



## wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 09:08 PM UTC

PDB ID : 5AA0 / pdb\_00005aa0  
EMDB ID : EMD-6397  
Title : Complex of Thermosus thermophilus ribosome (A-and P-site tRNA) bound to BipA-GDPCP  
Authors : Kumar, V.; Chen, Y.; Ahmed, T.; Tan, J.; Ero, R.; Bhushan, S.; Gao, Y.-G.  
Deposited on : 2015-07-23  
Resolution : 5.00 Å(reported)  
Based on initial model : 4V4Y

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:

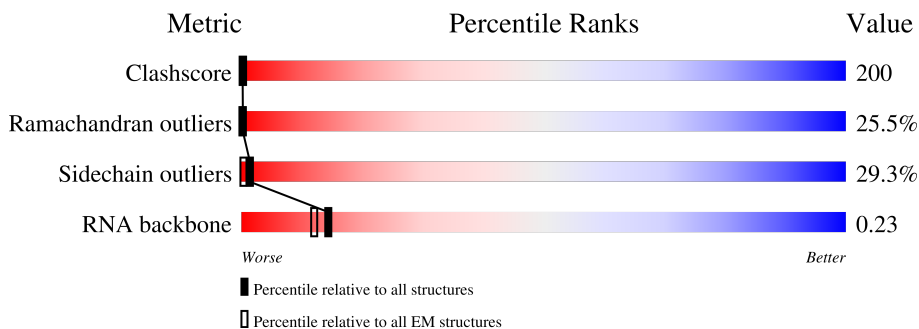
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 5.00 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	2889	
2	AB	123	
3	AC	228	
4	AD	272	
5	AE	206	
6	AF	208	
7	AG	182	

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Mol	Chain	Length	Quality of chain
8	AH	174	5% 47% 37% 11%
9	AK	139	32% 52% 16%
10	AL	122	28% 51% 20%
11	AM	145	36% 45% 15%
12	AN	136	29% 49% 21%
13	AO	117	52% 30% 16%
14	AP	110	39% 48% 11%
15	AQ	117	30% 50% 20%
16	AR	117	44% 41% 14%
17	AS	101	43% 36% 21%
18	AT	110	55% 34% 11%
19	AU	94	53% 36% 10%
20	AV	110	5% 44% 44% 8%
21	AW	180	42% 42% 13%
22	AX	85	56% 29% 11%
23	AY	67	55% 39% 6%
24	AZ	59	39% 46% 12%
25	Aa	71	20% 55% 24%
26	Ab	57	28% 51% 19%
27	Ac	49	16% 55% 27%
28	Ad	49	45% 47% 8%
29	Ae	64	34% 48% 17%
30	Af	37	5% 54% 30% 11%
31	AI	153	42% 46% 11%
32	AJ	134	7% 57% 28% 9%


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Mol	Chain	Length	Quality of chain
33	Ag	128	51% 49%
34	BA	1515	57% 33% 9%
35	BF	234	42% 43% 14%
36	BG	206	50% 39% 6%
37	BH	208	48% 39% 11%
38	BI	150	56% 35% 8%
39	BJ	101	50% 40% 8%
40	BK	155	50% 37% 9%
41	BL	138	50% 39% 9%
42	BM	127	56% 35% 6%
43	BN	98	48% 44% 6%
44	BO	119	55% 41% 6%
45	BP	124	39% 48% 9%
46	BQ	114	11% 56% 28% 5%
47	BR	60	7% 48% 30% 15%
48	BS	88	59% 33% 6%
49	BT	83	49% 40% 11%
50	BU	104	44% 43% 9%
51	BV	73	56% 29% 14%
52	BW	80	55% 38% 6%
53	BX	99	5% 51% 38% 6%
54	BY	24	63% 29% 8%
55	BC	76	11% 57% 33%
56	BD	75	16% 48% 35%
56	BE	75	15% 55% 31%

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Mol	Chain	Length	Quality of chain
57	BZ	605	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	8AN	AA	3002	-	-	X	-
59	8AN	AA	3003	-	-	X	-
60	GCP	BZ	701	-	-	X	-

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 155482 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	2889	62218	27691	11629	20009	2889	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	1134	G	UNK	conflict	GB 37223181

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	123	2641	1175	488	855	123	0	0

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	228	1742	1102	318	319	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	272	2124	1339	424	358	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	206	1578	997	302	273	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	208	1625	1034	303	286	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	182	1482	947	269	261	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AH	174	1328	844	248	235	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AM	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AN	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AO	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AP	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AQ	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AR	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AS	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AT	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AU	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AV	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AW	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AX	85	Total	C	N	O	S	0	0
			670	415	141	112	2		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AY	67	567	350	116	99	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	AZ	59	469	298	90	81	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Aa	71	581	364	108	104	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Ab	57	445	279	87	74	5	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ac	49	426	265	87	70	4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Ad	49	430	263	108	57	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ae	64	515	331	102	79	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Af	37	307	188	68	47	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	AI	153	752	446	153	153	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AJ	134	993	632	175	181	5	0	0

- Molecule 33 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Ag	128	620	369	128	123	0	5

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	BA	1515	32554	14490	6022	10527	1515	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BF	234	1900	1213	341	341	5	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BG	206	1612	1016	314	281	1	0	0

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BH	208	1703	1066	339	291	7	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	BI	150	1146	724	217	201	4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BJ	101	843	531	155	154	3	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BK	155	1257	781	252	218	6	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BL	138	1116	705	215	193	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	BM	127	1010	639	197	174	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BN	98	794	499	156	138	1	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BO	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BP	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BQ	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BR	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BS	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BT	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BU	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	BV	73	597	380	118	99	0	0

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	BW	80	647	414	119	112	2	0	0

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	BX	99	763	470	162	129	2	0	0

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	BY	24	208	128	50	30	0	0

- Molecule 55 is a RNA chain called tRNA chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	BC	76	1619	723	290	531	75	0	0

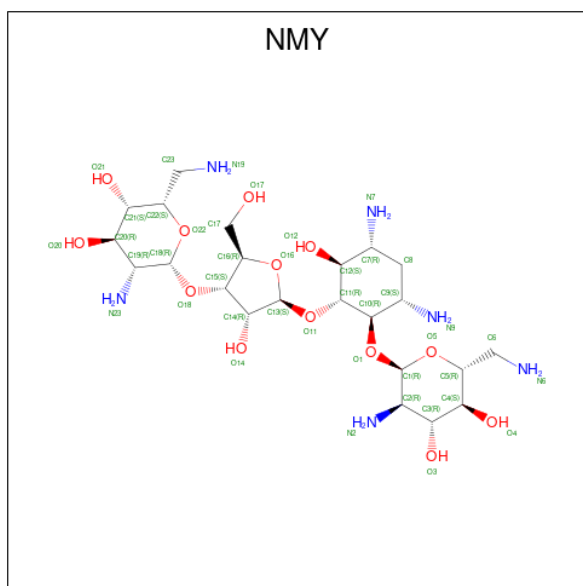
- Molecule 56 is a RNA chain called tRNA chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	BD	75	1597	713	285	525	74	0	0
56	BE	75	1597	713	285	525	74	0	0

- Molecule 57 is a protein called GTP-binding protein.

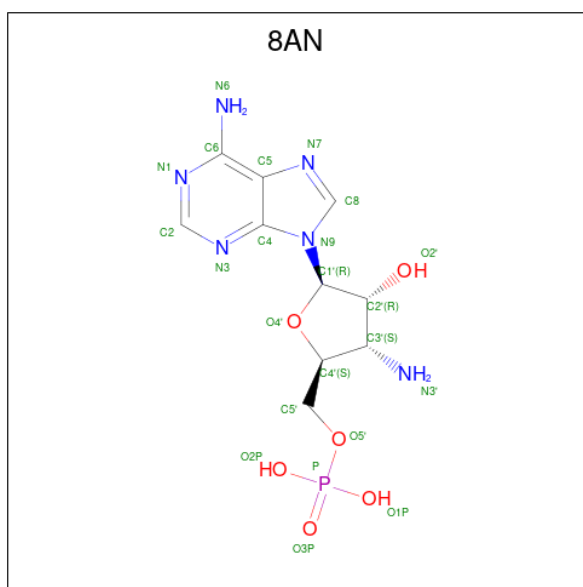
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BZ	605	4610	2902	807	883	18	0	0

- Molecule 58 is NEOMYCIN (CCD ID: NMY) (formula:  $C_{23}H_{46}N_6O_{13}$ ).



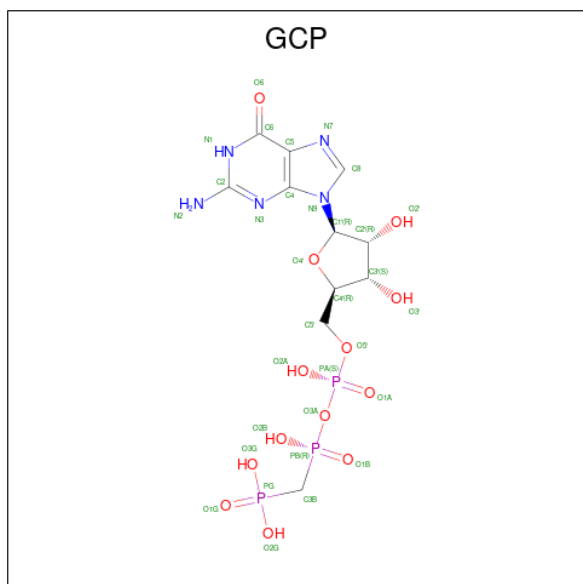
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	AA	1	42	23	6	13	0
58	BA	1	42	23	6	13	0

- Molecule 59 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula:  $C_{10}H_{15}N_6O_6P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	AA	1	22	10	6	5	1	0
59	AA	1	22	10	6	5	1	0

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).

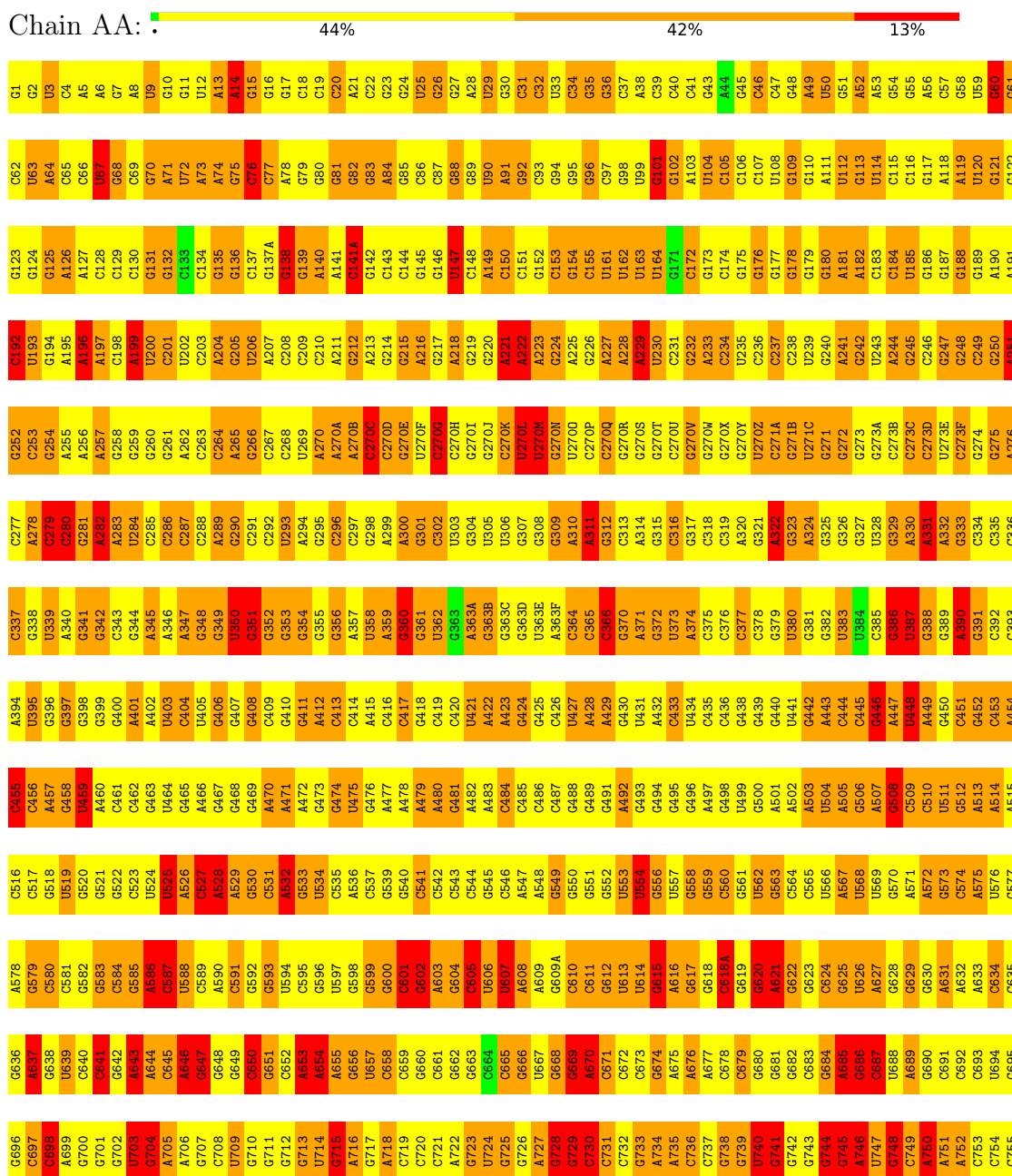


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	BZ	1	32	11	5	13	3	0

### 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: 23S ribosomal RNA

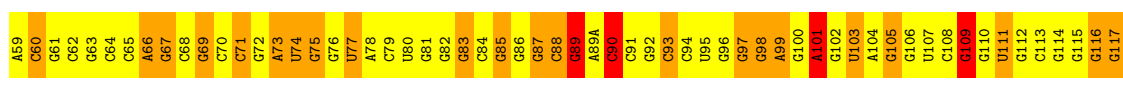
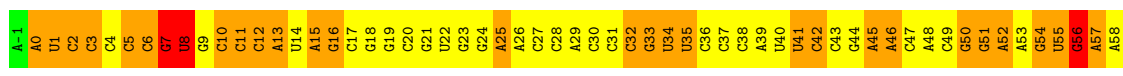
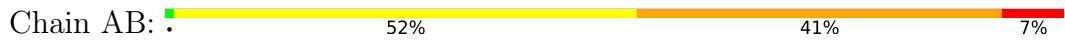


G1726	C1657	C1598	G1538	A1477	G1418	G1358	C1298	G1288	A1177	G1117	A1057	G997	G938	C876	C816	C756
U1727	C1658	C1599	G1539	G1478	A1419	A1389	G1299	G1289	C1178	C1118	G1058	C998	G939	U877	C817	U757
G1728	C1659	C1600	G1540	G1479	U1420	A1360	U1300	U1240	C1179	C1119	G1059	U999	G940	C818	C818	C758
A1729	C1660	G1601	G1541	G1480	A1421	G1361	A1301	A1241	C1180	G1120	U1060	A1000	A941	G879	A819	G759
U1730	C1661	U1602	G1542	U1482	G1422	C1362	A1302	G1242	C1181	G1121	U1061	A1001	G942	G880	A820	G760
G1731	C1662	A1603	G1543	U1483	G1423	C1363	G1303	G1243	C1182	G1122	G1062	G1002	U943	G881	A821	A761
A1732	C1663	C1604	G1544	G1484	U1424	G1364	C1304	G1244	G1183	C1123	G1063	G1003	G944	G882	U822	U762
G1733	A1664	C1605	A1545	G1485	G1425	A1365	C1305	G1245	G1184	C1124	U1064	C1004	A945	G883	U823	G763
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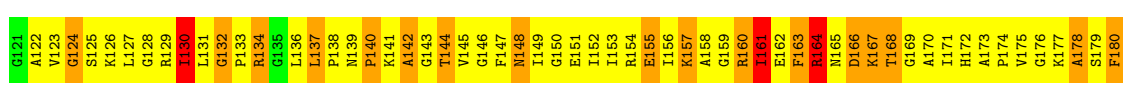
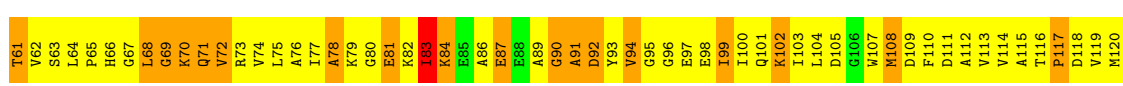
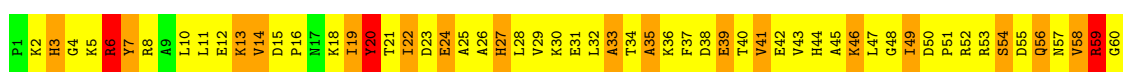
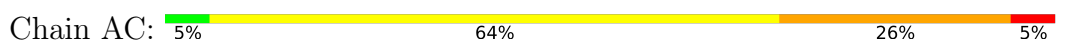
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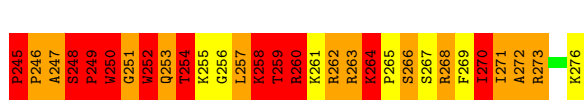
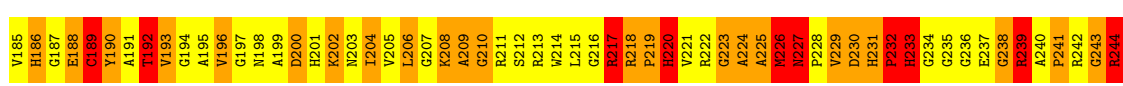
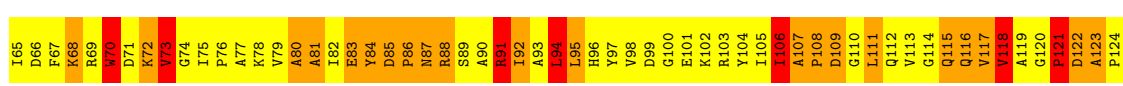
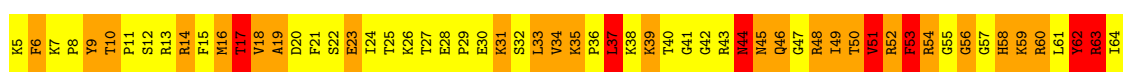
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L1



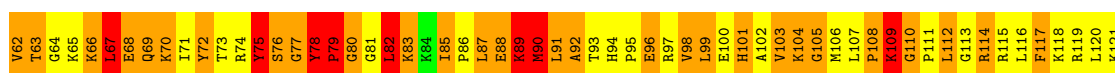
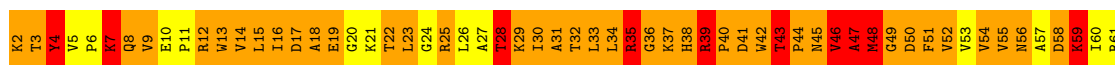
• Molecule 4: 50S ribosomal protein L2



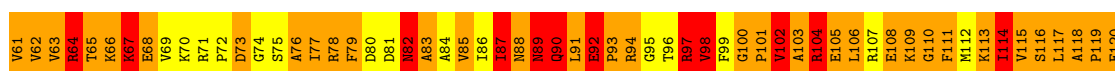




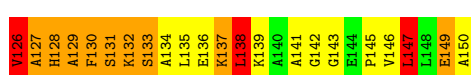
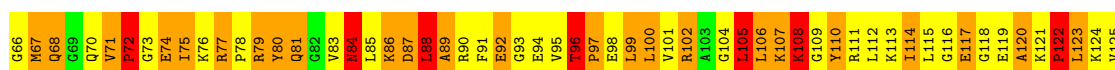
• Molecule 9: 50S ribosomal protein L13



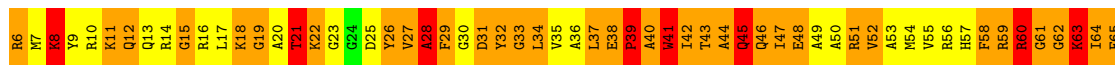
• Molecule 10: 50S ribosomal protein L14

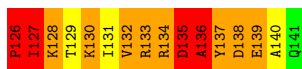


• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16





- Molecule 13: 50S ribosomal protein L17

Chain AO: 52% 30% 16%



- Molecule 14: 50S ribosomal protein L18

Chain AP: 39% 48% 11%



- Molecule 15: 50S ribosomal protein L19

Chain AQ: 30% 50% 20%



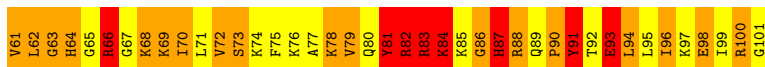
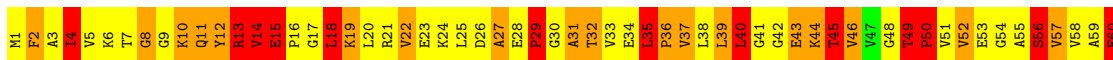
- Molecule 16: 50S ribosomal protein L20

Chain AR: 44% 41% 14%



- Molecule 17: 50S ribosomal protein L21

Chain AS: 43% 36% 21%



- Molecule 18: 50S ribosomal protein L22





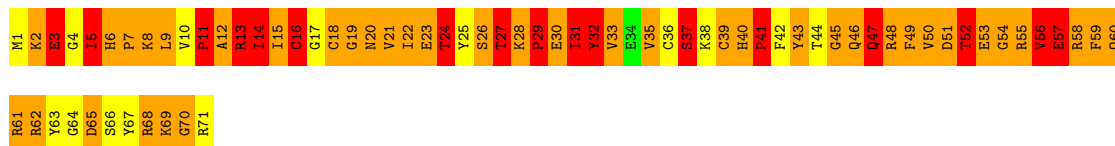
- Molecule 24: 50S ribosomal protein L30

Chain AZ: 39% 46% 12%



- Molecule 25: 50S ribosomal protein L31

Chain Aa: 20% 55% 24%



- Molecule 26: 50S ribosomal protein L32

Chain Ab: 28% 51% 19%



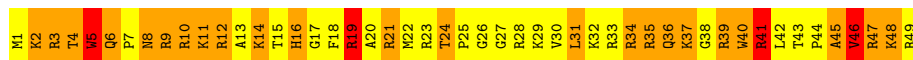
- Molecule 27: 50S ribosomal protein L33

Chain Ac: 16% 55% 27%



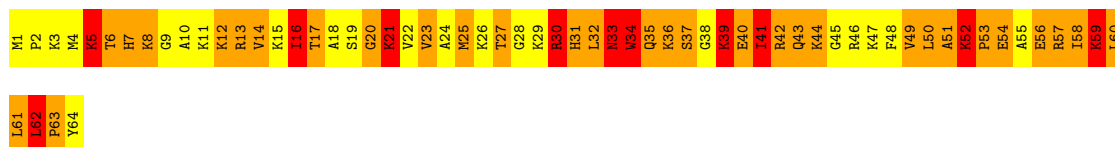
- Molecule 28: 50S ribosomal protein L34

Chain Ad: 45% 47% 8%

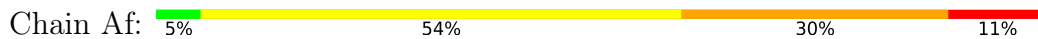


- Molecule 29: 50S ribosomal protein L35

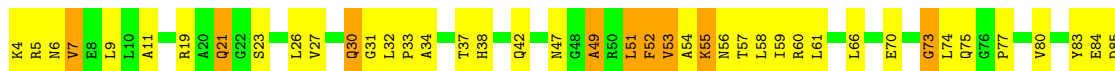
Chain Ae: 34% 48% 17%



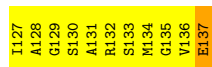
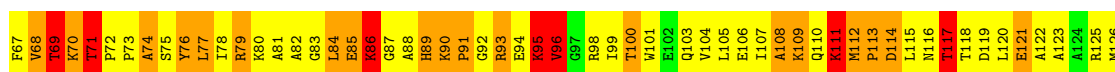
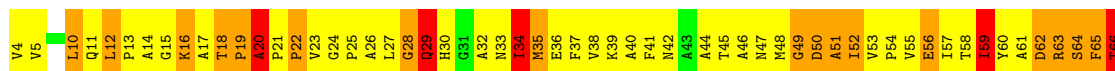
- Molecule 30: 50S ribosomal protein L36



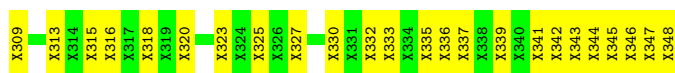
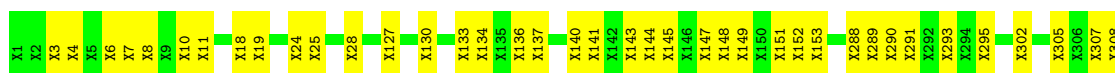
• Molecule 31: 50S ribosomal protein L10



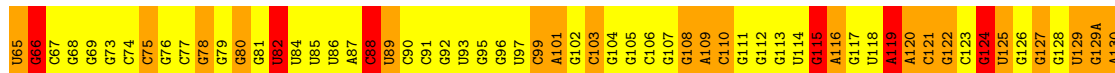
• Molecule 32: 50S ribosomal protein L11



• Molecule 33: Unknown peptide



• Molecule 34: 16S ribosomal RNA



A1225	C1265	G371	A431	C503	A563	C623	G683	U743	G803	G869	G929	C989	A1044	G1104	G1184	A1225
C1226	U252	C372	A432	C504	C564	C624	A684	C744	U804	U870	C930	C990	C1045	A1105	C1165	C1226
A1227	U253	A373	A433	G505	U565	G625	G685	C745	C805	U871	C931	U991	C1046	A1106	G1166	A1227
C1228	G254	A374	U434	G506	G566	U626	U686	A746	C806	A872	C932	U992	C1047	C1107	G1167	C1228
A1229	U255	G375	U435	C507	G567	G627	G687	A747	A807	A873	C933	U993	U1048	G1108	G1168	A1229
C1230	G256	G376	C436	C508	G568	G628	G688	C748	C808	G874	C934	U994	U1049	C1109	G1169	C1230
G1231	U257	G377	U437	A509	C569	G629	C689	C749	G809	C875	A935	C995	G1050	A1110	G1170	G1231
U1232	G258	G378	A438	A510	G570	G630	G690	U750	C810	G876	C936	U996	G1051	A1111	C1171	U1232
G1233	U259	C379	A439	G831	U571	G631	G691	U751	C811	G877	A937	U997	G1052	C1112	G1172	G1233
C1234	G260	C380	A440	U512	A572	G632	G692	U752	G812	G878	C938	U998	G1053	C1113	G1173	C1234
A1235	U261	C381	C442	C513	A573	G633	G693	U753	U813	G879	C939	G998A	C1054	C1114	G1174	A1235
C1236	A262	C382	C443	C514	A574	G634	G694	U754	A814	C880	C940	U999	U1055	C1115	G1175	C1236
G1237	A263	C383	C444	C515	A575	G635	A695	U755	A815	G881	C941	U1000	U1056	C1116	G1176	G1237
A1238	U264	G384	G445	U516	G576	U636	A696	C756	A816	C882	C942	G1001	G1057	C1117	G1177	A1238
A1239	G265	C385	G446	G517	G577	U637	U697	U757	C817	G883	U943	U1002	G1058	C1118	A1179	A1239
U1240	C266	C386	G447	C518	C578	G638	G698	U758	C818	U884	C944	G1003	G1059	C1119	A1180	U1240
G1241	U267	U387	A448	A520	G579	G639	G699	U759	A819	G885	C945	A1005	C1060	C1120	G1181	G1241
C1242	C268	C388	C449	A521	U580	A640	G700	U760	A820	G886	C946	U1006	U1061	C1121	A1182	C1242
G1243	C269	A389	A450	G521	G581	U641	C701	U761	G821	G887	C947	C1007	U1062	C1122	A1183	C1243
A1244	C270	C390	A451	C522	U582	A642	A702	C762	C822	G888	C948	C1008	C1063	C1123	A1184	A1244
C1245	G271	G391	A452	A523	C583	G643	G703	C763	G823	A889	C949	C1009	C1064	C1124	G1185	C1245
U1246	C272	C392	G453	G524	G584	G644	A704	C764	C824	G890	U950	G1010	U1065	C1125	G1186	U1246
G1247	A273	A393	A454	C525	G585	U645	U705	C765	G825	U891	C951	G1011	C1066	C1126	G1187	G1247
A1248	C274	C394	C455	C526	C586	U646	A706	U766	C826	U892	U952	U1012	A1067	C1127	A1188	A1248
C1249	A275	G395	C456	G527	C587	C647	C707	U767	C827	C893	C953	U1013	U1068	C1128	C1189	C1249
A1250	G276	G396	C457	C528	G588	A648	C708	U768	A828	G894	C954	G1014	C1069	C1129	G1190	A1250
A1251	C277	A397	A458	G529	C589	G649	G709	U769	G829	G895	U955	U1015	U1070	C1130	A1191	A1251
C1252	C278	C398	G459	G530	C590	G650	G710	C770	G830	C896	U956	A1016	C1071	C1131	C1192	C1252
G1253	C279	G399	A465	U531	U591	U651	A711	C771	U831	C897	U957	G1017	C1072	C1132	G1193	G1253
C1254	C280	C400	C466	C532	G592	U652	A712	U772	C832	U958	C958	G1018	U1073	C1133	U1194	C1254
G1255	G281	C401	G467	A533	C593	G653	G713	C773	U833	C899	C959	C1019	G1074	C1134	A1195	G1255
A1256	A282	G402	A468	U534	G594	U654	A714	U774	C834	A900	U960	U1020	C1075	C1135	U1196	A1256
U1257	C283	C403	G474	A535	G595	A655	A715	C775	U835	A901	U961	U1021	C1076	C1136	G1197	U1257
G1258	G284	U404	G475	C536	C596	G656	A716	C776	G836	G902	C962	G1022	C1077	C1137	U1198	G1258
C1259	G285	G405	G476	G537	U597	U657	C717	U777	G837	G903	C963	G1023	U1078	C1138	U1199	C1259
U1260	G286	C406	C477	G538	U598	G658	G718	C778	U838	C904	A964	G1024	G1079	C1139	G1200	U1260
A1261	G287	G407	A478	A539	C599	U659	C719	U779	U839	U905	A965	G1025	A1080	C1140	A1201	A1261
C1262	A288	A408	C479	G540	C600	G660	C720	U780	C842	G906	C966	U1026	G1081	C1141	G1202	C1262
C1263	G289	G409	U480	G541	C601	G661	G721	U781	U843	A907	C967	G1027	G1082	C1142	C1203	C1263
G1264	C290	G410	G481	G542	A602	G662	A722	U782	C844	A908	A968	C1028	U1083	G1143	A1204	G1264
C1265	G291	C411	A482	C543	U603	A663	C723	U783	C845	A909	A969	U1028A	U1084	C1144	U1205	C1265
G1266	A292	G412	C483	G544	G604	G664	G724	C784	U850	C910	C970	C1028B	U1085	C1145	G1206	G1266
C1267	G293	A413	G484	C545	U605	A665	G725	U785	G851	U911	G971	G1029	U1086	C1146	G1207	C1267
A1268	U294	G414	G485	G546	G606	G666	C726	U786	G852	C912	C972	G1030	G1087	C1147	C1208	A1268
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G1273	A300	U420	G490	U551	A611	G671	C731	U791	C857	G917	A977	G1032B	U1092	A1152	A1213	G1273
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G1276	A303	G362	G493	C554	A614	G674	A734	U794	A860	U920	C980	A1035	U1095	G1155	G1216	G1276
C1277	G304	A363	U494	C555	C615	A675	C735	U795	G861	U921	U981	G1036	U1096	C1156	C1217	C1277
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A1279	G306	U365	A496	G557	G617	U677	A737	U797	U863	A923	U983	C1038	U1098	C1158	U1219	A1279
U1280	C307	C366	U497	G558	C618	U678	C738	U798	A864	C924	C984	C1039	G1099	U1159	U1220	U1280
G1281	G308	U367	A498	A559	U619	C679	C739	U799	A865	G925	C985	U1040	C1100	G1160	G1221	U1281
C1282	C309	U368	G428	U560	G620	U740	C866	U800	G866	G926	A986	A1041	U1101	C1161	G1222	A1282
A1283	G309	U369	U429	U561	A621	C681	G867	U801	G867	G927	G987	G1042	A1102	C1162	C1223	C1283
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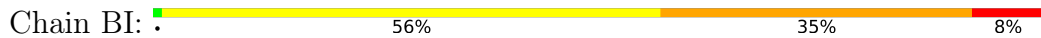


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R122	R123	R124	R125	R126	R127	R128	R129	R130	R131	R132	R133	R134	R135	R136	R137	R138	R139	R140	R141	R142	R143	R144	R145	R146	R147	R148	R149	R150	R151	R152	R153	R154	R155	R156	R157	R158	R159	R160	R161	R162	R163	R164	R165	R166	R167	R168	R169	R170	R171	R172	R173	R174	R175	R176	R177	R178	R179	R180	R181
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K182	G183	K184	F185	L186	R187	L188	P189	D190	R191	E192	D193	L194	A195	L196	V197	N198	N199	E200	Q201	L202	V203	I204	E205	F206	Y207	S208	R209
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• Molecule 38: 30S ribosomal protein S5



D5	F6	E7	E8	K9	M10	L11	L12	L13	R14	R15	T16	A17	R18	M19	Q20	A21	G22	G23	R24	R25	F26	R27	F28	G29	A30	R31	V32	V33	V34	G35	D36	R37	Q38	G39	R40	V100	V41	G42	L43	G44	F45	G46	K47	A48	P49	E50	V51	P52	L53	A54	V55	Q56	K57	A58	G59	Y60	Y61	A62	R63	R64
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M65	M66	V67	E68	V69	P70	L71	Q72	M73	G74	R75	I76	P77	H78	E79	R80	E81	V82	E83	F84	G85	A86	S87	K88	I89	V90	L91	K92	P93	A94	A95	P96	G97	T98	G99	V100	I101	A102	G103	A104	V105	P106	R107	A108	L109	L110	E111	L112	A113	G114	V115	T116	D117	I118	L119	T120	K121	E122	L123	G124
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S125	R126	M127	P128	I129	M130	I131	A132	Y133	A134	T135	M136	E137	A138	L139	R140	Q141	L142	R143	T144	R145	A146	D147	V148	E149	R150	L151	R152	K153	G154
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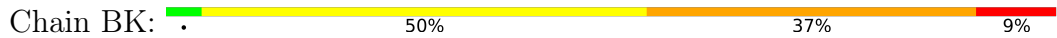
• Molecule 39: 30S ribosomal protein S6



M1	R2	Y4	E5	V6	M7	I8	V9	L10	N11	M12	M13	L14	D15	Q16	S17	E18	L19	A20	L21	E22	K23	E24	I25	I26	Q27	R28	A29	L30	E31	N32	Y33	G34	A35	R36	V37	E38	K39	V40	E41	E42	L43	G44	L45	R46	R47	L48	A49	Y50	P51	L52	A53	K54	D55	P56	Q57	G58	F60
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L61	M62	Y63	Q64	V65	E66	M67	P68	E69	D70	R71	V72	M73	D74	A75	A76	R77	E78	L79	R80	L81	R82	D83	N84	V85	R86	R87	V88	M89	V90	V91	K92	S93	G94	Q95	E96	P96	F97	L98	A99	M100	A101
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• Molecule 40: 30S ribosomal protein S7



A2	R3	R4	R5	R6	A7	E8	V9	R10	Q11	L12	Q13	D15	L16	V17	Y18	G19	D20	V21	L22	V23	T24	A25	F26	L27	N28	K29	S92	I30	M31	R32	R33	G34	K35	R36	N37	L38	A39	A40	R41	L42	F43	Y44	D45	A46	C47	R48	I50	I51	T54	G55	Q56	E57	P58	V61	F62	R63
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Q64	A65	V66	E67	M68	V69	K70	F71	R72	M73	E74	V75	S76	S77	R78	R79	V80	G81	G82	A83	R84	Y85	Q86	V87	P88	H89	E90	V91	S92	P93	R94	R95	Q96	Q97	S98	L99	A100	L101	R102	V103	L104	V105	Q106	A107	A108	M109	Q110	R111	P112	E113	R114	R115	G55	A116	A117	V118	R119	L120	A121	H122	E123
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L124	M125	D126	A127	Y128	E129	G130	K131	G132	G133	A134	V135	K136	K137	K138	E139	D140	V141	E142	R143	M144	A145	E146	A147	M148	R149	A150	Y151	A152	H153	Y154	R155	M156
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• Molecule 41: 30S ribosomal protein S8



M1	L2	T3	D4	F5	V6	A7	D8	M9	L10	T11	R12	L13	R14	M15	A16	T17	R18	V19	Y20	K21	E22	S23	T24	D25	V26	P27	A28	S29	R30	F31	K32	E33	E34	I35	L36	R37	L38	L39	A40	R41	E42	G43	F44	L45	K46	G47	Y48	E49	R50	V51	D52	V53	D54	G55	K56	P57	V58	L59	R60
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V61	V62	L63	K64	Y65	G66	P67	R68	R69	Q70	G71	F72	D73	F74	R75	E76	E77	Q78	V79	R80	H81	H82	L83	R84	R85	L86	S87	K88	S89	R90	R91	R92	V93	Y94	V95	G96	Y97	K98	E99	T100	R101	R102	G103	R104	R105	G106	L107	G108	I109	A110	L111	L112	S113	T114	S115	K116	G117	V118	L119	L120	T120
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D121  
R122  
A123  
A124  
R125  
K126  
L127  
G128  
V129  
G130  
G131  
E132  
L133  
L134  
C135  
E136  
V137  
W138

- Molecule 42: 30S ribosomal protein S9

Chain BM:  56% 35% 6%

E2 Q3 Y4 Y5 Y6 G6 T7 G8 R9 R10 K11 E12 A13 V14 A15 R16 R17 V17 F18 F19 L19 R20 R21 G22 G23 N23 G24 A25 K25 V26 V27 T27 V28 N29 R30 G30 P30 Q31 Q32 Y32 G33 F33 R34 N34 E35 Y36 Y37 F37 F38 Q38 G39 L40 L41 V41 R42 R43 A43 A44 V44 A45 A46 R47 E48 E49 P49 L50 L51 R51 A52 A53 V53 D54 A55 G55 L56 G57 H58 F59 D60 A61

Y62 I63 T64 Y65 V65 G66 G67 G68 G69 K70 S71 G72 G73 A74 I74 D75 A76 R77 I77 K78 L79 G80 R81 A82 A83 N83 G84 L85 K85 V86 Q87 Y88 N89 P90 G90 D91 Y92 R93 A94 K95 L96 L97 P98 R99 L99 G100 L101 F101 T102 L103 R104 A105 A106 R107 V108 V109 E110 R111 R112 K113 K114 G115 G116 H117 K118 A119 R120 R121

A122  
P123  
Q124  
Y125  
S126  
K127  
R128

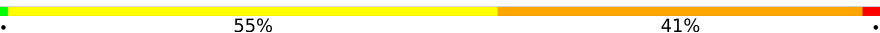
- Molecule 43: 30S ribosomal protein S10

Chain BN:  48% 44% 6%

K3 L4 I5 I6 K7 L8 R9 G10 F11 D12 H13 H14 K15 T15 L16 D17 A18 S19 S20 A20 Q21 K22 I23 V24 E25 A26 A27 R28 R29 S30 G31 P31 A32 A33 Q33 Y34 S35 G36 G37 I38 P39 L40 P41 T42 R43 V44 R45 R46 F47 T48 I49 I50 R51 G52 P53 F54 K55 H56 K57 S58 R60 E61 H62

F63 E64 L65 R66 T67 H68 N69 R70 L71 V72 D73 I74 I75 N76 P77 N78 R79 K80 T81 R82 E83 Q84 L85 M86 T87 L88 D89 R90 P91 T92 G93 G94 E95 I96 E97 I98 K99 T100

- Molecule 44: 30S ribosomal protein S11

Chain BO:  55% 41% 6%

K11 R12 Q13 V14 A15 S16 G17 R18 A19 I20 I21 I22 H23 A24 S24 Y25 N26 N27 N28 T28 I29 V30 T31 I32 I33 Q33 A34 P35 D36 G37 R38 R39 P39 I40 T41 T42 S43 S44 G45 G46 K46 V47 I48 G49 Y50 K51 G52 G53 S53 R54 K55 G56 T57 P58 Y59 A60 A61 Q62 L63 A64 A65 A66 D67 A68 A69 K70

K71 A72 M73 A74 Y75 G76 M77 Q78 S79 V80 D81 V82 I83 V84 R85 G86 T87 G88 A89 G90 R91 E92 Q93 A94 I95 R96 A97 L98 Q99 A100 S101 G102 L103 Q104 V105 K106 I107 I108 V109 D110 D111 T112 P113 V114 P115 H116 G118 C119 R120 P121 K122 K123 K124 F125 R126 L127 A128 S129

- Molecule 45: 30S ribosomal protein S12


Chain BP:  39% 48% 9%

P5 T6 N7 N8 Q9 L10 V11 R12 K13 G14 R15 E16 K17 V18 R19 G20 K21 S22 R23 V24 P25 A26 L27 L28 K28 G29 A30 P31 F32 F33 R34 R35 G35 V36 C37 T38 V39 R40 R41 R42 V43 V44 P45 K46 K47 P48 M49 S50 A51 L52 R53 K54 V55 A56 K57 V58 R59 L60 T61 S62 G63 Y64

E65 V66 T67 A68 Y69 I70 P71 G72 E73 H75 N76 L77 Q78 E79 H80 S81 V82 V83 L84 R85 R86 G87 G88 R89 V90 R91 D92 F93 P94 R95 G95 V96 R97 Y98 H99 I100 V101 R102 G103 V104 Y105 D106 A107 A108 G109 V110 K111 D112 R113 K114 K115 S116 R117 S118 K119 Y120 G121 T122 K123 K124

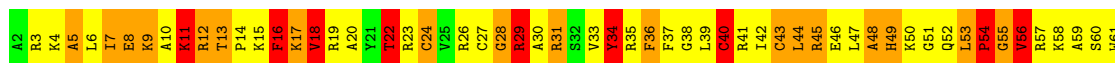
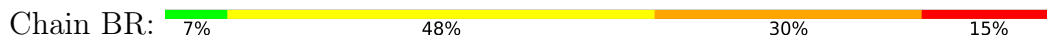
P125  
K126  
E127  
A128

- Molecule 46: 30S ribosomal protein S13

Chain BQ:  11% 56% 28% 5%



- Molecule 47: 30S ribosomal protein S14 type Z



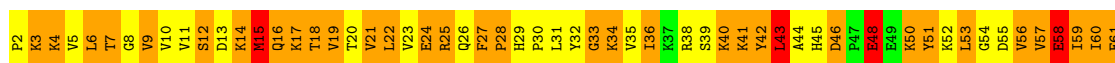
- Molecule 48: 30S ribosomal protein S15



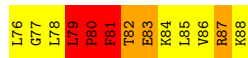
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17

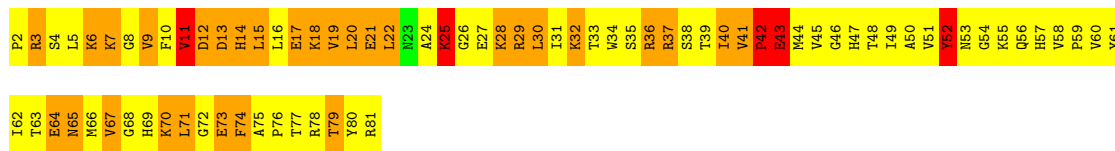


- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19

Chain BW: 55% 38% 6%



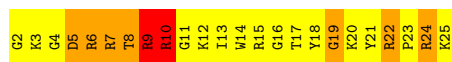
• Molecule 53: 30S ribosomal protein S20

Chain BX: 5% 51% 38% 6%



• Molecule 54: 30S ribosomal protein Thx

Chain BY: 63% 29% 8%



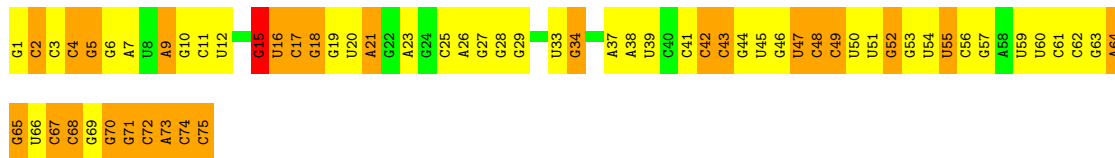
• Molecule 55: tRNA chain 1

Chain BC: 11% 57% 33%



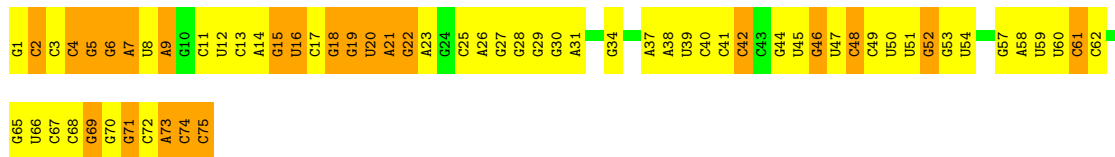
• Molecule 56: tRNA chain 2

Chain BD: 16% 48% 35%



• Molecule 56: tRNA chain 2

Chain BE: 15% 55% 31%



● Molecule 57: GTP-binding protein

Chain BZ: 8% 55% 31% 5%

M1	A63	P123	M183	E243	P305	E571	D432	Q493	E553
I2	I64	I124	T184	G244	T306	N372	G433	G494	A554
E3	K65	V125	P185	K245	V307	M373	R434	K495	V555
K4	W66	L126	L186	T246	S308	R374	G435	A496	V556
L5	Y67	I127	Y187	R247	M309	R375	R436	V497	L557
R6	Y68	M128	N248	N248	F310	E376	V437	A498	V558
N7	R69	K129	A249	A249	F311	G377	R438	F499	P559
I8	I70	V130	K250	K250	C312	F378	L439	A500	P560
A9	N71	D131	V191	V251	V313	E379	D440	L501	P561
I10	I72	R132	H192	G252	N314	L380	Y441	F502	R562
I11	I73	P133	H193	K253	T315	A381	Y442	G503	M563
A12	D74	G134	V194	V254	S316	R382	I443	L504	T564
H13	T75	A135	P195	L255	P317	S383	P444	Q505	L565
V14	P76	R136	A196	G256	F318	R384	S445	D506	E566
D15	G77	P137	P197	H257	C319	P385	R446	R507	Q567
H16	H78	D138	D198	L258	G320	K386	G447	G508	A568
G17	A79	M139	V199	G259	K321	V387	L448	K509	L569
K18	D80	V140	D200	L260	E322	I388	I449	L510	E570
T19	F81	V141	L201	E261	G323	F389	G450	F511	F571
T20	G82	D142	D202	R262	K324	R390	F451	L512	I572
L21	G83	Q143	G203	T265	F325	E391	R452	G513	D573
V22	E84	V144	F204	T266	V326	I392	S453	H514	D574
D23	V85	F145	F205	D266	T327	D393	E454	G515	D575
K24	E86	L146	Q206	L267	S328	G394	F455	A516	E576
L25	R87	L147	M207	A268	R329	R395	M456	E517	L577
L26	V88	F148	Q208	E269	Q330	K396	T457	V518	V578
Q27	M89	V149	I209	A270	I331	Q397	M458	Y519	E579
S28	S90	M150	Q211	G271	L332	E398	T459	E520	E580
S29	M91	L151	Q211	D272	D333	P399	S460	G521	T581
G30	V92	D152	D213	I273	D333	Y400	G461	Q522	P582
T31	D93	D154	D214	V274	E338	E401	T462	I523	T583
F32	S94	T154	Y214	A275	L339	M402	G463	I524	S584
D33	V95	D156	M215	T276	V340	M403	L464	G525	S585
S34	S96	L156	E216	T277	H341	T404	L465	I526	R586
A36	L97	Q157	V217	G278	H341	L405	Y466	H527	I587
A37	V98	L158	V218	L279	V342	D406	S467	S528	R588
E37	V99	D159	G219	G280	A344	V407	T468	R529	K589
T38	D100	F160	V220	E281	L345	E408	F469	S530	R590
Q39	A101	A161	I221	L282	R346	E409	S470	M531	H591
E40	F102	I162	G222	N283	E351	Q410	H471	D532	L592
R41	D103	V163	I223	I284	D352	H411	Y472	L533	T593
V42	G104	Y164	G224	S285	E352	Q412	D473	T534	L534
M43	P105	A165	R225	D286	A353	G413	D474	V535	V536
D44	M106	S166	I226	T287	D354	S414	V475	M536	R597
L48	P107	A167	K227	V288	A355	V415	R476	C537	R598
E49	Q108	L168	R228	C289	F356	M416	P477	L538	R599
E51	T109	M169	G229	D290	R357	Q417	V480	T539	A600
R52	R110	G170	K230	T291	V358	A418	G481	G540	N601
G53	F111	I171	V231	Q292	N293	L419	G482	K541	R602
R54	K114	G173	P233	V294	G360	G361	R483	K542	A603
T55	K115	L174	M234	E295	R362	R422	Q484	L543	P604
L56	D175	H176	Q235	A296	E363	K423	M485	T544	K605
L57	H177	H176	Q236	L297	L364	G424	G486	M545	
A58	F117	E177	V237	L297	H365	D425	V487	M546	
K59	A118	D178	T238	L300	L366	K427	L488	R547	
N60	Y119	M179	I239	S301	S367	M428	I489	A548	
T61	G120	A180	I240	S302	V368	M429	S490	S549	
A62	K122	E181	D241	V303	L369	M430	G492	A551	
				E304	I370	P431		D552	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77127	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	73684	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, GCP, NMY

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	0.69	17/69678 (0.0%)	1.05	364/108758 (0.3%)
2	AB	0.56	0/2954	0.95	5/4606 (0.1%)
3	AC	0.79	0/1772	1.35	32/2383 (1.3%)
4	AD	0.97	1/2174 (0.0%)	1.76	56/2927 (1.9%)
5	AE	1.06	5/1611 (0.3%)	1.66	43/2171 (2.0%)
6	AF	0.83	0/1660	1.51	35/2247 (1.6%)
7	AG	0.83	1/1507 (0.1%)	1.53	34/2027 (1.7%)
8	AH	0.82	2/1354 (0.1%)	1.48	28/1831 (1.5%)
9	AK	1.03	1/1140 (0.1%)	1.64	30/1537 (2.0%)
10	AL	1.23	3/942 (0.3%)	1.97	48/1268 (3.8%)
11	AM	1.00	2/1123 (0.2%)	1.63	33/1493 (2.2%)
12	AN	0.99	0/1100	1.76	35/1470 (2.4%)
13	AO	0.98	1/974 (0.1%)	1.60	27/1302 (2.1%)
14	AP	1.00	0/887	1.66	28/1180 (2.4%)
15	AQ	1.14	2/990 (0.2%)	1.85	35/1325 (2.6%)
16	AR	1.03	1/982 (0.1%)	1.50	21/1306 (1.6%)
17	AS	1.16	2/790 (0.3%)	1.93	32/1057 (3.0%)
18	AT	0.89	1/886 (0.1%)	1.52	17/1189 (1.4%)
19	AU	0.77	0/756	1.38	16/1015 (1.6%)
20	AV	0.75	0/857	1.57	21/1142 (1.8%)
21	AW	0.92	1/1467 (0.1%)	1.78	53/1992 (2.7%)
22	AX	0.86	0/679	1.59	20/902 (2.2%)
23	AY	0.83	0/569	1.31	8/751 (1.1%)
24	AZ	0.86	1/474 (0.2%)	1.62	13/635 (2.0%)
25	Aa	1.10	0/594	1.85	26/795 (3.3%)
26	Ab	1.03	2/459 (0.4%)	1.76	20/621 (3.2%)
27	Ac	1.10	0/433	1.88	15/576 (2.6%)
28	Ad	0.97	0/438	1.35	4/575 (0.7%)
29	Ae	0.83	0/523	1.62	18/690 (2.6%)
30	Af	0.81	0/310	1.56	6/407 (1.5%)
31	AI	0.67	1/751 (0.1%)	1.20	6/1042 (0.6%)
32	AJ	0.56	1/1012 (0.1%)	0.91	4/1373 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
34	BA	0.65	3/36437 (0.0%)	0.99	134/56865 (0.2%)
35	BF	0.87	1/1935 (0.1%)	1.50	38/2609 (1.5%)
36	BG	0.70	0/1636	1.33	21/2205 (1.0%)
37	BH	0.89	3/1733 (0.2%)	1.42	27/2318 (1.2%)
38	BI	0.86	0/1162	1.48	22/1564 (1.4%)
39	BJ	0.85	0/856	1.28	7/1154 (0.6%)
40	BK	0.77	0/1276	1.37	21/1709 (1.2%)
41	BL	0.85	0/1136	1.34	13/1527 (0.9%)
42	BM	0.75	0/1029	1.16	9/1379 (0.7%)
43	BN	0.70	0/807	1.33	10/1085 (0.9%)
44	BO	0.85	0/900	1.58	22/1213 (1.8%)
45	BP	0.78	0/986	1.49	21/1320 (1.6%)
46	BQ	0.36	0/924	0.68	0/1238
47	BR	0.72	0/501	1.34	8/664 (1.2%)
48	BS	0.83	0/745	1.33	9/992 (0.9%)
49	BT	0.87	0/716	1.35	12/963 (1.2%)
50	BU	0.99	1/870 (0.1%)	1.51	20/1159 (1.7%)
51	BV	0.79	0/603	1.61	13/799 (1.6%)
52	BW	0.63	1/661 (0.2%)	1.31	4/890 (0.4%)
53	BX	0.94	0/765	1.27	8/1007 (0.8%)
54	BY	0.57	0/212	1.26	3/277 (1.1%)
55	BC	0.42	0/1809	0.64	0/2819
56	BD	0.44	0/1784	0.66	2/2780 (0.1%)
56	BE	0.38	0/1784	0.65	0/2780
57	BZ	0.39	1/4678 (0.0%)	0.74	5/6310 (0.1%)
All	All	0.73	55/167791 (0.0%)	1.16	1562/250219 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	432
2	AB	0	17
3	AC	0	1
5	AE	0	1
6	AF	0	1
9	AK	0	1
12	AN	0	1
15	AQ	0	1
17	AS	0	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
25	Aa	0	1
26	Ab	0	1
31	AI	0	2
34	BA	0	170
37	BH	0	1
39	BJ	0	1
44	BO	0	1
47	BR	0	1
All	All	0	634

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1060	U	O3'-P	-64.22	0.64	1.61
34	BA	1317	C	O3'-P	-56.08	0.77	1.61
1	AA	1203	G	O3'-P	-27.80	1.19	1.61
34	BA	1167	A	O3'-P	16.69	1.86	1.61
31	AI	153	LEU	C-N	-15.30	1.11	1.33

The worst 5 of 1562 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1317	C	P-O3'-C3'	-39.35	61.17	120.20
34	BA	1317	C	O3'-P-O5'	38.74	162.11	104.00
1	AA	1060	U	O3'-P-O5'	36.33	158.49	104.00
1	AA	2448	A	C5'-C4'-O4'	-21.84	76.34	109.10
1	AA	1203	G	P-O3'-C3'	21.81	152.91	120.20

There are no chirality outliers.

5 of 634 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	A	Sidechain
1	AA	25	U	Sidechain
1	AA	3	U	Sidechain
1	AA	31	C	Sidechain
1	AA	9	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62218	0	31250	16555	0
2	AB	2641	0	1337	611	0
3	AC	1742	0	1779	1085	0
4	AD	2124	0	2207	1519	0
5	AE	1578	0	1647	1107	0
6	AF	1625	0	1666	835	0
7	AG	1482	0	1546	904	0
8	AH	1328	0	1407	738	0
9	AK	1113	0	1183	795	0
10	AL	932	0	992	757	0
11	AM	1106	0	1183	814	0
12	AN	1080	0	1127	756	0
13	AO	960	0	1021	619	0
14	AP	877	0	938	530	0
15	AQ	976	0	1031	671	0
16	AR	964	0	1022	743	0
17	AS	779	0	852	577	0
18	AT	876	0	941	473	0
19	AU	742	0	800	369	0
20	AV	844	0	930	440	0
21	AW	1435	0	1463	759	0
22	AX	670	0	700	387	0
23	AY	567	0	621	324	0
24	AZ	469	0	518	328	0
25	Aa	581	0	577	399	0
26	Ab	445	0	459	289	0
27	Ac	426	0	452	288	0
28	Ad	430	0	480	284	0
29	Ae	515	0	587	409	0
30	Af	307	0	335	156	0
31	AI	752	0	363	210	0
32	AJ	993	0	1019	756	0
33	Ag	620	0	132	151	0
34	BA	32554	0	16390	7469	0
35	BF	1900	0	1951	1096	0
36	BG	1612	0	1677	747	0
37	BH	1703	0	1763	883	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BI	1146	0	1207	606	0
39	BJ	843	0	857	410	0
40	BK	1257	0	1296	587	0
41	BL	1116	0	1177	740	0
42	BM	1010	0	1035	516	0
43	BN	794	0	840	381	0
44	BO	885	0	904	480	0
45	BP	970	0	1057	529	0
46	BQ	914	0	954	650	0
47	BR	492	0	529	288	0
48	BS	734	0	771	363	0
49	BT	700	0	720	359	0
50	BU	857	0	930	472	0
51	BV	597	0	666	390	0
52	BW	647	0	653	545	0
53	BX	763	0	857	418	0
54	BY	208	0	221	91	0
55	BC	1619	0	819	220	0
56	BD	1597	0	802	301	0
56	BE	1597	0	799	356	0
57	BZ	4610	0	4492	2755	0
58	AA	42	0	46	20	0
58	BA	42	0	46	15	0
59	AA	44	0	18	80	0
60	BZ	32	0	14	39	0
All	All	155482	0	106056	52024	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 200.

The worst 5 of 52024 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)
32:AJ:112:MET:SD	32:AJ:122:ALA:HB2	1.28	1.70
3:AC:171:ILE:CD1	3:AC:192:PHE:CZ	1.75	1.70
34:BA:1226:C:C4	46:BQ:104:ARG:HG3	1.16	1.69
1:AA:716:A:C2	48:BS:44:LYS:HG3	1.30	1.67
32:AJ:75:SER:HB3	32:AJ:130:SER:CB	1.24	1.66

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	220/228 (96%)	153 (70%)	39 (18%)	28 (13%)	0	4
4	AD	270/272 (99%)	125 (46%)	59 (22%)	86 (32%)	0	0
5	AE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
6	AF	206/208 (99%)	109 (53%)	46 (22%)	51 (25%)	0	1
7	AG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0
8	AH	172/174 (99%)	80 (46%)	46 (27%)	46 (27%)	0	0
9	AK	137/139 (99%)	64 (47%)	28 (20%)	45 (33%)	0	0
10	AL	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
11	AM	143/145 (99%)	57 (40%)	36 (25%)	50 (35%)	0	0
12	AN	134/136 (98%)	49 (37%)	33 (25%)	52 (39%)	0	0
13	AO	115/117 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
14	AP	108/110 (98%)	48 (44%)	28 (26%)	32 (30%)	0	0
15	AQ	115/117 (98%)	52 (45%)	26 (23%)	37 (32%)	0	0
16	AR	115/117 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
17	AS	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
18	AT	108/110 (98%)	63 (58%)	24 (22%)	21 (19%)	0	2
19	AU	92/94 (98%)	57 (62%)	16 (17%)	19 (21%)	0	1
20	AV	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
21	AW	178/180 (99%)	96 (54%)	43 (24%)	39 (22%)	0	1
22	AX	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	4
23	AY	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	3
24	AZ	57/59 (97%)	34 (60%)	8 (14%)	15 (26%)	0	1
25	Aa	69/71 (97%)	23 (33%)	15 (22%)	31 (45%)	0	0
26	Ab	55/57 (96%)	14 (26%)	19 (34%)	22 (40%)	0	0
27	Ac	47/49 (96%)	14 (30%)	7 (15%)	26 (55%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ad	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
29	Ae	62/64 (97%)	23 (37%)	17 (27%)	22 (36%)	0	0
30	Af	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
31	AI	151/153 (99%)	89 (59%)	33 (22%)	29 (19%)	0	2
32	AJ	132/134 (98%)	56 (42%)	44 (33%)	32 (24%)	0	1
35	BF	232/234 (99%)	114 (49%)	41 (18%)	77 (33%)	0	0
36	BG	204/206 (99%)	107 (52%)	46 (22%)	51 (25%)	0	1
37	BH	206/208 (99%)	95 (46%)	58 (28%)	53 (26%)	0	1
38	BI	148/150 (99%)	93 (63%)	38 (26%)	17 (12%)	0	5
39	BJ	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
40	BK	153/155 (99%)	73 (48%)	45 (29%)	35 (23%)	0	1
41	BL	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	1
42	BM	125/127 (98%)	62 (50%)	33 (26%)	30 (24%)	0	1
43	BN	96/98 (98%)	52 (54%)	20 (21%)	24 (25%)	0	1
44	BO	117/119 (98%)	65 (56%)	29 (25%)	23 (20%)	0	2
45	BP	122/124 (98%)	50 (41%)	30 (25%)	42 (34%)	0	0
46	BQ	112/114 (98%)	64 (57%)	28 (25%)	20 (18%)	0	2
47	BR	58/60 (97%)	24 (41%)	16 (28%)	18 (31%)	0	0
48	BS	86/88 (98%)	36 (42%)	35 (41%)	15 (17%)	0	2
49	BT	81/83 (98%)	42 (52%)	24 (30%)	15 (18%)	0	2
50	BU	102/104 (98%)	62 (61%)	23 (22%)	17 (17%)	0	3
51	BV	71/73 (97%)	26 (37%)	26 (37%)	19 (27%)	0	0
52	BW	78/80 (98%)	30 (38%)	25 (32%)	23 (30%)	0	0
53	BX	97/99 (98%)	38 (39%)	32 (33%)	27 (28%)	0	0
54	BY	22/24 (92%)	9 (41%)	6 (27%)	7 (32%)	0	0
57	BZ	603/605 (100%)	280 (46%)	200 (33%)	123 (20%)	0	1
All	All	6575/6683 (98%)	3224 (49%)	1675 (26%)	1676 (26%)	0	1

5 of 1676 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	35	ALA
3	AC	39	GLU

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Mol	Chain	Res	Type
3	AC	54	SER
3	AC	61	THR
3	AC	72	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	180/180 (100%)	147 (82%)	33 (18%)	2	9
4	AD	215/215 (100%)	151 (70%)	64 (30%)	0	2
5	AE	166/166 (100%)	102 (61%)	64 (39%)	0	1
6	AF	164/164 (100%)	103 (63%)	61 (37%)	0	1
7	AG	156/156 (100%)	111 (71%)	45 (29%)	0	3
8	AH	143/143 (100%)	101 (71%)	42 (29%)	0	3
9	AK	118/118 (100%)	73 (62%)	45 (38%)	0	1
10	AL	100/100 (100%)	62 (62%)	38 (38%)	0	1
11	AM	111/111 (100%)	74 (67%)	37 (33%)	0	2
12	AN	106/106 (100%)	65 (61%)	41 (39%)	0	1
13	AO	100/100 (100%)	70 (70%)	30 (30%)	0	2
14	AP	87/87 (100%)	63 (72%)	24 (28%)	0	3
15	AQ	105/105 (100%)	67 (64%)	38 (36%)	0	1
16	AR	93/93 (100%)	64 (69%)	29 (31%)	0	2
17	AS	82/82 (100%)	58 (71%)	24 (29%)	0	3
18	AT	90/90 (100%)	62 (69%)	28 (31%)	0	2
19	AU	76/76 (100%)	54 (71%)	22 (29%)	0	3
20	AV	91/91 (100%)	72 (79%)	19 (21%)	1	6
21	AW	159/159 (100%)	116 (73%)	43 (27%)	0	3
22	AX	67/67 (100%)	49 (73%)	18 (27%)	0	3
23	AY	62/62 (100%)	44 (71%)	18 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AZ	51/51 (100%)	36 (71%)	15 (29%)	0	3
25	Aa	63/63 (100%)	43 (68%)	20 (32%)	0	2
26	Ab	50/50 (100%)	33 (66%)	17 (34%)	0	2
27	Ac	48/48 (100%)	31 (65%)	17 (35%)	0	1
28	Ad	42/42 (100%)	30 (71%)	12 (29%)	0	3
29	Ae	54/54 (100%)	39 (72%)	15 (28%)	0	3
30	Af	34/34 (100%)	28 (82%)	6 (18%)	2	10
32	AJ	101/101 (100%)	68 (67%)	33 (33%)	0	2
35	BF	202/202 (100%)	133 (66%)	69 (34%)	0	2
36	BG	160/160 (100%)	121 (76%)	39 (24%)	1	4
37	BH	180/180 (100%)	129 (72%)	51 (28%)	0	3
38	BI	115/115 (100%)	76 (66%)	39 (34%)	0	2
39	BJ	90/90 (100%)	62 (69%)	28 (31%)	0	2
40	BK	126/126 (100%)	93 (74%)	33 (26%)	0	3
41	BL	119/119 (100%)	85 (71%)	34 (29%)	0	3
42	BM	98/98 (100%)	74 (76%)	24 (24%)	1	4
43	BN	88/88 (100%)	67 (76%)	21 (24%)	1	5
44	BO	90/90 (100%)	75 (83%)	15 (17%)	2	11
45	BP	104/104 (100%)	79 (76%)	25 (24%)	1	5
46	BQ	92/92 (100%)	66 (72%)	26 (28%)	0	3
47	BR	49/49 (100%)	37 (76%)	12 (24%)	1	4
48	BS	79/79 (100%)	62 (78%)	17 (22%)	1	6
49	BT	72/72 (100%)	47 (65%)	25 (35%)	0	2
50	BU	96/96 (100%)	69 (72%)	27 (28%)	0	3
51	BV	64/64 (100%)	51 (80%)	13 (20%)	1	7
52	BW	71/71 (100%)	53 (75%)	18 (25%)	0	4
53	BX	76/76 (100%)	59 (78%)	17 (22%)	1	6
54	BY	19/19 (100%)	17 (90%)	2 (10%)	6	22
57	BZ	486/514 (95%)	340 (70%)	146 (30%)	0	2
All	All	5390/5418 (100%)	3811 (71%)	1579 (29%)	1	3

5 of 1579 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	BF	91	PRO
40	BK	113	GLU
35	BF	185	ILE
35	BF	84	GLU
37	BH	141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
37	BH	154	ASN
43	BN	56	HIS
38	BI	65	ASN
40	BK	106	GLN
44	BO	38	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2883/2889 (99%)	1269 (44%)	254 (8%)
2	AB	122/123 (99%)	46 (37%)	3 (2%)
34	BA	1514/1515 (99%)	484 (31%)	140 (9%)
55	BC	75/76 (98%)	26 (34%)	0
56	BD	74/75 (98%)	31 (41%)	2 (2%)
56	BE	74/75 (98%)	23 (31%)	1 (1%)
All	All	4742/4753 (99%)	1879 (39%)	400 (8%)

5 of 1879 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	13	A
1	AA	14	A
1	AA	15	G
1	AA	20	C
1	AA	26	G

5 of 400 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	2609	U
34	BA	308	C
56	BE	5	G

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Mol	Chain	Res	Type
1	AA	2689	U
34	BA	31	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands 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
58	NMY	AA	3001	-	43,45,45	0.49	0	62,67,67	1.21	7 (11%)
59	8AN	AA	3003	56	21,24,25	1.59	4 (19%)	26,35,38	2.30	10 (38%)
60	GCP	BZ	701	-	32,34,34	1.76	8 (25%)	49,54,54	1.83	8 (16%)
59	8AN	AA	3002	-	21,24,25	1.58	4 (19%)	26,35,38	2.28	10 (38%)
58	NMY	BA	1601	-	43,45,45	0.48	0	62,67,67	1.07	6 (9%)

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
58	NMY	AA	3001	-	-	4/18/94/94	1/4/4/4
59	8AN	AA	3003	56	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GCP	BZ	701	-	-	4/19/38/38	0/3/3/3
59	8AN	AA	3002	-	-	4/7/25/26	0/3/3/3
58	NMY	BA	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BZ	701	GCP	PG-O1G	5.57	1.61	1.50
59	AA	3003	8AN	C5-C4	4.75	1.47	1.39
59	AA	3002	8AN	C5-C4	4.68	1.47	1.39
60	BZ	701	GCP	C5-C4	3.22	1.47	1.38
60	BZ	701	GCP	PG-O2G	-2.94	1.48	1.55

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BZ	701	GCP	C5-C4-N3	-6.20	118.52	128.39
59	AA	3003	8AN	C5-C4-N3	-5.84	118.68	126.72
59	AA	3002	8AN	C5-C4-N3	-5.83	118.68	126.72
60	BZ	701	GCP	C2-N3-C4	5.10	121.09	112.30
59	AA	3003	8AN	N3-C4-N9	4.62	135.02	127.17

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C19-C18-O18-C15
58	BA	1601	NMY	O5-C5-C6-N6
58	BA	1601	NMY	C14-C13-O11-C11
59	AA	3003	8AN	C4'-C5'-O5'-P
59	AA	3003	8AN	O4'-C4'-C5'-O5'

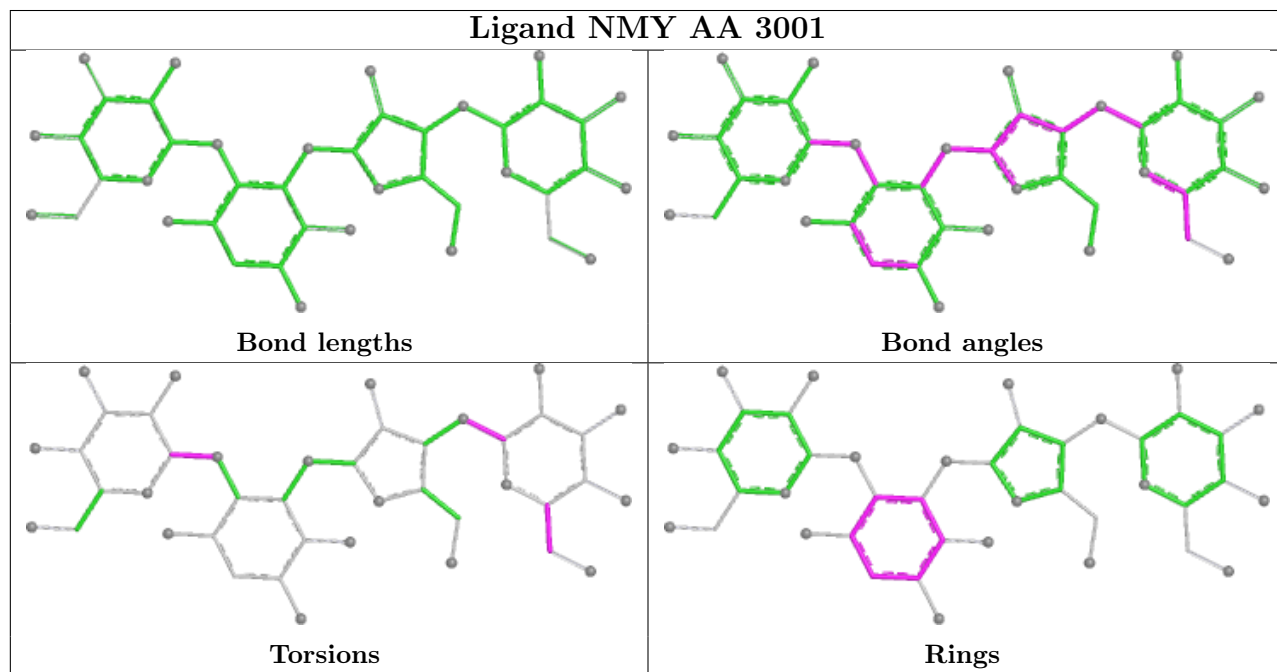
All (1) ring outliers are listed below:

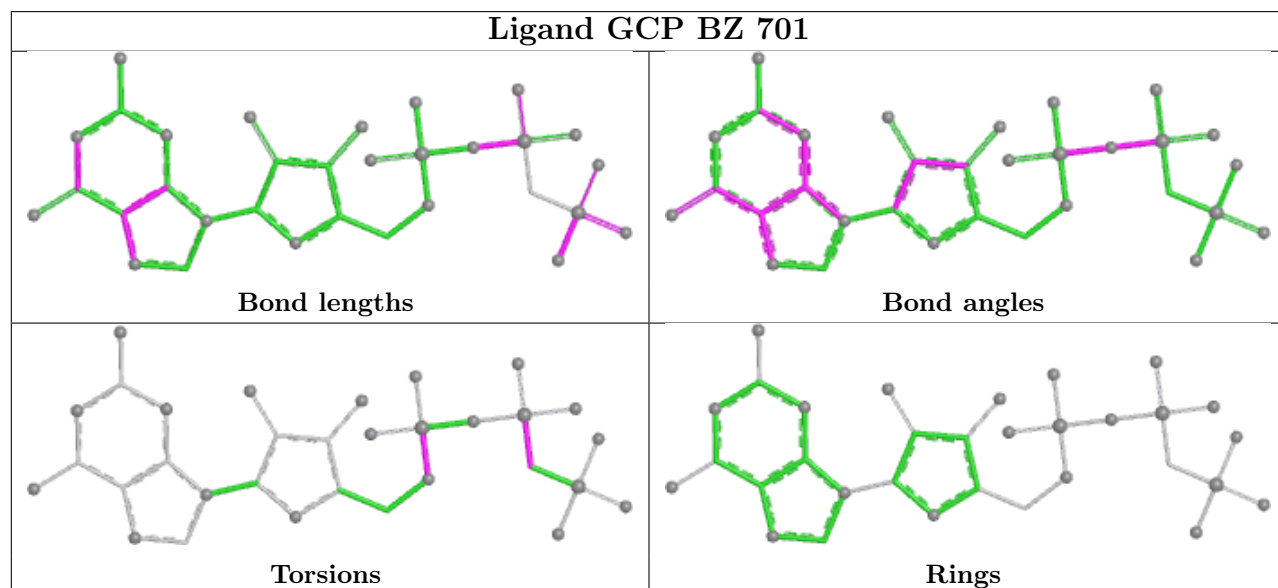
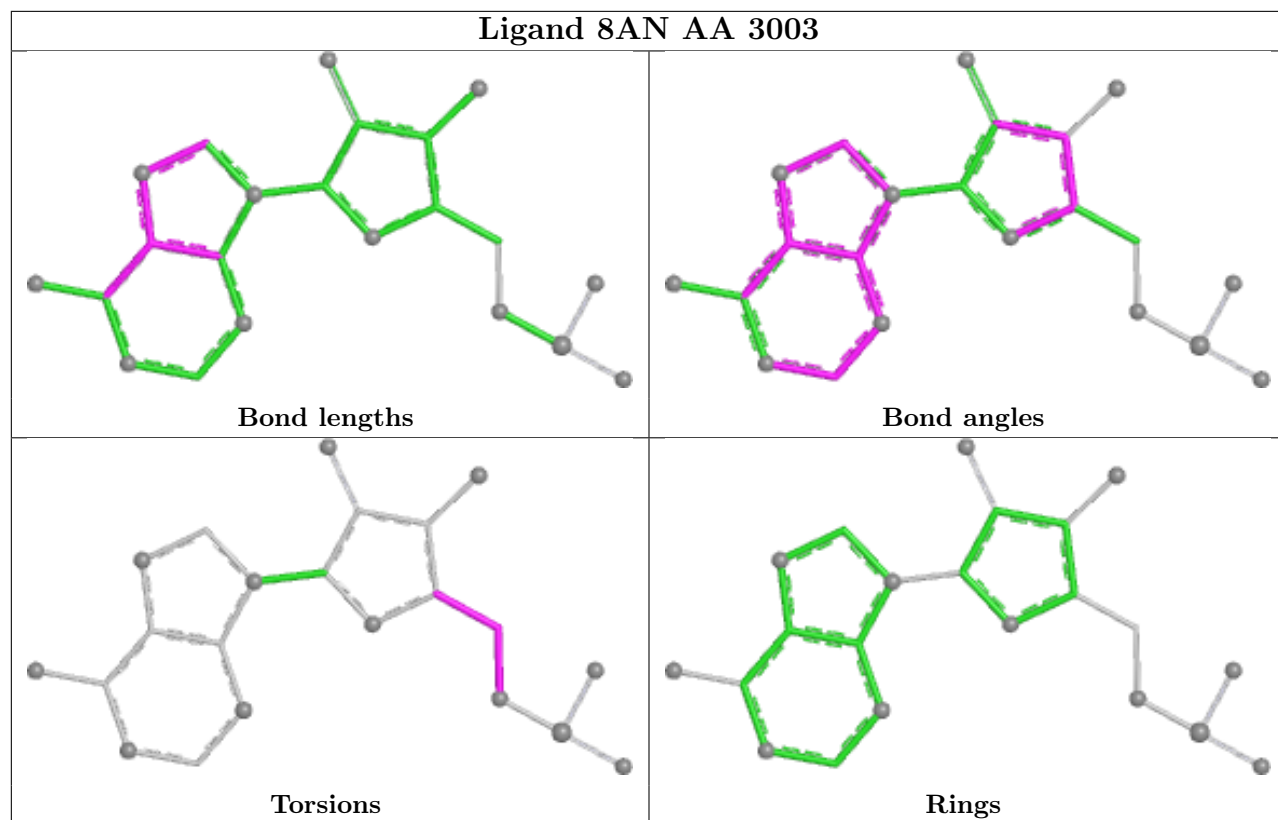
Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C10-C11-C12-C7-C8-C9

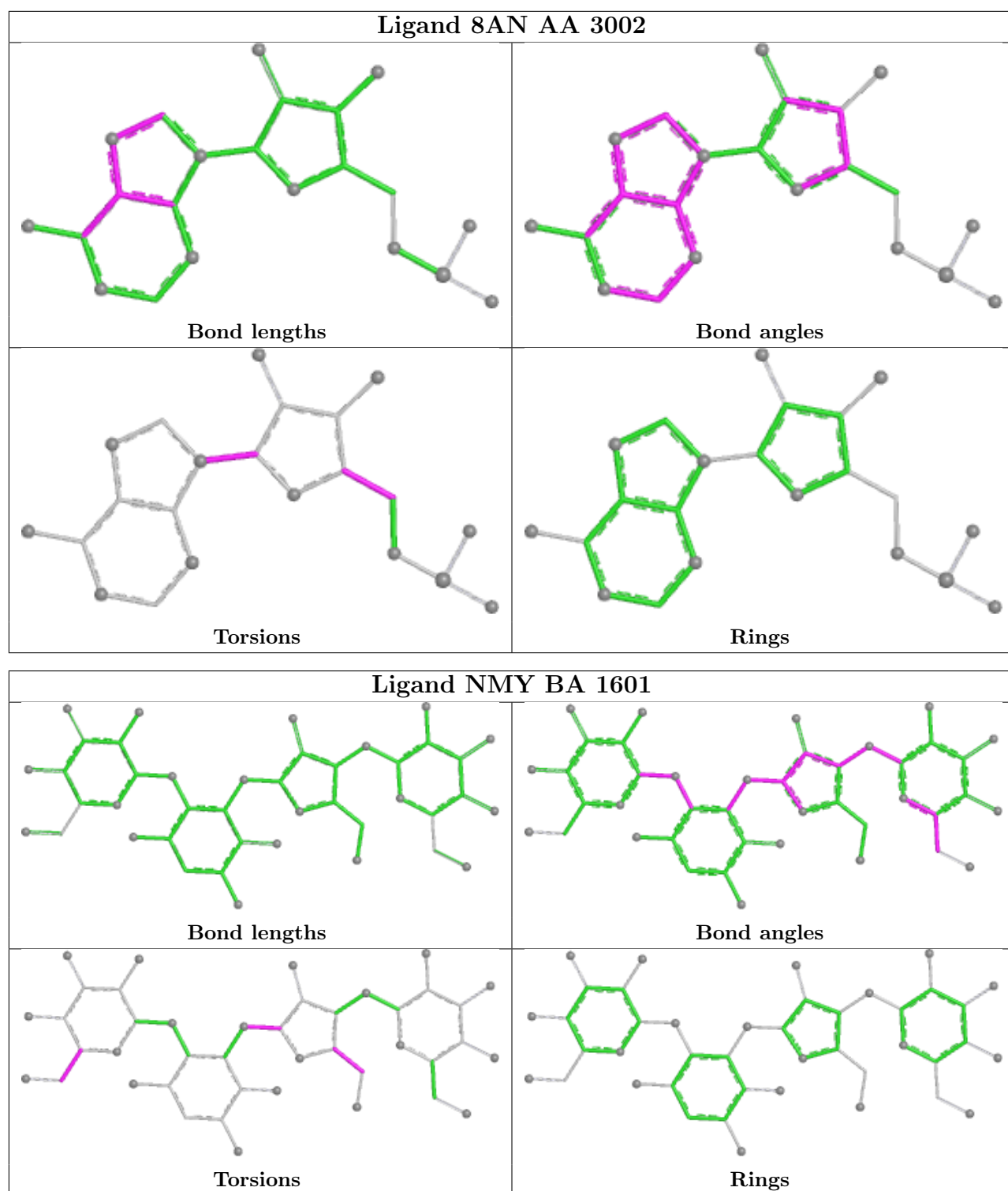
5 monomers are involved in 154 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AA	3001	NMY	20	0
59	AA	3003	8AN	35	0
60	BZ	701	GCP	39	0
59	AA	3002	8AN	45	0
58	BA	1601	NMY	15	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	10
3	AC	3
34	BA	3
33	Ag	2
31	AI	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ag	30:UNK	C	123:UNK	N	31.39
1	AA	164:U	O3'	171:G	P	7.68
1	AA	2893:G	O3'	2894:G	P	5.34
1	AA	2107:C	O3'	2108:C	P	4.97
1	AC	180:PHE	C	181:PRO	N	4.62

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6397. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.