



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:00 PM BST

PDB ID : 4V6N
EMDB ID: : EMD-5361
Title : Structural characterization of mRNA-tRNA translocation intermediates (50S ribosome of class2 of the six classes)
Authors : Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-12-07
Resolution : 12.10 Å (reported)
Based on PDB ID : 1ZAV, 1MZP, 2I2V

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

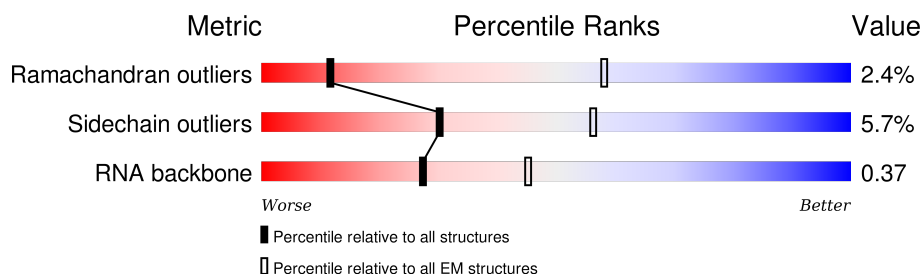
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 12.10 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)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	AA	120	35% 55% 10%
2	AB	2904	33% 54% 12%
3	AC	234	81% 18% .
4	AD	272	78% 18% .
5	AE	209	76% 18% . .
6	AF	201	78% 16% 5%
7	AG	178	66% 28% 7%
8	AH	176	81% 16% . .
9	AI	149	81% 15% 5%



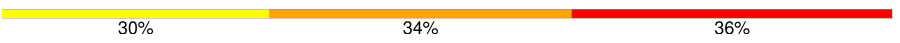







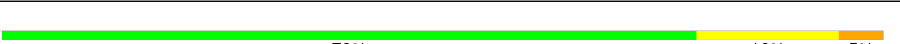
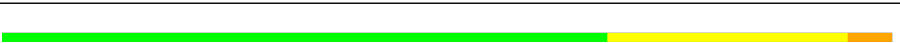




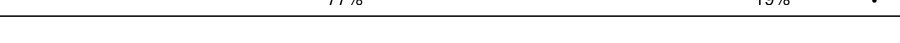
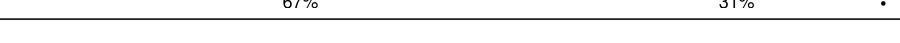
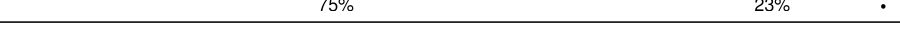
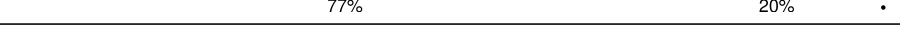

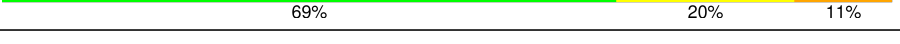


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Mol	Chain	Length	Quality of chain
10	AJ	164	 80% 18% .
11	AK	141	 84% 14% .
12	AL	142	 70% 25% 5%
13	AM	123	 74% 22% .
14	AN	144	 78% 20% .
15	AO	136	 79% 17% .
16	AP	127	 78% 20% .
17	AQ	117	 78% 20% .
18	AR	114	 74% 21% . .
19	AS	117	 78% 17% 5%
20	AT	103	 74% 23% .
21	AU	110	 72% 25% .
22	AV	100	 78% 21% .
23	AW	103	 77% 20% . .
24	AX	94	 84% 14% .
25	AY	84	 77% 18% 5%
26	AZ	77	 70% 25% 5%
27	A0	63	 79% 17% .
28	A1	58	 78% 21% .
29	A2	70	 77% 14% 9%
30	A3	56	 70% 21% 9%
31	A4	54	 72% 22% 6%
32	A5	46	 63% 33% .
33	A6	64	 80% 14% 6%
34	A7	38	 71% 29%

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Mol	Chain	Length	Quality of chain
35	BA	1542	
36	BB	76	
37	BC	47	
38	BD	77	
39	BE	240	
40	BF	232	
41	BG	205	
42	BH	166	
43	BI	135	
44	BJ	178	
45	BK	129	
46	BL	129	
47	BM	103	
48	BN	128	
49	BO	123	
50	BP	117	
51	BQ	100	
52	BR	88	
53	BS	82	
54	BT	83	
55	BU	74	
56	BV	91	
57	BW	86	
58	BX	70	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152351 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 36 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	BB	76	Total	C	N	O	P	S	0	0
			1627	731	287	532	75	2		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 38 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BD	77	Total	C	N	O	P	S	0	0
			1641	734	297	533	76	1		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BL	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BP	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

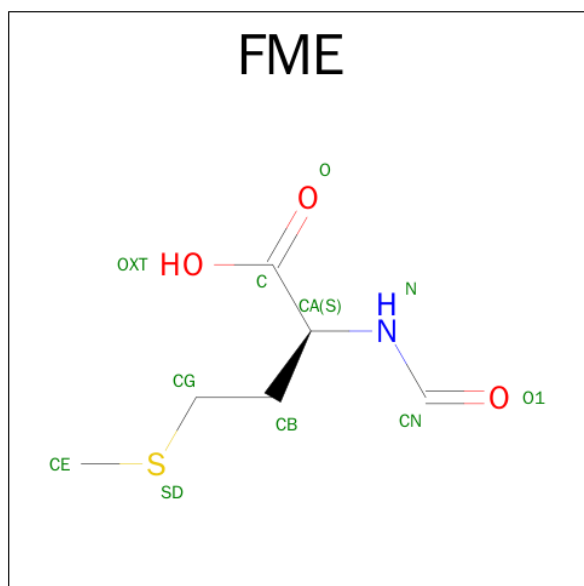
- Molecule 57 is a protein called 30S ribosomal protein S20.

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

- Molecule 58 is a protein called 30S ribosomal protein S21.

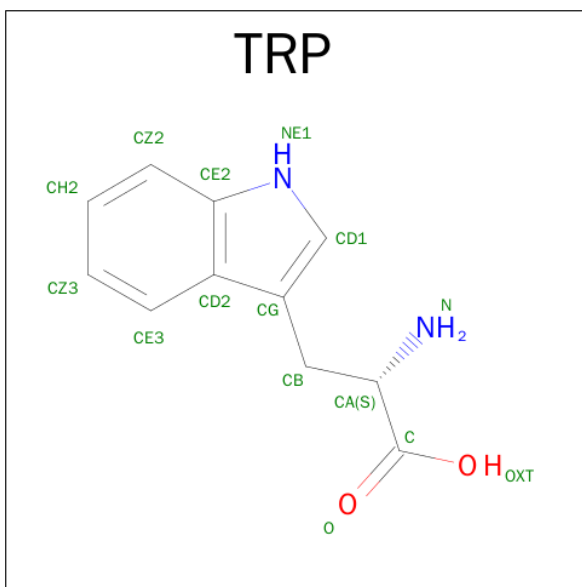
Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
59	AB	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).

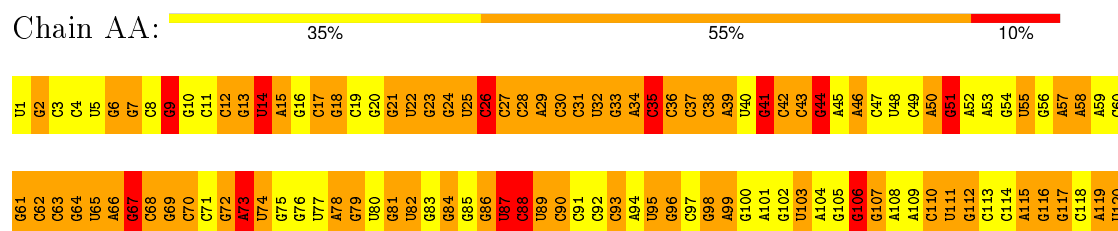


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	BB	1	14	11	2	1	0

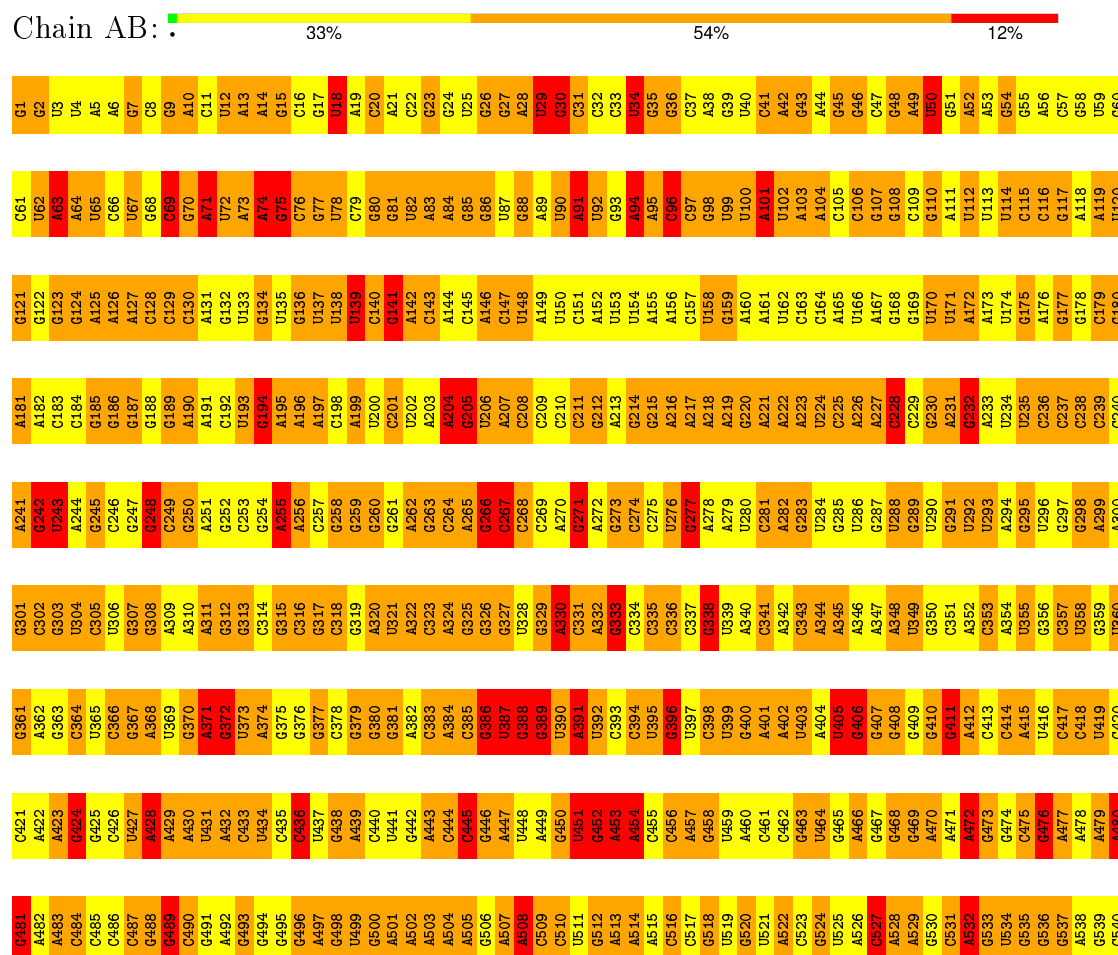
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5S ribosomal RNA

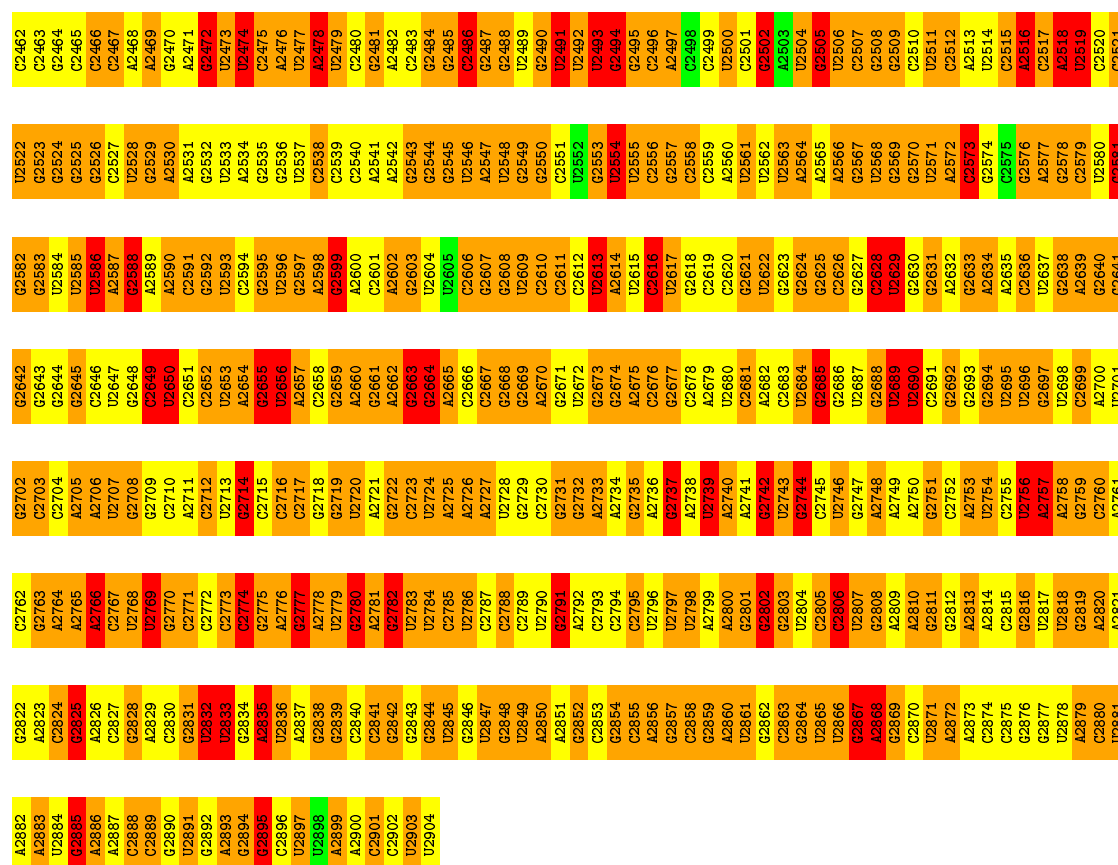


- Molecule 2: 23S ribosomal RNA

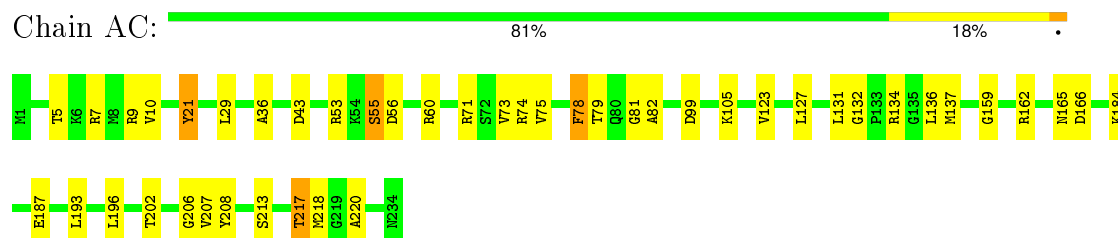


U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842	A782	A721	A661	G601	A541
U1443	A1383	C1323	U1263	U1203	A1143	U1083	U1023	U963	C903	G843	A783	A722	G662	A602	C541
U1444	A1384	A1264	A1264	A1204	A1144	A1084	G1024	C964	G904	A844	G784	C723	G663	A603	C543
G1445	A1385	U1325	A1265	A1205	C1145	A1085	G1025	C965	G905	A845	G785	U724	G664	G604	C544
U1446	C1386	G1326	G1266	G1206	C1146	A1086	A1026	G966	G906	U846	C786	G725	U665	G605	U545
G1447	A1387	A1327	U1267	G1207	A1147	G1087	G1027	U967	U907	U847	C787	G726	U666	U606	U546
U1448	A1388	A1328	A1268	C1208	U1148	A1088	A1028	C968	C908	C848	A788	A727	U667	U607	A547
G1449	G1389	A1329	A1269	U1209	G1149	A1089	C1029	G969	A909	U849	A789	G728	A668	A608	G548
G1450	U1390	C1330	C1270	G1210	C1150	A1090	A1030	U970	A910	U850	U790	G729	G669	A609	G549
C1451	U1391	G1331	G1271	C1211	A1151	G1091	G1031	G971	A911	C851	C791	A731	A670	C610	C550
A1453	A1392	A1332	A1272	G1212	C1152	C1092	A1032	A972	C912	U852	A792	C731	G671	C611	G551
C1454	A1393	G1333	U1273	A1213	G1153	U1093	U1033	A973	U913	C853	A793	G732	G672	G612	U552
U1455	G1394	G1334	A1274	A1214	G1154	U1094	G1034	G974	G914	C854	A794	G733	C673	A613	G553
A1456	A1395	C1335	A1275	G1215	A1155	A1095	U1035	A975	C915	G855	C795	A734	G674	A614	U554
G1457	U1396	A1336	G1276	G1216	A1156	A1096	G1036	G976	G916	G856	C796	A735	A675	U615	G555
U1458	G1397	G1337	A1277	U1217	G1157	U1097	G1037	G977	A917	C857	A797	G736	A676	A616	A556
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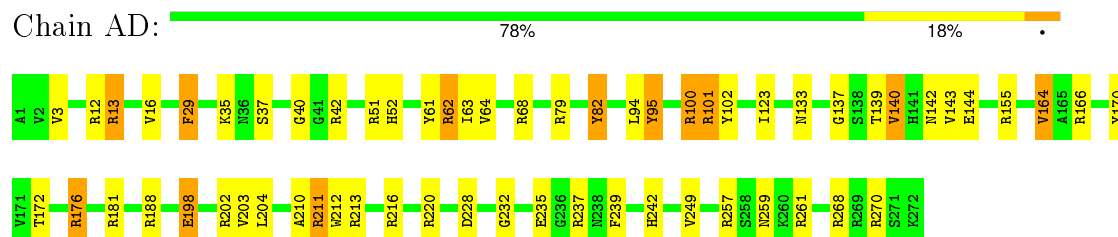
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G2445	G2385	G2325	U2265	A2205	C2145	U2085	C2025	G1965	G1845	A1785	A1665	C1605	A1545
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• Molecule 3: 50S ribosomal protein L1

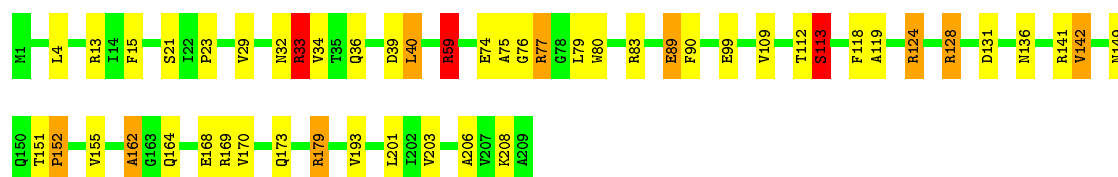


• Molecule 4: 50S ribosomal protein L2



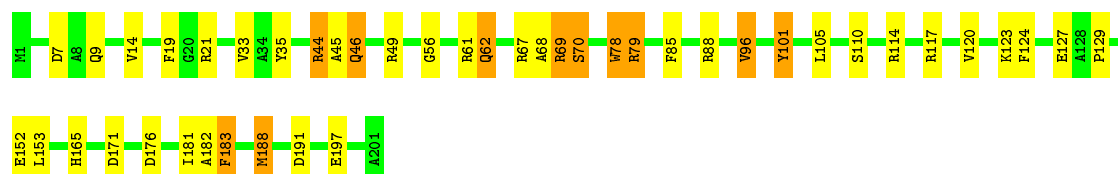
• Molecule 5: 50S ribosomal protein L3





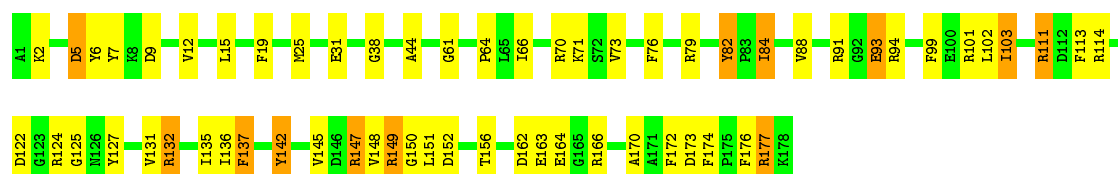
- Molecule 6: 50S ribosomal protein L4

Chain AF: 78% 16% 5%



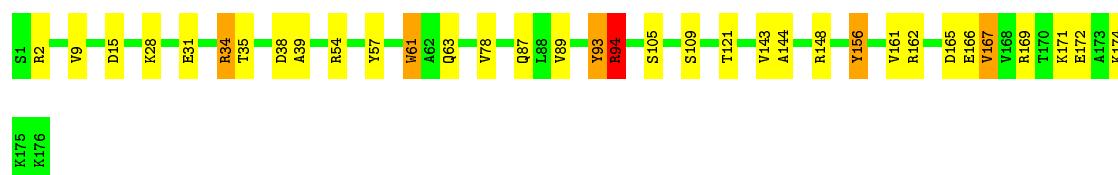
- Molecule 7: 50S ribosomal protein L5

Chain AG: 66% 28% 7%



- Molecule 8: 50S ribosomal protein L6

Chain AH: 81% 16% 3%



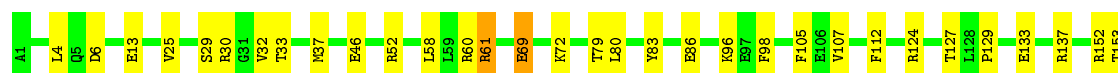
- Molecule 9: 50S ribosomal protein L9

Chain AI: 81% 15% 5%



- Molecule 10: 50S ribosomal protein L10

Chain AJ: 80% 18% 2%





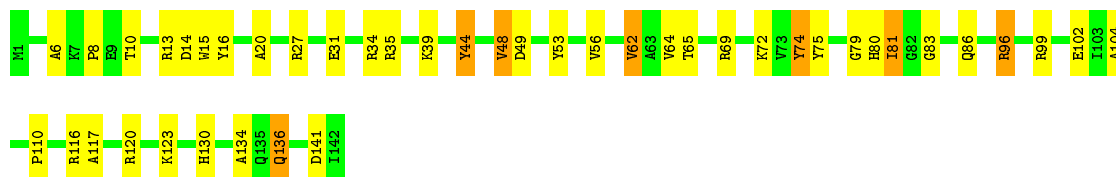
- Molecule 11: 50S ribosomal protein L11

Chain AK: 84% 14%



- Molecule 12: 50S ribosomal protein L13

Chain AL: 70% 25% 5%



- Molecule 13: 50S ribosomal protein L14

Chain AM: 74% 22%



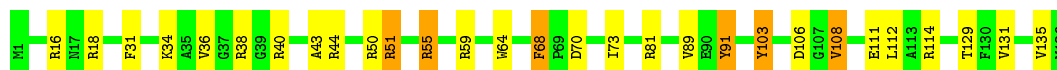
- Molecule 14: 50S ribosomal protein L15

Chain AN: 78% 20%



- Molecule 15: 50S ribosomal protein L16

Chain AO: 79% 17%



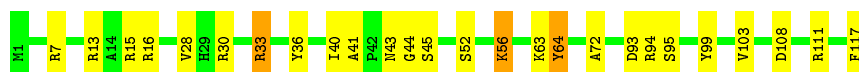
- Molecule 16: 50S ribosomal protein L17

Chain AP: 78% 20%



- Molecule 17: 50S ribosomal protein L18

Chain AQ: 78% 20%



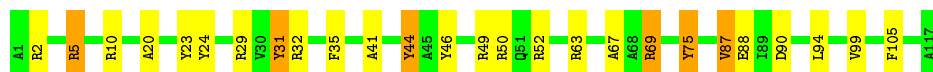
- Molecule 18: 50S ribosomal protein L19

Chain AR: 74% 21%



- Molecule 19: 50S ribosomal protein L20

Chain AS: 78% 17% 5%



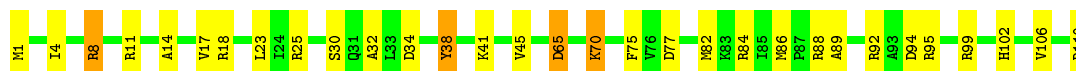
- Molecule 20: 50S ribosomal protein L21

Chain AT: 74% 23%



- Molecule 21: 50S ribosomal protein L22

Chain AU: 72% 25%



- Molecule 22: 50S ribosomal protein L23

Chain AV: 78% 21%



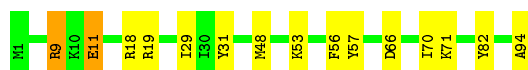
- Molecule 23: 50S ribosomal protein L24

Chain AW: 77% 20%

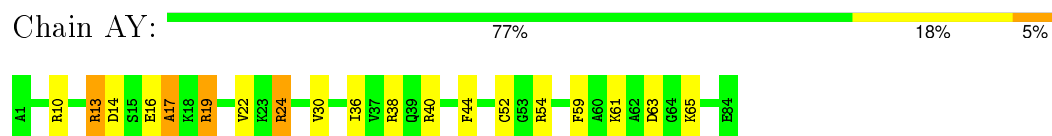


- Molecule 24: 50S ribosomal protein L25

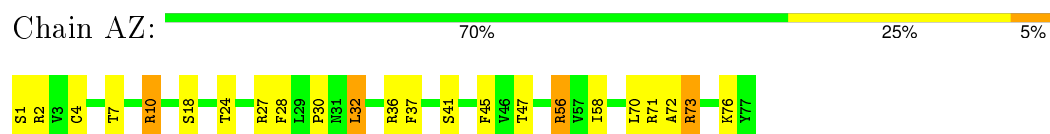
Chain AX: 84% 14%



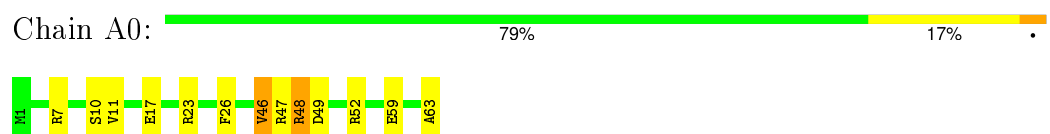
- Molecule 25: 50S ribosomal protein L27



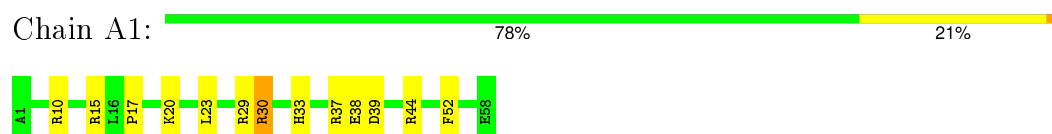
- Molecule 26: 50S ribosomal protein L28



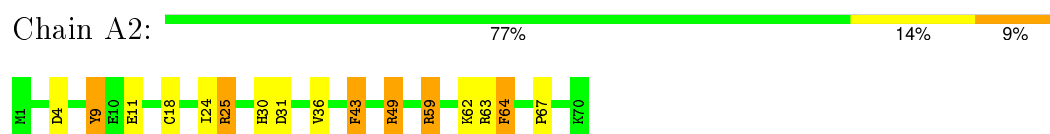
- Molecule 27: 50S ribosomal protein L29



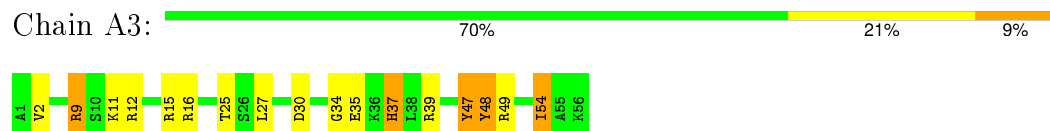
- Molecule 28: 50S ribosomal protein L30



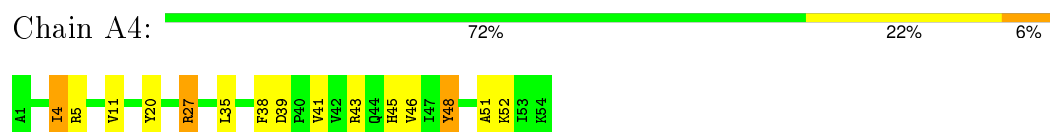
- Molecule 29: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33



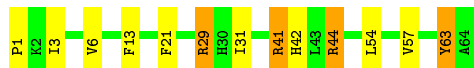
- Molecule 32: 50S ribosomal protein L34





- Molecule 33: 50S ribosomal protein L35

Chain A6: 80% 14% 6%



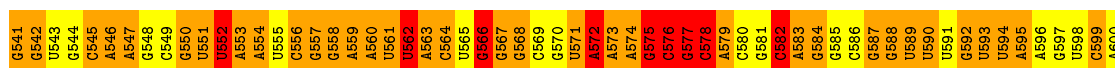
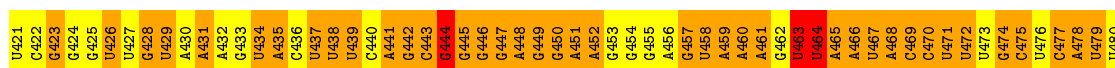
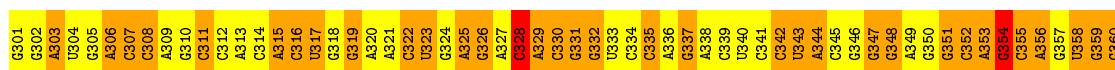
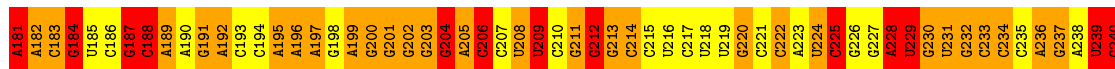
- Molecule 34: 50S ribosomal protein L36

Chain A7: 71% 29%



- Molecule 35: 16S ribosomal RNA

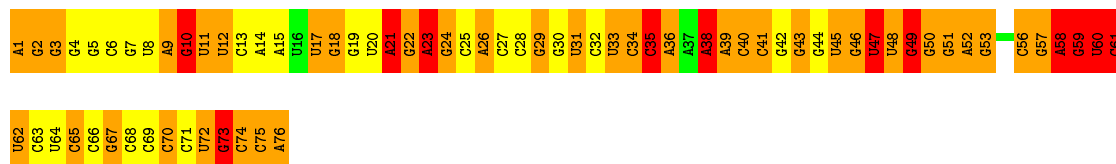
Chain BA: 32% 54% 14%



G1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C841	A781	G721	G661	G601
A1502	G1442	C1382	C1322	C1262	U1202	G1142	A1082	A1022	C962	G902	U842	A782	G722	U662	A602
G1503	C1443	C1383	G1323	C1263	U1203	G1143	U1083	U1023	G963	G903	U843	C783	U723	A663	U603
G1504	U1444	C1384	A1324	U1264	A1204	G1144	U1084	G1024	A964	U904	G844	A784	G724	G664	G604
G1505	U1445	G1385	C1325	C1265	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725	A665	U605
U1506	A1446	G1386	U1326	G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G786	G726	G666	G606
A1507	U1447	G1387	C1327	U1267	G1207	U1147	U1087	C1027	G967	A907	G847	A787	G727	G667	A607
A1508	C1448	C1388	A1328	G1268	C1208	U1148	U1088	C1028	A968	A908	C848	U788	A728	G668	A608
G1509	C1449	A1389	A1329	A1269	C1209	C1149	G1089	U1029	A969	A909	G849	A789	A729	G669	A609
C1510	U1450	U1390	U1330	C1270	C1210	A1150	U1090	U1030	C970	U910	U850	A790	G730	G670	U610
G1511	U1451	G1391	G1331	A1271	C1211	A1151	U1091	C1031	G971	U911	G851	A791	G731	G671	C611
U1512	C1452	G1392	A1332	C1272	U1212	A1152	A1092	G1032	G972	C912	G852	A792	C732	U672	C612
A1513	G1453	A1393	C1333	C1273	C1213	A1153	A1093	G1033	G973	A913	C853	U793	G733	A673	C613
G1514	G1454	A1394	G1334	A1274	C1214	G1154	G1094	G1034	A974	A914	U854	A794	G734	G674	C614
G1515	G1455	U1395	U1335	G1275	G1215	A1155	U1095	A1035	A975	A915	U855	C795	G735	A675	G615
G1516	A1456	A1396	C1336	G1276	A1216	G1156	C1096	A1036	G976	U916	C856	C796	C736	A676	G616
G1517	G1457	G1397	G1337	C1277	C1217	A1157	U1097	C1037	A977	G917	C857	C797	C737	U677	G617
G1520	G1459	A1398	G1338	G1278	C1218	G1158	C1098	C1038	A978	A918	G858	U798	C738	U678	C618
C1521	G1459	C1399	A1339	G1279	C1219	U1159	G1099	G1039	C979	A919	G859	C799	C739	G679	U619
U1522	C1460	A1400	A1340	A1280	G1220	G1160	C1100	U1040	C980	U920	A860	G800	U740	C680	G620
G1523	U1461	U1341	U1341	C1281	G1221	C1161	A1101	G1041	U981	U921	G861	U801	G741	A681	A621
G1524	C1462	C1342	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	C862	A802	G742	G682	A622
G1525	U1463	C1343	C1343	U1283	C1223	A1163	C1103	G1043	U983	A923	U863	G803	A743	G683	G623
G1526	U1464	C1344	C1344	U1284	U1224	G1164	A1104	A1044	C984	G924	A864	U804	G744	U684	C624
U1527	A1465	U1345	U1345	A1285	A1225	U1165	A1105	C1045	C985	G925	A865	C805	G745	G685	U625
U1528	C1466	U1406	A1346	U1286	C1226	G1166	G1106	A1046	U986	G926	C866	C806	A746	U686	G626
G1529	U1467	G1407	G1347	A1287	A1227	A1167	C1107	G1047	G987	G927	G867	A807	A747	A687	G627
G1530	A1468	A1408	U1348	A1288	C1228	U1168	G1108	G1048	G988	G928	C868	C808	G748	G688	G628
A1531	C1469	C1409	A1349	A1289	A1229	A1169	C1109	U1049	U989	G929	G869	G809	A749	C689	A629
U1532	U1470	A1410	A1350	G1290	C1230	A1170	A1110	G1050	C990	C930	U870	C810	C750	G690	A630
C1533	U1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	U871	C811	U751	G691	C631
A1534	U1472	C1412	C1352	C1292	G1232	C1172	C1112	U1052	U992	C932	A872	C812	G752	U692	U632
C1535	G1473	A1413	G1353	C1293	G1233	U1173	C1113	G1053	G993	G933	A873	C813	A753	G693	G633
G1536	U1474	U1414	U1354	U1294	C1234	G1174	C1114	C1054	A994	C934	G874	A814	C754	A694	C634
U1537	G1475	G1415	G1355	U1295	U1235	G1175	A1115	A1055	C995	A935	U875	A815	G755	A695	A635
C1538	A1476	G1416	G1356	C1296	A1236	A1176	U1116	U1056	A996	C936	C876	A816	C756	A696	U636
C1539	U1477	G1417	A1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G877	C817	U757	U697	C637
U1540	U1478	A1418	U1358	U1298	A1238	G1178	U1118	G1058	C998	A938	A878	C818	C758	G698	U638
U1541	C1479	G1419	C1359	A1299	A1239	A1179	C1119	C1059	C999	G939	C879	A819	A759	C699	G639
A1542	A1480	U1420	A1360	G1300	U1240	A1180	C1120	U1060	A1000	C940	U820	U820	G760	G700	A640
G1481	U1481	G1421	G1361	U1301	G1241	G1181	U1121	G1061	C1001	G941	C881	G821	G761	U701	U641
G1482	G1482	G1422	A1362	C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	U822	U762	A702	A642
A1483	G1483	G1423	C1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	G823	G763	G703	C643
U1484	U1484	U1424	U1364	G1304	G1244	G1184	U1124	G1064	A1004	G944	U884	G824	C764	A704	U644
U1485	U1485	U1425	G1365	C1305	C1245	G1185	U1125	U1065	A1005	G945	G885	A825	G765	G705	G645
G1486	G1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	C826	A766	A706	G646
G1487	G1487	C1427	C1367	U1307	U1247	G1187	G1127	A1067	U1007	G947	G887	U827	A767	U707	C647
G1488	G1488	A1428	A1368	U1308	A1248	A1188	C1128	G1068	U1008	C948	G888	U828	A768	C708	A648
U1489	G1489	A1429	C1369	G1309	C1249	U1189	C1129	C1069	U1009	A949	A889	G829	G769	U709	A649
U1490	U1490	A1430	G1370	G1310	A1250	G1190	A1130	U1070	U1010	U950	G890	G830	C770	G710	G650
G1491	G1491	A1431	G1371	A1311	A1251	A1191	G1131	C1071	C1011	G951	U891	A831	U771	G711	C651
A1492	A1492	G1432	U1372	G1312	A1252	A1192	C1132	G1072	A1012	U952	A892	G832	U772	A712	U652
A1493	A1493	C1373	G1373	G1253	G1253	G1193	G1133	U1073	G1013	G953	C893	G833	G773	G713	U653
G1494	G1494	A1434	A1374	C1314	C1254	U1194	G1134	G1074	A1014	G954	G894	U834	G774	G714	G654
U1495	U1495	G1435	A1375	G1315	G1255	C1195	U1135	U1075	G1015	U955	G895	U835	G775	A715	A655
C1496	U1496	U1436	G1376	G1316	A1256	A1196	C1136	U1076	U1016	U956	C896	G836	G776	A716	G656
G1497	G1497	A1437	A1377	C1317	A1257	A1197	C1137	G1077	U1017	U957	C897	U837	A777	U717	U657
U1498	U1498	G1378	C1378	G1258	G1258	G1198	G1138	U1078	G1018	A958	G898	G838	G778	A718	C658
G1499	G1499	G1439	G1379	A1319	C1259	U1199	G1139	G1079	A1019	A959	C899	G839	C779	A719	U659
A1500	A1500	U1440	U1380	C1320	G1260	C1200	C1140	A1080	G1020	U960	A900	C840	A780	C720	G660

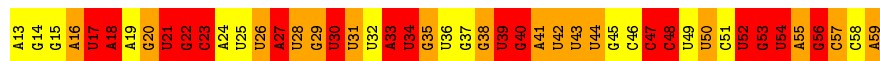
• Molecule 36: A site tRNA

Chain BB:  5% 30% 49% 16%



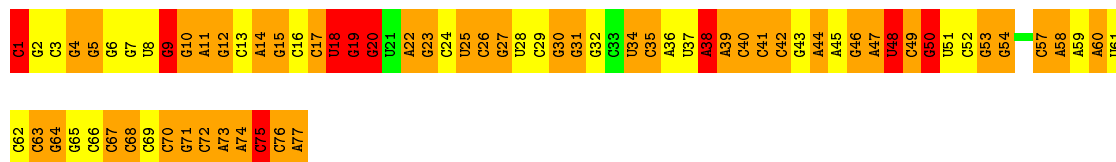
- Molecule 37: mRNA

Chain BC:  30% 34% 36%




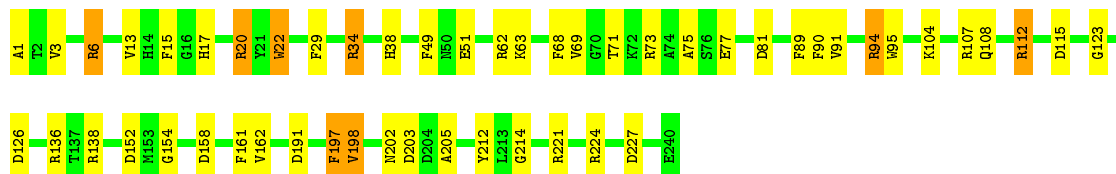
- Molecule 38: P site tRNA

Chain BD:  5% 30% 53% 12%




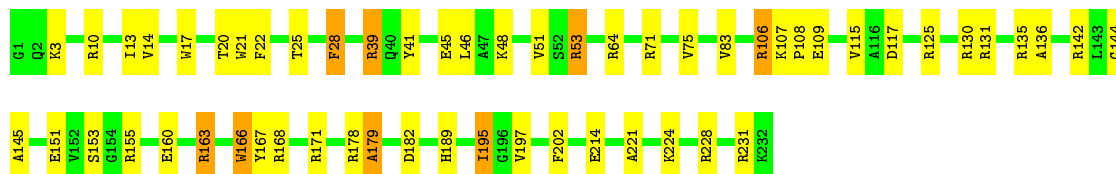
- Molecule 39: 30S ribosomal protein S2

Chain BE:  78% 18%




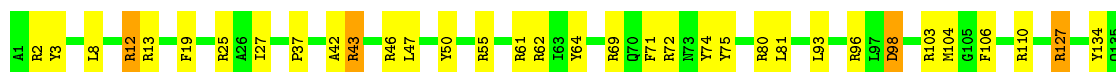
- Molecule 40: 30S ribosomal protein S3

Chain BF:  76% 21%



- Molecule 41: 30S ribosomal protein S4

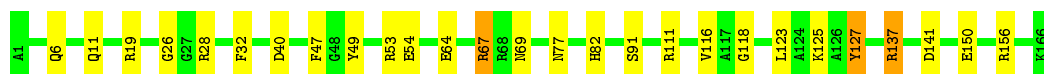
Chain BG:  76% 21%





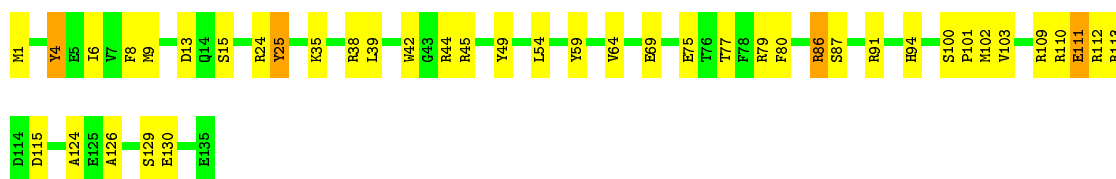
- Molecule 42: 30S ribosomal protein S5

Chain BH: 84% 14% •



- Molecule 43: 30S ribosomal protein S6

Chain BI: 69% 28% •



- Molecule 44: 30S ribosomal protein S7

Chain BJ: 75% 23% ••



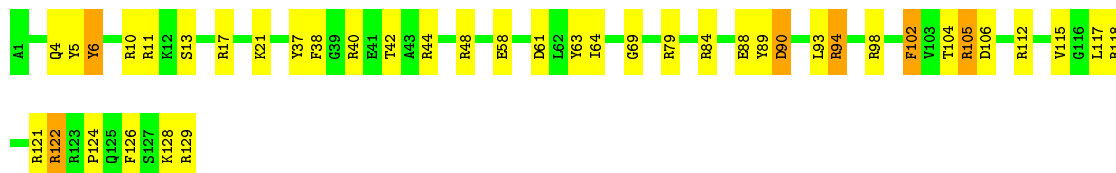
- Molecule 45: 30S ribosomal protein S8

Chain BK: 78% 16% 5%



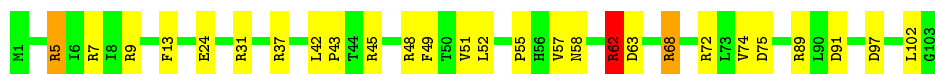
- Molecule 46: 30S ribosomal protein S9

Chain BL: 68% 27% 5%



- Molecule 47: 30S ribosomal protein S10

Chain BM: 74% 23% ••



- Molecule 48: 30S ribosomal protein S11

Chain BN: 77% 18% 5%



- Molecule 49: 30S ribosomal protein S12

Chain BO: 74% 23% 3%



- Molecule 50: 30S ribosomal protein S13

Chain BP: 77% 19% 4%



- Molecule 51: 30S ribosomal protein S14

Chain BQ: 67% 31% 2%



- Molecule 52: 30S ribosomal protein S15

Chain BR: 75% 23% 2%



- Molecule 53: 30S ribosomal protein S16

Chain BS: 77% 20% 3%

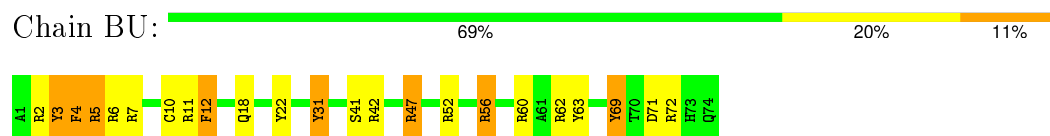


- Molecule 54: 30S ribosomal protein S17

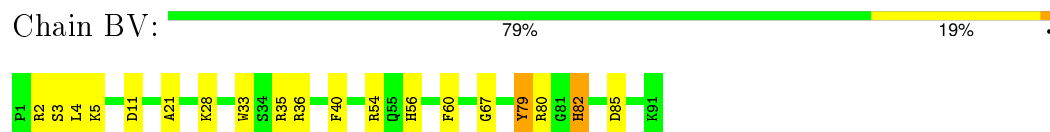
Chain BT: 75% 24% 1%



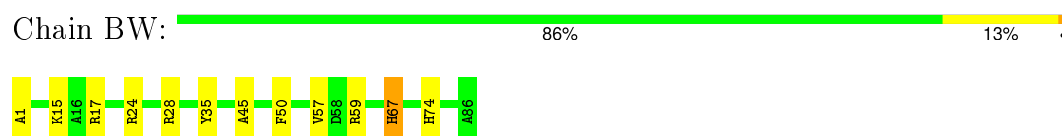
- Molecule 55: 30S ribosomal protein S18



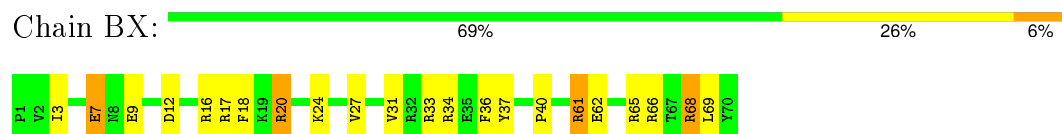
- Molecule 56: 30S ribosomal protein S19



- Molecule 57: 30S ribosomal protein S20



- Molecule 58: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	36204	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TemCam-F415 (CCD)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MU, CH, OMG, OMU, MA6, MIA, OMC, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, FME, 4SU, 7MG, 1MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	AA	3.14	330/2869 (11.5%)	3.60	681/4474 (15.2%)
10	AJ	1.56	7/1247 (0.6%)	1.92	21/1679 (1.3%)
11	AK	1.50	3/1046 (0.3%)	1.84	19/1410 (1.3%)
12	AL	1.52	7/1152 (0.6%)	1.94	33/1551 (2.1%)
13	AM	1.41	1/956 (0.1%)	1.89	24/1279 (1.9%)
14	AN	1.52	2/1062 (0.2%)	1.98	27/1413 (1.9%)
15	AO	1.48	2/1093 (0.2%)	2.19	34/1460 (2.3%)
16	AP	1.48	4/1021 (0.4%)	2.00	21/1364 (1.5%)
17	AQ	1.49	3/910 (0.3%)	1.93	24/1219 (2.0%)
18	AR	1.56	6/929 (0.6%)	2.07	25/1242 (2.0%)
19	AS	1.57	5/960 (0.5%)	2.21	34/1278 (2.7%)
2	AB	3.07	7254/69257 (10.5%)	3.51	15515/108040 (14.4%)
20	AT	1.56	1/829 (0.1%)	1.93	19/1107 (1.7%)
21	AU	1.47	4/864 (0.5%)	2.01	27/1156 (2.3%)
22	AV	1.49	4/794 (0.5%)	1.86	17/1060 (1.6%)
23	AW	1.53	4/797 (0.5%)	1.94	20/1062 (1.9%)
24	AX	1.46	2/766 (0.3%)	1.80	14/1025 (1.4%)
25	AY	1.51	0/642	1.97	16/848 (1.9%)
26	AZ	1.57	3/635 (0.5%)	2.13	20/848 (2.4%)
27	A0	1.51	1/510 (0.2%)	1.90	10/677 (1.5%)
28	A1	1.41	1/453 (0.2%)	2.05	17/605 (2.8%)
29	A2	1.55	1/559 (0.2%)	2.18	16/745 (2.1%)
3	AC	1.50	7/1748 (0.4%)	1.83	37/2355 (1.6%)
30	A3	1.53	4/450 (0.9%)	2.15	17/599 (2.8%)
31	A4	1.50	0/448	1.96	12/594 (2.0%)
32	A5	1.49	4/380 (1.1%)	2.28	17/498 (3.4%)
33	A6	1.49	3/513 (0.6%)	1.89	11/676 (1.6%)
34	A7	1.42	1/303 (0.3%)	2.16	11/397 (2.8%)
35	BA	3.10	3971/36769 (10.8%)	3.53	8378/57354 (14.6%)
36	BB	3.03	178/1600 (11.1%)	3.53	372/2492 (14.9%)
37	BC	3.13	119/1108 (10.7%)	3.48	238/1724 (13.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BD	3.05	179/1721 (10.4%)	3.56	400/2683 (14.9%)
39	BE	1.49	8/1904 (0.4%)	1.96	46/2565 (1.8%)
4	AD	1.51	4/2131 (0.2%)	1.99	62/2863 (2.2%)
40	BF	1.49	6/1852 (0.3%)	1.99	48/2490 (1.9%)
41	BG	1.57	9/1665 (0.5%)	2.08	56/2227 (2.5%)
42	BH	1.50	5/1239 (0.4%)	1.87	27/1664 (1.6%)
43	BI	1.55	5/1121 (0.4%)	2.04	41/1509 (2.7%)
44	BJ	1.54	8/1422 (0.6%)	1.94	39/1908 (2.0%)
45	BK	1.42	7/989 (0.7%)	1.98	21/1326 (1.6%)
46	BL	1.56	8/1048 (0.8%)	2.24	44/1394 (3.2%)
47	BM	1.49	3/835 (0.4%)	2.00	25/1127 (2.2%)
48	BN	1.48	2/982 (0.2%)	2.08	28/1323 (2.1%)
49	BO	1.52	4/969 (0.4%)	1.90	23/1300 (1.8%)
5	AE	1.50	6/1586 (0.4%)	1.92	28/2134 (1.3%)
50	BP	1.52	5/919 (0.5%)	2.05	25/1226 (2.0%)
51	BQ	1.62	9/817 (1.1%)	2.10	30/1088 (2.8%)
52	BR	1.47	1/724 (0.1%)	2.09	29/966 (3.0%)
53	BS	1.52	1/659 (0.2%)	2.18	22/884 (2.5%)
54	BT	1.55	4/681 (0.6%)	2.06	19/913 (2.1%)
55	BU	1.55	4/637 (0.6%)	2.18	28/851 (3.3%)
56	BV	1.52	2/744 (0.3%)	1.90	13/995 (1.3%)
57	BW	1.49	2/676 (0.3%)	1.78	7/895 (0.8%)
58	BX	1.58	2/598 (0.3%)	2.02	22/792 (2.8%)
6	AF	1.47	5/1571 (0.3%)	1.92	37/2113 (1.8%)
7	AG	1.60	10/1444 (0.7%)	2.03	49/1937 (2.5%)
8	AH	1.53	3/1343 (0.2%)	1.92	28/1816 (1.5%)
9	AI	1.45	3/1122 (0.3%)	1.96	24/1515 (1.6%)
All	All	2.70	12237/164069 (7.5%)	3.17	26948/244735 (11.0%)

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	68
10	AJ	0	3
11	AK	0	2
12	AL	0	4
13	AM	0	5
14	AN	0	4
15	AO	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	AP	0	8
17	AQ	0	2
18	AR	0	7
19	AS	0	5
2	AB	0	1652
20	AT	0	5
21	AU	0	2
22	AV	0	1
23	AW	0	1
24	AX	0	1
25	AY	0	7
26	AZ	0	2
27	A0	0	4
28	A1	0	1
29	A2	0	3
3	AC	0	2
30	A3	0	3
31	A4	0	2
33	A6	0	5
35	BA	0	910
36	BB	0	37
37	BC	0	28
38	BD	0	45
39	BE	0	4
4	AD	0	11
40	BF	0	7
41	BG	0	2
42	BH	0	3
43	BI	0	5
44	BJ	0	6
45	BK	0	4
46	BL	0	4
47	BM	0	2
48	BN	0	3
49	BO	0	8
5	AE	0	11
50	BP	0	2
51	BQ	0	3
52	BR	0	1
53	BS	0	4
54	BT	0	1
55	BU	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	BV	0	4
57	BW	0	2
58	BX	0	3
6	AF	0	3
7	AG	0	8
8	AH	0	5
9	AI	0	3
All	All	0	2936

The worst 5 of 12237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	2225	A	N3-C4	18.05	1.45	1.34
2	AB	2615	U	C2-N3	17.29	1.49	1.37
35	BA	729	A	P-O5'	15.61	1.75	1.59
2	AB	1970	A	N9-C4	15.52	1.47	1.37
2	AB	1008	A	N3-C4	15.09	1.44	1.34

The worst 5 of 26948 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2855	C	N3-C4-C5	-23.45	112.52	121.90
2	AB	1264	A	N9-C4-C5	22.40	114.76	105.80
29	A2	25	ARG	NE-CZ-NH1	21.63	131.12	120.30
2	AB	248	G	C2-N3-C4	20.59	122.19	111.90
2	AB	6	A	C8-N9-C4	-20.57	97.57	105.80

There are no chirality outliers.

5 of 2936 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	C	Sidechain
1	AA	2	G	Sidechain
1	AA	6	G	Sidechain
1	AA	7	G	Sidechain
1	AA	9	G	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2566	0	1294	0	0
2	AB	62351	0	31238	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1233	0	1283	0	0
11	AK	1032	0	1088	0	0
12	AL	1129	0	1162	0	0
13	AM	947	0	1023	0	0
14	AN	1053	0	1129	0	0
15	AO	1074	0	1157	0	0
16	AP	1008	0	1045	0	0
17	AQ	900	0	935	0	0
18	AR	917	0	965	0	0
19	AS	947	0	1022	0	0
20	AT	816	0	839	0	0
21	AU	857	0	922	0	0
22	AV	787	0	846	0	0
23	AW	789	0	847	0	0
24	AX	753	0	780	0	0
25	AY	634	0	656	0	0
26	AZ	625	0	655	0	0
27	A0	509	0	543	0	0
28	A1	449	0	491	0	0
29	A2	549	0	552	0	0
30	A3	444	0	461	0	0
31	A4	441	0	485	0	0
32	A5	377	0	418	0	0
33	A6	504	0	574	0	0
34	A7	302	0	343	0	0
35	BA	33089	0	16604	0	0
36	BB	1627	0	845	0	0
37	BC	993	0	499	0	0
38	BD	1641	0	841	0	0
39	BE	1872	0	1885	0	0
40	BF	1822	0	1913	0	0
41	BG	1643	0	1710	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BH	1225	0	1273	0	0
43	BI	1101	0	1050	0	0
44	BJ	1400	0	1449	0	0
45	BK	979	0	1034	0	0
46	BL	1036	0	1084	0	0
47	BM	825	0	865	0	0
48	BN	965	0	997	0	0
49	BO	955	0	1019	0	0
50	BP	910	0	981	0	0
51	BQ	805	0	847	0	0
52	BR	716	0	742	0	0
53	BS	649	0	666	0	0
54	BT	672	0	716	0	0
55	BU	626	0	651	0	0
56	BV	727	0	768	0	0
57	BW	670	0	722	0	0
58	BX	590	0	631	0	0
59	AB	10	0	10	0	0
60	BB	14	0	9	0	0
All	All	152351	0	103775	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	232/234 (99%)	214 (92%)	12 (5%)	6 (3%)	7 45
4	AD	270/272 (99%)	237 (88%)	24 (9%)	9 (3%)	5 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	207/209 (99%)	171 (83%)	28 (14%)	8 (4%)	4	36
6	AF	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	33
7	AG	176/178 (99%)	151 (86%)	16 (9%)	9 (5%)	2	30
8	AH	174/176 (99%)	158 (91%)	13 (8%)	3 (2%)	11	55
9	AI	147/149 (99%)	131 (89%)	10 (7%)	6 (4%)	3	35
10	AJ	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	30	74
11	AK	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
12	AL	140/142 (99%)	119 (85%)	16 (11%)	5 (4%)	4	38
13	AM	121/123 (98%)	107 (88%)	9 (7%)	5 (4%)	3	35
14	AN	142/144 (99%)	127 (89%)	12 (8%)	3 (2%)	9	50
15	AO	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	49
16	AP	125/127 (98%)	114 (91%)	10 (8%)	1 (1%)	24	69
17	AQ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
18	AR	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	11	53
19	AS	115/117 (98%)	107 (93%)	4 (4%)	4 (4%)	4	39
20	AT	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9	51
21	AU	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	6	44
22	AV	98/100 (98%)	75 (76%)	20 (20%)	3 (3%)	5	42
23	AW	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	9	51
24	AX	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	17	63
25	AY	82/84 (98%)	63 (77%)	17 (21%)	2 (2%)	7	47
26	AZ	75/77 (97%)	66 (88%)	7 (9%)	2 (3%)	6	45
27	A0	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	56
28	A1	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
29	A2	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	13	57
30	A3	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	28
31	A4	52/54 (96%)	49 (94%)	1 (2%)	2 (4%)	4	37
32	A5	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	3	33
33	A6	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	12	56
34	A7	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	28
39	BE	238/240 (99%)	220 (92%)	12 (5%)	6 (2%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BF	230/232 (99%)	217 (94%)	8 (4%)	5 (2%)	8	49
41	BG	203/205 (99%)	189 (93%)	11 (5%)	3 (2%)	13	57
42	BH	164/166 (99%)	149 (91%)	13 (8%)	2 (1%)	16	61
43	BI	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	24	69
44	BJ	176/178 (99%)	164 (93%)	9 (5%)	3 (2%)	11	55
45	BK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	24	69
46	BL	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	7	47
47	BM	101/103 (98%)	90 (89%)	6 (6%)	5 (5%)	3	31
48	BN	126/128 (98%)	112 (89%)	11 (9%)	3 (2%)	7	47
49	BO	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	11	55
50	BP	115/117 (98%)	110 (96%)	3 (3%)	2 (2%)	11	55
51	BQ	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2	30
52	BR	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	16	61
53	BS	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
54	BT	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	16	61
55	BU	72/74 (97%)	62 (86%)	7 (10%)	3 (4%)	3	34
56	BV	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	17	63
57	BW	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	16	61
58	BX	68/70 (97%)	61 (90%)	4 (6%)	3 (4%)	3	33
All	All	6319/6423 (98%)	5710 (90%)	457 (7%)	152 (2%)	12	47

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	217	THR
4	AD	94	LEU
6	AF	62	GLN
6	AF	188	MET
7	AG	136	ILE

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	
3	AC	181/181 (100%)	177 (98%)	4 (2%)	60	83
4	AD	217/217 (100%)	212 (98%)	5 (2%)	58	83
5	AE	164/164 (100%)	148 (90%)	16 (10%)	10	39
6	AF	165/165 (100%)	156 (94%)	9 (6%)	27	63
7	AG	149/149 (100%)	140 (94%)	9 (6%)	24	60
8	AH	137/137 (100%)	125 (91%)	12 (9%)	12	45
9	AI	114/114 (100%)	107 (94%)	7 (6%)	23	60
10	AJ	122/122 (100%)	111 (91%)	11 (9%)	12	44
11	AK	109/109 (100%)	104 (95%)	5 (5%)	33	68
12	AL	116/116 (100%)	104 (90%)	12 (10%)	9	37
13	AM	104/104 (100%)	96 (92%)	8 (8%)	16	52
14	AN	103/103 (100%)	98 (95%)	5 (5%)	31	67
15	AO	109/109 (100%)	106 (97%)	3 (3%)	51	78
16	AP	103/103 (100%)	100 (97%)	3 (3%)	50	78
17	AQ	87/87 (100%)	81 (93%)	6 (7%)	19	56
18	AR	99/99 (100%)	91 (92%)	8 (8%)	15	50
19	AS	89/89 (100%)	87 (98%)	2 (2%)	60	83
20	AT	84/84 (100%)	77 (92%)	7 (8%)	14	49
21	AU	93/93 (100%)	87 (94%)	6 (6%)	21	58
22	AV	84/84 (100%)	80 (95%)	4 (5%)	31	67
23	AW	84/84 (100%)	79 (94%)	5 (6%)	24	60
24	AX	78/78 (100%)	74 (95%)	4 (5%)	29	66
25	AY	62/62 (100%)	60 (97%)	2 (3%)	46	76
26	AZ	67/67 (100%)	61 (91%)	6 (9%)	12	44
27	A0	55/55 (100%)	52 (94%)	3 (6%)	27	63
28	A1	48/48 (100%)	46 (96%)	2 (4%)	36	70
29	A2	62/62 (100%)	56 (90%)	6 (10%)	10	40
30	A3	47/47 (100%)	45 (96%)	2 (4%)	35	70
31	A4	48/48 (100%)	44 (92%)	4 (8%)	14	49
32	A5	38/38 (100%)	34 (90%)	4 (10%)	8	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	A6	51/51 (100%)	50 (98%)	1 (2%)	63	85
34	A7	34/34 (100%)	33 (97%)	1 (3%)	50	78
39	BE	198/198 (100%)	187 (94%)	11 (6%)	26	62
40	BF	189/189 (100%)	176 (93%)	13 (7%)	19	56
41	BG	172/172 (100%)	165 (96%)	7 (4%)	37	71
42	BH	125/125 (100%)	120 (96%)	5 (4%)	38	71
43	BI	116/116 (100%)	109 (94%)	7 (6%)	24	60
44	BJ	146/146 (100%)	138 (94%)	8 (6%)	27	63
45	BK	104/104 (100%)	93 (89%)	11 (11%)	8	36
46	BL	106/106 (100%)	99 (93%)	7 (7%)	21	57
47	BM	90/90 (100%)	87 (97%)	3 (3%)	45	76
48	BN	98/98 (100%)	93 (95%)	5 (5%)	29	66
49	BO	103/103 (100%)	96 (93%)	7 (7%)	20	57
50	BP	95/95 (100%)	90 (95%)	5 (5%)	28	64
51	BQ	83/83 (100%)	81 (98%)	2 (2%)	57	82
52	BR	76/76 (100%)	74 (97%)	2 (3%)	54	80
53	BS	65/65 (100%)	64 (98%)	1 (2%)	72	88
54	BT	77/77 (100%)	72 (94%)	5 (6%)	21	58
55	BU	64/64 (100%)	61 (95%)	3 (5%)	32	68
56	BV	78/78 (100%)	73 (94%)	5 (6%)	22	58
57	BW	65/65 (100%)	63 (97%)	2 (3%)	47	77
58	BX	60/60 (100%)	56 (93%)	4 (7%)	20	57
All	All	5213/5213 (100%)	4918 (94%)	295 (6%)	30	62

5 of 295 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	AU	4	ILE
29	A2	24	ILE
51	BQ	45	LEU
21	AU	102	HIS
24	AX	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	17 (14%)	10 (8%)
2	AB	2898/2904 (99%)	529 (18%)	183 (6%)
35	BA	1538/1542 (99%)	299 (19%)	117 (7%)
36	BB	74/76 (97%)	25 (33%)	5 (6%)
37	BC	46/47 (97%)	16 (34%)	7 (15%)
38	BD	77/77 (100%)	14 (18%)	2 (2%)
All	All	4752/4766 (99%)	900 (18%)	324 (6%)

5 of 900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	G
1	AA	14	U
1	AA	25	U
1	AA	26	C

5 of 324 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AB	2236	U
2	AB	2756	U
35	BA	1347	G
2	AB	2263	C
2	AB	2440	C

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

49 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
2	6MZ	AB	1618	2	17,25,26	1.38	2 (11%)	15,36,39	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MG	AB	1835	2	18,26,27	1.93	4 (22%)	21,38,41	3.39	5 (23%)
2	PSU	AB	1911	2	15,21,22	1.86	5 (33%)	16,30,33	3.90	6 (37%)
2	3TD	AB	1915	2	15,22,23	1.85	5 (33%)	17,32,35	2.28	5 (29%)
2	PSU	AB	1917	2	15,21,22	2.07	4 (26%)	16,30,33	3.70	6 (37%)
2	5MU	AB	1939	2	13,22,23	1.96	4 (30%)	16,32,35	3.95	5 (31%)
2	5MC	AB	1962	2	14,22,23	2.13	3 (21%)	17,32,35	2.28	4 (23%)
2	6MZ	AB	2030	2	17,25,26	1.35	3 (17%)	15,36,39	2.40	4 (26%)
2	7MG	AB	2069	2	20,26,27	2.78	8 (40%)	23,39,42	2.95	7 (30%)
2	OMG	AB	2251	2	18,26,27	1.64	3 (16%)	21,38,41	2.90	8 (38%)
2	2MG	AB	2445	2	18,26,27	2.04	8 (44%)	21,38,41	3.09	8 (38%)
2	H2U	AB	2449	2	17,21,22	1.47	3 (17%)	23,30,33	1.46	4 (17%)
2	PSU	AB	2457	2	15,21,22	2.40	6 (40%)	16,30,33	4.51	5 (31%)
2	OMC	AB	2498	2	15,22,23	1.37	1 (6%)	20,31,34	1.67	4 (20%)
2	2MA	AB	2503	2	17,25,26	1.23	1 (5%)	18,37,40	2.54	4 (22%)
2	PSU	AB	2504	2	15,21,22	2.06	5 (33%)	16,30,33	3.94	5 (31%)
2	OMU	AB	2552	2	14,22,23	2.03	4 (28%)	19,31,34	2.52	6 (31%)
2	CH	AB	2575	2	14,21,22	1.28	1 (7%)	18,30,33	1.74	3 (16%)
2	PSU	AB	2580	2	15,21,22	2.05	5 (33%)	16,30,33	4.71	7 (43%)
2	PSU	AB	2605	2	15,21,22	1.85	4 (26%)	16,30,33	3.98	3 (18%)
2	1MG	AB	745	2	17,26,27	1.77	5 (29%)	19,39,42	1.73	7 (36%)
2	PSU	AB	746	2	15,21,22	1.77	2 (13%)	16,30,33	4.33	3 (18%)
2	5MU	AB	747	2	13,22,23	2.10	4 (30%)	16,32,35	4.22	5 (31%)
2	PSU	AB	955	2	15,21,22	2.07	4 (26%)	16,30,33	4.80	5 (31%)
35	2MG	BA	1207	35	18,26,27	1.87	7 (38%)	21,38,41	2.74	8 (38%)
35	4OC	BA	1402	35	15,23,24	1.77	4 (26%)	21,32,35	3.17	6 (28%)
35	5MC	BA	1407	35	14,22,23	1.71	4 (28%)	17,32,35	1.75	4 (23%)
35	UR3	BA	1498	35	13,22,23	1.88	2 (15%)	18,32,35	1.67	3 (16%)
35	2MG	BA	1516	35	18,26,27	1.80	4 (22%)	21,38,41	2.58	8 (38%)
35	MA6	BA	1518	35	18,26,27	1.39	2 (11%)	15,38,41	1.87	4 (26%)
35	MA6	BA	1519	35	18,26,27	1.42	4 (22%)	15,38,41	1.68	2 (13%)
35	PSU	BA	516	35	15,21,22	2.48	5 (33%)	16,30,33	4.07	8 (50%)
35	7MG	BA	527	35	20,26,27	3.04	5 (25%)	23,39,42	2.34	3 (13%)
35	2MG	BA	966	35	18,26,27	2.15	6 (33%)	21,38,41	3.11	6 (28%)
35	5MC	BA	967	35	14,22,23	1.61	2 (14%)	17,32,35	1.22	2 (11%)
36	H2U	BB	16	36	17,21,22	1.40	3 (17%)	23,30,33	1.44	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	H2U	BB	17	36	17,21,22	1.37	4 (23%)	23,30,33	2.23	9 (39%)
36	H2U	BB	20	36	17,21,22	1.93	6 (35%)	23,30,33	1.90	6 (26%)
36	OMC	BB	32	36	15,22,23	1.58	3 (20%)	20,31,34	1.94	6 (30%)
36	MIA	BB	37	36	22,31,32	1.85	5 (22%)	26,44,47	1.96	5 (19%)
36	7MG	BB	46	36	20,26,27	3.18	6 (30%)	23,39,42	2.85	7 (30%)
36	5MU	BB	54	36	13,22,23	1.89	3 (23%)	16,32,35	4.41	2 (12%)
36	PSU	BB	55	36	15,21,22	1.95	6 (40%)	16,30,33	4.90	8 (50%)
36	4SU	BB	8	36	12,21,22	2.46	2 (16%)	15,30,33	1.43	4 (26%)
38	H2U	BD	21	38	17,21,22	1.12	1 (5%)	23,30,33	1.81	5 (21%)
38	OMC	BD	33	38	15,22,23	1.56	3 (20%)	20,31,34	1.70	5 (25%)
38	5MU	BD	55	38	13,22,23	1.88	4 (30%)	16,32,35	4.54	4 (25%)
38	PSU	BD	56	38	15,21,22	2.38	4 (26%)	16,30,33	3.45	6 (37%)
38	4SU	BD	8	38	12,21,22	1.45	1 (8%)	15,30,33	1.78	2 (13%)

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
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/3/25/26	0/2/2/2
2	5MC	AB	1962	2	-	0/3/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	0/5/27/28	0/3/3/3
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	2498	2	-	0/5/27/28	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2504	2	-	0/7/25/26	0/2/2/2
2	OMU	AB	2552	2	-	0/5/27/28	0/2/2/2
2	CH	AB	2575	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	746	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	747	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
35	2MG	BA	1207	35	-	0/5/27/28	0/3/3/3
35	4OC	BA	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	BA	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	BA	1498	35	-	0/3/25/26	0/2/2/2
35	2MG	BA	1516	35	-	0/5/27/28	0/3/3/3
35	MA6	BA	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	BA	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	BA	516	35	-	0/7/25/26	0/2/2/2
35	7MG	BA	527	35	-	0/7/37/38	0/3/3/3
35	2MG	BA	966	35	-	0/5/27/28	0/3/3/3
35	5MC	BA	967	35	-	0/3/25/26	0/2/2/2
36	H2U	BB	16	36	-	0/7/38/39	0/2/2/2
36	H2U	BB	17	36	-	0/7/38/39	0/2/2/2
36	H2U	BB	20	36	-	0/7/38/39	0/2/2/2
36	OMC	BB	32	36	-	0/5/27/28	0/2/2/2
36	MIA	BB	37	36	-	0/11/33/34	0/3/3/3
36	7MG	BB	46	36	-	0/7/37/38	0/3/3/3
36	5MU	BB	54	36	-	0/3/25/26	0/2/2/2
36	PSU	BB	55	36	-	0/7/25/26	0/2/2/2
36	4SU	BB	8	36	-	0/3/25/26	0/2/2/2
38	H2U	BD	21	38	-	0/7/38/39	0/2/2/2
38	OMC	BD	33	38	-	0/5/27/28	0/2/2/2
38	5MU	BD	55	38	-	0/3/25/26	0/2/2/2
38	PSU	BD	56	38	-	0/7/25/26	0/2/2/2
38	4SU	BD	8	38	-	0/3/25/26	0/2/2/2

The worst 5 of 190 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	46	7MG	C8-N9	-11.38	1.29	1.45
35	BA	527	7MG	C8-N9	-9.08	1.32	1.45
2	AB	2069	7MG	C8-N9	-8.91	1.32	1.45
35	BA	516	PSU	C5-C1'	-7.24	1.45	1.52
2	AB	2580	PSU	O4'-C1'	-4.87	1.36	1.44

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	54	5MU	C5-C4-N3	-12.78	114.62	125.35
2	AB	747	5MU	C5-C4-N3	-12.21	115.10	125.35
38	BD	55	5MU	C5-C4-N3	-11.55	115.65	125.35
2	AB	1939	5MU	C5-C4-N3	-10.71	116.36	125.35
2	AB	1835	2MG	C5-C6-N1	-9.78	110.73	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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
59	FME	AB	3001	60	8,9,10	1.81	3 (37%)	5,9,11	2.29	2 (40%)
60	TRP	BB	101	59,36	12,15,16	1.39	1 (8%)	9,20,22	1.89	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	AB	3001	60	-	1/6/9/11	0/0/0/0
60	TRP	BB	101	59,36	-	0/3/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	3001	FME	CA-N	-4.05	1.40	1.46
59	AB	3001	FME	CB-CA	2.05	1.57	1.53
59	AB	3001	FME	O-C	2.06	1.29	1.19
60	BB	101	TRP	CD1-NE1	2.37	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BB	101	TRP	CB-CG-CD1	-4.76	122.09	127.97
59	AB	3001	FME	O-C-CA	-4.35	113.79	125.69
59	AB	3001	FME	CG-CB-CA	2.05	119.22	113.07
60	BB	101	TRP	CZ2-CE2-NE1	2.35	137.38	130.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AB	3001	FME	O1-CN-N-CA

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](#)

There are no chain breaks in this entry.