



wwPDB EM Validation Summary Report ⓘ

Sep 18, 2021 – 09:48 am BST

PDB ID : 7O1C
EMDB ID : EMD-12695
Title : Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome-RF2 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 : 2.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

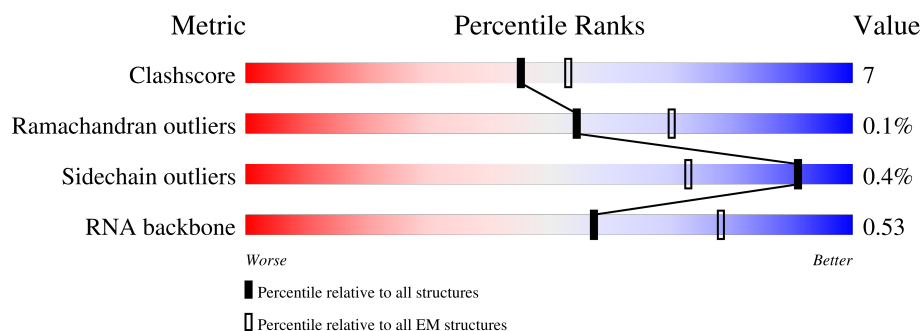
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	1534	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	









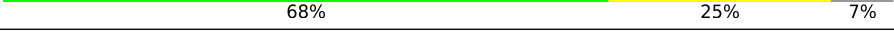
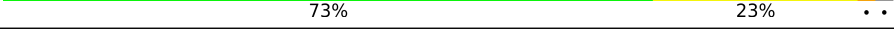
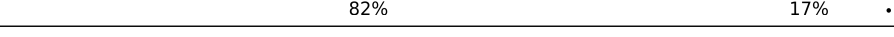

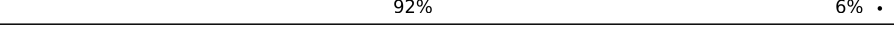
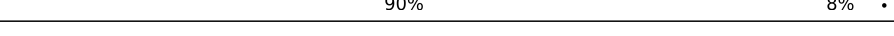
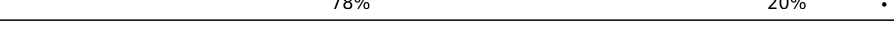


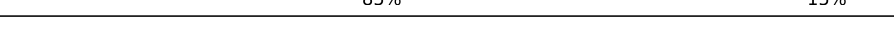
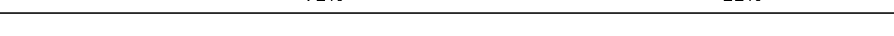

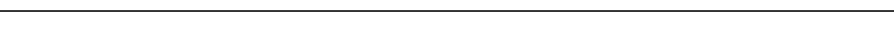

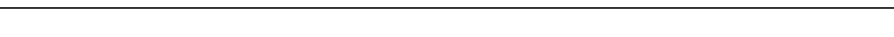
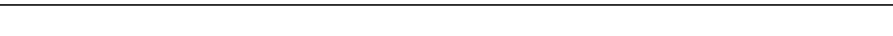
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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	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	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	B5	17	
54	B7	10	
55	B8	77	
56	B9	365	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148175 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-(R23F) - Tryptophanase leader peptide.

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	10	Total	C	N	O	P	0	0
			211	94	36	71	10		

- 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
			1646	733	295	541	77		

- Molecule 56 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B9	348	Total	C	N	O	S	0	0
			2768	1705	482	571	10		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	87	Total	Mg	0
			87	87	
57	BA	243	Total	Mg	0
			243	243	
57	BB	1	Total	Mg	0
			1	1	
57	BC	1	Total	Mg	0
			1	1	
57	BD	2	Total	Mg	0
			2	2	
57	BL	3	Total	Mg	0
			3	3	
57	B8	2	Total	Mg	0
			2	2	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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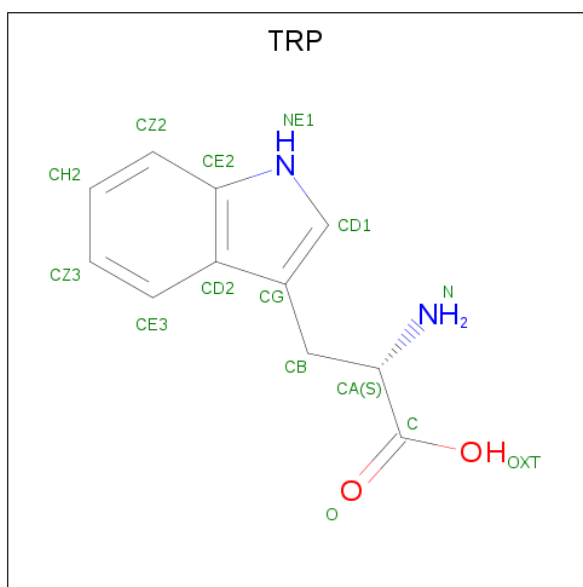
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Mol	Chain	Residues	Atoms		AltConf
58	BM	1	Total	K	0
			1	1	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 60 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	AA	167	Total	O	0
			167	167	
61	AK	1	Total	O	0
			1	1	

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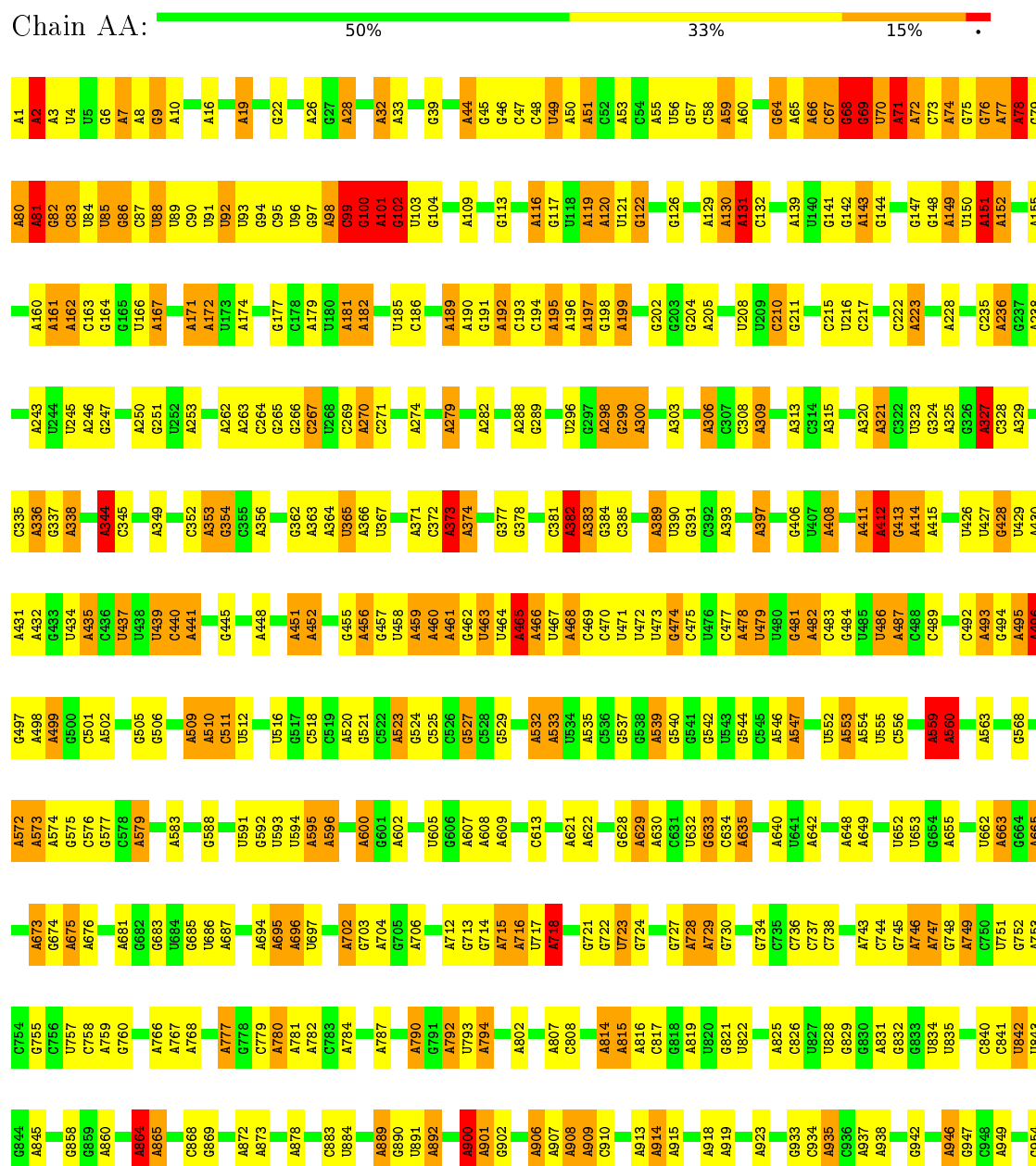
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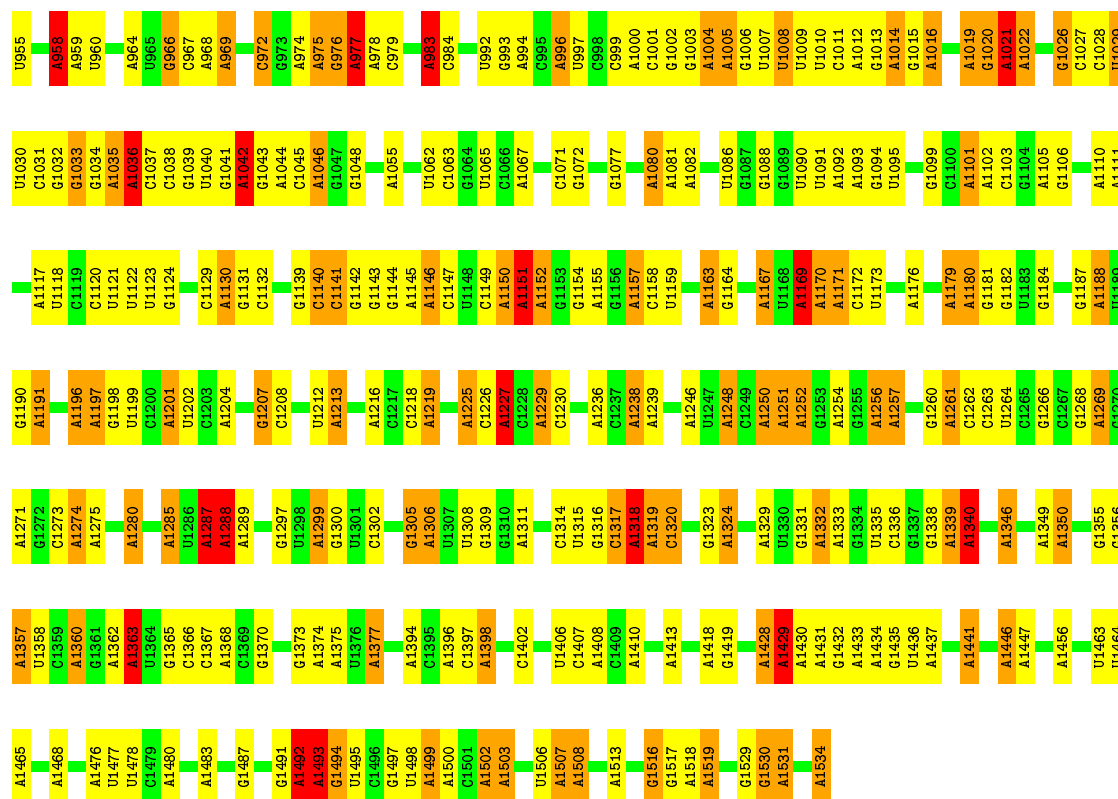
Mol	Chain	Residues	Atoms		AltConf
61	AM	1	Total 1	O 1	0
61	AN	3	Total 3	O 3	0
61	BA	617	Total 617	O 617	0
61	BC	6	Total 6	O 6	0
61	BD	2	Total 2	O 2	0
61	BN	3	Total 3	O 3	0

3 Residue-property plots

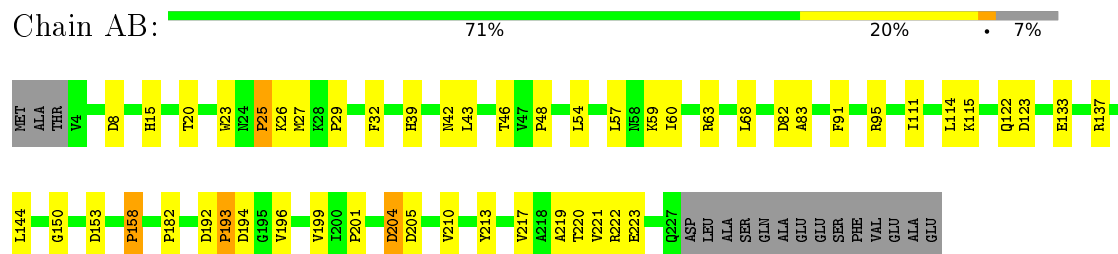
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

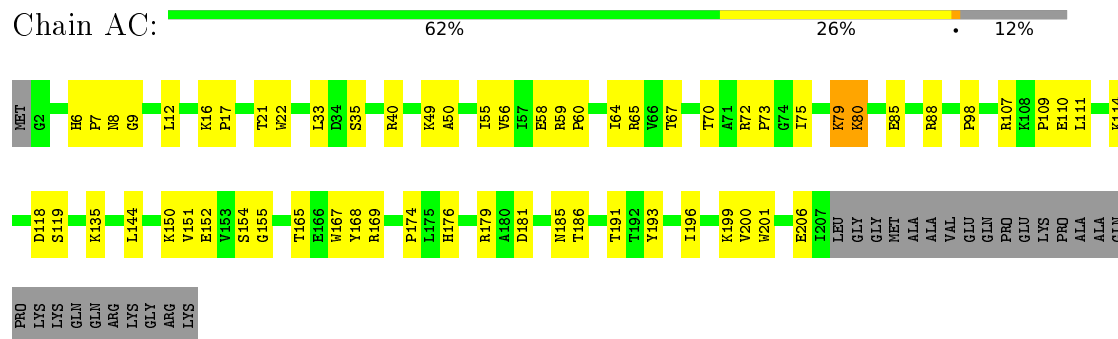




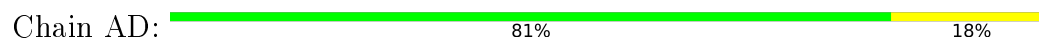
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



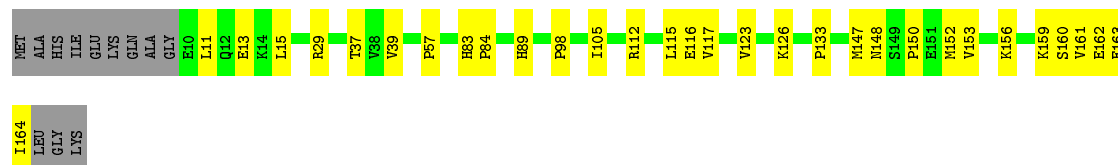
• Molecule 4: 30S ribosomal protein S4





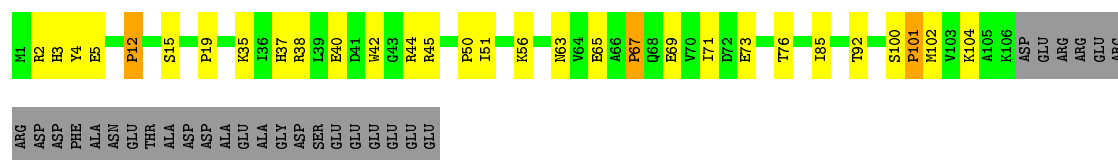
- Molecule 5: 30S ribosomal protein S5

Chain AE: 74% 19% 7%



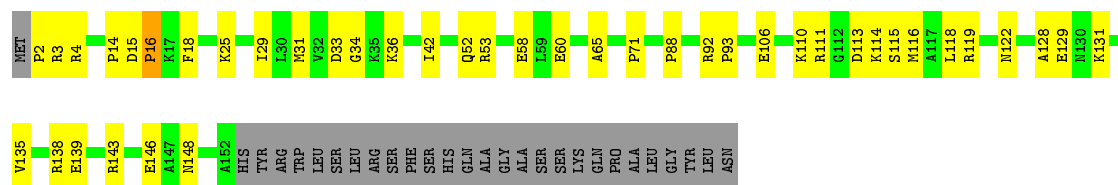
- Molecule 6: 30S ribosomal protein S6

Chain AF: 56% 20% 21%



- Molecule 7: 30S ribosomal protein S7

Chain AG: 61% 23% 16%



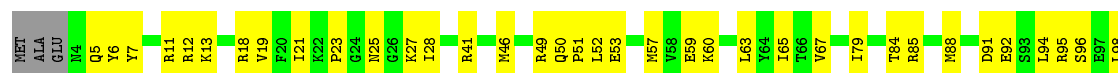
- Molecule 8: 30S ribosomal protein S8

Chain AH: 75% 23% ..



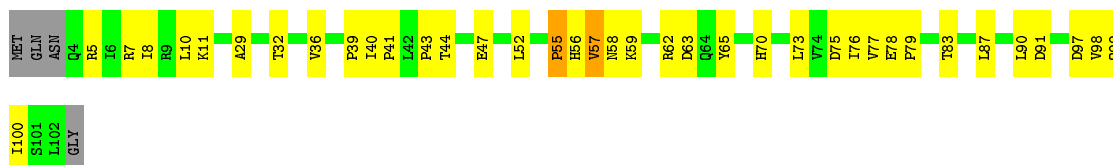
- Molecule 9: 30S ribosomal protein S9

Chain AI: 62% 35% ..

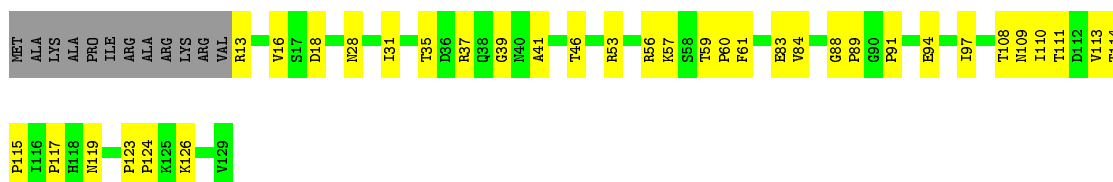




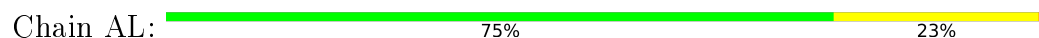
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

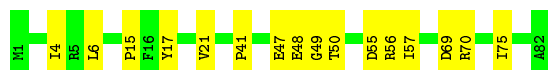
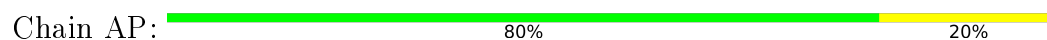


- Molecule 15: 30S ribosomal protein S15

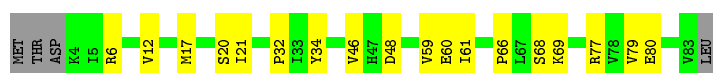
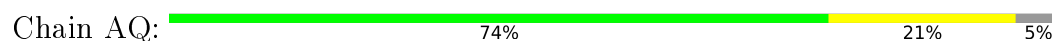




- Molecule 16: 30S ribosomal protein S16



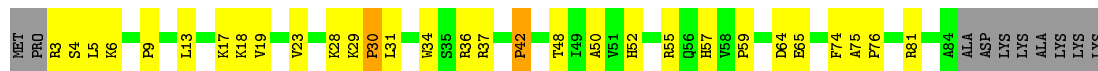
- Molecule 17: 30S ribosomal protein S17



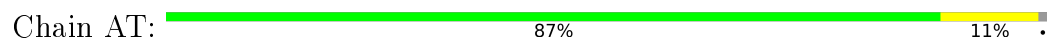
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

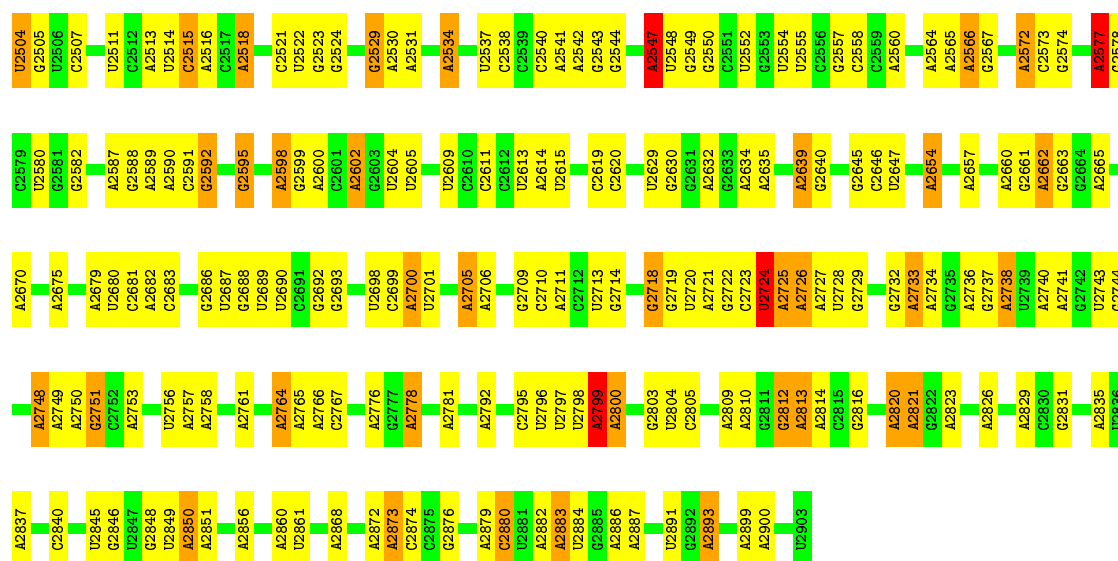


- Molecule 22: Ribosomal RNA 23S



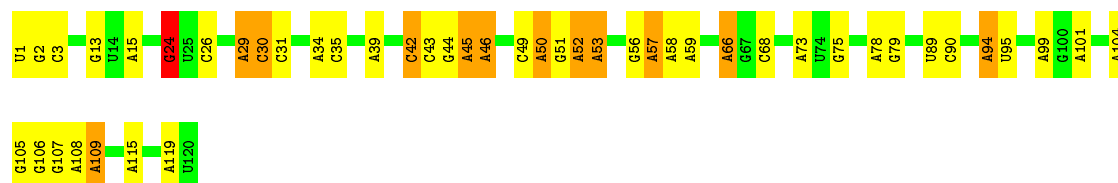
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A1175	C1092	A1020	A849	C786	A689	G533	U448	U365	G273	U193	A95	G2
G1177	U1093	G942	U850	G770	G690	U534	A449	A368	C274	G194	A101	U3
C1178	U1094	A1021	C851	G771	C691	C691	A453	A371	C275	A195	U102	U4
A1179	A1095	G1022	G856	G775	C692	A538	A454	G372	U276	A196	A103	A5
U1180	A1096	G1025	G857	G776	A693	A541	A457	U373	A277	A197	A104	A6
U1181	C946	G1026	G858	G777	U615	U546	G458	A374	A278	C198	A111	A10
G1182	C947	G1027	G859	G780	A616	U546	U459	C378	U279	U200	A112	C11
U1183	A948	A1028	U860	A781	A621	U546	U460	A379	C281	U201	G117	U12
U1184	C1102	A1029	A861	A782	U626	U547	A460	C378	A282	U202	A118	A13
G1185	A1103	G952	G862	G783	A627	G548	A466	A382	A283	A203	A119	A14
U1186	U955	U955	A863	G784	A627	G549	A466	C383	A284	A204	U120	G15
G1187	U955	U955	A863	A705	A627	C550	A466	C383	G285	G205	A125	U18
U1188	A959	A960	A866	A706	A631	G551	A466	A384	U286	U206	A126	A19
A1189	A960	A960	A866	A706	A631	U552	A470	A385	G287	C208	A127	C20
G1190	G961	C961	U871	A788	A632	U553	A471	G386	A294	A209	A131	C22
U1191	C962	A1039	U872	A789	A633	U554	A472	A391	A299	G213	A132	G23
A1194	G962	A1040	U873	A790	C634	U555	A472	A391	A300	G214	A133	G24
G1197	U963	U963	C876	C791	C635	G555	A477	A400	G301	G215	A134	C27
U1201	C964	C964	A877	A792	G636	U556	A478	A401	G302	A216	U138	A28
G1202	G966	G966	A878	A793	U639	U557	A479	A402	C303	A217	U139	G27
U1203	U967	U967	A878	A794	U639	A563	A480	A403	G303	A218	G140	A28
A1204	C968	C968	G881	G799	C640	C564	A481	U403	A309	A219	A141	A38
G1205	G971	G971	G882	A800	A643	C565	A482	U404	A310	G220	A142	A42
A1206	A972	A972	G883	G801	A644	U567	A483	U405	A311	A221	C143	G43
G1207	C973	C973	U884	U802	A645	U568	A484	U406	A312	A222	A144	A44
U1208	A974	A974	C885	U803	U646	U569	A485	U407	A320	A223	A145	G45
A1209	G974	G974	U886	U804	U647	U570	A486	A408	A321	U224	A146	G46
G1210	A975	A975	C887	C805	U648	U571	A487	A409	A322	C225	A149	A49
U1211	G976	G976	U888	C806	U649	U572	A488	A410	A323	A226	A152	U50
A1212	U977	U977	G889	U807	U650	A573	A489	A411	A330	A227	A153	G51
G1213	C977	C977	G890	U808	U651	A574	A490	A412	A331	A231	A154	A52
A1214	A978	A978	U891	G809	A654	A575	A491	C413	A332	G232	A155	A53
G1215	C978	C978	U892	U810	A655	U576	A492	C414	A340	A233	A156	A56
U1216	A979	A979	G893	U811	U656	U577	A493	U415	A341	C239	A160	A61
A1217	C979	C979	U894	C812	U657	G578	A494	U416	A342	C240	U162	C61
G1218	G980	G980	A900	G813	U658	A582	A495	C417	A343	A241	C163	U62
U1219	A981	A981	A901	U814	A661	A583	A496	C418	A344	A242	A164	A63
A1220	C981	C981	U902	A815	A662	C584	A497	A421	A345	A243	A165	A64
G1221	U982	U982	G903	U816	A663	C585	A498	A422	A346	A244	U166	A65
U1222	A983	A983	U904	U817	A664	C586	A499	A423	A347	G247	A167	A66
A1223	C982	C982	U905	U818	A665	C587	A500	A424	A348	C248	A172	A71
G1224	G983	G983	A906	U819	A666	C588	A501	A425	A349	G249	A173	U72
U1225	A984	A984	U906	U820	A667	C589	A502	A426	A350	C250	A174	A73
A1226	C984	C984	U907	U821	A668	C590	A503	A427	A351	A251	A175	A74
G1227	U985	U985	G908	U822	A669	C591	A504	A428	A352	A252	A176	G75
U1228	A986	A986	U909	U823	A670	C592	A505	A429	A353	A253	A177	A83
A1229	C985	C985	U910	U824	A671	C593	A506	A430	A354	A254	A181	A84
G1230	G986	G986	A911	A825	A672	C594	A507	A431	A355	A255	A182	G85
U1231	U987	U987	U911	U826	A673	C595	A508	A432	A356	A256	C183	A89
A1232	C986	C986	U912	U827	A674	C596	A509	A433	A357	A257	A190	U90
G1233	A987	A987	U913	U828	A675	C597	A510	A434	A358	A258	A191	A91
U1234	U988	U988	U914	U829	A676	C598	A511	A435	A359	A259	G189	G189
A1235	C987	C987	U915	U830	A677	C599	A512	A436	A360	A260	A190	A91
G1236	G988	G988	A916	U831	A678	C600	A513	A437	A361	A261	A191	A91
U1237	U989	U989	U916	U832	A679	C601	A514	A438	A362	A262	A192	A91
A1238	A989	A989	U917	U833	A680	C602	A515	A439	A363	A263	A193	A91
G1239	C988	C988	U918	U834	A681	C603	A516	A440	A364	A264	A194	A91
U1240	U990	U990	U919	U835	A682	C604	A517	A441	A365	A265	A195	A91
A1241	A991	A991	U920	U836	A683	C605	A518	A442	A366	A266	A196	A91
G1242	G989	G989	A921	U837	A684	C606	A519	A443	A367	A267	A197	A91
U1243	U991	U991	U921	U838	A685	C607	A520	A444	A368	A268	A198	A91
A1244	C989	C989	U922	U839	A686	C608	A521	A445	A369	A269	A199	A91
G1245	A992	A992	U923	U840	A687	C609	A522	A446	A370	A270	A199	A91
U1246	U993	U993	U924	U841	A688	C610	A523	A447	A371	A271	A199	A91
A1247	C990	C990	U925	U842	A689	C611	A524	A448	A372	A272	A199	A91
G1248	G991	G991	A926	U843	A690	C612	A525	A449	A373	A273	A199	A91
U1249	U992	U992	U926	U844	A691	C613	A526	A450	A374	A274	A199	A91
A1250	A993	A993	U927	U845	A692	C614	A527	A451	A375	A275	A199	A91
G1251	C991	C991	U928	U846	A693	C615	A528	A452	A376	A276	A199	A91
U1252	U994	U994	U929	U847	A694	C616	A529	A453	A377	A277	A199	A91
A1253	A995	A995	U930	U848	A695	C617	A530	A454	A378	A278	A199	A91
G1254	C992	C992	U931	U849	A696	C618	A531	A455	A379	A279	A199	A91
U1255	U995	U995	U932	U850	A697	C619	A532	A456	A380	A280	A199	A91
A1256	A996	A996	U933	U851	A698	C620	A533	A457	A381	A281	A199	A91
G1257	C993	C993	U934	U852	A699	C621	A534	A458	A382	A282	A199	A91
U1258	U996	U996	U935	U853	A700	C622	A535	A459	A383	A283	A199	A91
A1259	A997	A997	U936	U854	A701	C623	A536	A460	A384	A284	A199	A91
G1260	C994	C994	U937	U855	A702	C624	A537	A461	A385	A285	A199	A91
U1261	U997	U997	U938	U856	A703	C625	A538	A462	A386	A286	A199	A91
A1262	A998	A998	U939	U857	A704	C626	A539	A463	A387	A287	A199	A91
G1263	C995	C995	U940	U858	A705	C627	A540	A464	A388	A288	A199	A91
U1264	U998	U998	U941	U859	A706	C628	A541	A465	A389	A289	A199	A91
A1265	A999	A999	U942	U860	A707	C629	A542	A466	A390	A290	A199	A91
G1266	C996	C996	U943	U861	A708	C630	A543	A467	A391	A291	A199	A91
U1267	U999	U999	U944	U862	A709	C631	A544	A468	A392	A292	A199	A91
A1268	A1000	A1000	U945	U863	A710	C632	A545	A469	A393	A293	A199	A91
G1269	C1001	C1001	U946	U864	A711	C633	A546	A470	A394	A294	A199	A91
U1270	U1001	U1001	U947	U865	A712	C634	A547	A471	A395	A295	A199	A91
A1271	A1002	A1002	U948	U866	A713	C635	A548	A472	A396	A296	A199	A91
G1272	C1002	C1002	U949	U867	A714	C636	A549	A473	A397	A297	A199	A91
U1273	U1003	U1003	U950	U868	A715	C637	A550	A474	A398	A298	A199	A91
A1274	A1004	A1004	U951	U869	A716	C638	A551	A475	A399	A299	A199	A91
G1275	C1003	C1003	U952	U870	A717	C639	A552	A476	A400	A300	A199	A91
U1276	U1005	U1005	U953	U871	A718	C640	A553	A477	A401	A301	A199	A91
A1277	A1006	A1006	U954	U872	A719	C641	A554	A478	A402	A302	A199	A91
G1278	C1004	C1004	U955	U873	A720	C642	A555	A479	A403	A303	A199	A91
U1279	U1007	U1007	U956	U874	A721	C643	A556	A480	A404	A304	A199	A91
A1280	A1008	A1008	U957	U875	A722	C644	A557	A481	A405	A305	A199	A91
G1281	C1005	C1005	U958	U876	A723	C645	A558	A482	A406	A306	A199	A91
U1282	U1009	U1009	U959	U877	A724	C646	A559	A483	A407	A307	A199	A91
A1283	A1010	A1010	U960	U878	A725	C647	A560	A484	A408	A308	A199	A91
G1284	C1006	C1006	U961	U879	A726	C648	A561	A485	A409	A309	A199	A91
U1285	U1011	U1011	U962	U880	A727	C649	A562	A486	A410	A310	A199	A91
A1286	A1012	A1012	U963	U881	A728	C650	A563	A487	A411	A311	A199	A91
G1287	C1007	C1007	U964	U882	A729	C651	A564	A488	A412	A312	A199	A91
U1288	U1013	U1013	U965	U883	A730	C652	A565	A489	A413	A313	A199	A91
A1289	A1014	A1014	U966	U884	A731	C653	A566	A490	A414	A314	A199	A91
G1290	C1008	C1008	U967	U885	A732	C654	A567	A491	A415	A315	A199	A91
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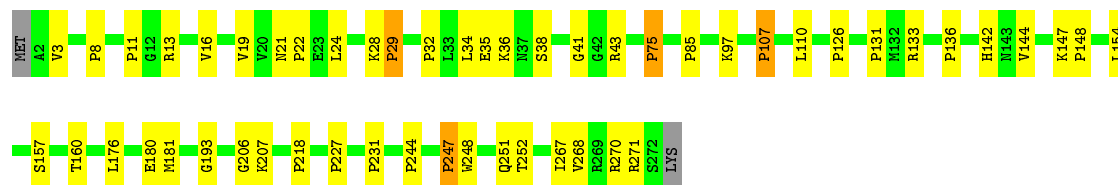
• Molecule 23: Ribosomal RNA 5S

Chain BB: 61% 28% 10% .



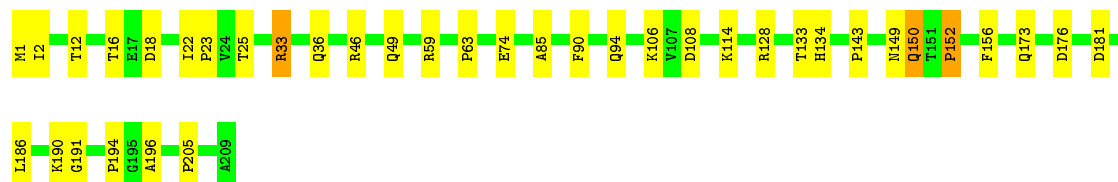
• Molecule 24: 50S ribosomal protein L2

Chain BC: 80% 18% ..



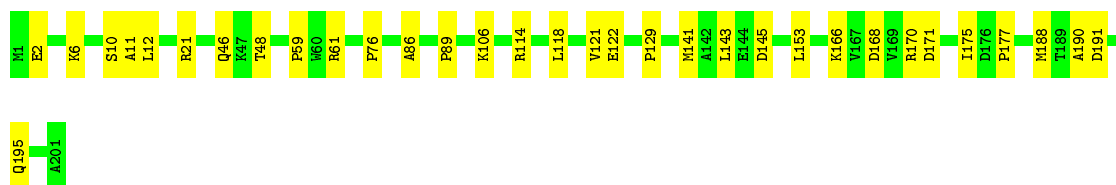
• Molecule 25: 50S ribosomal protein L3

Chain BD: 82% 17% .



• Molecule 26: 50S ribosomal protein L4

Chain BE: 84% 16%



- Molecule 27: 50S ribosomal protein L5

Chain BF: 72% 27% ..



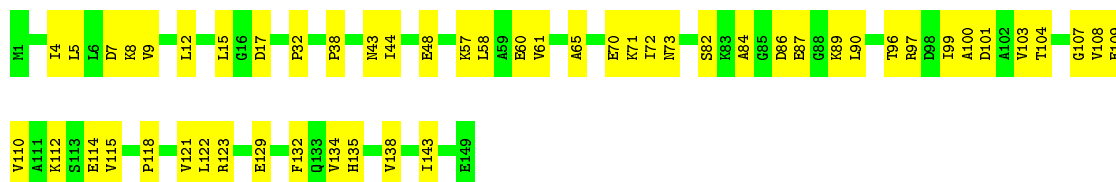
- Molecule 28: 50S ribosomal protein L6

Chain BG: 82% 16% ..



- Molecule 29: 50S ribosomal protein L9

Chain BH: 65% 35%



- Molecule 30: 50S ribosomal protein L31

Chain BI: 53% 40% 6%




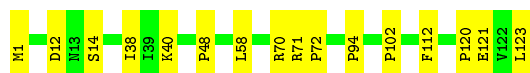
- Molecule 31: 50S ribosomal protein L13

Chain BJ: 84% 15%




- Molecule 32: 50S ribosomal protein L14

Chain BK:  87% 13%




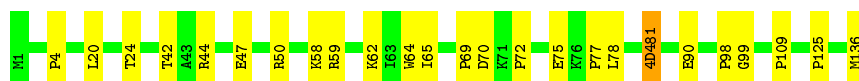
- Molecule 33: 50S ribosomal protein L15

Chain BL:  84% 15%



- Molecule 34: 50S ribosomal protein L16

Chain BM:  82% 18%



- Molecule 35: 50S ribosomal protein L17

Chain BN:  83% 9% 7%




- Molecule 36: 50S ribosomal protein L18

Chain BO:  89% 10%



- Molecule 37: 50S ribosomal protein L19

Chain BP:  83% 17%




- Molecule 38: 50S ribosomal protein L20

Chain BQ:  91% 8%




- Molecule 39: 50S ribosomal protein L21

Chain BR:  87% 13%



- Molecule 40: 50S ribosomal protein L22

Chain BS:  81% 19%



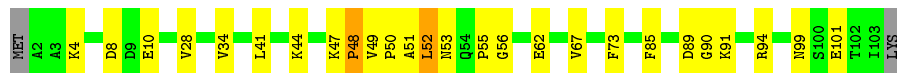
- Molecule 41: 50S ribosomal protein L23

Chain BT:  68% 25% 7%




- Molecule 42: 50S ribosomal protein L24

Chain BU:  73% 23% ..




- Molecule 43: 50S ribosomal protein L25

Chain BV:  82% 17% .



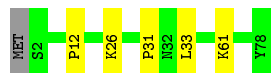
- Molecule 44: 50S ribosomal protein L27

Chain BW:  73% 16% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX:  92% 6% .




- Molecule 46: 50S ribosomal protein L29

Chain BY:  90% 8% .




- Molecule 47: 50S ribosomal protein L30

Chain BZ:  78% 20% .



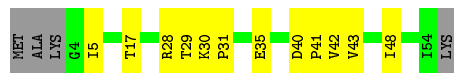
- Molecule 48: 50S ribosomal protein L32

Chain B0:  81% 18% .




- Molecule 49: 50S ribosomal protein L33

Chain B1:  71% 22% 7%



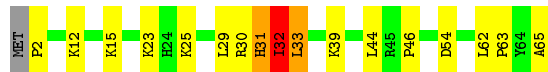
- Molecule 50: 50S ribosomal protein L34

Chain B2:  85% 15%




- Molecule 51: 50S ribosomal protein L35

Chain B3:  72% 22% . . .



- Molecule 52: 50S ribosomal protein L36

Chain B4:  87% 13%



- Molecule 53: TnaC-(R23F) - Tryptophanase leader peptide

Chain B5:  59% 35% 6%

V8
T9
S10
K11
F12
F13
H14
I15
P24

- Molecule 54: mRNA

Chain B7:  30% 60% 10%

C1
G2
C3
C4
G8
A9
U10

- Molecule 55: P-site tRNA-Pro

Chain B8:  42% 39% 18%

C1
G2
G3
U4
G5
A6
A14
C17
U17A
G18
G19
U20
A21
C23
G24
C25
A26
C30
G31
U32
U33
C34
A38
A41
E32
A42
G46
U47
A51
G52
C56
G57
A58
A59
C62
U63
C64
U65
A66
U67
C68
A69
C70
C71
G72
A73
C74
C75
A76

- Molecule 56: Peptide chain release factor RF2

Chain B9:  61% 33% 5%

MET
PHE
GLU
ILE
ASN
P6
V7
M8
N9
R10
I11
Q12
L84
D13
L14
T15
E16
R17
S18
D19
V20
L21
R22
L25
D26
Y27
D28
A29
K30
K31
E32
R33
L34
E40
L41
E42
Q43
P44
E49
P50
E51
R52
A53
Q54
A55
L56
E59
R60
S61
S62
L63
E64
A65
R66
V67
D68
T69
L70
M73
K74
L77
E78
D79
V80
L83
E84
E85
L86
A87
V88
E89
A90
D91
D92
E93
E94
T95
F96
N97
E98
A99
L103
D104
E107
E108
K109
L110
A111
R116
R117
M118
G121
E122
Y123
D124
Y129
E140
W144
W155
E170
I176
Y187
E195
R200
L201
P206
P224
E225
T230
P236
A237
D238
V243
Y244
G248
ALA
GLY
GLY
GLN
HIS
VAL
ASN
ARG
THR
E258
V261
R262
H265
I266
P267
T268
G269
I270
D277
Q280
H281
K282
N283
K284
A287
M288
K289
Q290
M291
K294
E299
K302
K303
S315
Q322
I323
R324
D330
S331
R332
I333
T338
G339
T342
R343
N344
T345
L349
L353
I357
E358
K362
ALA
GLY
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40, 44	Depositor
Minimum defocus (nm)	-1000, -400	Depositor
Maximum defocus (nm)	-2000, -1600	Depositor
Magnification	55127, 59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), 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: OMU, 3TD, 5MU, OMC, MA6, UR3, PSU, 1MG, OMG, 2MG, 5MC, 2MA, G7M, D2T, MEQ, MG, 4OC, ZN, 6MZ, 4D4, 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	1.65	964/36593 (2.6%)	3.44	4347/57081 (7.6%)
2	AB	0.82	7/1784 (0.4%)	0.56	1/2403 (0.0%)
3	AC	0.86	7/1651 (0.4%)	0.62	2/2225 (0.1%)
4	AD	0.81	6/1665 (0.4%)	0.51	0/2227
5	AE	0.90	5/1157 (0.4%)	0.60	0/1557
6	AF	1.01	5/881 (0.6%)	0.56	0/1189
7	AG	0.96	7/1195 (0.6%)	0.54	0/1602
8	AH	0.94	5/989 (0.5%)	0.62	1/1326 (0.1%)
9	AI	0.76	3/1034 (0.3%)	0.56	0/1375
10	AJ	1.05	6/805 (0.7%)	0.59	0/1089
11	AK	1.11	7/893 (0.8%)	0.62	0/1205
12	AL	1.18	8/960 (0.8%)	0.65	0/1286
13	AM	0.93	5/892 (0.6%)	0.58	0/1193
14	AN	0.89	4/811 (0.5%)	0.55	0/1081
15	AO	0.44	0/722	0.48	0/964
16	AP	0.76	2/659 (0.3%)	0.60	0/884
17	AQ	0.83	2/657 (0.3%)	0.55	0/881
18	AR	0.97	2/462 (0.4%)	0.58	0/621
19	AS	1.09	5/672 (0.7%)	0.65	0/904
20	AT	0.60	1/676 (0.1%)	0.46	0/895
21	AU	1.09	4/472 (0.8%)	0.53	0/627
22	BA	2.12	2046/69120 (3.0%)	3.57	8225/107824 (7.6%)
23	BB	1.74	59/2872 (2.1%)	3.03	258/4478 (5.8%)
24	BC	1.29	23/2121 (1.1%)	0.68	0/2852
25	BD	1.05	11/1576 (0.7%)	0.64	0/2119
26	BE	0.91	6/1571 (0.4%)	0.60	0/2113
27	BF	0.89	6/1434 (0.4%)	0.56	0/1926
28	BG	1.03	8/1343 (0.6%)	0.60	0/1816
29	BH	0.73	3/1121 (0.3%)	0.54	0/1515
30	BI	0.82	2/531 (0.4%)	0.55	0/709
31	BJ	1.09	7/1152 (0.6%)	0.62	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	1.08	5/955 (0.5%)	0.68	0/1279
33	BL	0.95	5/1062 (0.5%)	0.67	0/1413
34	BM	1.16	8/1081 (0.7%)	0.66	0/1443
35	BN	1.07	5/958 (0.5%)	0.68	0/1281
36	BO	0.81	2/910 (0.2%)	0.57	1/1219 (0.1%)
37	BP	0.99	3/929 (0.3%)	0.62	0/1242
38	BQ	0.93	0/960	0.58	0/1278
39	BR	0.91	2/829 (0.2%)	0.64	0/1107
40	BS	0.84	3/864 (0.3%)	0.60	0/1156
41	BT	0.79	1/744 (0.1%)	0.63	0/994
42	BU	0.96	3/787 (0.4%)	0.68	1/1051 (0.1%)
43	BV	1.06	4/766 (0.5%)	0.61	0/1025
44	BW	0.91	1/587 (0.2%)	0.63	0/776
45	BX	0.96	3/635 (0.5%)	0.66	1/848 (0.1%)
46	BY	0.55	0/502	0.56	0/667
47	BZ	0.97	2/453 (0.4%)	0.64	0/605
48	B0	0.89	2/450 (0.4%)	0.61	0/599
49	B1	1.09	2/421 (0.5%)	0.64	0/561
50	B2	0.97	1/380 (0.3%)	0.64	0/498
51	B3	1.21	4/513 (0.8%)	0.82	1/676 (0.1%)
52	B4	1.02	1/303 (0.3%)	0.67	0/397
53	B5	1.33	2/151 (1.3%)	0.81	0/205
54	B7	1.47	3/233 (1.3%)	2.72	14/358 (3.9%)
55	B8	1.87	57/1839 (3.1%)	2.96	169/2866 (5.9%)
56	B9	0.73	8/2806 (0.3%)	0.55	0/3778
All	All	1.72	3353/158589 (2.1%)	3.01	13021/236840 (5.5%)

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
5	AE	0	1
51	B3	0	1
All	All	0	2

The worst 5 of 3353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-22.33	1.28	1.53
22	BA	2449	U	C5-C6	18.12	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	O4'-C1'	16.77	1.63	1.41
55	B8	59	A	C6-N6	16.71	1.47	1.33
55	B8	58	A	C6-N6	16.69	1.47	1.33

The worst 5 of 13021 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	752	A	N1-C6-N6	-27.47	102.12	118.60
22	BA	2872	A	N1-C6-N6	-24.44	103.94	118.60
22	BA	1668	A	N1-C6-N6	-24.16	104.11	118.60
22	BA	2062	A	N1-C2-N3	-23.43	117.58	129.30
22	BA	1668	A	N1-C2-N3	-23.24	117.68	129.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16583	454	0
2	AB	1753	0	1780	34	0
3	AC	1624	0	1696	33	0
4	AD	1643	0	1707	20	0
5	AE	1144	0	1185	18	0
6	AF	862	0	864	21	0
7	AG	1181	0	1238	28	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	39	0
10	AJ	795	0	836	25	0
11	AK	877	0	887	19	0
12	AL	957	0	1017	19	0
13	AM	883	0	941	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	799	0	841	23	0
15	AO	714	0	734	2	0
16	AP	649	0	666	9	0
17	AQ	648	0	691	10	0
18	AR	455	0	478	10	0
19	AS	656	0	680	24	0
20	AT	670	0	719	7	0
21	AU	465	0	491	11	0
22	BA	62209	0	31287	446	0
23	BB	2569	0	1301	19	0
24	BC	2082	0	2154	26	0
25	BD	1566	0	1618	18	0
26	BE	1552	0	1619	18	0
27	BF	1410	0	1444	38	0
28	BG	1323	0	1371	14	0
29	BH	1110	0	1148	31	0
30	BI	522	0	520	23	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	8	0
33	BL	1053	0	1128	15	0
34	BM	1075	0	1155	13	0
35	BN	945	0	989	7	0
36	BO	900	0	935	7	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	11	0
39	BR	816	0	839	7	0
40	BS	857	0	922	12	0
41	BT	738	0	807	17	0
42	BU	779	0	831	18	0
43	BV	753	0	780	10	0
44	BW	580	0	594	11	0
45	BX	625	0	652	2	0
46	BY	501	0	531	4	0
47	BZ	449	0	488	8	0
48	B0	444	0	458	7	0
49	B1	414	0	442	6	0
50	B2	377	0	418	3	0
51	B3	504	0	572	16	0
52	B4	302	0	340	3	0
53	B5	146	0	139	5	0
54	B7	211	0	110	5	0
55	B8	1646	0	831	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B9	2768	0	2666	86	0
57	AA	87	0	0	0	0
57	B8	2	0	0	0	0
57	BA	243	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	2	0	0	0	0
57	BL	3	0	0	0	0
58	AA	38	0	0	0	0
58	AM	1	0	0	0	0
58	BA	104	0	0	0	0
58	BB	1	0	0	0	0
58	BC	1	0	0	0	0
58	BD	1	0	0	0	0
58	BM	1	0	0	0	0
59	AB	1	0	0	0	0
59	B4	1	0	0	0	0
59	BI	1	0	0	0	0
60	BA	15	0	9	0	0
61	AA	167	0	0	0	0
61	AK	1	0	0	0	0
61	AM	1	0	0	0	0
61	AN	3	0	0	0	0
61	BA	617	0	0	3	0
61	BC	6	0	0	0	0
61	BD	2	0	0	0	0
61	BN	3	0	0	0	0
All	All	148175	0	99399	1626	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 7.

The worst 5 of 1626 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)
55:B8:1:C:H5'	56:B9:282:LYS:NZ	1.70	1.05
22:BA:2185:U:C4	22:BA:2186:G:O6	2.13	1.00
1:AA:1088:G:N2	1:AA:1167:A:H61	1.59	1.00
1:AA:1026:G:C6	1:AA:1035:A:N6	2.32	0.98
22:BA:884:U:O4	22:BA:892:A:C5	2.21	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	AD	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	AE	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	AF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	AG	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	7	13
11	AK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	AL	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
13	AM	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
14	AN	99/102 (97%)	84 (85%)	15 (15%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
35	BN	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	BO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	BP	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	15	32
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%)	69 (92%)	6 (8%)	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%)	52 (96%)	2 (4%)	0	100	100
49	B1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	6
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
56	B9	344/365 (94%)	325 (94%)	19 (6%)	0	100	100
All	All	5934/6296 (94%)	5626 (95%)	302 (5%)	6 (0%)	54	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN

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	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	168 (99%)	2 (1%)	71	87
4	AD	172/173 (99%)	171 (99%)	1 (1%)	86	95
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	76	90
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	89 (99%)	1 (1%)	73	88
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	78 (99%)	1 (1%)	69	86
15	AO	76/77 (99%)	75 (99%)	1 (1%)	69	86
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	47 (98%)	1 (2%)	53	77
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	85
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	161 (99%)	2 (1%)	71	87
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	91
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	86 (99%)	1 (1%)	73	88
37	BP	99/100 (99%)	98 (99%)	1 (1%)	76	90
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	37 (97%)	1 (3%)	46	72
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19	39
56	B9	298/311 (96%)	296 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4948/5155 (96%)	4930 (100%)	18 (0%)	91 97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	B2	41	ARG
56	B9	116	ARG
56	B9	33	ARG
19	AS	81	ARG
37	BP	37	LYS

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

Mol	Chain	Res	Type
56	B9	281	HIS
41	BT	48	GLN
11	AK	119	ASN
8	AH	118	GLN
26	BE	97	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	241 (15%)	8 (0%)
22	BA	2890/2897 (99%)	438 (15%)	24 (0%)
23	BB	119/120 (99%)	15 (12%)	1 (0%)
54	B7	8/10 (80%)	2 (25%)	0
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4623/4638 (99%)	708 (15%)	35 (0%)

5 of 708 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	19	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2474	U
22	BA	2518	A
23	BB	66	A
22	BA	685	A
22	BA	276	U

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

37 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
25	MEQ	BD	150	25	8,9,10	1.43	2 (25%)	5,10,12	1.50	1 (20%)
22	PSU	BA	2605	22	17,21,22	2.93	9 (52%)	20,30,33	3.03	5 (25%)
22	OMC	BA	2498	57,22	15,22,23	2.61	5 (33%)	17,31,34	1.12	1 (5%)
22	PSU	BA	2580	22	17,21,22	2.92	8 (47%)	20,30,33	3.08	9 (45%)
22	1MG	BA	745	22	18,26,27	3.39	6 (33%)	19,39,42	1.54	4 (21%)
1	5MC	AA	967	1	15,22,23	2.83	5 (33%)	19,32,35	1.39	4 (21%)
1	MA6	AA	1519	1	19,26,27	1.38	3 (15%)	18,38,41	3.80	2 (11%)
1	5MC	AA	1407	1	15,22,23	2.54	5 (33%)	19,32,35	1.32	3 (15%)
22	2MG	BA	2445	22	19,26,27	3.37	8 (42%)	21,38,41	3.16	6 (28%)
22	PSU	BA	746	57,22	17,21,22	3.34	9 (52%)	20,30,33	3.27	7 (35%)
22	PSU	BA	955	22	17,21,22	2.93	9 (52%)	20,30,33	2.68	5 (25%)
22	6MZ	BA	1618	22	18,25,26	2.84	5 (27%)	16,36,39	2.95	4 (25%)
22	6MZ	BA	2030	22	18,25,26	2.87	6 (33%)	16,36,39	2.91	4 (25%)
22	PSU	BA	1911	22	17,21,22	3.23	8 (47%)	20,30,33	2.81	6 (30%)
12	D2T	AL	89	12	4,9,10	1.09	0	3,11,13	2.96	1 (33%)
22	PSU	BA	1917	22	17,21,22	3.22	9 (52%)	20,30,33	2.96	5 (25%)
22	OMG	BA	2251	58,22,55	18,26,27	3.01	7 (38%)	20,38,41	2.09	7 (35%)
22	PSU	BA	2457	22	17,21,22	2.83	8 (47%)	20,30,33	2.50	6 (30%)
1	UR3	AA	1498	1	14,22,23	2.54	5 (35%)	15,32,35	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	BA	2504	58,22	17,21,22	2.91	8 (47%)	20,30,33	3.34	6 (30%)
22	OMU	BA	2552	57,22	14,22,23	2.86	5 (35%)	14,31,34	0.82	0
1	4OC	AA	1402	57,1	16,23,24	2.97	6 (37%)	17,32,35	1.51	1 (5%)
34	4D4	BM	81	34	9,11,12	2.44	4 (44%)	8,13,15	1.26	1 (12%)
22	G7M	BA	2069	58,22	20,26,27	2.93	6 (30%)	20,39,42	3.01	7 (35%)
22	2MG	BA	1835	22	19,26,27	3.48	8 (42%)	21,38,41	2.50	6 (28%)
22	3TD	BA	1915	22,56	17,22,23	4.83	8 (47%)	19,32,35	1.32	2 (10%)
1	2MG	AA	966	1	19,26,27	4.21	8 (42%)	21,38,41	2.27	8 (38%)
1	G7M	AA	527	58,1	20,26,27	3.35	7 (35%)	20,39,42	2.84	5 (25%)
22	5MU	BA	1939	58,22	15,22,23	1.19	2 (13%)	16,32,35	2.56	1 (6%)
22	5MC	BA	1962	58,22	15,22,23	2.38	5 (33%)	19,32,35	1.19	2 (10%)
1	PSU	AA	516	57,1	17,21,22	3.34	8 (47%)	20,30,33	3.18	7 (35%)
1	MA6	AA	1518	1	19,26,27	1.45	5 (26%)	18,38,41	3.42	2 (11%)
22	2MA	BA	2503	57,58,22	17,25,26	3.30	6 (35%)	19,37,40	2.25	4 (21%)
1	2MG	AA	1207	58,1	19,26,27	4.20	8 (42%)	21,38,41	2.18	8 (38%)
22	PSU	BA	2604	22	17,21,22	2.77	8 (47%)	20,30,33	2.59	6 (30%)
22	5MU	BA	747	22,40	15,22,23	1.18	2 (13%)	16,32,35	2.54	1 (6%)
1	2MG	AA	1516	1	19,26,27	3.72	8 (42%)	21,38,41	2.65	5 (23%)

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
25	MEQ	BD	150	25	-	4/8/9/11	-
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	57,22	-	0/7/27/28	0/2/2/2
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	746	57,22	-	4/7/25/26	0/2/2/2
22	PSU	BA	955	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	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/3/12/14	-
22	PSU	BA	1917	22	-	1/7/25/26	0/2/2/2
22	OMG	BA	2251	58,22,55	-	2/5/27/28	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
22	PSU	BA	2504	58,22	-	2/7/25/26	0/2/2/2
22	OMU	BA	2552	57,22	-	0/7/27/28	0/2/2/2
1	4OC	AA	1402	57,1	-	2/9/29/30	0/2/2/2
34	4D4	BM	81	34	-	2/11/12/14	-
22	G7M	BA	2069	58,22	-	2/3/25/26	0/3/3/3
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
22	3TD	BA	1915	22,56	-	3/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	G7M	AA	527	58,1	-	2/3/25/26	0/3/3/3
22	5MU	BA	1939	58,22	-	0/5/25/26	0/2/2/2
22	5MC	BA	1962	58,22	-	2/5/25/26	0/2/2/2
1	PSU	AA	516	57,1	-	1/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	2MA	BA	2503	57,58,22	-	2/3/25/26	0/3/3/3
1	2MG	AA	1207	58,1	-	0/5/27/28	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	5MU	BA	747	22,40	-	3/5/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C5-C1'	-16.01	1.38	1.52
1	AA	966	2MG	C2-N2	13.13	1.45	1.34
1	AA	1207	2MG	C2-N2	12.59	1.44	1.34
1	AA	1516	2MG	C2-N2	10.85	1.43	1.34
22	BA	2030	6MZ	C6-N6	10.36	1.52	1.35

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-14.58	101.71	117.06
1	AA	1518	MA6	N1-C6-N6	-13.26	103.10	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	746	PSU	N1-C2-N3	-11.63	119.19	128.43
22	BA	2504	PSU	N1-C2-N3	-11.09	119.61	128.43
1	AA	516	PSU	N1-C2-N3	-10.75	119.88	128.43

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
25	BD	150	MEQ	O-C-CA-CB
22	BA	746	PSU	O4'-C1'-C5-C4

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BD	150	MEQ	1	0
22	BA	2498	OMC	1	0
1	AA	1519	MA6	1	0
22	BA	2030	6MZ	2	0
22	BA	2251	OMG	1	0
34	BM	81	4D4	1	0
1	AA	1207	2MG	1	0
1	AA	1516	2MG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 489 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	$\# Z > 2$
60	TRP	BA	3001	-	12,16,16	0.66	0	12,22,22	0.83	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
60	TRP	BA	3001	-	-	0/3/8/8	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	2
54	B7	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	13.97
1	BA	2099:U	O3'	2100:G	P	3.25
1	B7	7:U	O3'	8:G	P	2.92