



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 02:20 pm GMT

PDB ID : 7O1A  
EMDB ID : EMD-12694  
Title : Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome complex stalled in response to L-tryptophan  
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.  
Deposited on : 2021-03-29  
Resolution : 2.40 Å(reported)  
Based on initial model : 6TBV

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.41



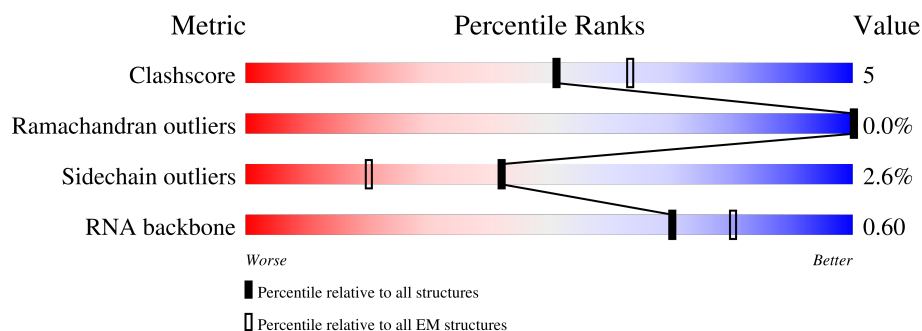
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	1534	 55% 32% 12% .
2	AB	240	 58% 32% . . 7%
3	AC	233	 61% 25% . 12%
4	AD	206	 74% 23% .
5	AE	167	 73% 19% . 7%
6	AF	135	 59% 19% . 21%
7	AG	179	 57% 25% . 16%

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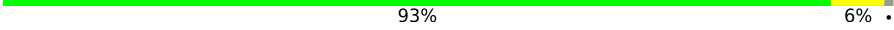





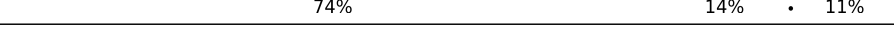

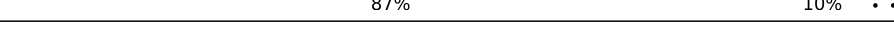







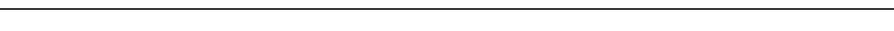

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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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Mol	Chain	Length	Quality of chain
33	BL	144	 88% 11% .
34	BM	136	 79% 19% .
35	BN	127	 80% 13% 7%
36	BO	117	 87% 12% .
37	BP	115	 87% 11% ..
38	BQ	118	 93% 6% .
39	BR	103	 91% 9%
40	BS	110	 91% 9%
41	BT	100	 74% 18% . 7%
42	BU	104	 83% 15% .
43	BV	94	 77% 23%
44	BW	85	 74% 14% . 11%
45	BX	78	 87% 10% ..
46	BY	63	 87% 10% ..
47	BZ	59	 90% 8% .
48	B0	57	 77% 21% .
49	B1	55	 58% 35% 7%
50	B2	46	 83% 17%
51	B3	65	 86% 12% .
52	B4	38	 82% 18%
53	B5	17	 76% 18% 6%
54	B7	9	 56% 11% 33%
55	B8	77	 42% 35% 19% .



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 146602 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 Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		



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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

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

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



Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.



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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.



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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.



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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	51	Total	C	N	O		0	0
			414	266	76	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called TnaC - Tryptophanase leader peptide - R23F.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	9	Total	C	N	O	P	0	0
			191	85	34	63	9		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.



Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1648	735	295	541	77		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	86	Total	Mg	0
			86	86	
56	BA	233	Total	Mg	0
			233	233	
56	BB	1	Total	Mg	0
			1	1	
56	BC	1	Total	Mg	0
			1	1	
56	BD	2	Total	Mg	0
			2	2	
56	BL	1	Total	Mg	0
			1	1	
56	B8	2	Total	Mg	0
			2	2	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

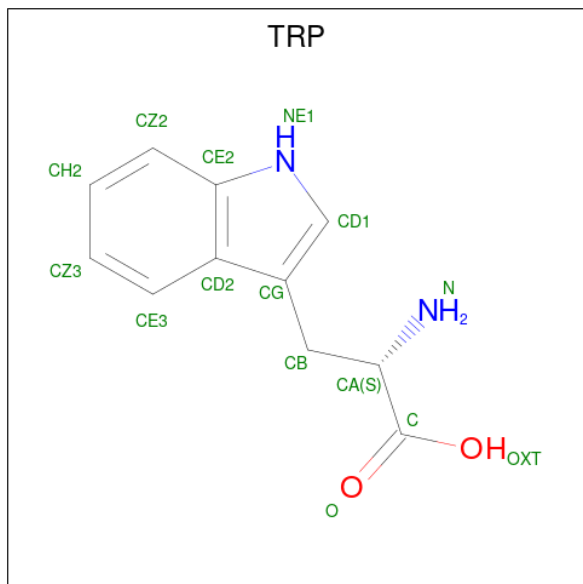
Mol	Chain	Residues	Atoms		AltConf
57	AA	38	Total	K	0
			38	38	
57	AM	1	Total	K	0
			1	1	
57	BA	104	Total	K	0
			104	104	
57	BB	1	Total	K	0
			1	1	
57	BC	1	Total	K	0
			1	1	
57	BD	1	Total	K	0
			1	1	
57	BM	1	Total	K	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		AltConf
58	AB	1	Total	Zn	0
			1	1	
58	BI	1	Total	Zn	0
			1	1	
58	B4	1	Total	Zn	0
			1	1	

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				AltConf
59	BA	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	AA	184	Total	O	0
			184	184	
60	AK	1	Total	O	0
			1	1	
60	AN	1	Total	O	0
			1	1	
60	BA	1672	Total	O	0
			1672	1672	
60	BB	2	Total	O	0
			2	2	
60	BC	38	Total	O	0
			38	38	

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Mol	Chain	Residues	Atoms		AltConf
60	BD	14	Total 14	O 14	0
60	BE	21	Total 21	O 21	0
60	BF	1	Total 1	O 1	0
60	BJ	2	Total 2	O 2	0
60	BK	3	Total 3	O 3	0
60	BL	14	Total 14	O 14	0
60	BM	2	Total 2	O 2	0
60	BN	9	Total 9	O 9	0
60	BO	1	Total 1	O 1	0
60	BP	2	Total 2	O 2	0
60	BQ	12	Total 12	O 12	0
60	BR	4	Total 4	O 4	0
60	BS	7	Total 7	O 7	0
60	BT	3	Total 3	O 3	0
60	BU	1	Total 1	O 1	0
60	BW	5	Total 5	O 5	0
60	BX	4	Total 4	O 4	0
60	B0	4	Total 4	O 4	0
60	B2	6	Total 6	O 6	0
60	B3	7	Total 7	O 7	0
60	B4	1	Total 1	O 1	0

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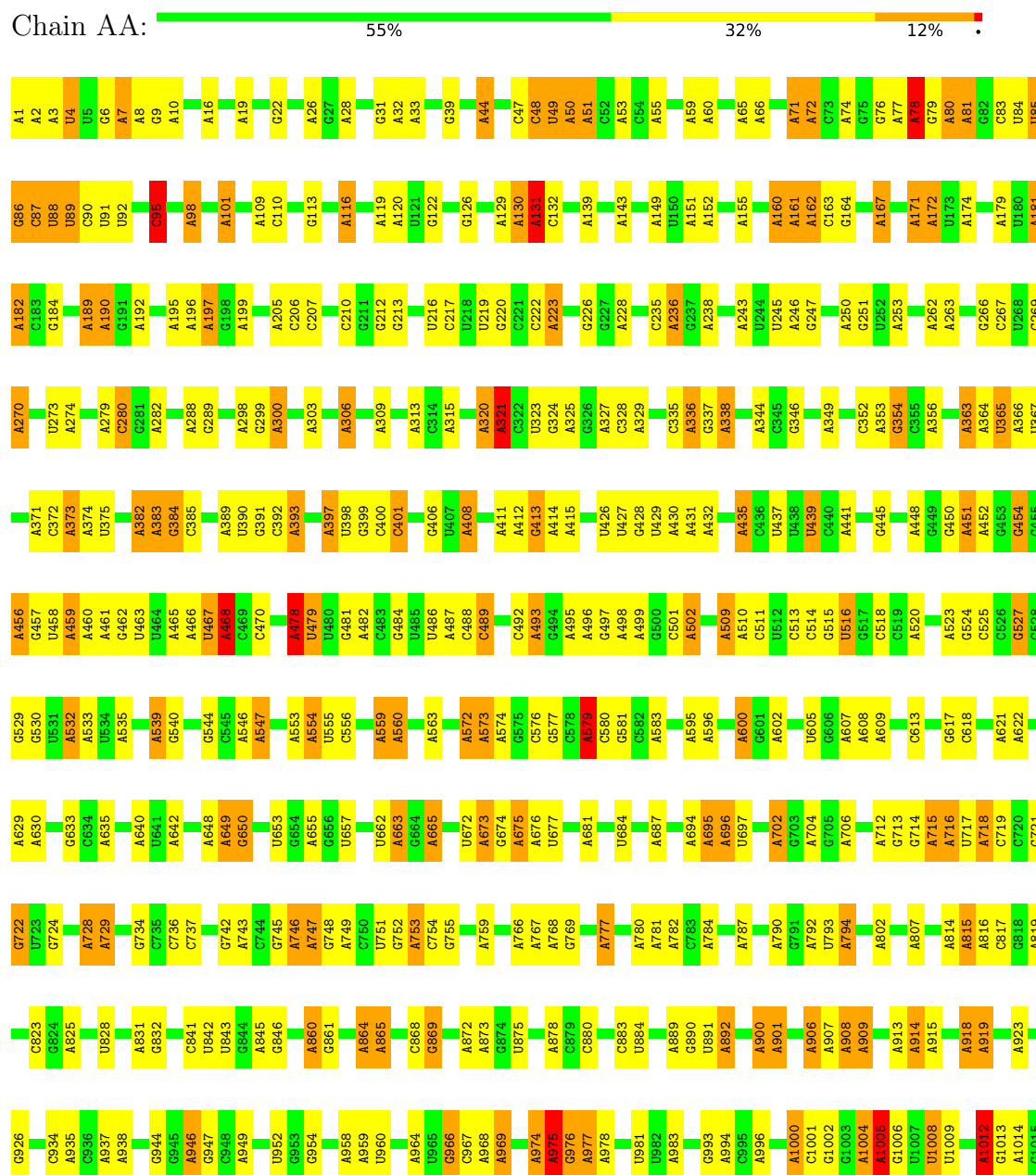
Mol	Chain	Residues	Atoms		AltConf
60	B5	2	Total	O	0
			2	2	
60	B8	3	Total	O	0
			3	3	



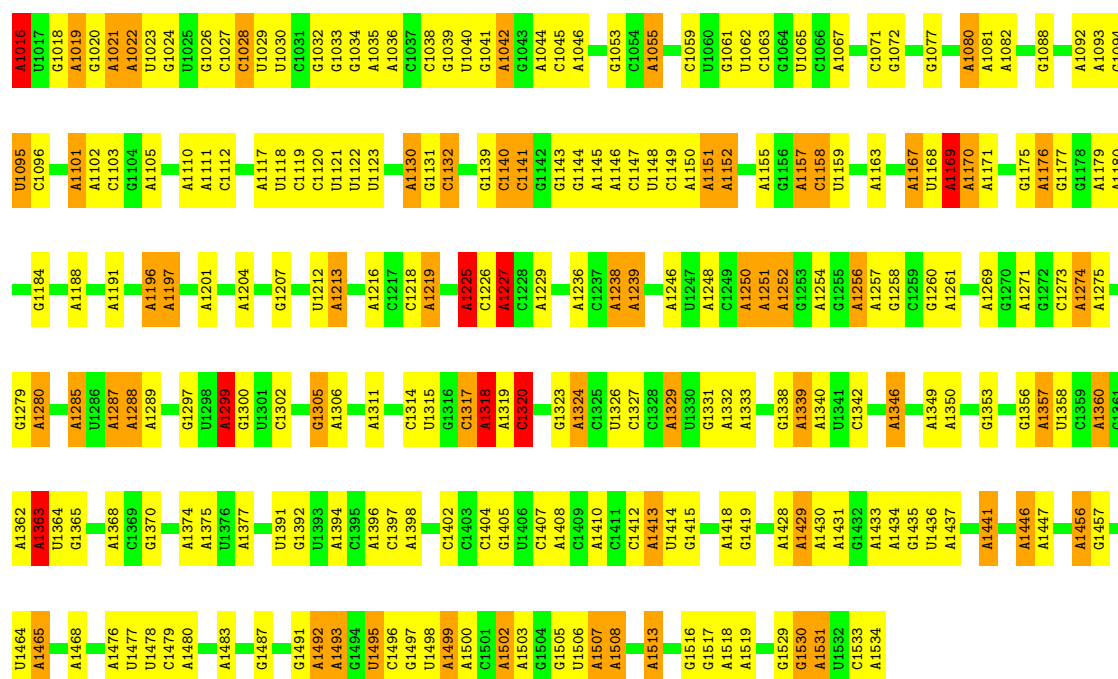
### 3 Residue-property plots [i](#)

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: Ribosomal RNA 16S

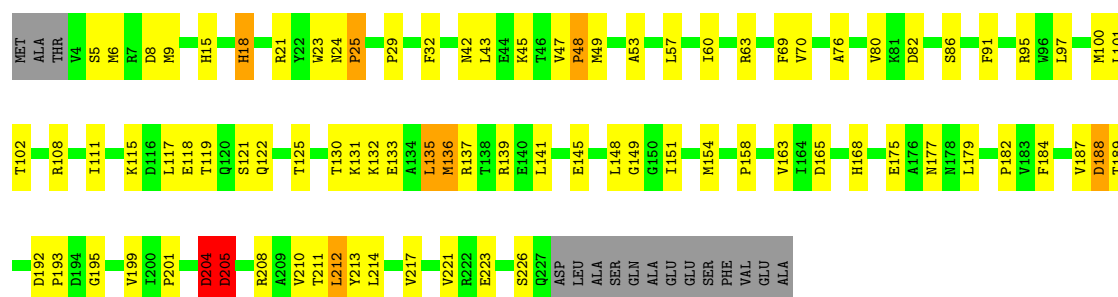






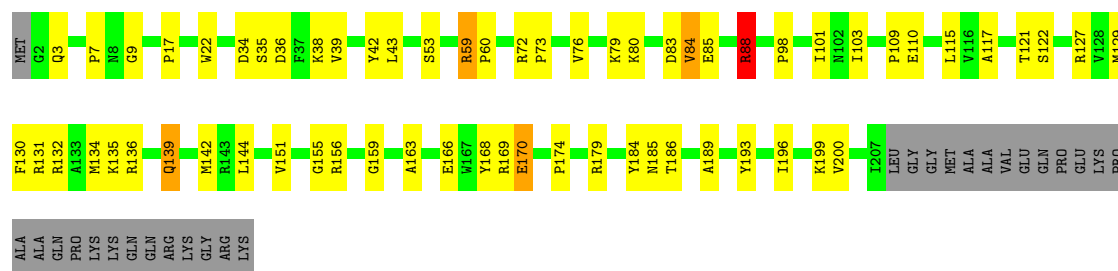
### • Molecule 2: 30S ribosomal protein S2

Chain AB: 58% 32% 7%



### • Molecule 3: 30S ribosomal protein S3

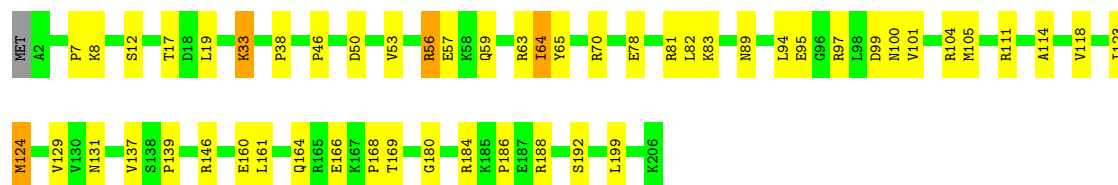
Chain AC: 61% 25% 12%



### • Molecule 4: 30S ribosomal protein S4

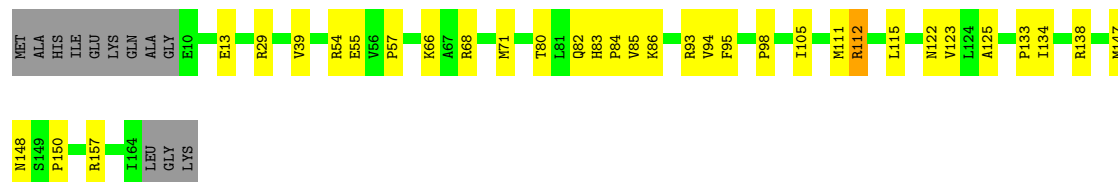
Chain AD: 74% 23% 3%





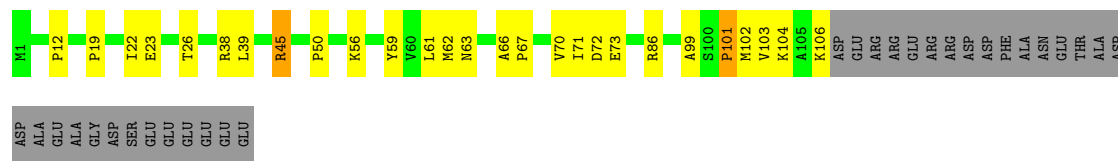
• Molecule 5: 30S ribosomal protein S5

Chain AE: 73% 19% 7%



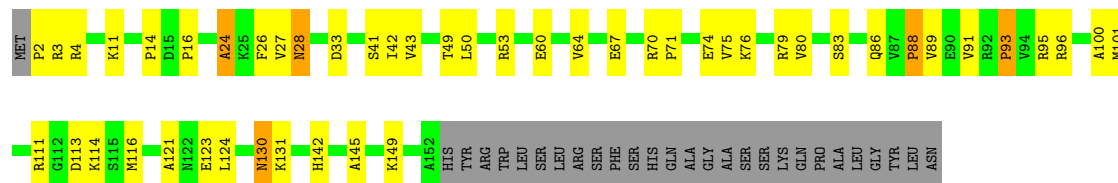
• Molecule 6: 30S ribosomal protein S6

Chain AF: 59% 19% 21%



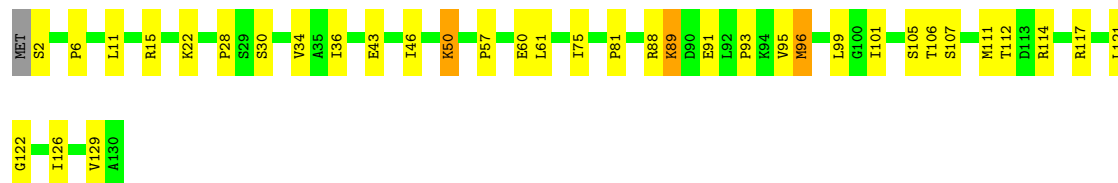
• Molecule 7: 30S ribosomal protein S7

Chain AG: 57% 25% 16%



• Molecule 8: 30S ribosomal protein S8

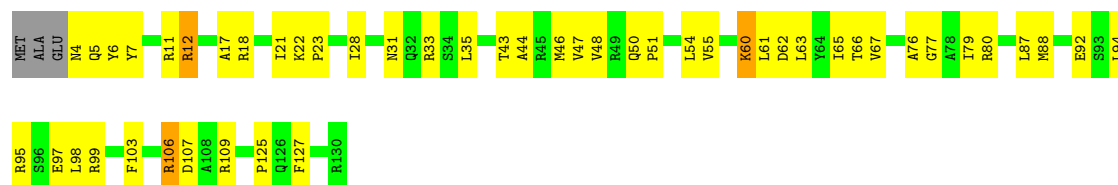
Chain AH: 72% 25% 3%



• Molecule 9: 30S ribosomal protein S9

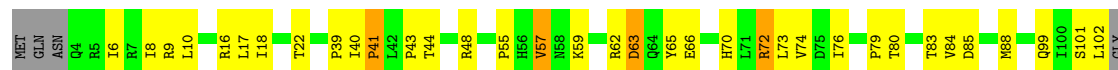
Chain AI: 60% 35% 5%





- Molecule 10: 30S ribosomal protein S10

Chain AJ: 62% 30%



- Molecule 11: 30S ribosomal protein S11

Chain AK: 74% 17% 9%



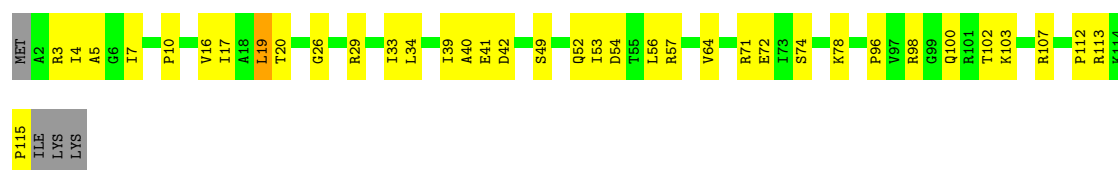
- Molecule 12: 30S ribosomal protein S12

Chain AL: 80% 18%



- Molecule 13: 30S ribosomal protein S13

Chain AM: 65% 31%



- Molecule 14: 30S ribosomal protein S14

Chain AN: 71% 26%



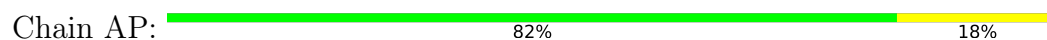
- Molecule 15: 30S ribosomal protein S15

Chain AO: 74% 24%

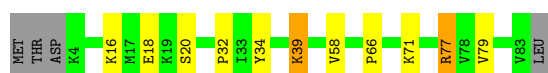
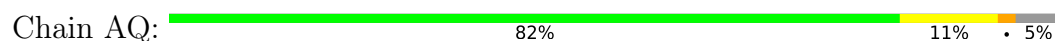




- Molecule 16: 30S ribosomal protein S16



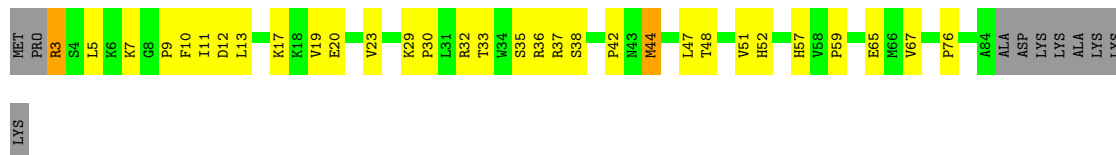
- Molecule 17: 30S ribosomal protein S17



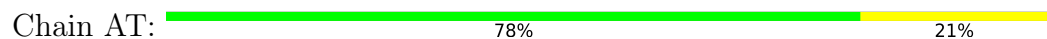
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: Ribosomal RNA 23S

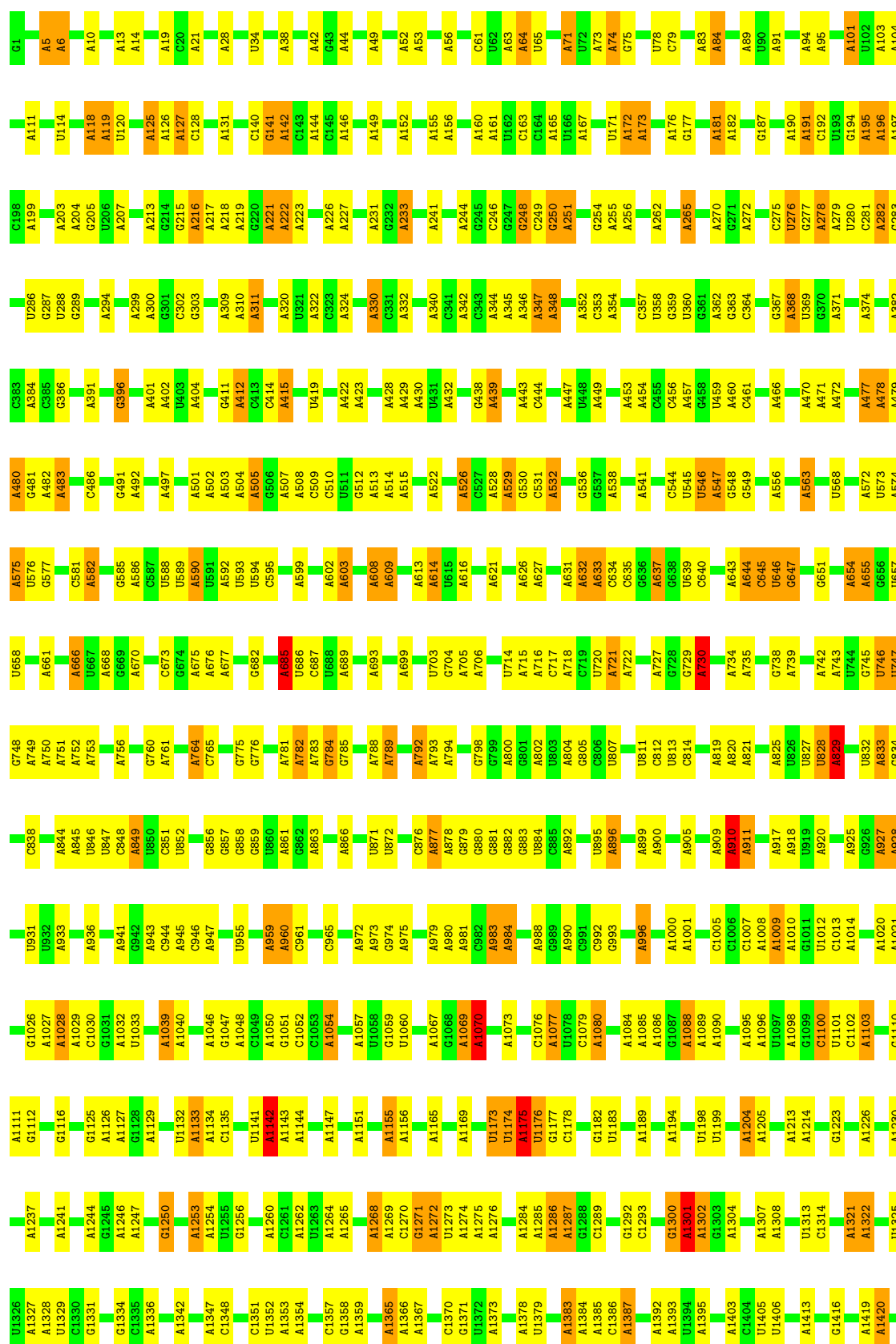


Chain BA:

57%

33%

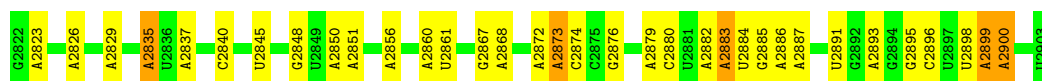
9%





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		A2641	A2568	A2479	A2383	U2299	A2215	A2068				A1584	





• Molecule 23: Ribosomal RNA 5S



• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3



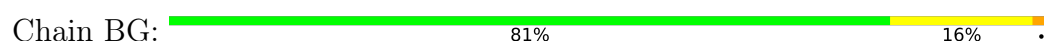
• Molecule 26: 50S ribosomal protein L4



• Molecule 27: 50S ribosomal protein L5



• Molecule 28: 50S ribosomal protein L6

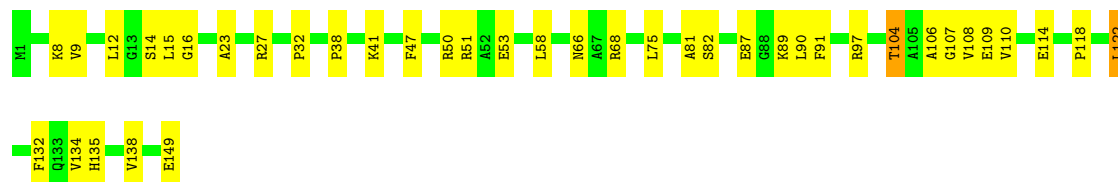






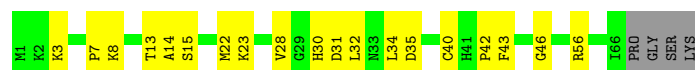
- Molecule 29: 50S ribosomal protein L9

Chain BH: 73% 26%



- Molecule 30: 50S ribosomal protein L31

Chain BI: 67% 27% 6%



- Molecule 31: 50S ribosomal protein L13

Chain BJ: 82% 18%



- Molecule 32: 50S ribosomal protein L14

Chain BK: 81% 19%



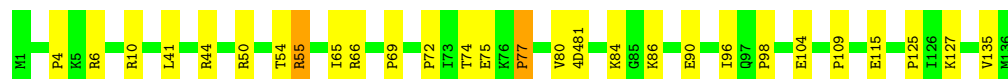
- Molecule 33: 50S ribosomal protein L15

Chain BL: 88% 11%




- Molecule 34: 50S ribosomal protein L16

Chain BM: 79% 19%




- Molecule 35: 50S ribosomal protein L17



Chain BN:  80% 13% 7%



- Molecule 36: 50S ribosomal protein L18

Chain BO:  87% 12% .



- Molecule 37: 50S ribosomal protein L19

Chain BP:  87% 11% ..



- Molecule 38: 50S ribosomal protein L20

Chain BQ:  93% 6% .



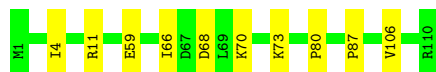
- Molecule 39: 50S ribosomal protein L21

Chain BR:  91% 9%




- Molecule 40: 50S ribosomal protein L22

Chain BS:  91% 9%




- Molecule 41: 50S ribosomal protein L23

Chain BT:  74% 18% . 7%




- Molecule 42: 50S ribosomal protein L24



Chain BU:  83% 15% .




- Molecule 43: 50S ribosomal protein L25

Chain BV:  77% 23%




- Molecule 44: 50S ribosomal protein L27

Chain BW:  74% 14% . 11%




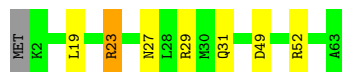
- Molecule 45: 50S ribosomal protein L28

Chain BX:  87% 10% ..



- Molecule 46: 50S ribosomal protein L29

Chain BY:  87% 10% ..




- Molecule 47: 50S ribosomal protein L30

Chain BZ:  90% 8% .



- Molecule 48: 50S ribosomal protein L32

Chain B0:  77% 21% .



- Molecule 49: 50S ribosomal protein L33



MT	ALA	LYS	G4	I5	R6	E7	R8	I9	K10	L11	V12	S13	T24	K27	R28	P31	E32	K33	L34	E35	L36	K37	P41	H46	V47	I48	Y49	R50	E51	I54	LYS
----	-----	-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- 
- A diagram showing a sequence of 10 nodes: M1, T4, P7, R12, K25, N26, R41, V44, S45, and K46. The nodes are arranged in a horizontal line, connected by vertical lines. The nodes are colored in a repeating pattern of yellow and light blue.

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- A diagram of the 5-Region Model showing five regions: V8 (green), N14 (yellow), N17 (yellow), V20 (yellow), and P24 (red). The regions are connected by horizontal lines, with V8 and P24 at the ends and N14, N17, and V20 in the middle.

- 
- ```

graph TD
    C1[C1] --- C4[C4]
    C4 --- U7[U7]
    C4 --- G8[G8]
    C4 --- A9[A9]
  
```

- |    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 | C9 | C10 | C11 | C12 | C13 | C14 | C15 | C16 | C17 | C18 | C19 | C20 | C21 | C22 | C23 | C24 | C25 | C26 | C27 | C28 | C29 | C30 | C31 | C32 | C33 | C34 | C35 | C36 | C37 | C38 | C39 | C40 | C41 | C42 | C43 | C44 | C45 | C46 | C47 | C48 | C49 | C50 | C51 | C52 | C53 | C54 | C55 | C56 | C57 | C58 | C59 | C60 | C61 | C62 | C63 | C64 | C65 | C66 | C67 | C68 | C69 | C70 | C71 | C72 | C73 | C74 | C75 | C76 | C77 | C78 | C79 | C80 | C81 | C82 | C83 | C84 | C85 | C86 | C87 | C88 | C89 | C90 | C91 | C92 | C93 | C94 | C95 | C96 | C97 | C98 | C99 | C100 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 191230                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44                                      | Depositor |
| Minimum defocus (nm)                 | -400                                    | Depositor |
| Maximum defocus (nm)                 | -1600                                   | Depositor |
| Magnification                        | 59880                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 1MG, PSU, 3TD, OMC, UR3, 4D4, 2MG, D2T, MEQ, ZN, 6MZ, MA6, 5MU, 2MA, OMU, G7M, MG, OMG, 5MC, K

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   | AA    | 1.48         | 1296/36593 (3.5%) | 3.33        | 3996/57081 (7.0%)  |
| 2   | AB    | 0.90         | 9/1784 (0.5%)     | 1.10        | 13/2403 (0.5%)     |
| 3   | AC    | 0.86         | 7/1651 (0.4%)     | 0.69        | 3/2225 (0.1%)      |
| 4   | AD    | 0.80         | 6/1665 (0.4%)     | 0.65        | 2/2227 (0.1%)      |
| 5   | AE    | 0.87         | 5/1157 (0.4%)     | 0.61        | 1/1557 (0.1%)      |
| 6   | AF    | 0.94         | 5/881 (0.6%)      | 0.58        | 0/1189             |
| 7   | AG    | 0.99         | 8/1195 (0.7%)     | 0.70        | 1/1602 (0.1%)      |
| 8   | AH    | 0.96         | 6/989 (0.6%)      | 0.69        | 2/1326 (0.2%)      |
| 9   | AI    | 0.73         | 3/1034 (0.3%)     | 0.72        | 2/1375 (0.1%)      |
| 10  | AJ    | 1.08         | 6/805 (0.7%)      | 0.74        | 0/1089             |
| 11  | AK    | 1.12         | 7/893 (0.8%)      | 0.67        | 0/1205             |
| 12  | AL    | 1.09         | 8/960 (0.8%)      | 0.62        | 0/1286             |
| 13  | AM    | 0.91         | 5/892 (0.6%)      | 0.74        | 2/1193 (0.2%)      |
| 14  | AN    | 0.90         | 4/811 (0.5%)      | 0.63        | 1/1081 (0.1%)      |
| 15  | AO    | 0.32         | 0/722             | 0.53        | 0/964              |
| 16  | AP    | 0.73         | 2/659 (0.3%)      | 0.57        | 0/884              |
| 17  | AQ    | 0.73         | 2/657 (0.3%)      | 0.77        | 2/881 (0.2%)       |
| 18  | AR    | 0.84         | 2/462 (0.4%)      | 0.58        | 0/621              |
| 19  | AS    | 1.08         | 5/672 (0.7%)      | 0.78        | 2/904 (0.2%)       |
| 20  | AT    | 0.56         | 1/676 (0.1%)      | 0.47        | 0/895              |
| 21  | AU    | 1.15         | 5/472 (1.1%)      | 0.62        | 0/627              |
| 22  | BA    | 1.57         | 2305/69121 (3.3%) | 3.43        | 7802/107828 (7.2%) |
| 23  | BB    | 1.34         | 75/2872 (2.6%)    | 2.95        | 243/4478 (5.4%)    |
| 24  | BC    | 1.14         | 17/2121 (0.8%)    | 0.65        | 0/2852             |
| 25  | BD    | 0.86         | 8/1576 (0.5%)     | 0.56        | 0/2119             |
| 26  | BE    | 0.76         | 5/1571 (0.3%)     | 0.55        | 0/2113             |
| 27  | BF    | 0.84         | 6/1434 (0.4%)     | 0.63        | 2/1926 (0.1%)      |
| 28  | BG    | 0.98         | 8/1343 (0.6%)     | 0.59        | 0/1816             |
| 29  | BH    | 0.71         | 3/1121 (0.3%)     | 0.67        | 2/1515 (0.1%)      |
| 30  | BI    | 0.82         | 2/531 (0.4%)      | 0.70        | 1/709 (0.1%)       |
| 31  | BJ    | 0.92         | 6/1152 (0.5%)     | 0.55        | 0/1551             |



| Mol | Chain | Bond lengths |                    | Bond angles |                     |
|-----|-------|--------------|--------------------|-------------|---------------------|
|     |       | RMSZ         | # Z  >5            | RMSZ        | # Z  >5             |
| 32  | BK    | 0.93         | 5/955 (0.5%)       | 0.63        | 0/1279              |
| 33  | BL    | 0.83         | 4/1062 (0.4%)      | 0.58        | 0/1413              |
| 34  | BM    | 1.02         | 7/1081 (0.6%)      | 0.59        | 0/1443              |
| 35  | BN    | 0.86         | 4/958 (0.4%)       | 0.61        | 0/1281              |
| 36  | BO    | 0.65         | 2/910 (0.2%)       | 0.50        | 0/1219              |
| 37  | BP    | 0.80         | 3/929 (0.3%)       | 0.56        | 0/1242              |
| 38  | BQ    | 0.38         | 0/960              | 0.50        | 0/1278              |
| 39  | BR    | 0.63         | 2/829 (0.2%)       | 0.56        | 0/1107              |
| 40  | BS    | 0.69         | 2/864 (0.2%)       | 0.59        | 0/1156              |
| 41  | BT    | 0.64         | 1/744 (0.1%)       | 0.78        | 4/994 (0.4%)        |
| 42  | BU    | 0.82         | 3/787 (0.4%)       | 0.58        | 0/1051              |
| 43  | BV    | 0.92         | 4/766 (0.5%)       | 0.56        | 0/1025              |
| 44  | BW    | 0.64         | 1/587 (0.2%)       | 0.55        | 0/776               |
| 45  | BX    | 0.77         | 2/635 (0.3%)       | 0.55        | 0/848               |
| 46  | BY    | 0.30         | 0/502              | 0.45        | 0/667               |
| 47  | BZ    | 0.84         | 2/453 (0.4%)       | 0.54        | 0/605               |
| 48  | B0    | 0.65         | 1/450 (0.2%)       | 0.58        | 0/599               |
| 49  | B1    | 0.92         | 2/421 (0.5%)       | 0.60        | 0/561               |
| 50  | B2    | 0.75         | 1/380 (0.3%)       | 0.56        | 0/498               |
| 51  | B3    | 1.13         | 4/513 (0.8%)       | 0.61        | 0/676               |
| 52  | B4    | 0.79         | 1/303 (0.3%)       | 0.55        | 0/397               |
| 53  | B5    | 1.33         | 2/151 (1.3%)       | 0.90        | 1/205 (0.5%)        |
| 54  | B7    | 1.51         | 6/212 (2.8%)       | 2.52        | 12/328 (3.7%)       |
| 55  | B8    | 1.53         | 41/1765 (2.3%)     | 3.06        | 169/2750 (6.1%)     |
| All | All   | 1.38         | 3927/155689 (2.5%) | 2.93        | 12263/232920 (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 |
|-----|-------|---------------------|---------------------|
| 2   | AB    | 0                   | 2                   |
| 7   | AG    | 0                   | 1                   |
| 29  | BH    | 0                   | 2                   |
| 43  | BV    | 0                   | 1                   |
| All | All   | 0                   | 6                   |

The worst 5 of 3927 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | BA    | 2449 | U    | C5-C6 | 23.39 | 1.55        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 55  | B8    | 20  | U    | C5-C6 | 22.49 | 1.54        | 1.34     |
| 10  | AJ    | 41  | PRO  | N-CD  | 12.96 | 1.66        | 1.47     |
| 7   | AG    | 2   | PRO  | N-CD  | 12.92 | 1.66        | 1.47     |
| 21  | AU    | 2   | PRO  | N-CD  | 12.52 | 1.65        | 1.47     |

The worst 5 of 12263 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22  | BA    | 2872 | A    | N1-C6-N6 | -26.13 | 102.92      | 118.60   |
| 22  | BA    | 1848 | A    | N1-C6-N6 | -22.75 | 104.95      | 118.60   |
| 22  | BA    | 1285 | A    | N1-C6-N6 | -22.74 | 104.95      | 118.60   |
| 22  | BA    | 1253 | A    | N1-C6-N6 | -22.72 | 104.97      | 118.60   |
| 1   | AA    | 1299 | A    | N1-C6-N6 | -22.71 | 104.97      | 118.60   |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | AB    | 204 | ASP  | Sidechain |
| 2   | AB    | 205 | ASP  | Sidechain |
| 7   | AG    | 24  | ALA  | Mainchain |
| 29  | BH    | 104 | THR  | Peptide   |
| 29  | BH    | 66  | ASN  | Peptide   |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32930 | 0        | 16580    | 240     | 0            |
| 2   | AB    | 1753  | 0        | 1780     | 60      | 0            |
| 3   | AC    | 1624  | 0        | 1696     | 41      | 0            |
| 4   | AD    | 1643  | 0        | 1707     | 38      | 0            |
| 5   | AE    | 1144  | 0        | 1185     | 25      | 0            |
| 6   | AF    | 862   | 0        | 864      | 34      | 0            |
| 7   | AG    | 1181  | 0        | 1238     | 31      | 0            |
| 8   | AH    | 979   | 0        | 1031     | 29      | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | AJ    | 795   | 0        | 836      | 26      | 0            |
| 11  | AK    | 877   | 0        | 887      | 16      | 0            |
| 12  | AL    | 957   | 0        | 1017     | 12      | 0            |
| 13  | AM    | 883   | 0        | 941      | 25      | 0            |
| 14  | AN    | 799   | 0        | 841      | 23      | 0            |
| 15  | AO    | 714   | 0        | 734      | 18      | 0            |
| 16  | AP    | 649   | 0        | 666      | 10      | 0            |
| 17  | AQ    | 648   | 0        | 691      | 12      | 0            |
| 18  | AR    | 455   | 0        | 478      | 13      | 0            |
| 19  | AS    | 656   | 0        | 680      | 25      | 0            |
| 20  | AT    | 670   | 0        | 719      | 10      | 0            |
| 21  | AU    | 465   | 0        | 491      | 9       | 0            |
| 22  | BA    | 62209 | 0        | 31290    | 320     | 0            |
| 23  | BB    | 2569  | 0        | 1301     | 7       | 0            |
| 24  | BC    | 2082  | 0        | 2154     | 27      | 0            |
| 25  | BD    | 1566  | 0        | 1617     | 12      | 0            |
| 26  | BE    | 1552  | 0        | 1619     | 10      | 0            |
| 27  | BF    | 1410  | 0        | 1444     | 26      | 0            |
| 28  | BG    | 1323  | 0        | 1371     | 18      | 0            |
| 29  | BH    | 1110  | 0        | 1148     | 28      | 0            |
| 30  | BI    | 522   | 0        | 520      | 13      | 0            |
| 31  | BJ    | 1129  | 0        | 1162     | 14      | 0            |
| 32  | BK    | 946   | 0        | 1023     | 13      | 0            |
| 33  | BL    | 1053  | 0        | 1128     | 12      | 0            |
| 34  | BM    | 1075  | 0        | 1155     | 14      | 0            |
| 35  | BN    | 945   | 0        | 989      | 9       | 0            |
| 36  | BO    | 900   | 0        | 935      | 8       | 0            |
| 37  | BP    | 917   | 0        | 962      | 9       | 0            |
| 38  | BQ    | 947   | 0        | 1019     | 7       | 0            |
| 39  | BR    | 816   | 0        | 839      | 7       | 0            |
| 40  | BS    | 857   | 0        | 922      | 7       | 0            |
| 41  | BT    | 738   | 0        | 807      | 10      | 0            |
| 42  | BU    | 779   | 0        | 831      | 11      | 0            |
| 43  | BV    | 753   | 0        | 780      | 9       | 0            |
| 44  | BW    | 580   | 0        | 594      | 21      | 0            |
| 45  | BX    | 625   | 0        | 652      | 4       | 0            |
| 46  | BY    | 501   | 0        | 531      | 5       | 0            |
| 47  | BZ    | 449   | 0        | 488      | 1       | 0            |
| 48  | B0    | 444   | 0        | 458      | 5       | 0            |
| 49  | B1    | 414   | 0        | 442      | 12      | 0            |
| 50  | B2    | 377   | 0        | 418      | 5       | 0            |
| 51  | B3    | 504   | 0        | 572      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52  | B4    | 302   | 0        | 340      | 4       | 0            |
| 53  | B5    | 146   | 0        | 139      | 3       | 0            |
| 54  | B7    | 191   | 0        | 99       | 0       | 0            |
| 55  | B8    | 1648  | 0        | 833      | 27      | 0            |
| 56  | AA    | 86    | 0        | 0        | 0       | 0            |
| 56  | B8    | 2     | 0        | 0        | 0       | 0            |
| 56  | BA    | 233   | 0        | 0        | 0       | 0            |
| 56  | BB    | 1     | 0        | 0        | 0       | 0            |
| 56  | BC    | 1     | 0        | 0        | 0       | 0            |
| 56  | BD    | 2     | 0        | 0        | 0       | 0            |
| 56  | BL    | 1     | 0        | 0        | 0       | 0            |
| 57  | AA    | 38    | 0        | 0        | 0       | 0            |
| 57  | AM    | 1     | 0        | 0        | 0       | 0            |
| 57  | BA    | 104   | 0        | 0        | 1       | 0            |
| 57  | BB    | 1     | 0        | 0        | 0       | 0            |
| 57  | BC    | 1     | 0        | 0        | 0       | 0            |
| 57  | BD    | 1     | 0        | 0        | 0       | 0            |
| 57  | BM    | 1     | 0        | 0        | 0       | 0            |
| 58  | AB    | 1     | 0        | 0        | 0       | 0            |
| 58  | B4    | 1     | 0        | 0        | 0       | 0            |
| 58  | BI    | 1     | 0        | 0        | 0       | 0            |
| 59  | BA    | 15    | 0        | 9        | 0       | 0            |
| 60  | AA    | 184   | 0        | 0        | 1       | 0            |
| 60  | AK    | 1     | 0        | 0        | 0       | 0            |
| 60  | AN    | 1     | 0        | 0        | 0       | 0            |
| 60  | B0    | 4     | 0        | 0        | 0       | 0            |
| 60  | B2    | 6     | 0        | 0        | 0       | 0            |
| 60  | B3    | 7     | 0        | 0        | 0       | 0            |
| 60  | B4    | 1     | 0        | 0        | 0       | 0            |
| 60  | B5    | 2     | 0        | 0        | 1       | 0            |
| 60  | B8    | 3     | 0        | 0        | 1       | 0            |
| 60  | BA    | 1672  | 0        | 0        | 25      | 0            |
| 60  | BB    | 2     | 0        | 0        | 0       | 0            |
| 60  | BC    | 38    | 0        | 0        | 1       | 0            |
| 60  | BD    | 14    | 0        | 0        | 0       | 0            |
| 60  | BE    | 21    | 0        | 0        | 2       | 0            |
| 60  | BF    | 1     | 0        | 0        | 0       | 0            |
| 60  | BJ    | 2     | 0        | 0        | 0       | 0            |
| 60  | BK    | 3     | 0        | 0        | 0       | 0            |
| 60  | BL    | 14    | 0        | 0        | 0       | 0            |
| 60  | BM    | 2     | 0        | 0        | 0       | 0            |
| 60  | BN    | 9     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | BO    | 1      | 0        | 0        | 0       | 0            |
| 60  | BP    | 2      | 0        | 0        | 0       | 0            |
| 60  | BQ    | 12     | 0        | 0        | 0       | 0            |
| 60  | BR    | 4      | 0        | 0        | 0       | 0            |
| 60  | BS    | 7      | 0        | 0        | 0       | 0            |
| 60  | BT    | 3      | 0        | 0        | 0       | 0            |
| 60  | BU    | 1      | 0        | 0        | 0       | 0            |
| 60  | BW    | 5      | 0        | 0        | 3       | 0            |
| 60  | BX    | 4      | 0        | 0        | 0       | 0            |
| All | All   | 146602 | 0        | 96723    | 1260    | 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 1260 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) |
|------------------|------------------|--------------------------|-------------------|
| 6:AF:39:LEU:HD11 | 6:AF:62:MET:CE   | 1.55                     | 1.34              |
| 6:AF:39:LEU:CD1  | 6:AF:62:MET:CE   | 2.07                     | 1.33              |
| 42:BU:10:GLU:OE2 | 42:BU:73:PHE:HB3 | 1.34                     | 1.23              |
| 6:AF:39:LEU:CD1  | 6:AF:62:MET:HE2  | 1.65                     | 1.19              |
| 6:AF:39:LEU:HD12 | 6:AF:62:MET:HG2  | 1.27                     | 1.14              |

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    | 222/240 (92%) | 211 (95%) | 11 (5%) | 0        | 100         | 100 |
| 3   | AC    | 204/233 (88%) | 193 (95%) | 11 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 4   | AD    | 203/206 (98%) | 196 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 5   | AE    | 153/167 (92%) | 146 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 6   | AF    | 104/135 (77%) | 102 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 7   | AG    | 149/179 (83%) | 136 (91%)  | 13 (9%)  | 0        | 100         | 100 |
| 8   | AH    | 127/130 (98%) | 124 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 9   | AI    | 125/130 (96%) | 114 (91%)  | 11 (9%)  | 0        | 100         | 100 |
| 10  | AJ    | 97/103 (94%)  | 92 (95%)   | 4 (4%)   | 1 (1%)   | 13          | 20  |
| 11  | AK    | 115/129 (89%) | 109 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 12  | AL    | 120/124 (97%) | 115 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 13  | AM    | 112/118 (95%) | 108 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 14  | AN    | 99/102 (97%)  | 91 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 15  | AO    | 86/89 (97%)   | 83 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 16  | AP    | 80/82 (98%)   | 77 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 17  | AQ    | 78/84 (93%)   | 77 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 18  | AR    | 53/75 (71%)   | 51 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 19  | AS    | 80/92 (87%)   | 74 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 20  | AT    | 84/87 (97%)   | 81 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 21  | AU    | 54/71 (76%)   | 52 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 24  | BC    | 269/273 (98%) | 263 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 25  | BD    | 206/209 (99%) | 198 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 26  | BE    | 199/201 (99%) | 195 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 27  | BF    | 175/179 (98%) | 169 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 28  | BG    | 174/177 (98%) | 173 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 29  | BH    | 147/149 (99%) | 132 (90%)  | 15 (10%) | 0        | 100         | 100 |
| 30  | BI    | 64/70 (91%)   | 54 (84%)   | 10 (16%) | 0        | 100         | 100 |
| 31  | BJ    | 140/142 (99%) | 140 (100%) | 0        | 0        | 100         | 100 |
| 32  | BK    | 121/123 (98%) | 118 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 33  | BL    | 142/144 (99%) | 135 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 34  | BM    | 133/136 (98%) | 131 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 35  | BN    | 116/127 (91%) | 112 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 36  | BO    | 115/117 (98%) | 114 (99%)  | 1 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 37  | BP    | 112/115 (97%)   | 110 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 38  | BQ    | 115/118 (98%)   | 115 (100%) | 0        | 0        | 100         | 100 |
| 39  | BR    | 101/103 (98%)   | 99 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 40  | BS    | 108/110 (98%)   | 106 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 41  | BT    | 91/100 (91%)    | 87 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 42  | BU    | 100/104 (96%)   | 98 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 43  | BV    | 92/94 (98%)     | 89 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 44  | BW    | 74/85 (87%)     | 71 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 45  | BX    | 75/78 (96%)     | 75 (100%)  | 0        | 0        | 100         | 100 |
| 46  | BY    | 60/63 (95%)     | 59 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 47  | BZ    | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 48  | B0    | 54/57 (95%)     | 54 (100%)  | 0        | 0        | 100         | 100 |
| 49  | B1    | 49/55 (89%)     | 48 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 50  | B2    | 44/46 (96%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 51  | B3    | 62/65 (95%)     | 57 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 52  | B4    | 36/38 (95%)     | 36 (100%)  | 0        | 0        | 100         | 100 |
| 53  | B5    | 15/17 (88%)     | 14 (93%)   | 1 (7%)   | 0        | 100         | 100 |
| All | All   | 5590/5930 (94%) | 5381 (96%) | 208 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AJ    | 57  | VAL  |

### 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   | AB    | 186/198 (94%) | 182 (98%) | 4 (2%)   | 47          | 67 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 3   | AC    | 170/190 (90%)  | 163 (96%) | 7 (4%)   | 26          | 44  |
| 4   | AD    | 172/173 (99%)  | 167 (97%) | 5 (3%)   | 37          | 58  |
| 5   | AE    | 118/126 (94%)  | 115 (98%) | 3 (2%)   | 42          | 63  |
| 6   | AF    | 92/116 (79%)   | 91 (99%)  | 1 (1%)   | 70          | 84  |
| 7   | AG    | 124/147 (84%)  | 115 (93%) | 9 (7%)   | 11          | 20  |
| 8   | AH    | 104/105 (99%)  | 101 (97%) | 3 (3%)   | 37          | 58  |
| 9   | AI    | 105/107 (98%)  | 101 (96%) | 4 (4%)   | 28          | 47  |
| 10  | AJ    | 87/90 (97%)    | 82 (94%)  | 5 (6%)   | 17          | 29  |
| 11  | AK    | 90/99 (91%)    | 89 (99%)  | 1 (1%)   | 70          | 84  |
| 12  | AL    | 102/103 (99%)  | 97 (95%)  | 5 (5%)   | 21          | 36  |
| 13  | AM    | 92/96 (96%)    | 92 (100%) | 0        | 100         | 100 |
| 14  | AN    | 79/84 (94%)    | 76 (96%)  | 3 (4%)   | 28          | 47  |
| 15  | AO    | 76/77 (99%)    | 74 (97%)  | 2 (3%)   | 41          | 62  |
| 16  | AP    | 65/65 (100%)   | 65 (100%) | 0        | 100         | 100 |
| 17  | AQ    | 74/78 (95%)    | 72 (97%)  | 2 (3%)   | 40          | 60  |
| 18  | AR    | 48/65 (74%)    | 46 (96%)  | 2 (4%)   | 25          | 43  |
| 19  | AS    | 71/79 (90%)    | 70 (99%)  | 1 (1%)   | 62          | 79  |
| 20  | AT    | 65/66 (98%)    | 65 (100%) | 0        | 100         | 100 |
| 21  | AU    | 48/61 (79%)    | 45 (94%)  | 3 (6%)   | 15          | 25  |
| 24  | BC    | 216/218 (99%)  | 213 (99%) | 3 (1%)   | 62          | 79  |
| 25  | BD    | 163/163 (100%) | 157 (96%) | 6 (4%)   | 29          | 48  |
| 26  | BE    | 165/165 (100%) | 162 (98%) | 3 (2%)   | 54          | 73  |
| 27  | BF    | 148/150 (99%)  | 142 (96%) | 6 (4%)   | 26          | 44  |
| 28  | BG    | 137/138 (99%)  | 134 (98%) | 3 (2%)   | 47          | 67  |
| 29  | BH    | 114/114 (100%) | 112 (98%) | 2 (2%)   | 54          | 73  |
| 30  | BI    | 59/62 (95%)    | 57 (97%)  | 2 (3%)   | 32          | 52  |
| 31  | BJ    | 116/116 (100%) | 114 (98%) | 2 (2%)   | 56          | 75  |
| 32  | BK    | 104/104 (100%) | 101 (97%) | 3 (3%)   | 37          | 58  |
| 33  | BL    | 103/103 (100%) | 102 (99%) | 1 (1%)   | 73          | 86  |
| 34  | BM    | 108/108 (100%) | 104 (96%) | 4 (4%)   | 29          | 48  |
| 35  | BN    | 98/103 (95%)   | 98 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 36  | BO    | 87/87 (100%)    | 84 (97%)   | 3 (3%)   | 32          | 52  |
| 37  | BP    | 99/100 (99%)    | 96 (97%)   | 3 (3%)   | 36          | 57  |
| 38  | BQ    | 89/90 (99%)     | 88 (99%)   | 1 (1%)   | 70          | 84  |
| 39  | BR    | 84/84 (100%)    | 82 (98%)   | 2 (2%)   | 44          | 64  |
| 40  | BS    | 93/93 (100%)    | 93 (100%)  | 0        | 100         | 100 |
| 41  | BT    | 80/84 (95%)     | 78 (98%)   | 2 (2%)   | 42          | 63  |
| 42  | BU    | 83/85 (98%)     | 82 (99%)   | 1 (1%)   | 67          | 82  |
| 43  | BV    | 78/78 (100%)    | 76 (97%)   | 2 (3%)   | 41          | 62  |
| 44  | BW    | 57/63 (90%)     | 55 (96%)   | 2 (4%)   | 31          | 51  |
| 45  | BX    | 67/68 (98%)     | 66 (98%)   | 1 (2%)   | 60          | 77  |
| 46  | BY    | 54/55 (98%)     | 53 (98%)   | 1 (2%)   | 52          | 72  |
| 47  | BZ    | 48/49 (98%)     | 47 (98%)   | 1 (2%)   | 48          | 69  |
| 48  | B0    | 47/48 (98%)     | 44 (94%)   | 3 (6%)   | 14          | 24  |
| 49  | B1    | 45/49 (92%)     | 44 (98%)   | 1 (2%)   | 47          | 67  |
| 50  | B2    | 38/38 (100%)    | 36 (95%)   | 2 (5%)   | 19          | 33  |
| 51  | B3    | 51/52 (98%)     | 50 (98%)   | 1 (2%)   | 50          | 70  |
| 52  | B4    | 34/34 (100%)    | 33 (97%)   | 1 (3%)   | 37          | 58  |
| 53  | B5    | 17/17 (100%)    | 16 (94%)   | 1 (6%)   | 16          | 28  |
| All | All   | 4650/4843 (96%) | 4527 (97%) | 123 (3%) | 42          | 62  |

5 of 123 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AU    | 25  | LYS  |
| 44  | BW    | 81  | SER  |
| 26  | BE    | 168 | ASP  |
| 44  | BW    | 44  | LYS  |
| 50  | B2    | 25  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BG    | 38  | ASN  |
| 50  | B2    | 26  | ASN  |
| 50  | B2    | 29  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AI    | 50  | GLN  |
| 5   | AE    | 135 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1530/1534 (99%) | 180 (11%)         | 1 (0%)          |
| 22  | BA    | 2891/2897 (99%) | 295 (10%)         | 15 (0%)         |
| 23  | BB    | 119/120 (99%)   | 7 (5%)            | 0               |
| 54  | B7    | 8/9 (88%)       | 4 (50%)           | 0               |
| 55  | B8    | 76/77 (98%)     | 14 (18%)          | 4 (5%)          |
| All | All   | 4624/4637 (99%) | 500 (10%)         | 20 (0%)         |

5 of 500 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | U    |
| 1   | AA    | 7   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 22  | G    |
| 1   | AA    | 39  | G    |

5 of 20 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 2518 | A    |
| 55  | B8    | 3    | G    |
| 55  | B8    | 20   | U    |
| 55  | B8    | 19   | G    |
| 22  | BA    | 1608 | A    |

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection.



RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | AA    | 967  | 1        | 18,22,23     | 3.50 | 7 (38%)  | 26,32,35    | 0.98 | 1 (3%)   |
| 22  | OMU  | BA    | 2552 | 22,56    | 19,22,23     | 2.83 | 7 (36%)  | 26,31,34    | 1.72 | 5 (19%)  |
| 22  | G7M  | BA    | 2069 | 22,57    | 20,26,27     | 2.39 | 6 (30%)  | 17,39,42    | 1.21 | 3 (17%)  |
| 12  | D2T  | AL    | 89   | 12       | 7,9,10       | 1.09 | 0        | 6,11,13     | 2.51 | 3 (50%)  |
| 22  | OMG  | BA    | 2251 | 22,57,55 | 18,26,27     | 2.46 | 8 (44%)  | 19,38,41    | 1.89 | 8 (42%)  |
| 22  | PSU  | BA    | 2580 | 22,57    | 18,21,22     | 4.19 | 8 (44%)  | 22,30,33    | 2.02 | 6 (27%)  |
| 22  | 2MA  | BA    | 2503 | 22,57,56 | 19,25,26     | 3.29 | 6 (31%)  | 21,37,40    | 1.75 | 3 (14%)  |
| 55  | G7M  | B8    | 46   | 55       | 20,26,27     | 2.30 | 6 (30%)  | 17,39,42    | 1.34 | 2 (11%)  |
| 1   | MA6  | AA    | 1519 | 1        | 18,26,27     | 1.18 | 1 (5%)   | 19,38,41    | 3.50 | 2 (10%)  |
| 22  | 2MG  | BA    | 1835 | 22       | 18,26,27     | 2.36 | 7 (38%)  | 16,38,41    | 1.45 | 3 (18%)  |
| 22  | PSU  | BA    | 1911 | 22       | 18,21,22     | 4.28 | 7 (38%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 22  | PSU  | BA    | 955  | 22       | 18,21,22     | 4.18 | 7 (38%)  | 22,30,33    | 1.50 | 4 (18%)  |
| 1   | UR3  | AA    | 1498 | 1        | 19,22,23     | 3.02 | 8 (42%)  | 26,32,35    | 1.42 | 2 (7%)   |
| 55  | PSU  | B8    | 55   | 55       | 18,21,22     | 4.26 | 8 (44%)  | 22,30,33    | 1.94 | 5 (22%)  |
| 34  | 4D4  | BM    | 81   | 34       | 9,11,12      | 2.52 | 3 (33%)  | 8,13,15     | 1.06 | 0        |
| 22  | 5MU  | BA    | 747  | 22       | 19,22,23     | 0.78 | 0        | 28,32,35    | 1.10 | 2 (7%)   |
| 22  | 5MU  | BA    | 1939 | 22,57    | 19,22,23     | 0.75 | 0        | 28,32,35    | 1.19 | 4 (14%)  |
| 22  | 3TD  | BA    | 1915 | 22       | 18,22,23     | 4.17 | 8 (44%)  | 22,32,35    | 1.65 | 3 (13%)  |
| 22  | 5MC  | BA    | 1962 | 22,57    | 18,22,23     | 3.39 | 7 (38%)  | 26,32,35    | 1.15 | 2 (7%)   |
| 25  | MEQ  | BD    | 150  | 25       | 8,9,10       | 1.64 | 2 (25%)  | 5,10,12     | 1.76 | 2 (40%)  |
| 22  | PSU  | BA    | 2457 | 22       | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.70 | 5 (22%)  |
| 1   | 4OC  | AA    | 1402 | 1,56     | 20,23,24     | 3.13 | 8 (40%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 1   | 2MG  | AA    | 1207 | 57,1     | 18,26,27     | 2.57 | 7 (38%)  | 16,38,41    | 1.42 | 3 (18%)  |
| 22  | PSU  | BA    | 2605 | 22       | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.71 | 3 (13%)  |
| 22  | 6MZ  | BA    | 1618 | 22       | 18,25,26     | 2.91 | 4 (22%)  | 16,36,39    | 1.95 | 3 (18%)  |
| 22  | PSU  | BA    | 2504 | 22,57    | 18,21,22     | 4.25 | 7 (38%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 22  | 2MG  | BA    | 2445 | 22       | 18,26,27     | 2.43 | 7 (38%)  | 16,38,41    | 1.39 | 2 (12%)  |
| 1   | 5MC  | AA    | 1407 | 1        | 18,22,23     | 3.53 | 7 (38%)  | 26,32,35    | 1.02 | 1 (3%)   |
| 22  | PSU  | BA    | 746  | 22,56    | 18,21,22     | 4.26 | 8 (44%)  | 22,30,33    | 1.81 | 4 (18%)  |
| 1   | 2MG  | AA    | 1516 | 1        | 18,26,27     | 2.47 | 7 (38%)  | 16,38,41    | 1.44 | 3 (18%)  |
| 22  | PSU  | BA    | 1917 | 22       | 18,21,22     | 4.24 | 7 (38%)  | 22,30,33    | 1.71 | 5 (22%)  |
| 22  | 1MG  | BA    | 745  | 22       | 18,26,27     | 2.50 | 7 (38%)  | 19,39,42    | 1.64 | 4 (21%)  |
| 55  | 1MG  | B8    | 37   | 55       | 18,26,27     | 2.48 | 5 (27%)  | 19,39,42    | 1.34 | 3 (15%)  |



| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | PSU  | BA    | 2604 | 22    | 18,21,22     | 4.11 | 6 (33%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 1   | 2MG  | AA    | 966  | 1     | 18,26,27     | 2.49 | 7 (38%)  | 16,38,41    | 1.38 | 3 (18%)  |
| 22  | 6MZ  | BA    | 2030 | 22    | 18,25,26     | 2.75 | 5 (27%)  | 16,36,39    | 2.70 | 4 (25%)  |
| 1   | G7M  | AA    | 527  | 1     | 20,26,27     | 2.57 | 6 (30%)  | 17,39,42    | 1.11 | 1 (5%)   |
| 22  | OMC  | BA    | 2498 | 22,56 | 19,22,23     | 2.91 | 8 (42%)  | 26,31,34    | 1.17 | 2 (7%)   |
| 1   | MA6  | AA    | 1518 | 1     | 18,26,27     | 1.21 | 1 (5%)   | 19,38,41    | 3.42 | 2 (10%)  |
| 1   | PSU  | AA    | 516  | 1,56  | 18,21,22     | 4.35 | 7 (38%)  | 22,30,33    | 1.66 | 4 (18%)  |

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   |
|-----|------|-------|------|----------|---------|------------|---------|
| 1   | 5MC  | AA    | 967  | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | OMU  | BA    | 2552 | 22,56    | -       | 1/9/27/28  | 0/2/2/2 |
| 22  | G7M  | BA    | 2069 | 22,57    | -       | 2/3/25/26  | 0/3/3/3 |
| 12  | D2T  | AL    | 89   | 12       | -       | 1/7/12/14  | -       |
| 22  | OMG  | BA    | 2251 | 22,57,55 | -       | 3/5/27/28  | 0/3/3/3 |
| 22  | PSU  | BA    | 2580 | 22,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 2MA  | BA    | 2503 | 22,57,56 | -       | 2/3/25/26  | 0/3/3/3 |
| 55  | G7M  | B8    | 46   | 55       | -       | 0/3/25/26  | 0/3/3/3 |
| 1   | MA6  | AA    | 1519 | 1        | -       | 2/7/29/30  | 0/3/3/3 |
| 22  | 2MG  | BA    | 1835 | 22       | -       | 0/5/27/28  | 0/3/3/3 |
| 22  | PSU  | BA    | 1911 | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | PSU  | BA    | 955  | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | UR3  | AA    | 1498 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | B8    | 55   | 55       | -       | 2/7/25/26  | 0/2/2/2 |
| 34  | 4D4  | BM    | 81   | 34       | -       | 3/11/12/14 | -       |
| 22  | 5MU  | BA    | 747  | 22       | -       | 1/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | BA    | 1939 | 22,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 3TD  | BA    | 1915 | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MC  | BA    | 1962 | 22,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | MEQ  | BD    | 150  | 25       | -       | 3/8/9/11   | -       |
| 22  | PSU  | BA    | 2457 | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | AA    | 1402 | 1,56     | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | 2MG  | AA    | 1207 | 57,1     | -       | 0/5/27/28  | 0/3/3/3 |
| 22  | PSU  | BA    | 2605 | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 6MZ  | BA    | 1618 | 22       | -       | 0/5/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 22  | PSU  | BA    | 2504 | 22,57 | -       | 2/7/25/26 | 0/2/2/2 |
| 22  | 2MG  | BA    | 2445 | 22    | -       | 1/5/27/28 | 0/3/3/3 |
| 1   | 5MC  | AA    | 1407 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 22  | PSU  | BA    | 746  | 22,56 | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | 2MG  | AA    | 1516 | 1     | -       | 0/5/27/28 | 0/3/3/3 |
| 22  | PSU  | BA    | 1917 | 22    | -       | 0/7/25/26 | 0/2/2/2 |
| 22  | 1MG  | BA    | 745  | 22    | -       | 0/3/25/26 | 0/3/3/3 |
| 55  | 1MG  | B8    | 37   | 55    | -       | 0/3/25/26 | 0/3/3/3 |
| 22  | PSU  | BA    | 2604 | 22    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 2MG  | AA    | 966  | 1     | -       | 2/5/27/28 | 0/3/3/3 |
| 22  | 6MZ  | BA    | 2030 | 22    | -       | 2/5/27/28 | 0/3/3/3 |
| 1   | G7M  | AA    | 527  | 1     | -       | 2/3/25/26 | 0/3/3/3 |
| 22  | OMC  | BA    | 2498 | 22,56 | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | MA6  | AA    | 1518 | 1     | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | PSU  | AA    | 516  | 1,56  | -       | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 234 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | BA    | 1915 | 3TD  | C6-C5 | 11.97 | 1.49        | 1.35     |
| 22  | BA    | 746  | PSU  | C6-C5 | 11.78 | 1.49        | 1.35     |
| 22  | BA    | 2504 | PSU  | C6-C5 | 11.65 | 1.48        | 1.35     |
| 1   | AA    | 516  | PSU  | C6-C5 | 11.65 | 1.48        | 1.35     |
| 22  | BA    | 2580 | PSU  | C6-C5 | 11.49 | 1.48        | 1.35     |

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

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1   | AA    | 1519 | MA6  | N1-C6-N6 | -13.93 | 102.40      | 117.06   |
| 1   | AA    | 1518 | MA6  | N1-C6-N6 | -13.60 | 102.74      | 117.06   |
| 22  | BA    | 2030 | 6MZ  | C9-N6-C6 | -7.09  | 116.76      | 122.87   |
| 22  | BA    | 2503 | 2MA  | C2-N3-C4 | 6.00   | 120.39      | 115.52   |
| 1   | AA    | 1518 | MA6  | N3-C2-N1 | -5.56  | 119.99      | 128.68   |

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | AA    | 527 | G7M  | C3'-C4'-C5'-O5' |
| 1   | AA    | 966 | 2MG  | O4'-C4'-C5'-O5' |
| 1   | AA    | 966 | 2MG  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | AA    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 12  | AL    | 89   | D2T  | CG-CB-SB-CB1    |

There are no ring outliers.

11 monomers are involved in 15 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | BA    | 2552 | OMU  | 1       | 0            |
| 22  | BA    | 2251 | OMG  | 1       | 0            |
| 22  | BA    | 2503 | 2MA  | 1       | 0            |
| 55  | B8    | 46   | G7M  | 3       | 0            |
| 55  | B8    | 55   | PSU  | 1       | 0            |
| 22  | BA    | 1915 | 3TD  | 1       | 0            |
| 25  | BD    | 150  | MEQ  | 1       | 0            |
| 22  | BA    | 2504 | PSU  | 1       | 0            |
| 22  | BA    | 746  | PSU  | 1       | 0            |
| 55  | B8    | 37   | 1MG  | 2       | 0            |
| 22  | BA    | 2030 | 6MZ  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 477 ligands modelled in this entry, 476 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 | $\# Z  > 2$ |
| 59  | TRP  | BA    | 3001 | -    | 14,16,16     | 0.98 | 0           | 16,22,22    | 0.97 | 0           |

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   |
|-----|------|-------|------|------|---------|----------|---------|
| 59  | TRP  | BA    | 3001 | -    | -       | 0/7/8/8  | 0/2/2/2 |

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 22  | BA    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | BA    | 885:C     | O3'    | 892:A     | P      | 13.28        |