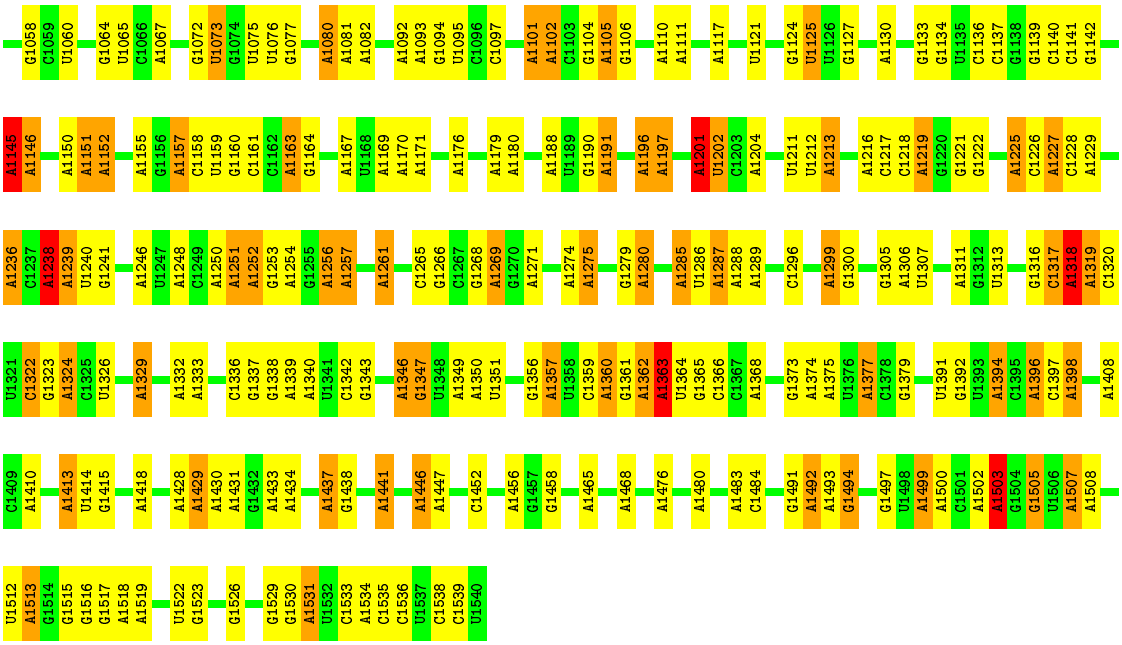
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

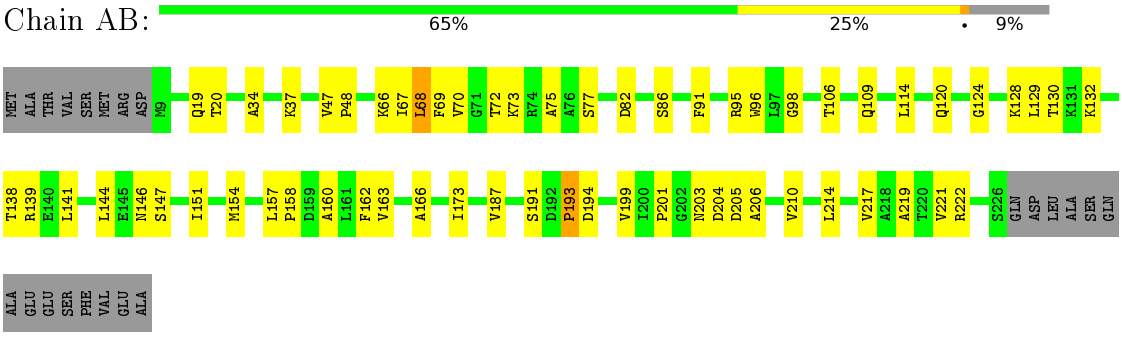
Chain AA: 53% 35% 11%





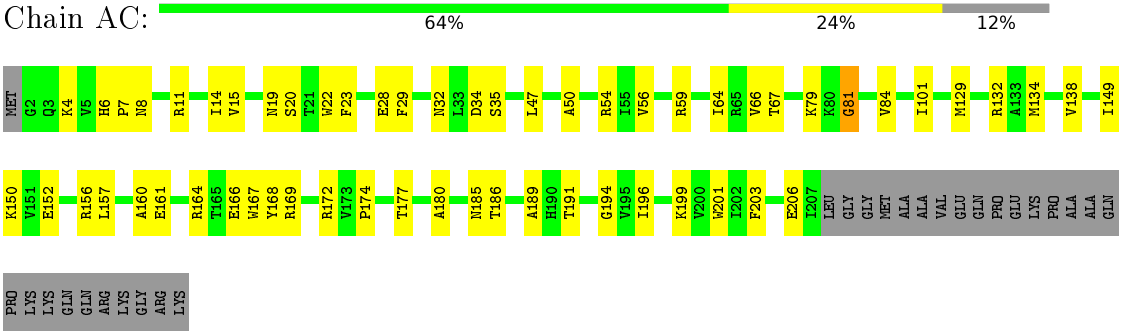
• Molecule 2: 30S ribosomal protein S2

Chain AB:



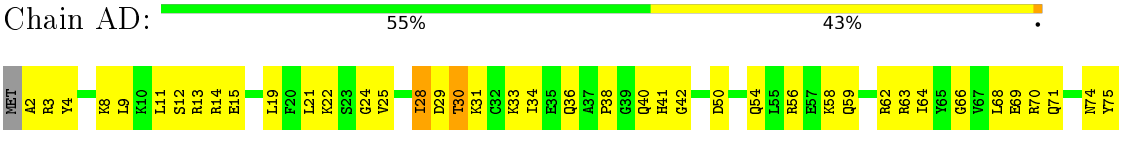
• Molecule 3: 30S ribosomal protein S3

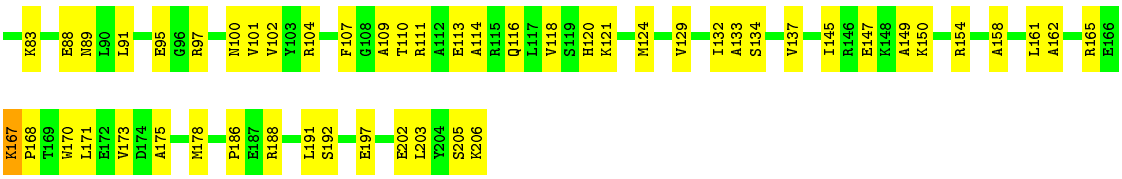
Chain AC:



• Molecule 4: 30S ribosomal protein S4

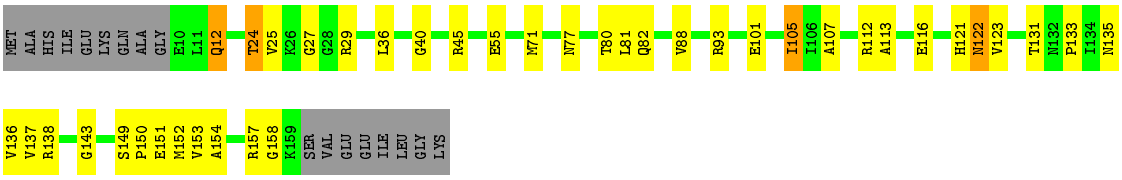
Chain AD:





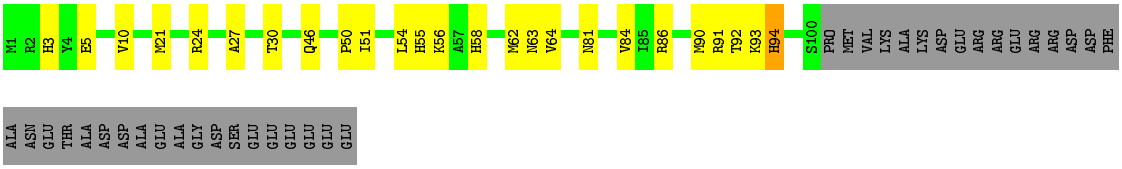
- Molecule 5: 30S ribosomal protein S5

Chain AE:



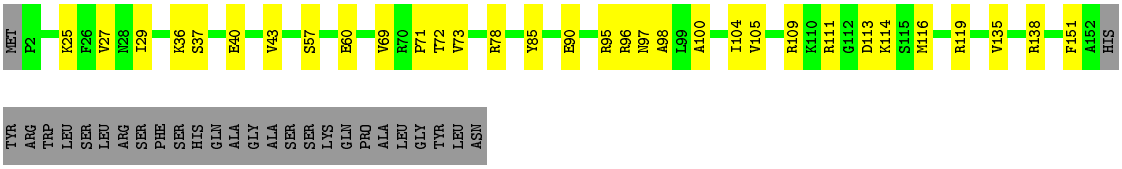
- Molecule 6: 30S ribosomal protein S6

Chain AF:



- Molecule 7: 30S ribosomal protein S7

Chain AG:

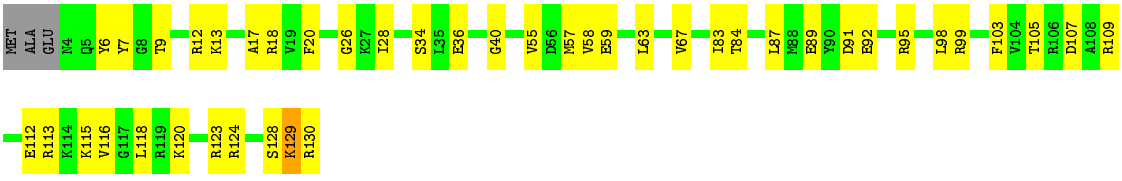


- Molecule 8: 30S ribosomal protein S8

Chain AH:

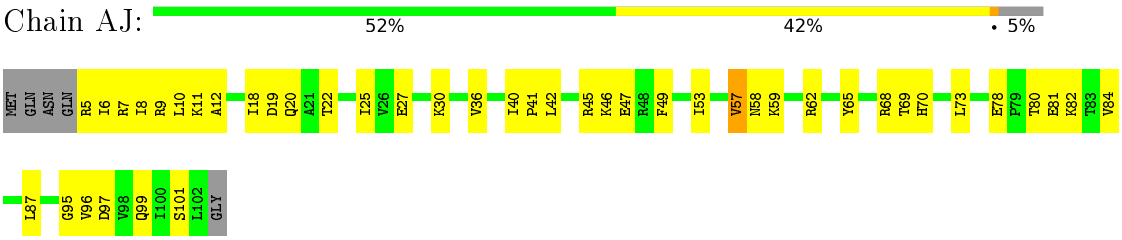
- Molecule 9: 30S ribosomal protein S9

Chain AI:



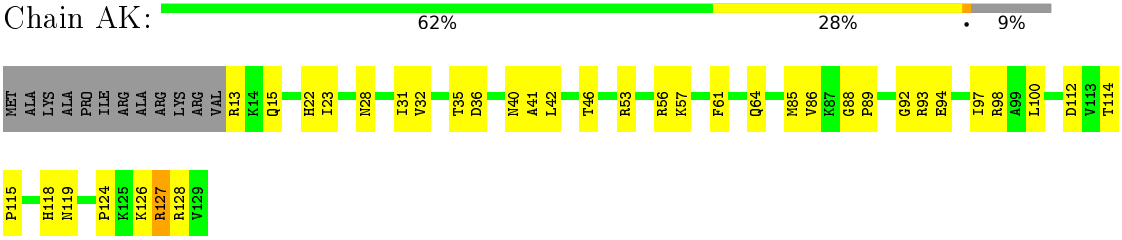
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



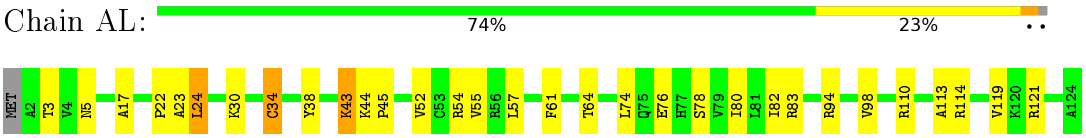
- Molecule 11: 30S ribosomal protein S11

Chain AK:



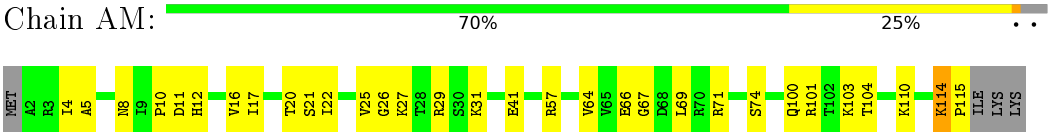
- Molecule 12: 30S ribosomal protein S12

Chain AL:



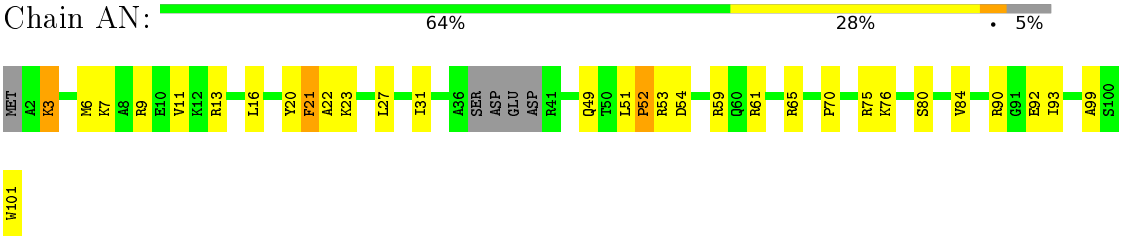
- Molecule 13: 30S ribosomal protein S13

Chain AM:



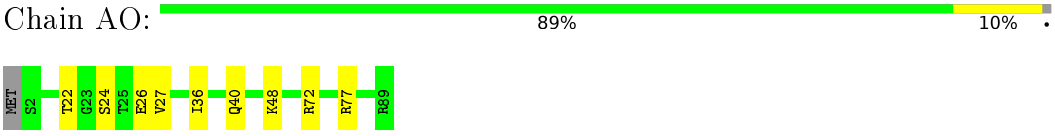
- Molecule 14: 30S ribosomal protein S14

Chain AN:



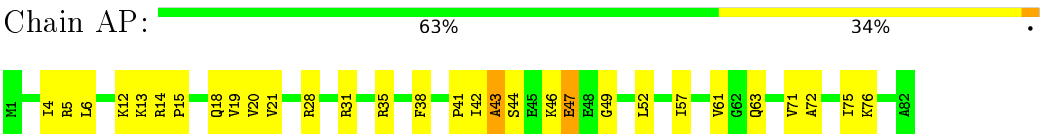
- Molecule 15: 30S ribosomal protein S15

Chain AO:



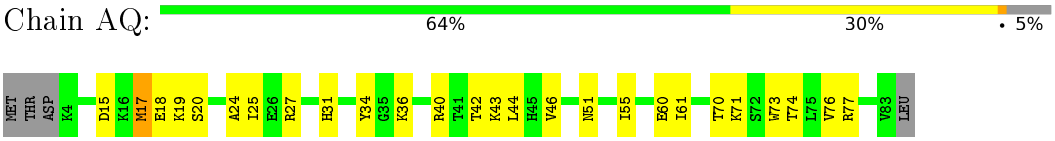
- Molecule 16: 30S ribosomal protein S16

Chain AP:



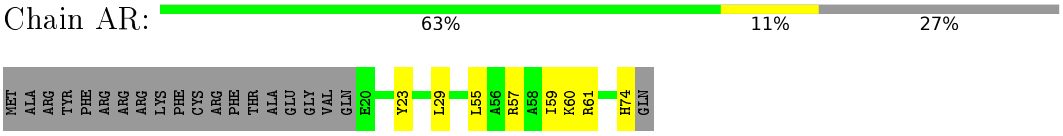
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



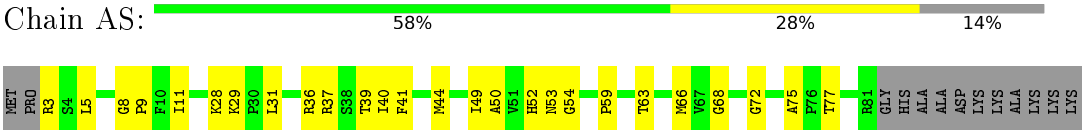
• Molecule 18: 30S ribosomal protein S18

Chain AR:



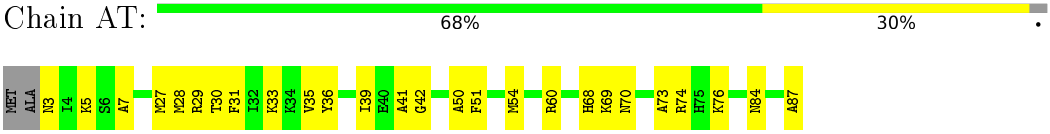
• Molecule 19: 30S ribosomal protein S19

Chain AS:



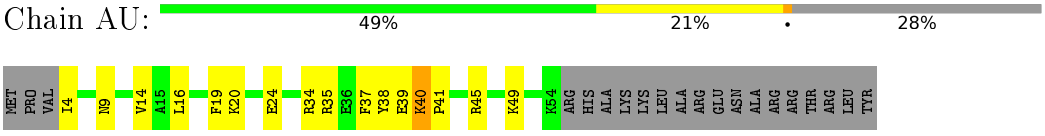
• Molecule 20: 30S ribosomal protein S20

Chain AT:



• Molecule 21: 30S ribosomal protein S21

Chain AU:

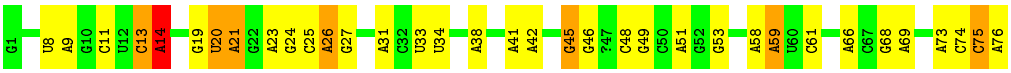


• Molecule 22: mRNA

Chain AV:

• Molecule 23: A-site Lysine tRNA Lysine

Chain AW:

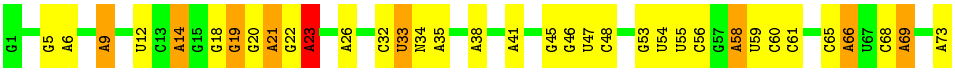


• Molecule 24: P-site tRNA Aspartate

Chain AX:

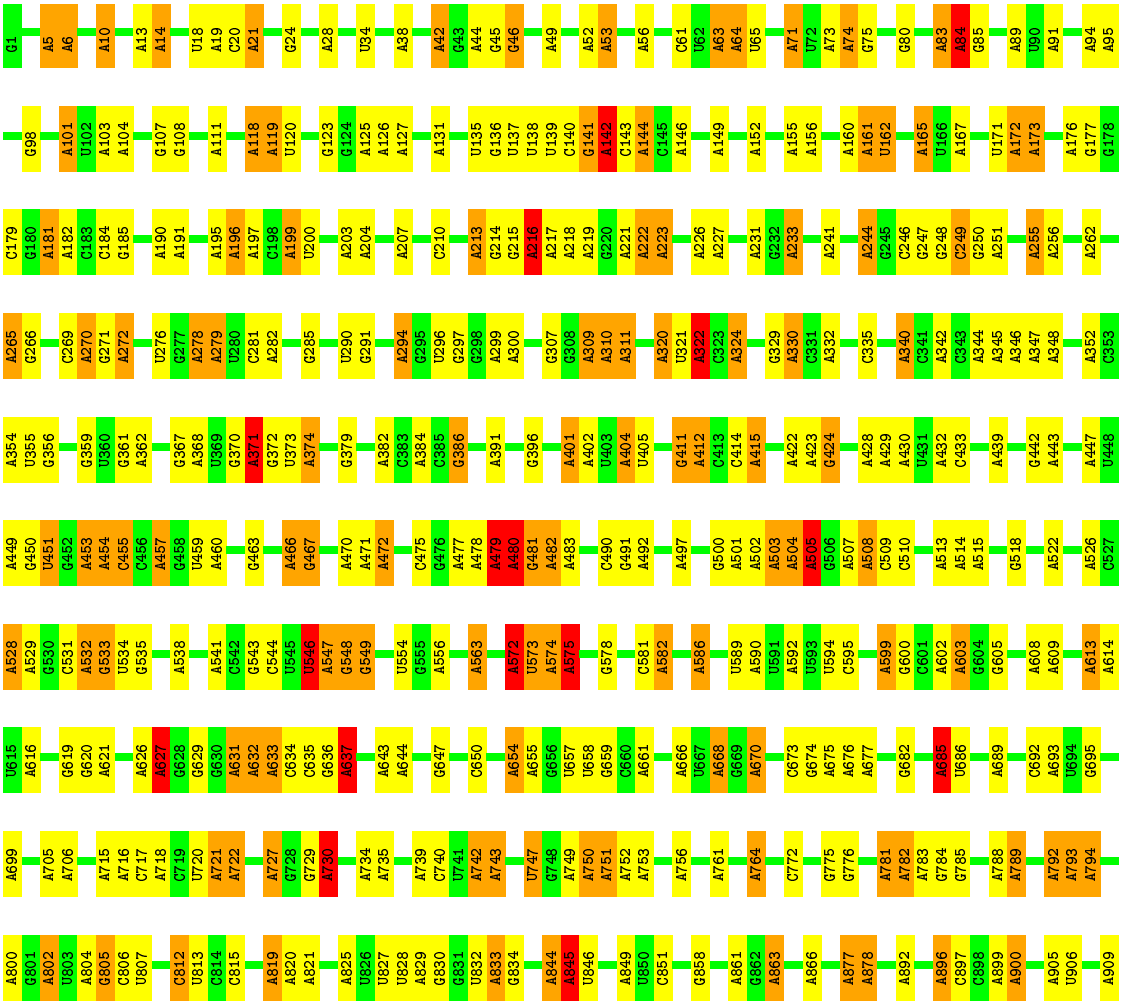
• Molecule 25: E-site tRNA Valine

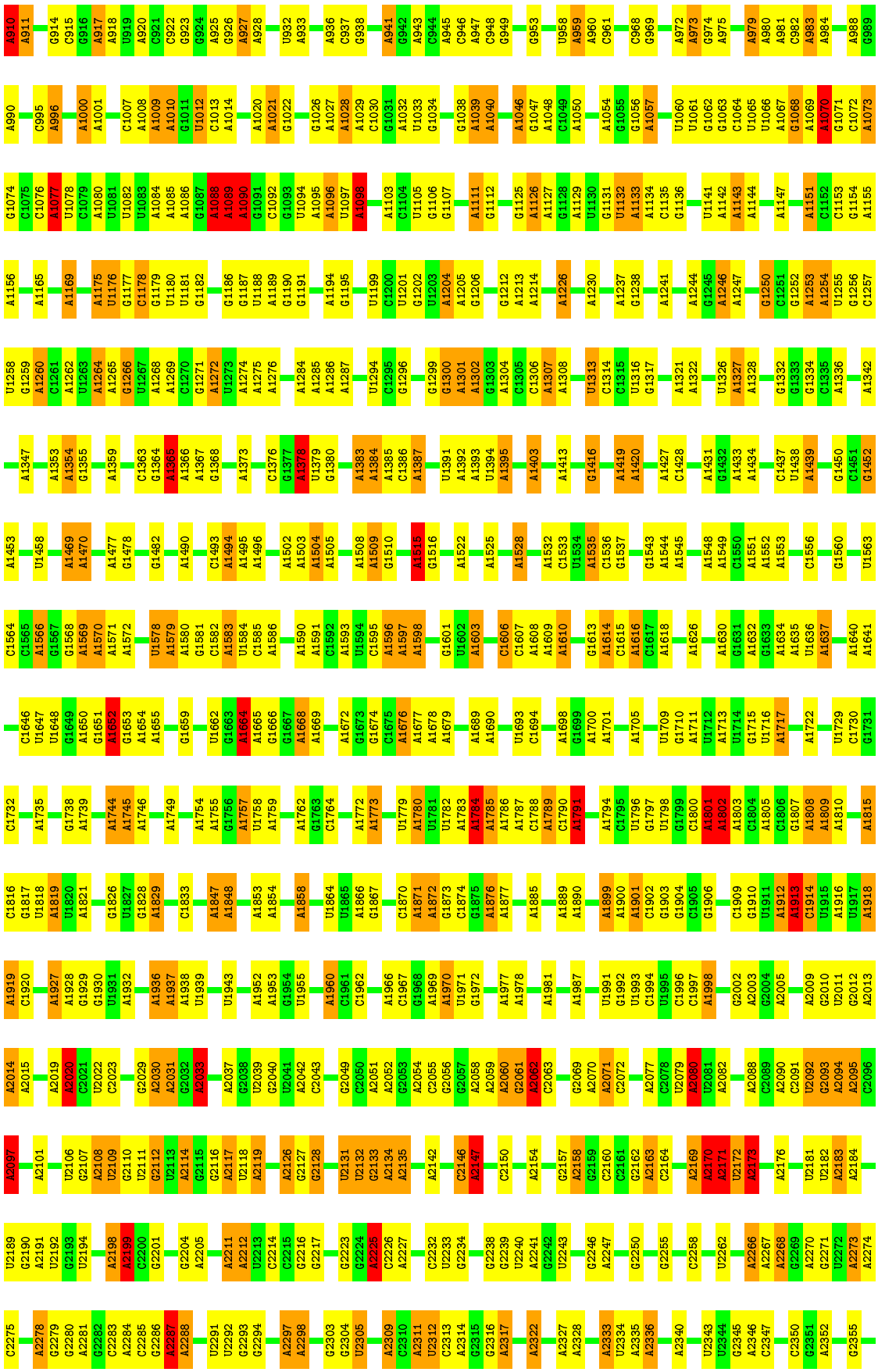
Chain AY:

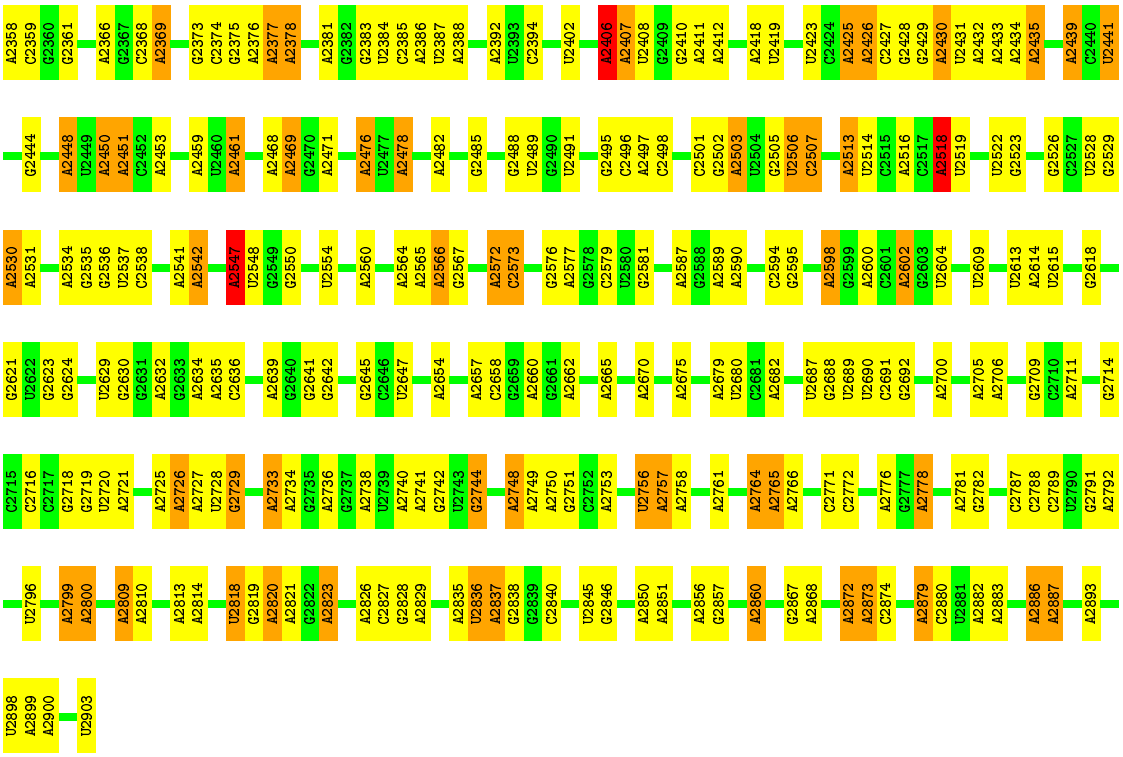


• Molecule 26: 23S ribosomal RNA

Chain BA:

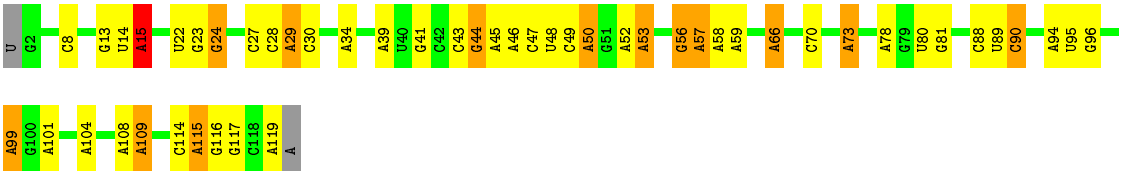






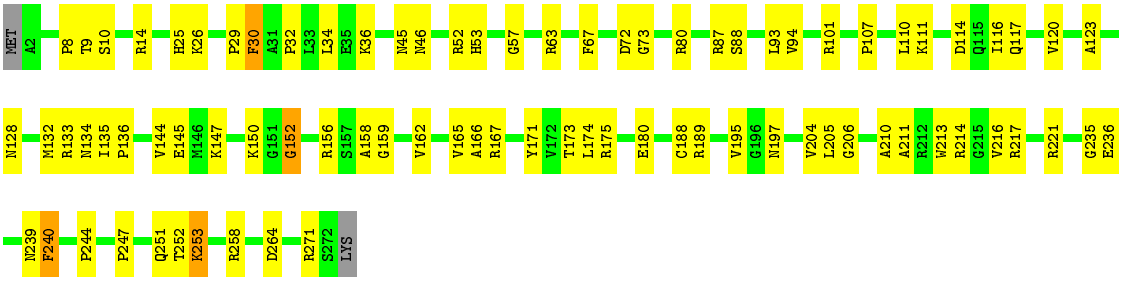
- Molecule 27: 5S ribosomal RNA

Chain BB:



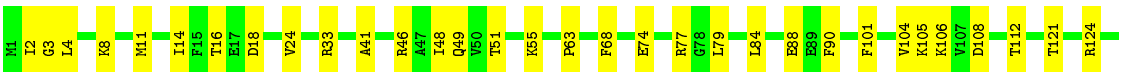
- Molecule 28: 50S ribosomal protein L2

Chain BC:



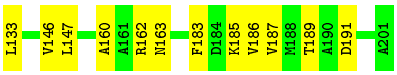
- Molecule 29: 50S ribosomal protein L3

Chain BD:



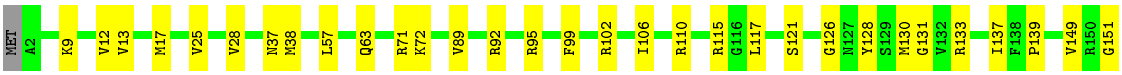
• Molecule 30: 50S ribosomal protein L4

Chain BE:



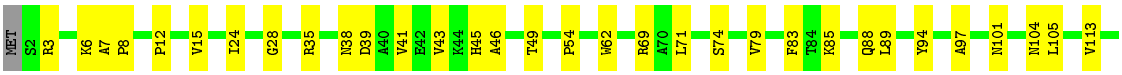
• Molecule 31: 50S ribosomal protein L5

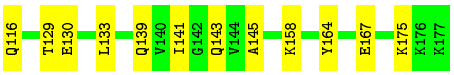
Chain BF:



• Molecule 32: 50S ribosomal protein L6

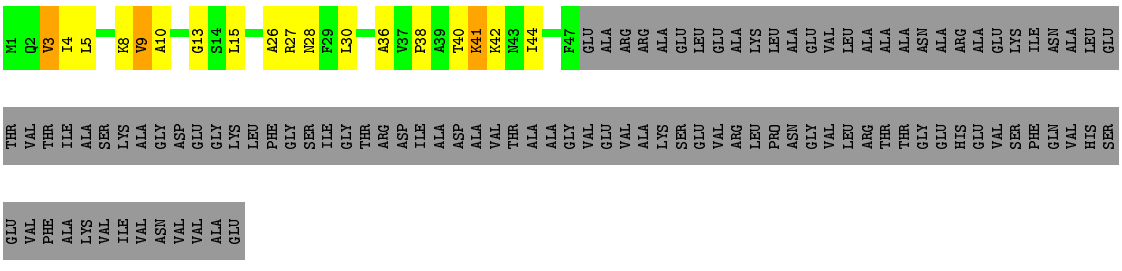
Chain BG:





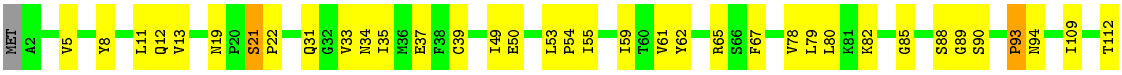
• Molecule 33: 50S ribosomal protein L9

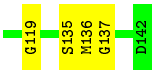
Chain BH:



• Molecule 34: 50S ribosomal protein L11

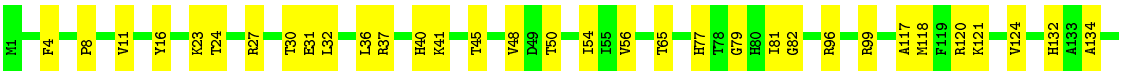
Chain BI:





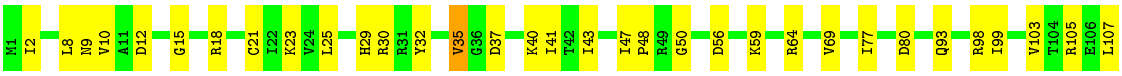
• Molecule 35: 50S ribosomal protein L13

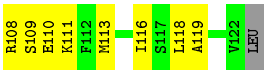
Chain BJ:



• Molecule 36: 50S ribosomal protein L14

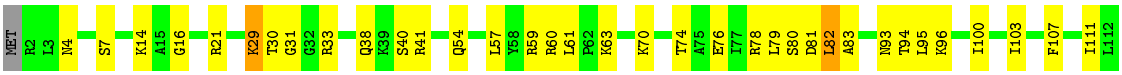
Chain BK:

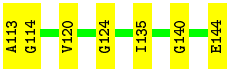




• Molecule 37: 50S ribosomal protein L15

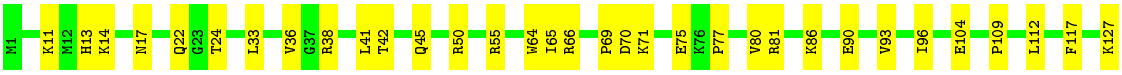
Chain BL:





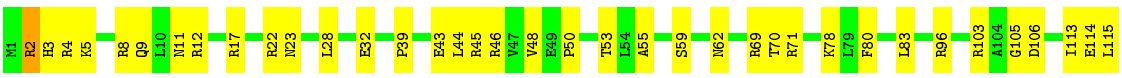
• Molecule 38: 50S ribosomal protein L16

Chain BM:



• Molecule 39: 50S ribosomal protein L17

Chain BN:

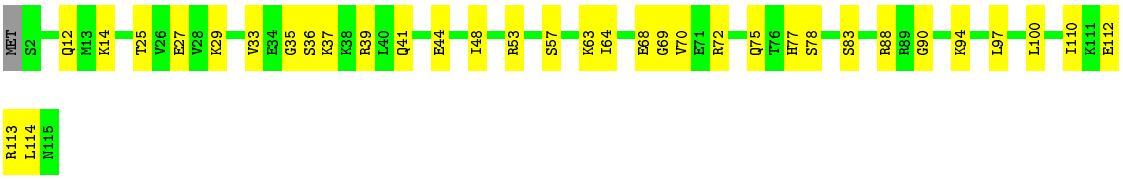


- Molecule 40: 50S ribosomal protein L18

Chain BO:

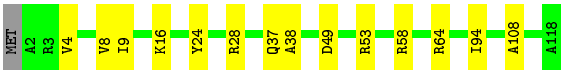
- Molecule 41: 50S ribosomal protein L19

Chain BP:



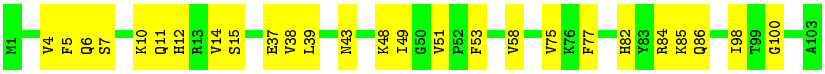
- Molecule 42: 50S ribosomal protein L20

Chain BQ:



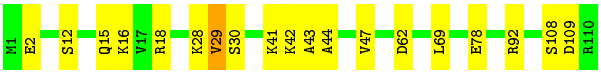
- Molecule 43: 50S ribosomal protein L21

Chain BR:



- Molecule 44: 50S ribosomal protein L22

Chain BS:

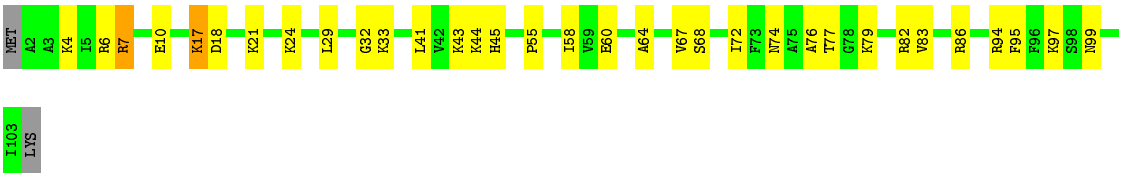


- Molecule 45: 50S ribosomal protein L23

Chain BT:

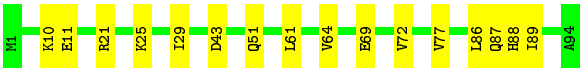
- Molecule 46: 50S ribosomal protein L24

Chain BU:



- Molecule 47: 50S ribosomal protein L25

Chain BV:

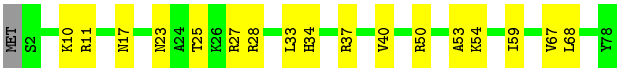


- Molecule 48: 50S ribosomal protein L27

Chain BW:

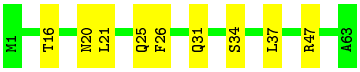
- Molecule 49: 50S ribosomal protein L28

Chain BX:



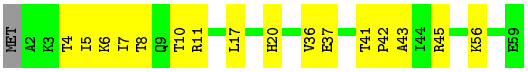
- Molecule 50: 50S ribosomal protein L29

Chain BY:



- Molecule 51: 50S ribosomal protein L30

Chain BZ:

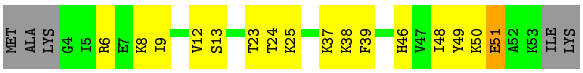


- Molecule 52: 50S ribosomal protein L32

Chain B0:

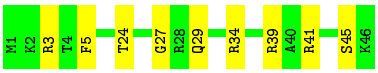
- Molecule 53: 50S ribosomal protein L33

Chain B1:



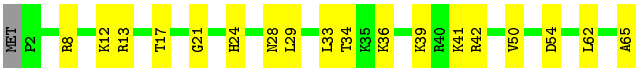
- Molecule 54: 50S ribosomal protein L34

Chain B2:



- Molecule 55: 50S ribosomal protein L35

Chain B3:



- Molecule 56: 50S ribosomal protein L36

Chain B4:

- Molecule 57: ErmBL

Chain B5:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	85393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, U8U, 7MG, ERY, PSU, 2MA, 6MZ, 3AU, 4SU, T6A, QUO, CM0

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	AA	2.20	1353/36965 (3.7%)	3.39	4664/57662 (8.1%)
10	AJ	0.31	0/796	0.53	0/1077
11	AK	0.25	0/893	0.44	0/1205
12	AL	0.25	0/969	0.45	0/1300
13	AM	0.27	0/892	0.49	0/1193
14	AN	0.24	0/785	0.42	0/1043
15	AO	0.28	0/718	0.45	0/959
16	AP	0.26	0/659	0.44	0/884
17	AQ	0.26	0/657	0.49	0/881
18	AR	0.27	0/462	0.44	0/621
19	AS	0.26	0/652	0.43	0/877
2	AB	0.30	0/1735	0.49	0/2338
20	AT	0.25	0/671	0.43	0/888
21	AU	0.25	0/430	0.50	0/570
22	AV	3.36	21/245 (8.6%)	5.13	72/380 (18.9%)
23	AW	2.30	58/1569 (3.7%)	3.39	201/2437 (8.2%)
24	AX	2.07	48/1668 (2.9%)	2.69	139/2593 (5.4%)
25	AY	1.97	44/1554 (2.8%)	3.05	157/2416 (6.5%)
26	BA	2.25	2626/69659 (3.8%)	3.46	9154/108672 (8.4%)
27	BB	1.94	79/2828 (2.8%)	3.00	278/4410 (6.3%)
28	BC	0.25	0/2121	0.45	0/2852
29	BD	0.27	0/1586	0.45	0/2134
3	AC	0.25	0/1651	0.44	0/2225
30	BE	0.27	0/1571	0.45	0/2113
31	BF	0.30	0/1434	0.47	0/1926
32	BG	0.27	0/1343	0.44	0/1816
33	BH	0.29	0/364	0.52	0/490
34	BI	0.28	0/1046	0.49	0/1410
35	BJ	0.27	0/1152	0.44	0/1551
36	BK	0.26	0/947	0.46	0/1268
37	BL	0.24	0/1054	0.44	0/1403
38	BM	0.26	0/1093	0.43	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	BN	0.25	0/973	0.43	0/1301
4	AD	0.27	0/1665	0.47	0/2227
40	BO	0.25	0/902	0.40	0/1209
41	BP	0.24	0/929	0.43	0/1242
42	BQ	0.24	0/960	0.38	0/1278
43	BR	0.25	0/829	0.43	0/1107
44	BS	0.29	0/864	0.48	0/1156
45	BT	0.23	0/744	0.43	0/994
46	BU	0.28	0/787	0.45	0/1051
47	BV	0.27	0/766	0.44	0/1025
48	BW	0.25	0/576	0.39	0/762
49	BX	0.23	0/635	0.39	0/848
5	AE	0.24	0/1118	0.46	0/1504
50	BY	0.22	0/510	0.38	0/677
51	BZ	0.23	0/453	0.44	0/605
52	B0	0.27	0/450	0.44	0/599
53	B1	0.24	0/416	0.43	0/554
54	B2	0.20	0/380	0.37	0/498
55	B3	0.22	0/513	0.41	0/676
56	B4	0.23	0/303	0.39	0/397
57	B5	0.36	0/74	0.59	0/98
6	AF	0.25	0/835	0.46	0/1128
7	AG	0.25	0/1195	0.42	0/1602
8	AH	0.27	0/989	0.45	0/1326
9	AI	0.28	0/1034	0.48	0/1375
All	All	1.89	4229/159069 (2.7%)	2.97	14665/238293 (6.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
29	BD	0	1

The worst 5 of 4229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	20	U	C5-C6	23.31	1.55	1.34
23	AW	20	U	C5-C6	23.29	1.55	1.34
24	AX	16	U	C5-C6	23.26	1.55	1.34
24	AX	19	U	C5-C6	23.18	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	454	A	C6-N6	17.20	1.47	1.33

The worst 5 of 14665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	278	A	C2-N3-C4	20.42	120.81	110.60
1	AA	983	A	C2-N3-C4	20.30	120.75	110.60
26	BA	2114	A	C2-N3-C4	20.19	120.70	110.60
26	BA	514	A	C2-N3-C4	19.99	120.60	110.60
26	BA	2451	A	N1-C6-N6	-19.89	106.67	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	BD	151	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33015	0	16618	252	0
2	AB	1704	0	1732	31	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	74	0
5	AE	1105	0	1148	24	0
6	AF	817	0	808	12	0
7	AG	1181	0	1238	21	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	25	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	25	0
12	AL	955	0	1016	20	0
13	AM	883	0	941	22	0
14	AN	774	0	824	26	0
15	AO	710	0	728	7	0
16	AP	649	0	666	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AQ	648	0	691	17	0
18	AR	455	0	478	7	0
19	AS	637	0	665	15	0
20	AT	665	0	714	18	0
21	AU	425	0	449	7	0
22	AV	218	0	109	3	0
23	AW	1593	0	820	8	0
24	AX	1656	0	849	10	0
25	AY	1525	0	780	11	0
26	BA	62195	0	31280	431	0
27	BB	2529	0	1281	22	0
28	BC	2082	0	2154	53	0
29	BD	1565	0	1616	40	0
30	BE	1552	0	1619	32	0
31	BF	1410	0	1444	23	0
32	BG	1323	0	1371	27	0
33	BH	359	0	381	13	0
34	BI	1032	0	1085	26	0
35	BJ	1129	0	1162	22	0
36	BK	938	0	1012	26	0
37	BL	1045	0	1117	26	0
38	BM	1074	0	1157	25	0
39	BN	960	0	1000	29	0
40	BO	892	0	923	21	0
41	BP	917	0	962	22	0
42	BQ	947	0	1019	11	0
43	BR	816	0	839	15	0
44	BS	857	0	922	13	0
45	BT	738	0	807	14	0
46	BU	779	0	831	23	0
47	BV	753	0	780	9	0
48	BW	569	0	581	15	0
49	BX	625	0	652	13	0
50	BY	509	0	543	8	0
51	BZ	449	0	488	10	0
52	B0	444	0	458	8	0
53	B1	409	0	440	12	0
54	B2	377	0	418	7	0
55	B3	504	0	572	15	0
56	B4	302	0	343	8	0
57	B5	74	0	74	23	0
58	AW	9	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BA	51	0	67	12	0
All	All	146760	0	97903	1470	0

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

The worst 5 of 1470 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)
59:BA:9000:ERY:C27	57:B5:-2:ASN:ND2	2.18	1.07
59:BA:9000:ERY:H271	57:B5:-2:ASN:HD21	1.13	1.06
59:BA:9000:ERY:H271	57:B5:-2:ASN:ND2	1.74	1.01
59:BA:9000:ERY:C27	57:B5:-2:ASN:HD21	1.72	0.98
58:AW:101:LYS:N	24:AX:76:A:HO2'	1.69	0.91

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	5 42
3	AC	204/233 (88%)	180 (88%)	20 (10%)	4 (2%)	9 53
4	AD	203/206 (98%)	188 (93%)	8 (4%)	7 (3%)	5 41
5	AE	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	3 30
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	2 28
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	26 72
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	24 69
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	3 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	2 23
11	AK	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	7 46
12	AL	121/124 (98%)	108 (89%)	6 (5%)	7 (6%)	2 25
13	AM	112/118 (95%)	104 (93%)	7 (6%)	1 (1%)	21 67
14	AN	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	2 27
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100 100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7 48
17	AQ	78/84 (93%)	64 (82%)	11 (14%)	3 (4%)	4 37
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100 100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	15 60
20	AT	83/87 (95%)	76 (92%)	4 (5%)	3 (4%)	4 39
21	AU	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	1 11
28	BC	269/273 (98%)	247 (92%)	16 (6%)	6 (2%)	8 51
29	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	19 66
30	BE	199/201 (99%)	188 (94%)	9 (4%)	2 (1%)	19 66
31	BF	175/179 (98%)	154 (88%)	16 (9%)	5 (3%)	6 44
32	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	11 55
33	BH	45/149 (30%)	37 (82%)	4 (9%)	4 (9%)	1 13
34	BI	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	2 25
35	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	26 72
36	BK	120/123 (98%)	106 (88%)	9 (8%)	5 (4%)	3 33
37	BL	141/144 (98%)	117 (83%)	16 (11%)	8 (6%)	2 25
38	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8 51
39	BN	118/127 (93%)	104 (88%)	9 (8%)	5 (4%)	3 33
40	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	7 46
41	BP	112/115 (97%)	105 (94%)	5 (4%)	2 (2%)	11 54
42	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100 100
43	BR	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	4 35
44	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	10 53
45	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	8 51
46	BU	100/104 (96%)	82 (82%)	13 (13%)	5 (5%)	3 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100 100
48	BW	73/85 (86%)	69 (94%)	4 (6%)	0	100 100
49	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100 100
50	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100 100
51	BZ	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	11 54
52	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
53	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	9 52
54	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8 50
55	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100 100
56	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
57	B5	7/9 (78%)	3 (43%)	3 (43%)	1 (14%)	0 5
All	All	5522/5993 (92%)	4968 (90%)	406 (7%)	148 (3%)	10 46

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
12	AL	23	ALA
17	AQ	17	MET

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
2	AB	180/198 (91%)	180 (100%)	0	100 100
3	AC	170/190 (90%)	170 (100%)	0	100 100
4	AD	172/173 (99%)	172 (100%)	0	100 100
5	AE	113/126 (90%)	113 (100%)	0	100 100
6	AF	87/116 (75%)	87 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
28	BC	216/218 (99%)	216 (100%)	0	100	100
29	BD	164/164 (100%)	164 (100%)	0	100	100
30	BE	165/165 (100%)	165 (100%)	0	100	100
31	BF	148/150 (99%)	148 (100%)	0	100	100
32	BG	137/138 (99%)	137 (100%)	0	100	100
33	BH	38/114 (33%)	38 (100%)	0	100	100
34	BI	109/110 (99%)	109 (100%)	0	100	100
35	BJ	116/116 (100%)	116 (100%)	0	100	100
36	BK	103/104 (99%)	103 (100%)	0	100	100
37	BL	102/103 (99%)	102 (100%)	0	100	100
38	BM	109/109 (100%)	109 (100%)	0	100	100
39	BN	100/103 (97%)	100 (100%)	0	100	100
40	BO	86/87 (99%)	86 (100%)	0	100	100
41	BP	99/100 (99%)	99 (100%)	0	100	100
42	BQ	89/90 (99%)	89 (100%)	0	100	100
43	BR	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BS	93/93 (100%)	93 (100%)	0	100	100
45	BT	80/84 (95%)	80 (100%)	0	100	100
46	BU	83/85 (98%)	83 (100%)	0	100	100
47	BV	78/78 (100%)	78 (100%)	0	100	100
48	BW	56/63 (89%)	56 (100%)	0	100	100
49	BX	67/68 (98%)	67 (100%)	0	100	100
50	BY	55/55 (100%)	55 (100%)	0	100	100
51	BZ	48/49 (98%)	48 (100%)	0	100	100
52	B0	47/48 (98%)	47 (100%)	0	100	100
53	B1	45/49 (92%)	45 (100%)	0	100	100
54	B2	38/38 (100%)	38 (100%)	0	100	100
55	B3	51/52 (98%)	51 (100%)	0	100	100
56	B4	34/34 (100%)	34 (100%)	0	100	100
57	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
29	BD	164	GLN
32	BG	116	GLN
50	BY	25	GLN
30	BE	41	GLN
30	BE	97	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	218 (14%)	4 (0%)
22	AV	9/10 (90%)	0	0
23	AW	70/74 (94%)	13 (18%)	1 (1%)
24	AX	74/77 (96%)	6 (8%)	0
25	AY	67/71 (94%)	13 (19%)	1 (1%)
26	BA	2895/2897 (99%)	425 (14%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	BB	117/120 (97%)	13 (11%)	0
All	All	4769/4788 (99%)	688 (14%)	16 (0%)

5 of 688 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	32	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	404	A
26	BA	479	A
26	BA	2146	C
26	BA	271	G
26	BA	2225	A

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

21 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	$\#\|Z\| > 2$
23	U8U	AW	34	22,23	15,24,25	1.54	1 (6%)	17,34,37	3.48	2 (11%)
23	T6A	AW	37	23	23,34,35	1.19	2 (8%)	26,49,52	1.89	6 (23%)
23	PSU	AW	39	23	15,21,22	2.03	4 (26%)	16,30,33	2.85	5 (31%)
23	7MG	AW	46	23	20,26,27	1.85	5 (25%)	23,39,42	1.86	4 (17%)
23	3AU	AW	47	23	16,28,29	1.18	2 (12%)	16,40,43	0.78	1 (6%)
23	5MU	AW	54	23	13,22,23	1.42	1 (7%)	16,32,35	3.61	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	AW	55	23	15,21,22	2.05	4 (26%)	16,30,33	2.88	5 (31%)
23	4SU	AW	8	23	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)
24	QUO	AX	34	24,22	27,35,36	1.66	4 (14%)	30,52,55	2.89	5 (16%)
24	2MA	AX	37	24	17,25,26	1.73	4 (23%)	18,37,40	1.63	1 (5%)
24	7MG	AX	46	24	20,26,27	1.89	5 (25%)	23,39,42	1.86	4 (17%)
24	5MU	AX	54	24	13,22,23	1.42	1 (7%)	16,32,35	3.59	2 (12%)
24	PSU	AX	55	24	15,21,22	2.03	4 (26%)	16,30,33	2.88	5 (31%)
24	PSU	AX	65	24	15,21,22	1.96	3 (20%)	16,30,33	2.88	3 (18%)
24	4SU	AX	8	24	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)
25	CM0	AY	34	25	15,26,27	1.64	2 (13%)	18,37,40	2.72	3 (16%)
25	6MZ	AY	37	25	17,25,26	1.25	4 (23%)	15,36,39	0.93	1 (6%)
25	7MG	AY	46	25	20,26,27	1.87	5 (25%)	23,39,42	1.88	4 (17%)
25	5MU	AY	54	25	13,22,23	1.42	1 (7%)	16,32,35	3.61	2 (12%)
25	PSU	AY	55	25	15,21,22	2.00	4 (26%)	16,30,33	2.86	5 (31%)
25	4SU	AY	8	25	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)

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
23	U8U	AW	34	22,23	-	0/5/28/29	0/2/2/2
23	T6A	AW	37	23	-	0/15/41/42	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	3AU	AW	47	23	-	0/8/34/35	0/2/2/2
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	QUO	AX	34	24,22	-	0/6/43/44	0/4/4/4
24	2MA	AX	37	24	-	0/3/25/26	0/3/3/3
24	7MG	AX	46	24	-	0/7/37/38	0/3/3/3
24	5MU	AX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	65	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
25	CM0	AY	34	25	-	0/6/30/31	0/2/2/2
25	6MZ	AY	37	25	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	AY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	55	PSU	C5-C1'	-2.77	1.49	1.52
23	AW	39	PSU	C5-C1'	-2.65	1.49	1.52
24	AX	55	PSU	C5-C1'	-2.63	1.49	1.52
24	AX	65	PSU	C6-C5	-2.48	1.35	1.38
23	AW	39	PSU	C6-C5	-2.48	1.35	1.38

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	34	QUO	C5-C6-N1	-14.01	113.38	124.15
23	AW	34	U8U	C5-C4-N3	-11.78	114.62	125.19
23	AW	54	5MU	C5-C4-N3	-10.41	116.61	125.35
25	AY	54	5MU	C5-C4-N3	-10.38	116.63	125.35
24	AX	54	5MU	C5-C4-N3	-10.35	116.66	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	34	U8U	1	0
25	AY	34	CM0	1	0
25	AY	55	PSU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\|>2$
58	LYS	AW	101	23	6,8,9	0.79	0	6,8,10	1.55	1 (16%)
59	ERY	BA	9000	-	53,53,53	1.14	5 (9%)	82,82,82	1.66	22 (26%)

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
58	LYS	AW	101	23	-	0/5/7/9	0/0/0/0
59	ERY	BA	9000	-	-	0/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BA	9000	ERY	O9-C26	-2.84	1.39	1.44
59	BA	9000	ERY	O13-C12	-2.84	1.39	1.44
59	BA	9000	ERY	O10-C6	-2.50	1.40	1.44
59	BA	9000	ERY	O2-C13	-2.45	1.42	1.46
59	BA	9000	ERY	C15-C14	2.01	1.56	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	BA	9000	ERY	C34-C10-C11	-3.58	109.62	114.44
59	BA	9000	ERY	C36-C13-C12	-3.48	107.79	115.13
58	AW	101	LYS	O-C-CA	-3.16	117.24	125.72
59	BA	9000	ERY	C12-C11-C10	-3.15	112.18	116.51
59	BA	9000	ERY	C16-C15-C14	-3.08	109.66	115.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AW	101	LYS	3	0
59	BA	9000	ERY	12	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	1
23	AW	1
25	AY	1
26	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.72
1	AW	15:G	O3'	18:G	P	9.77
1	AY	15:G	O3'	18:G	P	6.82
1	AA	99:C	O3'	100:G	P	4.17