



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:57 am GMT

PDB ID : 3J9W
EMDB ID: : EMD-6306
Title : Cryo-EM structure of the Bacillus subtilis MifM-stalled ribosome complex
Authors : Sohmen, D.; Chiba, S.; Shimokawa-Chiba, N.; Innis, C.A.; Berninghausen, O.; Beckmann, R.; Ito, K.; Wilson, D.N.
Deposited on : 2015-03-16
Resolution : 3.90 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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

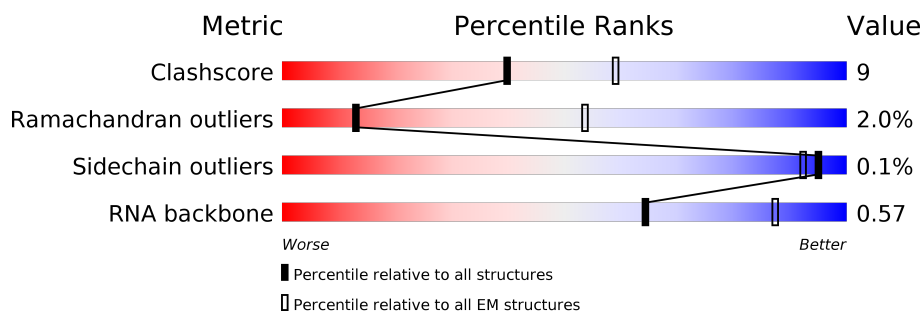
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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




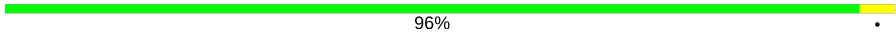

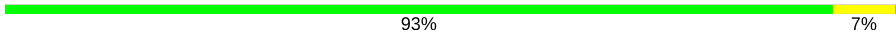


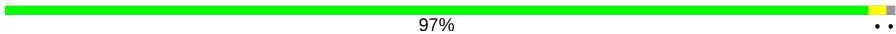
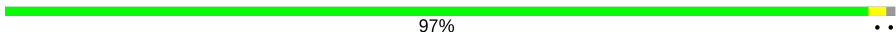
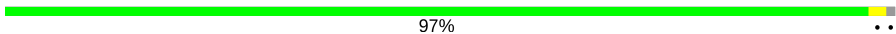
















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	AA	1555	51% 34% 12% ..
2	AB	246	88% 9%
3	AC	218	94% ..
4	AD	200	97% ..
5	AE	166	96% ..
6	AF	95	98% .
7	AG	156	96% ..
8	AH	132	98% ..
















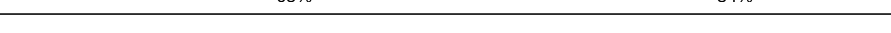

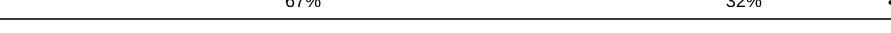

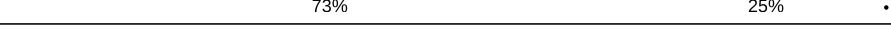

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Mol	Chain	Length	Quality of chain
9	AI	130	
10	AJ	102	
11	AK	131	
12	AL	138	
13	AM	121	
14	AN	61	
15	AO	89	
16	AP	90	
17	AQ	87	
18	AR	79	
19	AS	92	
20	AT	88	
21	AX	77	
22	AY	19	
23	AZ	95	
24	B0	62	
25	B1	66	
26	B2	59	
27	B3	66	
28	B4	59	
29	B5	49	
30	B6	44	
31	B7	66	
32	B8	37	
33	BA	2928	

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Mol	Chain	Length	Quality of chain
34	BB	119	
35	BD	277	
36	BE	209	
37	BF	207	
38	BG	179	
39	BH	179	
40	BJ	166	
41	BK	141	
42	BM	145	
43	BN	122	
44	BO	146	
45	BP	144	
46	BQ	120	
47	BR	120	
48	BS	115	
49	BT	119	
50	BU	102	
51	BV	113	
52	BW	95	
53	BX	103	
54	BZ	94	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 135425 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	AA	1544	Total	C	N	O	P	0	0
			33115	14768	6067	10736	1544		

- Molecule 2 is a protein called 30S ribosomal protein uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	AB	224	Total	C	N	O	0	0
			896	448	224	224		

- Molecule 3 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AC	210	Total	C	N	O	0	0
			840	420	210	210		

- Molecule 4 is a protein called 30S ribosomal protein uS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AD	199	Total	C	N	O	0	0
			797	398	199	200		

- Molecule 5 is a protein called 30S ribosomal protein uS5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	165	Total	C	N	O	0	0
			661	330	165	166		

- Molecule 6 is a protein called 30S ribosomal protein bS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AF	95	Total	C	N	O	0	0
			381	190	95	96		

- Molecule 7 is a protein called 30S ribosomal protein uS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	153	Total	C	N	O	0	0
			613	306	153	154		

- Molecule 8 is a protein called 30S ribosomal protein uS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	131	Total	C	N	O	0	0
			525	262	131	132		

- Molecule 9 is a protein called 30S ribosomal protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AI	130	Total	C	N	O	0	0
			521	260	130	131		

- Molecule 10 is a protein called 30S ribosomal protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AJ	102	Total	C	N	O	0	0
			409	204	102	103		

- Molecule 11 is a protein called 30S ribosomal protein uS11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AK	118	Total	C	N	O	0	0
			472	236	118	118		

- Molecule 12 is a protein called 30S ribosomal protein uS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AL	137	Total	C	N	O	0	0
			549	274	137	138		

- Molecule 13 is a protein called 30S ribosomal protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AM	119	Total	C	N	O	0	0
			476	238	119	119		

- Molecule 14 is a protein called 30S ribosomal protein uS14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AN	60	Total	C	N	O	0	0
			241	120	60	61		

- Molecule 15 is a protein called 30S ribosomal protein uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AO	88	Total	C	N	O	0	0
			353	176	88	89		

- Molecule 16 is a protein called 30S ribosomal protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AP	89	Total	C	N	O	0	0
			357	178	89	90		

- Molecule 17 is a protein called 30S ribosomal protein uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AQ	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 18 is a protein called 30S ribosomal protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	71	Total	C	N	O	0	0
			285	142	71	72		

- Molecule 19 is a protein called 30S ribosomal protein uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AS	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 20 is a protein called 30S ribosomal protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	AT	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 21 is a RNA chain called tRNA-Asp.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AX	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AY	19	Total	C	N	O	P	0	0
			415	185	82	129	19		

- Molecule 23 is a protein called MifM.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AZ	24	Total	C	N	O	S	0	0
			107	64	28	14	1		

- Molecule 24 is a protein called 50S ribosomal protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B0	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 25 is a protein called 50S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B1	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B2	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 27 is a protein called 50S ribosomal protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B3	64	Total	C	N	O	S	0	0
			503	314	92	92	5		

- Molecule 28 is a protein called 50S ribosomal protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B4	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 29 is a protein called 50S ribosomal protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B5	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 30 is a protein called 50S ribosomal protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B6	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 31 is a protein called 50S ribosomal protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B7	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 32 is a protein called 50S ribosomal protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B8	36	Total	C	N	O	S	0	0
			288	181	59	44	4		

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BA	2923	Total	C	N	O	P	0	0
			62767	28002	11589	20253	2923		

- Molecule 34 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BB	112	Total	C	N	O	P	0	0
			2395	1068	435	780	112		

- Molecule 35 is a protein called 50S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BD	275	Total	C	N	O	S	0	0
			2111	1312	416	377	6		

- Molecule 36 is a protein called 50S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BE	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 37 is a protein called 50S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BF	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 38 is a protein called 50S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BG	178	Total	C	N	O	S	0	0
			1404	893	245	259	7		

- Molecule 39 is a protein called 50S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BH	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 40 is a protein called 50S ribosomal protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BJ	123	Total	C	N	O	S	0	0
			955	602	163	189	1		

- Molecule 41 is a protein called 50S ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BK	133	Total	C	N	O	S	0	0
			981	617	173	185	6		

- Molecule 42 is a protein called 50S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BM	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 43 is a protein called 50S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BN	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 44 is a protein called 50S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BO	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 45 is a protein called 50S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BP	138	Total	C	N	O	S	0	0
			1097	703	208	181	5		

- Molecule 46 is a protein called 50S ribosomal protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BQ	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 47 is a protein called 50S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BR	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 48 is a protein called 50S ribosomal protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	BS	114	Total	C	N	O	0	0
			936	595	184	157		

- Molecule 49 is a protein called 50S ribosomal protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BT	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 50 is a protein called 50S ribosomal protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BU	101	Total	C	N	O	S	0	0
			786	501	139	146			

- Molecule 51 is a protein called 50S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BV	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 52 is a protein called 50S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BW	93	Total	C	N	O	S	0	0
			752	472	137	139	4		

- Molecule 53 is a protein called 50S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BX	100	Total	C	N	O	S	0	0
			754	473	141	137	3		

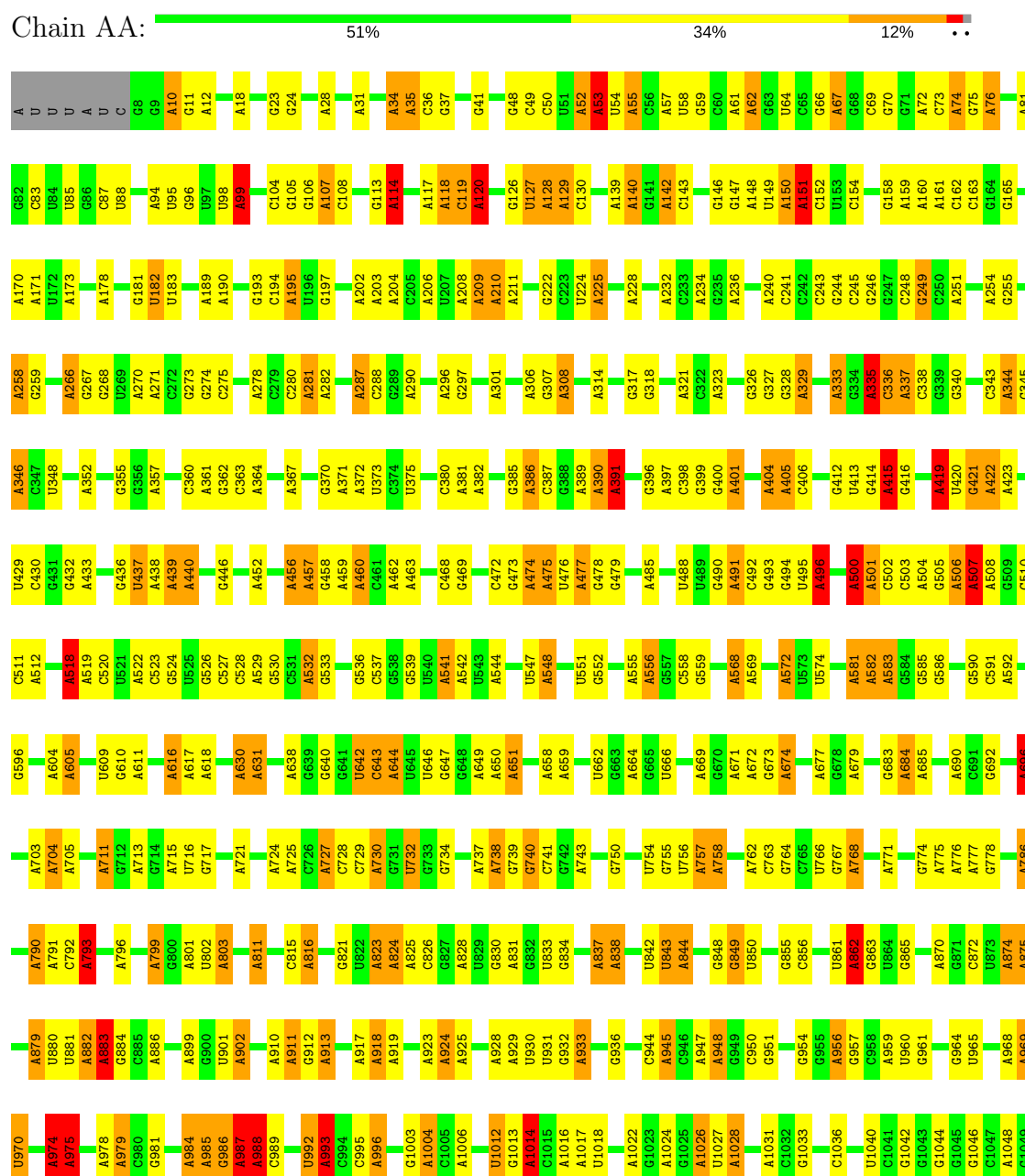
- Molecule 54 is a protein called 50S ribosomal protein bL27.

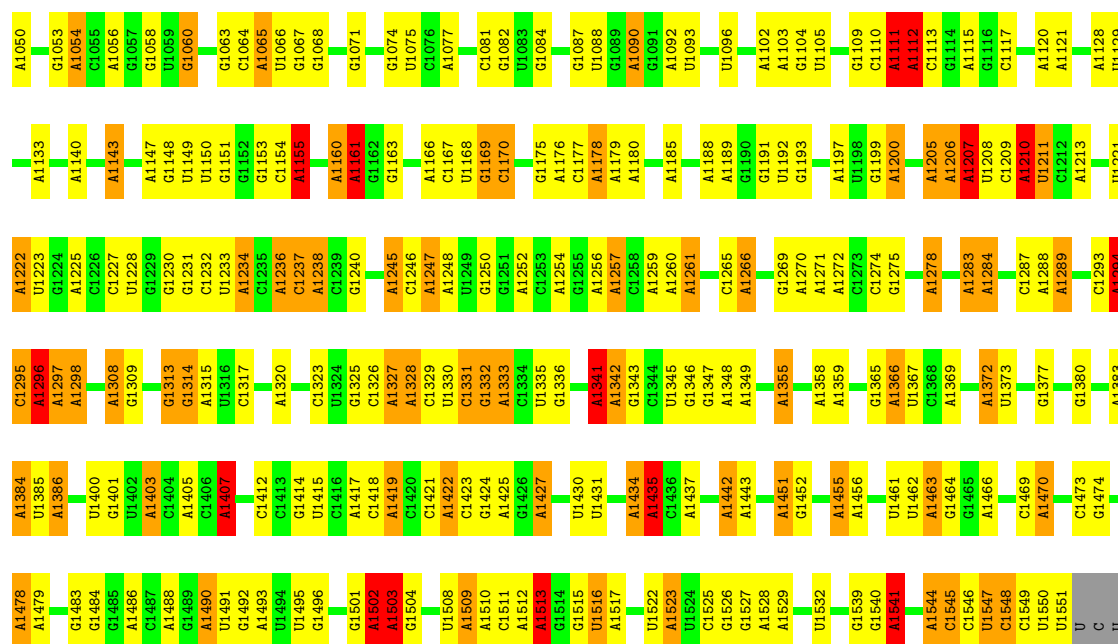
Mol	Chain	Residues	Atoms					AltConf	Trace
54	BZ	82	Total	C	N	O	S	0	0
			630	390	123	117			

3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA





A

- Molecule 2: 30S ribosomal protein uS2

Chain AB: 88% 9%



- Molecule 3: 30S ribosomal protein uS3

Chain AC: 94%



- Molecule 4: 30S ribosomal protein uS4

Chain AD: 97%



- Molecule 5: 30S ribosomal protein uS5

Chain AE: 96%



- Molecule 6: 30S ribosomal protein bS6

Chain AF:  98% .



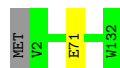
- Molecule 7: 30S ribosomal protein uS7

Chain AG:  96% . .



- Molecule 8: 30S ribosomal protein uS8

Chain AH:  98% . .



- Molecule 9: 30S ribosomal protein uS9

Chain AI:  93% 5% .




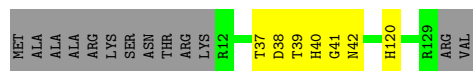
- Molecule 10: 30S ribosomal protein uS10

Chain AJ:  96% .



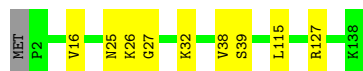
- Molecule 11: 30S ribosomal protein uS11

Chain AK:  85% 5% 10%



- Molecule 12: 30S ribosomal protein uS12

Chain AL:  93% 7% .



- Molecule 13: 30S ribosomal protein uS13

Chain AM:  89% 7% . .



- Molecule 14: 30S ribosomal protein uS14

Chain AN: 90% 7% ..



- Molecule 15: 30S ribosomal protein uS15

Chain AO: 97% ..



- Molecule 16: 30S ribosomal protein bS16

Chain AP: 97% ..



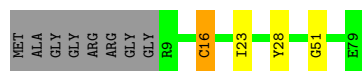
- Molecule 17: 30S ribosomal protein uS17

Chain AQ: 97% ..



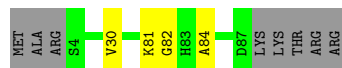
- Molecule 18: 30S ribosomal protein bS18

Chain AR: 85% 10% ..



- Molecule 19: 30S ribosomal protein uS19

Chain AS: 87% 9% ..

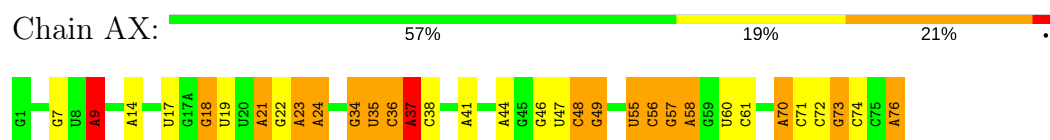


- Molecule 20: 30S ribosomal protein bS20

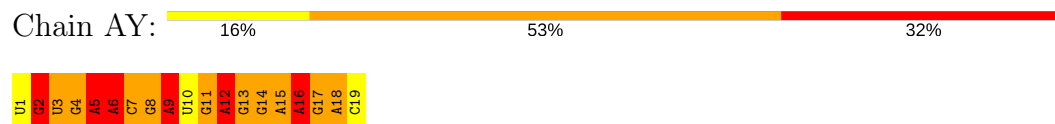
Chain AT: 92% 6% ..



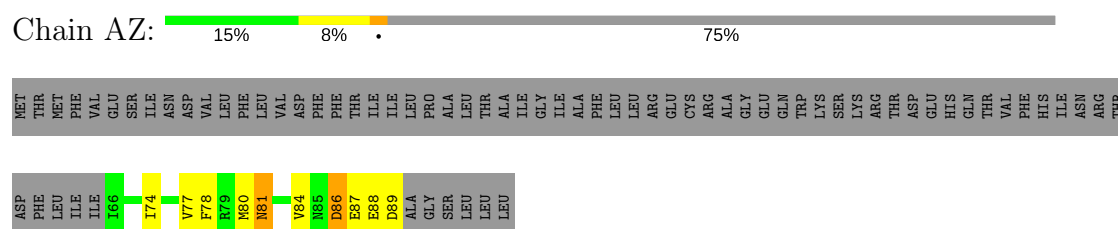
- Molecule 21: tRNA-Asp



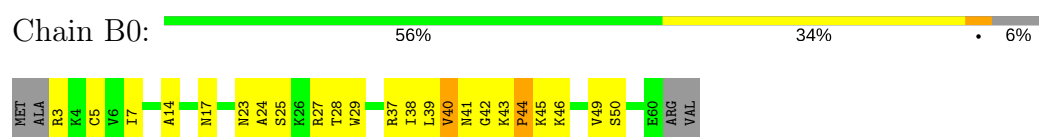
- Molecule 22: mRNA



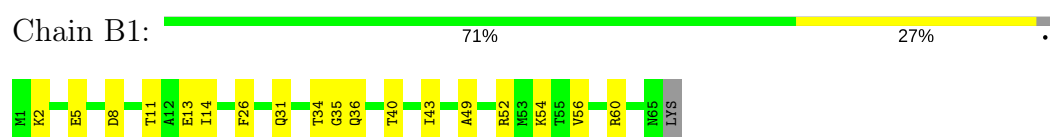
- Molecule 23: MifM



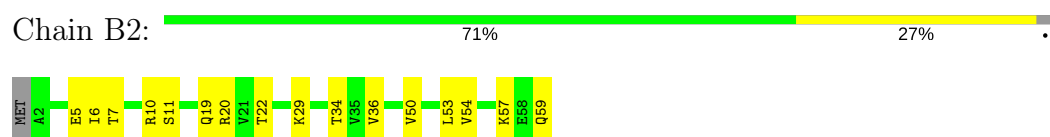
- Molecule 24: 50S ribosomal protein bL28



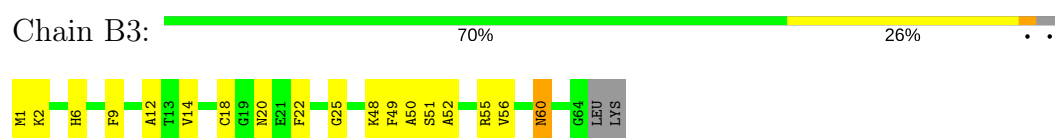
- Molecule 25: 50S ribosomal protein uL29



- Molecule 26: 50S ribosomal protein uL30



- Molecule 27: 50S ribosomal protein bL31



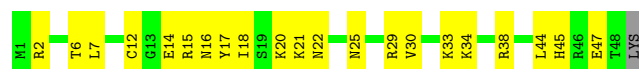
- Molecule 28: 50S ribosomal protein bL32

Chain B4: 




- Molecule 29: 50S ribosomal protein bL33

Chain B5: 



- Molecule 30: 50S ribosomal protein bL34

Chain B6: 




- Molecule 31: 50S ribosomal protein bL35

Chain B7: 



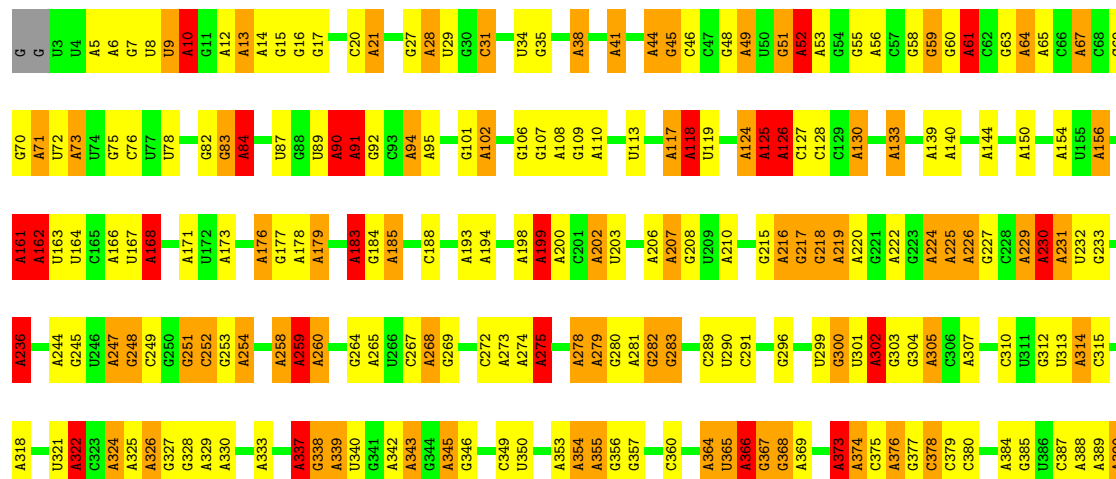
- Molecule 32: 50S ribosomal protein bL36

Chain B8: 



- Molecule 33: 23S ribosomal RNA

Chain BA: 

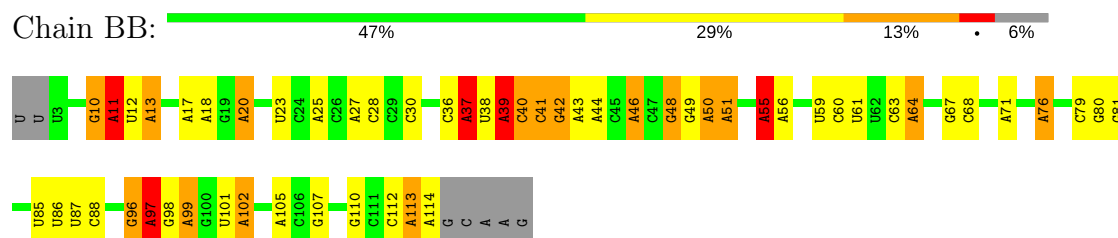



WORLDWIDE PDB
 PROTEIN DATA BANK

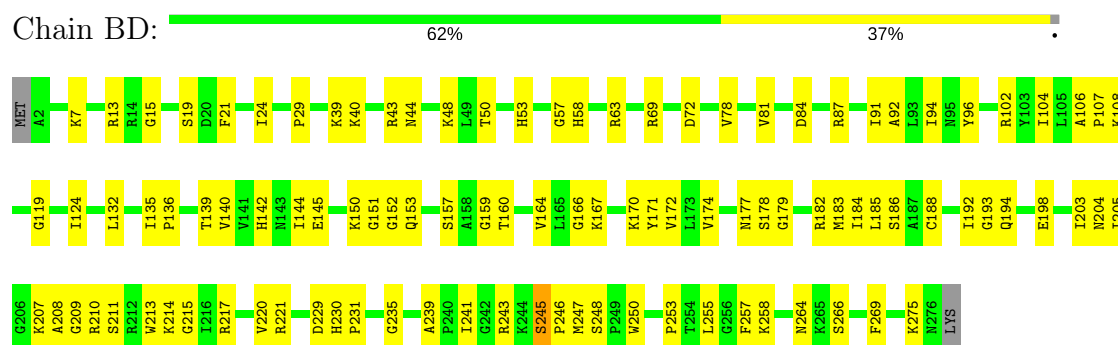
EMDataBank
 Unified Data Resource for 3DEM

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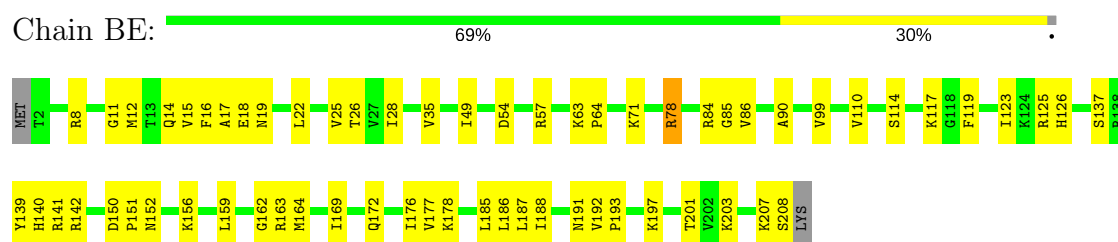
- Molecule 34: 5S ribosomal RNA



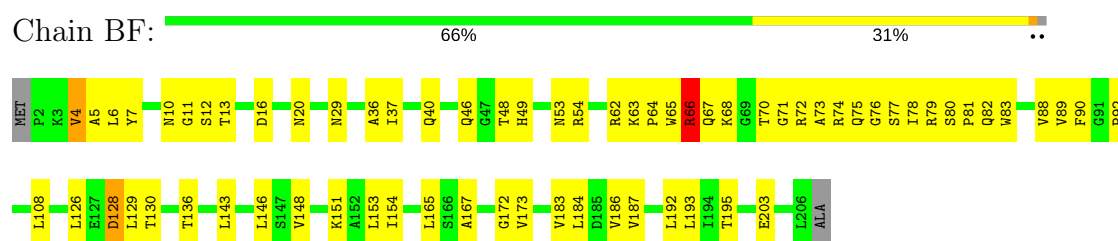
- Molecule 35: 50S ribosomal protein uL2



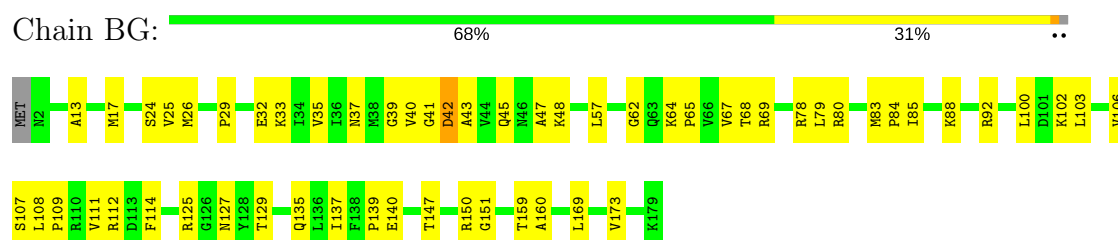
- Molecule 36: 50S ribosomal protein uL3



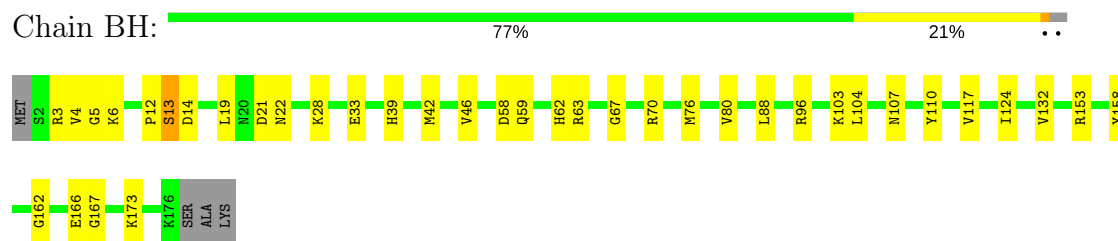
- Molecule 37: 50S ribosomal protein uL4



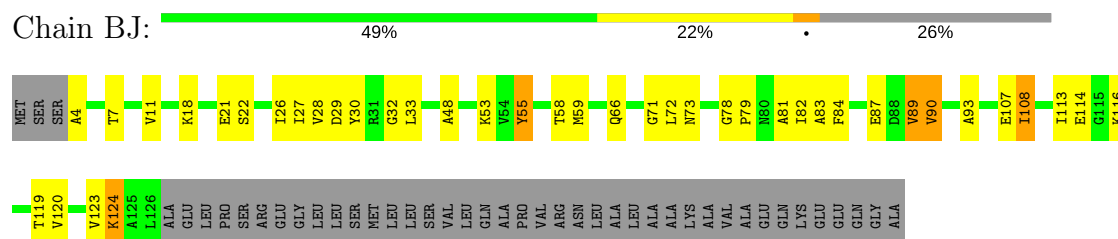
- Molecule 38: 50S ribosomal protein uL5



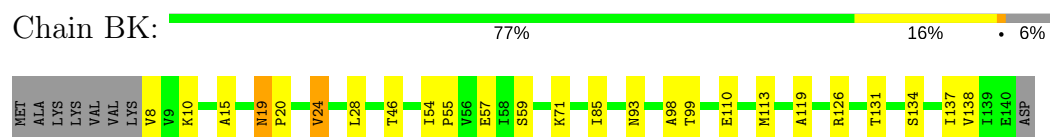
- Molecule 39: 50S ribosomal protein uL6



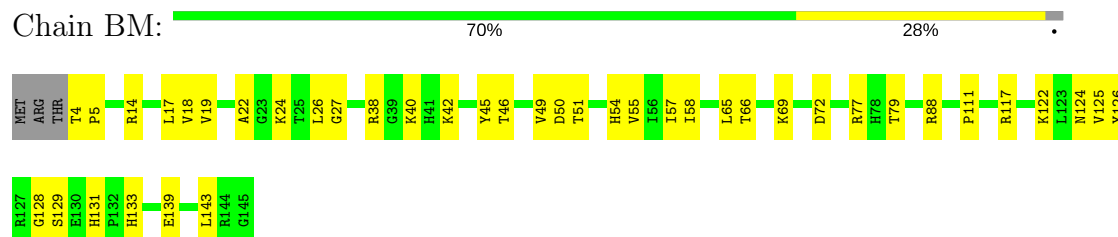
- Molecule 40: 50S ribosomal protein uL10



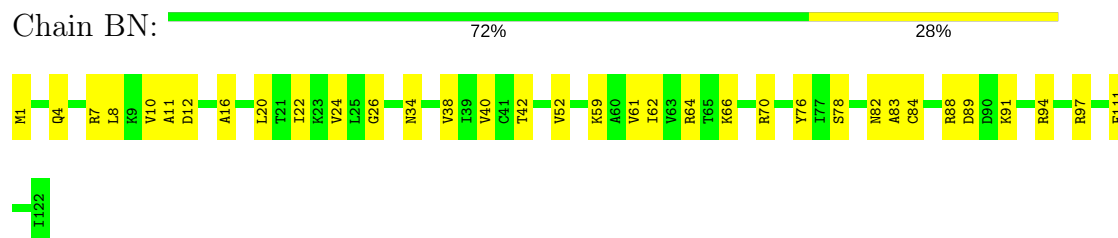
- Molecule 41: 50S ribosomal protein uL11



- Molecule 42: 50S ribosomal protein uL13

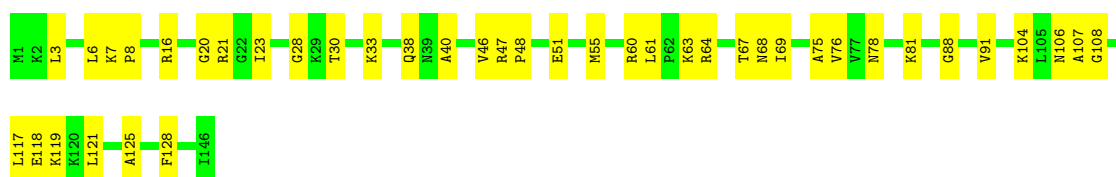


- Molecule 43: 50S ribosomal protein uL14



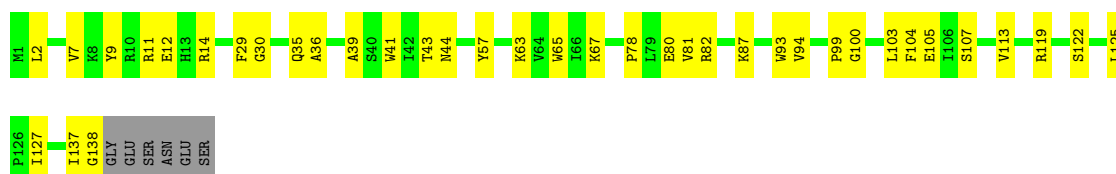
- Molecule 44: 50S ribosomal protein uL15





- Molecule 45: 50S ribosomal protein uL16

Chain BP: 69% 26%



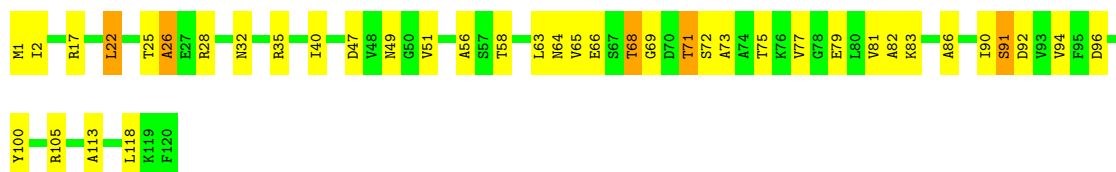
- Molecule 46: 50S ribosomal protein bL17

Chain BQ: 73% 25%



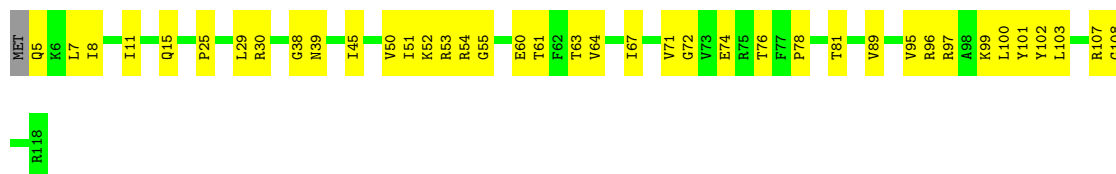
- Molecule 47: 50S ribosomal protein uL18

Chain BR: 67% 29%



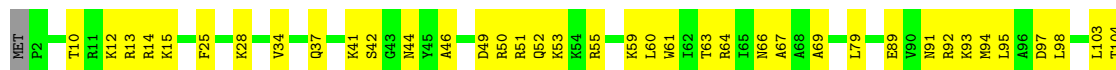
- Molecule 48: 50S ribosomal protein bL19

Chain BS: 65% 34%



- Molecule 49: 50S ribosomal protein bL20

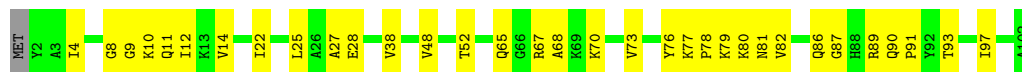
Chain BT: 64% 34%





- Molecule 50: 50S ribosomal protein bL21

Chain BU: 67% 32%



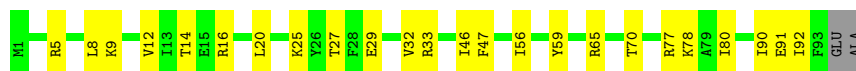
- Molecule 51: 50S ribosomal protein uL22

Chain BV: 61% 31%



- Molecule 52: 50S ribosomal protein uL23

Chain BW: 73% 25%



- Molecule 53: 50S ribosomal protein uL24

Chain BX: 58% 38%



- Molecule 54: 50S ribosomal protein bL27

Chain BZ: 64% 23% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	305045	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.36	984/37074 (2.7%)	2.90	3806/57834 (6.6%)
10	AJ	0.28	0/408	0.39	0/507
11	AK	0.22	0/471	0.42	0/587
12	AL	0.24	0/548	0.50	0/682
13	AM	0.30	0/475	0.52	0/592
14	AN	0.21	0/240	0.48	0/297
15	AO	0.27	0/352	0.41	0/437
16	AP	0.27	0/356	0.41	0/442
17	AQ	0.27	0/344	0.44	0/427
18	AR	0.31	0/284	0.43	0/352
19	AS	0.33	0/335	0.46	0/417
2	AB	0.31	0/895	0.40	0/1117
20	AT	0.26	0/344	0.40	0/427
21	AX	1.03	30/1834 (1.6%)	2.18	104/2858 (3.6%)
22	AY	0.38	0/466	0.93	2/726 (0.3%)
23	AZ	0.50	0/106	1.02	0/122
24	B0	0.30	0/448	0.58	0/596
25	B1	0.24	0/531	0.47	0/707
26	B2	0.24	0/457	0.44	0/613
27	B3	0.27	0/513	0.43	0/683
28	B4	0.23	0/433	0.48	0/574
29	B5	0.25	0/406	0.44	0/540
3	AC	0.29	0/839	0.38	0/1047
30	B6	0.20	0/370	0.44	0/483
31	B7	0.23	0/519	0.48	0/680
32	B8	0.19	0/291	0.36	0/383
33	BA	1.40	1948/70307 (2.8%)	2.98	7636/109687 (7.0%)
34	BB	1.30	66/2678 (2.5%)	2.78	248/4174 (5.9%)
35	BD	0.27	0/2148	0.48	0/2881
36	BE	0.27	0/1597	0.47	0/2140
37	BF	0.26	0/1580	0.50	0/2132
38	BG	0.29	0/1423	0.50	0/1910
39	BH	0.23	0/1360	0.43	0/1832
4	AD	0.25	0/796	0.41	0/992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	BJ	0.26	0/963	0.49	0/1298
41	BK	0.26	0/995	0.48	0/1346
42	BM	0.25	0/1146	0.49	0/1542
43	BN	0.28	0/927	0.47	0/1245
44	BO	0.23	0/1093	0.44	0/1457
45	BP	0.20	0/1120	0.38	0/1496
46	BQ	0.26	0/960	0.50	0/1284
47	BR	0.30	0/921	0.54	1/1236 (0.1%)
48	BS	0.24	0/949	0.44	0/1269
49	BT	0.26	0/952	0.45	0/1266
5	AE	0.26	0/660	0.46	0/822
50	BU	0.28	0/797	0.53	0/1070
51	BV	0.34	0/851	0.59	0/1146
52	BW	0.29	0/759	0.47	0/1011
53	BX	0.26	0/764	0.52	0/1022
54	BZ	0.30	0/638	0.49	0/847
6	AF	0.31	0/380	0.41	0/472
7	AG	0.26	0/612	0.39	0/762
8	AH	0.24	0/524	0.43	0/652
9	AI	0.26	0/520	0.51	0/647
All	All	1.20	3028/147759 (2.0%)	2.62	11797/221768 (5.3%)

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
1	AA	0	36
21	AX	0	2
22	AY	0	7
33	BA	0	84
34	BB	0	2
37	BF	0	1
51	BV	0	2
All	All	0	134

The worst 5 of 3028 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	508	A	C8-N7	8.50	1.37	1.31
1	AA	439	A	C8-N7	8.28	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1188	A	C8-N7	8.21	1.37	1.31
1	AA	1372	A	C8-N7	8.18	1.37	1.31
33	BA	526	A	C8-N7	8.14	1.37	1.31

The worst 5 of 11797 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1134	A	C2-N3-C4	20.56	120.88	110.60
33	BA	226	A	C2-N3-C4	20.47	120.84	110.60
33	BA	1691	A	C2-N3-C4	20.46	120.83	110.60
1	AA	1308	A	C2-N3-C4	20.36	120.78	110.60
1	AA	195	A	C2-N3-C4	20.24	120.72	110.60

There are no chirality outliers.

5 of 134 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	209	A	Sidechain
1	AA	308	A	Sidechain
1	AA	335	A	Sidechain
1	AA	53	A	Sidechain
1	AA	76	A	Sidechain

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	AA	33115	0	16676	250	0
2	AB	896	0	244	2	0
3	AC	840	0	241	3	0
4	AD	797	0	224	3	0
5	AE	661	0	197	1	0
6	AF	381	0	104	0	0
7	AG	613	0	164	1	0
8	AH	525	0	146	0	0
9	AI	521	0	155	4	0
10	AJ	409	0	104	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AK	472	0	135	7	0
12	AL	549	0	157	1	0
13	AM	476	0	137	2	0
14	AN	241	0	62	2	0
15	AO	353	0	94	0	0
16	AP	357	0	95	0	0
17	AQ	345	0	90	1	0
18	AR	285	0	76	1	0
19	AS	336	0	93	2	0
20	AT	345	0	89	2	0
21	AX	1643	0	830	30	0
22	AY	415	0	207	80	0
23	AZ	107	0	58	9	0
24	B0	444	0	486	61	0
25	B1	530	0	568	12	0
26	B2	455	0	491	12	0
27	B3	503	0	494	12	0
28	B4	426	0	445	14	0
29	B5	401	0	413	18	0
30	B6	367	0	410	20	0
31	B7	512	0	564	31	0
32	B8	288	0	330	3	0
33	BA	62767	0	31584	776	0
34	BB	2395	0	1212	21	0
35	BD	2111	0	2200	85	0
36	BE	1575	0	1642	48	0
37	BF	1561	0	1647	92	0
38	BG	1404	0	1467	44	0
39	BH	1342	0	1388	26	0
40	BJ	955	0	990	24	0
41	BK	981	0	1020	27	0
42	BM	1123	0	1162	31	0
43	BN	920	0	977	21	0
44	BO	1081	0	1132	40	0
45	BP	1097	0	1165	25	0
46	BQ	953	0	983	28	0
47	BR	912	0	947	36	0
48	BS	936	0	1008	31	0
49	BT	940	0	1005	41	0
50	BU	786	0	826	40	0
51	BV	842	0	899	46	0
52	BW	752	0	802	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	BX	754	0	809	31	0
54	BZ	630	0	644	16	0
All	All	135425	0	80088	1864	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 9.

The worst 5 of 1864 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)
23:AZ:74:ILE:CA	51:BV:85:PHE:HE2	1.11	1.60
23:AZ:74:ILE:CA	51:BV:85:PHE:CE2	1.99	1.44
24:B0:37:ARG:NH1	24:B0:44:PRO:HG3	1.37	1.40
37:BF:80:SER:OG	37:BF:81:PRO:HD2	1.30	1.29
41:BK:15:ALA:HB1	41:BK:46:THR:CG2	1.62	1.28

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	222/246 (90%)	204 (92%)	13 (6%)	5 (2%)	7	46
3	AC	208/218 (95%)	193 (93%)	14 (7%)	1 (0%)	32	73
4	AD	197/200 (98%)	191 (97%)	4 (2%)	2 (1%)	18	61
5	AE	163/166 (98%)	150 (92%)	9 (6%)	4 (2%)	6	44
6	AF	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	8	47
7	AG	151/156 (97%)	144 (95%)	6 (4%)	1 (1%)	25	67
8	AH	129/132 (98%)	123 (95%)	5 (4%)	1 (1%)	22	65
9	AI	128/130 (98%)	113 (88%)	10 (8%)	5 (4%)	3	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	3	34
11	AK	116/131 (88%)	106 (91%)	9 (8%)	1 (1%)	20	63
12	AL	135/138 (98%)	119 (88%)	9 (7%)	7 (5%)	2	28
13	AM	117/121 (97%)	94 (80%)	13 (11%)	10 (8%)	1	16
14	AN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	28
15	AO	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	7	46
16	AP	87/90 (97%)	82 (94%)	3 (3%)	2 (2%)	7	46
17	AQ	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
18	AR	69/79 (87%)	64 (93%)	2 (3%)	3 (4%)	3	32
19	AS	82/92 (89%)	75 (92%)	5 (6%)	2 (2%)	7	45
20	AT	84/88 (96%)	77 (92%)	6 (7%)	1 (1%)	15	58
23	AZ	22/95 (23%)	17 (77%)	2 (9%)	3 (14%)	0	5
24	B0	56/62 (90%)	53 (95%)	1 (2%)	2 (4%)	4	37
25	B1	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
26	B2	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	10	51
27	B3	62/66 (94%)	56 (90%)	4 (6%)	2 (3%)	5	40
28	B4	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	9	50
29	B5	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	B6	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
31	B7	62/66 (94%)	56 (90%)	5 (8%)	1 (2%)	11	53
32	B8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
35	BD	273/277 (99%)	264 (97%)	8 (3%)	1 (0%)	38	76
36	BE	205/209 (98%)	189 (92%)	11 (5%)	5 (2%)	7	45
37	BF	203/207 (98%)	184 (91%)	16 (8%)	3 (2%)	12	54
38	BG	176/179 (98%)	154 (88%)	18 (10%)	4 (2%)	7	46
39	BH	173/179 (97%)	165 (95%)	7 (4%)	1 (1%)	28	70
40	BJ	121/166 (73%)	97 (80%)	14 (12%)	10 (8%)	1	16
41	BK	131/141 (93%)	122 (93%)	7 (5%)	2 (2%)	12	54
42	BM	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	25	67
43	BN	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	11	52
44	BO	144/146 (99%)	132 (92%)	10 (7%)	2 (1%)	13	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BP	136/144 (94%)	129 (95%)	7 (5%)	0	100	100
46	BQ	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	20	63
47	BR	118/120 (98%)	106 (90%)	7 (6%)	5 (4%)	3	32
48	BS	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
49	BT	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
50	BU	99/102 (97%)	82 (83%)	15 (15%)	2 (2%)	9	49
51	BV	107/113 (95%)	96 (90%)	8 (8%)	3 (3%)	6	43
52	BW	91/95 (96%)	86 (94%)	5 (6%)	0	100	100
53	BX	98/103 (95%)	87 (89%)	8 (8%)	3 (3%)	5	40
54	BZ	80/94 (85%)	77 (96%)	3 (4%)	0	100	100
All	All	5563/5920 (94%)	5116 (92%)	336 (6%)	111 (2%)	13	49

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	4	ILE
6	AF	70	ALA
12	AL	127	ARG
13	AM	101	ASN
23	AZ	78	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AZ	6/87 (7%)	4 (67%)	2 (33%)	0	2
24	B0	47/50 (94%)	47 (100%)	0	100	100
25	B1	56/57 (98%)	56 (100%)	0	100	100
26	B2	52/53 (98%)	52 (100%)	0	100	100
27	B3	53/55 (96%)	53 (100%)	0	100	100
28	B4	48/53 (91%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	B5	46/47 (98%)	46 (100%)	0	100	100
30	B6	39/39 (100%)	39 (100%)	0	100	100
31	B7	54/56 (96%)	54 (100%)	0	100	100
32	B8	34/35 (97%)	34 (100%)	0	100	100
35	BD	223/225 (99%)	223 (100%)	0	100	100
36	BE	168/170 (99%)	168 (100%)	0	100	100
37	BF	169/170 (99%)	168 (99%)	1 (1%)	89	95
38	BG	153/154 (99%)	153 (100%)	0	100	100
39	BH	148/151 (98%)	148 (100%)	0	100	100
40	BJ	105/138 (76%)	105 (100%)	0	100	100
41	BK	103/110 (94%)	103 (100%)	0	100	100
42	BM	120/123 (98%)	120 (100%)	0	100	100
43	BN	101/101 (100%)	101 (100%)	0	100	100
44	BO	110/110 (100%)	110 (100%)	0	100	100
45	BP	111/116 (96%)	111 (100%)	0	100	100
46	BQ	99/100 (99%)	99 (100%)	0	100	100
47	BR	93/93 (100%)	93 (100%)	0	100	100
48	BS	99/100 (99%)	99 (100%)	0	100	100
49	BT	96/98 (98%)	96 (100%)	0	100	100
50	BU	83/84 (99%)	83 (100%)	0	100	100
51	BV	90/93 (97%)	89 (99%)	1 (1%)	78	89
52	BW	84/85 (99%)	84 (100%)	0	100	100
53	BX	84/87 (97%)	84 (100%)	0	100	100
54	BZ	64/74 (86%)	64 (100%)	0	100	100
All	All	2738/2914 (94%)	2734 (100%)	4 (0%)	95	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	AZ	81	ASN
23	AZ	86	ASP
37	BF	66	ARG
51	BV	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
37	BF	67	GLN
39	BH	62	HIS
53	BX	39	ASN
37	BF	75	GLN
37	BF	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1543/1555 (99%)	235 (15%)	0
21	AX	76/77 (98%)	15 (19%)	0
22	AY	18/19 (94%)	14 (77%)	0
33	BA	2922/2928 (99%)	791 (27%)	0
34	BB	111/119 (93%)	32 (28%)	0
All	All	4670/4698 (99%)	1087 (23%)	0

5 of 1087 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	11	G
1	AA	34	A
1	AA	41	G
1	AA	49	C

There are no RNA pucker outliers to report.

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 ⓘ

There are no ligands in this entry.

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.