



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 20, 2016 – 02:59 PM EST

PDB ID : 5LI0
EMDB ID: : EMD-4050
Title : 70S ribosome from Staphylococcus aureus
Authors : Khusainov, I.; Vicens, Q.; Bochler, A.; Grosse, F.; Myasnikov, A.; Menetret, J.F.; Chicher, J.; Marzi, S.; Romby, P.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2016-07-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
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-20028442

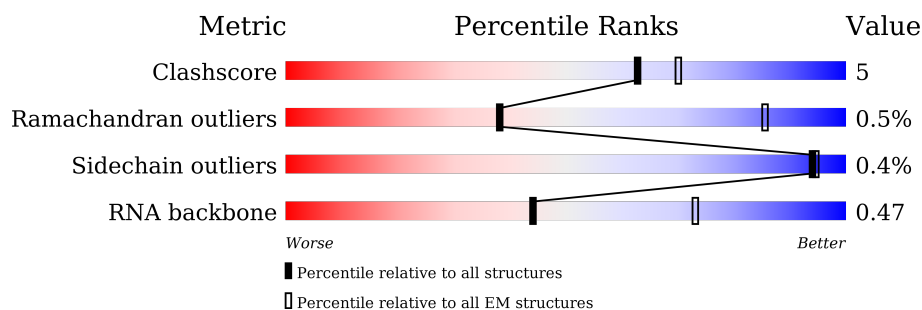
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	1547	79% 20% .
2	b	255	87% 12%
3	c	217	95% . .
4	d	199	98% ..
5	e	165	99% .
6	f	96	100%
7	g	150	96% ...
8	h	131	98% .











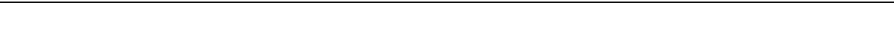

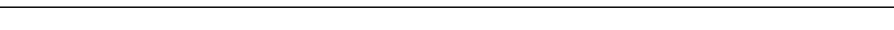
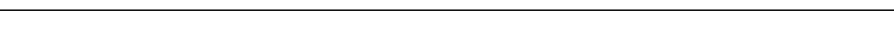
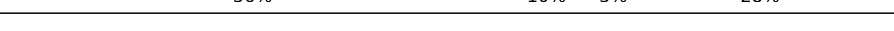


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	128	99% .
10	j	102	100%
11	k	118	100%
12	l	135	100%
13	m	119	96% . .
14	n	60	97% .
15	o	88	100%
16	p	90	100%
17	q	86	95% . .
18	r	71	100%
19	s	84	96% .
20	t	80	100%
21	A	2918	60% 31% 8% .
22	B	114	58% 36% 6%
23	D	275	82% 17% .
24	E	218	87% 11% .
25	F	199	89% 10% .
26	G	166	95% 5%
27	H	164	87% 13%
28	M	145	94% 6%
29	N	122	84% 16% .
30	O	131	90% 8% .
31	P	141	91% 9%
32	Q	119	87% 13%
33	R	119	79% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	S	110	 89% 11%
35	T	116	 89% 11%
36	U	102	 93% 7%
37	V	112	 90% 10%
38	W	89	 93% 6% .
39	X	100	 84% . 13%
40	Y	94	 80% 19% .
41	Z	82	 82% 18%
42	0	46	 83% 17%
43	1	65	 83% 17%
44	2	57	 95% 5%
45	3	84	 54% 36% 10% .
46	4	56	 89% 11%
47	5	39	 56% 10% 5% 28%
48	6	44	 75% 23% .
49	7	60	 77% 23%
50	8	37	 84% 16%

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140825 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
1	a	1547	Total	C	N	O	P	0	0
			33126	14790	6036	10753	1547		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1802	1147	315	333	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	208	Total	C	N	O	S	0	0
			1638	1032	306	298	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	197	Total	C	N	O	S	0	0
			1600	1009	300	289	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	165	Total	C	N	O	S	0	0
			1239	775	229	233	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	96	Total	C	N	O	S	0	0
			799	503	139	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	147	Total	C	N	O	S	0	0
			1189	744	227	214	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	102	Total	C	N	O	S	0	0
			813	512	148	150	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	118	Total	C	N	O	S	0	0
			881	543	169	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1063	658	218	185	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	119	Total	C	N	O	S	0	0
			946	581	188	176	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	86	Total	C	N	O	S	0	0
			707	447	126	133	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	71	Total	C	N	O	S	0	0
			590	372	115	100	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			678	434	120	122	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	367	119	119	2		

- Molecule 21 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	2914	Total	C	N	O	P	0	0
			62475	27892	11424	20245	2914		

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	114	Total	C	N	O	P	0	0
			2427	1086	436	792	113		

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	275	Total	C	N	O	S	0	0
			2104	1309	417	373	5		

- Molecule 24 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	218	Total	C	N	O	S	0	0
			1649	1030	304	310	5		

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	199	Total	C	N	O	S	0	0
			1525	955	281	287	2		

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	166	Total	C	N	O	S	0	0
			1312	832	223	251	6		

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	164	Total	C	N	O	S	0	0
			1285	799	232	251	3		

- Molecule 28 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	O	131	Total	C	N	O	S	0	0
			998	618	197	182	1		

- Molecule 31 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	141	Total	C	N	O	S	0	0
			1122	717	211	190	4		

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Q	119	Total	C	N	O	S	0	0
			940	575	181	183	1		

- Molecule 33 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 34 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S	110	Total	C	N	O	S	0	0
			886	557	177	151	1		

- Molecule 35 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	116	Total	C	N	O	S	0	0
			944	593	189	158	4		

- Molecule 36 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	U	102	Total	C	N	O	S	0	0
			799	506	142	150	1		

- Molecule 37 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	112	Total	C	N	O	S	0	0
			863	537	164	159	3		

- Molecule 38 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W	89	Total	C	N	O	S	0	0
			726	457	130	135	4		

- Molecule 39 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	X	87	Total	C	N	O	S	0	0
			669	423	122	123	1		

- Molecule 40 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Z	82	Total	C	N	O	0	0
			627	386	122	119		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	0	46	Total	C	N	O	0	0
			374	231	83	60		

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	1	65	Total	C	N	O	0	0
			537	330	101	106		

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2	57	Total	C	N	O	0	0
			442	274	83	85		

- Molecule 45 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	83	Total	C	N	O	S	0	0
			677	430	116	128	3		

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	56	Total	C	N	O	S	0	0
			444	268	92	79	5		

- Molecule 47 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	60	Total	C	N	O	S	0	0
			488	300	108	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	A	29	Total	Mg	0
			29	29	
51	a	2	Total	Mg	0
			2	2	

- Molecule 52 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		AltConf
52	A	9	Total	O	0
			9	9	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	8	1	Total	Zn	0
			1	1	

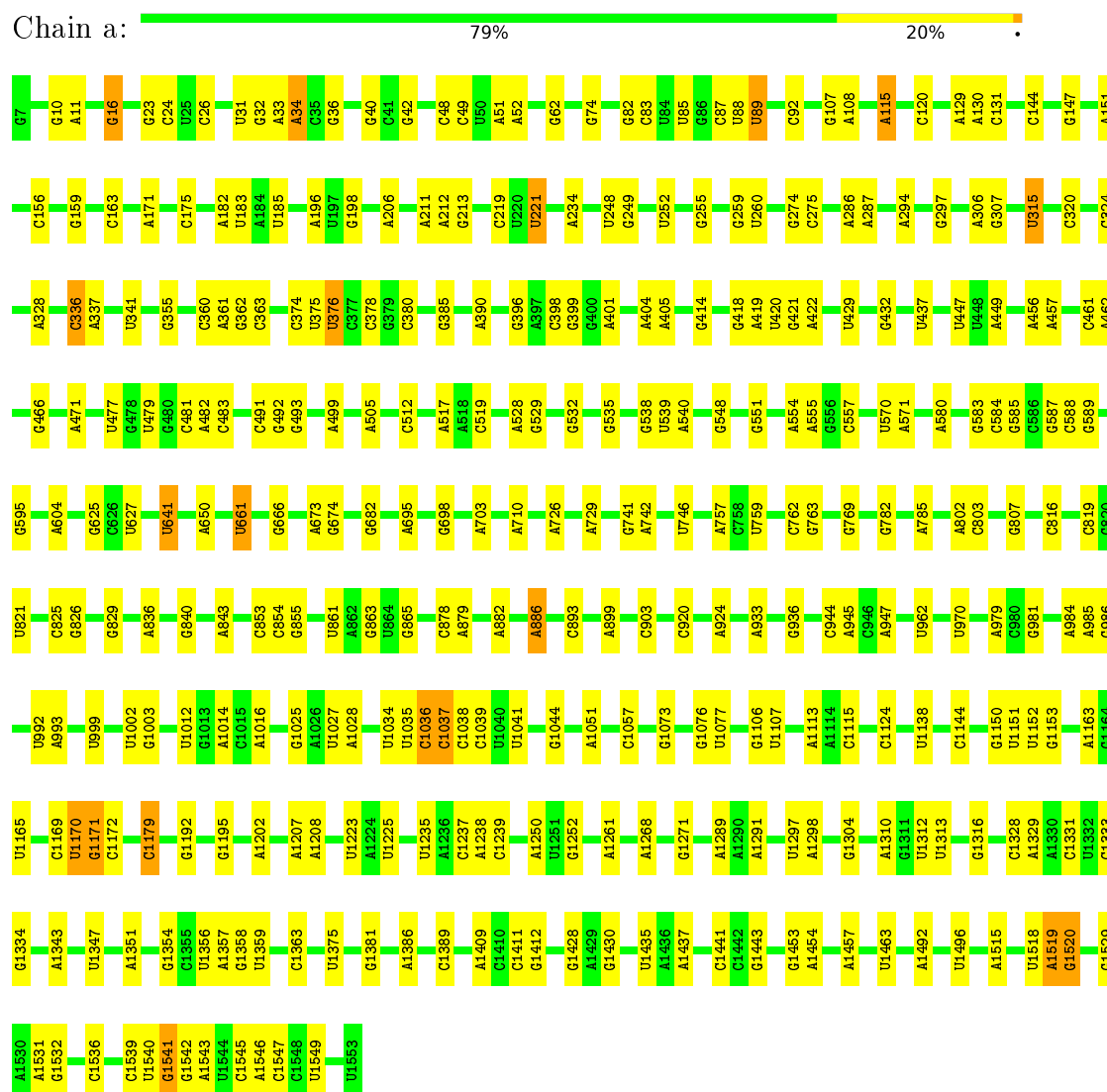
- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	a	12	Total	O	0
			12	12	
54	A	143	Total	O	0
			143	143	
54	D	4	Total	O	0
			4	4	
54	T	2	Total	O	0
			2	2	
54	U	1	Total	O	0
			1	1	

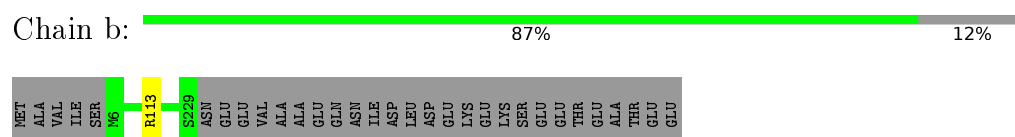
3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

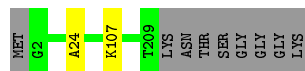


• Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

Chain c:  95% ..



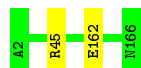
- Molecule 4: 30S ribosomal protein S4

Chain d:  98% ..



- Molecule 5: 30S ribosomal protein S5

Chain e:  99% .



- Molecule 6: 30S ribosomal protein S6

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S ribosomal protein S7

Chain g:  96% ...



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  99% .



- Molecule 10: 30S ribosomal protein S10

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 30S ribosomal protein S11

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 30S ribosomal protein S12

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S13

Chain m:  96% . .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain n:  97% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 30S ribosomal protein S16

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S ribosomal protein S17

Chain q:  95% . .

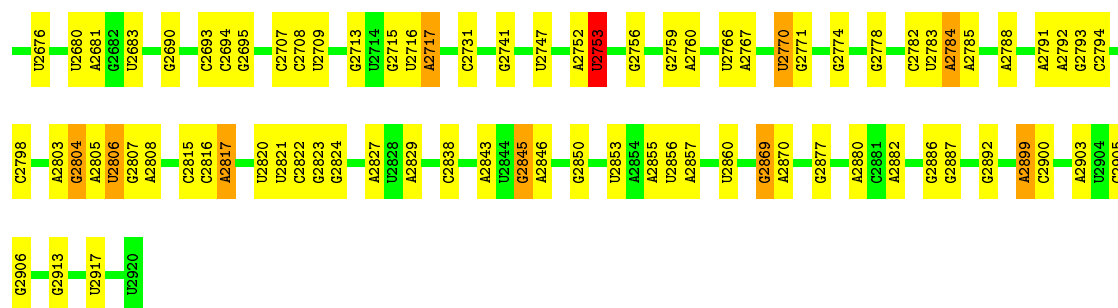


- Molecule 18: 30S ribosomal protein S18

Chain r:  100%

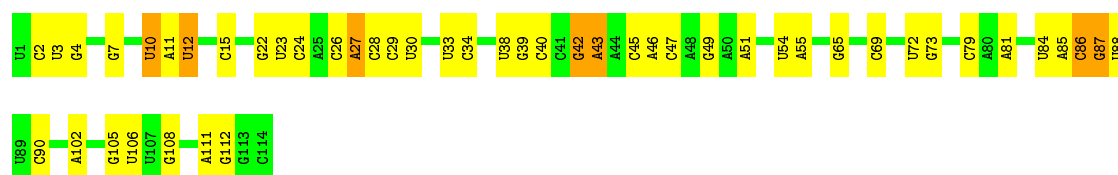
There are no outlier residues recorded for this chain.





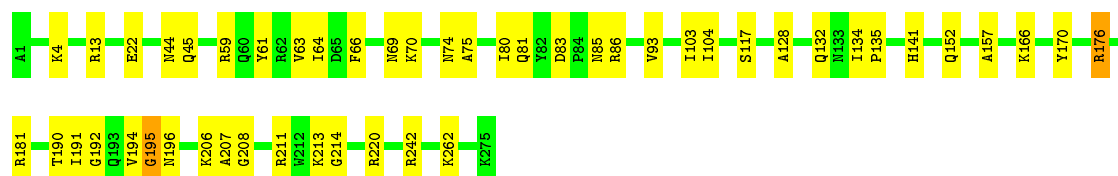
- Molecule 22: 5S ribosomal RNA

Chain B: 58% 36% 6%



- Molecule 23: 50S ribosomal protein L2

Chain D: 82% 17%



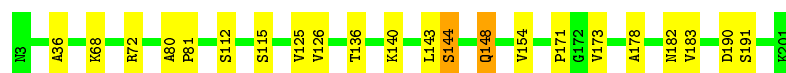
- Molecule 24: 50S ribosomal protein L3

Chain E: 87% 11%



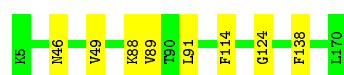
- Molecule 25: 50S ribosomal protein L4

Chain F: 89% 10%




- Molecule 26: 50S ribosomal protein L5

Chain G: 95% 5%



- Molecule 27: 50S ribosomal protein L6

Chain H:  87% 13%




- Molecule 28: 50S ribosomal protein L13

Chain M:  94% 6%



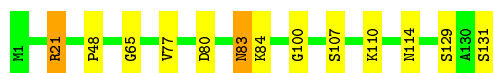
- Molecule 29: 50S ribosomal protein L14

Chain N:  84% 16%



- Molecule 30: 50S ribosomal protein L15

Chain O:  90% 8%




- Molecule 31: 50S ribosomal protein L16

Chain P:  91% 9%




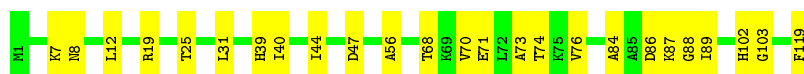
- Molecule 32: 50S ribosomal protein L17

Chain Q:  87% 13%




- Molecule 33: 50S ribosomal protein L18

Chain R:  79% 21%



- Molecule 34: 50S ribosomal protein L19

Chain S:  89% 11%



- Molecule 35: 50S ribosomal protein L20

Chain T: 89% 11%



- Molecule 36: 50S ribosomal protein L21

Chain U: 93% 7%



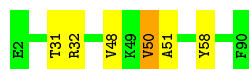
- Molecule 37: 50S ribosomal protein L22

Chain V: 90% 10%



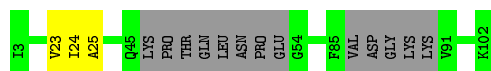
- Molecule 38: 50S ribosomal protein L23

Chain W: 93% 6%



- Molecule 39: 50S ribosomal protein L24

Chain X: 84% 13%



- Molecule 40: 50S ribosomal protein L25

Chain Y: 80% 19%




- Molecule 41: 50S ribosomal protein L27

Chain Z: 82% 18%




- Molecule 42: 50S ribosomal protein L28

Chain 0:  83% 17%



- Molecule 43: 50S ribosomal protein L29

Chain 1:  83% 17%



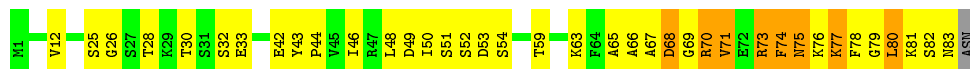
- Molecule 44: 50S ribosomal protein L30

Chain 2:  95% 5%



- Molecule 45: 50S ribosomal protein L31 type B

Chain 3:  54% 36% 10%



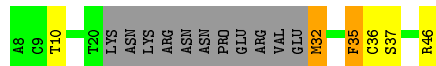
- Molecule 46: 50S ribosomal protein L32

Chain 4:  89% 11%



- Molecule 47: 50S ribosomal protein L33 2

Chain 5:  56% 10% 5% 28%




- Molecule 48: 50S ribosomal protein L34

Chain 6:  75% 23%




- Molecule 49: 50S ribosomal protein L35

Chain 7:  77% 23%



- Molecule 50: 50S ribosomal protein L36

Chain 8:  84% 16%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	110000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, O

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	a	0.89	0/37086	1.18	125/57833 (0.2%)
10	j	0.43	0/825	0.67	0/1110
11	k	0.46	0/896	0.69	0/1207
12	l	0.53	0/1080	0.78	0/1445
13	m	0.41	0/953	0.77	0/1275
14	n	0.54	0/512	0.70	0/678
15	o	0.51	0/747	0.68	0/996
16	p	0.55	0/723	0.67	0/971
17	q	0.57	0/715	0.79	0/955
18	r	0.45	0/599	0.72	0/797
19	s	0.41	0/696	0.73	0/934
2	b	0.39	0/1829	0.63	1/2454 (0.0%)
20	t	0.44	0/607	0.61	0/810
21	A	2.04	70/69965 (0.1%)	1.80	586/109115 (0.5%)
22	B	0.85	0/2714	1.14	4/4228 (0.1%)
23	D	0.73	0/2139	0.75	0/2869
24	E	0.67	0/1673	0.69	0/2243
25	F	0.62	0/1548	0.66	0/2088
26	G	0.42	0/1327	0.70	1/1780 (0.1%)
27	H	0.47	0/1303	0.65	0/1757
28	M	0.65	0/1173	0.65	0/1578
29	N	0.71	0/927	0.76	0/1243
3	c	0.44	0/1661	0.64	0/2233
30	O	0.60	0/1011	0.80	1/1344 (0.1%)
31	P	0.66	0/1146	0.75	0/1536
32	Q	0.56	0/943	0.69	0/1259
33	R	0.53	0/931	0.69	0/1244
34	S	0.66	0/898	0.72	0/1199
35	T	0.73	0/956	0.77	1/1265 (0.1%)
36	U	0.63	0/809	0.69	1/1080 (0.1%)
37	V	0.63	0/871	0.76	0/1171
38	W	0.60	0/734	0.71	0/978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	X	0.49	0/673	0.64	0/893
4	d	0.51	0/1629	0.68	0/2185
40	Y	0.50	0/746	0.69	0/1000
41	Z	0.72	0/633	0.77	0/838
42	0	0.54	0/379	0.78	0/504
43	1	0.49	0/538	0.63	0/714
44	2	0.58	0/444	0.66	0/597
45	3	0.46	0/694	0.74	1/930 (0.1%)
46	4	0.65	0/451	0.73	0/599
47	5	0.51	0/230	0.79	0/303
48	6	0.72	0/377	0.79	0/491
49	7	0.61	0/492	0.87	0/643
5	e	0.55	0/1253	0.69	0/1687
50	8	0.73	0/300	0.72	1/393 (0.3%)
6	f	0.60	0/810	0.63	0/1085
7	g	0.41	0/1207	0.65	0/1625
8	h	0.57	0/1044	0.72	0/1401
9	i	0.41	0/1033	0.70	0/1386
All	All	1.48	70/152930 (0.0%)	1.43	722/228949 (0.3%)

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
13	m	0	5
14	n	0	2
17	q	0	3
19	s	0	3
23	D	0	1
24	E	0	6
25	F	0	5
26	G	0	4
28	M	0	2
29	N	0	1
3	c	0	2
30	O	0	4
31	P	0	1
33	R	0	2
34	S	0	1
35	T	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
36	U	0	1
38	W	0	2
40	Y	0	1
41	Z	0	4
45	3	0	3
46	4	0	2
47	5	0	1
48	6	0	2
49	7	0	2
5	e	0	1
7	g	0	3
8	h	0	2
All	All	0	67

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1288	G	C6-N1	171.20	2.59	1.39
21	A	1288	G	N3-C4	147.91	2.38	1.35
21	A	857	C	C5-C6	139.70	2.46	1.34
21	A	1288	G	N1-C2	138.56	2.48	1.37
21	A	1288	G	C2-N3	124.17	2.32	1.32

The worst 5 of 722 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	N3-C4-C5	-238.20	26.62	121.90
21	A	857	C	C6-N1-C2	-227.33	29.37	120.30
21	A	2230	G	C8-N9-C4	-102.39	65.45	106.40
21	A	857	C	C2-N3-C4	83.55	161.67	119.90
21	A	857	C	C5-C6-N1	82.07	162.03	121.00

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	107	LYS	Peptide
3	c	24	ALA	Peptide
5	e	162	GLU	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33126	0	16679	0	0
2	b	1802	0	1861	0	0
3	c	1638	0	1702	0	0
4	d	1600	0	1628	0	0
5	e	1239	0	1298	0	0
6	f	799	0	794	0	0
7	g	1189	0	1218	0	0
8	h	1032	0	1082	0	0
9	i	1017	0	1039	0	0
10	j	813	0	859	0	0
11	k	881	0	899	0	0
12	l	1063	0	1130	0	0
13	m	946	0	1001	0	0
14	n	502	0	527	0	0
15	o	738	0	769	0	0
16	p	712	0	744	0	0
17	q	707	0	749	0	0
18	r	590	0	628	0	0
19	s	678	0	672	0	0
20	t	607	0	650	0	0
21	A	62475	0	31402	495	0
22	B	2427	0	1230	24	0
23	D	2104	0	2221	35	0
24	E	1649	0	1689	15	0
25	F	1525	0	1570	12	0
26	G	1312	0	1366	1	0
27	H	1285	0	1301	13	0
28	M	1151	0	1145	5	0
29	N	920	0	981	10	0
30	O	998	0	1044	6	0
31	P	1122	0	1185	8	0
32	Q	940	0	990	12	0
33	R	922	0	968	14	0
34	S	886	0	957	6	0
35	T	944	0	1014	8	0
36	U	799	0	836	3	0
37	V	863	0	920	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	726	0	761	3	0
39	X	669	0	725	2	0
40	Y	738	0	787	11	0
41	Z	627	0	645	11	0
42	0	374	0	407	5	0
43	1	537	0	567	8	0
44	2	442	0	478	3	0
45	3	677	0	655	55	0
46	4	444	0	453	2	0
47	5	229	0	224	15	0
48	6	373	0	420	6	0
49	7	488	0	548	9	0
50	8	297	0	339	5	0
51	A	29	0	0	0	0
51	a	2	0	0	0	0
52	A	9	0	0	1	0
53	8	1	0	0	0	0
54	A	143	0	0	13	0
54	D	4	0	0	0	0
54	T	2	0	0	0	0
54	U	1	0	0	1	0
54	a	12	0	0	0	0
All	All	140825	0	93757	732	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 5.

The worst 5 of 732 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)
21:A:1828:U:C6	21:A:1828:U:C5	2.07	1.42
21:A:2230:G:N9	21:A:2230:G:C4	1.68	1.39
21:A:857:C:C6	21:A:857:C:N3	1.94	1.34
21:A:1828:U:C5	21:A:1828:U:C4	2.18	1.31
21:A:1288:G:C5	21:A:1288:G:C4	2.24	1.23

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	b	222/255 (87%)	199 (90%)	23 (10%)	0	100	100
3	c	206/217 (95%)	172 (84%)	34 (16%)	0	100	100
4	d	193/199 (97%)	171 (89%)	21 (11%)	1 (0%)	34	77
5	e	163/165 (99%)	140 (86%)	23 (14%)	0	100	100
6	f	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
7	g	143/150 (95%)	124 (87%)	17 (12%)	2 (1%)	14	59
8	h	129/131 (98%)	109 (84%)	19 (15%)	1 (1%)	24	70
9	i	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
10	j	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
11	k	116/118 (98%)	99 (85%)	17 (15%)	0	100	100
12	l	133/135 (98%)	103 (77%)	30 (23%)	0	100	100
13	m	117/119 (98%)	92 (79%)	23 (20%)	2 (2%)	11	56
14	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	o	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
16	p	88/90 (98%)	74 (84%)	14 (16%)	0	100	100
17	q	84/86 (98%)	66 (79%)	17 (20%)	1 (1%)	16	63
18	r	69/71 (97%)	58 (84%)	11 (16%)	0	100	100
19	s	82/84 (98%)	66 (80%)	16 (20%)	0	100	100
20	t	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
23	D	273/275 (99%)	236 (86%)	36 (13%)	1 (0%)	39	80
24	E	216/218 (99%)	181 (84%)	33 (15%)	2 (1%)	21	68
25	F	197/199 (99%)	166 (84%)	30 (15%)	1 (0%)	34	77
26	G	164/166 (99%)	132 (80%)	31 (19%)	1 (1%)	30	74
27	H	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
28	M	143/145 (99%)	126 (88%)	17 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	N	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	7	49
30	O	129/131 (98%)	90 (70%)	39 (30%)	0	100	100
31	P	139/141 (99%)	106 (76%)	33 (24%)	0	100	100
32	Q	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
33	R	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
34	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
35	T	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
36	U	100/102 (98%)	82 (82%)	18 (18%)	0	100	100
37	V	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
38	W	87/89 (98%)	75 (86%)	10 (12%)	2 (2%)	8	51
39	X	81/100 (81%)	66 (82%)	15 (18%)	0	100	100
40	Y	92/94 (98%)	73 (79%)	17 (18%)	2 (2%)	8	52
41	Z	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
42	0	44/46 (96%)	30 (68%)	14 (32%)	0	100	100
43	1	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	2	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
45	3	81/84 (96%)	54 (67%)	24 (30%)	3 (4%)	4	40
46	4	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
47	5	24/39 (62%)	15 (62%)	9 (38%)	0	100	100
48	6	42/44 (96%)	35 (83%)	5 (12%)	2 (5%)	3	32
49	7	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
50	8	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	5292/5466 (97%)	4481 (85%)	787 (15%)	24 (0%)	38	77

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	13	LEU
8	h	99	ASN
38	W	50	VAL
45	3	12	VAL
45	3	68	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	194/221 (88%)	194 (100%)	0	100	100
3	c	169/175 (97%)	169 (100%)	0	100	100
4	d	172/174 (99%)	172 (100%)	0	100	100
5	e	130/130 (100%)	129 (99%)	1 (1%)	86	94
6	f	84/84 (100%)	84 (100%)	0	100	100
7	g	126/127 (99%)	126 (100%)	0	100	100
8	h	112/112 (100%)	112 (100%)	0	100	100
9	i	106/106 (100%)	105 (99%)	1 (1%)	84	93
10	j	91/91 (100%)	91 (100%)	0	100	100
11	k	94/94 (100%)	94 (100%)	0	100	100
12	l	117/117 (100%)	117 (100%)	0	100	100
13	m	102/102 (100%)	102 (100%)	0	100	100
14	n	52/52 (100%)	52 (100%)	0	100	100
15	o	80/80 (100%)	80 (100%)	0	100	100
16	p	76/76 (100%)	76 (100%)	0	100	100
17	q	81/81 (100%)	80 (99%)	1 (1%)	78	91
18	r	63/63 (100%)	63 (100%)	0	100	100
19	s	73/73 (100%)	73 (100%)	0	100	100
20	t	67/67 (100%)	67 (100%)	0	100	100
23	D	222/222 (100%)	221 (100%)	1 (0%)	92	97
24	E	175/175 (100%)	175 (100%)	0	100	100
25	F	163/163 (100%)	163 (100%)	0	100	100
26	G	147/147 (100%)	147 (100%)	0	100	100
27	H	144/144 (100%)	144 (100%)	0	100	100
28	M	123/123 (100%)	123 (100%)	0	100	100
29	N	100/100 (100%)	100 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	O	104/104 (100%)	104 (100%)	0	100	100
31	P	116/116 (100%)	116 (100%)	0	100	100
32	Q	100/100 (100%)	100 (100%)	0	100	100
33	R	95/95 (100%)	95 (100%)	0	100	100
34	S	96/96 (100%)	96 (100%)	0	100	100
35	T	96/96 (100%)	96 (100%)	0	100	100
36	U	86/86 (100%)	86 (100%)	0	100	100
37	V	91/91 (100%)	91 (100%)	0	100	100
38	W	80/80 (100%)	80 (100%)	0	100	100
39	X	73/85 (86%)	73 (100%)	0	100	100
40	Y	83/83 (100%)	83 (100%)	0	100	100
41	Z	64/64 (100%)	64 (100%)	0	100	100
42	0	39/39 (100%)	39 (100%)	0	100	100
43	1	59/59 (100%)	59 (100%)	0	100	100
44	2	51/51 (100%)	51 (100%)	0	100	100
45	3	74/75 (99%)	65 (88%)	9 (12%)	6	34
46	4	49/49 (100%)	49 (100%)	0	100	100
47	5	26/37 (70%)	23 (88%)	3 (12%)	7	37
48	6	39/39 (100%)	39 (100%)	0	100	100
49	7	52/52 (100%)	52 (100%)	0	100	100
50	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4571/4631 (99%)	4555 (100%)	16 (0%)	94	97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	3	75	ASN
45	3	76	LYS
45	3	83	ASN
45	3	74	PHE
47	5	32	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
18	r	57	GLN
19	s	43	ASN
40	Y	38	ASN
15	o	9	ASN
40	Y	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1546/1547 (99%)	268 (17%)	0
21	A	2910/2918 (99%)	631 (21%)	8 (0%)
22	B	113/114 (99%)	18 (15%)	0
All	All	4569/4579 (99%)	917 (20%)	8 (0%)

5 of 917 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	G
1	a	11	A
1	a	16	G
1	a	23	G
1	a	31	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	661	U
21	A	2230	G
21	A	1938	U
21	A	377	U
21	A	1127	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 41 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.