



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:32 AM UTC

PDB ID : 4V8O / pdb_00004v8o
Title : Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3
Authors : Jin, H.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2011-07-26
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

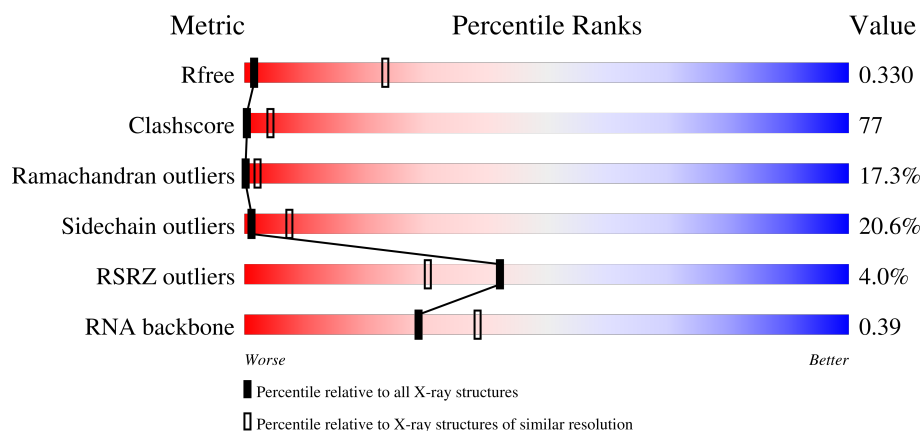
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	3% 11% 63% 19% 5%
2	AB	256	% 7% 42% 34% 9% 8%
3	AC	239	15% 45% 23% 13%
4	AD	209	4% 16% 54% 26%

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	9	
24	AY	529	
25	B0	85	
26	B1	98	
27	B2	72	
28	B3	60	
29	B4	71	

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Mol	Chain	Length	Quality of chain
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

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Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	GCP	AY	1000	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 151017 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	expression tag	UNP P17293
AL	2	VAL	-	expression tag	UNP P17293
AL	3	ALA	-	expression tag	UNP P17293
AL	4	LEU	-	expression tag	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	318	319	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	19	ILE	VAL	conflict	UNP Q5SLP7
BC	27	HIS	ARG	conflict	UNP Q5SLP7
BC	127	MET	LEU	conflict	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	156	Total	C	N	O	S	0	0	1
			1189	752	222	214	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	131	Total	C	N	O		0	0	1
			654	393	131	130				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	141	Total	C	N	O		0	0	1
			701	420	141	140				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O	S	0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

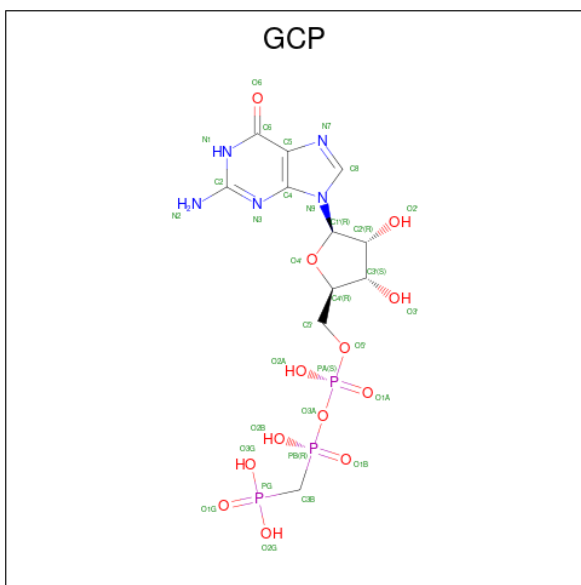
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

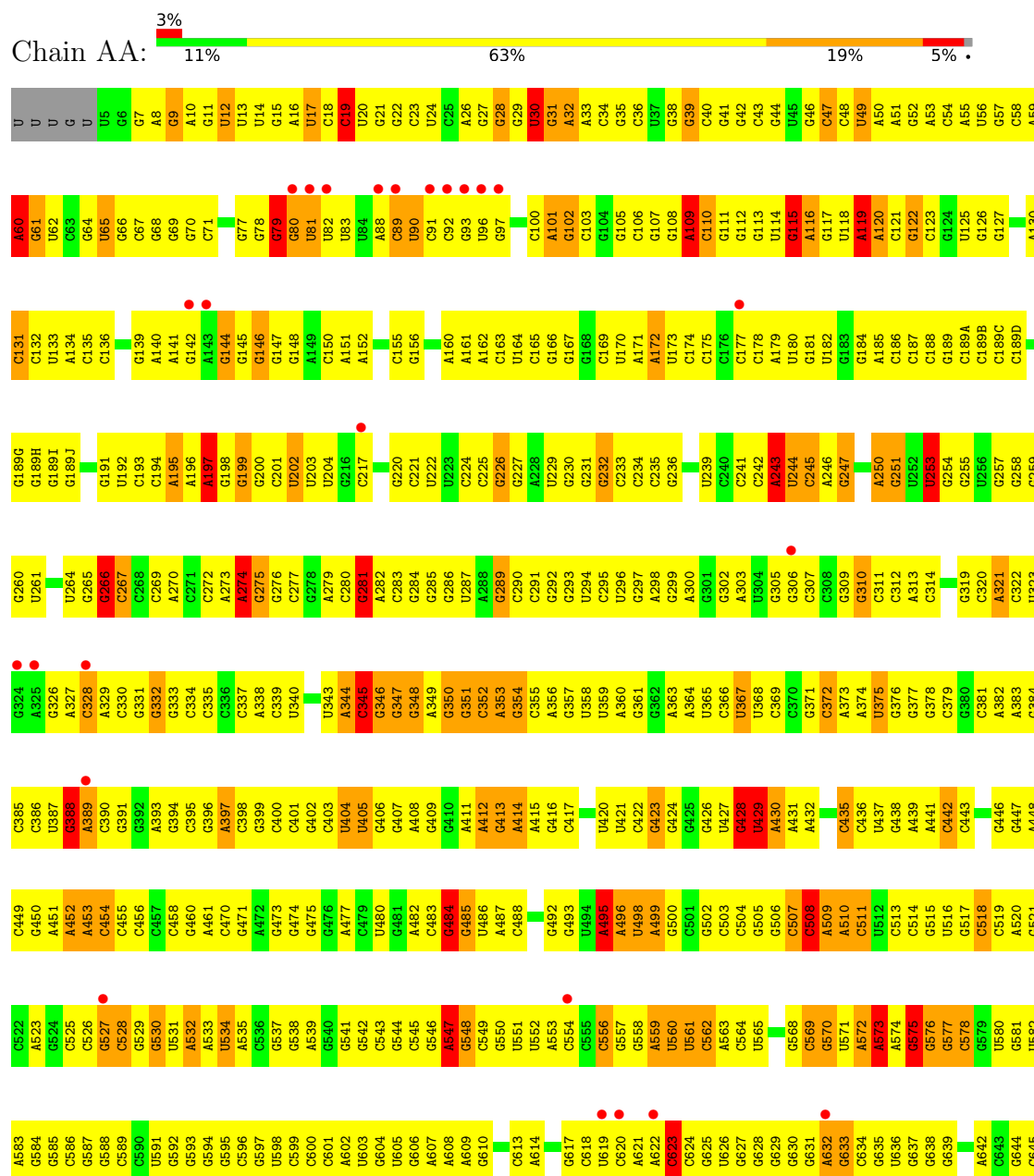


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

3 Residue-property plots

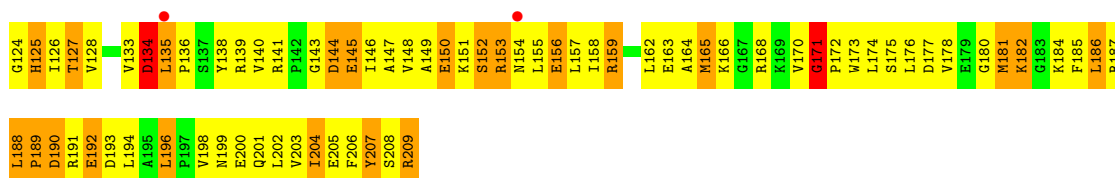
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 rRNA

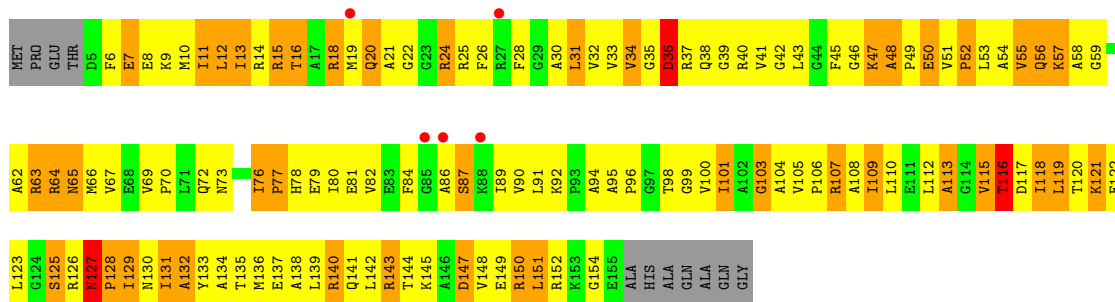
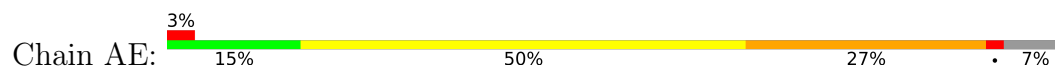


C1440	C1441	G1442	G1442A	A1442B	G1443	C1444	C1445	A1446	A1447	C1452	C1456	G1457	C1458	C1459	A1460	G1461	G1462	C1463	G1464	C1465	C1466	G1467	A1468	G1469	C1470	G1471	A1472	G1473	G1474	G1475	G1476	G1477	C1478	C1479	C1480	G1481	A1482	A1483	C1484	G1485	G1486	G1487	G1488	G1489	C1490	G1491	A1492	A1493	G1494	C1495	G1497	G1498	A1499	C1501	A1502	A1503														
A1377	C1378	G1379	A1380	G1381	C1382	C1383	C1384	C1385	G1386	G1387	C1388	C1389	A1390	A1391	G1392	A1393	C1394	C1395	G1396	C1397	A1398	C1399	C1400	G1401	C1402	C1403	C1404	G1405	A1406	C1407	A1408	C1409	G1410	C1411	C1412	C1413	A1414	G1415	C1416	G1417	A1418	G1419			C1420	A1421	A1422	A1423	C1424	C1425	A1426	A1427		C1430	A1431	G1432	A1433	A1434	C1435	A1436	C1437	A1438	C1439							
A1318	A1319	C1320	C1321	C1322	C1323	A1324	C1325	C1326	C1327	C1328	A1329	A1330	G1331	A1332	A1333	A1334	C1335	C1336	G1337	G1338	A1339	A1340	A1341	C1342	G1343	C1344	G1345	A1346	G1347	A1348	A1349	C1350	A1351	C1352	G1353	C1354	G1355	C1356	A1357	A1358	C1359	A1360	G1361	C1362	C1363	A1363A	G1364	G1365	C1366	C1367	A1368	C1369	G1370	A1371	A1372	C1373	A1374	A1375	A1376											
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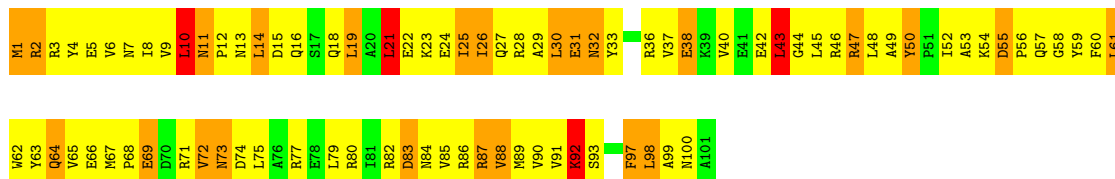
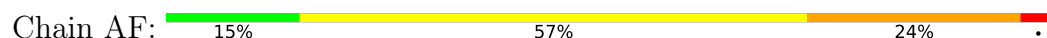
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MET		G2	G3	Y4	T5	G6	P7	V8	C9	R10	L11	C12	R13	R14	E15	G16	V17	K18	L19	Y20	L21	K22	G23	E24	R25	C26	Y27	S28	P29	K30	C31	A32	M33	E34	R35	R36	P37	X38	P39	P40	C41	Q42	H43		K46	R47	A48	R49	R50	P51	S52	P53	Y54	A55	V56	R57	L58	R59	Z60	F61



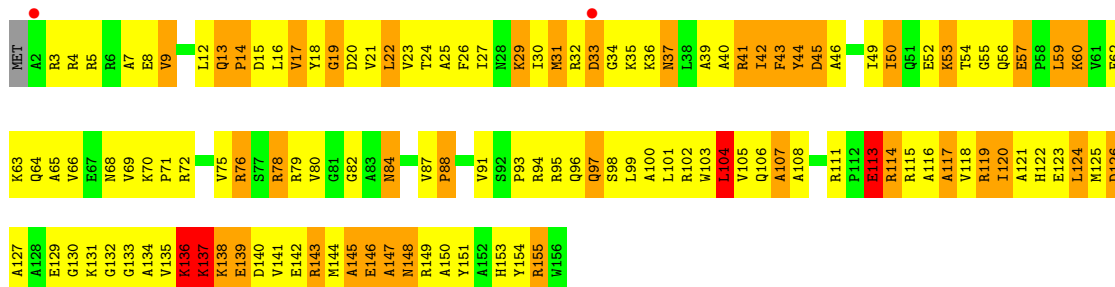
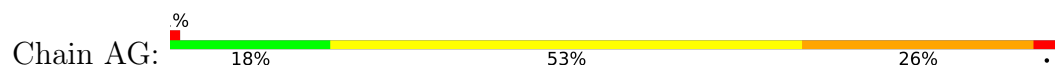
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



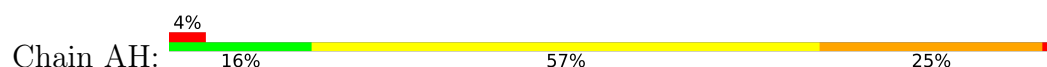
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

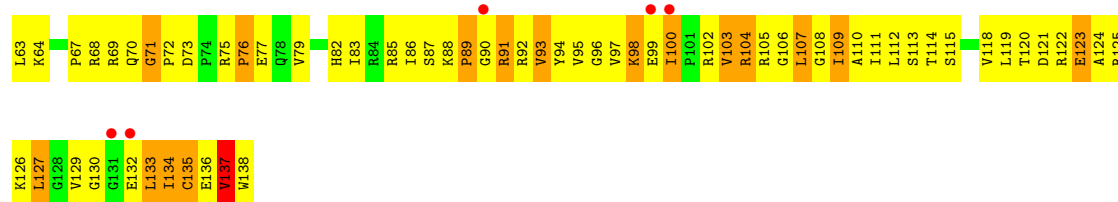


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

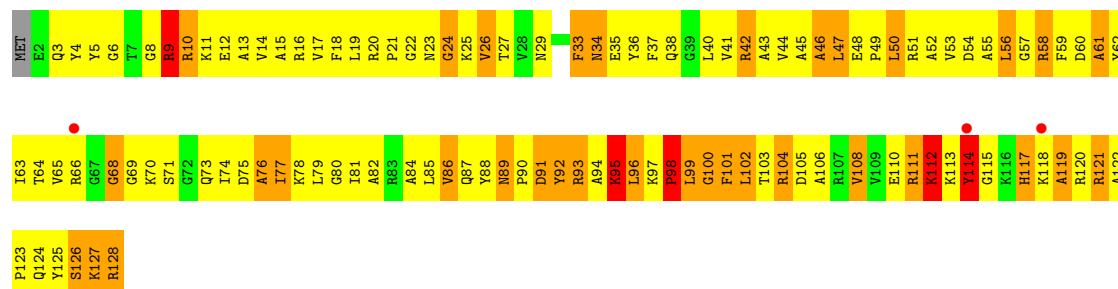
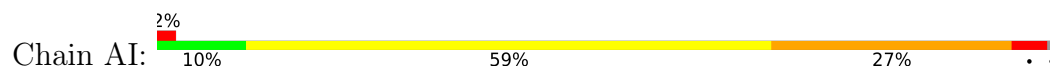


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

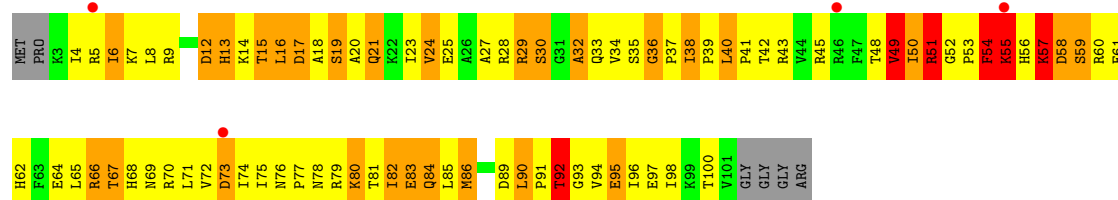
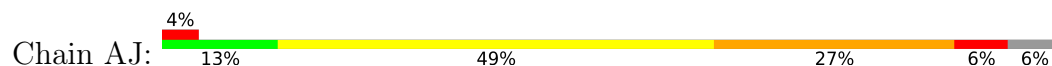




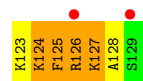
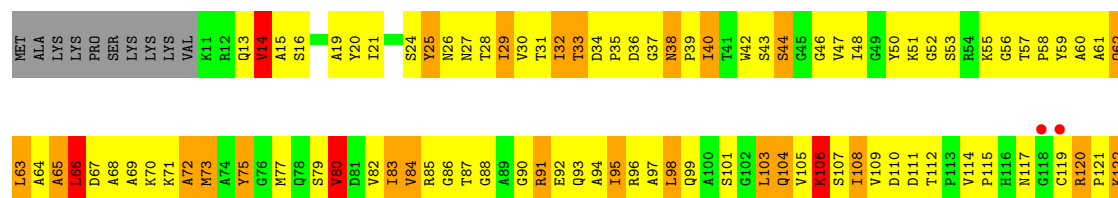
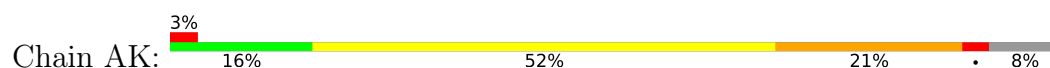
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



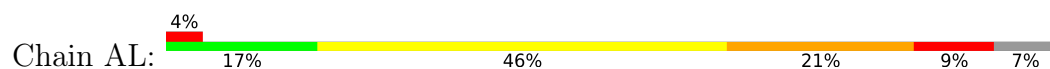
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

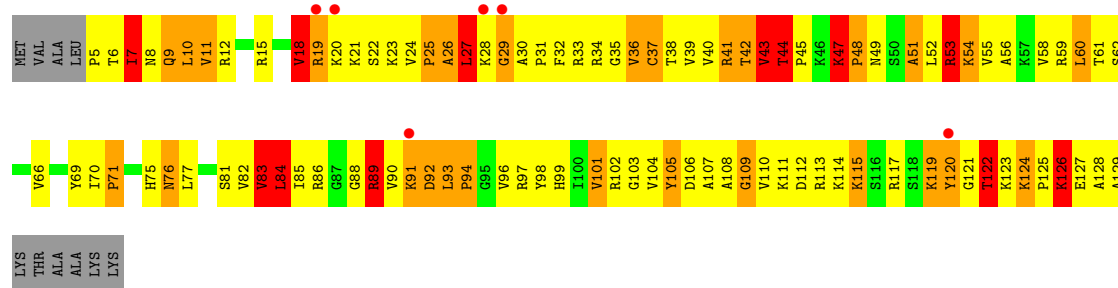


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

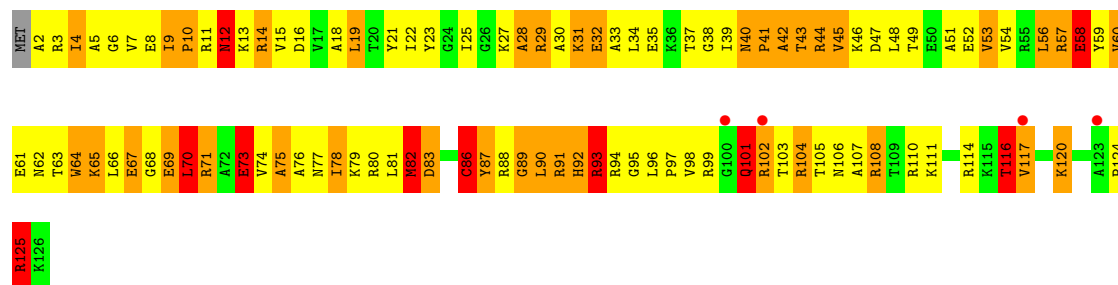
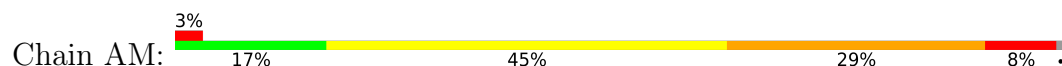


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

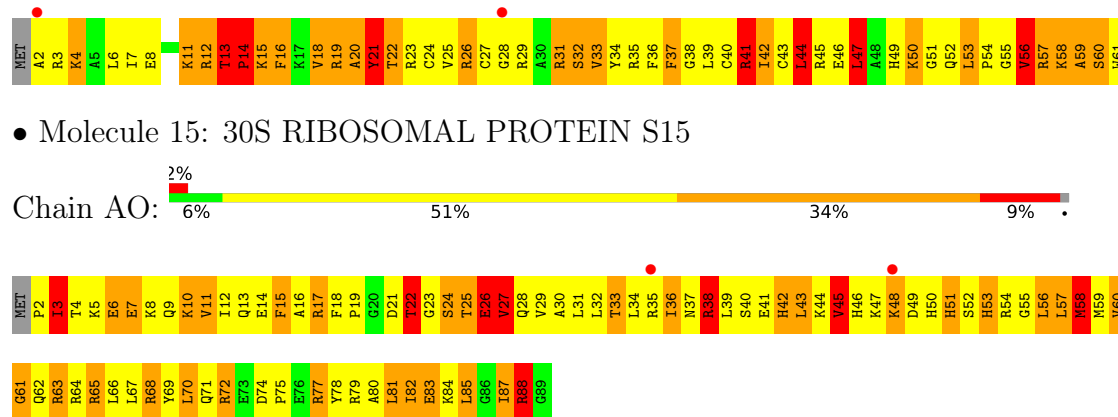




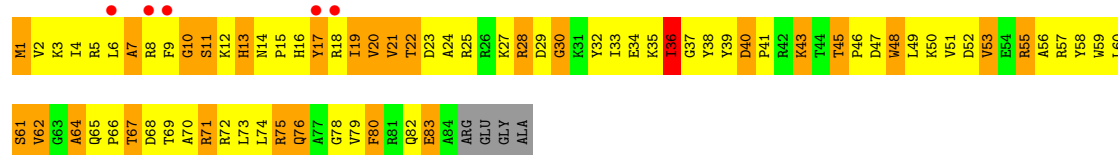
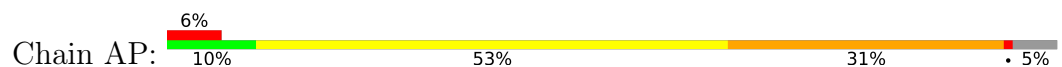
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



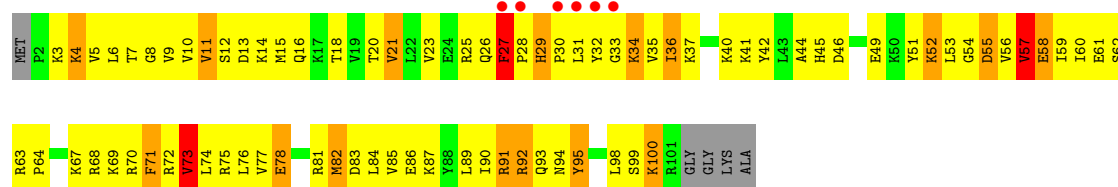
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



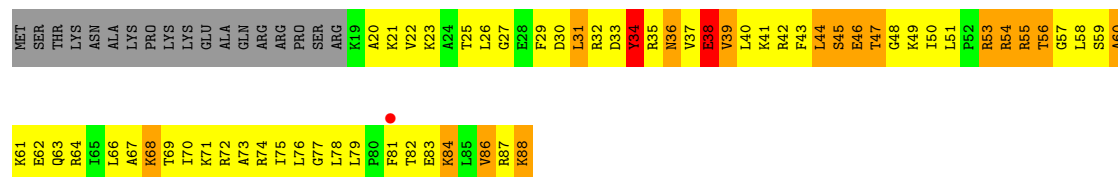
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



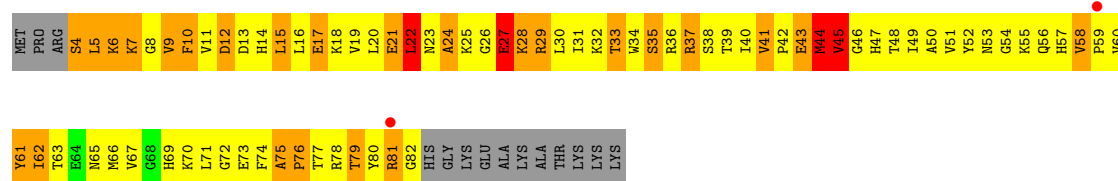
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



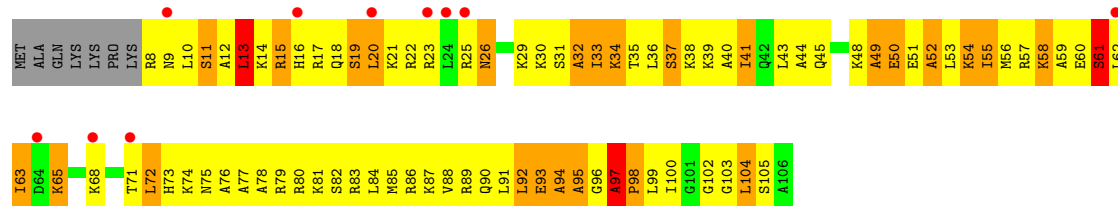
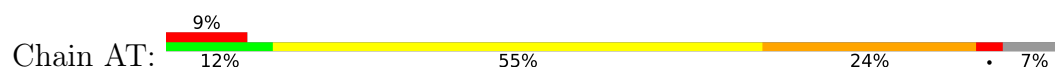
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



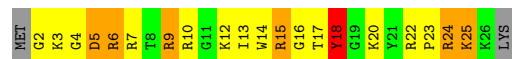
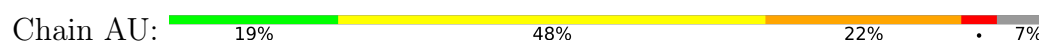
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

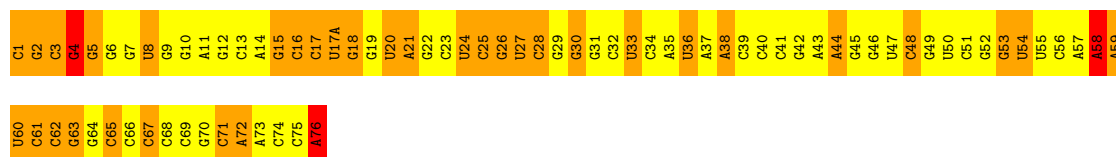


• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: PE HYBRID STATE TRNA FMET





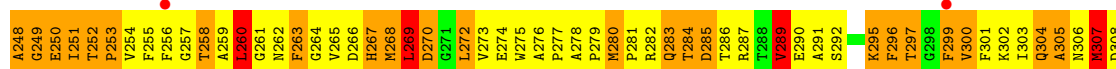
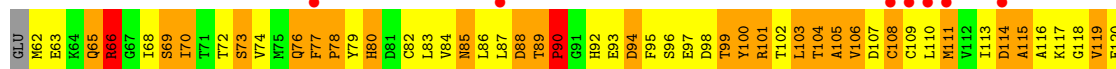
- Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

Chain AX: 11% 44% 44%



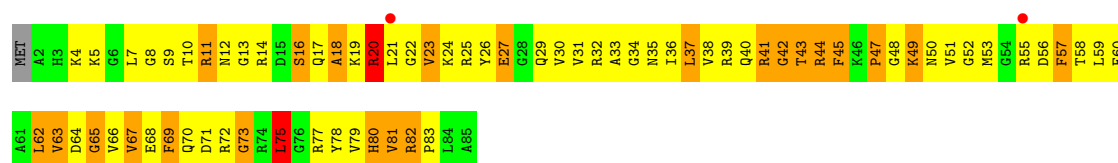
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

Chain AY: 3% 12% 43% 32% 7% 6%

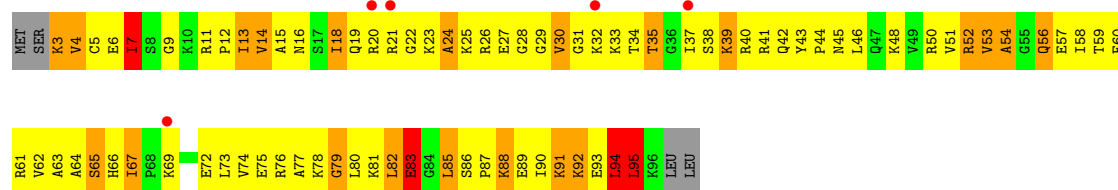
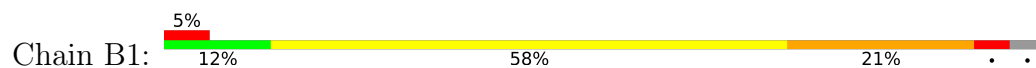


- Molecule 25: 50S RIBOSOMAL PROTEIN L27

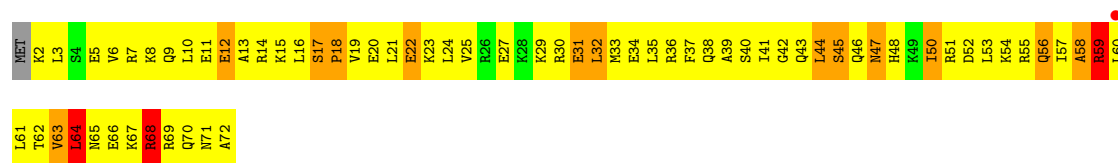
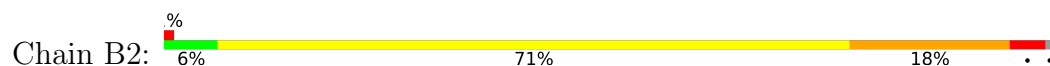
Chain B0: 2% 14% 55% 27% ..



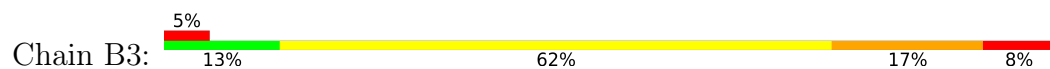
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



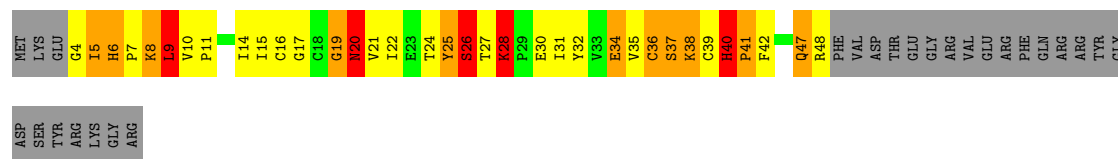
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



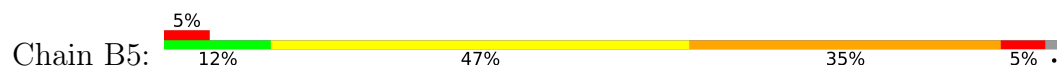
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



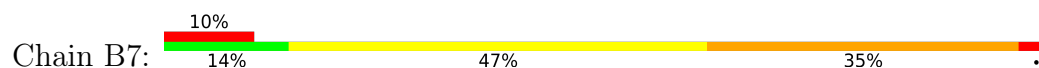
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



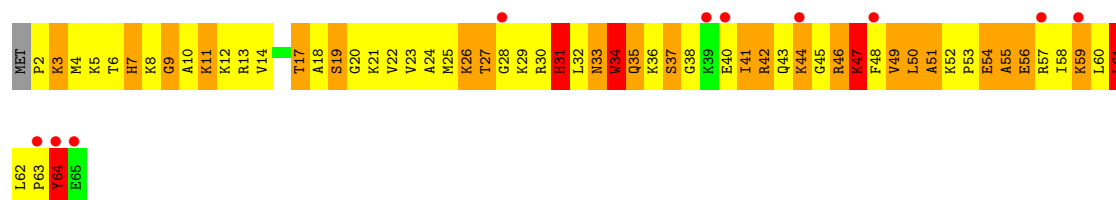
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L34



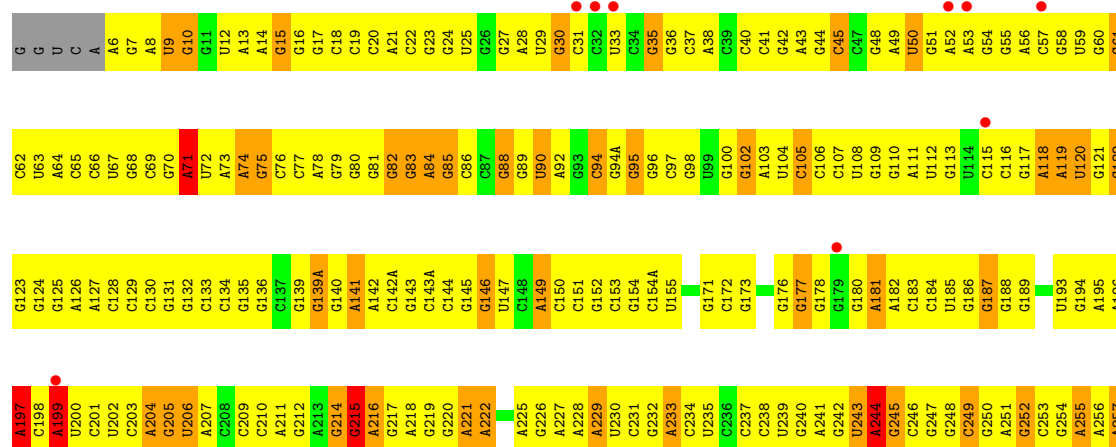
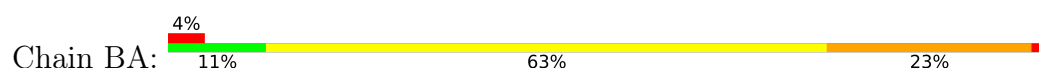
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L36



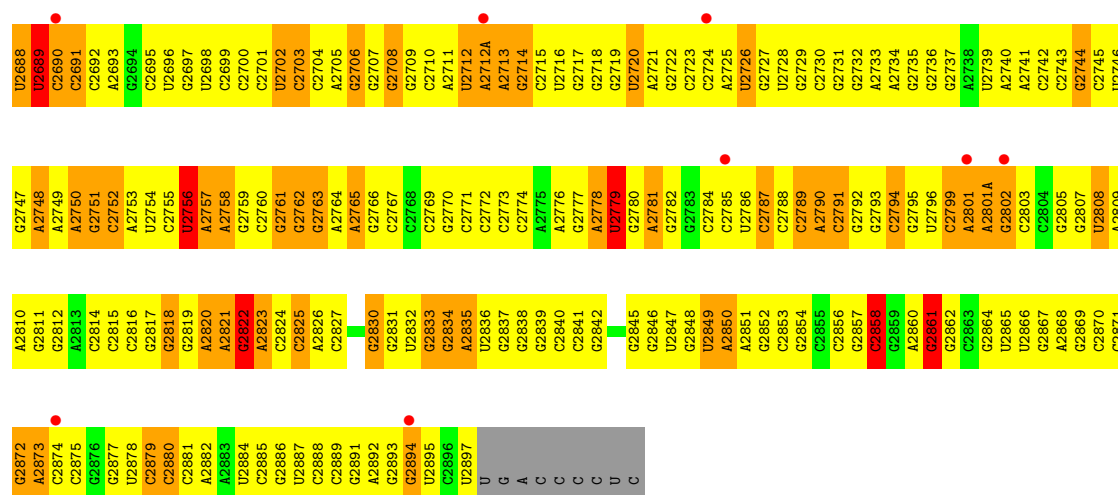
• Molecule 35: 23S RIBOSOMAL RNA



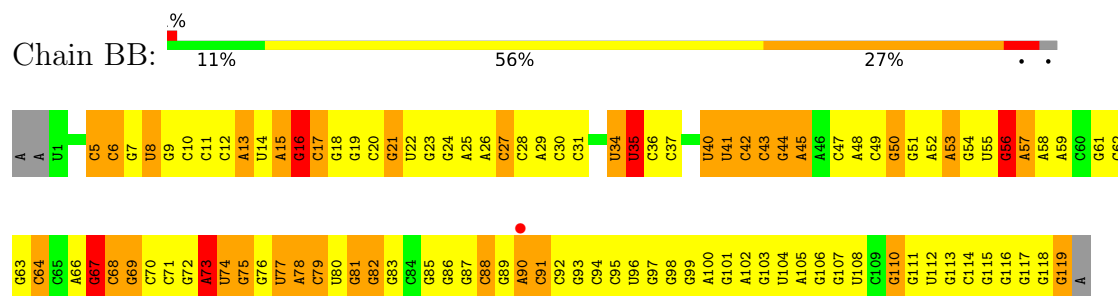
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C1004	A945	G881	A820	C755	G695	G654C	G596	U534	A470	U405	A346	C285	G259
C1005	G946	C884	G823	C756	G696	G654D	U597	C535	A471	G406	A347	G286	G260
C1006	G947	C885	A824	U761	G697	G654E	G598	A636	A472	G407	G348	C287	G261
C1007	G948	C886	C825	A762	G698	G654F	G599	G537	G473	G408	G349	C288	A262
A1008	G949	C887	G826	U763	A699	G654G	G600	G538	G474	C409	G350	A289	G263
A1009	G950	C888	U826	G763	G700	G654H	C501	G539	U475	G410	G351	C290	C264
A1010	C951	C889	U827	G764	G701	G654I	G602	C540	G476	G411	G352	G265	A266
G1011	G952	C890	U828	G765	G702	A654J	A603	C541	A477	A412	G353	C291	G266
C1012	A953	A890	A829	C766	U703	G654K	G604	C542	A478	C413	G354	U293	C267
C1013	G954	G830	G830	U767	G704	G654L	C605	C543	A479	C414	G355	A294	C268
A1014	G955	C893	G831	G768	A705	G654M	U606	G544	A480	C419	G356	U295	G269
G1015	G956	C894	G832	G769	A706	U607	U607	G545	G481	C420	A357	A270	A271
	A957	U895	U833	G770	G707	A654N	A608	A547	A482		U358	C296	
C1018	U958	A896	C834	G771	C708	G654P	A609	A548	A483	A423	A359	C297	
U1019	A959	C897	A835	C772	U709	G654Q		G549	C484		G360	G298	A271A
A1020	A960	C898	G836	U773	G710	G654R	G613	G551	C485	G424	G361	A299	C271B
A1021	C961	A899	C837	A774	G711	G654S	G614	G552	C486	G425	U362	A300	C271C
G1022	G962	A900	C838	G775	G712	G654T	U614	G553		C426	G363	G301	G271D
U1023	U963	A901	U839	G776	G713	A654U	U614A	U554	G489	U427	A363A	C302	U271E
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U1026	G966	C904	G842	U779	A716	G656	G615	U557	G493	G430	U363E	U305	G271H
A1027	G967	U905	G843	G780	G717	U657	G616	G558	G494	U431	A363F	U306	G271I
A1028	G968	G906	C844	A781	A718	C658	C618	G559	G495	A432	C364	G307	C271J
A1029	U969	U907	G845	A782	C719	C659	G619	C560	G496	C433	C365	G308	U271K
G1030	C970	C908	C846	A783	C720	G660	G620	G561	A497	U434	C366	G309	U271L
G1031	C971	A909	U847	A784	G721	C661	A621	U562	G498	U435	C367	A310	U271M
A1032	G972	A910	G848	G785	A722	G662	G663	G563	U500	C436	A371	A311	U271N
U1033	A973	A911	A849	G786	G723	G663	G623	C564	G500	G437	G372	G312	C271O
G1034	G974	C912	C850	U787	U724	C664	G624	C565	A501	G438	U373	G313	C271P
U1035	C975	U913	U851	A788	G725	G665	G625	U566	A502	G440	A374	A314	G271Q
G1036	G975A	C914	G852	A789	G726	G666	U626	A567	A505	U441	C375	G315	G271R
U1037	C976	C915	G853	C790	A727	U667	A627	U568	G506	G442	C376	G316	G271S
G1038	G977	G916	G854	C791	G728	G668	G628	U569	G507	G443	C377	G317	C271T
U1039	G978	A917	G855	G792	G729	G669	G629	G570	A507	C444	C378	G318	G271U
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U1042	C981	G920	U858	C797	C732	C672	A632	G573	C510	A447	G381	A322	U271Y
C1043	C982	G921	G859	C797	G733	C673	A633	C574	U511	U448	G382	G323	C271Z
A1044	A983	U922	U860	G798	A734	G674	C634	A575	G512	A449	U383	A324	G272
A1045	C985	C923	A861	A735	A735	A675	C635	U576	A513	G450	U384	G325	U272A
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G1047	C987	C925	A863	C737	C737	A677	A637	A578	A515	G452	G386	G327	G272C
A1048	G987	A926	G864	U803	G738	C678	G638	G579	C516	C453	U387	U328	G272D
C1049	A988	G927	C865	A804	G739	C679	U639	G580	C517	C454	G388	G329	G272E
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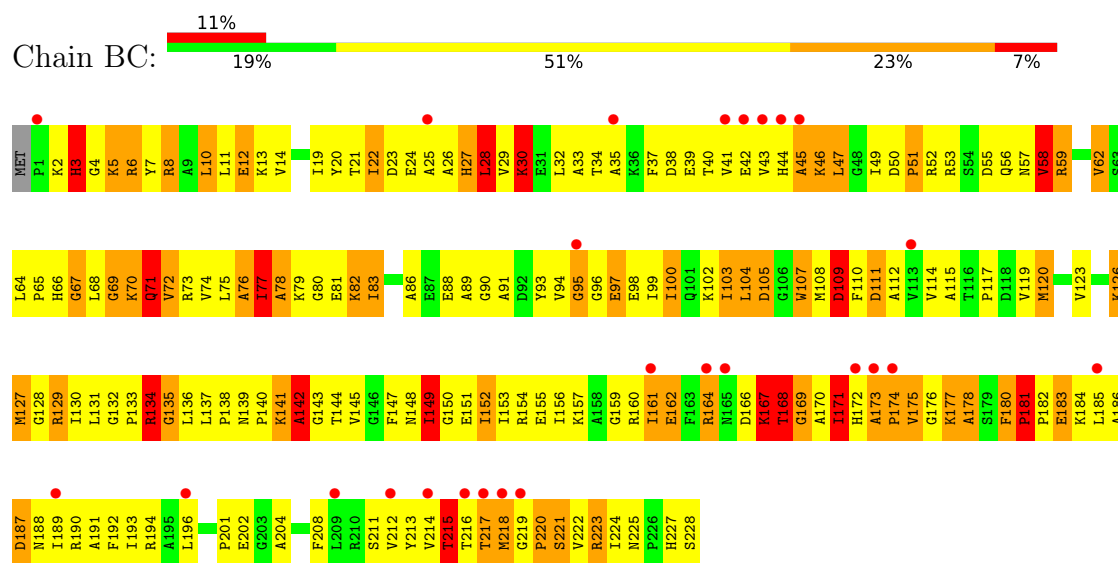
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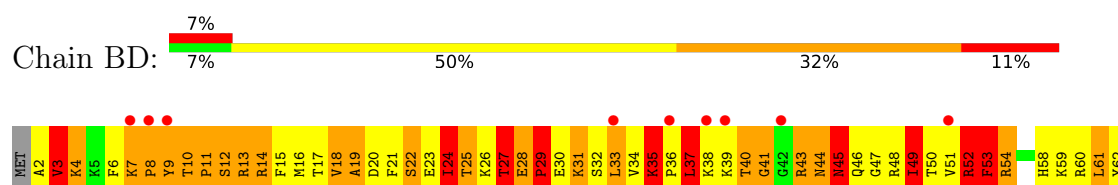
• Molecule 36: 5S RIBOSOMAL RNA

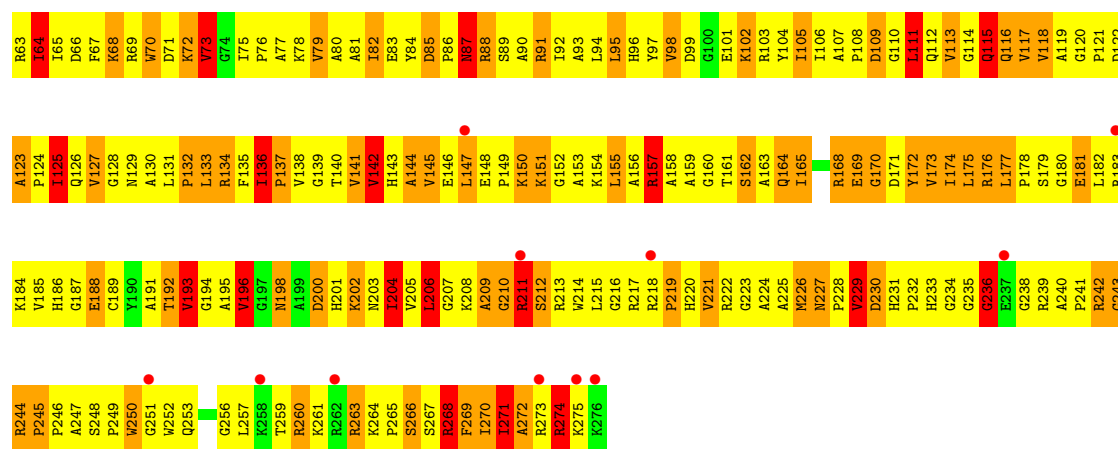


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

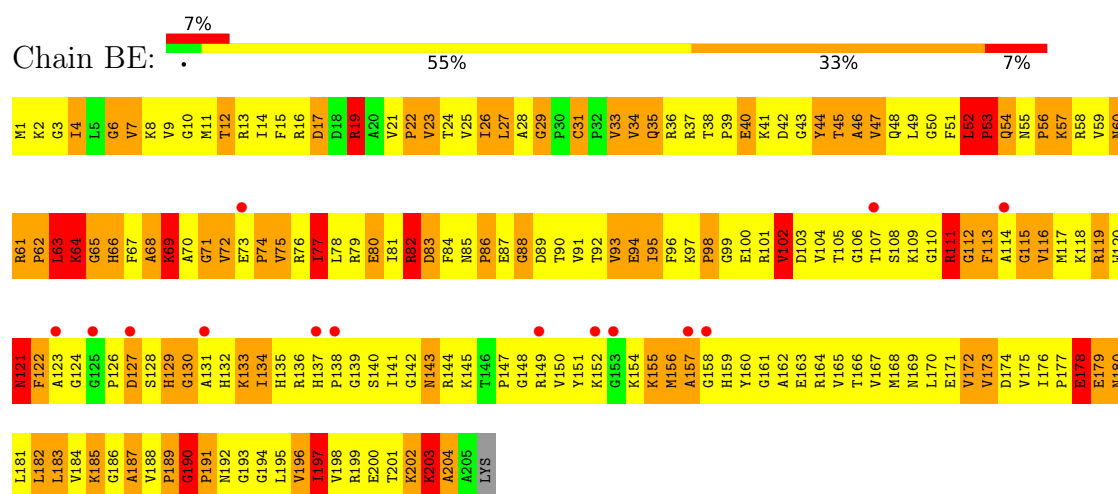


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

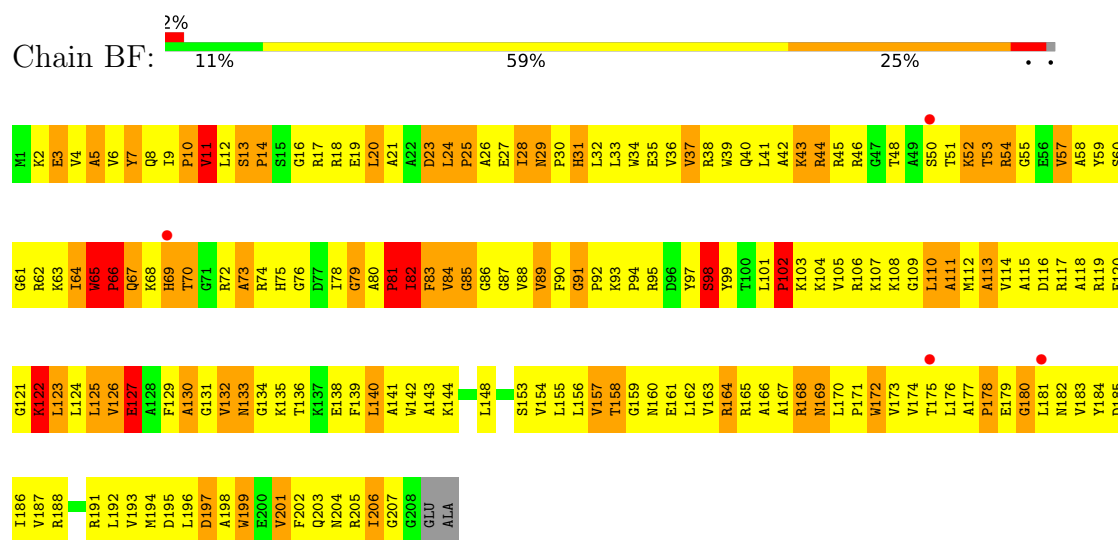




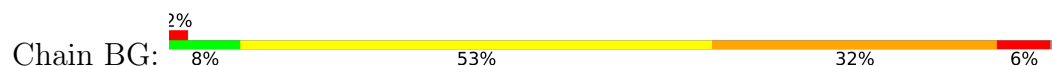
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

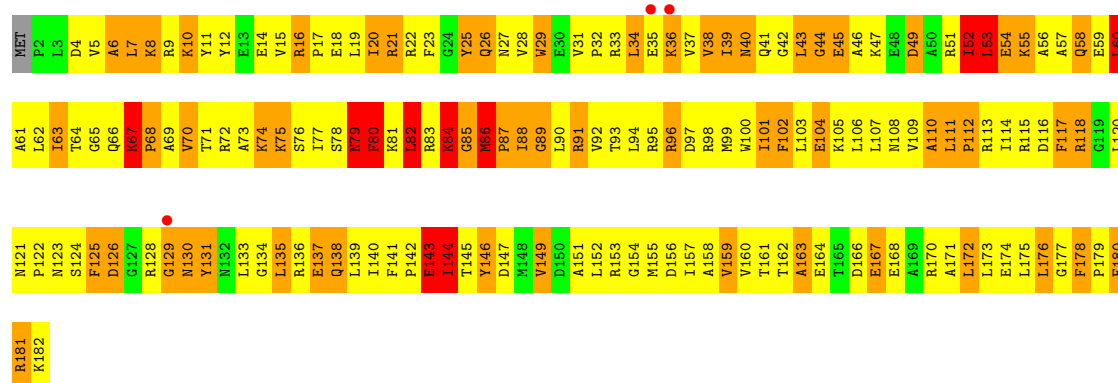


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

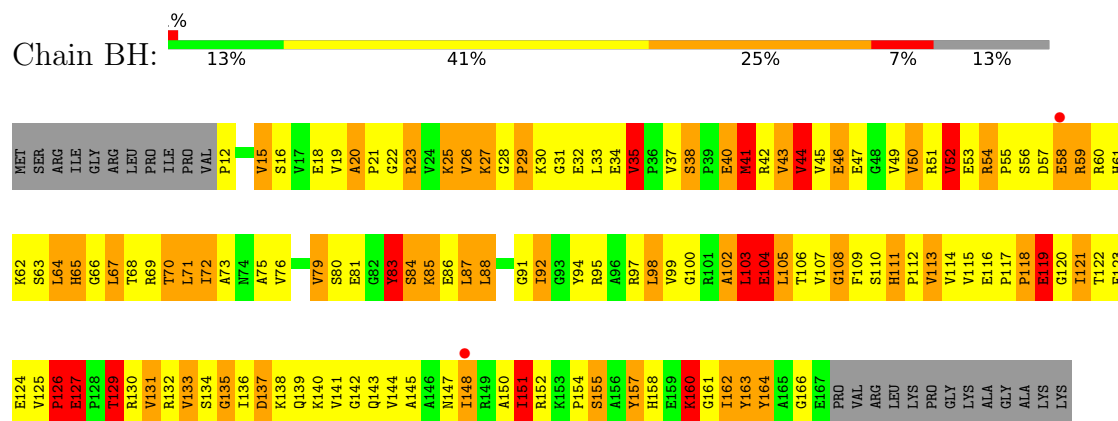


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

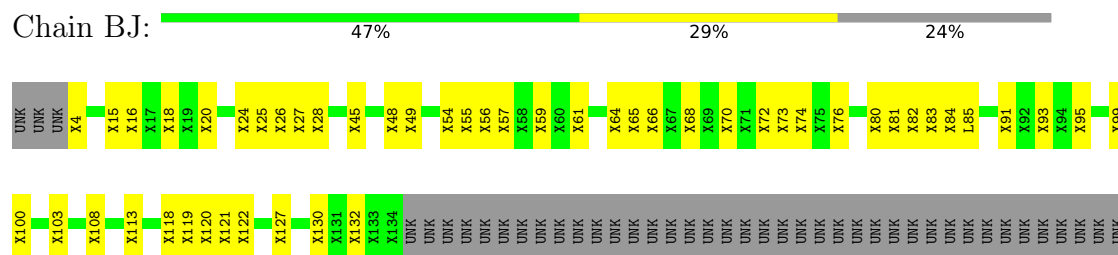




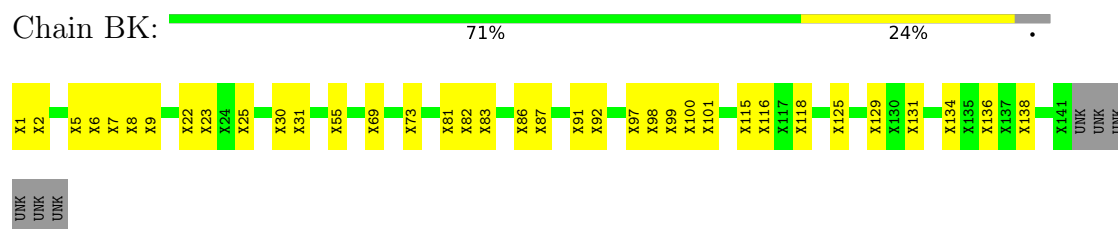
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L10

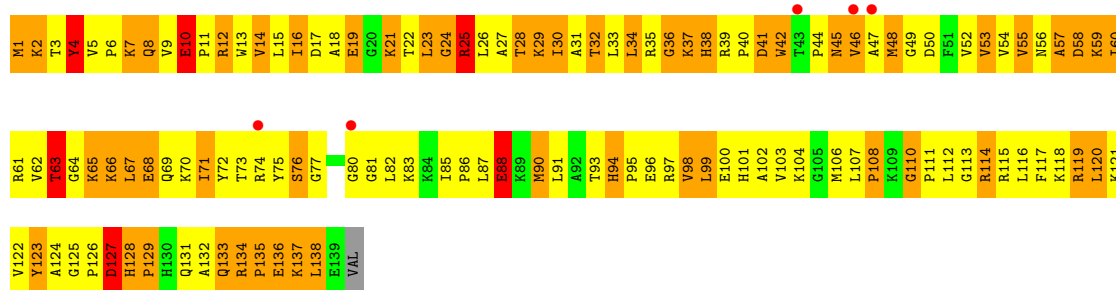


• Molecule 44: 50S RIBOSOMAL PROTEIN L11

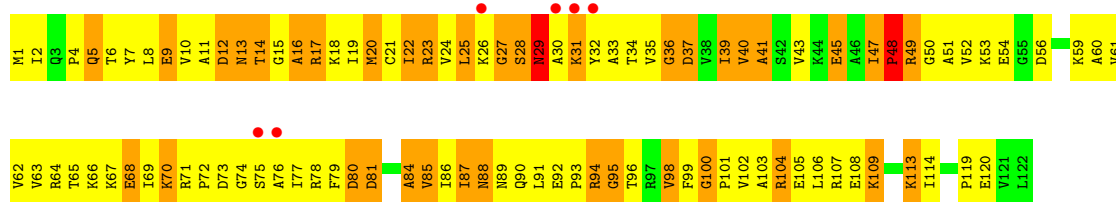
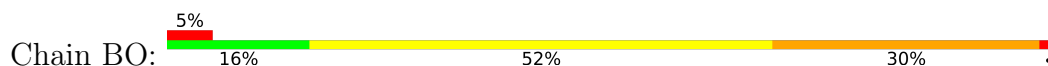


• Molecule 45: 50S RIBOSOMAL PROTEIN L13

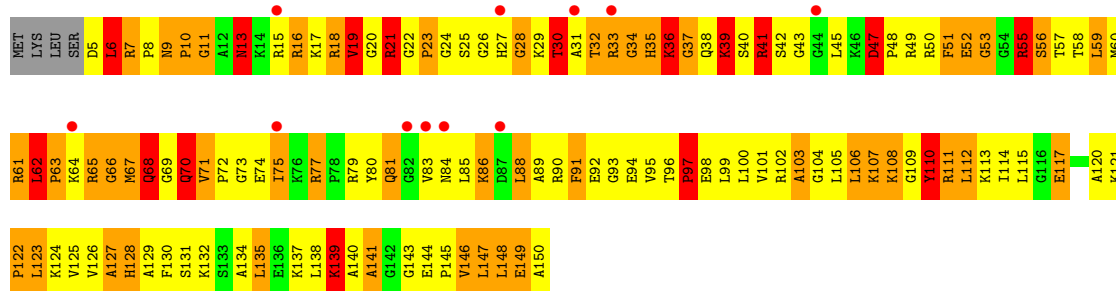




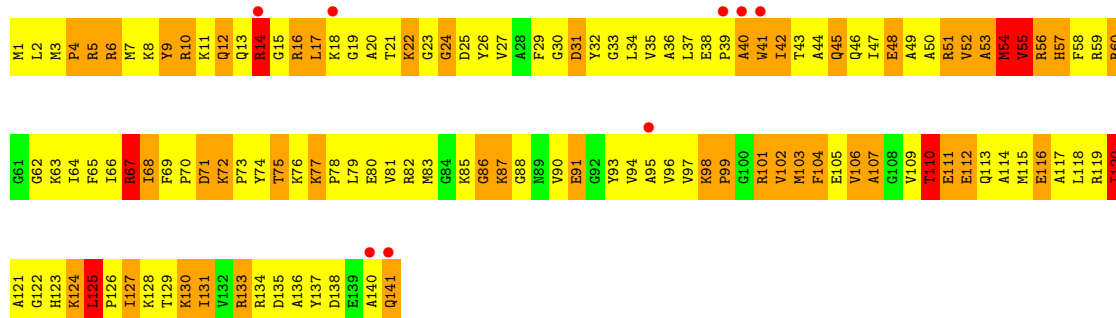
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



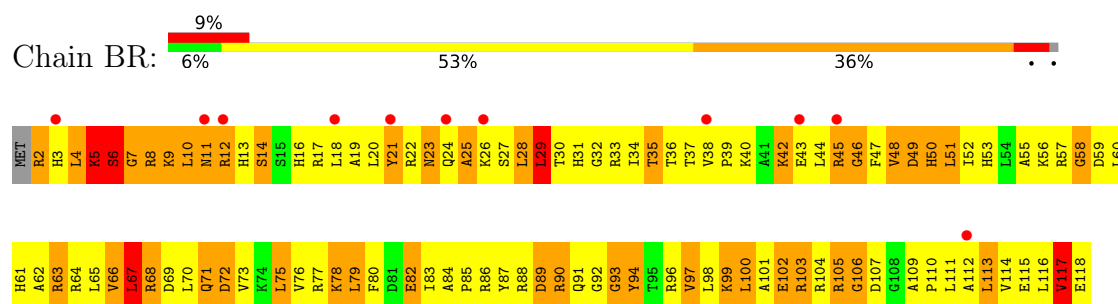
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



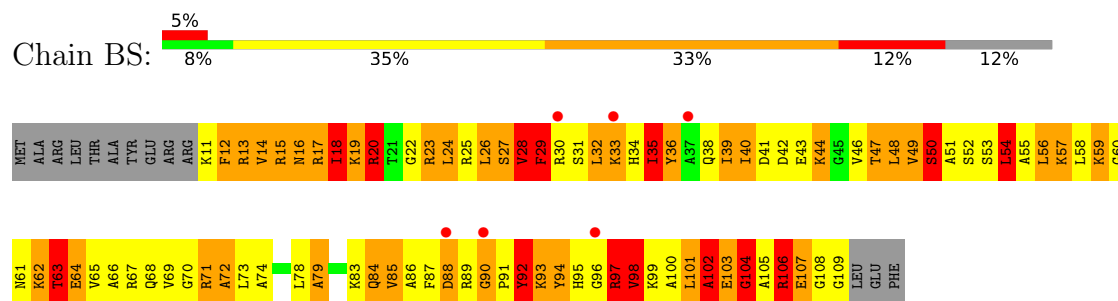
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



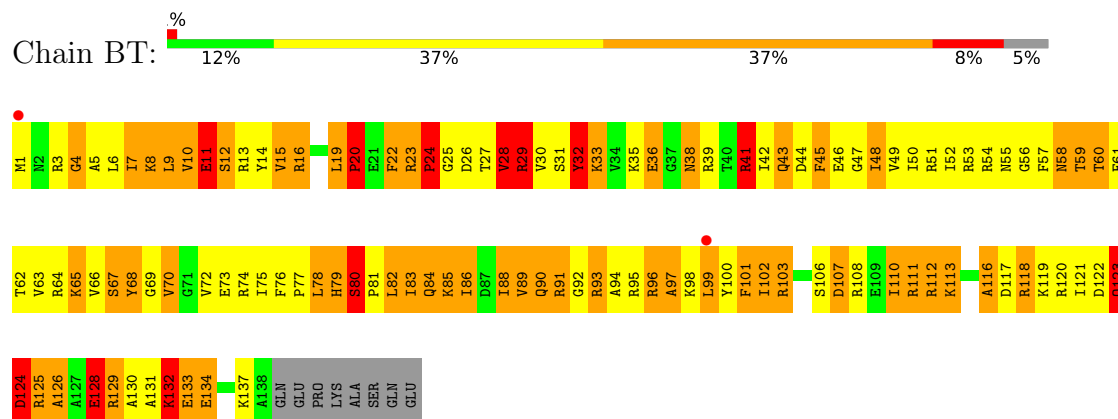
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



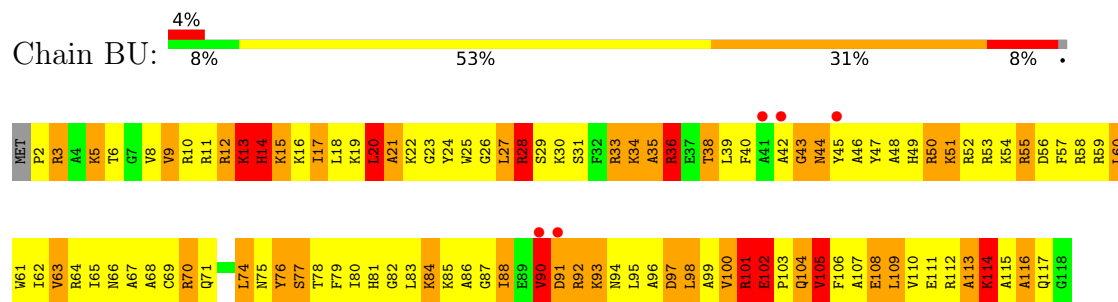
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



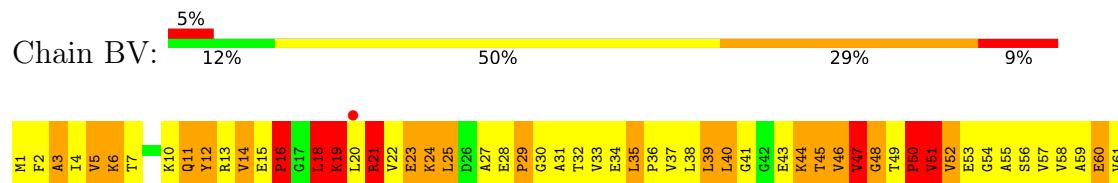
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

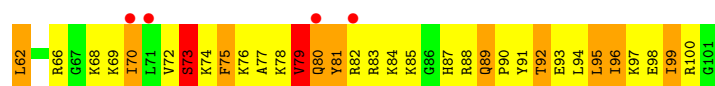


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

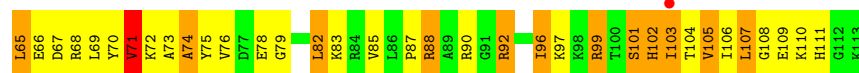
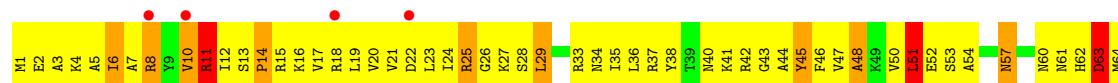


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

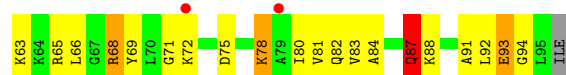
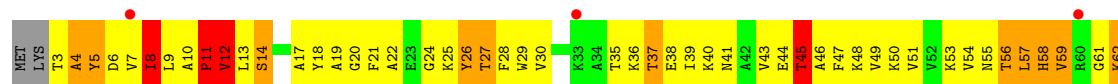




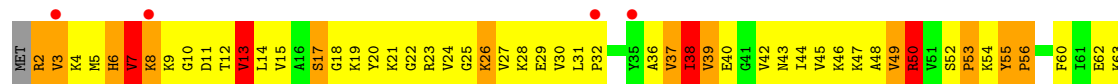
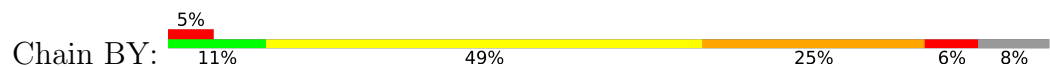
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



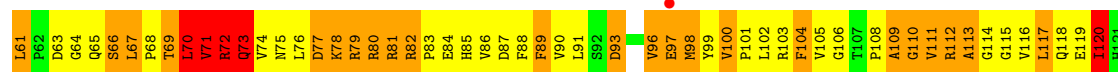
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.90 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 98.7 (44.90-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.351 0.278 , 0.330	Depositor DCC
R_{free} test set	53888 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	110.2	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.65	2/36190 (0.0%)	0.87	93/56486 (0.2%)
2	AB	0.76	2/1936 (0.1%)	1.35	29/2611 (1.1%)
3	AC	0.76	3/1637 (0.2%)	1.33	22/2207 (1.0%)
4	AD	0.60	0/1733	1.36	34/2318 (1.5%)
5	AE	0.80	1/1163 (0.1%)	1.40	22/1566 (1.4%)
6	AF	0.64	0/856	1.35	16/1154 (1.4%)
7	AG	0.72	0/1276	1.27	15/1709 (0.9%)
8	AH	0.72	0/1136	1.42	18/1527 (1.2%)
9	AI	0.64	0/1029	1.23	11/1378 (0.8%)
10	AJ	0.76	1/808 (0.1%)	1.39	16/1087 (1.5%)
11	AK	0.74	1/900 (0.1%)	1.27	9/1213 (0.7%)
12	AL	0.75	1/987 (0.1%)	1.54	20/1322 (1.5%)
13	AM	0.76	1/999 (0.1%)	1.37	15/1338 (1.1%)
14	AN	0.85	1/501 (0.2%)	1.47	11/664 (1.7%)
15	AO	0.85	2/745 (0.3%)	1.27	13/992 (1.3%)
16	AP	0.64	1/717 (0.1%)	1.29	9/965 (0.9%)
17	AQ	0.77	1/837 (0.1%)	1.41	13/1119 (1.2%)
18	AR	0.71	0/579	1.26	6/768 (0.8%)
19	AS	0.83	2/643 (0.3%)	1.27	6/867 (0.7%)
20	AT	0.62	0/765	1.22	8/1007 (0.8%)
21	AU	0.83	1/213 (0.5%)	1.23	1/279 (0.4%)
22	AV	0.56	1/1832 (0.1%)	0.82	2/2855 (0.1%)
23	AX	0.53	0/216	0.74	0/335
24	AY	1.26	31/4005 (0.8%)	1.44	65/5407 (1.2%)
25	B0	0.75	0/671	1.36	11/892 (1.2%)
26	B1	0.64	2/739 (0.3%)	1.24	8/983 (0.8%)
27	B2	0.63	0/600	1.20	8/793 (1.0%)
28	B3	0.76	1/473 (0.2%)	1.45	8/636 (1.3%)
29	B4	0.94	2/350 (0.6%)	1.25	4/476 (0.8%)
30	B5	0.83	0/473	1.36	8/639 (1.3%)
31	B6	0.91	0/440	1.50	8/586 (1.4%)
32	B7	0.64	1/427 (0.2%)	1.22	7/563 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.81	1/516 (0.2%)	1.29	5/681 (0.7%)
34	B9	0.70	0/310	1.10	1/407 (0.2%)
35	BA	0.64	4/69976 (0.0%)	0.85	130/109244 (0.1%)
36	BB	0.62	0/2853	0.92	12/4451 (0.3%)
37	BC	1.17	8/1775 (0.5%)	1.48	38/2392 (1.6%)
38	BD	0.91	2/2195 (0.1%)	1.61	58/2955 (2.0%)
39	BE	0.79	4/1597 (0.3%)	1.42	29/2155 (1.3%)
40	BF	0.72	1/1659 (0.1%)	1.35	25/2246 (1.1%)
41	BG	0.70	0/1499	1.26	20/2016 (1.0%)
42	BH	0.87	1/1211 (0.1%)	1.33	19/1636 (1.2%)
43	BJ	0.54	0/7	0.37	0/8
45	BN	0.71	1/1132 (0.1%)	1.33	17/1527 (1.1%)
46	BO	0.76	0/943	1.40	21/1269 (1.7%)
47	BP	0.71	0/1131	1.50	23/1504 (1.5%)
48	BQ	0.77	1/1143 (0.1%)	1.48	18/1527 (1.2%)
49	BR	0.62	0/974	1.30	16/1302 (1.2%)
50	BS	0.83	1/779 (0.1%)	1.49	16/1038 (1.5%)
51	BT	0.78	1/1156 (0.1%)	1.38	26/1544 (1.7%)
52	BU	0.72	0/975	1.28	13/1297 (1.0%)
53	BV	0.71	0/790	1.27	13/1057 (1.2%)
54	BW	0.73	0/907	1.23	10/1216 (0.8%)
55	BX	0.82	2/740 (0.3%)	1.28	11/995 (1.1%)
56	BY	0.79	1/789 (0.1%)	1.37	9/1053 (0.9%)
57	BZ	0.75	0/1435	1.33	25/1949 (1.3%)
All	All	0.70	86/162368 (0.1%)	1.03	1071/242211 (0.4%)

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	3	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	444	LEU	C-N	-16.31	1.12	1.34
24	AY	504	ILE	C-N	-15.36	1.11	1.33
24	AY	502	ALA	C-N	9.94	1.46	1.33
24	AY	149	ARG	C-O	9.11	1.34	1.24
37	BC	127	MET	CG-SD	9.04	2.03	1.80

The worst 5 of 1071 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	504	ILE	CA-C-N	-17.65	91.26	122.32
24	AY	504	ILE	C-N-CA	-17.65	91.26	122.32
1	AA	1498	U	C2'-C3'-O3'	17.28	135.42	109.50
8	AH	79	VAL	N-CA-C	-15.22	96.89	110.74
50	BS	54	LEU	N-CA-C	-15.00	94.08	112.38

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	2585	0
2	AB	1901	0	1951	544	1
3	AC	1613	0	1677	321	0
4	AD	1703	0	1767	353	0
5	AE	1147	0	1207	235	0
6	AF	843	0	857	147	0
7	AG	1257	0	1296	193	0
8	AH	1116	0	1177	210	0
9	AI	1011	0	1043	211	0
10	AJ	795	0	840	200	0
11	AK	885	0	904	165	0
12	AL	971	0	1057	224	0
13	AM	988	0	1059	204	0
14	AN	492	0	533	153	0
15	AO	734	0	771	244	0
16	AP	701	0	720	135	0
17	AQ	824	0	891	157	0
18	AR	574	0	644	136	0
19	AS	630	0	652	215	0
20	AT	763	0	861	157	0
21	AU	209	0	221	50	0
22	AV	1640	0	837	196	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1280	0
25	B0	662	0	688	141	0
26	B1	732	0	808	135	0
27	B2	598	0	653	130	0
28	B3	468	0	523	111	0
29	B4	341	0	339	94	0
30	B5	459	0	480	136	0
31	B6	433	0	461	112	0
32	B7	419	0	467	116	0
33	B8	508	0	576	158	0
34	B9	307	0	338	71	0
35	BA	62477	0	31497	5289	0
36	BB	2551	0	1295	230	0
37	BC	1742	0	1794	387	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	794	0
39	BE	1564	0	1629	467	0
40	BF	1624	0	1677	432	0
41	BG	1474	0	1535	351	0
42	BH	1189	0	1247	290	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	285	0
46	BO	933	0	996	190	0
47	BP	1114	0	1187	370	0
48	BQ	1122	0	1179	308	0
49	BR	960	0	1021	245	0
50	BS	771	0	832	214	0
51	BT	1142	0	1202	336	0
52	BU	958	0	1015	323	0
53	BV	779	0	852	217	0
54	BW	896	0	953	175	0
55	BX	726	0	778	118	0
56	BY	776	0	870	200	0
57	BZ	1403	0	1432	385	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	19390	1

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 77.

The worst 5 of 19390 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)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:62:ALA:O	37:BC:30:LYS:O[2_656]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0	0
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0	2
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	0	4
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1	13
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	10
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	2
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	4
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0	2
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0	3
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0	5
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0	1
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0	0
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0	1
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	1	12
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0	4
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	1	14
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0	1
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0	1
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0	1
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0	2
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0	2
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0	5
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	3
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	3
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0	1
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0	1
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0	0
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	2
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0	0
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0	2
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	3
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0	4
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0	0
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0	2
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0	1
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0	3
43	BJ	1/173 (1%)	1 (100%)	0	0	100	100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0	0
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	5
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0	0
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0	3
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	2
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	1
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0	0
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0	1
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0	4
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	0	7
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0	0
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0	1
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0	2

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	202/220 (92%)	150 (74%)	52 (26%)	0	3
3	AC	160/188 (85%)	134 (84%)	26 (16%)	2	14
4	AD	180/181 (99%)	153 (85%)	27 (15%)	3	16
5	AE	115/123 (94%)	93 (81%)	22 (19%)	1	9
6	AF	90/90 (100%)	73 (81%)	17 (19%)	1	10
7	AG	126/127 (99%)	111 (88%)	15 (12%)	5	22
8	AH	119/119 (100%)	102 (86%)	17 (14%)	3	17
9	AI	98/99 (99%)	76 (78%)	22 (22%)	1	5
10	AJ	88/92 (96%)	70 (80%)	18 (20%)	1	7
11	AK	90/99 (91%)	72 (80%)	18 (20%)	1	8
12	AL	104/111 (94%)	87 (84%)	17 (16%)	2	14
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1	8
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	3
15	AO	79/80 (99%)	49 (62%)	30 (38%)	0	0
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3	16
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	38
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	23
19	AS	69/80 (86%)	57 (83%)	12 (17%)	2	12
20	AT	76/82 (93%)	68 (90%)	8 (10%)	6	26
21	AU	19/22 (86%)	17 (90%)	2 (10%)	6	26
24	AY	427/453 (94%)	309 (72%)	118 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B0	66/67 (98%)	50 (76%)	16 (24%)	1	4
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	13
27	B2	66/67 (98%)	61 (92%)	5 (8%)	12	37
28	B3	51/52 (98%)	41 (80%)	10 (20%)	1	8
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0	3
30	B5	51/52 (98%)	44 (86%)	7 (14%)	3	18
31	B6	49/52 (94%)	34 (69%)	15 (31%)	0	1
32	B7	41/42 (98%)	34 (83%)	7 (17%)	2	13
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	7
34	B9	34/34 (100%)	27 (79%)	7 (21%)	1	7
37	BC	180/181 (99%)	149 (83%)	31 (17%)	2	13
38	BD	217/218 (100%)	142 (65%)	75 (35%)	0	1
39	BE	165/166 (99%)	138 (84%)	27 (16%)	2	14
40	BF	165/166 (99%)	141 (86%)	24 (14%)	3	17
41	BG	155/156 (99%)	122 (79%)	33 (21%)	1	6
42	BH	128/148 (86%)	81 (63%)	47 (37%)	0	0
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	95 (81%)	22 (19%)	1	10
46	BO	100/100 (100%)	83 (83%)	17 (17%)	2	13
47	BP	112/116 (97%)	85 (76%)	27 (24%)	1	4
48	BQ	111/111 (100%)	86 (78%)	25 (22%)	1	5
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	5
50	BS	77/88 (88%)	56 (73%)	21 (27%)	0	3
51	BT	120/127 (94%)	91 (76%)	29 (24%)	1	4
52	BU	92/94 (98%)	75 (82%)	17 (18%)	1	11
53	BV	82/82 (100%)	64 (78%)	18 (22%)	1	5
54	BW	91/92 (99%)	80 (88%)	11 (12%)	5	21
55	BX	74/78 (95%)	64 (86%)	10 (14%)	4	19
56	BY	84/91 (92%)	70 (83%)	14 (17%)	2	13
57	BZ	155/179 (87%)	119 (77%)	36 (23%)	1	5
All	All	5271/5546 (95%)	4185 (79%)	1086 (21%)	1	7

5 of 1086 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BR	99	LYS
51	BT	20	PRO
49	BR	97	VAL
56	BY	11	ASP
24	AY	141	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
38	BD	227	ASN
47	BP	70	GLN
39	BE	66	HIS
41	BG	40	ASN
49	BR	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	276 (18%)	58 (3%)
22	AV	76/77 (98%)	36 (47%)	3 (3%)
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	658 (22%)	73 (2%)
36	BB	118/122 (96%)	24 (20%)	1 (0%)
All	All	4605/4645 (99%)	999 (21%)	135 (2%)

5 of 999 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 135 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	1996	C
35	BA	2126	A

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Mol	Chain	Res	Type
35	BA	2689	U
1	AA	1285	A
1	AA	1283	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	GCP	AY	1000	-	32,34,34	2.01	9 (28%)	49,54,54	1.08	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	AY	1000	-	-	10/19/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PB-O3A	5.83	1.64	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	C6-N1	4.68	1.47	1.38
58	AY	1000	GCP	C4-N3	3.75	1.42	1.34
58	AY	1000	GCP	C2-N3	3.53	1.41	1.33
58	AY	1000	GCP	PG-O2G	-2.90	1.48	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	O3G-PG-O2G	2.77	115.84	107.96
58	AY	1000	GCP	O3G-PG-O1G	-2.73	105.32	112.39
58	AY	1000	GCP	O2G-PG-O1G	-2.43	106.11	112.39
58	AY	1000	GCP	PB-O3A-PA	-2.34	124.74	132.37
58	AY	1000	GCP	O2'-C2'-C3'	2.01	118.27	111.82

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

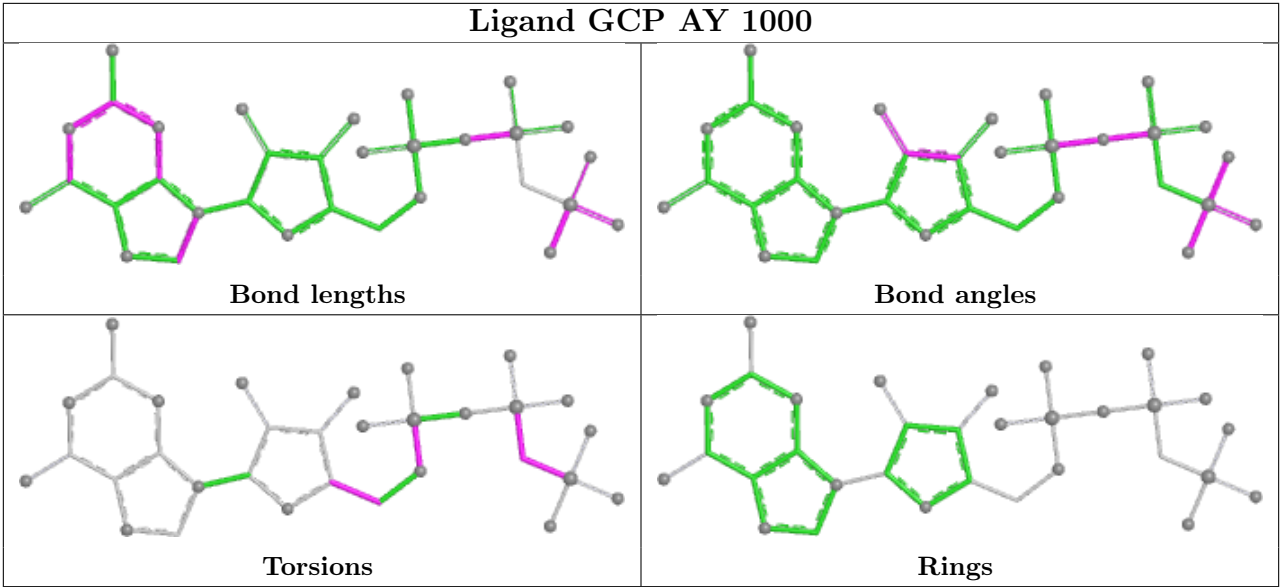
Mol	Chain	Res	Type	Atoms
58	AY	1000	GCP	PB-C3B-PG-O1G
58	AY	1000	GCP	PB-C3B-PG-O2G
58	AY	1000	GCP	PG-C3B-PB-O1B
58	AY	1000	GCP	PG-C3B-PB-O3A
58	AY	1000	GCP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AY	1000	GCP	11	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	AY	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AY	444:LEU	C	445:GLN	N	1.12
1	AY	504:ILE	C	505:ALA	N	1.11

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.04	42 (2%) 55 38	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.17	3 (1%) 75 53	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.37	1 (0%) 87 71	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.13	9 (4%) 40 28	48, 158, 200, 200	0
5	AE	151/162 (93%)	-0.15	5 (3%) 49 34	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.31	0 100 100	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.18	2 (1%) 75 53	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.22	6 (4%) 40 28	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.04	3 (2%) 59 41	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.10	4 (4%) 42 30	32, 125, 191, 200	0
11	AK	119/129 (92%)	-0.21	4 (3%) 48 33	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.14	6 (4%) 35 26	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.01	4 (3%) 50 35	64, 127, 200, 200	0
14	AN	60/61 (98%)	0.18	2 (3%) 49 34	28, 104, 172, 200	0
15	AO	88/89 (98%)	-0.09	2 (2%) 61 42	59, 130, 188, 200	0
16	AP	84/88 (95%)	0.30	5 (5%) 27 22	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.19	6 (6%) 27 22	66, 141, 200, 200	0
18	AR	70/88 (79%)	-0.15	1 (1%) 73 51	59, 124, 176, 200	0
19	AS	79/93 (84%)	-0.21	2 (2%) 58 40	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.49	10 (10%) 12 14	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.40	0 100 100	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.31	0 100 100	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.42	0 100 100	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.00	14 (2%) 55 38	71, 170, 202, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	84/85 (98%)	0.12	2 (2%) 59 41	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.18	5 (5%) 32 24	65, 143, 197, 200	0
27	B2	71/72 (98%)	-0.28	1 (1%) 73 51	101, 153, 200, 200	0
28	B3	60/60 (100%)	-0.02	3 (5%) 34 25	54, 126, 198, 200	0
29	B4	45/71 (63%)	-0.51	0 100 100	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.29	3 (5%) 33 25	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.13	1 (2%) 65 44	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.61	5 (10%) 12 14	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.77	10 (15%) 5 8	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.12	10 (27%) 1 3	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.17	118 (4%) 41 30	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.23	1 (0%) 82 62	66, 123, 172, 190	0
37	BC	228/229 (99%)	0.76	26 (11%) 10 13	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.27	20 (7%) 21 19	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.22	14 (6%) 23 20	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.10	4 (1%) 66 45	51, 156, 200, 200	0
41	BG	181/182 (99%)	-0.05	3 (1%) 69 47	47, 134, 194, 200	0
42	BH	156/180 (86%)	-0.04	2 (1%) 75 53	78, 165, 200, 200	0
43	BJ	1/173 (0%)	0.29	0 100 100	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-
45	BN	139/140 (99%)	0.09	5 (3%) 46 32	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.13	6 (4%) 35 26	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.27	11 (7%) 20 18	65, 147, 200, 200	0
48	BQ	141/141 (100%)	-0.03	8 (5%) 29 23	20, 107, 171, 200	0
49	BR	117/118 (99%)	0.36	11 (9%) 14 16	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.25	6 (6%) 27 22	49, 123, 194, 200	0
51	BT	138/146 (94%)	-0.14	2 (1%) 73 51	89, 162, 200, 200	0
52	BU	117/118 (99%)	0.12	5 (4%) 40 28	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.16	5 (4%) 34 25	42, 146, 200, 200	0
54	BW	113/113 (100%)	0.32	5 (4%) 39 28	78, 165, 200, 200	0
55	BX	93/96 (96%)	0.33	5 (5%) 31 24	38, 167, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BY	101/110 (91%)	0.24	6 (5%) 28 23	86, 169, 200, 200	0
57	BZ	176/206 (85%)	-0.24	2 (1%) 78 56	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.09	436 (3%) 42 30	20, 146, 200, 202	0

The worst 5 of 436 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	BD	276	LYS	14.1
37	BC	165	ASN	8.8
11	AK	126	ARG	7.8
38	BD	36	PRO	7.0
41	BG	35	GLU	6.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

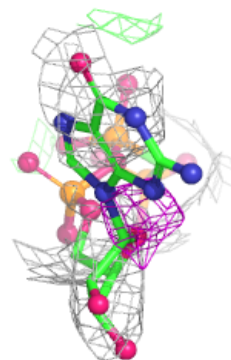
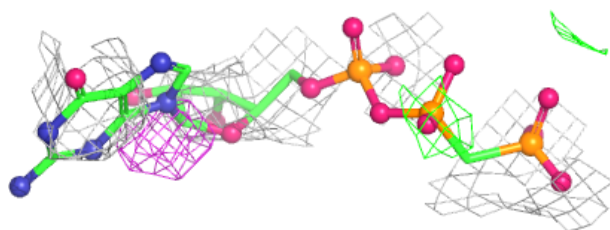
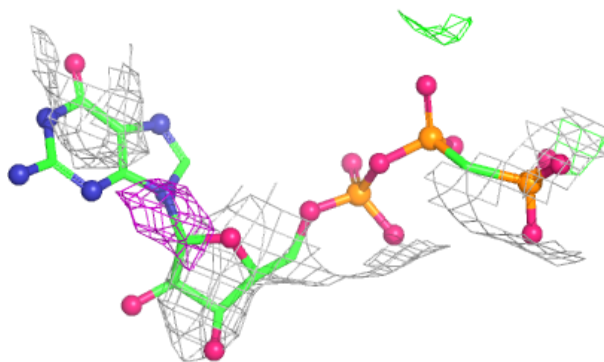
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	GCP	AY	1000	32/32	0.86	0.08	95,109,121,122	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GCP AY 1000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.