



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:09 PM BST

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 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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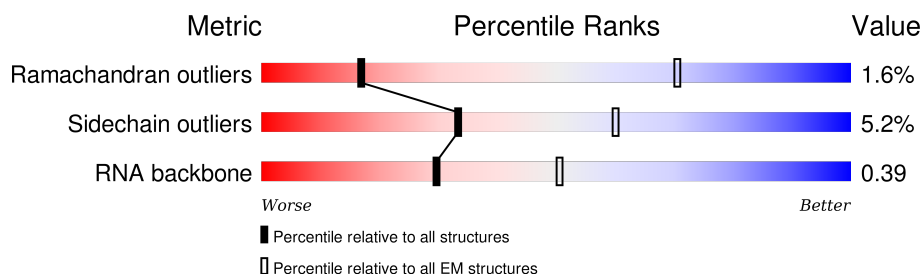
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 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.








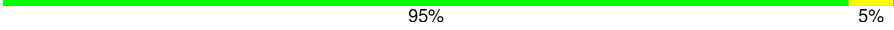

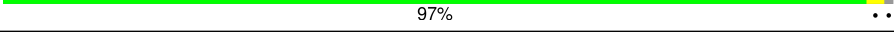


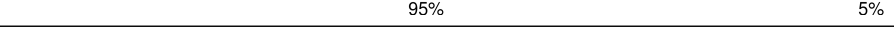
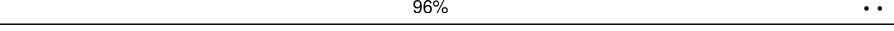

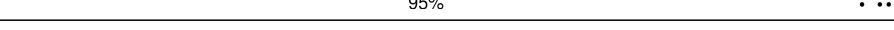
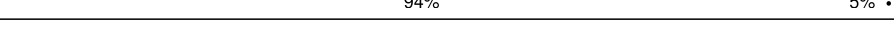



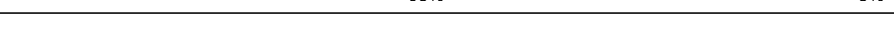
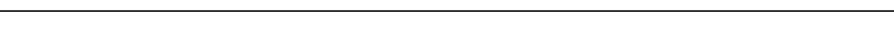

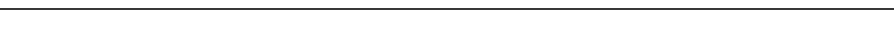
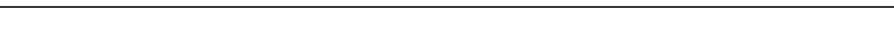


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	
2	AB	76	
2	AE	76	
3	AC	393	
4	AD	24	
5	AF	241	
6	AG	233	
7	AH	206	
8	AI	167	

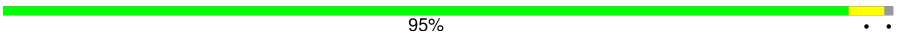
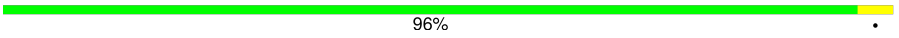

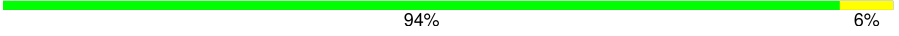
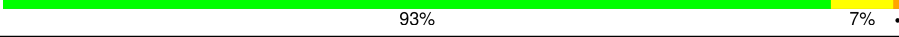
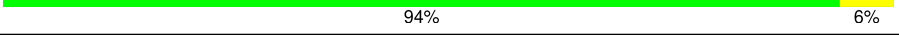
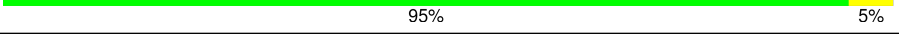

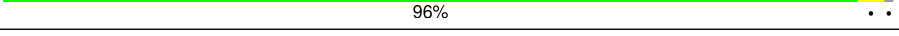
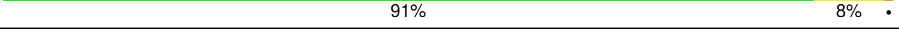
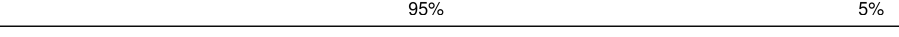
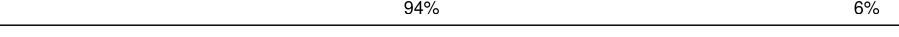
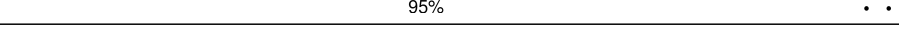
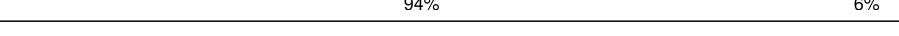
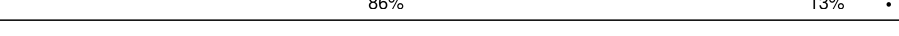

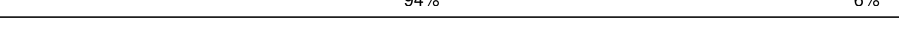
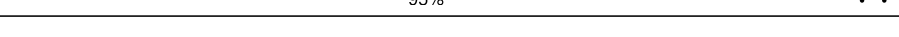
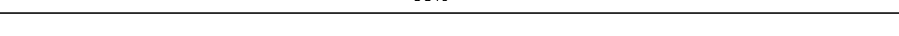

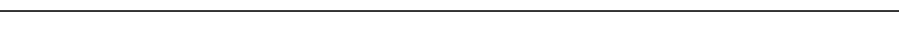

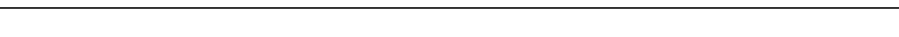
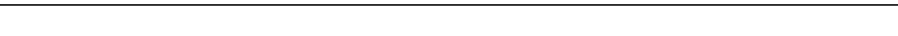
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Mol	Chain	Length	Quality of chain
9	AJ	135	 89% 10% .
10	AK	179	 92% 7% .
11	AL	130	 93% 6% .
12	AM	130	 91% 8% .
13	AN	103	 90% 9% .
14	AO	129	 95% 5% .
15	AP	124	 90% 9% .
16	AQ	118	 97% ..
17	AR	101	 85% 14% .
18	AS	89	 92% 7% .
19	AT	82	 95% 5%
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% 50% 25% .
26	BB	2904	 21% 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		

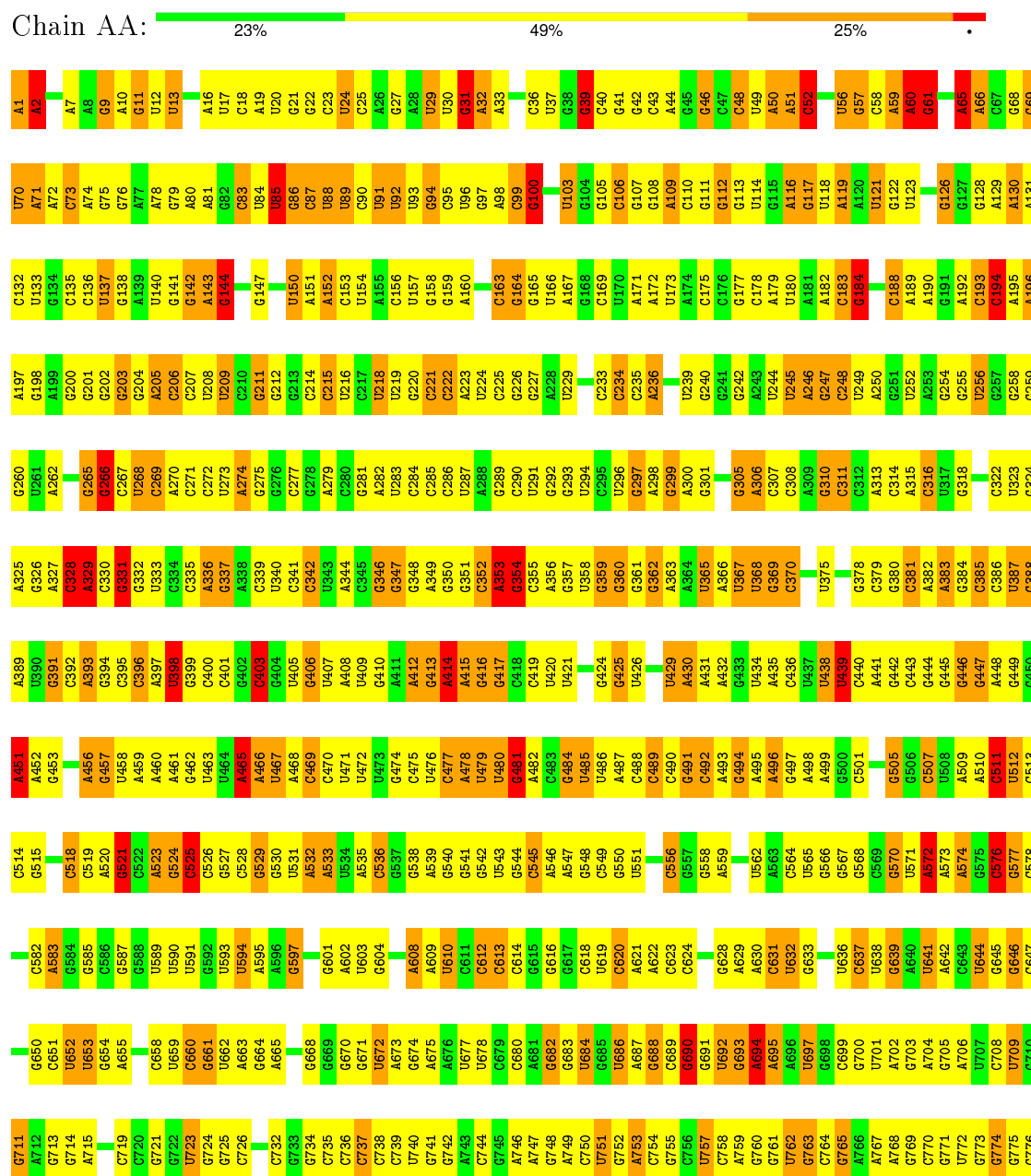
- Molecule 57 is a protein called 50S ribosomal protein L36.

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 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: 16S ribosomal RNA



A1483	G1353	A1285	G1220	A1155	A1092	U1029	G966	A900	G838	A777
C1484	U1354	A1288	G1221	G1156	A1093	U1030	C967	A901	C839	G778
U1485	G1355	A1288	G1222	A1157	G1094	G1031	A968	G902	C840	C779
G1486	G1356	A1289	C1223	G1158	U1095	G1032	A969	G903	C841	A780
G1487	U1357	U1290	U1224	U1159	C1096	G1033	C970	U904	U842	A781
G1488	U1358	U1291	A1225	G1160	C1097	G1034	G971	U905	U843	A782
G1489	C1359	G1292	C1226	C1161	C1098	A1035	G972	A906	G844	C783
U1490	U1360	C1293	C1227	C1162	G1099	C1036	G973	A907	A845	A784
A1491	G1361	U1294	C1228	A1163	C1100	C1037	A974	A908	G846	G785
A1492	A1362	A1362	C1229	G1164	A1101	C1038	A975	A909	G847	G786
G1493	U1363	U1295	C1230	U1165	A1102	G1039	G976	C910	C848	A787
G1494	U1364	U1298	U1231	A1169	C1103	U1040	A977	U911	G849	U788
G1495	G1365	U1299	U1232	A1170	G1104	G1041	A978	G912	U850	U789
G1496	C1366	G1300	G1233	C1172	A1105	A1042	G979	A913	G851	A790
G1497	C1366	U1301	U1234	C1173	C1109	U1043	C980	A914	U854	G791
G1498	C1369	U1302	U1235	U1174	C1110	A1044	U981	A915	U854	A792
A1499	G1370	G1303	A1236	G1175	A1111	C1046	A983	U916	U855	U793
A1500	G1371	G1304	C1237	G1176	C1112	U1047	C984	G917	C856	A794
G1501	U1372	G1305	G1241	A1177	G1113	G1048	C985	U920	G858	C795
A1502	G1373	A1306	G1242	G1178	C1114	U1049	U986	U921	G858	C796
A1503	A1374	U1307	U1243	G1179	U1115	C1051	G987	A923	A860	U798
G1504	U1375	U1308	G1244	A1180	U1116	U1052	U989	G928	C862	G800
G1505	G1376	G1309	G1245	G1181	U1117	G1053	C990	G929	U863	U801
U1506	A1377	G1310	A1246	G1182	U1118	C1054	U991	A935	A864	A802
U1507	U1444	U1311	U1247	U1183	G1119	U1055	U992	C930	C866	G803
A1508	G1378	U1312	A1248	G1184	C1120	U1056	A994	C931	C867	U804
G1509	G1379	U1313	C1249	G1185	U1121	G1057	G995	G932	C868	C806
G1510	U1380	U1314	A1250	G1186	U1122	G1058	A996	G933	C869	A807
G1511	C1382	U1315	U1251	G1187	U1123	C1059	U997	A936	U870	G808
A1512	C1383	G1316	G1253	U1188	G1124	U1060	C998	C937	A872	C810
G1513	C1384	C1317	A1254	U1189	U1125	U1061	C999	A938	A873	C811
G1514	G1385	A1318	G1255	U1190	U1126	U1062	G1001	G941	G874	U813
G1517	C1388	A1319	U1256	A1191	G1127	C1063	G1002	G942	C876	A814
C1520	U1389	C1320	A1257	U1192	C1128	G1064	G1003	U943	G877	A815
G1521	U1390	U1321	G1258	G1193	C1129	U1065	G1004	U944	A878	A816
U1522	U1391	G1322	G1259	U1194	A1130	C1066	G1006	G945	C879	C817
G1523	G1392	A1324	G1260	C1195	G1131	C1067	U1007	A946	C880	C818
G1526	C1395	U1325	U1264	A1196	C1132	A1068	U1008	G947	G881	A819
U1527	A1396	U1326	C1265	U1197	G1133	G1068	U1009	C948	C882	U820
U1528	C1397	G1327	G1266	G1198	G1134	C1069	C1011	A949	U884	G821
G1529	C1397	U1328	U1267	U1199	U1135	U1070	A1012	U950	U885	C823
G1530	A1398	A1329	G1268	C1200	C1136	C1071	G1013	U951	G886	G824
U1531	C1399	U1330	A1269	U1201	C1137	G1072	G1014	G952	G887	A825
U1532	C1400	A1333	U1270	U1202	G1138	U1073	G1015	U953	G888	C826
C1533	G1401	C1325	G1271	C1203	C1139	G1074	A1016	U954	A889	U827
A1534	G1405	G1337	U1272	A1204	C1140	U1075	U1017	U955	G890	U828
U1535	U1406	G1338	C1273	U1205	C1141	U1076	G1018	U956	U891	A830
C1536	U1407	A1339	A1274	C1208	G1142	G1077	U1083	A957	C893	G833
U1537	A1408	U1340	A1275	C1209	G1143	U1078	U1084	A959	C896	U834
C1538	C1409	U1341	G1276	U1212	A1145	U1085	G1085	U960	C897	U835
U1539	A1410	G1342	G1277	A1213	C1146	U1086	G1086	U961	C898	G836
U1540	C1411	G1343	G1278	A1214	C1147	U1087	U1087	C962	C899	U837
U1541	C1412	A1346	U1279	G1215	U1148	G1087	U1088	G963		
U1542	A1413	A1347	U1280	G1216	U1149	G1088	U1089			
	U1470	U1406	C1281	A1217	A1151	G1088	G1090			
	U1471	U1407	U1282	C1217	A1152	G1089	U1091			
	U1472	A1408	U1283	C1218	A1153	G1090				
	U1473	C1409	U1284	C1219	A1154					
	U1474	U1341								
		G1342								
		G1343								
	U1477	C1411								
	U1478	C1412								
	U1479	A1413								
	U1480	U1414								
	U1481	G1415								
	U1482	U1416								

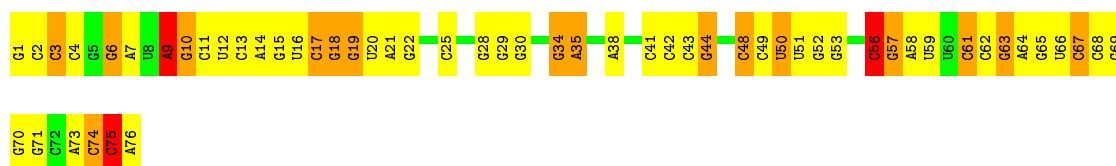
• Molecule 2: A/T-site tRNA Phe

Chain AB:  29% 45% 25%

G1	G69	G68
G2	G70	G69
G3	G71	G70
G4	G72	G71
G5	G73	G72
G6	G74	G73
G7	G75	G74
G8	G76	G75
G9	G77	G76
G10	G78	G77
G11	G79	G78
G12	G80	G79
G13	G81	G80
G14	G82	G81
G15	G83	G82
G16	G84	G83
G17	G85	G84
G18	G86	G85
G19	G87	G86
G20	G88	G87
G21	G89	G88
G22	G90	G89
G23	G91	G90
G24	G92	G91
G25	G93	G92
G26	G94	G93
G27	G95	G94
G28	G96	G95
G29	G97	G96
G30	G98	G97
G31	G99	G98
G32	G100	G99
G33	G101	G100
G34	G102	G101
G35	G103	G102
G36	G104	G103
G37	G105	G104
G38	G106	G105
G39	G107	G106
G40	G108	G107
G41	G109	G108
G42	G110	G109
G43	G111	G110
G44	G112	G111
G45	G113	G112
G46	G114	G113
G47	G115	G114
G48	G116	G115
G49	G117	G116
G50	G118	G117
G51	G119	G118
G52	G120	G119
G53	G121	G120
G54	G122	G121
G55	G123	G122
G56	G124	G123
G57	G125	G124
G58	G126	G125
G59	G127	G126
G60	G128	G127
G61	G129	G128
G62	G130	G129
G63	G131	G130
G64	G132	G131
G65	G133	G132
G66	G134	G133
G67	G135	G134

• Molecule 2: A/T-site tRNA Phe

Chain AE:  26% 49% 21%



- Molecule 3: Elongation factor Tu 2

Chain AC: 95% 5%



- Molecule 4: mRNA

Chain AD: 13% 50% 29% 8%



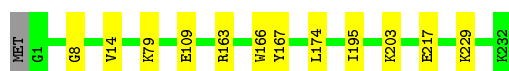
- Molecule 5: 30S ribosomal protein S2

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%

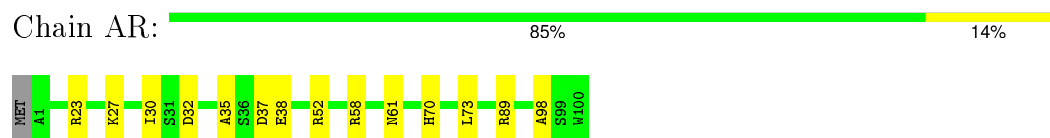


- Molecule 16: 30S ribosomal protein S13

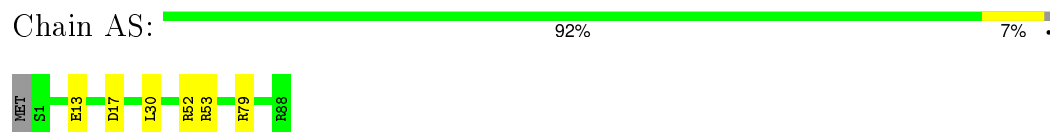
Chain AQ: 97%



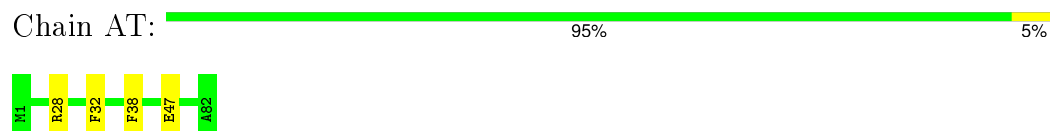
- Molecule 17: 30S ribosomal protein S14



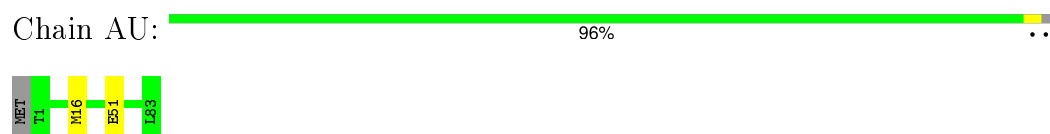
- Molecule 18: 30S ribosomal protein S15



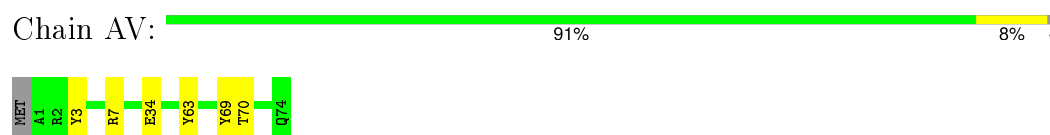
- Molecule 19: 30S ribosomal protein S16



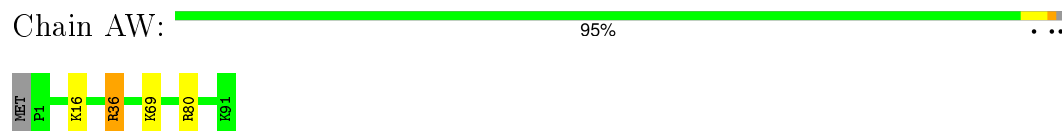
- Molecule 20: 30S ribosomal protein S17



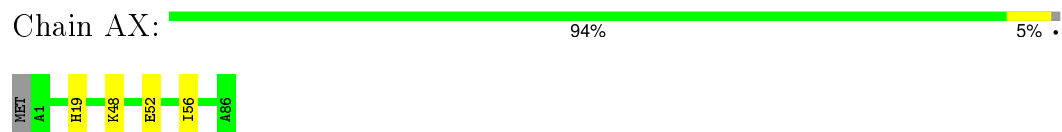
- Molecule 21: 30S ribosomal protein S18



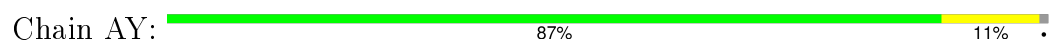
- Molecule 22: 30S ribosomal protein S19



- Molecule 23: 30S ribosomal protein S20



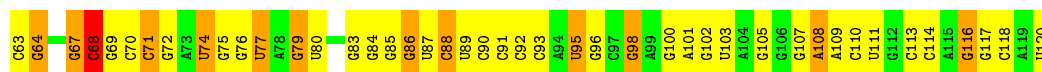
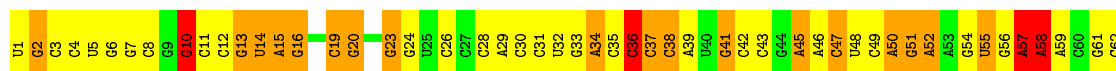
- Molecule 24: 30S ribosomal protein S21





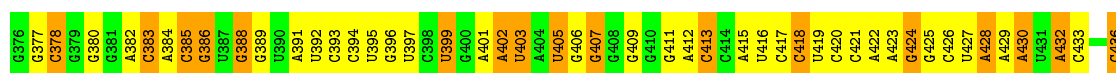
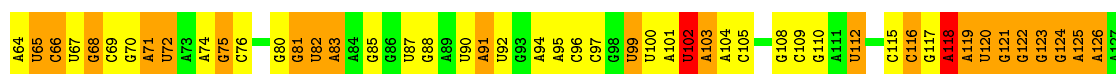
• Molecule 25: 50S ribosomal RNA 5S

Chain BA: 21% 50% 25%



• Molecule 26: 50S ribosomal RNA 23S

Chain BB: 21% 49% 26%



G1691	A1630	G1668	U1506	U1440	U1375	U1313	C1251	U1188	G1124	G1062	U999	C937	G874	U813	A752
U1692	G1631	A1669	C1507	G1441	C1376	C1314	G1252	A1189	G1125	G1063	A1000	G938	G875	C814	A753
U1693	A1632	A1570	A1508	U1442	G1377	C1315	A1253	G1190	A1126	C1064	A1001	G939	C876	C815	
C1694	G1633	A1571	A1509	U1443	A1378	U1316	A1254	G1191	A1127	U1065	G1002	G940	A877	C816	A756
G1695	A1634	A1572	G1510	G1444	U1379	G1317	U1255	G1192	U1066	U1067	G1003	A941	A878	C817	G757
G1696	A1635	G1573	G1511	G1445	U1380	U1318	G1256	G1193	A1128	A1068	U1004	G942	A879	C818	C758
G1697	G1636	G1574	C1512	G1446	G1381		C1257	A1194	U1130	G1069	C1005	A943	C880	A819	G759
A1698	A1637	C1575	U1513	C1447	G1382	A1321	U1258	G1195	G1131	A1069	C1006	G944	G881	A820	G760
G1699	G1638	U1576	G1514	A1448	A1383		G1259	C1196	U1132	A1070	C1007	A945	G882	A821	A761
A1700	C1639	U1577	A1515	G1449	A1384	G1325	A1260	G1197	A1133	G1072		C946	G883	G822	G762
A1701	A1640	U1578	G1516	G1450	A1385	U1326	C1261	U1198	A1134	U1073	G1015	G951	U884	C823	G763
G1702	A1641	G1579	G1451	G1452	U1386	U1326	A1262	U1199	G1135	A1073	G1011	C948	C885	U824	A764
G1703	G1642	A1580	G1452	G1453	A1387	A1327	U1263		G1136	G1074	U1012	G949	A886	A825	G765
C1704	G1643	G1581	U1519	A1454	G1388	A1328	A1264	G1202	G1137	C1075	C1013	G950	U887	U826	G766
A1705	G1644		G1520	G1455	U1389	U1329	G1265	U1203	G1138	A1076	A1014	C952	C888	U827	G767
G1706	G1645	U1584	A1521	G1456	G1390	U1330	A1266	U1204	G1139	A1077	U1015	G953	C889	U828	G768
G1707	C1646	A1585	U1523		U1391	G1331	U1267	A1205	A1140	C1078	G1016	G954	C890	A829	U769
G1708	A1647	A1586	G1524	U1458	A1392	G1332	A1268	G1206	U1141	C1079	G1017		C891	G830	G770
U1709	U1648	G1587	A1525	G1459	U1393	G1333	A1269	C1207	U1142	A1080	U1018		A892	G831	G771
G1710	G1649		U1526	U1460	A1394	G1334	C1270	C1208	A1143	U1081	U1019	C957	C893	U832	C772
A1711	A1650		G1527	U1461	U1395	C1335	G1271	U1209	A1144	U1082	U1020	U958	U894	A833	C773
	G1651	A1591	A1528	C1462	U1396	A1336	A1272	G1210	C1145	U1083	A1021	A959	U895	G834	G774
G1714	A1652	C1592	G1529	C1463	U1397	G1337	U1273	C1211	A1146	A1084	G1022	A960	A896	C835	G775
G1715	G1653	A1593	U1530	C1463	C1398	G1338	A1274	G1212	A1147	A1085	U1023	C961	C897	G836	G776
U1716	A1654	U1466	G1531	U1466	G1399	G1339	A1275	A1213	U1148	A1086	G1024	G962	C898	C837	G777
A1717	A1655	U1467	A1532	U1467		U1340	A1276	A1214	G1149	G1087	G1025	U863	A899	C838	G778
G1718	C1656		A1533		U1402	G1341	G1277	G1215	C1150	A1088	G1026	C964	U979	U839	G779
U1719	U1657	A1596	U1534	C1472	A1403	A1342	C1278	G1216	A1151	A1089	A1027	C965	C902	C840	G780
G1720	C1658	A1597	A1535	G1473	U1404	G1343	G1279	G1217	C1152	A1090	A1028	G966	C903	G841	A781
G1721	G1659	U1599	A1536	U1474	U1405	U1344	G1280	G1218	C1153	A1091	A1029	U967	G904	U842	A782
A1722	C1660	G1600	G1537	G1475	U1406	G1345	G1281	U1219	G1154	C1092	C1030	C968	A905	G843	A783
G1723	G1661	G1601	G1538	U1476	G1407	G1346	U1282	G1220		G1093	G1031	C969	U906	A844	G784
G1724	U1662	U1602	U1539	A1477	A1408	A1347	G1283	C1221	C1156	U1094	A1032	U970	C907	A845	G785
G1725	G1663	G1603	G1540	G1478	U1409	C1348	A1284	U1222	G1159	A1095	U1033	G971	C908	C848	G786
A1664	A1665	C1604	C1541	G1479	G1410	C1349	A1285	G1223	G1160	A1096	G1034	A972	A909	C787	
C1727	G1666	G1605	U1542	U1480	U1411	C1350	A1286		G1161	U1097	U1035	A973	A910	A849	
G1728		C1606	G1543	U1481		C1351	A1287	A1226	G1162	A1098	G1036	G974	A911	U850	A788
U1729	G1667	G1607	A1544	G1482	G1414	U1352	G1288	G1227		G1099	G1037	A975	C912	C851	U790
C1730		A1608	A1545		U1415	A1353	C1289		A1165	C1100	G1038	G976	U913	U852	C791
G1731	U1670	U1609	G1546	U1483	G1416	C1354	C1290	A1230	G1166	U1101		G977	U914	C853	A792
C1732	U1671	C1610	C1547	U1484	C1417	G1355	C1291	U1231	C1167	A1102	G1041	G978	C915	C854	A793
G1733	A1672	A1611	A1548	U1485	G1418	G1356	G1292	G1232		A1103	G1042	A979	G916	G855	A794
G1734	G1673	U1487	A1549	U1486	A1419	C1357	C1293	C1233	G1170	C1104	C1043	A980	A917	G856	C795
A1735	G1674	G1612	C1550	A1420	U1420	G1358	U1294	U1234	G1171	U1105	C1044	A981	A918	G857	C796
U1736	C1675	A1613	A1551	G1421	A1421	A1359	C1295	G1235	C1172	G1106	C1045	C982	U919	G858	G797
G1737	A1676	G1615	A1552	G1422	G1360	G1361	G1296	G1236	U1173	A1107	A1046	A983	A920	G859	G798
G1738	G1677	U1553	G1423	G1423	C1361	U1237	C1297	U1237	U1174	U1108	G1047	A984	C921	U860	G799
A1739	A1678	U1554	G1424	G1424	C1362	G1362	C1298	G1238	A1175	C1109	A1048		C922	A861	A800
G1740	U1680	U1618	G1425	G1425	C1363	G1363	G1299	U1239	U1176	G1110		C987	G923	G862	G801
C1741		A1692	G1426	G1426	G1364	U1240	G1300	U1240	G1177	A1113	C1049	A988	G924	A863	A802
U1742	G1681		A1427	A1427	A1365	A1241	A1301	A1241	C1176	G1112		G989	A925	G864	U803
G1743	U1682	U1559			A1366	U1242	A1302	U1242	G1179	U1113	C1052	A990	G926	C865	A804
A1744	U1683	G1560	A1431	C1498	A1367	C1243	G1303	C1243	U1180	C1114	C1053	C991		A866	G805
A1745	G1684	C1561	C1499	C1499	G1368	A1304	A1304	A1244	U1181	G1115	A1054	C992	G930	C867	C806
A1746	C1685	U1562	G1500	G1500	A1433	G1369	C1305	G1245	G1182	G1116	G1056	G993	U931	U868	U807
U1747	G1686	G1501	U1563	G1501	A1434	C1370	C1306	A1246	U1183	C1117	A1057	C994	U932	G869	G808
C1748	G1687	A1502	C1564	A1502	A1434	G1371	A1307	A1247	U1184	C1118	U1058	C995	A933	U870	G809
A1749	U1688	U1565	C1565	A1503	U1437	A1372	A1308	G1248	G1185	U1119	G1059	A996	U934	U871	U810
G1750	A1689	A1566	U1566	U1504	U1438	C1373	G1309	U1249	G1186		U1060	G997	C935	U872	U811
U1751	A1690	U1629	G1567	A1505	A1439	G1374		G1250	G1187	C1123	U1061	C998	A936	C873	C812

C2723	G2659	U2593	A2530	C2466	G2331	A2266	G2204	G2141	A2077	G2012	C1947	U1883	A1819	C1752
U2724	A2660	C2594	A2531	C2467	C2332	A2267	A2205	A2142	C2078	A2013	U1951	G1884	A1819	G1753
A2725	G2661	G2595	G2532	A2468	U2333	G2268	C2206	G2143	U2079	A2014	U1951	A1885	C1822	A1754
A2726	A2662	U2533	U2533	A2469	U2334	G2269	C2207	G2144	A2080	A2015	U1952	U1886	C1822	
A2727	G2663	A2534	A2534	G2470	A2335	A2271	C2208	C2145	U2081	U2016	G1953	C1887	U1825	U1757
A2728	G2664	G2535	G2535	A2471	A2336	G2270		C2146	A2082	U2017	G1954	C1888	U1826	U1758
G2729	A2665	G2536	G2536	G2472	G2337	U2272		A2147	G2083	G2018	U1955	A1889	U1827	A1759
G2730	C2667	G2603	U2537	U2473	C2338	A2273		G2148	U2085	A2019	U1956	A1890	C1828	C1760
G2731	G2668	G2604	C2538	A2406	A2339	A2274	U2212	U2149	U2086	A2020	G1961	C1831	G1831	C1761
A2732			C2539	C2475	A2340	C2275	C2214	C2150	C2087	U2022	C1962	C1832	C1832	A1762
A2733			C2540	A2476	G2341	G2276	C2215	U2151	G2087	G2023	U1963	C1894	C1833	C1763
G2734			U2403	U2477	G2342	G2277	G2216	G2152	A2088	G2024	U1964	C1895	U1834	C1764
G2735	U2672	C2610	A2541	U2478	C2343	A2278	G2217		C2089	G2025	C1965	G1896	C1766	C1765
A2736	G2673	C2612	G2542	U2479	U2344		G2218	U2155	A2090	C2025	C1966	G1897	C1767	G1766
G2737		U2613	G2543	C2480	G2345	A2281	U2219	G2156	C2091	U2026	U1967	G1897	C1837	C1768
A2738	G2676	G2614	G2546		A2346	G2282	U2220	U2157	U2092	U2027	C1967	U1898	C1838	C1769
U2739	C2678	U2546	G2415	G2485	C2347	C2283	G2221	A2158	G1968	U2028	A1899	C1839	C1839	U1769
A2740	A2679	A2547	C2416	C2486	U2348	A2284	G2222	G2159	G2093	G2029	A1900	G1840	G1840	U1770
A2741	U2680	U2548	C2417	G2487	G2349	C2285	G2223	C2160	A2094	U2030	A1901	U1841	U1841	A1772
G2742	C2681	G2615	A2418	U2488	C2350	G2286	G2224	C2161	A2097	A2031	U1971	C1842	C1842	A1773
U2743	A2682	C2620	U2419	G2489	C2351	A2287	A2225	C2162	U2098	G2032	G1972	C1843	C1843	C1774
G2744	C2683	G2621	C2420	C2490	A2352	A2288	C2226	A2163	U2099	U2034	G1974	C1844	C1844	U1775
C2745	U2684	U2622	G2421	U2491			A2227	C2164			G1975	G1845	G1845	G1776
U2746	G2685	U2622									G1975	G1846	G1846	U1777
G2747	G2686	G2623	G2553	U2492	G2357		G2228	G2102		U2039	U1976	C1908	G1847	U1778
A2748	U2687	U2624	U2554	U2493	G2357		G2229	C2103		G2040	U1977	C1909	A1847	U1779
U2749	G2688	G2625	U2555	C2494	C2362		G2230	A2168			A1977	A1848	A1848	
A2750	U2689	C2626	G2557	G2495	G2363		U2231	A2170	U2106	U2041	U1978	G1849	G1849	A1780
G2751	C2690	G2627	A2426	C2496	C2364		C2232	A2171	G2107	A2042	A1979	G1850	G1850	U1781
C2752	U2691	U2628	C2427	A2497	G2365		U2233	U2172	A2108	C2043	G1980	C1914	U1851	U1782
A2753	G2692	G2629	G2428	G2498	A2366		G2234	U2109	U2109	C2044	A1981	G1915	U1852	A1783
U2754	C2693	U2630	G2429	G2499	G2367		G2235	C2174	G2111	C2045	U1982	A1916	A1853	A1784
G2755	G2694	G2631	A2430	U2500	C2368		U2236	C2175	U2111	G2046	G1983	U1917	A1854	A1785
A2756	U2695	A2632	U2431	C2501	C2369		G2237	A2176	G1984	C2047	U1918	A1855	A1855	A1786
A2757	G2696	G2633	A2432	G2502	G2370		G2238	C2177	U2113	G2048	A1919	C1856	C1856	A1787
G2758	C2697	A2634	A2433	A2503	G2371		U2239	C2178	A2114	C2049	C1986	G1857	G1857	C1788
U2759	U2698	A2635	A2434	U2504	G2372		G2240	C2179	G2115	C2050	A1987	G1921	A1858	
C2760	G2699	C2636	U2438	G2506	G2373		G2242	U2180	G2116	A2051	G1988	G1922	U1859	A1791
A2761	U2700	U2637	A2439	C2507	G2374		U2243	U2181	A2117	G2053	G1923	U1923	G1860	G1792
G2762	G2701	G2638	C2440	G2508	G2375		U2244	U2182	U2118	A2054	C1990	C1924	C1861	C1793
G2763	C2702	A2639	U2441	G2509	A2376		U2245	A2183	A2119	G2055	U1991	C1925	G1862	
A2764	C2703	G2640	C2442	U2510	G2378		G2246	A2184	G2120	C2056	G1992	U1926	G1863	U1796
A2765	C2704	U2511	G2443	U2511	G2379			U2185	G2121	G2057	A1927	U1864	G1864	G1797
U2766	G2705	G2642	G2444	C2512	G2380		U2249	G2186	U2122	G2057	C1994	U1865	U1865	U1798
G2767	A2706	G2643	G2445	G2513	A2381		G2250	U2187	G2123	A2058	U1995	G1923	A1866	G1799
U2768	U2707	G2644	G2446	U2514	G2382		G2251	G2188	G2124	A2059	C1996	G1867	C1867	C1800
U2769	G2708	G2645	G2447	G2515	G2383		G2252	U2189	G2125	A2060	C1997	C1868	A1801	A1802
G2770	C2709	A2646	A2448	A2516	U2384		G2253	A2190	A2126	G2061	A1998	G1869	G1869	
G2771	G2710	G2579	U2449	G2517	C2385		G2254	A2191	G2127	A2062	C1999	G1933	C1870	A1806
C2772	A2711	G2580	U2450	U2459	G2386		G2255	U2192	G2128	C2063	C2000	C1934	A1871	G1807
		G2581	G2451	G2459	U2387		G2256	G2193	C2129	C2064	C2001	G1935	G1872	G1807
		G2582	G2455	U2459	A2388		G2257	U2194	U2130	C2065	G2002	A1936	G1873	A1808
		G2583	G2456	C2456	G2389		G2258	U2195	U2131	C2066	A2003	C1937	C1874	A1809
		G2584	G2457	U2457	U2390		G2259	C2196	U2132	G2067	A1938	C1875	G1875	A1810
		G2585	G2458	G2458	G2391		U2259	U2197	G2133	U2068	A2005	A1876	G1811	G1811
		G2586	A2459	A2459	A2392		C2261	A2198	A2134	C2006	U1940	A1877	U1812	U1812
		G2587	U2460	U2460	U2393		U2262	A2199	A2135	C2072	U2007	G1878	G1813	G1813
		G2588	A2461	A2461	A2394		U2263	C2200	C2008	C2073	C1942	C1879	G1814	G1814
		G2589	C2462	C2462	C2395		G2264	G2201	U2139	U2074	U1943	U1880	C1881	A1815
		G2592			G2397		U2265	U2202	G2140	U2075	U2011	C1882	C1816	C1816



- 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%



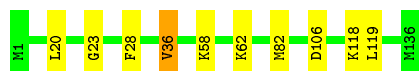
- Molecule 37: 50S ribosomal protein L15

Chain BM: 94%



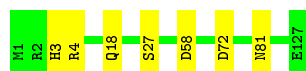
- Molecule 38: 50S ribosomal protein L16

Chain BN: 93%



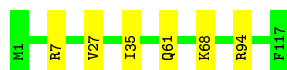
- Molecule 39: 50S ribosomal protein L17

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%



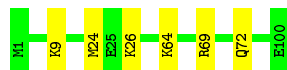
- Molecule 44: 50S ribosomal protein L22

Chain BT:  95% 5%



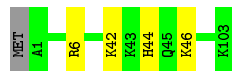
- Molecule 45: 50S ribosomal protein L23

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%



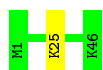
- Molecule 54: 50S ribosomal protein L33

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 images	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

*Continued on next page...*

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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%)	24	69
5	AF	238/241 (99%)	215 (90%)	21 (9%)	2 (1%)	24	69
6	AG	230/233 (99%)	210 (91%)	18 (8%)	2 (1%)	21	67
7	AH	203/206 (98%)	189 (93%)	12 (6%)	2 (1%)	19	65
8	AI	164/167 (98%)	143 (87%)	18 (11%)	3 (2%)	11	53
9	AJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	13	57
10	AK	176/179 (98%)	159 (90%)	15 (8%)	2 (1%)	17	63
11	AL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	12	56
12	AM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	12	56
13	AN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	4	35
14	AO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	12	56
15	AP	121/124 (98%)	103 (85%)	13 (11%)	5 (4%)	3	35
16	AQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
17	AR	98/101 (97%)	82 (84%)	9 (9%)	7 (7%)	1	22
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%)	14	58
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%)	13	57
27	BC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	15	60
28	BD	270/273 (99%)	239 (88%)	22 (8%)	9 (3%)	5	40
29	BE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	6	43
30	BF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	13	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BG	176/179 (98%)	148 (84%)	25 (14%)	3 (2%)	11	55
32	BH	174/177 (98%)	162 (93%)	9 (5%)	3 (2%)	11	55
33	BI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	5	40
34	BJ	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	26	71
35	BK	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
36	BL	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	11	55
37	BM	142/144 (99%)	124 (87%)	16 (11%)	2 (1%)	14	58
38	BN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	8	49
39	BO	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	24	69
40	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21	67
41	BQ	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	11	53
42	BR	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	21	67
43	BS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	42
44	BT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	21	67
45	BU	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	19	65
46	BV	101/104 (97%)	90 (89%)	10 (10%)	1 (1%)	19	65
47	BW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8	49
48	BX	82/85 (96%)	68 (83%)	11 (13%)	3 (4%)	4	38
49	BY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	6	45
50	BZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	3	31
51	Ba	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	11	53
52	Bb	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	57
53	Bc	54/57 (95%)	46 (85%)	6 (11%)	2 (4%)	4	38
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	44
All	All	6548/6682 (98%)	5895 (90%)	547 (8%)	106 (2%)	17	56

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%)	33	68
5	AF	198/199 (100%)	188 (95%)	10 (5%)	29	66
6	AG	189/190 (100%)	180 (95%)	9 (5%)	31	67
7	AH	172/173 (99%)	164 (95%)	8 (5%)	32	68
8	AI	125/126 (99%)	122 (98%)	3 (2%)	57	82
9	AJ	116/116 (100%)	104 (90%)	12 (10%)	9	37
10	AK	146/147 (99%)	136 (93%)	10 (7%)	20	57
11	AL	104/105 (99%)	99 (95%)	5 (5%)	31	67
12	AM	106/107 (99%)	98 (92%)	8 (8%)	17	53
13	AN	90/90 (100%)	85 (94%)	5 (6%)	26	62
14	AO	98/99 (99%)	95 (97%)	3 (3%)	47	77
15	AP	103/104 (99%)	98 (95%)	5 (5%)	31	67
16	AQ	95/96 (99%)	93 (98%)	2 (2%)	61	84
17	AR	83/84 (99%)	79 (95%)	4 (5%)	31	67
18	AS	76/77 (99%)	71 (93%)	5 (7%)	21	57
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	77/78 (99%)	75 (97%)	2 (3%)	54	80
21	AV	64/65 (98%)	60 (94%)	4 (6%)	22	59
22	AW	78/79 (99%)	74 (95%)	4 (5%)	29	66
23	AX	65/66 (98%)	61 (94%)	4 (6%)	23	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AY	60/61 (98%)	55 (92%)	5 (8%)	14	49
27	BC	181/181 (100%)	176 (97%)	5 (3%)	51	78
28	BD	217/218 (100%)	210 (97%)	7 (3%)	46	76
29	BE	164/164 (100%)	153 (93%)	11 (7%)	20	57
30	BF	165/165 (100%)	156 (94%)	9 (6%)	27	63
31	BG	149/150 (99%)	138 (93%)	11 (7%)	17	54
32	BH	137/138 (99%)	128 (93%)	9 (7%)	21	57
33	BI	114/114 (100%)	109 (96%)	5 (4%)	35	69
34	BJ	109/110 (99%)	104 (95%)	5 (5%)	33	68
35	BK	116/116 (100%)	110 (95%)	6 (5%)	29	65
36	BL	104/104 (100%)	96 (92%)	8 (8%)	16	52
37	BM	103/103 (100%)	97 (94%)	6 (6%)	25	61
38	BN	109/109 (100%)	101 (93%)	8 (7%)	17	54
39	BO	103/103 (100%)	97 (94%)	6 (6%)	25	61
40	BP	87/87 (100%)	82 (94%)	5 (6%)	25	62
41	BQ	99/100 (99%)	93 (94%)	6 (6%)	23	60
42	BR	89/90 (99%)	88 (99%)	1 (1%)	80	91
43	BS	84/84 (100%)	78 (93%)	6 (7%)	18	55
44	BT	93/93 (100%)	88 (95%)	5 (5%)	27	64
45	BU	84/84 (100%)	79 (94%)	5 (6%)	24	60
46	BV	84/85 (99%)	81 (96%)	3 (4%)	42	74
47	BW	78/78 (100%)	74 (95%)	4 (5%)	29	66
48	BX	62/63 (98%)	55 (89%)	7 (11%)	7	33
49	BY	67/68 (98%)	64 (96%)	3 (4%)	34	69
50	BZ	55/55 (100%)	54 (98%)	1 (2%)	66	87
51	Ba	48/49 (98%)	47 (98%)	1 (2%)	61	84
52	Bb	62/62 (100%)	60 (97%)	2 (3%)	46	76
53	Bc	47/48 (98%)	46 (98%)	1 (2%)	61	84
54	Bd	48/49 (98%)	48 (100%)	0	100	100
55	Be	38/38 (100%)	37 (97%)	1 (3%)	54	80
56	Bf	51/52 (98%)	49 (96%)	2 (4%)	39	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	Bg	34/34 (100%)	30 (88%)	4 (12%)	6 32
All	All	5417/5447 (99%)	5138 (95%)	279 (5%)	33 65

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	1539/1542 (99%)	193 (12%)	73 (4%)
2	AB	73/76 (96%)	12 (16%)	2 (2%)
2	AE	73/76 (96%)	13 (17%)	6 (8%)
25	BA	119/120 (99%)	15 (12%)	4 (3%)
26	BB	2898/2904 (99%)	401 (13%)	137 (4%)
4	AD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4726/4742 (99%)	638 (13%)	227 (4%)

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

5 of 227 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	227	A
26	BB	786	C

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Mol	Chain	Res	Type
26	BB	2602	A
26	BB	332	A
26	BB	574	A

## 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	18,26,27	1.29	2 (11%)	21,38,41	2.60	3 (14%)
1	4OC	AA	1402	1	15,23,24	1.04	2 (13%)	21,32,35	1.78	3 (14%)
1	5MC	AA	1407	1	14,22,23	0.90	1 (7%)	17,32,35	0.87	0
1	UR3	AA	1498	1	13,22,23	0.84	0	18,32,35	1.44	4 (22%)
1	2MG	AA	1516	1	18,26,27	1.23	2 (11%)	21,38,41	2.73	6 (28%)
1	MA6	AA	1518	1	18,26,27	0.91	1 (5%)	15,38,41	1.78	4 (26%)
1	MA6	AA	1519	1	18,26,27	0.84	1 (5%)	15,38,41	1.86	5 (33%)
1	PSU	AA	516	1	15,21,22	1.32	1 (6%)	16,30,33	3.60	5 (31%)
1	7MG	AA	527	1	20,26,27	2.22	4 (20%)	23,39,42	2.39	2 (8%)
1	2MG	AA	966	1	18,26,27	1.28	2 (11%)	21,38,41	2.97	8 (38%)
1	5MC	AA	967	1	14,22,23	0.95	1 (7%)	17,32,35	0.80	1 (5%)
2	H2U	AB	16	2	17,21,22	0.83	0	23,30,33	1.39	2 (8%)
2	H2U	AB	20	2	17,21,22	0.80	0	23,30,33	1.13	1 (4%)
2	PSU	AB	32	2	15,21,22	1.29	2 (13%)	16,30,33	3.58	4 (25%)
2	MIA	AB	37	2	22,31,32	1.04	3 (13%)	26,44,47	1.70	6 (23%)
2	PSU	AB	39	2	15,21,22	1.27	1 (6%)	16,30,33	3.61	4 (25%)
2	7MG	AB	46	2	20,26,27	2.21	3 (15%)	23,39,42	2.54	2 (8%)
2	3AU	AB	47	-	15,28,29	0.89	0	17,40,43	0.88	1 (5%)
2	5MU	AB	54	2	13,22,23	1.25	1 (7%)	16,32,35	4.85	3 (18%)
2	PSU	AB	55	2	15,21,22	1.31	2 (13%)	16,30,33	3.45	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	4SU	AB	8	2	12,21,22	1.01	1 (8%)	15,30,33	1.68	1 (6%)
2	H2U	AE	16	2	17,21,22	0.80	0	23,30,33	1.00	1 (4%)
2	H2U	AE	20	2	17,21,22	0.81	0	23,30,33	1.06	1 (4%)
2	PSU	AE	32	2	15,21,22	1.32	1 (6%)	16,30,33	3.47	4 (25%)
2	MIA	AE	37	2	22,31,32	1.05	4 (18%)	26,44,47	1.68	5 (19%)
2	PSU	AE	39	2	15,21,22	1.23	1 (6%)	16,30,33	3.57	4 (25%)
2	7MG	AE	46	2	20,26,27	2.18	3 (15%)	23,39,42	2.43	4 (17%)
2	3AU	AE	47	-	15,28,29	0.83	0	17,40,43	1.31	1 (5%)
2	5MU	AE	54	2	13,22,23	1.23	1 (7%)	16,32,35	4.89	2 (12%)
2	PSU	AE	55	2	15,21,22	1.33	1 (6%)	16,30,33	3.52	3 (18%)
2	4SU	AE	8	2	12,21,22	0.95	0	15,30,33	1.64	2 (13%)
26	6MZ	BB	1618	26	17,25,26	0.88	1 (5%)	15,36,39	1.33	1 (6%)
26	2MG	BB	1835	26	18,26,27	1.32	1 (5%)	21,38,41	2.43	5 (23%)
26	PSU	BB	1911	26	15,21,22	1.32	1 (6%)	16,30,33	3.35	2 (12%)
26	3TD	BB	1915	26	15,22,23	0.98	0	17,32,35	1.66	4 (23%)
26	PSU	BB	1917	26	15,21,22	1.36	1 (6%)	16,30,33	3.61	4 (25%)
26	5MU	BB	1939	26	13,22,23	1.24	1 (7%)	16,32,35	4.44	2 (12%)
26	5MC	BB	1962	26	14,22,23	0.97	1 (7%)	17,32,35	1.00	1 (5%)
26	6MZ	BB	2030	26	17,25,26	0.93	1 (5%)	15,36,39	1.57	3 (20%)
26	7MG	BB	2069	26	20,26,27	2.21	3 (15%)	23,39,42	2.31	3 (13%)
26	OMG	BB	2251	26	18,26,27	1.29	1 (5%)	21,38,41	2.65	5 (23%)
26	2MG	BB	2445	26	18,26,27	1.28	2 (11%)	21,38,41	2.47	5 (23%)
26	H2U	BB	2449	26	17,21,22	0.79	0	23,30,33	1.23	2 (8%)
26	PSU	BB	2457	26	15,21,22	1.32	1 (6%)	16,30,33	3.67	6 (37%)
26	OMC	BB	2498	26	15,22,23	0.87	0	20,31,34	1.18	1 (5%)
26	2MA	BB	2503	26	17,25,26	1.10	3 (17%)	18,37,40	1.85	2 (11%)
26	PSU	BB	2504	26	15,21,22	1.33	1 (6%)	16,30,33	3.62	5 (31%)
26	OMU	BB	2552	26	14,22,23	1.26	2 (14%)	19,31,34	2.84	4 (21%)
26	CH	BB	2575	26	14,21,22	0.99	1 (7%)	18,30,33	0.96	1 (5%)
26	PSU	BB	2580	26	15,21,22	1.39	1 (6%)	16,30,33	3.48	3 (18%)
26	PSU	BB	2605	26	15,21,22	1.27	1 (6%)	16,30,33	3.62	4 (25%)
26	1MG	BB	745	26	17,26,27	0.95	1 (5%)	19,39,42	1.61	2 (10%)
26	PSU	BB	746	26	15,21,22	1.35	1 (6%)	16,30,33	3.46	4 (25%)
26	5MU	BB	747	26	13,22,23	1.19	1 (7%)	16,32,35	4.70	3 (18%)
26	PSU	BB	955	26	15,21,22	1.28	1 (6%)	16,30,33	3.56	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 68 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
26	BB	2069	7MG	C8-N7	-2.79	1.30	1.43

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	54	5MU	C5-C4-N3	-13.67	113.88	125.35
2	AB	54	5MU	C5-C4-N3	-13.43	114.08	125.35
26	BB	747	5MU	C5-C4-N3	-13.18	114.28	125.35
26	BB	1939	5MU	C5-C4-N3	-12.79	114.62	125.35
1	AA	1516	2MG	C5-C6-N1	-8.60	112.27	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 [i](#)

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.