



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:44 pm GMT

PDB ID : 4V6L
EMDB ID: : EMD-1850
Title : Structural insights into cognate vs. near-cognate discrimination during decoding.
Authors : Agirrezabala, X.; Schreiner, E.; Trabuco, L.G.; Lei, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-01-07
Resolution : 13.20 Å(reported)
Based on PDB ID : 3FIH, 2I2U

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

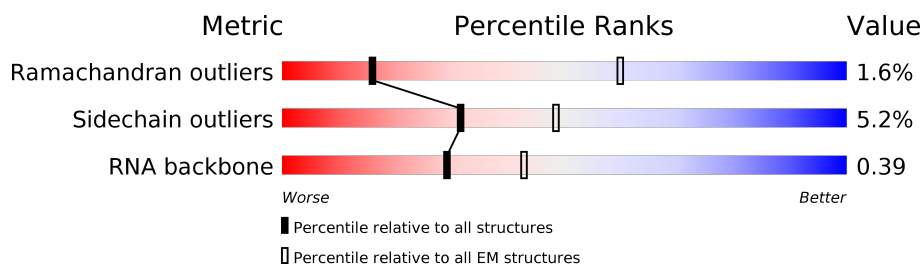
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.20 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.








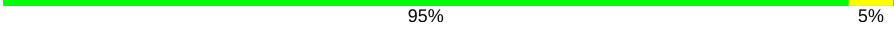

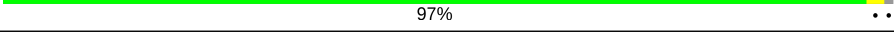


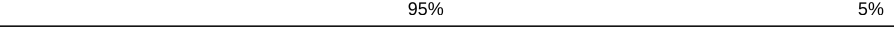
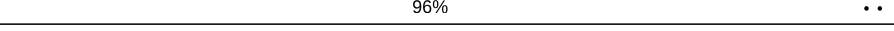

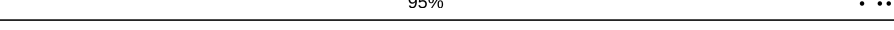
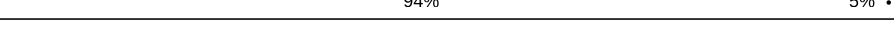

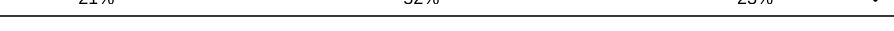
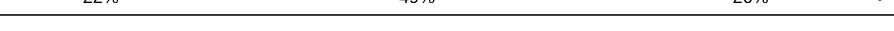
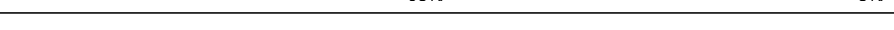
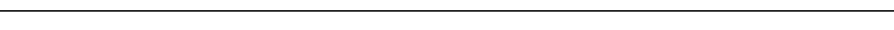
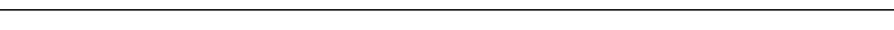
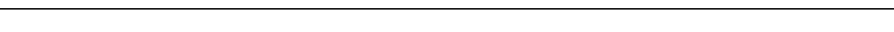
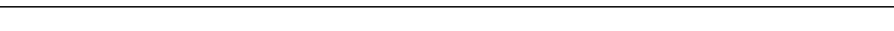
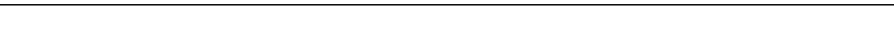

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	AA	1542	24% 50% 24% .
2	AB	76	30% 45% 24% .
2	AE	76	26% 50% 21% .
3	AC	393	95% 5%
4	AD	24	17% 58% 17% 8%
5	AF	241	94% 5%
6	AG	233	94% 5%
7	AH	206	94% 5%
8	AI	167	93% 6% .

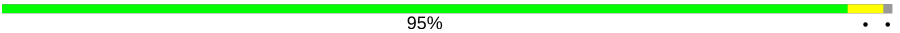
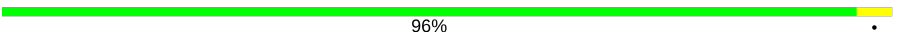

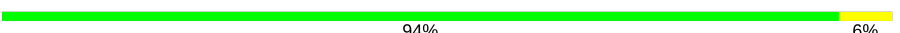









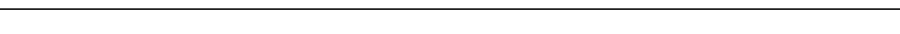

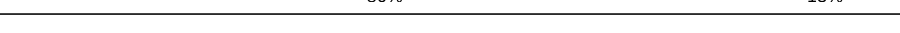

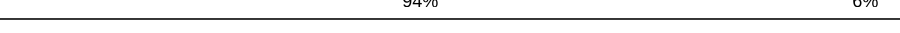
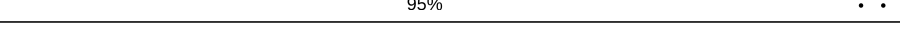
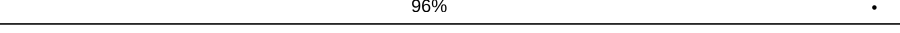

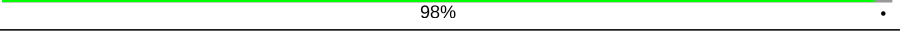
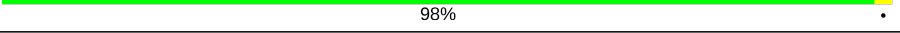
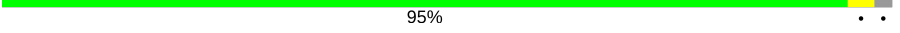
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Mol	Chain	Length	Quality of chain
9	AJ	135	 89% 10% .
10	AK	179	 92% 7% .
11	AL	130	 93% 6% .
12	AM	130	 91% 8% .
13	AN	103	 90% 9% .
14	AO	129	 95% 5% .
15	AP	124	 90% 9% .
16	AQ	118	 97% ..
17	AR	101	 85% 14% .
18	AS	89	 92% 7% .
19	AT	82	 95% 5%
20	AU	84	 96% ..
21	AV	75	 91% 8% .
22	AW	92	 95% ...
23	AX	87	 94% 5% .
24	AY	71	 87% 11% .
25	BA	120	 21% 52% 23% .
26	BB	2904	 22% 49% 26% .
27	BC	234	 95% 5%
28	BD	273	 93% 7%
29	BE	209	 91% 8%
30	BF	201	 93% 6%
31	BG	179	 92% 7% ..
32	BH	177	 91% 8% ..
33	BI	149	 93% 7% .

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Mol	Chain	Length	Quality of chain
34	BJ	142	 95% . .
35	BK	142	 96% .
36	BL	123	 93% 7% .
37	BM	144	 94% 6%
38	BN	136	 93% 7% .
39	BO	127	 94% 6%
40	BP	117	 95% 5%
41	BQ	115	 91% 8% .
42	BR	118	 96% . .
43	BS	103	 91% 8% .
44	BT	110	 95% 5%
45	BU	100	 94% 6%
46	BV	104	 95% . .
47	BW	94	 94% 6%
48	BX	85	 86% 13% .
49	BY	78	 91% 6% . .
50	BZ	63	 94% 6%
51	Ba	59	 95% . .
52	Bb	70	 96% .
53	Bc	57	 91% 7% .
54	Bd	55	 98% .
55	Be	46	 98% .
56	Bf	65	 95% . .
57	Bg	38	 87% 13%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 2 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		
2	AE	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		

- Molecule 3 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	393	Total	C	N	O	S	0	0
			3036	1918	523	582	13		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	24	Total	C	N	O	P	0	0
			495	222	68	181	24		

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein S21.

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

- Molecule 25 is a RNA chain called 50S ribosomal RNA 5S.

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

- Molecule 26 is a RNA chain called 50S ribosomal RNA 23S.

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

- Molecule 27 is a protein called 50S ribosomal protein L1.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	103	Total	C	N	O		0	0
			789	498	148	143			

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L31.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

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

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

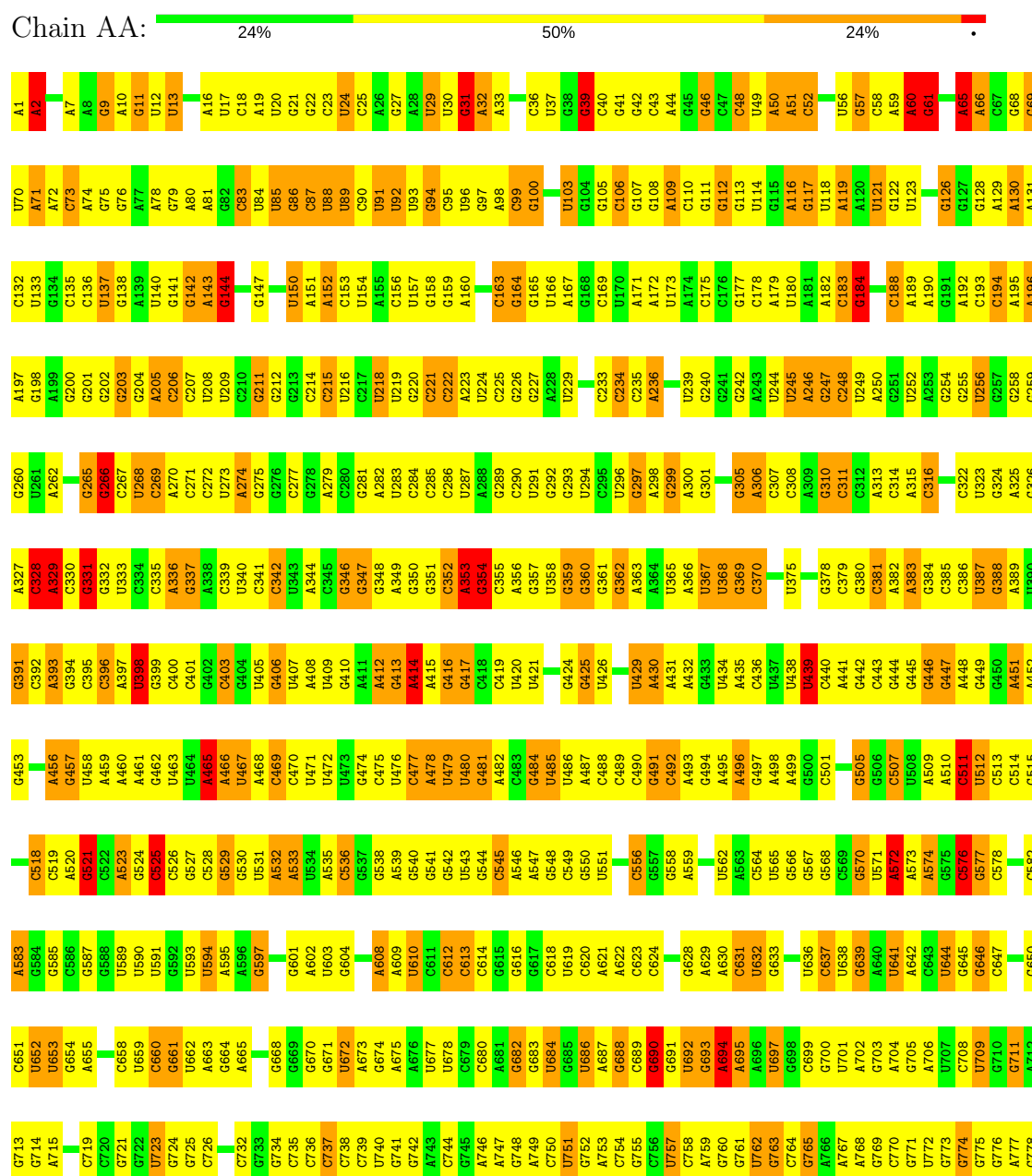
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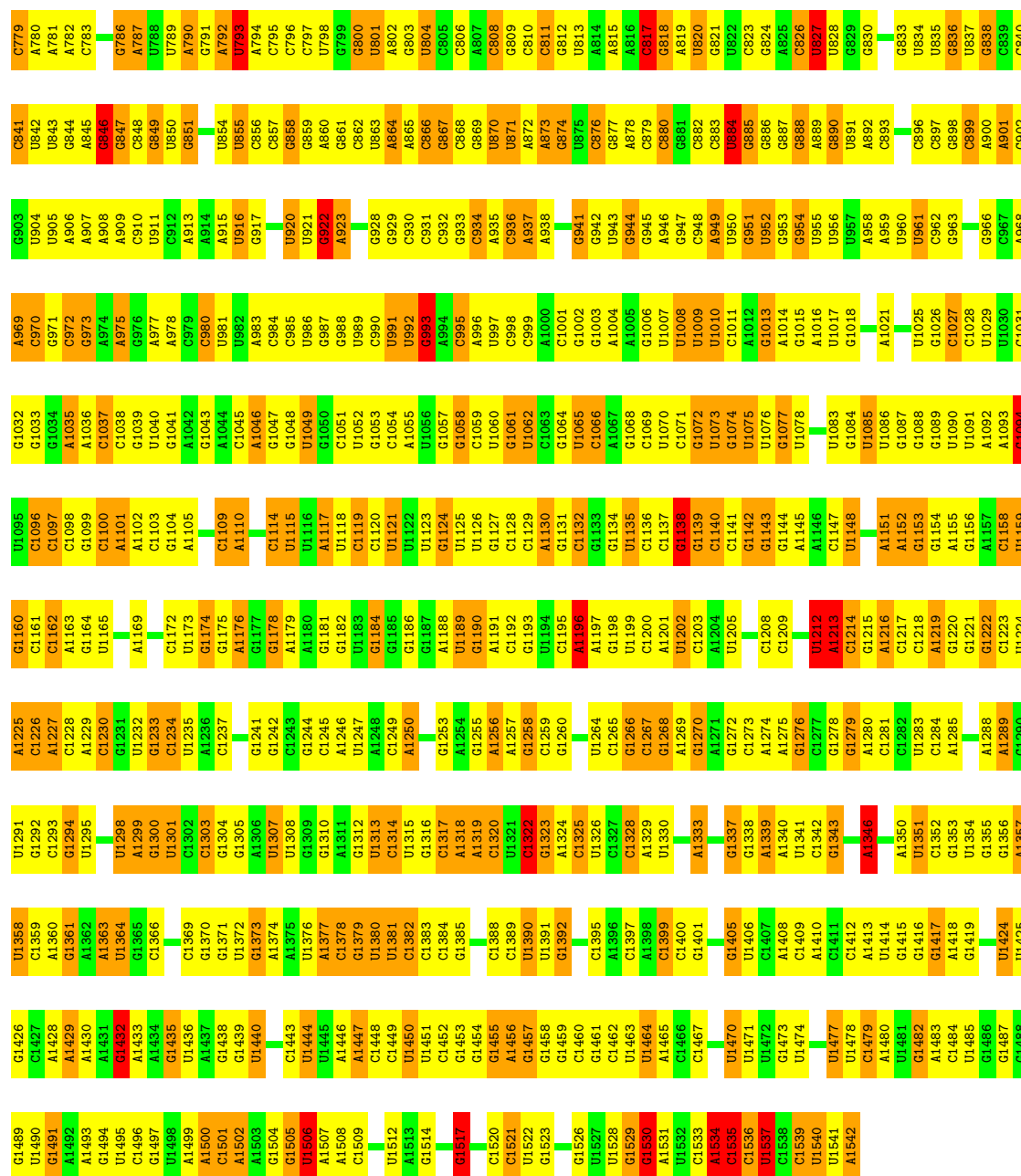
Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bg	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

3 Residue-property plots

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

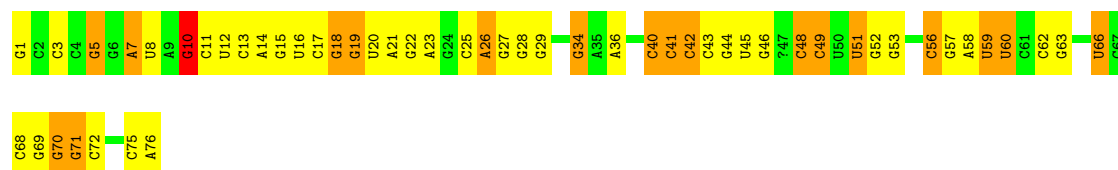
• Molecule 1: 16S ribosomal RNA





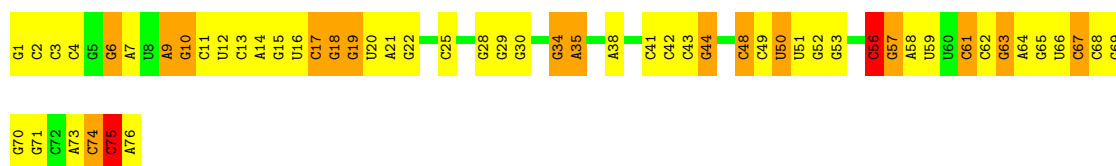
- Molecule 2: A/T-site tRNA Phe

Chain AB: 



- Molecule 2: A/T-site tRNA Phe

Chain AE:  26% 50% 21% 3%



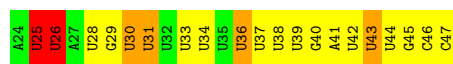
- Molecule 3: Elongation factor Tu 2

Chain AC: 95% 5%



- Molecule 4: mRNA

Chain AD: 17% 58% 17% 8%



- Molecule 5: 30S ribosomal protein S2

Chain AF: 94% 5%



- Molecule 6: 30S ribosomal protein S3

Chain AG: 94% 5%



- Molecule 7: 30S ribosomal protein S4

Chain AH: 94% 5%



- Molecule 8: 30S ribosomal protein S5

Chain AI: 93% 6% 1%



- Molecule 9: 30S ribosomal protein S6

Chain AJ: 89% 10% 1%



- Molecule 10: 30S ribosomal protein S7

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S8

Chain AL: 93% 6%



- Molecule 12: 30S ribosomal protein S9

Chain AM: 91% 8%



- Molecule 13: 30S ribosomal protein S10

Chain AN: 90% 9%



- Molecule 14: 30S ribosomal protein S11

Chain AO: 95% 5%



- Molecule 15: 30S ribosomal protein S12

Chain AP: 90% 9%

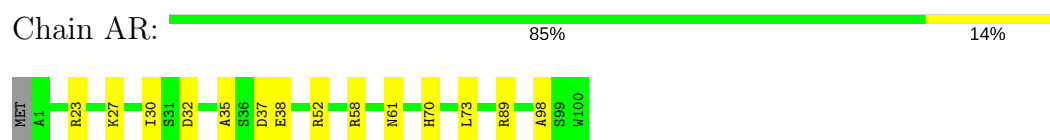


- Molecule 16: 30S ribosomal protein S13

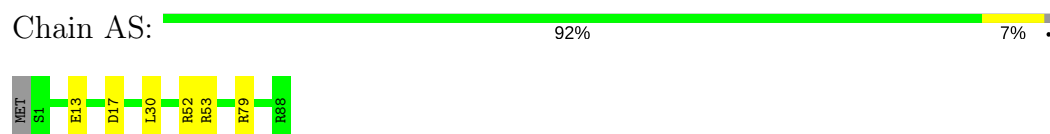
Chain AQ: 97% 2%



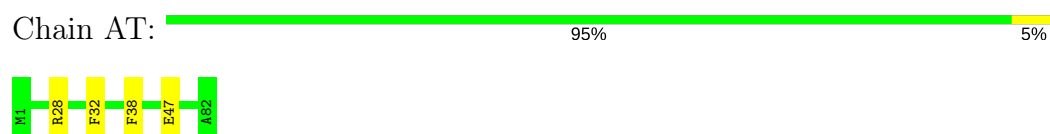
- Molecule 17: 30S ribosomal protein S14



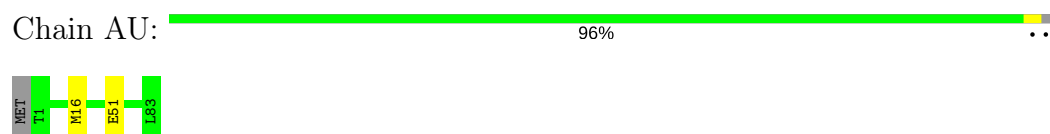
- Molecule 18: 30S ribosomal protein S15



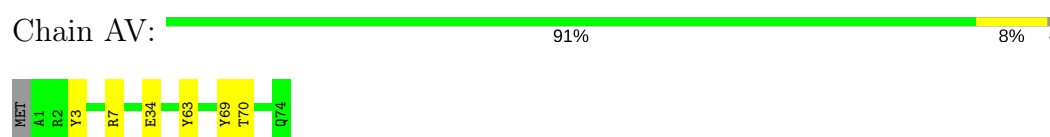
- Molecule 19: 30S ribosomal protein S16



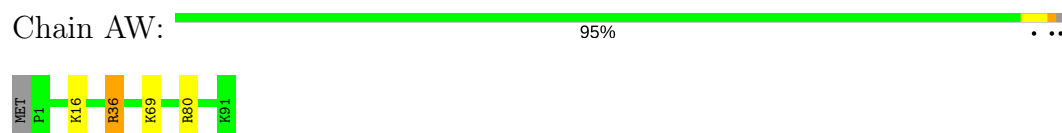
- Molecule 20: 30S ribosomal protein S17



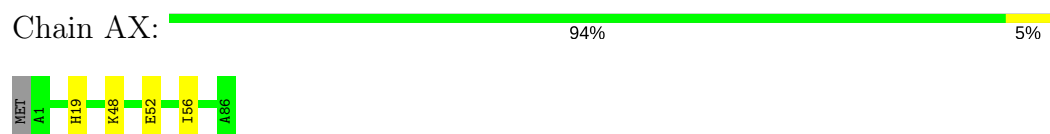
- Molecule 21: 30S ribosomal protein S18



- Molecule 22: 30S ribosomal protein S19



- Molecule 23: 30S ribosomal protein S20



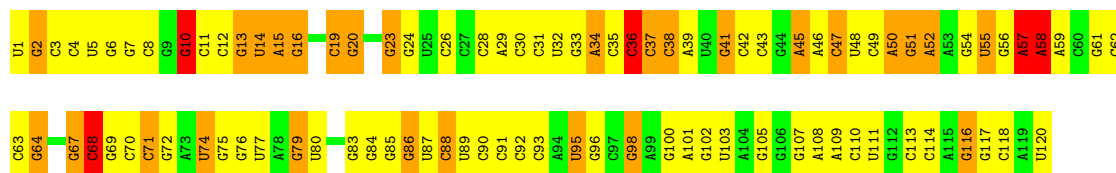
- Molecule 24: 30S ribosomal protein S21





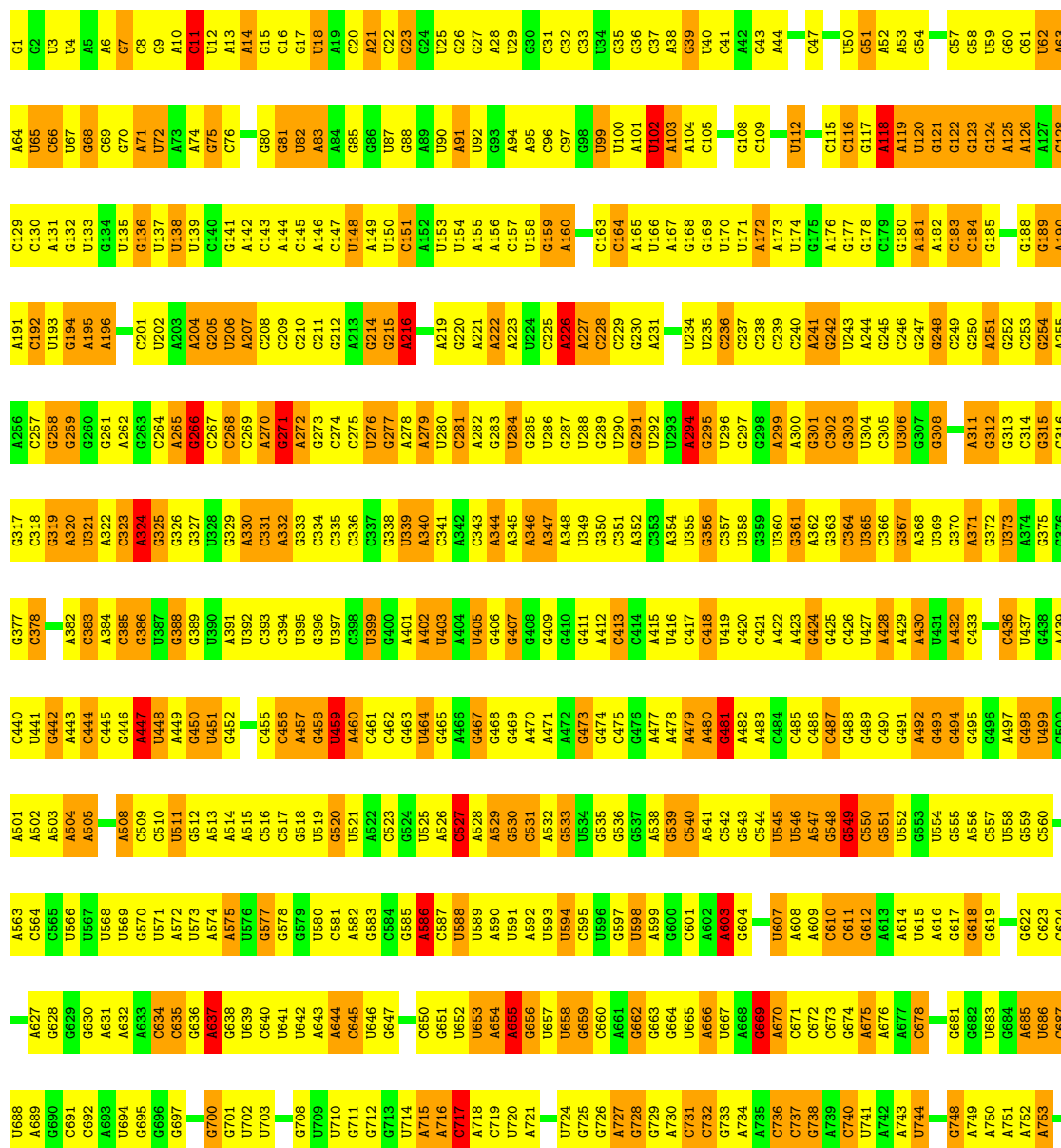
• Molecule 25: 50S ribosomal RNA 5S

Chain BA: 21% 52% 23%



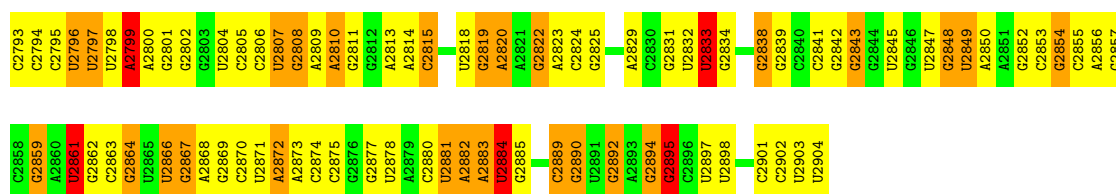
• Molecule 26: 50S ribosomal RNA 23S

Chain BB: 22% 49% 26%



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A1701	C1639	U1576	G1514	G1448	A1383	G1324	G1259	G1193	A1129	A1067	G1003	A941	C886	C824	G822	A762	G766	C765	C759	A757
G1702	A1640	C1577	A1515	G1449	A1384	G1324	A1260	A1194	U1130	A1068	U1004	G942	G879	A831	A820	A763	U766	G765	G759	
G1703	A1641	C1578	A1516	G1450	A1385	G1325	C1261	G1195	G1131	A1069	C1005	A943	G880	G881	A821	A764	U767			
G1704	G1642	A1579	G1519	G1451	A1386	G1326	A1262	C1196	U1132	A1070	C1006	C944	G882	G882	A822	A765	U768			
A1705	G1643	A1580	U1520	G1452	A1387	A1327	U1263	G1197	U1133	G1071	C1007	C945	G883	G883	G822	A766	U769			
G1706	C1644	G1581	U1521	A1453	G1388	A1328	A1264	U1198	A1134	C1072		C946	G884	G884	G822	A767	U770			
G1707	G1645	U1584	G1522	G1454	G1389	U1329	A1265	U1199	C1135	A1073	A1010	A947	C885	G823	G822	A768				
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	A1650	G1588	C1526	U1460	U1394	G1334	C1270	A1205	G1140	U1078	U1015	G952	C889	U828	U828	A773				
	G1651		G1527	G1461	A1395	G1335	G1271	G1206	U1141	C1079	G1016	G953	C890	U829	U829	A774				
U1714			A1528	U1462	U1396	A1336	A1272	C1207	A1142	A1080	G1017	G954	C891	A829	A829	A775				
G1715	G1652	A1591	U1528	C1463	U1397	G1337	U1273	C1208	A1143	A1081	U1018		A892	G830	G830	A776				
U1716	G1653	C1592	G1529	C1463	U1398	G1338	A1274	U1209	A1144	U1082	U1018		A893	G831	G831	A777				
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G1731		C1607	A1544	G1482	C1414	U1352	G1288	G1224	G1161	U1096	G1034	C972		G846	U846	A792				
C1732		A1608	U1545	G1483	U1415	A1353	C1289	A1226	G1162	U1097	U1035	A973		G847	U847	A793				
G1733	U1671	A1609	G1546	U1484	G1416	A1354	C1290	G1227		A1098	G1036	C974		G848	U848	A794				
G1734	A1672	C1610	C1547	U1485	C1417	G1355	C1291		A1165	C1099	G1037	C975		G849	U849	A795				
A1735	G1673	C1611	A1548	U1486	G1418	G1356	G1292		G1166	C1100	U1038	C976		G850	U850	A796				
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C2214	C2215	G2216	G2217	U2218	U2219	U2220	G2221	C2222	G2223	G2224	A2225	C2226	A2227	G2228	U2229	G2230	U2231	U2232	U2233	G2234	G2235	G2236	G2237	G2238	G2239	U2240	U2241	G2242	U2243	U2244	U2245	U2246	U2249	G2250	G2251	G2252	G2253	C2254	G2255	U2256	U2257	C2258	U2259	A2260	C2261	U2262	C2263	C2264	U2265	A2266	C2267	A2268	G2269	U2270	G2271	U2272	A2274										
C2150	U2151	G2152	U2155	C2156	G2157	A2158	C2159	C2160	C2161	G2162	A2163	C2164	G2168	A2169	A2170	U2171	U2172	A2173	G2174	C2175	A2176	C2177	C2178	C2179	U2180	G2181	U2182	U2183	A2184	U2185	U2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	C2196	U2197	A2198	A2199	C2200	G2201	U2202	G2203	C2204	A2205	C2206	C2207	C2208	A2211	U2212	U2213											
U2086	G2087	A2088	C2089	A2090	C2091	U2092	G2093	A2094	A2097	U2098	U2099	G2102	C2103	U2096	U2097	U2098	U2099	U2106	G2107	A2108	U2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	U2117	U2118	U2119	G2120	U2121	U2122	U2123	G2124	G2125	A2126	G2127	G2128	U2129	U2130	U2131	U2132	G2133	A2134	A2135	U2138	U2139	U2140	G2141	A2142	C2143	G2144	U2145	C2146	A2147	U2148	U2149								
C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	U2030	A2031	G2032	A2033	U2034	U2039	G2040	U2041	A2042	C2043	C2044	U2045	G2046	C2047	G2048	G2049	C2050	U2051	A2052	C2053	G2054	C2055	G2056	G2057	U2058	U2059	C2063	C2064	C2065	C2066	G2067	U2068	C2072	U2073	U2074	U2075	U2076	A2077	C2078	U2079	A2080	U2081	A2082	C2083	U2085														
C1961	C1962	C1963	C1964	C1965	A1966	C1967	U1968	A1969	U1970	U1971	G1972	C1902	C1903	G1904	C1905	G1906	G1907	C1908	C1909	U1976	A1977	U1978	U1979	G1980	U1981	U1982	G1983	U1917	G1984	U1985	U1986	G1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	A1998	C1999	C2000	C2001	G2002	A2003	C2004	A2005	C2006	U2007	C2008	C2009	U2010	U2011	U2012	C1947	U1951	A1885	U1952	U1886	C1887	G1888	A1889	U1955	U1956
G1831	C1832	C1833	U1834	C1837	C1838	G1839	G1840	U1841	C1842	C1843	C1844	G1845	U1846	U1847	A1848	G1849	U1850	U1851	U1852	A1783	U1854	U1855	U1856	A1786	C1788	A1791	G1792	C1793	U1796	G1797	U1798	G1799	C1800	A1801	A1802	C1806	G1807	A1808	A1809	A1810	G1811	U1812	G1813	U1814	A1815	C1816	A1819	C1822	U1825	G1826	U1827	U1828	G1829	U1830													



- Molecule 27: 50S ribosomal protein L1

Chain BC: 95% 5%



- Molecule 28: 50S ribosomal protein L2

Chain BD: 93% 7%



- Molecule 29: 50S ribosomal protein L3

Chain BE: 91% 8%



- Molecule 30: 50S ribosomal protein L4

Chain BF: 93% 6%



- Molecule 31: 50S ribosomal protein L5

Chain BG: 92% 7% ..



- Molecule 32: 50S ribosomal protein L6

Chain BH: 91% 8% ..



- Molecule 33: 50S ribosomal protein L9

Chain BI: 93% 7% .



- Molecule 34: 50S ribosomal protein L11

Chain BJ: 95%



- Molecule 35: 50S ribosomal protein L13

Chain BK: 96%



- Molecule 36: 50S ribosomal protein L14

Chain BL: 93%



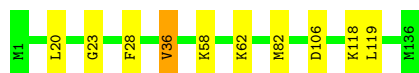
- Molecule 37: 50S ribosomal protein L15

Chain BM: 94%



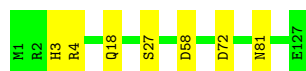
- Molecule 38: 50S ribosomal protein L16

Chain BN: 93%



- Molecule 39: 50S ribosomal protein L17

Chain BO: 94%



- Molecule 40: 50S ribosomal protein L18

Chain BP: 95%



- Molecule 41: 50S ribosomal protein L19

Chain BQ:  91% 8%



- Molecule 42: 50S ribosomal protein L20

Chain BR:  96%



- Molecule 43: 50S ribosomal protein L21

Chain BS:  91% 8%



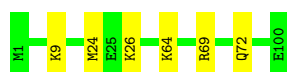
- Molecule 44: 50S ribosomal protein L22

Chain BT:  95% 5%



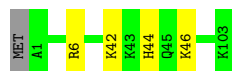
- Molecule 45: 50S ribosomal protein L23

Chain BU:  94% 6%



- Molecule 46: 50S ribosomal protein L24

Chain BV:  95%




- Molecule 47: 50S ribosomal protein L25

Chain BW:  94% 6%



- Molecule 48: 50S ribosomal protein L27

Chain BX:  86% 13%



- Molecule 49: 50S ribosomal protein L28

Chain BY:  91% 6%



- Molecule 50: 50S ribosomal protein L29

Chain BZ:  94% 6%



- Molecule 51: 50S ribosomal protein L30

Chain Ba:  95%



- Molecule 52: 50S ribosomal protein L31

Chain Bb:  96%



- Molecule 53: 50S ribosomal protein L32

Chain Bc:  91% 7%



- Molecule 54: 50S ribosomal protein L33

Chain Bd:  98%



- Molecule 55: 50S ribosomal protein L34

Chain Be:  98%



- Molecule 56: 50S ribosomal protein L35

Chain Bf: 95% . .



- Molecule 57: 50S ribosomal protein L36

Chain Bg: 87% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 3TD, CH, OMG, 5MC, 3AU, MA6, MIA, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 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	1.22	1/36769 (0.0%)	2.00	1273/57354 (2.2%)
10	AK	0.63	0/1422	1.07	1/1908 (0.1%)
11	AL	0.59	0/989	1.01	0/1326
12	AM	0.65	0/1048	1.05	1/1394 (0.1%)
13	AN	0.57	0/835	1.08	1/1127 (0.1%)
14	AO	0.61	0/982	1.04	0/1323
15	AP	0.62	0/969	1.12	0/1300
16	AQ	0.58	0/919	1.02	0/1226
17	AR	0.63	0/817	1.15	2/1088 (0.2%)
18	AS	0.59	0/724	0.96	1/966 (0.1%)
19	AT	0.63	0/659	1.08	1/884 (0.1%)
2	AB	1.25	0/1580	2.01	56/2459 (2.3%)
2	AE	1.26	0/1580	2.04	66/2459 (2.7%)
20	AU	0.58	0/681	0.97	0/913
21	AV	0.73	0/637	1.08	0/851
22	AW	0.60	0/744	1.00	1/995 (0.1%)
23	AX	0.58	0/676	0.98	0/895
24	AY	0.69	0/598	1.18	1/792 (0.1%)
25	BA	1.24	0/2869	2.16	127/4474 (2.8%)
26	BB	1.22	0/69257	2.02	2547/108040 (2.4%)
27	BC	0.55	0/1748	0.98	0/2355
28	BD	0.62	0/2131	1.09	0/2863
29	BE	0.59	0/1586	1.04	0/2134
3	AC	0.61	0/3092	0.97	1/4183 (0.0%)
30	BF	0.58	0/1571	1.01	1/2113 (0.0%)
31	BG	0.66	0/1444	1.10	0/1937
32	BH	0.59	0/1343	1.05	2/1816 (0.1%)
33	BI	0.58	0/1122	1.01	1/1515 (0.1%)
34	BJ	0.57	0/1046	0.93	0/1410
35	BK	0.64	0/1152	1.00	0/1551
36	BL	0.58	0/956	1.03	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
37	BM	0.62	0/1062	1.07	0/1413
38	BN	0.63	0/1093	1.04	0/1460
39	BO	0.62	0/1021	1.06	0/1364
4	AD	1.37	0/548	1.98	20/848 (2.4%)
40	BP	0.60	0/910	1.01	0/1219
41	BQ	0.63	0/929	1.05	0/1242
42	BR	0.67	0/960	1.03	1/1278 (0.1%)
43	BS	0.63	0/829	1.06	0/1107
44	BT	0.54	0/864	0.98	0/1156
45	BU	0.57	0/794	1.02	0/1060
46	BV	0.58	0/797	1.02	0/1062
47	BW	0.61	0/766	0.98	0/1025
48	BX	0.64	0/642	1.10	0/848
49	BY	0.64	0/635	1.10	1/848 (0.1%)
5	AF	0.60	0/1904	1.00	1/2565 (0.0%)
50	BZ	0.56	0/510	1.05	0/677
51	Ba	0.55	0/453	0.97	0/605
52	Bb	0.62	0/559	1.10	0/745
53	Bc	0.62	0/450	1.12	0/599
54	Bd	0.60	0/448	0.96	0/594
55	Be	0.64	0/380	1.04	0/498
56	Bf	0.60	0/513	1.02	0/676
57	Bg	0.55	0/303	1.09	0/397
6	AG	0.61	0/1852	1.04	0/2490
7	AH	0.64	0/1665	0.99	0/2227
8	AI	0.59	0/1239	1.07	1/1664 (0.1%)
9	AJ	0.62	0/1121	1.05	2/1509 (0.1%)
All	All	1.07	1/165193 (0.0%)	1.79	4109/246106 (1.7%)

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	502
11	AL	0	1
13	AN	0	1
14	AO	0	1
15	AP	0	1
17	AR	0	2
2	AB	0	19

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	AE	0	15
21	AV	0	1
24	AY	0	1
25	BA	0	37
26	BB	0	952
27	BC	0	3
28	BD	0	2
29	BE	0	2
3	AC	0	1
30	BF	0	2
32	BH	0	2
33	BI	0	1
4	AD	0	9
41	BQ	0	1
42	BR	0	1
43	BS	0	1
48	BX	0	1
49	BY	0	1
53	Bc	0	1
6	AG	0	1
7	AH	0	1
8	AI	0	3
9	AJ	0	1
All	All	0	1567

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	439	U	C2-N3	5.10	1.41	1.37

The worst 5 of 4109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2092	U	O4'-C1'-N1	16.66	121.53	108.20
25	BA	49	C	O4'-C1'-N1	15.19	120.35	108.20
1	AA	465	A	O4'-C1'-N9	14.84	120.07	108.20
26	BB	736	C	O4'-C1'-N1	12.90	118.52	108.20
26	BB	1535	A	O4'-C1'-N9	12.89	118.51	108.20

There are no chirality outliers.

5 of 1567 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	10	A	Sidechain
1	AA	11	G	Sidechain
1	AA	13	U	Sidechain
1	AA	2	A	Sidechain
1	AA	7	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33089	0	16678	0	0
2	AB	1635	0	849	0	0
2	AE	1635	0	849	0	0
3	AC	3036	0	3052	0	0
4	AD	495	0	249	0	0
5	AF	1872	0	1885	0	0
6	AG	1822	0	1913	0	0
7	AH	1643	0	1710	0	0
8	AI	1225	0	1273	0	0
9	AJ	1101	0	1050	0	0
10	AK	1400	0	1449	0	0
11	AL	979	0	1034	0	0
12	AM	1036	0	1084	0	0
13	AN	825	0	865	0	0
14	AO	965	0	997	0	0
15	AP	955	0	1019	0	0
16	AQ	910	0	981	0	0
17	AR	805	0	847	0	0
18	AS	716	0	742	0	0
19	AT	649	0	666	0	0
20	AU	672	0	716	0	0
21	AV	626	0	651	0	0
22	AW	727	0	769	0	0
23	AX	670	0	722	0	0
24	AY	590	0	631	0	0
25	BA	2566	0	1302	0	0
26	BB	62351	0	31387	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1032	0	1088	0	0
35	BK	1129	0	1162	0	0
36	BL	947	0	1023	0	0
37	BM	1053	0	1129	0	0
38	BN	1074	0	1157	0	0
39	BO	1008	0	1045	0	0
40	BP	900	0	935	0	0
41	BQ	917	0	965	0	0
42	BR	947	0	1022	0	0
43	BS	816	0	839	0	0
44	BT	857	0	922	0	0
45	BU	787	0	846	0	0
46	BV	789	0	847	0	0
47	BW	753	0	780	0	0
48	BX	634	0	656	0	0
49	BY	625	0	655	0	0
50	BZ	509	0	543	0	0
51	Ba	449	0	491	0	0
52	Bb	549	0	552	0	0
53	Bc	444	0	461	0	0
54	Bd	441	0	485	0	0
55	Be	377	0	418	0	0
56	Bf	504	0	574	0	0
57	Bg	302	0	343	0	0
All	All	153634	0	105519	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	391/393 (100%)	367 (94%)	21 (5%)	3 (1%)	22	67
5	AF	238/241 (99%)	215 (90%)	21 (9%)	2 (1%)	22	67
6	AG	230/233 (99%)	210 (91%)	18 (8%)	2 (1%)	20	63
7	AH	203/206 (98%)	189 (93%)	12 (6%)	2 (1%)	18	61
8	AI	164/167 (98%)	143 (87%)	18 (11%)	3 (2%)	10	49
9	AJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	12	53
10	AK	176/179 (98%)	159 (90%)	15 (8%)	2 (1%)	17	60
11	AL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	11	51
12	AM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	11	51
13	AN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	3	31
14	AO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	11	51
15	AP	121/124 (98%)	103 (85%)	13 (11%)	5 (4%)	3	30
16	AQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
17	AR	98/101 (97%)	82 (84%)	9 (9%)	7 (7%)	1	19
18	AS	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
19	AT	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
20	AU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
21	AV	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	13	54
22	AW	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
23	AX	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
24	AY	68/71 (96%)	62 (91%)	5 (7%)	1 (2%)	12	53
27	BC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	14	56
28	BD	270/273 (99%)	239 (88%)	22 (8%)	9 (3%)	4	35
29	BE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	5	38
30	BF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	12	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BG	176/179 (98%)	148 (84%)	25 (14%)	3 (2%)	11	50
32	BH	174/177 (98%)	162 (93%)	9 (5%)	3 (2%)	11	50
33	BI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	4	35
34	BJ	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	25	68
35	BK	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
36	BL	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	11	50
37	BM	142/144 (99%)	124 (87%)	16 (11%)	2 (1%)	13	54
38	BN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	8	44
39	BO	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	22	67
40	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	20	63
41	BQ	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	10	49
42	BR	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	20	63
43	BS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	37
44	BT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	20	63
45	BU	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	18	61
46	BV	101/104 (97%)	90 (89%)	10 (10%)	1 (1%)	18	61
47	BW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8	44
48	BX	82/85 (96%)	68 (83%)	11 (13%)	3 (4%)	4	33
49	BY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	6	40
50	BZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	27
51	Ba	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	10	49
52	Bb	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	12	53
53	Bc	54/57 (95%)	46 (85%)	6 (11%)	2 (4%)	4	33
54	Bd	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
55	Be	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
56	Bf	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
57	Bg	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	39
All	All	6548/6682 (98%)	5895 (90%)	547 (8%)	106 (2%)	16	51

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	18	LEU

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Mol	Chain	Res	Type
12	AM	3	ASN
13	AN	74	VAL
14	AO	118	ASN
15	AP	86	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	326/326 (100%)	311 (95%)	15 (5%)	31	62
5	AF	198/199 (100%)	188 (95%)	10 (5%)	28	60
6	AG	189/190 (100%)	180 (95%)	9 (5%)	30	61
7	AH	172/173 (99%)	164 (95%)	8 (5%)	30	62
8	AI	125/126 (99%)	122 (98%)	3 (2%)	54	78
9	AJ	116/116 (100%)	104 (90%)	12 (10%)	8	32
10	AK	146/147 (99%)	136 (93%)	10 (7%)	18	51
11	AL	104/105 (99%)	99 (95%)	5 (5%)	30	61
12	AM	106/107 (99%)	98 (92%)	8 (8%)	16	48
13	AN	90/90 (100%)	85 (94%)	5 (6%)	25	57
14	AO	98/99 (99%)	95 (97%)	3 (3%)	45	71
15	AP	103/104 (99%)	98 (95%)	5 (5%)	29	61
16	AQ	95/96 (99%)	93 (98%)	2 (2%)	59	80
17	AR	83/84 (99%)	79 (95%)	4 (5%)	30	61
18	AS	76/77 (99%)	71 (93%)	5 (7%)	19	52
19	AT	65/65 (100%)	62 (95%)	3 (5%)	31	62
20	AU	77/78 (99%)	75 (97%)	2 (3%)	51	75
21	AV	64/65 (98%)	60 (94%)	4 (6%)	21	53
22	AW	78/79 (99%)	74 (95%)	4 (5%)	28	60
23	AX	65/66 (98%)	61 (94%)	4 (6%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AY	60/61 (98%)	55 (92%)	5 (8%)	13	43
27	BC	181/181 (100%)	176 (97%)	5 (3%)	49	74
28	BD	217/218 (100%)	210 (97%)	7 (3%)	44	71
29	BE	164/164 (100%)	153 (93%)	11 (7%)	19	51
30	BF	165/165 (100%)	156 (94%)	9 (6%)	25	58
31	BG	149/150 (99%)	138 (93%)	11 (7%)	16	48
32	BH	137/138 (99%)	128 (93%)	9 (7%)	19	52
33	BI	114/114 (100%)	109 (96%)	5 (4%)	33	63
34	BJ	109/110 (99%)	104 (95%)	5 (5%)	31	62
35	BK	116/116 (100%)	110 (95%)	6 (5%)	27	59
36	BL	104/104 (100%)	96 (92%)	8 (8%)	15	47
37	BM	103/103 (100%)	97 (94%)	6 (6%)	23	56
38	BN	109/109 (100%)	101 (93%)	8 (7%)	16	49
39	BO	103/103 (100%)	97 (94%)	6 (6%)	23	56
40	BP	87/87 (100%)	82 (94%)	5 (6%)	24	56
41	BQ	99/100 (99%)	93 (94%)	6 (6%)	22	55
42	BR	89/90 (99%)	88 (99%)	1 (1%)	78	89
43	BS	84/84 (100%)	78 (93%)	6 (7%)	17	49
44	BT	93/93 (100%)	88 (95%)	5 (5%)	26	58
45	BU	84/84 (100%)	79 (94%)	5 (6%)	22	55
46	BV	84/85 (99%)	81 (96%)	3 (4%)	40	68
47	BW	78/78 (100%)	74 (95%)	4 (5%)	28	60
48	BX	62/63 (98%)	55 (89%)	7 (11%)	7	29
49	BY	67/68 (98%)	64 (96%)	3 (4%)	32	63
50	BZ	55/55 (100%)	54 (98%)	1 (2%)	64	84
51	Ba	48/49 (98%)	47 (98%)	1 (2%)	59	80
52	Bb	62/62 (100%)	60 (97%)	2 (3%)	44	71
53	Bc	47/48 (98%)	46 (98%)	1 (2%)	59	80
54	Bd	48/49 (98%)	48 (100%)	0	100	100
55	Be	38/38 (100%)	37 (97%)	1 (3%)	51	75
56	Bf	51/52 (98%)	49 (96%)	2 (4%)	37	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	Bg	34/34 (100%)	30 (88%)	4 (12%)	6 27
All	All	5417/5447 (99%)	5138 (95%)	279 (5%)	31 59

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	BC	8	MET
30	BF	155	GLU
48	BX	2	HIS
27	BC	164	ARG
29	BE	43	ASP

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	1538/1542 (99%)	193 (12%)	0
2	AB	73/76 (96%)	12 (16%)	0
2	AE	73/76 (96%)	13 (17%)	0
25	BA	119/120 (99%)	15 (12%)	0
26	BB	2898/2904 (99%)	401 (13%)	0
4	AD	23/24 (95%)	4 (17%)	0
All	All	4724/4742 (99%)	638 (13%)	0

5 of 638 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	AA	1207	1	19,26,27	1.37	3 (15%)	20,38,41	2.39	3 (15%)
1	4OC	AA	1402	1	16,23,24	1.17	3 (18%)	19,32,35	1.35	2 (10%)
1	5MC	AA	1407	1	15,22,23	1.13	2 (13%)	17,32,35	0.83	0
1	UR3	AA	1498	1	14,22,23	0.95	0	16,32,35	1.39	3 (18%)
1	2MG	AA	1516	1	19,26,27	1.36	3 (15%)	20,38,41	2.49	4 (20%)
1	MA6	AA	1518	1	16,26,27	0.94	1 (6%)	18,38,41	1.40	2 (11%)
1	MA6	AA	1519	1	16,26,27	0.87	1 (6%)	18,38,41	1.61	3 (16%)
1	PSU	AA	516	1	16,21,22	1.38	1 (6%)	20,30,33	6.01	9 (45%)
1	7MG	AA	527	1	20,26,27	2.26	4 (20%)	22,39,42	2.17	2 (9%)
1	2MG	AA	966	1	19,26,27	1.35	2 (10%)	20,38,41	2.84	7 (35%)
1	5MC	AA	967	1	15,22,23	1.11	2 (13%)	17,32,35	0.78	0
2	H2U	AB	16	2	17,21,22	1.00	1 (5%)	21,30,33	1.39	2 (9%)
2	H2U	AB	20	2	17,21,22	1.05	1 (5%)	21,30,33	1.03	0
2	PSU	AB	32	2	16,21,22	1.35	3 (18%)	20,30,33	6.13	7 (35%)
2	MIA	AB	37	2	23,31,32	1.12	3 (13%)	25,44,47	1.63	5 (20%)
2	PSU	AB	39	2	16,21,22	1.33	1 (6%)	20,30,33	6.16	7 (35%)
2	7MG	AB	46	2	20,26,27	2.24	3 (15%)	22,39,42	2.31	2 (9%)
2	3AU	AB	47	-	14,28,29	1.07	1 (7%)	14,40,43	0.75	0
2	5MU	AB	54	2	14,22,23	1.34	2 (14%)	16,32,35	4.20	4 (25%)
2	PSU	AB	55	2	16,21,22	1.34	1 (6%)	20,30,33	5.98	5 (25%)
2	4SU	AB	8	2	14,21,22	1.24	3 (21%)	15,30,33	2.28	2 (13%)
2	H2U	AE	16	2	17,21,22	0.89	0	21,30,33	0.89	0
2	H2U	AE	20	2	17,21,22	0.92	0	21,30,33	0.95	0
2	PSU	AE	32	2	16,21,22	1.36	1 (6%)	20,30,33	5.97	7 (35%)
2	MIA	AE	37	2	23,31,32	1.16	5 (21%)	25,44,47	1.50	4 (16%)
2	PSU	AE	39	2	16,21,22	1.30	2 (12%)	20,30,33	6.05	7 (35%)
2	7MG	AE	46	2	20,26,27	2.21	4 (20%)	22,39,42	2.20	3 (13%)
2	3AU	AE	47	-	14,28,29	1.00	0	14,40,43	1.31	2 (14%)
2	5MU	AE	54	2	14,22,23	1.31	2 (14%)	16,32,35	4.22	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	AE	55	2	16,21,22	1.39	2 (12%)	20,30,33	6.07	6 (30%)
2	4SU	AE	8	2	14,21,22	1.11	1 (7%)	15,30,33	2.05	3 (20%)
26	6MZ	BB	1618	26	18,25,26	0.99	1 (5%)	16,36,39	1.54	2 (12%)
26	2MG	BB	1835	26	19,26,27	1.36	2 (10%)	20,38,41	2.26	4 (20%)
26	PSU	BB	1911	26	16,21,22	1.35	1 (6%)	20,30,33	5.94	5 (25%)
26	3TD	BB	1915	26	16,22,23	1.09	0	19,32,35	2.02	6 (31%)
26	PSU	BB	1917	26	16,21,22	1.44	2 (12%)	20,30,33	6.16	7 (35%)
26	5MU	BB	1939	26	14,22,23	1.40	2 (14%)	16,32,35	3.83	2 (12%)
26	5MC	BB	1962	26	15,22,23	1.06	1 (6%)	17,32,35	0.97	1 (5%)
26	6MZ	BB	2030	26	18,25,26	1.08	2 (11%)	16,36,39	1.70	4 (25%)
26	7MG	BB	2069	26	20,26,27	2.23	3 (15%)	22,39,42	2.12	3 (13%)
26	OMG	BB	2251	26	18,26,27	1.44	3 (16%)	22,38,41	2.28	4 (18%)
26	2MG	BB	2445	26	19,26,27	1.42	3 (15%)	20,38,41	2.22	4 (20%)
26	H2U	BB	2449	26	17,21,22	0.96	1 (5%)	21,30,33	1.18	1 (4%)
26	PSU	BB	2457	26	16,21,22	1.37	1 (6%)	20,30,33	6.13	9 (45%)
26	OMC	BB	2498	26	15,22,23	1.00	1 (6%)	19,31,34	1.23	1 (5%)
26	2MA	BB	2503	26	18,25,26	1.20	4 (22%)	17,37,40	1.48	2 (11%)
26	PSU	BB	2504	26	16,21,22	1.37	1 (6%)	20,30,33	6.14	7 (35%)
26	OMU	BB	2552	26	14,22,23	1.44	2 (14%)	18,31,34	3.43	2 (11%)
26	CH	BB	2575	26	15,21,22	1.03	1 (6%)	16,30,33	1.02	0
26	PSU	BB	2580	26	16,21,22	1.45	2 (12%)	20,30,33	6.11	5 (25%)
26	PSU	BB	2605	26	16,21,22	1.38	2 (12%)	20,30,33	6.13	7 (35%)
26	1MG	BB	745	26	18,26,27	1.08	2 (11%)	18,39,42	1.56	1 (5%)
26	PSU	BB	746	26	16,21,22	1.42	2 (12%)	20,30,33	6.07	8 (40%)
26	5MU	BB	747	26	14,22,23	1.26	1 (7%)	16,32,35	4.05	3 (18%)
26	PSU	BB	955	26	16,21,22	1.40	2 (12%)	20,30,33	6.05	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	32	2	-	0/7/25/26	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
2	PSU	AB	39	2	-	0/7/25/26	0/2/2/2
2	7MG	AB	46	2	-	0/7/37/38	0/3/3/3
2	3AU	AB	47	-	-	0/8/34/35	0/2/2/2
2	5MU	AB	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AB	8	2	-	0/3/25/26	0/2/2/2
2	H2U	AE	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AE	20	2	-	0/7/38/39	0/2/2/2
2	PSU	AE	32	2	-	0/7/25/26	0/2/2/2
2	MIA	AE	37	2	-	0/11/33/34	0/3/3/3
2	PSU	AE	39	2	-	0/7/25/26	0/2/2/2
2	7MG	AE	46	2	-	0/7/37/38	0/3/3/3
2	3AU	AE	47	-	-	0/8/34/35	0/2/2/2
2	5MU	AE	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AE	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AE	8	2	-	0/3/25/26	0/2/2/2
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	BB	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	0/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/5/27/28	0/2/2/2
26	CH	BB	2575	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	746	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	46	7MG	C8-N9	-7.90	1.34	1.45
26	BB	2069	7MG	C8-N9	-7.81	1.34	1.45
1	AA	527	7MG	C8-N9	-7.79	1.34	1.45
2	AE	46	7MG	C8-N9	-7.57	1.34	1.45
2	AB	20	H2U	O5'-C5'	-2.92	1.40	1.44

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2580	PSU	N1-C2-N3	-19.71	114.23	128.40
26	BB	1917	PSU	N1-C2-N3	-19.57	114.32	128.40
2	AB	39	PSU	N1-C2-N3	-19.43	114.42	128.40
2	AB	32	PSU	N1-C2-N3	-19.28	114.53	128.40
26	BB	2605	PSU	N1-C2-N3	-19.21	114.58	128.40

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.