wwPDB EM Validation Summary Report

Apr 16, 2024 – 09:45 am BST

PDB ID	:	6ZTM
EMDB ID	:	EMD-11420
Title	:	E. coli 70S-RNAP expressome complex in collided state without NusG
Authors	:	Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on	:	2020-07-20
Resolution	:	3.30 Å(reported)
Based on initial models	:	6ALH, 4YBB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

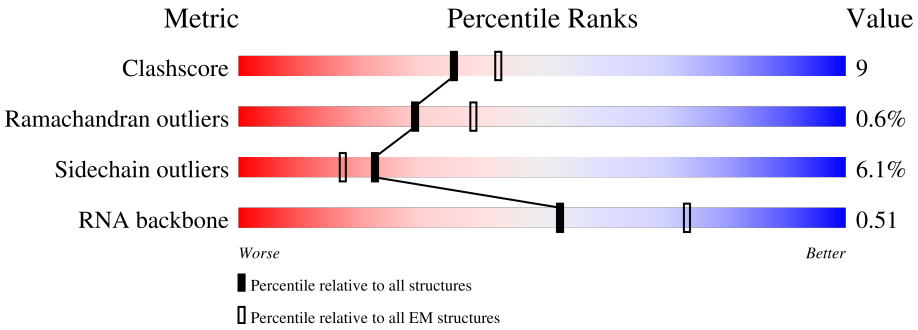
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	1542	58% 33% 7% ••
2	AB	241	71% 20% • 6%
3	AC	233	58% 27% 5% 10%
4	AD	206	66% 30% •
5	AE	167	65% 25% •• 7%
6	AF	131	49% 24% 6% 21%
7	AG	156	65% 29% • •

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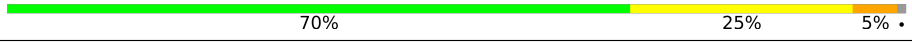
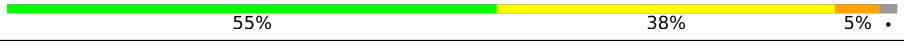
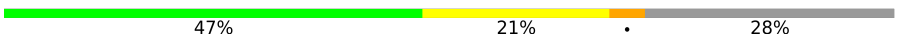
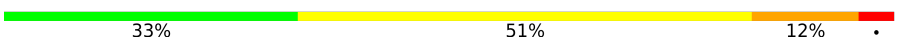
Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	57	
23	AW	77	
24	AX	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	

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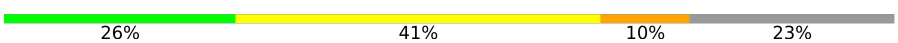
Mol	Chain	Length	Quality of chain
33	BK	142	
34	BL	123	
35	BM	144	
36	BN	136	
37	BO	127	
38	BP	117	
39	BQ	115	
40	BR	118	
41	BS	103	
42	BT	110	
43	BU	100	
44	BV	104	
45	BW	94	
46	BX	85	
47	BY	78	
48	BZ	63	
49	B1	59	
50	B2	57	
51	B3	55	
52	B4	46	
53	B5	65	
54	B6	50	
55	CN	39	
56	CT	39	
57	CA	329	

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Mol	Chain	Length	Quality of chain
57	CB	329	
58	CC	1342	
59	CD	1407	

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 171689 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
			Total	C	N	O	P		
1	AA	1533	32907	14682	6037	10655	1533	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	226	1765	1116	317	324	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	209	1640	1038	308	291	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	156	1148	715	217	210	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	100	Total	C	N	O	S	0	0
			800	500	153	146	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	116	Total	C	N	O	S	0	0
			866	534	170	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0
			949	587	195	163	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	54	Total	C	N	O	0	0
			443	281	81	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	30	Total	C	N	O	P	0	0
			636	285	115	206	30		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2901	Total	C	N	O	P	0	0
			62290	27795	11458	20136	2901		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	95	Total 757	C 479	N 141	O 135	S 2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total 582	C 360	N 117	O 104	S 1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 56 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
57	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	AA	119	Total	Mg	0
			119	119	
60	AW	2	Total	Mg	0
			2	2	

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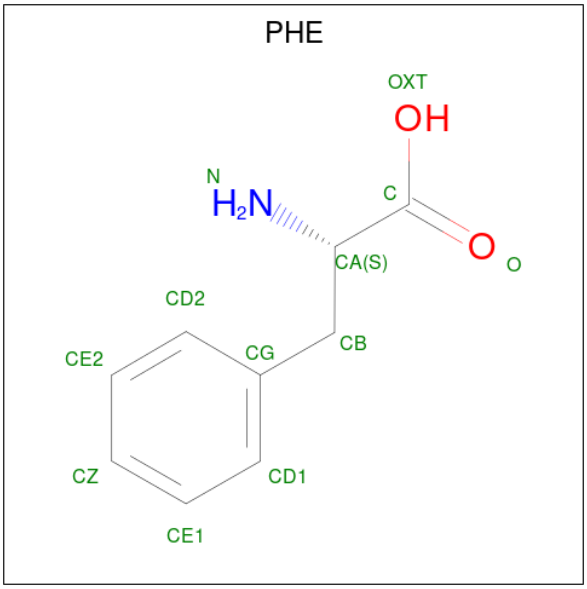
Mol	Chain	Residues	Atoms	AltConf
60	BA	294	Total Mg 294 294	0
60	BB	2	Total Mg 2 2	0
60	BC	1	Total Mg 1 1	0
60	BO	1	Total Mg 1 1	0
60	B2	1	Total Mg 1 1	0
60	CD	1	Total Mg 1 1	0

- Molecule 61 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	AltConf
61	AX	1	Total C N O 11 9 1 1	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

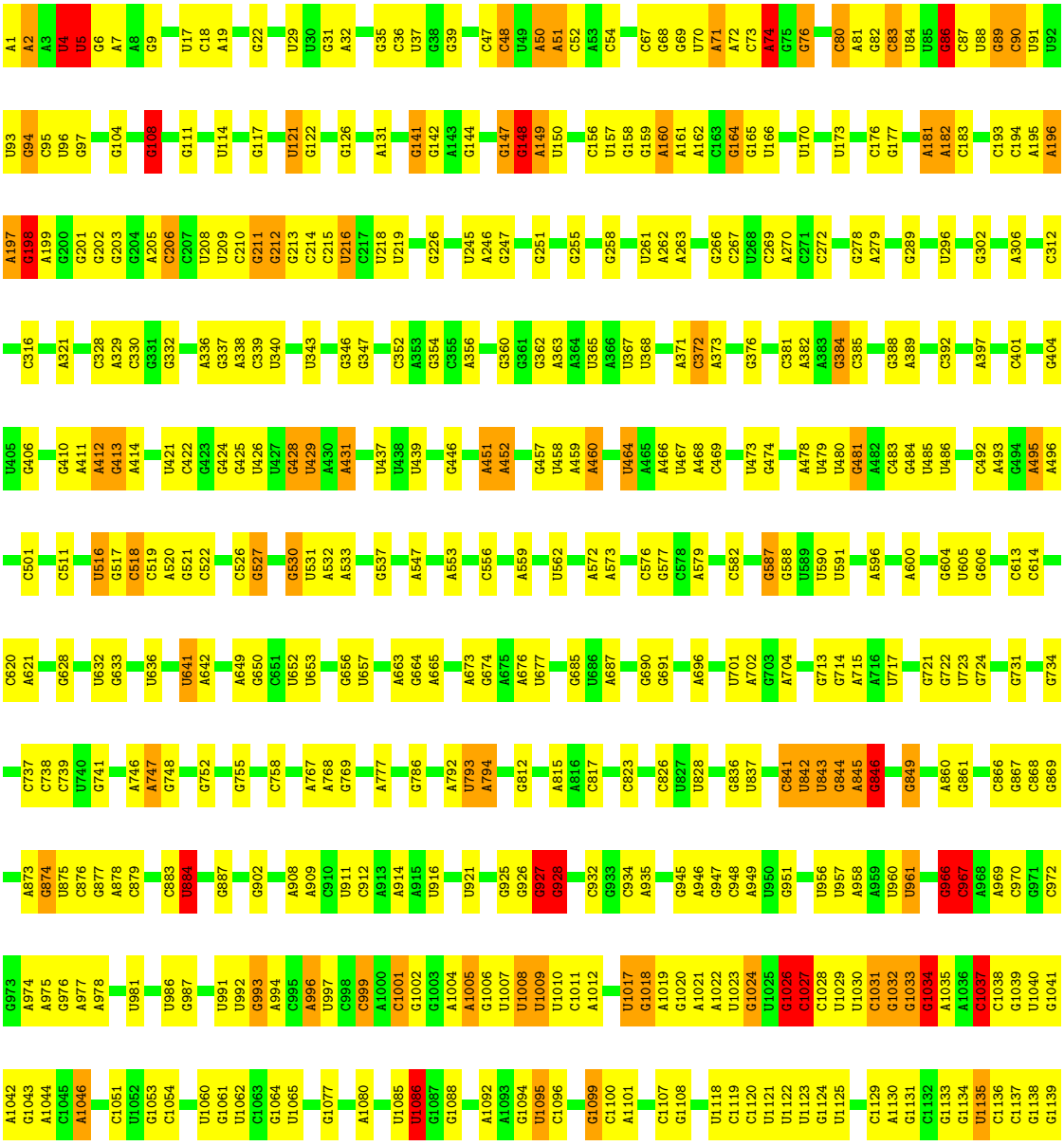
Mol	Chain	Residues	Atoms	AltConf
62	B6	1	Total Zn 1 1	0
62	CD	2	Total Zn 2 2	0

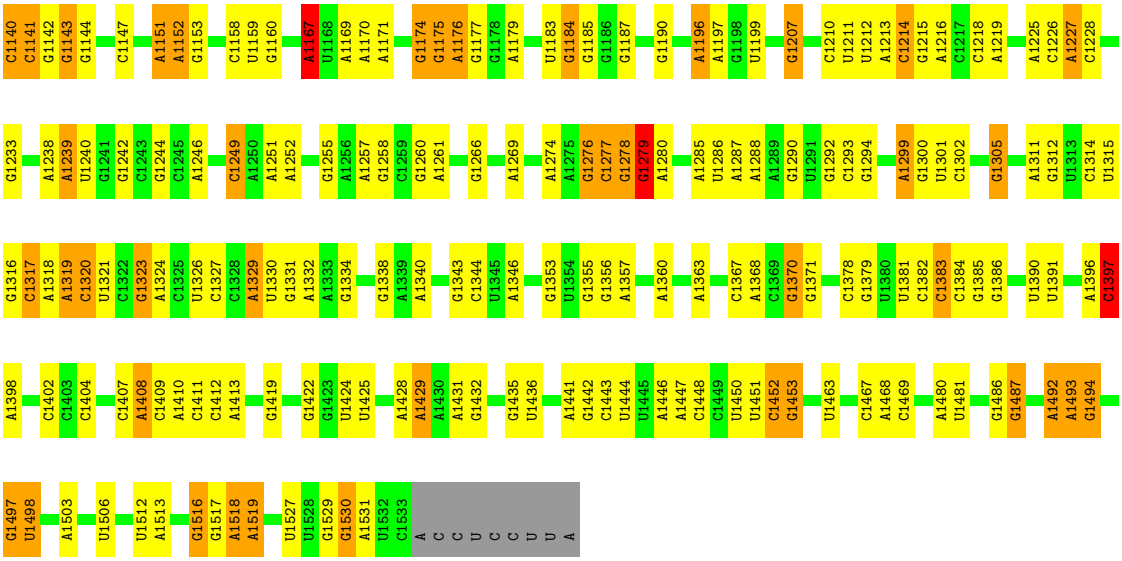
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

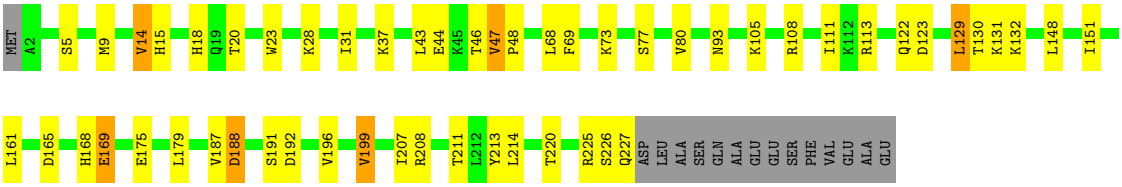
Chain AA: 58% 33% 7%





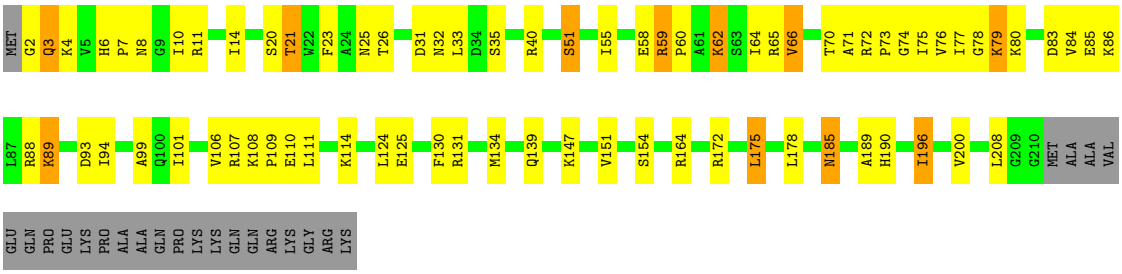
• Molecule 2: 30S ribosomal protein S2

Chain AB:



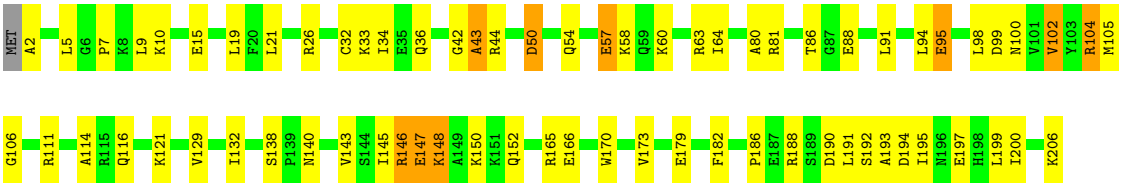
• Molecule 3: 30S ribosomal protein S3

Chain AC:



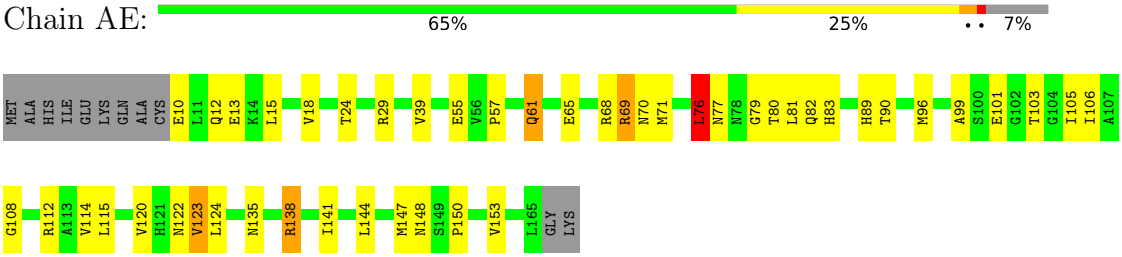
• Molecule 4: 30S ribosomal protein S4

Chain AD:



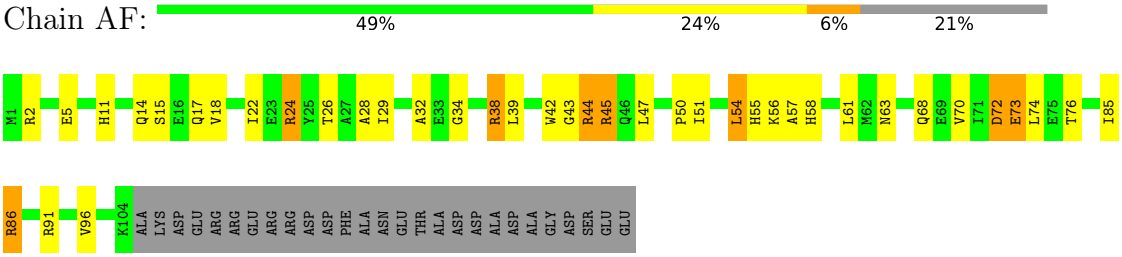
• Molecule 5: 30S ribosomal protein S5

Chain AE:



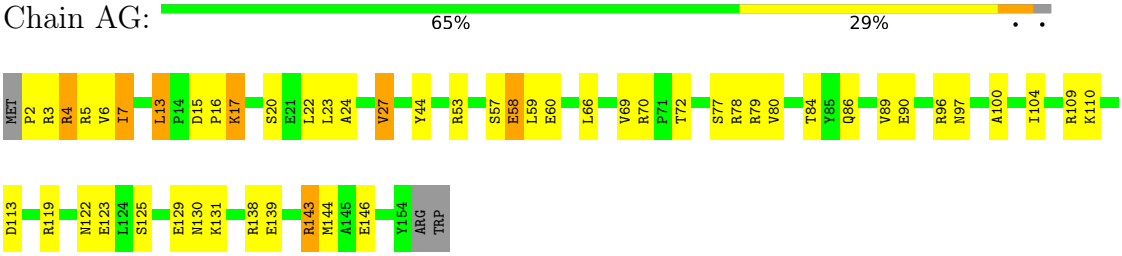
• Molecule 6: 30S ribosomal protein S6

Chain AF:



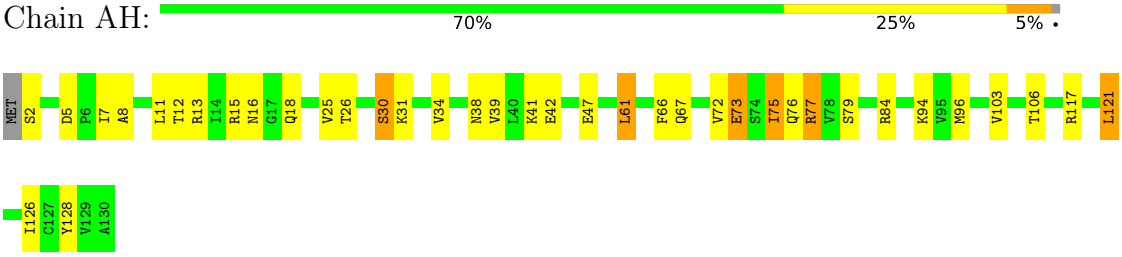
• Molecule 7: 30S ribosomal protein S7

Chain AG:



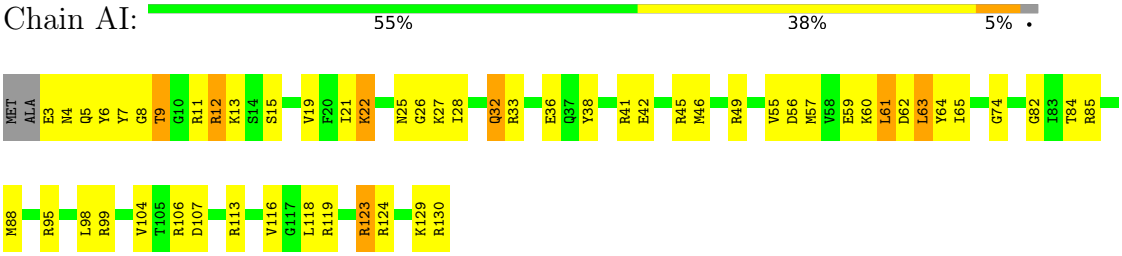
• Molecule 8: 30S ribosomal protein S8

Chain AH:



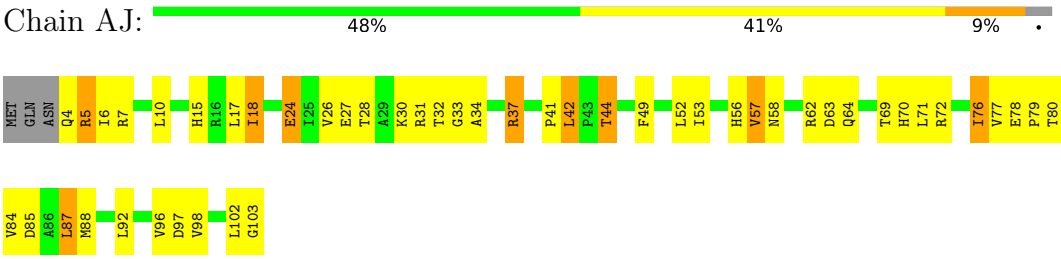
• Molecule 9: 30S ribosomal protein S9

Chain AI:



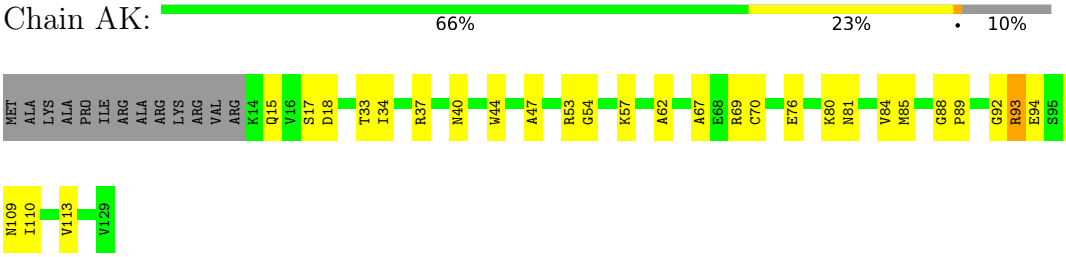
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



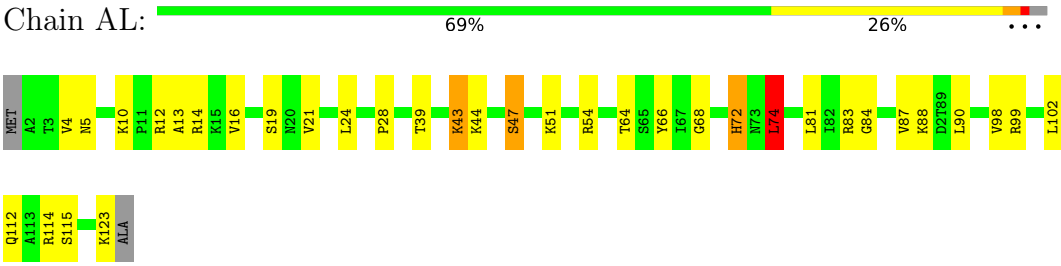
• Molecule 11: 30S ribosomal protein S11

Chain AK:



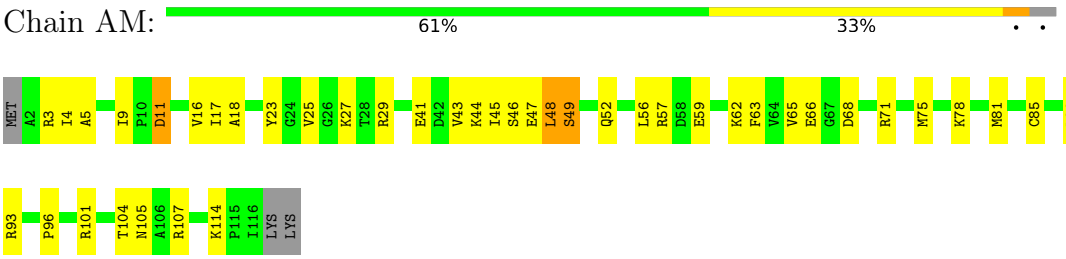
• Molecule 12: 30S ribosomal protein S12

Chain AL:



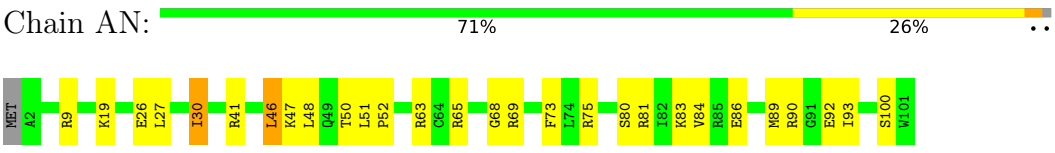
• Molecule 13: 30S ribosomal protein S13

Chain AM:



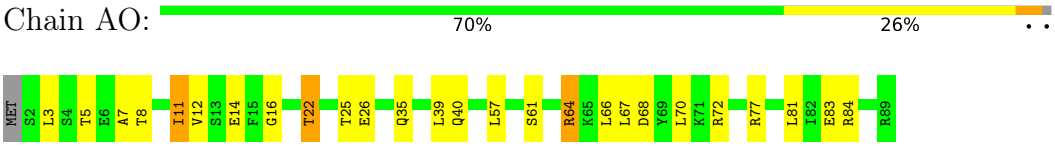
• Molecule 14: 30S ribosomal protein S14

Chain AN:



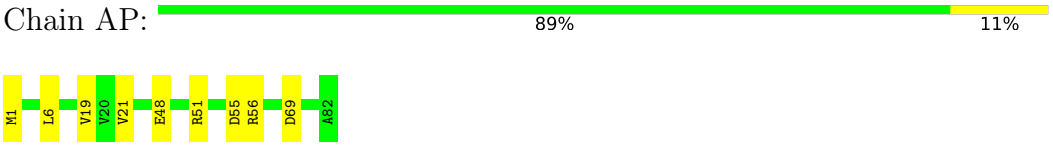
• Molecule 15: 30S ribosomal protein S15

Chain AO:



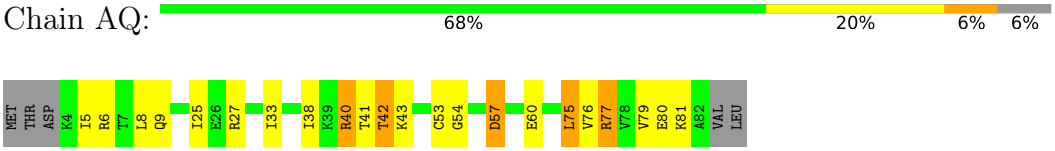
• Molecule 16: 30S ribosomal protein S16

Chain AP:



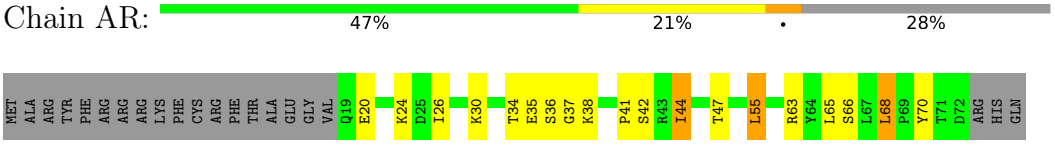
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



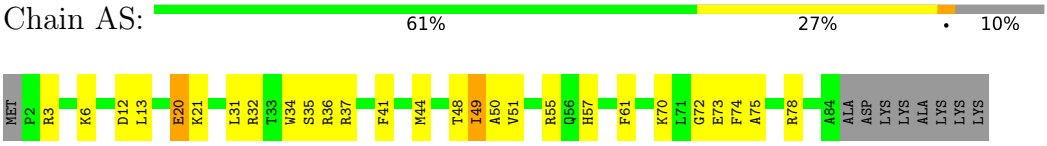
• Molecule 18: 30S ribosomal protein S18

Chain AR:



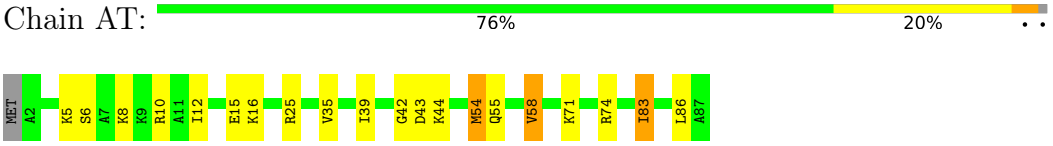
• Molecule 19: 30S ribosomal protein S19

Chain AS:



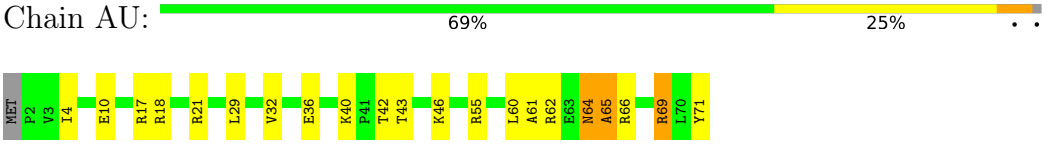
• Molecule 20: 30S ribosomal protein S20

Chain AT:



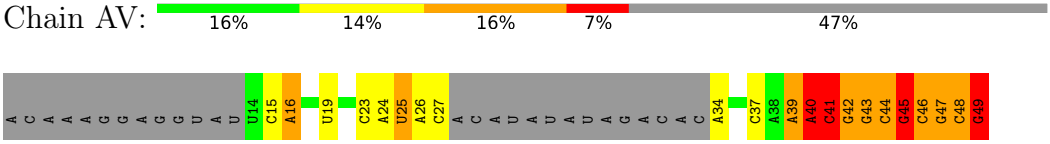
• Molecule 21: 30S ribosomal protein S21

Chain AU:



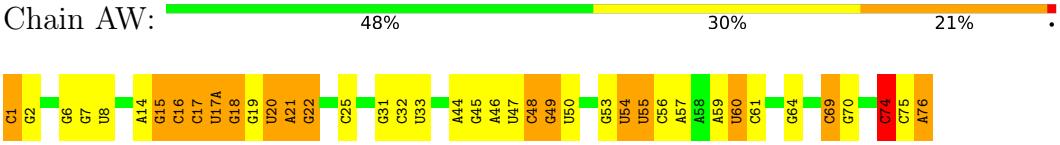
• Molecule 22: mRNA

Chain AV:



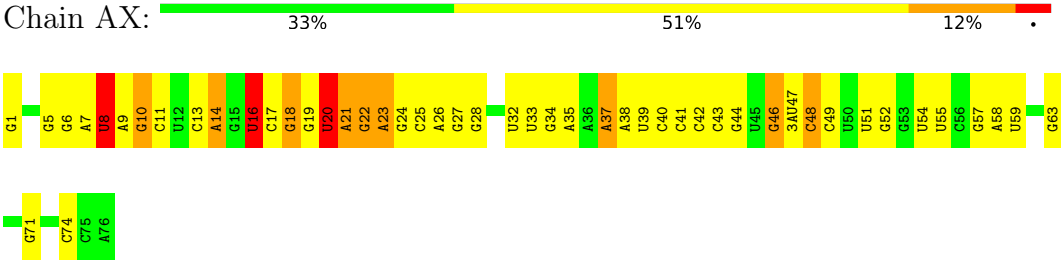
• Molecule 23: tRNA(fmet) P-site

Chain AW:



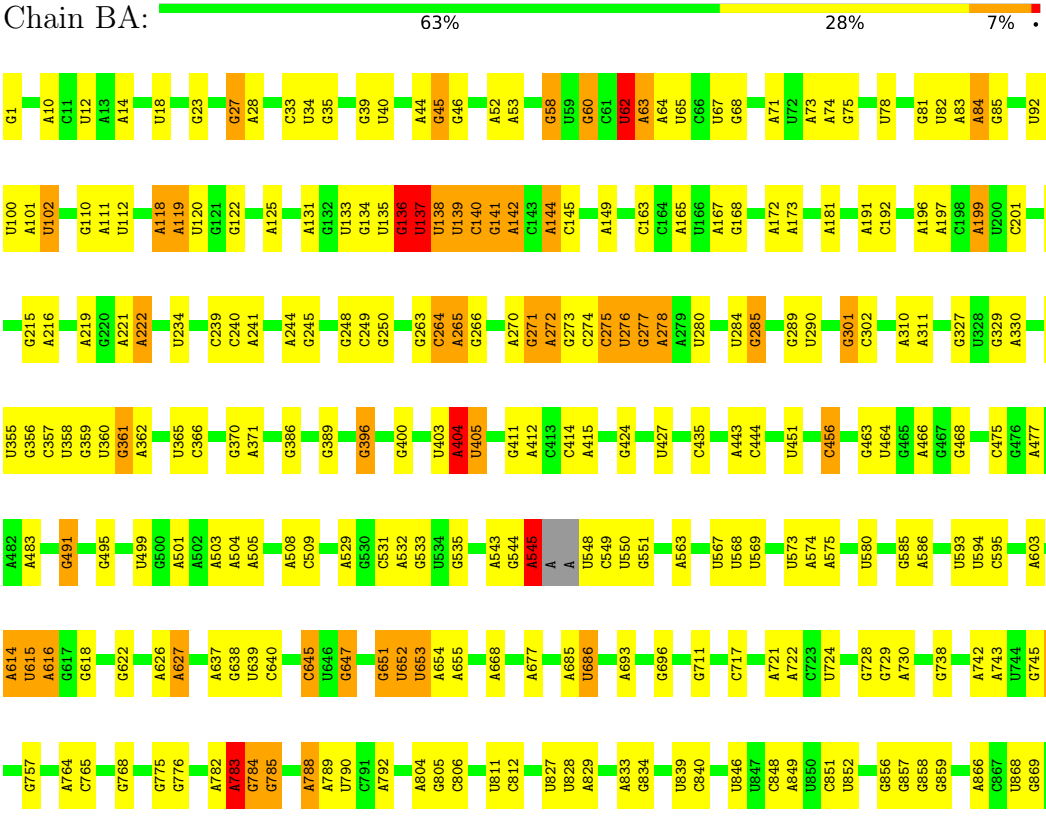
• Molecule 24: Phe-NH-tRNA(Phe) A-site

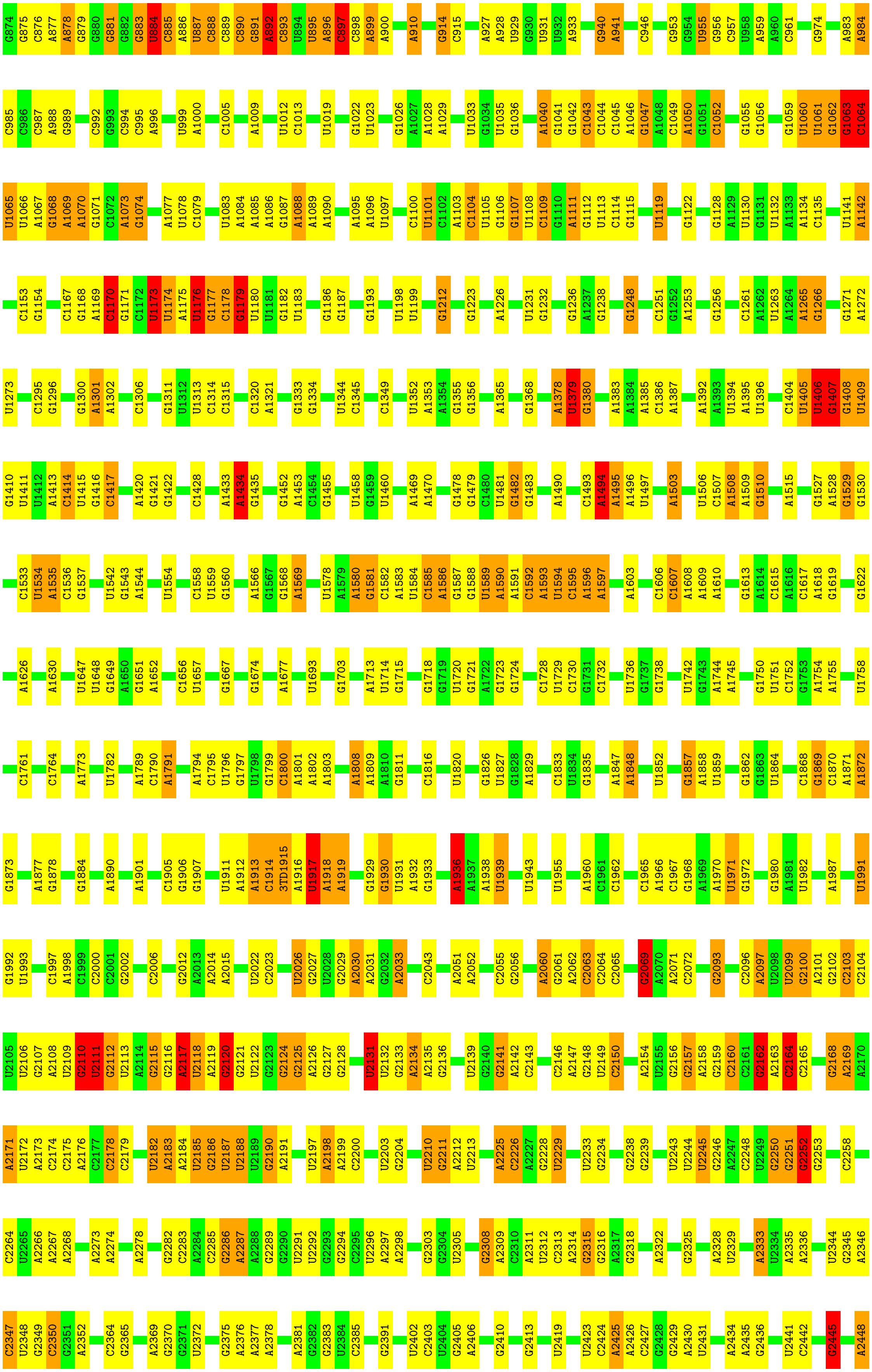
Chain AX:



• Molecule 25: 23S ribosomal RNA

Chain BA:

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C985 C986 C987 A988 G989 C992 G993 C994 C995 A996 U999 A1000 C1005 A1009 U1012 C1013 U1019 G1022 U1023 G1026 A1027 A1028 A1029 U1033 G1034 U1035 G1036 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 G1055 G1056 G1059 U1060 U1061 G1062 G1063 C1064
U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 A1077 U1078 C1079 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 A1095 A1096 U1097 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1119 G1122 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 U1141 A1142
C1153 G1154 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 G1186 G1187 G1193 U1198 U1199 G1212 G1223 A1226 U1231 G1232 G1236 A1237 G1238 G1248 C1251 G1252 A1253 G1256 C1261 A1262 U1263 A1264 A1265 G1266 G1271 A1272
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C1533 U1534 A1535 C1536 G1537 U1542 G1543 A1544 U1554 C1558 U1559 G1560 A1566 G1567 C1568 A1569 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1603 C1606 C1607 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1622
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G1873 A1877 G1878 G1884 A1890 A1901 C1905 G1906 G1907 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 U1943 U1955 A1960 C1961 C1962 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 G1980 A1981 U1982 A1987 U1991
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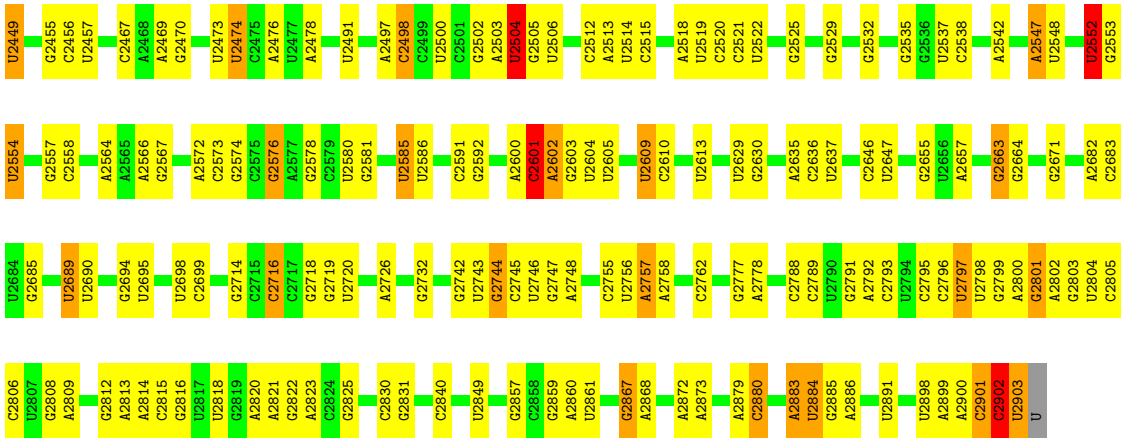
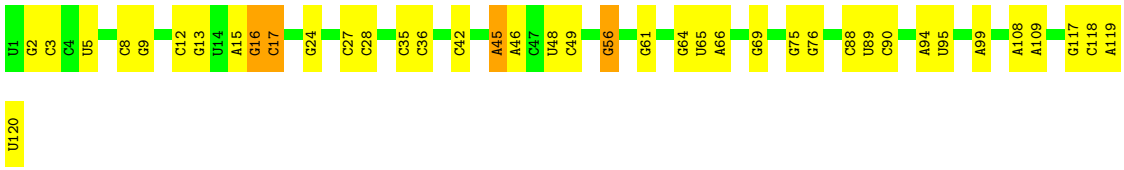
C2347 U2348 G2349 C2350 G2351 A2352 C2364 G2365 A2369 G2370 G2371 U2372 G2375 A2376 A2377 A2378 A2381 G2382 G2383 U2384 C2385 G2391 U2402 C2403 U2404 G2405 A2406 G2410 G2413 U2419 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2434 A2435 G2436 U2441 C2442 G2445 A2448



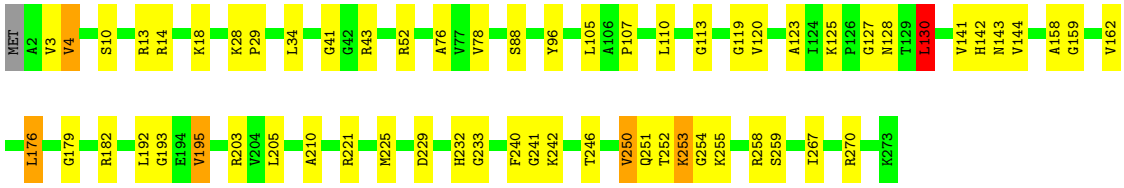
• Molecule 26: 5S ribosomal RNA

Chain BB:



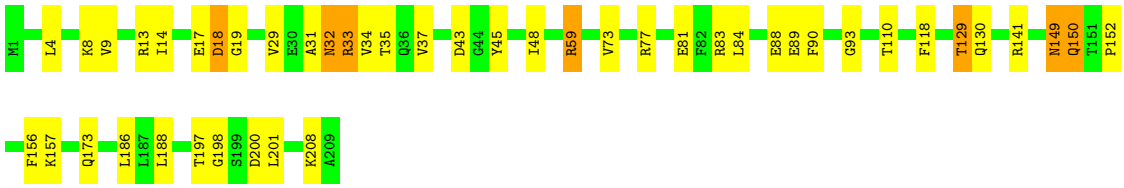
• Molecule 27: 50S ribosomal protein L2

Chain BC:



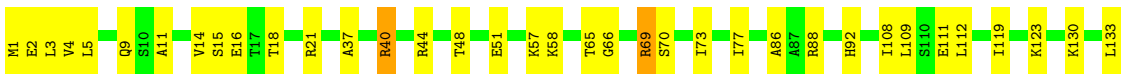
• Molecule 28: 50S ribosomal protein L3

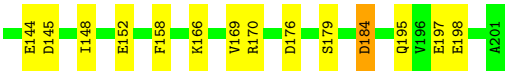
Chain BD:



• Molecule 29: 50S ribosomal protein L4

Chain BE:



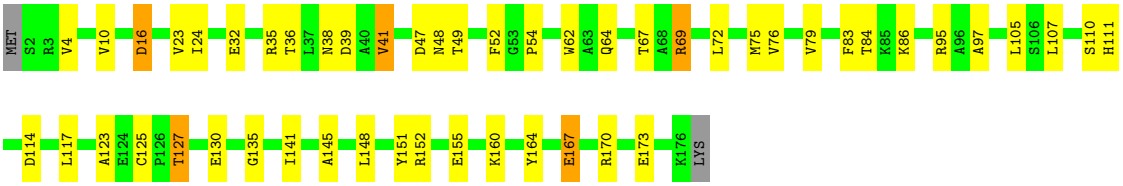


• Molecule 30: 50S ribosomal protein L5

Chain BF:

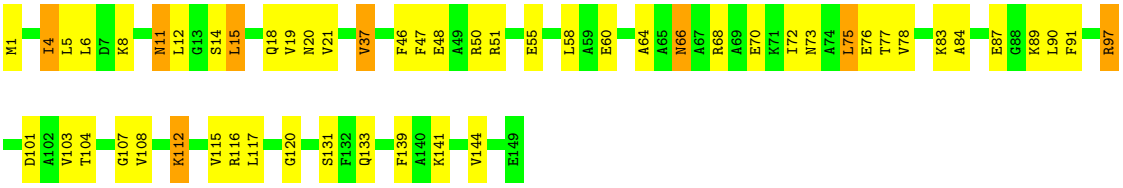
• Molecule 31: 50S ribosomal protein L6

Chain BG:



• Molecule 32: 50S ribosomal protein L9

Chain BH:



• Molecule 33: 50S ribosomal protein L13

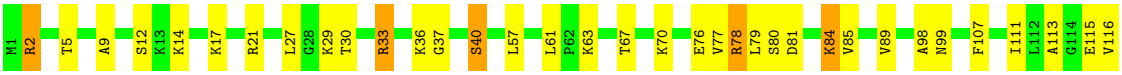
Chain BK:

• Molecule 34: 50S ribosomal protein L14

Chain BL:

• Molecule 35: 50S ribosomal protein L15

Chain BM:



• Molecule 36: 50S ribosomal protein L16

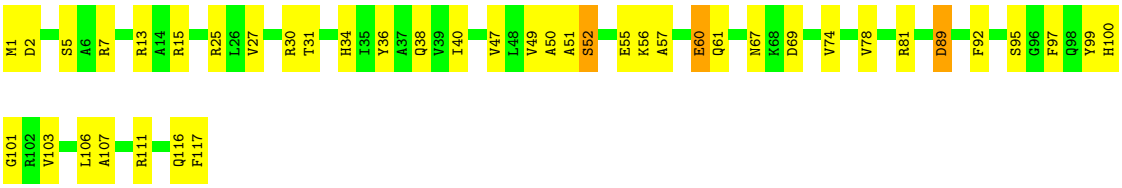
Chain BN:

• Molecule 37: 50S ribosomal protein L17

Chain BO:

• Molecule 38: 50S ribosomal protein L18

Chain BP:

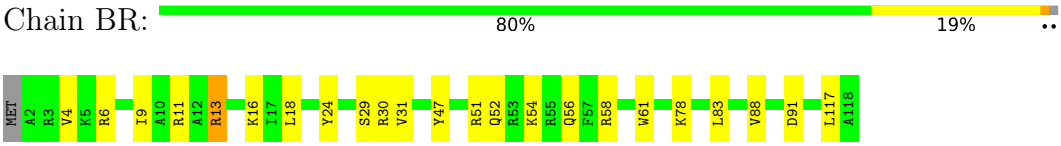


• Molecule 39: 50S ribosomal protein L19

Chain BQ:

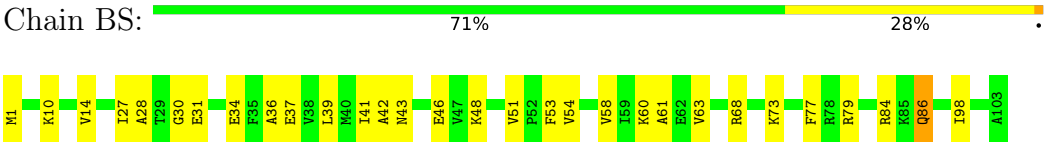
• Molecule 40: 50S ribosomal protein L20

Chain BR:



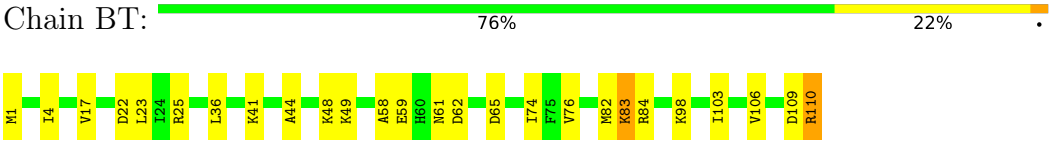
• Molecule 41: 50S ribosomal protein L21

Chain BS:



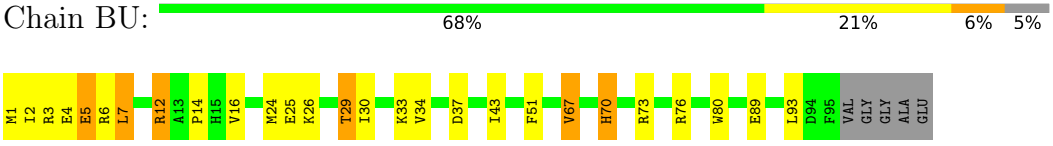
• Molecule 42: 50S ribosomal protein L22

Chain BT:



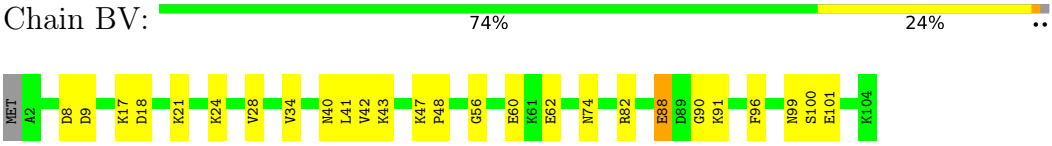
• Molecule 43: 50S ribosomal protein L23

Chain BU:



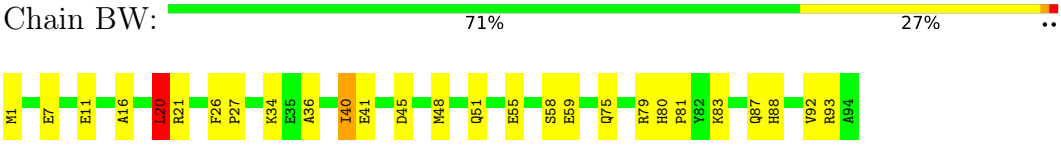
• Molecule 44: 50S ribosomal protein L24

Chain BV:



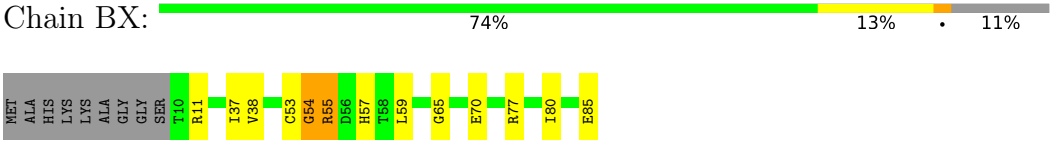
• Molecule 45: 50S ribosomal protein L25

Chain BW:



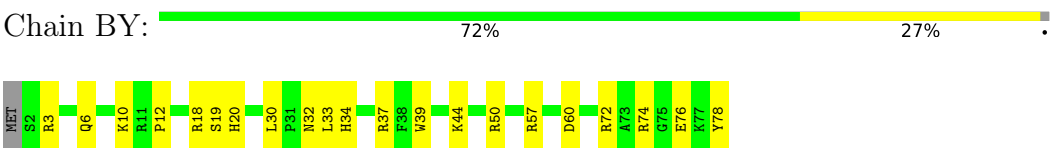
• Molecule 46: 50S ribosomal protein L27

Chain BX:



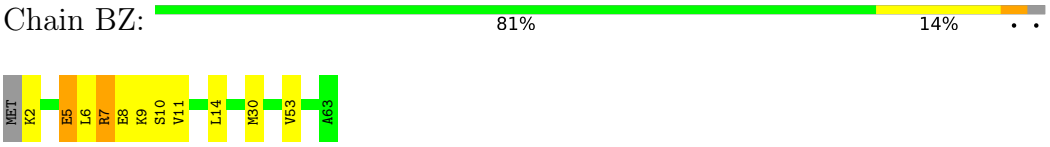
• Molecule 47: 50S ribosomal protein L28

Chain BY:



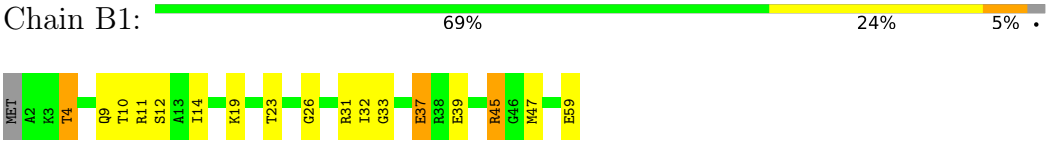
• Molecule 48: 50S ribosomal protein L29

Chain BZ:



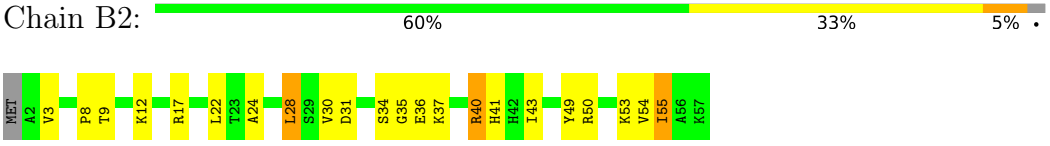
• Molecule 49: 50S ribosomal protein L30

Chain B1:



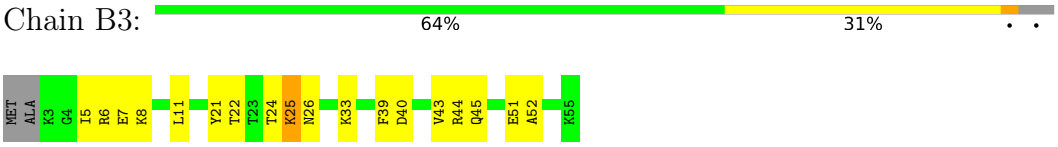
• Molecule 50: 50S ribosomal protein L32

Chain B2:



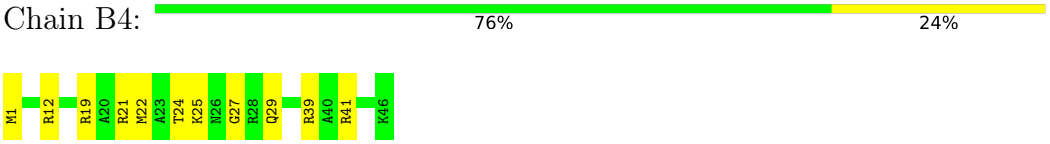
• Molecule 51: 50S ribosomal protein L33

Chain B3:



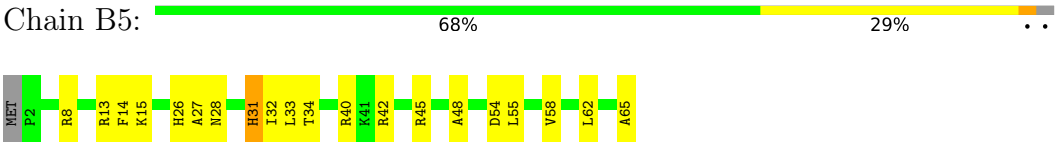
• Molecule 52: 50S ribosomal protein L34

Chain B4:



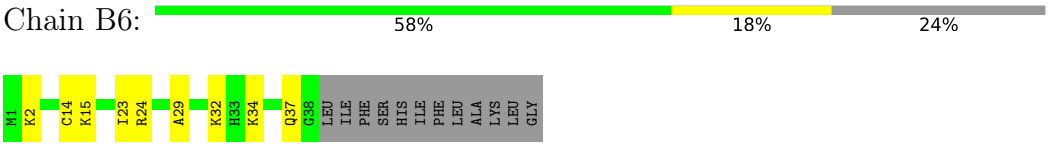
• Molecule 53: 50S ribosomal protein L35

Chain B5:



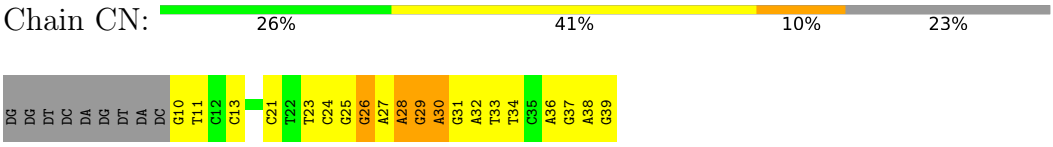
• Molecule 54: 50S ribosomal protein L36

Chain B6:



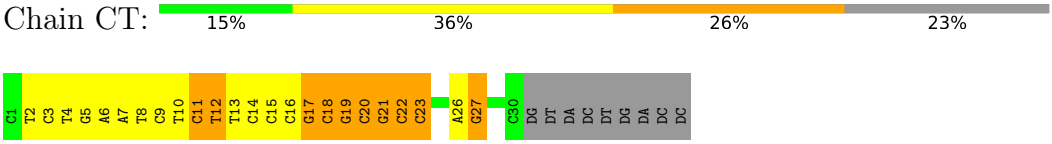
• Molecule 55: Non-template DNA strand

Chain CN:



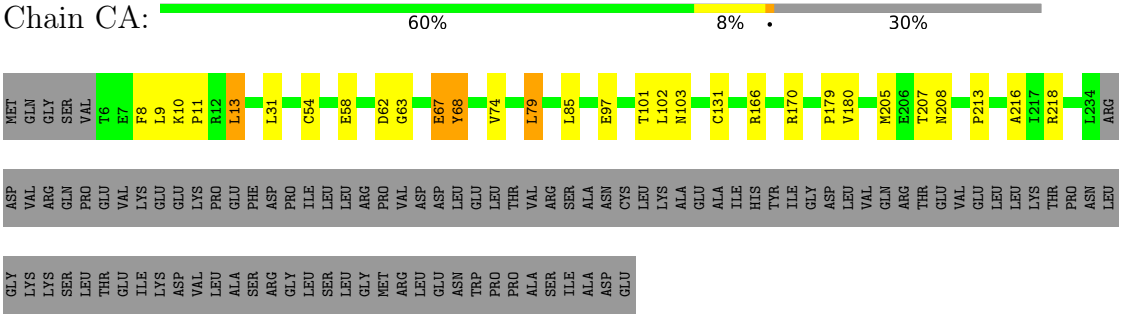
• Molecule 56: Template DNA strand

Chain CT:



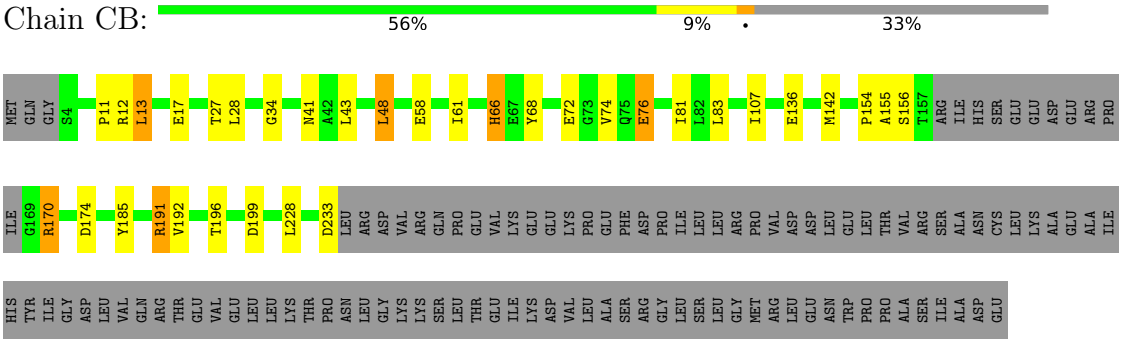
• Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain CA:



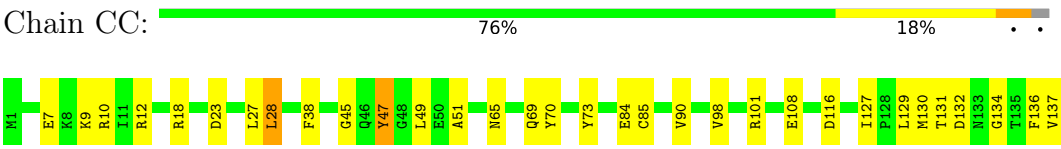
• Molecule 57: DNA-directed RNA polymerase subunit alpha

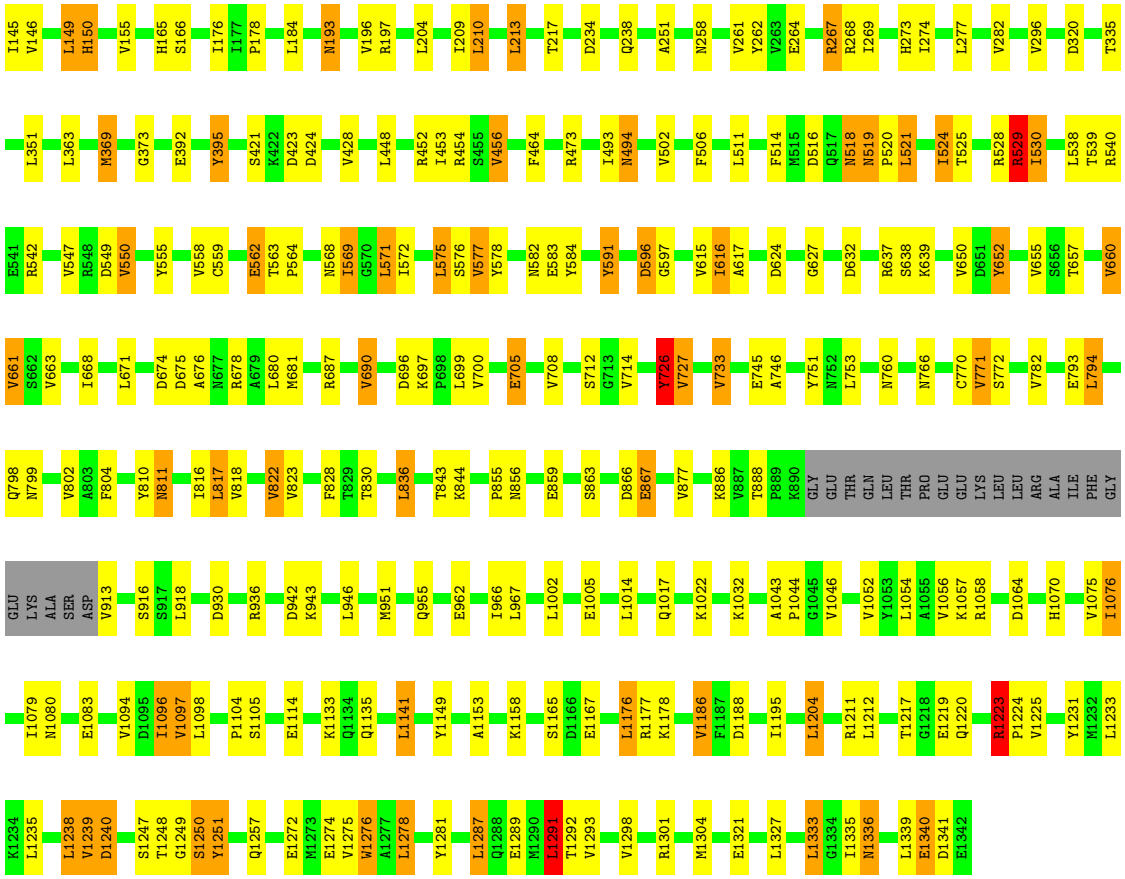
Chain CB:



• Molecule 58: DNA-directed RNA polymerase subunit beta

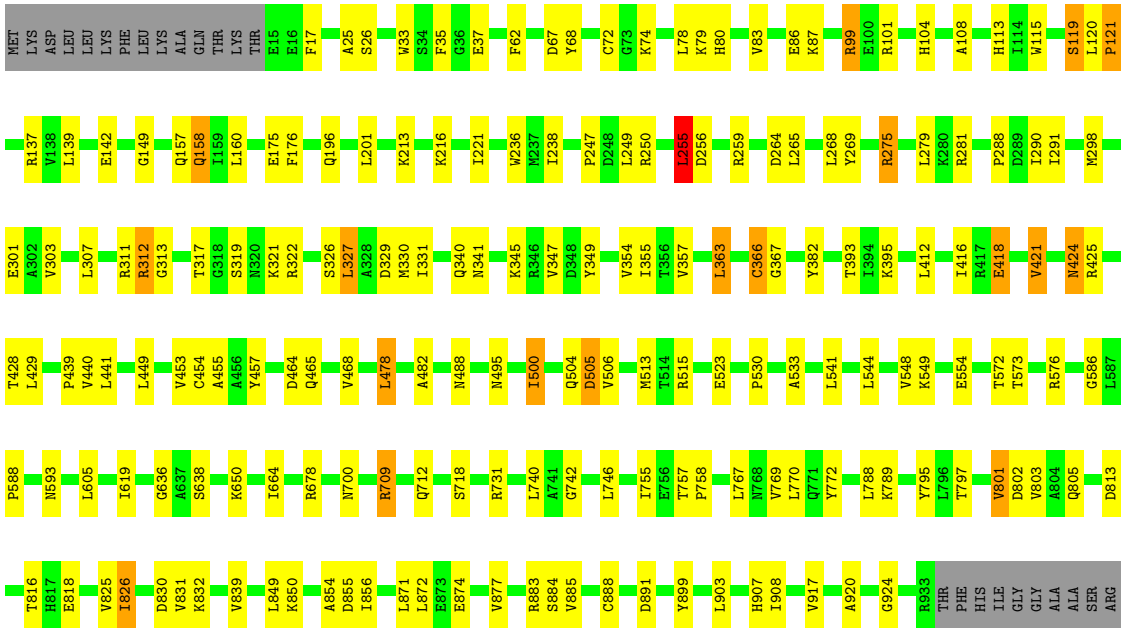
Chain CC:

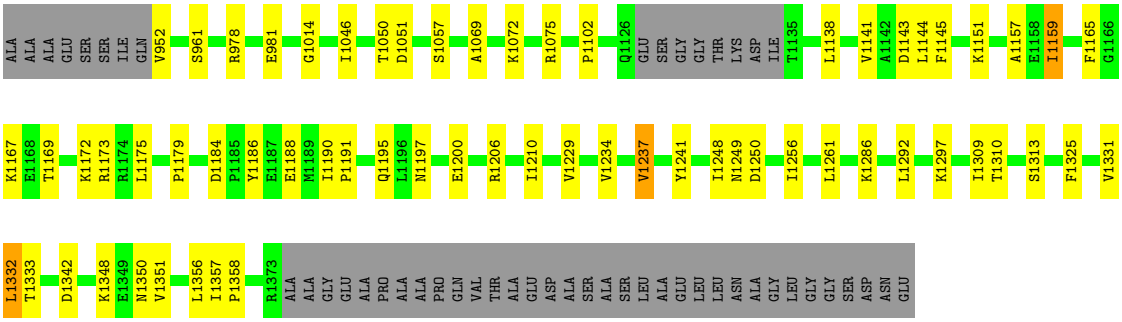




• Molecule 59: DNA-directed RNA polymerase subunit beta'

Chain CD:




ALA ALA ALA GLU SER SER ILE GLN V952
S961 R978 E981 G1014 I1046 T1050 D1051 S1057 A1069 K1072 R1075 P1102 Q1126 GLU SER GLY GLY THR LYS ASP ILE T1135 L1138 V1141 A1142 D1143 L1144 F1145 K1151 A1157 E1158 I1159 F1165 G1166
K1167 E1168 T1169 K1172 R1173 R1174 L1175 P1179 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 Q1195 L1196 N1197 E1200 R1206 I1210 V1229 V1234 V1237 Y1241 I1248 N1249 D1250 I1256 L1261 K1286 L1292 K1297 I1309 T1310 S1313 F1325 V1331
L1332 T1333 D1342 K1348 E1349 N1350 V1351 L1356 I1357 P1358 R1373 ALA ALA GLY GLU ALA PRO ALA ALA PRO GLN VAL THR ALA GLU ASP ALA SER ALA SER LEU ALA GLU LEU LEU ASN ALA GLY LEU GLY GLY SER ASP ASN GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, ZN, 5MC, MG, PSU, OMU, 4D4, MIA, 7MG, 3AU, H2U, 2MA, OMC, MEQ, D2T, G7M, 2MG, 1MG, OMG, 4OC, 3TD, UR3, 6MZ, 4SU, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	1.13	1/36569 (0.0%)	1.04	68/57044 (0.1%)
2	AB	0.35	0/1796	0.56	0/2420
3	AC	0.42	0/1667	0.58	0/2246
4	AD	0.51	0/1665	0.62	0/2227
5	AE	0.50	0/1161	0.68	1/1563 (0.1%)
6	AF	0.44	0/867	0.58	0/1171
7	AG	0.34	0/1219	0.61	1/1635 (0.1%)
8	AH	0.54	0/989	0.60	1/1326 (0.1%)
9	AI	0.43	0/1043	0.62	0/1387
10	AJ	0.41	0/810	0.70	1/1094 (0.1%)
11	AK	0.40	0/882	0.57	0/1191
12	AL	0.59	0/954	0.72	1/1279 (0.1%)
13	AM	0.36	0/900	0.55	0/1204
14	AN	0.40	0/817	0.52	0/1088
15	AO	0.45	0/722	0.56	0/964
16	AP	0.63	0/659	0.62	0/884
17	AQ	0.53	0/650	0.71	1/871 (0.1%)
18	AR	0.43	0/449	0.47	0/604
19	AS	0.42	0/680	0.58	0/915
20	AT	0.47	0/676	0.53	0/895
21	AU	0.37	0/598	0.57	1/792 (0.1%)
22	AV	1.89	28/709 (3.9%)	1.72	32/1099 (2.9%)
23	AW	0.73	1/1725 (0.1%)	1.04	2/2687 (0.1%)
24	AX	0.60	1/1584 (0.1%)	0.85	0/2463
25	BA	1.01	2/69187 (0.0%)	1.01	148/107927 (0.1%)
26	BB	0.72	0/2872	0.90	1/4478 (0.0%)
27	BC	0.50	0/2131	0.64	1/2863 (0.0%)
28	BD	0.47	0/1576	0.60	0/2119
29	BE	0.44	0/1571	0.65	2/2113 (0.1%)
30	BF	0.33	0/1444	0.59	0/1937
31	BG	0.38	0/1333	0.59	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BH	0.30	0/1122	0.65	2/1515 (0.1%)
33	BK	0.47	0/1152	0.54	0/1551
34	BL	0.46	0/956	0.62	0/1279
35	BM	0.44	0/1061	0.64	0/1412
36	BN	0.43	0/1081	0.57	0/1443
37	BO	0.46	0/973	0.62	0/1301
38	BP	0.36	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.58	0/1242
40	BR	0.59	0/960	0.56	0/1278
41	BS	0.48	0/829	0.67	0/1107
42	BT	0.43	0/864	0.58	0/1156
43	BU	0.41	0/764	0.57	0/1021
44	BV	0.41	0/797	0.58	0/1062
45	BW	0.42	0/766	0.61	1/1025 (0.1%)
46	BX	0.45	0/589	0.56	0/779
47	BY	0.46	0/635	0.52	0/848
48	BZ	0.34	0/502	0.51	0/667
49	B1	0.40	0/453	0.61	0/605
50	B2	0.47	0/450	0.73	0/599
51	B3	0.36	0/443	0.65	0/587
52	B4	0.48	0/380	0.61	0/498
53	B5	0.40	0/513	0.65	0/676
54	B6	0.47	0/302	0.65	0/397
55	CN	1.77	13/693 (1.9%)	1.24	3/1068 (0.3%)
56	CT	2.53	39/676 (5.8%)	1.33	9/1039 (0.9%)
57	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
57	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
58	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
59	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
All	All	0.98	271/183318 (0.1%)	0.94	327/270903 (0.1%)

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	3
10	AJ	0	1
12	AL	0	1
13	AM	0	2
22	AV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BA	0	2
27	BC	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	14

The worst 5 of 271 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.65	1.48	1.61
24	AX	1	G	OP3-P	-10.51	1.48	1.61
56	CT	18	DC	C3'-O3'	-10.28	1.30	1.44
59	CD	1357	ILE	C-N	-9.69	1.15	1.34
56	CT	14	DC	C3'-O3'	-9.60	1.31	1.44

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1027	C	C6-N1-C2	-25.80	109.98	120.30
1	AA	1027	C	C2-N1-C1'	18.88	139.57	118.80
1	AA	1027	C	C5-C6-N1	18.21	130.11	121.00
1	AA	1027	C	C6-N1-C1'	-15.29	102.45	120.80
25	BA	2131	U	O4'-C1'-N1	-14.14	96.89	108.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	884	U	Sidechain
10	AJ	42	LEU	Mainchain
12	AL	43	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32907	0	16571	400	0
2	AB	1765	0	1792	35	0
3	AC	1640	0	1713	99	0
4	AD	1643	0	1706	58	0
5	AE	1148	0	1195	40	0
6	AF	848	0	846	31	0
7	AG	1203	0	1254	34	0
8	AH	979	0	1031	26	0
9	AI	1031	0	1076	50	0
10	AJ	800	0	839	39	0
11	AK	866	0	874	17	0
12	AL	949	0	1008	24	0
13	AM	891	0	952	37	0
14	AN	805	0	844	21	0
15	AO	714	0	734	13	0
16	AP	649	0	666	4	0
17	AQ	641	0	682	13	0
18	AR	443	0	466	14	0
19	AS	663	0	688	21	0
20	AT	670	0	719	14	0
21	AU	590	0	629	19	0
22	AV	636	0	327	19	0
23	AW	1645	0	842	26	0
24	AX	1624	0	823	35	0
25	BA	62290	0	31344	614	0
26	BB	2569	0	1301	24	0
27	BC	2092	0	2167	40	0
28	BD	1566	0	1618	31	0
29	BE	1552	0	1618	28	0
30	BF	1420	0	1457	63	0
31	BG	1313	0	1358	34	0
32	BH	1111	0	1148	35	0
33	BK	1129	0	1162	17	0
34	BL	947	0	1023	25	0
35	BM	1052	0	1127	26	0
36	BN	1075	0	1153	23	0
37	BO	960	0	999	15	0
38	BP	900	0	935	26	0
39	BQ	917	0	962	23	0
40	BR	947	0	1019	20	0
41	BS	816	0	839	15	0
42	BT	857	0	922	17	0
43	BU	757	0	820	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	789	0	844	18	0
45	BW	753	0	780	17	0
46	BX	582	0	599	8	0
47	BY	625	0	652	13	0
48	BZ	501	0	531	7	0
49	B1	449	0	488	9	0
50	B2	444	0	458	17	0
51	B3	436	0	477	13	0
52	B4	377	0	418	10	0
53	B5	504	0	572	14	0
54	B6	301	0	341	7	0
55	CN	618	0	339	27	0
56	CT	606	0	338	36	0
57	CA	1775	0	1800	15	0
57	CB	1684	0	1713	19	0
58	CC	10415	0	10432	214	0
59	CD	10375	0	10597	176	0
60	AA	119	0	0	0	0
60	AW	2	0	0	0	0
60	B2	1	0	0	0	0
60	BA	294	0	0	0	0
60	BB	2	0	0	0	0
60	BC	1	0	0	0	0
60	BO	1	0	0	0	0
60	CD	1	0	0	0	0
61	AX	11	0	8	1	0
62	B6	1	0	0	0	0
62	CD	2	0	0	0	0
All	All	171689	0	122636	2452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2452 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:109:PRO:HD2	58:CC:859:GLU:CG	1.58	1.34
4:AD:193:ALA:CA	59:CD:86:GLU:OE2	1.73	1.32
5:AE:10:GLU:HG3	59:CD:78:LEU:CD1	1.77	1.15
3:AC:109:PRO:HD2	58:CC:859:GLU:HG3	1.21	1.15
4:AD:191:LEU:O	59:CD:86:GLU:OE1	1.60	1.15

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	224/241 (93%)	208 (93%)	15 (7%)	1 (0%)	34	66
3	AC	207/233 (89%)	194 (94%)	10 (5%)	3 (1%)	11	38
4	AD	203/206 (98%)	193 (95%)	9 (4%)	1 (0%)	29	61
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	25	57
6	AF	102/131 (78%)	95 (93%)	7 (7%)	0	100	100
7	AG	151/156 (97%)	142 (94%)	8 (5%)	1 (1%)	22	54
8	AH	127/130 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
9	AI	126/130 (97%)	115 (91%)	9 (7%)	2 (2%)	9	36
10	AJ	98/103 (95%)	88 (90%)	7 (7%)	3 (3%)	4	23
11	AK	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	48
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	9	35
13	AM	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	17	48
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
17	AQ	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
18	AR	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	68/71 (96%)	66 (97%)	1 (2%)	1 (2%)	10	38
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	14	45
28	BD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BE	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
30	BF	176/179 (98%)	162 (92%)	14 (8%)	0	100	100
31	BG	173/177 (98%)	158 (91%)	15 (9%)	0	100	100
32	BH	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	22	54
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
35	BM	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	11	38
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
37	BO	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
38	BP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	48
39	BQ	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
40	BR	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
41	BS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	46
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	93/100 (93%)	88 (95%)	5 (5%)	0	100	100
44	BV	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	46
45	BW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
51	B3	51/55 (93%)	49 (96%)	2 (4%)	0	100	100
52	B4	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
53	B5	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	9	36
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
57	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
57	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	29	61
58	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	22	54
59	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	19	51
All	All	8623/9235 (93%)	8034 (93%)	540 (6%)	49 (1%)	29	57

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AI	13	LYS
9	AI	56	ASP
11	AK	93	ARG
12	AL	88	LYS
27	BC	241	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	187/199 (94%)	175 (94%)	12 (6%)	17 46
3	AC	171/190 (90%)	153 (90%)	18 (10%)	7 25
4	AD	172/173 (99%)	154 (90%)	18 (10%)	7 25
5	AE	118/126 (94%)	107 (91%)	11 (9%)	9 30
6	AF	91/112 (81%)	83 (91%)	8 (9%)	10 33
7	AG	126/129 (98%)	111 (88%)	15 (12%)	5 21
8	AH	104/105 (99%)	97 (93%)	7 (7%)	16 45
9	AI	106/107 (99%)	97 (92%)	9 (8%)	10 35
10	AJ	87/90 (97%)	75 (86%)	12 (14%)	3 16
11	AK	89/99 (90%)	85 (96%)	4 (4%)	27 58
12	AL	102/103 (99%)	90 (88%)	12 (12%)	5 21
13	AM	93/96 (97%)	86 (92%)	7 (8%)	13 39
14	AN	83/84 (99%)	77 (93%)	6 (7%)	14 41
15	AO	76/77 (99%)	67 (88%)	9 (12%)	5 21
16	AP	65/65 (100%)	63 (97%)	2 (3%)	40 67
17	AQ	73/78 (94%)	63 (86%)	10 (14%)	3 16
18	AR	47/65 (72%)	43 (92%)	4 (8%)	10 35
19	AS	72/79 (91%)	69 (96%)	3 (4%)	30 60
20	AT	65/66 (98%)	58 (89%)	7 (11%)	6 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	60/61 (98%)	58 (97%)	2 (3%)	38	66
27	BC	217/218 (100%)	207 (95%)	10 (5%)	27	58
28	BD	163/163 (100%)	151 (93%)	12 (7%)	13	40
29	BE	165/165 (100%)	150 (91%)	15 (9%)	9	31
30	BF	149/150 (99%)	135 (91%)	14 (9%)	8	30
31	BG	136/138 (99%)	122 (90%)	14 (10%)	7	26
32	BH	114/114 (100%)	100 (88%)	14 (12%)	4	20
33	BK	116/116 (100%)	108 (93%)	8 (7%)	15	44
34	BL	104/104 (100%)	96 (92%)	8 (8%)	13	38
35	BM	103/103 (100%)	92 (89%)	11 (11%)	6	25
36	BN	108/108 (100%)	103 (95%)	5 (5%)	27	58
37	BO	100/103 (97%)	95 (95%)	5 (5%)	24	55
38	BP	87/87 (100%)	80 (92%)	7 (8%)	12	37
39	BQ	99/100 (99%)	91 (92%)	8 (8%)	11	36
40	BR	89/90 (99%)	84 (94%)	5 (6%)	21	52
41	BS	84/84 (100%)	78 (93%)	6 (7%)	14	42
42	BT	93/93 (100%)	88 (95%)	5 (5%)	22	53
43	BU	82/84 (98%)	73 (89%)	9 (11%)	6	24
44	BV	84/85 (99%)	81 (96%)	3 (4%)	35	63
45	BW	78/78 (100%)	72 (92%)	6 (8%)	13	38
46	BX	58/63 (92%)	55 (95%)	3 (5%)	23	54
47	BY	67/68 (98%)	66 (98%)	1 (2%)	65	81
48	BZ	54/55 (98%)	52 (96%)	2 (4%)	34	63
49	B1	48/49 (98%)	41 (85%)	7 (15%)	3	14
50	B2	47/48 (98%)	42 (89%)	5 (11%)	6	25
51	B3	48/49 (98%)	46 (96%)	2 (4%)	30	60
52	B4	38/38 (100%)	36 (95%)	2 (5%)	22	53
53	B5	51/52 (98%)	50 (98%)	1 (2%)	55	76
54	B6	34/44 (77%)	34 (100%)	0	100	100
57	CA	197/286 (69%)	193 (98%)	4 (2%)	55	76
57	CB	187/286 (65%)	177 (95%)	10 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	CC	1139/1157 (98%)	1096 (96%)	43 (4%)	33 62
59	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	57 77
All	All	7244/7650 (95%)	6802 (94%)	442 (6%)	22 48

5 of 442 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	BG	69	ARG
36	BN	127	LYS
59	CD	1167	LYS
58	CC	830	THR
31	BG	155	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	70	ASN
6	AF	11	HIS
9	AI	31	ASN
39	BQ	115	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	288 (18%)	32 (2%)
22	AV	28/57 (49%)	12 (42%)	1 (3%)
23	AW	76/77 (98%)	21 (27%)	6 (7%)
24	AX	73/76 (96%)	18 (24%)	0
25	BA	2895/2904 (99%)	552 (19%)	66 (2%)
26	BB	119/120 (99%)	15 (12%)	0
All	All	4720/4776 (98%)	906 (19%)	105 (2%)

5 of 906 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	19	A

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Mol	Chain	Res	Type
1	AA	22	G

5 of 105 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	884	U
25	BA	1344	U
25	BA	2601	C
25	BA	984	A
25	BA	1109	C

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

53 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	4OC	AA	1402	1,60	20,23,24	3.29	9 (45%)	26,32,35	1.05	3 (11%)
25	PSU	BA	746	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.04	6 (27%)
1	G7M	AA	527	1	20,26,27	2.24	8 (40%)	17,39,42	1.31	2 (11%)
24	H2U	AX	20	24	18,21,22	3.21	5 (27%)	21,30,33	1.90	5 (23%)
25	5MU	BA	747	25	19,22,23	1.41	4 (21%)	28,32,35	2.25	6 (21%)
25	G7M	BA	2069	25	20,26,27	2.21	8 (40%)	17,39,42	1.24	1 (5%)
24	PSU	AX	39	24	18,21,22	1.11	2 (11%)	22,30,33	1.86	4 (18%)
25	PSU	BA	2457	25	18,21,22	1.06	2 (11%)	22,30,33	2.09	6 (27%)
24	3AU	AX	47	24	18,21,29	3.41	8 (44%)	26,30,43	1.66	4 (15%)
24	H2U	AX	16	24	18,21,22	2.99	5 (27%)	21,30,33	1.94	5 (23%)
23	H2U	AW	20	23	18,21,22	3.05	5 (27%)	21,30,33	2.03	4 (19%)
1	5MC	AA	1407	1	18,22,23	3.75	7 (38%)	26,32,35	1.03	1 (3%)
25	5MC	BA	1962	25	18,22,23	3.70	7 (38%)	26,32,35	1.11	1 (3%)
25	PSU	BA	2580	25	18,21,22	1.09	2 (11%)	22,30,33	2.27	8 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	AA	1518	1	18,26,27	1.40	3 (16%)	19,38,41	3.96	2 (10%)
24	PSU	AX	32	24	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
24	7MG	AX	46	24	20,25,27	3.16	10 (50%)	27,37,42	2.05	7 (25%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.21	5 (19%)
25	2MG	BA	2445	29,25	18,26,27	2.18	7 (38%)	16,38,41	1.63	4 (25%)
1	MA6	AA	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.51	2 (10%)
1	2MG	AA	1516	1	18,26,27	2.20	7 (38%)	16,38,41	1.65	4 (25%)
25	OMU	BA	2552	25	19,22,23	2.80	6 (31%)	26,31,34	1.85	5 (19%)
1	PSU	AA	516	1,60	18,21,22	1.03	2 (11%)	22,30,33	2.04	7 (31%)
1	2MG	AA	966	1	18,25,27	2.54	8 (44%)	19,37,41	1.69	5 (26%)
1	5MC	AA	967	1	18,22,23	3.85	7 (38%)	26,32,35	1.11	2 (7%)
28	MEQ	BD	150	28	8,9,10	0.94	0	5,10,12	0.97	1 (20%)
25	6MZ	BA	1618	25	18,25,26	1.96	3 (16%)	16,36,39	2.19	3 (18%)
25	PSU	BA	2604	25	18,21,22	1.04	2 (11%)	22,30,33	1.90	5 (22%)
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.82	0
12	D2T	AL	89	12	6,7,10	1.02	0	5,8,13	1.07	0
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.88	3 (13%)
25	3TD	BA	1915	25	18,22,23	4.39	10 (55%)	22,32,35	2.04	4 (18%)
24	PSU	AX	55	24	18,21,22	1.01	1 (5%)	22,30,33	1.94	5 (22%)
24	4SU	AX	8	24	18,21,22	4.03	8 (44%)	26,30,33	2.20	4 (15%)
23	PSU	AW	55	23	18,21,22	1.03	1 (5%)	22,30,33	1.96	5 (22%)
25	5MU	BA	1939	25,60	19,22,23	1.45	3 (15%)	28,32,35	2.36	6 (21%)
25	PSU	BA	2504	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.11	6 (27%)
25	2MG	BA	1835	25	18,26,27	2.23	7 (38%)	16,38,41	1.57	4 (25%)
36	4D4	BN	81	36	9,11,12	2.47	3 (33%)	8,13,15	0.84	0
25	OMC	BA	2498	25,60	19,22,23	2.69	7 (36%)	26,31,34	0.84	1 (3%)
25	OMG	BA	2251	25,23	18,26,27	2.54	8 (44%)	19,38,41	1.48	4 (21%)
1	2MG	AA	1207	1	18,25,27	2.49	8 (44%)	19,37,41	1.66	5 (26%)
25	1MG	BA	745	25	18,26,27	2.55	4 (22%)	19,39,42	1.52	4 (21%)
25	6MZ	BA	2030	25	18,25,26	1.95	3 (16%)	16,36,39	2.61	4 (25%)
25	PSU	BA	1917	25	18,21,22	1.00	3 (16%)	22,30,33	1.90	5 (22%)
1	UR3	AA	1498	1	19,22,23	2.40	6 (31%)	26,32,35	1.29	1 (3%)
25	PSU	BA	955	25,36	18,21,22	1.17	3 (16%)	22,30,33	1.94	5 (22%)
25	PSU	BA	1911	25	18,21,22	1.11	2 (11%)	22,30,33	1.87	4 (18%)
24	MIA	AX	37	24	18,24,32	1.48	3 (16%)	18,35,47	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	H2U	BA	2449	25	18,21,22	2.74	5 (27%)	21,30,33	2.10	5 (23%)
24	5MU	AX	54	24	19,22,23	1.37	4 (21%)	28,32,35	2.11	6 (21%)
25	2MA	BA	2503	25,60	17,25,26	2.58	6 (35%)	17,37,40	1.45	4 (23%)
23	5MU	AW	54	23	19,22,23	1.38	5 (26%)	28,32,35	2.20	8 (28%)

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	4OC	AA	1402	1,60	-	0/9/29/30	0/2/2/2
25	PSU	BA	746	25,60	-	1/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	0/7/25/35	0/2/2/2
24	H2U	AX	16	24	-	1/7/38/39	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	3/7/29/30	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	4/7/34/38	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	2MG	BA	2445	29,25	-	2/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	6/7/29/30	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
1	PSU	AA	516	1,60	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/3/25/28	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	3/8/9/11	-
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
12	D2T	AL	89	12	-	1/5/6/14	-
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	3TD	BA	1915	25	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	1/7/25/26	0/2/2/2
25	5MU	BA	1939	25,60	-	2/7/25/26	0/2/2/2
25	PSU	BA	2504	25,60	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
36	4D4	BN	81	36	-	7/11/12/14	-
25	OMC	BA	2498	25,60	-	2/9/27/28	0/2/2/2
25	OMG	BA	2251	25,23	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	2/3/25/28	0/3/3/3
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	955	25,36	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/3/25/34	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	2MA	BA	2503	25,60	-	2/3/25/26	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2

The worst 5 of 255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.44	1.48	1.35
24	AX	20	H2U	C2-N1	10.34	1.50	1.35
25	BA	1915	3TD	C2-N1	9.65	1.49	1.37
23	AW	20	H2U	C2-N1	9.55	1.49	1.35
1	AA	967	5MC	C6-C5	9.49	1.50	1.34

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-18.57	97.51	117.06
1	AA	1518	MA6	N1-C6-N6	-16.24	99.97	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	8	4SU	C4-N3-C2	-7.77	119.79	127.34
24	AX	8	4SU	C4-N3-C2	-7.50	120.05	127.34
25	BA	2030	6MZ	C9-N6-C6	-7.37	116.52	122.87

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1518	MA6	C5-C6-N6-C9
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	2	0
24	AX	20	H2U	2	0
25	BA	747	5MU	1	0
25	BA	2069	G7M	1	0
24	AX	16	H2U	1	0
1	AA	1518	MA6	2	0
24	AX	46	7MG	1	0
25	BA	2445	2MG	1	0
1	AA	1519	MA6	1	0
1	AA	1516	2MG	1	0
25	BA	2552	OMU	3	0
1	AA	966	2MG	2	0
1	AA	967	5MC	1	0
28	BD	150	MEQ	3	0
25	BA	1915	3TD	3	0
24	AX	8	4SU	2	0
23	AW	55	PSU	1	0
25	BA	2504	PSU	1	0
1	AA	1207	2MG	2	0
25	BA	2030	6MZ	1	0
25	BA	1917	PSU	3	0
1	AA	1498	UR3	1	0
25	BA	955	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	37	MIA	2	0
25	BA	2449	H2U	2	0
23	AW	54	5MU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 425 ligands modelled in this entry, 424 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PHE	AX	101	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AX	101	PHE	CA-CB-CG-CD1
61	AX	101	PHE	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AX	101	PHE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11420. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.