wwPDB EM Validation Summary Report

Oct 28, 2024 – 02:39 pm GMT

PDB ID	:	7OOD
EMDB ID	:	EMD-11999
Title	:	Mycoplasma pneumoniae 50S subunit of ribosomes in chloramphenicol-treated cells
Authors	:	Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on	:	2021-05-27
Resolution	:	3.40 Å(reported)
Based on initial models	:	3J9W, 4YBB, 1DIV, 1ZAV

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 (i) 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 (1)) were used in the production of this report:

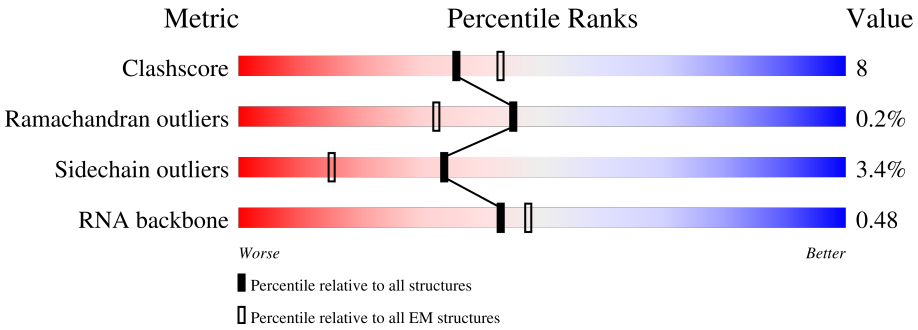
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5%

Mol	Chain	Length	Quality of chain
1	3	2907	64% 29% 6%
2	4	108	62% 27% 7%
3	w	111	85% 5% 11%
4	a	287	97%
5	c	212	95%
6	e	184	94%
7	k	151	95%

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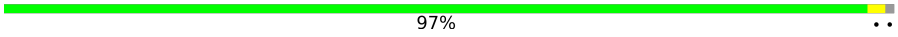
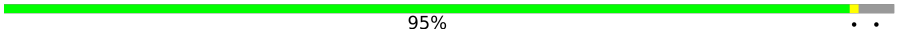
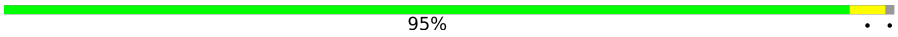
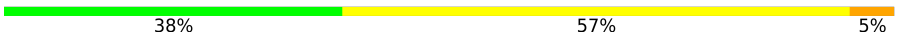
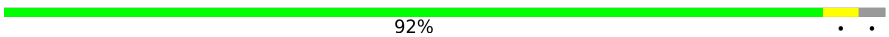
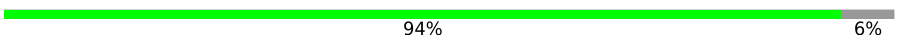
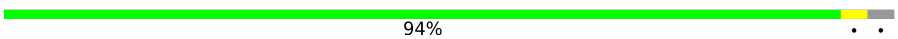
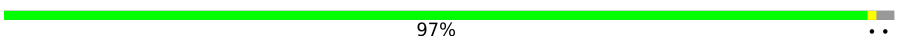
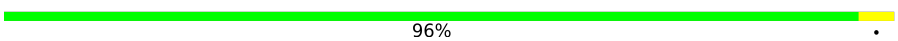
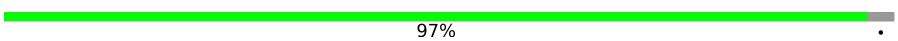
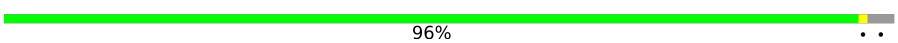
Mol	Chain	Length	Quality of chain
8	i	146	
9	m	124	
10	q	100	
11	u	104	
12	y	57	
13	0	48	
14	2	37	
15	1	59	
16	o	119	
17	s	237	
18	v	65	
19	x	97	
20	z	53	
21	d	180	
22	b	287	
23	l	139	
24	p	127	
25	j	122	
26	n	116	
27	t	111	
28	r	159	
29	f	149	
30	h	137	
31	g	161	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 89509 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	3	2879	61690	27566	11236	20009	2879	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	4	105	2245	1003	409	728	105	0	0

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	w	99	798	505	149	144	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	285	2199	1370	433	390	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	210	1613	1026	294	290	3	0	0

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	e	176	1349	867	240	242	0	0

- Molecule 7 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	k	148	Total	C	N	O	0	0
			1138	722	223	193		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	144	Total	C	N	O	S	0	0
			1158	733	212	208	5		

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	119	Total	C	N	O	S	0	0
			957	609	175	170	3		

- Molecule 10 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	99	Total	C	N	O	S	0	0
			809	525	148	133	3		

- Molecule 11 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	u	86	Total	C	N	O	S	0	0
			641	397	127	116	1		

- Molecule 12 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	y	56	Total	C	N	O	S	0	0
			436	262	96	73	5		

- Molecule 13 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0	47	Total	C	N	O	S	0	0
			377	234	81	61	1		

- Molecule 14 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	37	Total	C	N	O	S	0	0
			303	189	65	45	4		

- Molecule 15 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o	115	Total	C	N	O	S	0	0
			895	568	169	157	1		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	s	92	Total	C	N	O	S	0	0
			714	470	121	122	1		

- Molecule 18 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	v	63	Total	C	N	O	S	0	0
			504	312	107	84	1		

- Molecule 19 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	x	44	Total	C	N	O	0	0
			218	130	44	44		

- Molecule 20 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 21 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	175	Total	C	N	O	S	0	0
			1244	797	214	229	4		

- Molecule 22 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	229	Total	C	N	O	S	0	0
			1758	1116	317	318	7		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	136	Total	C	N	O	S	0	0
			1057	680	193	177	7		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	114	Total	C	N	O	S	0	0
			941	600	185	154	2		

- Molecule 25 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	112	Total	C	N	O	S	0	0
			853	534	169	149	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	96	Total	C	N	O	S	0	0
			706	449	132	122	3		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	144	Total	C	N	O	0	0
			713	425	144	144		

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	h	128	Total	C	N	O	0	0
			630	374	128	128		

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	g	125	Total	C	N	O	0	0
			617	367	125	125		

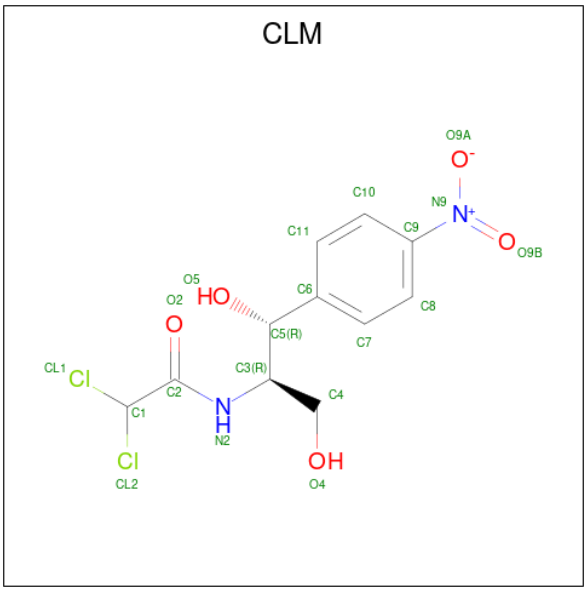
- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
32	3	1	Total	K	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	3	24	Total	Mg	0
			24	24	
33	y	1	Total	Mg	0
			1	1	

- Molecule 34 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					AltConf
34	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

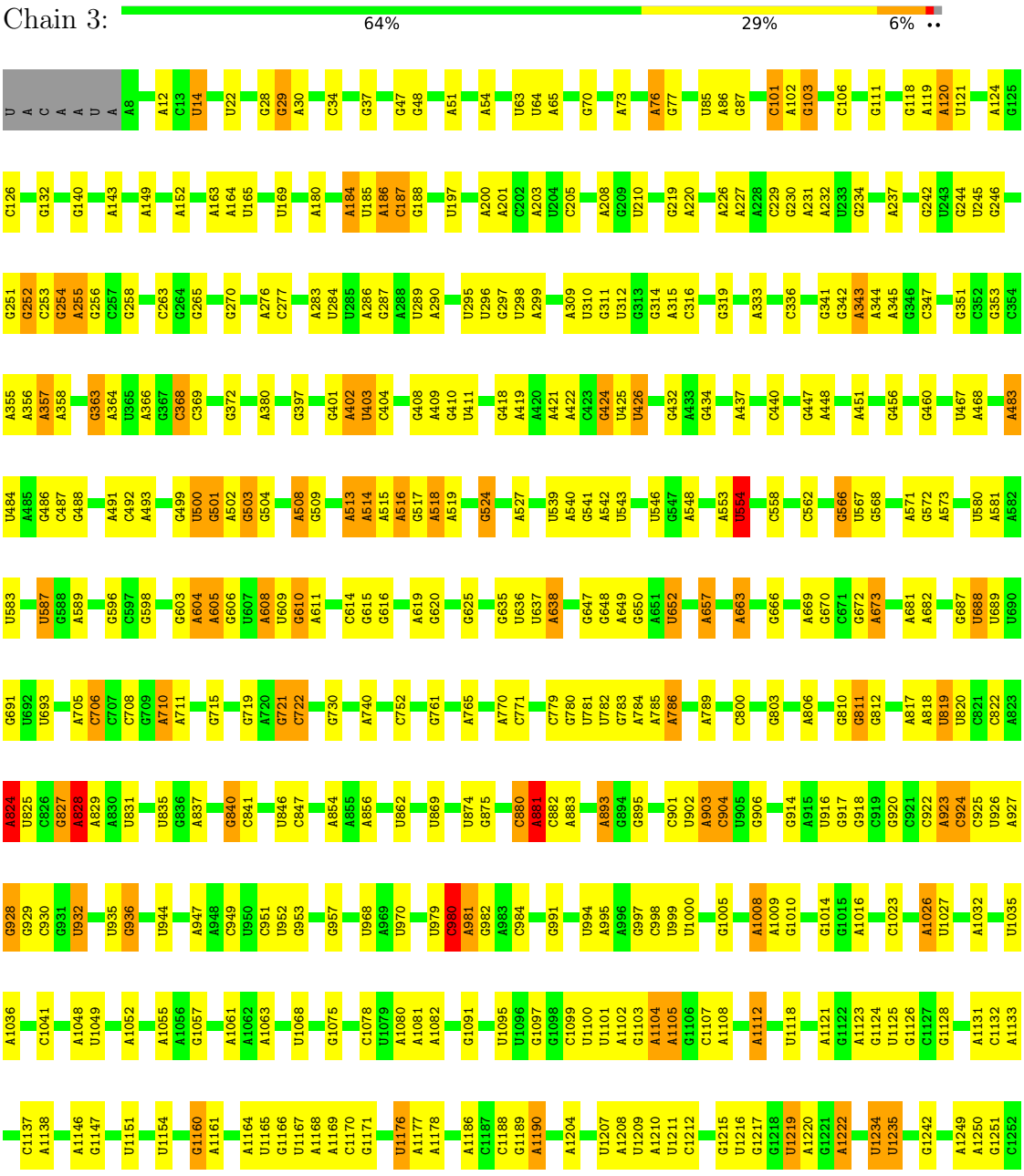
Mol	Chain	Residues	Atoms		AltConf
35	y	1	Total	Zn	0
			1	1	
35	2	1	Total	Zn	0
			1	1	
35	z	1	Total	Zn	0
			1	1	

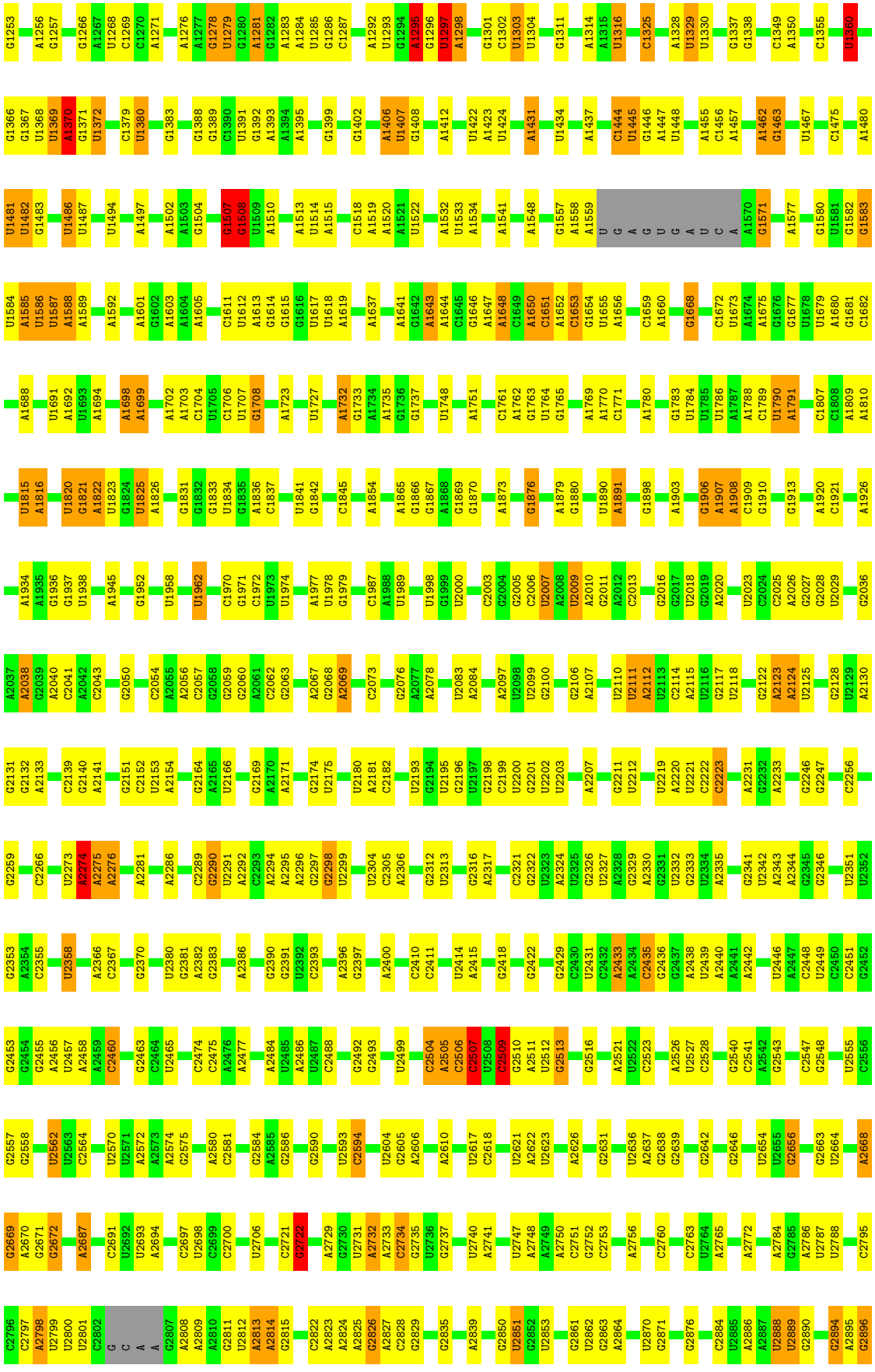
3 Residue-property plots (i)

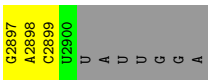
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Chain 3:

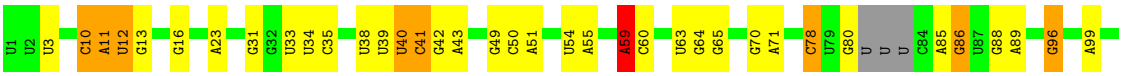






• Molecule 2: 5S ribosomal RNA

Chain 4:

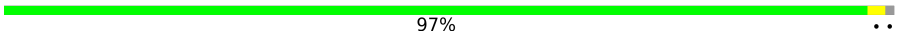


• Molecule 3: 50S ribosomal protein L29

Chain w:

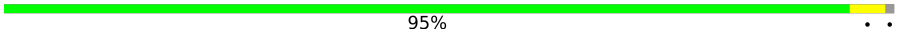
• Molecule 4: 50S ribosomal protein L2

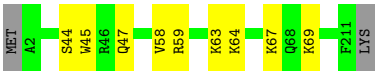
Chain a:



• Molecule 5: 50S ribosomal protein L4

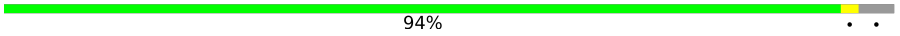
Chain c:

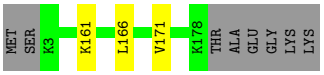




• Molecule 6: 50S ribosomal protein L6

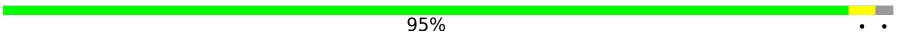
Chain e:

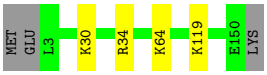




• Molecule 7: 50S ribosomal protein L15

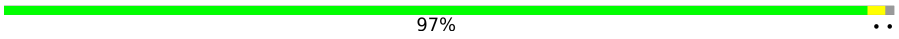
Chain k:





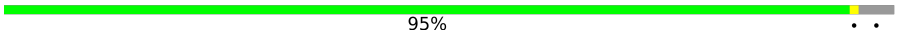
• Molecule 8: 50S ribosomal protein L13

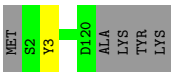
Chain i:



• Molecule 9: 50S ribosomal protein L17

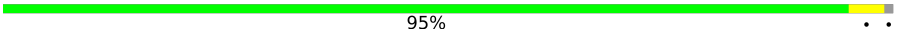
Chain m:





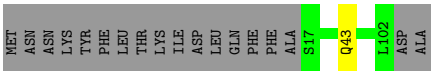
• Molecule 10: 50S ribosomal protein L21

Chain q:



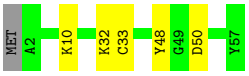
• Molecule 11: 50S ribosomal protein L27

Chain u:



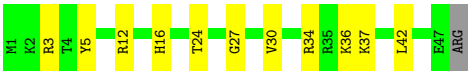
• Molecule 12: 50S ribosomal protein L32

Chain y:



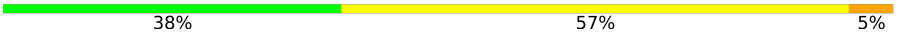
• Molecule 13: 50S ribosomal protein L34

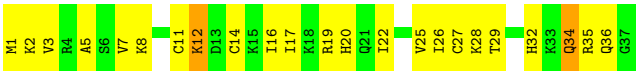
Chain 0:



• Molecule 14: 50S ribosomal protein L36

Chain 2:



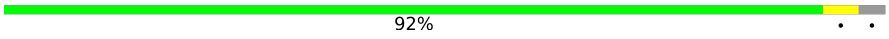


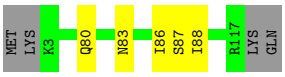
• Molecule 15: 50S ribosomal protein L35

Chain 1:

• Molecule 16: 50S ribosomal protein L19

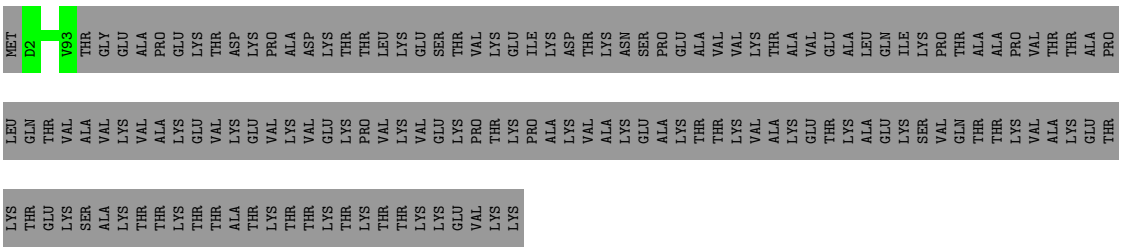
Chain o:





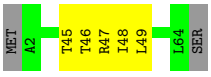
• Molecule 17: 50S ribosomal protein L23

Chain s:



• Molecule 18: 50S ribosomal protein L28

Chain v:

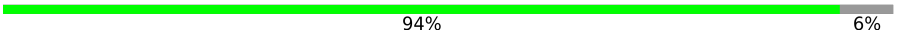


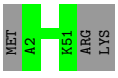
• Molecule 19: 50S ribosomal protein L31

Chain x:

• Molecule 20: 50S ribosomal protein L33 1

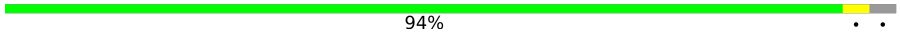
Chain z:





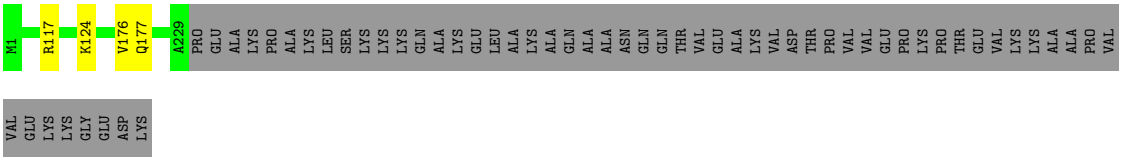
• Molecule 21: 50S ribosomal protein L5

Chain d:



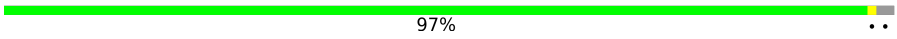
• Molecule 22: 50S ribosomal protein L3

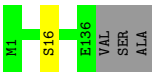
Chain b:



• Molecule 23: 50S ribosomal protein L16

Chain l:



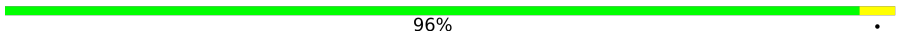


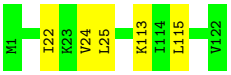
• Molecule 24: 50S ribosomal protein L20

Chain p:

• Molecule 25: 50S ribosomal protein L14

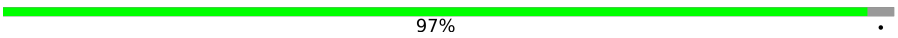
Chain j:





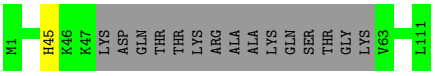
• Molecule 26: 50S ribosomal protein L18

Chain n:



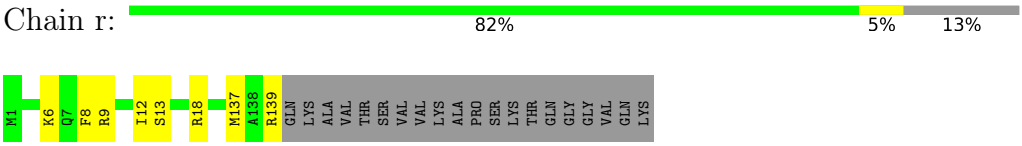
• Molecule 27: 50S ribosomal protein L24

Chain t:



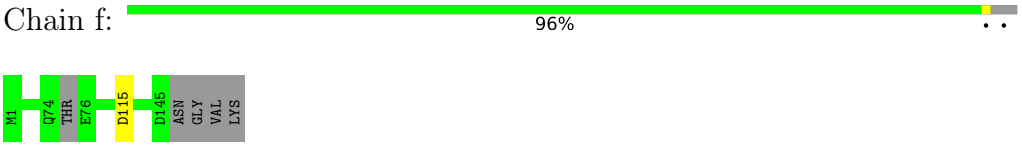
• Molecule 28: 50S ribosomal protein L22

Chain r:



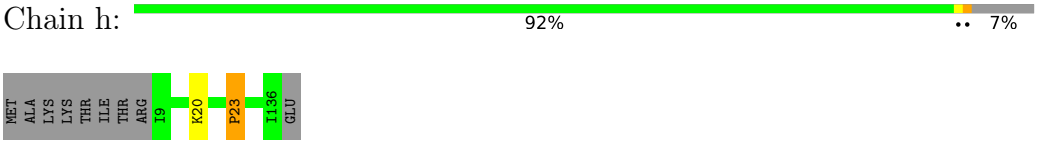
• Molecule 29: 50S ribosomal protein L9

Chain f:



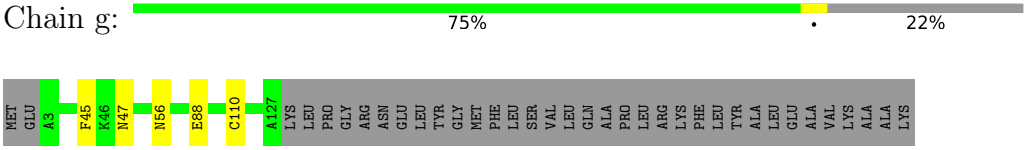
• Molecule 30: 50S ribosomal protein L11

Chain h:



• Molecule 31: 50S ribosomal protein L10

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	17890	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 ($e^-/Å^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (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: MG, K, CLM, ZN

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	3	0.89	68/69100 (0.1%)	0.93	141/107749 (0.1%)
2	4	0.60	0/2511	0.82	1/3910 (0.0%)
3	w	0.41	0/806	0.61	0/1080
4	a	0.46	1/2241 (0.0%)	0.59	0/3013
5	c	0.41	0/1639	0.65	1/2209 (0.0%)
6	e	0.36	0/1373	0.55	0/1854
7	k	0.40	0/1155	0.59	0/1541
8	i	0.43	0/1180	0.54	0/1585
9	m	0.41	0/972	0.55	0/1308
10	q	0.42	0/826	0.59	0/1109
11	u	0.45	0/649	0.55	0/867
12	y	0.48	0/440	0.79	1/582 (0.2%)
13	0	0.41	0/380	0.50	0/501
14	2	0.57	1/305 (0.3%)	0.77	2/401 (0.5%)
15	1	0.44	0/484	0.56	0/637
16	o	0.42	0/905	0.63	1/1211 (0.1%)
17	s	0.39	0/726	0.51	0/981
18	v	0.39	0/510	0.59	0/684
19	x	0.25	0/217	0.48	0/301
20	z	0.39	0/412	0.58	0/547
21	d	0.32	0/1264	0.57	1/1719 (0.1%)
22	b	0.42	0/1791	0.57	0/2408
23	l	0.45	0/1082	0.54	0/1456
24	p	0.49	0/955	0.55	0/1271
25	j	0.49	0/953	0.60	0/1275
26	n	0.35	0/861	0.51	0/1156
27	t	0.35	0/712	0.52	0/954
28	r	0.50	1/1077 (0.1%)	0.57	0/1441
29	f	0.44	0/711	0.78	0/988
30	h	0.62	0/629	1.00	1/873 (0.1%)
31	g	0.76	0/616	1.03	1/856 (0.1%)
All	All	0.79	71/97482 (0.1%)	0.86	150/146467 (0.1%)

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	89	ASP	C-N	8.41	1.50	1.34
1	3	2735	G	O3'-P	-7.74	1.51	1.61
1	3	611	A	P-OP2	7.73	1.62	1.49
1	3	1281	A	C5-C6	-7.67	1.34	1.41
1	3	2057	C	O3'-P	-7.63	1.51	1.61

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	2506	C	O5'-P-OP1	-12.90	94.09	105.70
1	3	1399	G	O5'-P-OP1	-12.79	94.19	105.70
1	3	205	C	O5'-P-OP1	-12.26	94.67	105.70
1	3	372	G	O5'-P-OP2	-11.34	95.49	105.70
1	3	2060	G	O5'-P-OP1	11.10	124.02	110.70

There are no chirality outliers.

There are no planarity outliers.

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	3	61690	0	30961	237	0
2	4	2245	0	1135	7	0
3	w	798	0	838	0	0
4	a	2199	0	2248	0	0
5	c	1613	0	1676	0	0
6	e	1349	0	1373	0	0
7	k	1138	0	1223	0	0
8	i	1158	0	1176	0	0
9	m	957	0	1008	0	0
10	q	809	0	852	0	0
11	u	641	0	650	0	0
12	y	436	0	441	0	0
13	0	377	0	422	14	0
14	2	303	0	348	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	1	477	0	530	30	0
16	o	895	0	932	0	0
17	s	714	0	785	0	0
18	v	504	0	542	0	0
19	x	218	0	90	0	0
20	z	408	0	436	0	0
21	d	1244	0	1160	0	0
22	b	1758	0	1797	0	0
23	l	1057	0	1088	0	0
24	p	941	0	1017	0	0
25	j	944	0	1019	0	0
26	n	853	0	873	0	0
27	t	706	0	726	0	0
28	r	1068	0	1150	0	0
29	f	713	0	313	0	0
30	h	630	0	309	0	0
31	g	617	0	308	0	0
32	3	1	0	0	0	0
33	3	24	0	0	0	0
33	y	1	0	0	0	0
34	3	20	0	10	4	0
35	2	1	0	0	0	0
35	y	1	0	0	0	0
35	z	1	0	0	0	0
All	All	89509	0	57436	272	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 8.

The worst 5 of 272 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)
14:2:11:CYS:SG	14:2:32:HIS:HE1	1.46	1.35
14:2:14:CYS:SG	14:2:27:CYS:HB2	1.99	1.03
1:3:254:G:OP2	15:1:10:ARG:NH2	2.01	0.93
1:3:253:C:O2	15:1:9:LYS:NZ	2.09	0.86
14:2:16:ILE:HG12	14:2:25:VAL:HG12	1.62	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	w	95/111 (86%)	89 (94%)	6 (6%)	0	100	100
4	a	283/287 (99%)	253 (89%)	30 (11%)	0	100	100
5	c	208/212 (98%)	186 (89%)	22 (11%)	0	100	100
6	e	174/184 (95%)	165 (95%)	9 (5%)	0	100	100
7	k	146/151 (97%)	126 (86%)	20 (14%)	0	100	100
8	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
9	m	117/124 (94%)	111 (95%)	6 (5%)	0	100	100
10	q	97/100 (97%)	85 (88%)	12 (12%)	0	100	100
11	u	84/104 (81%)	76 (90%)	8 (10%)	0	100	100
12	y	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
13	0	45/48 (94%)	43 (96%)	2 (4%)	0	100	100
14	2	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	1	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
16	o	113/119 (95%)	95 (84%)	18 (16%)	0	100	100
17	s	90/237 (38%)	82 (91%)	8 (9%)	0	100	100
18	v	61/65 (94%)	53 (87%)	8 (13%)	0	100	100
19	x	42/97 (43%)	31 (74%)	11 (26%)	0	100	100
20	z	48/53 (91%)	45 (94%)	3 (6%)	0	100	100
21	d	173/180 (96%)	154 (89%)	19 (11%)	0	100	100
22	b	227/287 (79%)	199 (88%)	28 (12%)	0	100	100
23	l	134/139 (96%)	118 (88%)	16 (12%)	0	100	100
24	p	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
25	j	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
26	n	108/116 (93%)	91 (84%)	17 (16%)	0	100	100
27	t	92/111 (83%)	84 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	r	137/159 (86%)	123 (90%)	14 (10%)	0	100 100
29	f	140/149 (94%)	121 (86%)	18 (13%)	1 (1%)	19 47
30	h	126/137 (92%)	116 (92%)	8 (6%)	2 (2%)	8 29
31	g	123/161 (76%)	115 (94%)	4 (3%)	4 (3%)	3 18
All	All	3383/3879 (87%)	3039 (90%)	337 (10%)	7 (0%)	45 72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	f	115	ASP
30	h	20	LYS
31	g	45	PHE
31	g	110	CYS
30	h	23	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
3	w	83/98 (85%)	78 (94%)	5 (6%)	16 41
4	a	233/243 (96%)	226 (97%)	7 (3%)	36 61
5	c	174/184 (95%)	166 (95%)	8 (5%)	23 49
6	e	138/159 (87%)	135 (98%)	3 (2%)	47 68
7	k	118/126 (94%)	114 (97%)	4 (3%)	32 57
8	i	124/128 (97%)	121 (98%)	3 (2%)	44 66
9	m	104/109 (95%)	103 (99%)	1 (1%)	73 83
10	q	88/91 (97%)	84 (96%)	4 (4%)	23 50
11	u	64/85 (75%)	63 (98%)	1 (2%)	58 75
12	y	45/49 (92%)	41 (91%)	4 (9%)	8 27
13	0	39/41 (95%)	39 (100%)	0	100 100
14	2	35/35 (100%)	32 (91%)	3 (9%)	8 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	1	51/51 (100%)	47 (92%)	4 (8%)	10 33
16	o	91/105 (87%)	87 (96%)	4 (4%)	24 50
17	s	80/208 (38%)	80 (100%)	0	100 100
18	v	55/60 (92%)	50 (91%)	5 (9%)	7 26
20	z	47/50 (94%)	47 (100%)	0	100 100
21	d	111/154 (72%)	107 (96%)	4 (4%)	30 56
22	b	185/233 (79%)	181 (98%)	4 (2%)	47 68
23	l	107/115 (93%)	106 (99%)	1 (1%)	75 86
24	p	99/108 (92%)	95 (96%)	4 (4%)	27 52
25	j	103/103 (100%)	98 (95%)	5 (5%)	21 48
26	n	85/99 (86%)	85 (100%)	0	100 100
27	t	69/96 (72%)	68 (99%)	1 (1%)	62 77
28	r	116/132 (88%)	109 (94%)	7 (6%)	16 41
All	All	2444/2862 (85%)	2362 (97%)	82 (3%)	34 57

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	d	94	GLU
25	j	25	LEU
21	d	99	PHE
24	p	50	ARG
28	r	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
26	n	38	HIS
15	1	28	HIS
6	e	24	HIS
6	e	21	GLN
7	k	134	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	2876/2907 (98%)	667 (23%)	58 (2%)
2	4	103/108 (95%)	32 (31%)	6 (5%)
All	All	2979/3015 (98%)	699 (23%)	64 (2%)

5 of 699 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	12	A
1	3	14	U
1	3	28	G
1	3	37	G
1	3	47	G

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	2897	G
2	4	34	U
1	3	1209	U
1	3	1048	A
2	4	38	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 29 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	$\#\|Z\|>2$
34	CLM	3	3026	-	19,20,20	2.42	7 (36%)	23,27,27	1.34	2 (8%)

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
34	CLM	3	3026	-	-	3/20/22/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	3	3026	CLM	O9B-N9	-5.97	1.12	1.22
34	3	3026	CLM	C2-N2	4.12	1.43	1.34
34	3	3026	CLM	C1-C2	3.80	1.58	1.53
34	3	3026	CLM	O2-C2	-3.42	1.16	1.23
34	3	3026	CLM	O5-C5	-3.12	1.36	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	3	3026	CLM	C4-C3-N2	-3.06	104.40	109.27
34	3	3026	CLM	C3-N2-C2	-2.79	118.14	123.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	3	3026	CLM	C3-C5-C6-C7
34	3	3026	CLM	C3-C5-C6-C11
34	3	3026	CLM	N2-C3-C4-O4

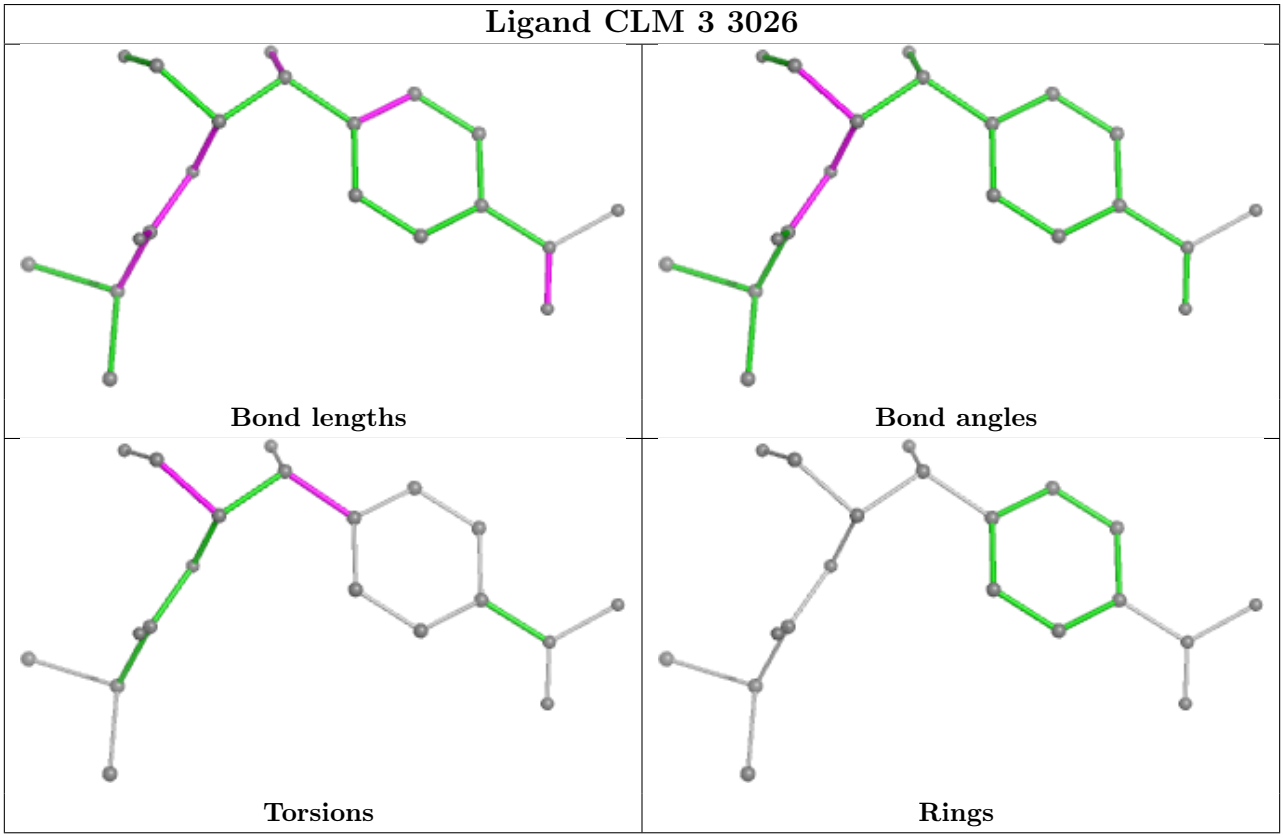
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	3	3026	CLM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11999. 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 (i)

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

9 Map-model fit

This section was not generated.