



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:28 PM UTC

PDB ID : 3DLL / pdb_00003dll
Title : The oxazolidinone antibiotics perturb the ribosomal peptidyl-transferase center and effect tRNA positioning
Authors : Wilson, D.N.; Schlutzen, F.; Harms, J.M.; Starosta, A.L.; Connell, S.R.; Fucini, P.
Deposited on : 2008-06-27
Resolution : 3.50 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

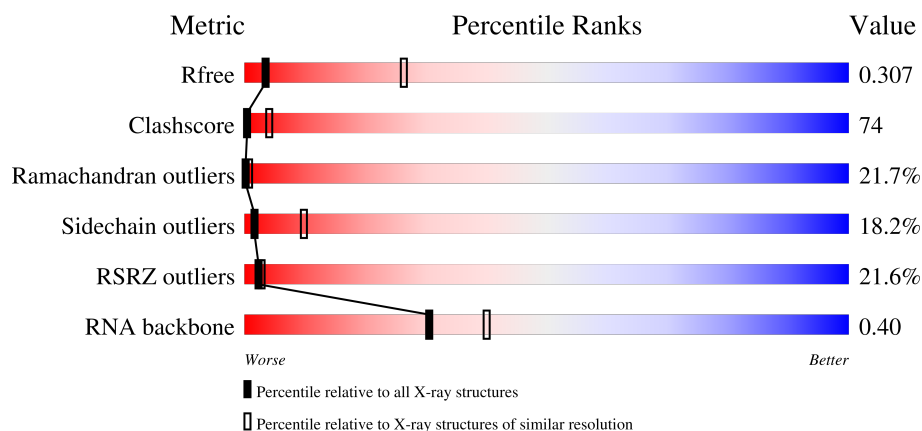
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

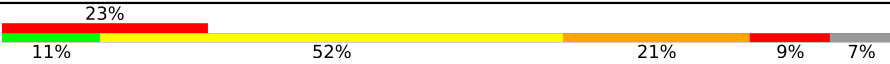
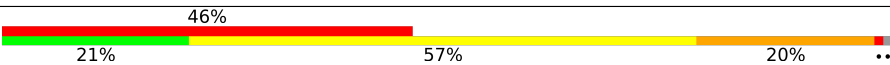
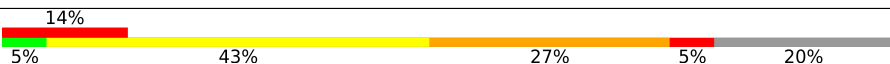
The reported resolution of this entry is 3.50 Å.

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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	X	2880	
2	Z	123	
3	A	274	

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Mol	Chain	Length	Quality of chain
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Y	60	
27	1	55	
28	2	47	

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Mol	Chain	Length	Quality of chain
29	3	66	95% 92% 5%
30	4	37	22% 5% 76% 19%

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
31	MG	M	167	-	-	-	X
31	MG	X	2882	-	-	-	X
31	MG	X	2898	-	-	-	X
31	MG	X	2902	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2908	-	-	-	X
32	ZLD	X	2911	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 83657 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 rRNA-23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called rRNA-5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	218	Total	C	N	O	S	0	0	0
			1637	1017	326	292	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	70	Total	C	N	O	S	0	0	0
			504	314	90	97	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O		0	0	0
			1067	655	216	196				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O		0	0	0
			741	465	139	137				

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	S	0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

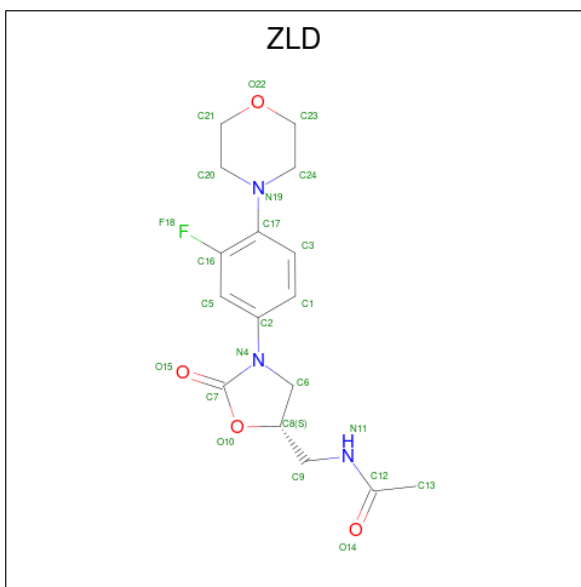
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Z	4	Total Mg 4 4	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

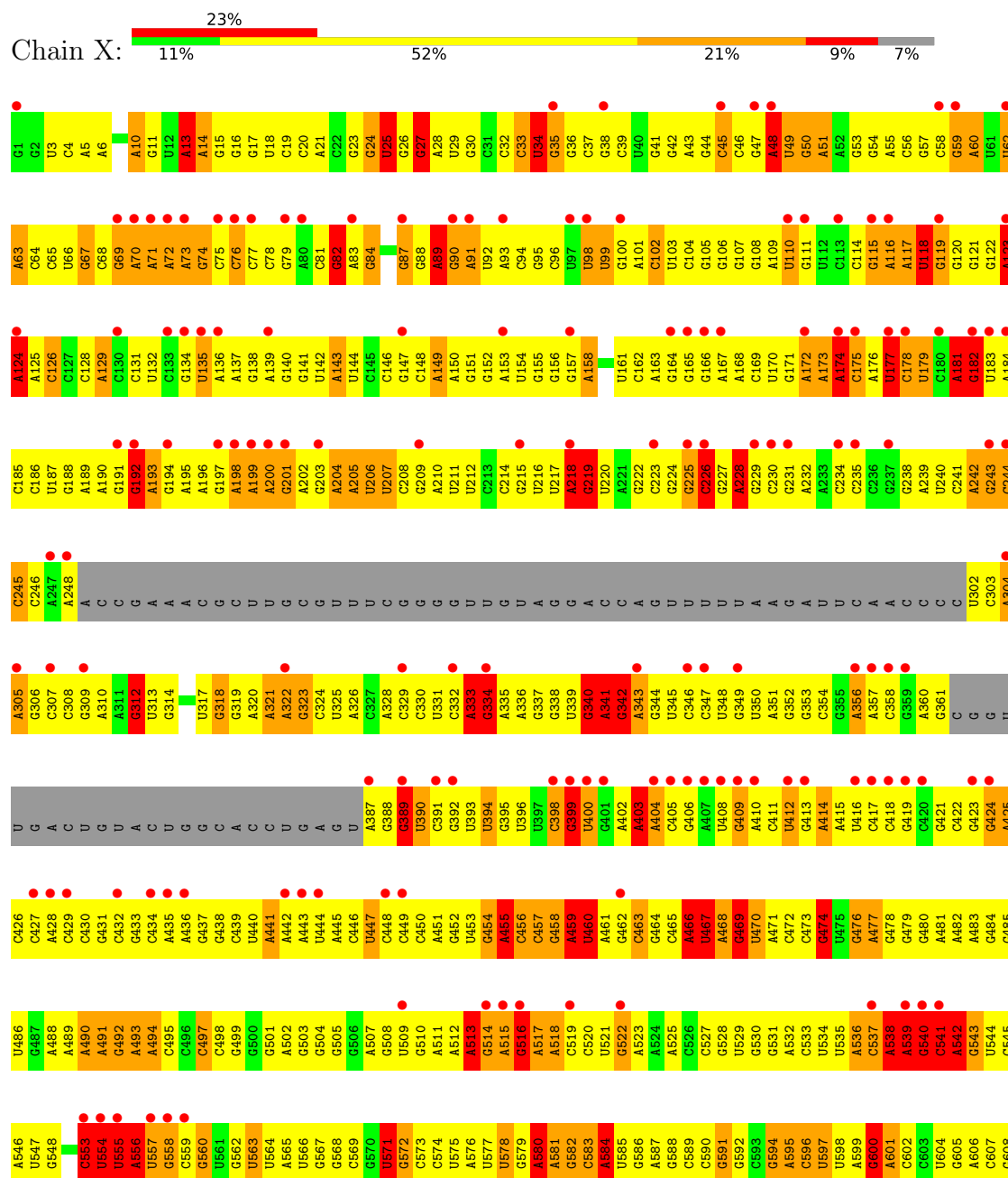
- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Y	1	Total	Zn	0	0
			1	1		
33	4	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

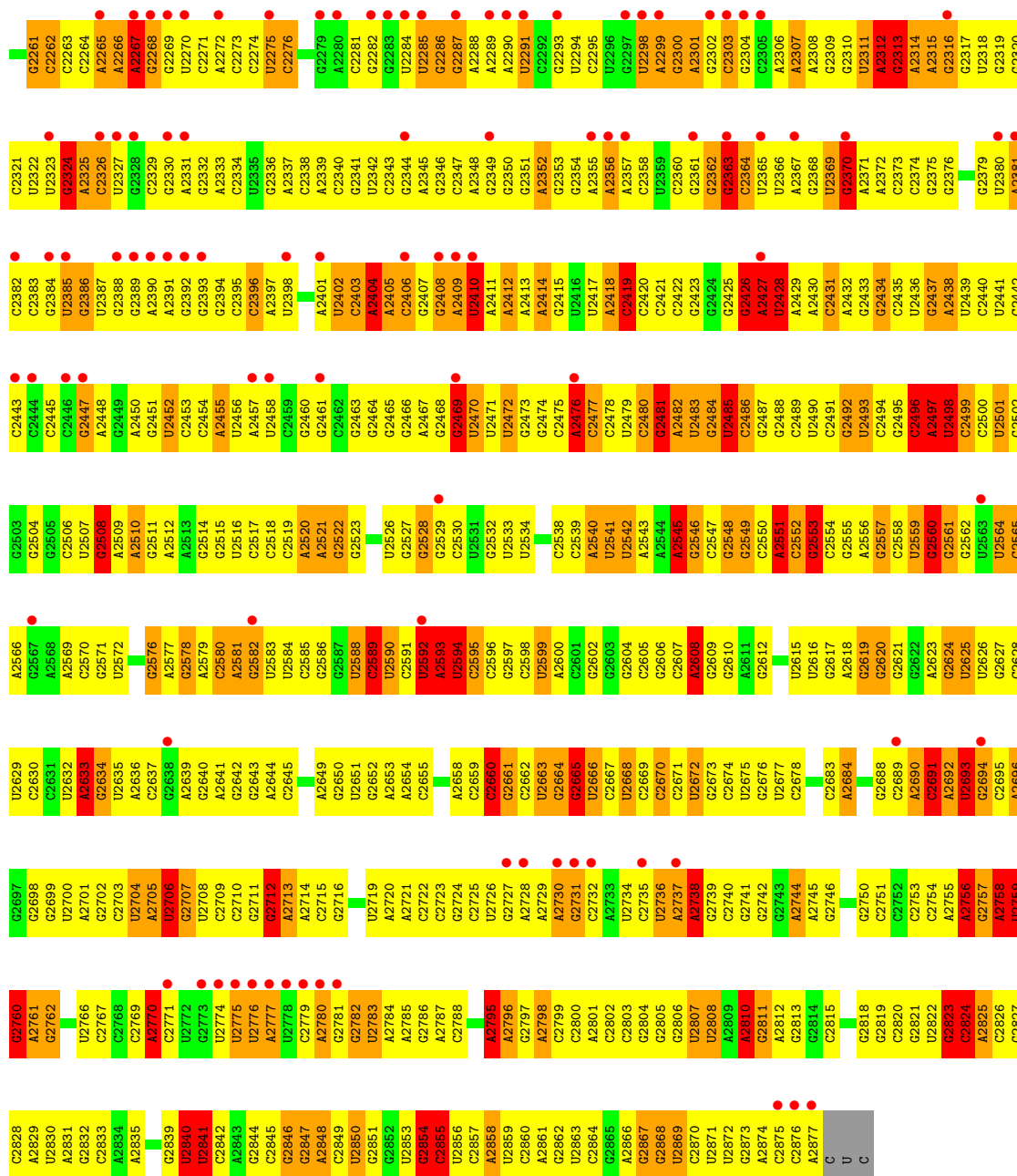
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: rRNA-23S ribosomal RNA

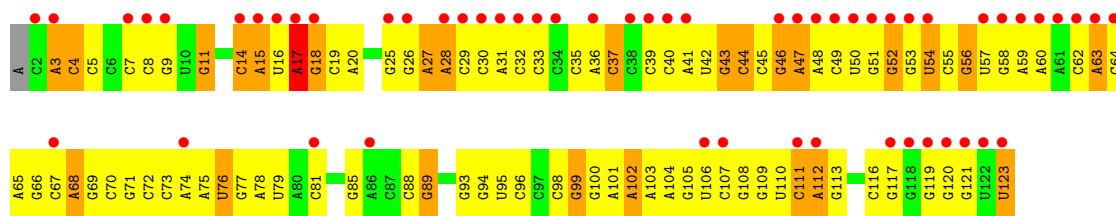


U1403	U1404	A1405	A1406	G1407	A1408	U1409	U1410	C1411	C1412	U1413	G1414	G1415	A1416	C1417	G1418	G1419	A1420	U1421	C1422	A1423	C1424	G1425	U1426	G1427	U1428	A1429	U1430	U1431	U1432	U1433	U1434	A1435	G1436	A1437	U1438	U1439	U1440	A1441	C1442	G1443	C1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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A1099	C1100	U1101	C1102	C1103	C1104	U1105	A1106	U1107	U1108	A1109	C1110	C1111	U1112	C1113	C1114	A1115	U1116	U1117	C1118	U1119	C1120	C1121	A1122	C1123	U1124	C1125	A1126	C1127	C1128	U1129	U1130	C1131	C1132	C1133	C1134	C1135	U1136	U1137	A1138	U1139	C1140	U1141	U1202	C1203	U1204	C1205	C1206	C1207	C1208	U1209	C1210	C1211	U1212	U1213	C1214	A1215	C1216	C1217	C1218	U1219	U1220	U1221	U1222	U1223	U1224																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U1038	A1039	U1040	G1041	G1042	U1043	U1044	U1045	U1046	U1047	C1048	C1049	C1050	U1051	C1052	C1053	C1054	A1055	U1056	U1057	C1058	A1059	C1060	U1061	C1062	C1063	C1064	A1065	C1066	C1067	U1068	C1069	U1070	U1071	U1072	C1073	C1074	C1075	U1076	U1077	U1078	A1079	C1080	U1081	C1082	C1083	U1084	C1085	C1086	C1087	U1088	C1089	U1090	C1091	U1092	U1093	C1094	U1095	A1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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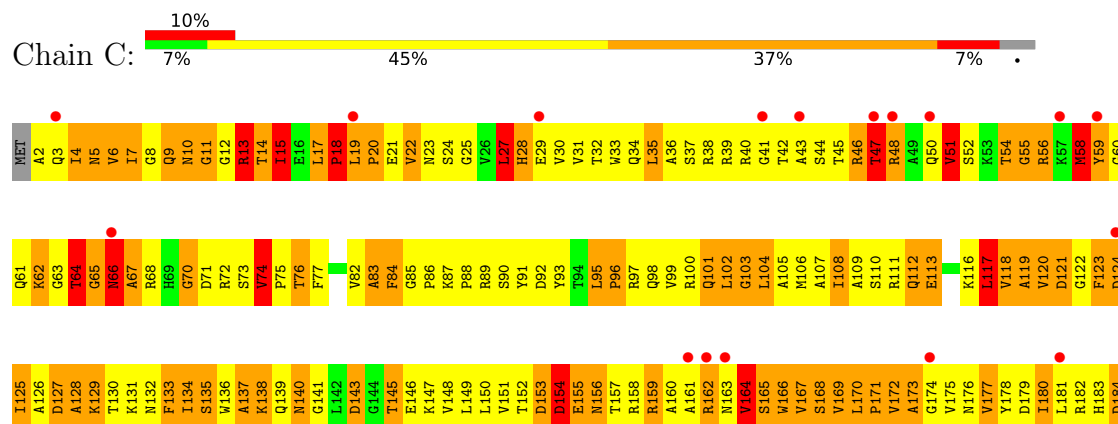
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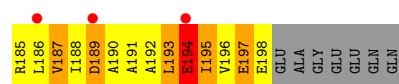


• Molecule 2: rRNA-5S ribosomal RNA

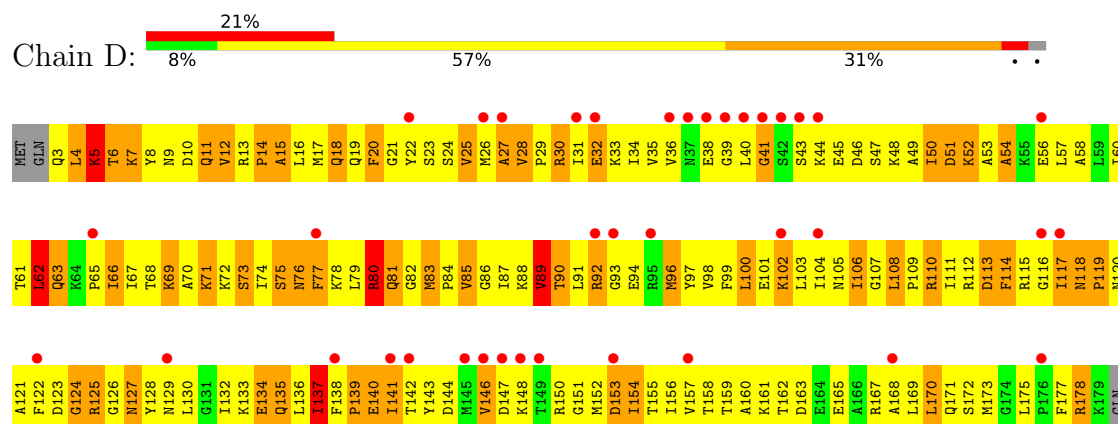


• Molecule 3: 50S ribosomal protein L2

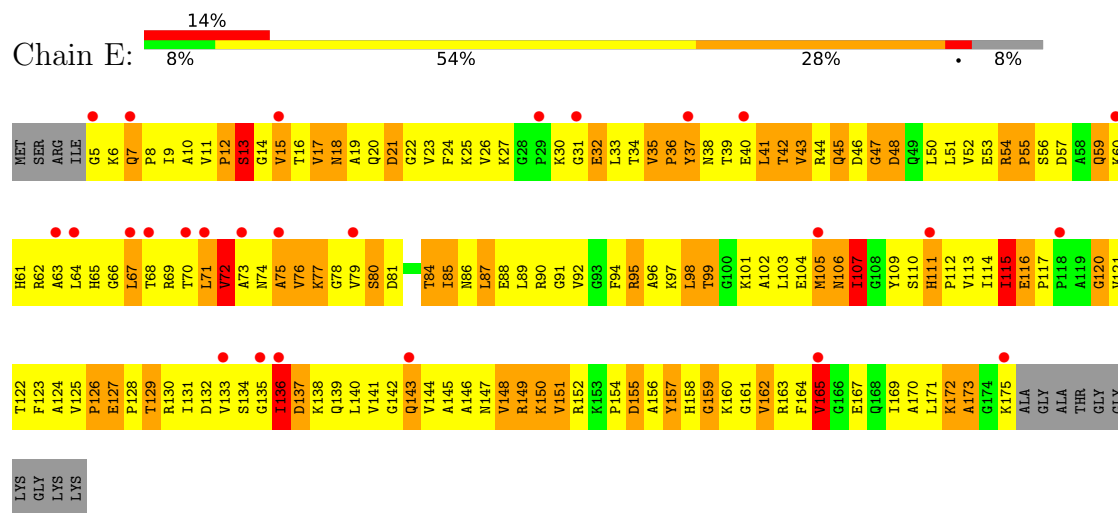




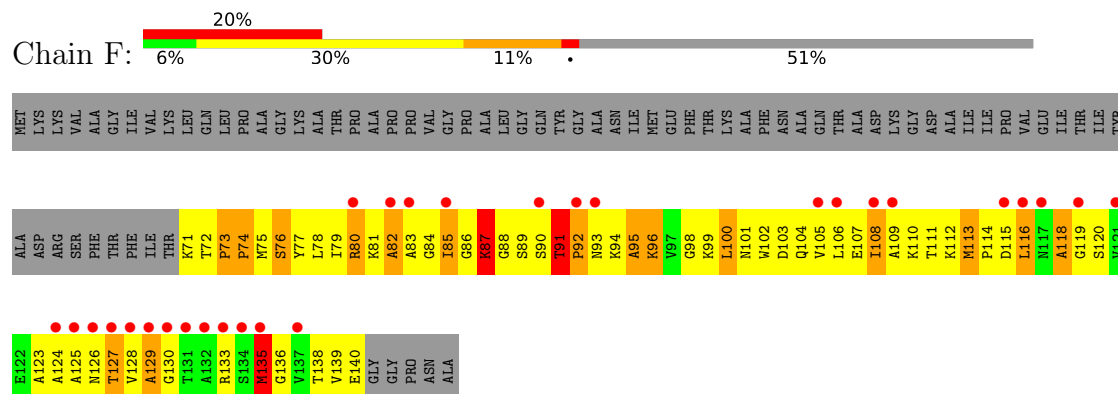
• Molecule 6: 50S ribosomal protein L5



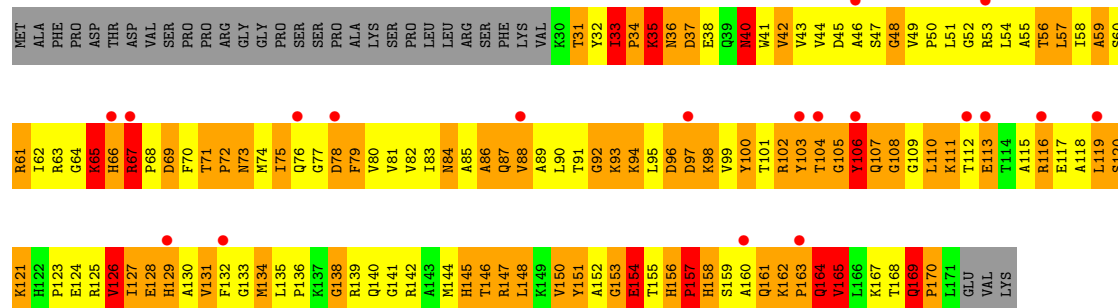
• Molecule 7: 50S ribosomal protein L6



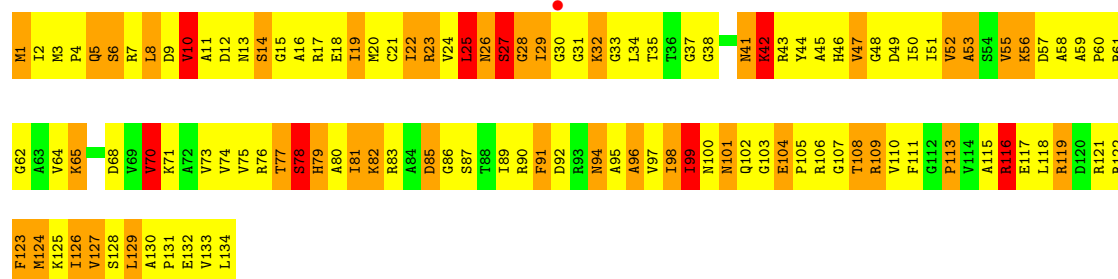
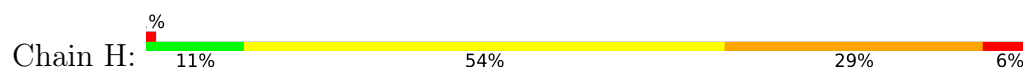
• Molecule 8: 50S ribosomal protein L11



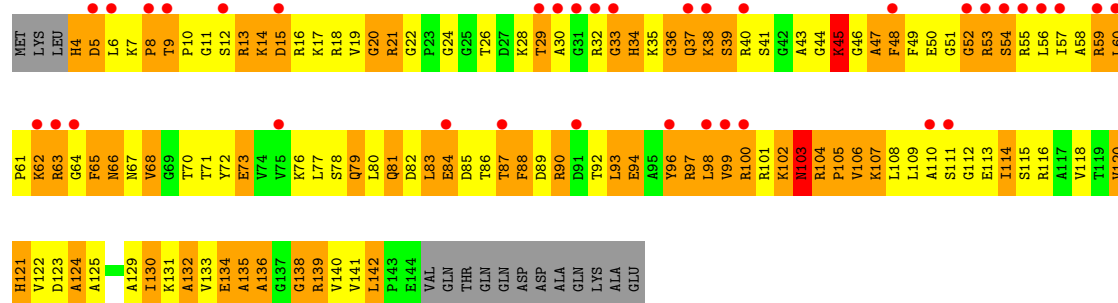
• Molecule 9: 50S ribosomal protein L13



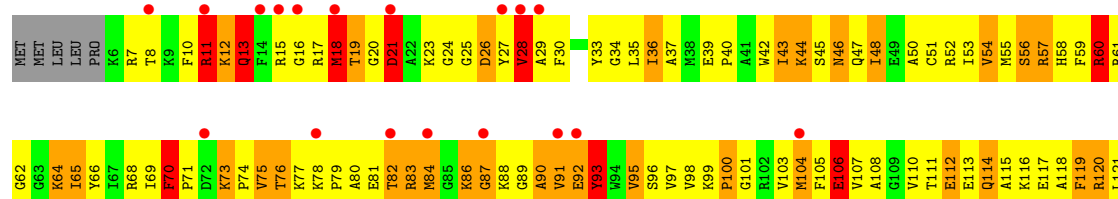
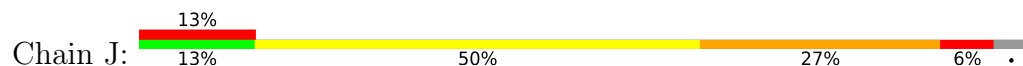
• Molecule 10: 50S ribosomal protein L14

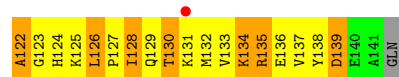


• Molecule 11: 50S ribosomal protein L15

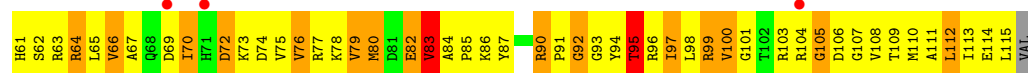
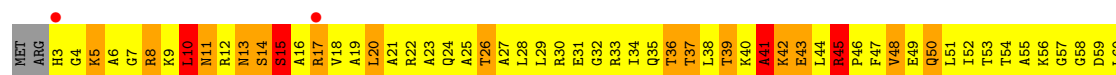
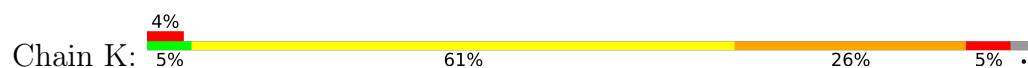


• Molecule 12: 50S ribosomal protein L16

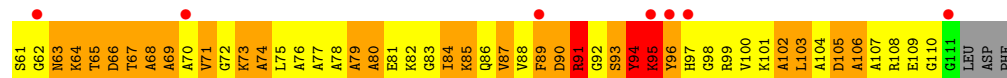
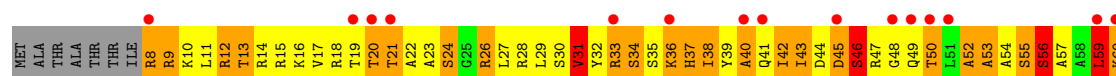




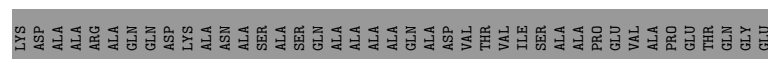
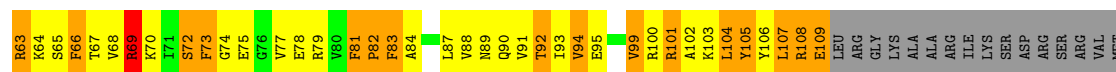
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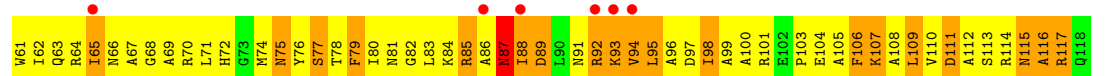
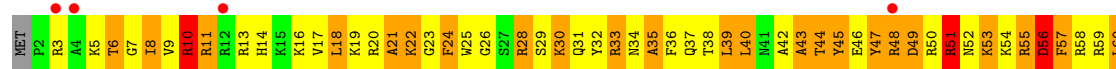
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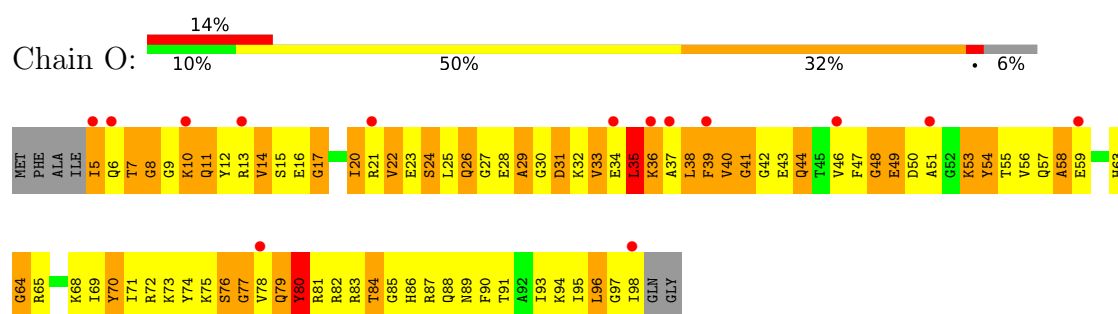
• Molecule 15: 50S ribosomal protein L19



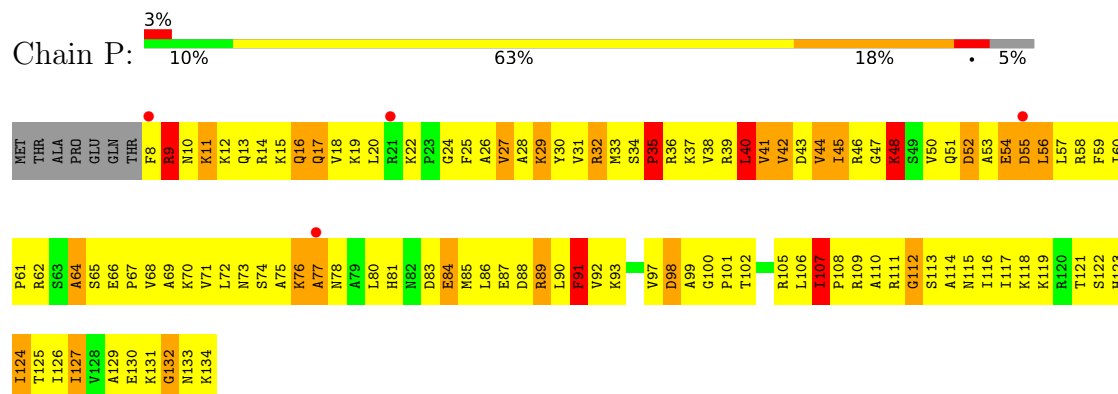
• Molecule 16: 50S ribosomal protein L20



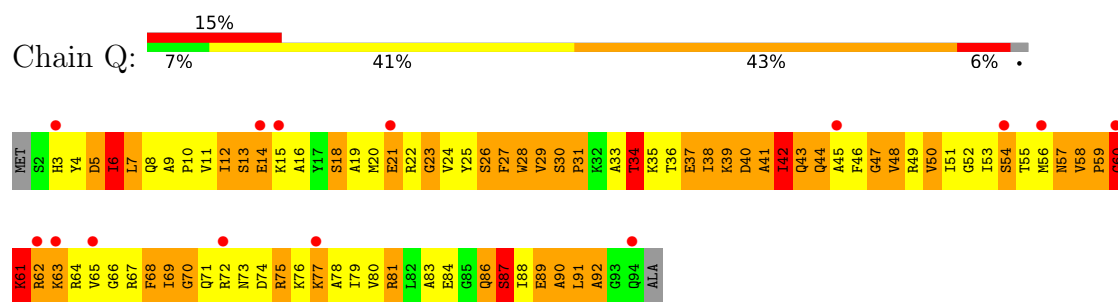
• Molecule 17: 50S ribosomal protein L21



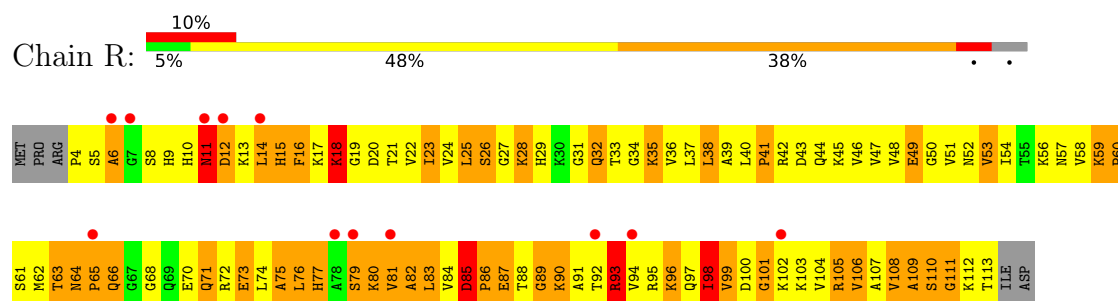
• Molecule 18: 50S ribosomal protein L22



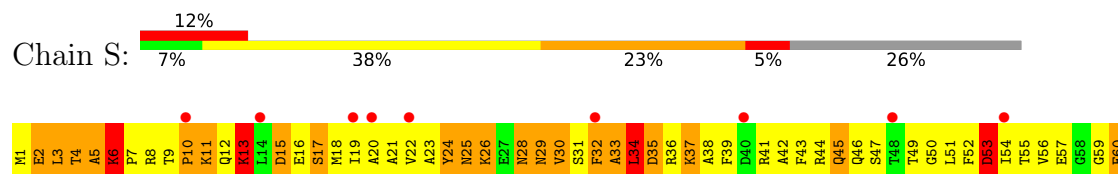
• Molecule 19: 50S ribosomal protein L23

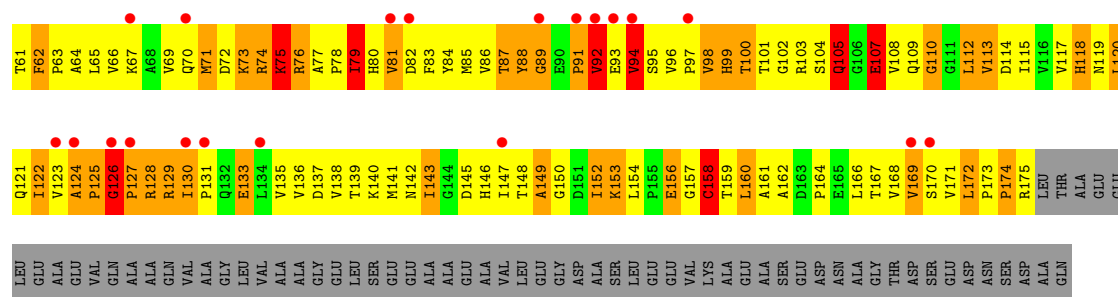


• Molecule 20: 50S ribosomal protein L24

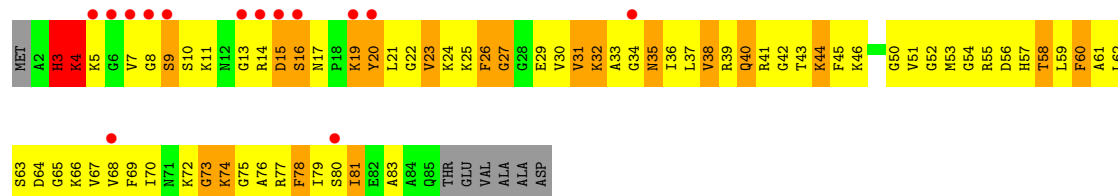
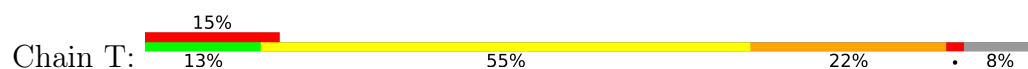


• Molecule 21: 50S ribosomal protein L25

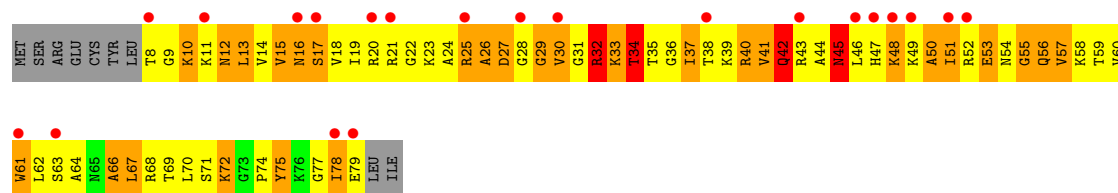




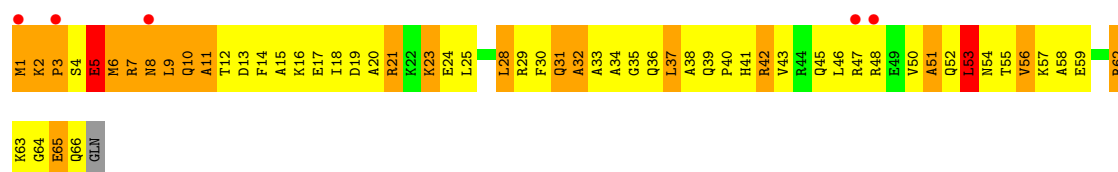
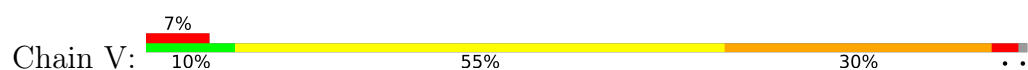
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28



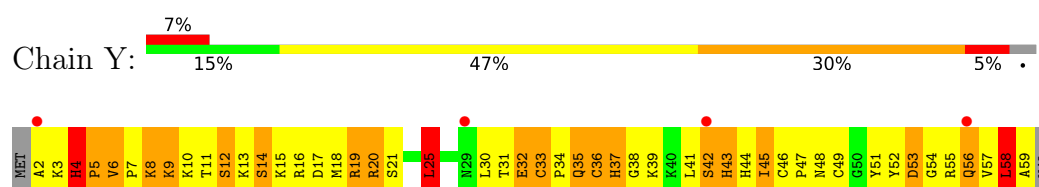
• Molecule 24: 50S ribosomal protein L29



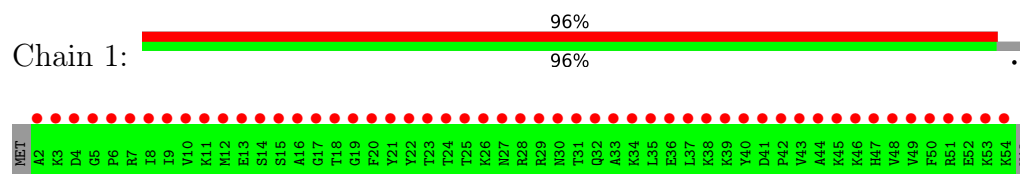
• Molecule 25: 50S ribosomal protein L30



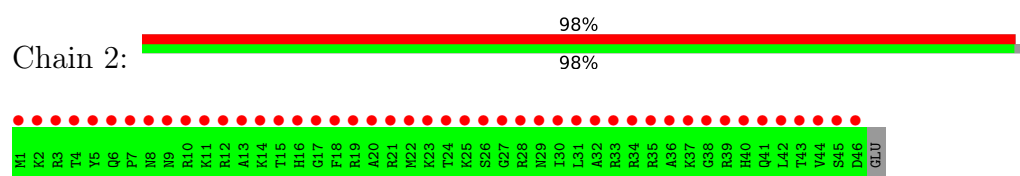
• Molecule 26: 50S ribosomal protein L32



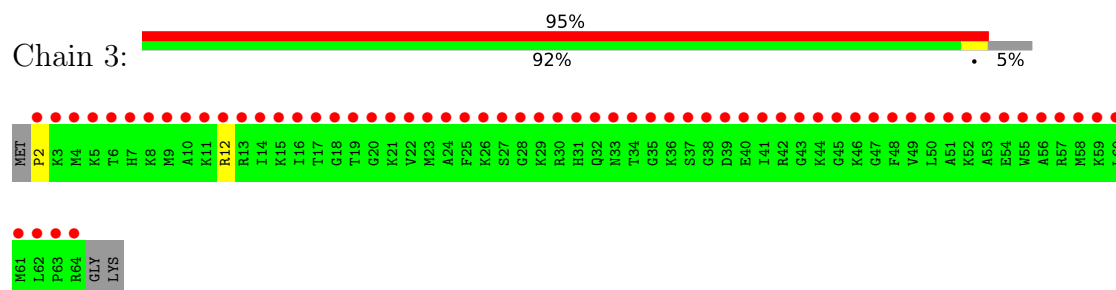
- Molecule 27: 50S ribosomal protein L33



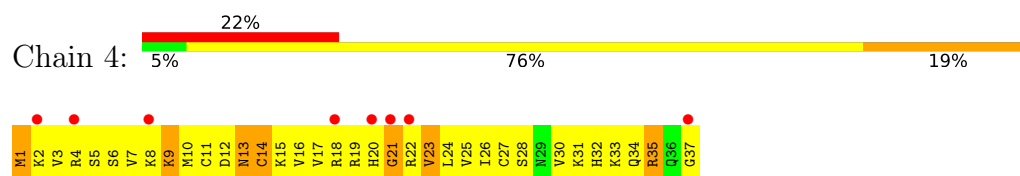
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.70Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.98-3.50) 90.2 (29.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.280 0.267 , 0.307	Depositor DCC
R_{free} test set	15358 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	83657	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: ZLD, MG, ZN

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	X	0.55	3/64561 (0.0%)	0.98	322/100708 (0.3%)
2	Z	0.42	0/2904	0.78	0/4525
3	A	0.79	0/1669	1.37	23/2254 (1.0%)
4	B	1.00	1/1567 (0.1%)	1.46	26/2105 (1.2%)
5	C	0.78	1/1529 (0.1%)	1.32	27/2070 (1.3%)
6	D	0.57	0/1419	1.21	17/1903 (0.9%)
7	E	0.60	0/1308	1.25	21/1771 (1.2%)
8	F	0.69	0/510	1.39	10/688 (1.5%)
9	G	0.78	1/1138 (0.1%)	1.39	23/1539 (1.5%)
10	H	1.03	2/1007 (0.2%)	1.43	18/1352 (1.3%)
11	I	0.84	2/1081 (0.2%)	1.44	18/1448 (1.2%)
12	J	0.82	3/1113 (0.3%)	1.29	17/1486 (1.1%)
13	K	1.16	0/886	1.50	15/1188 (1.3%)
14	L	0.65	0/785	1.18	10/1048 (1.0%)
15	M	0.96	0/884	2.02	30/1186 (2.5%)
16	N	0.81	0/994	1.15	6/1323 (0.5%)
17	O	0.69	0/750	1.27	7/1000 (0.7%)
18	P	0.98	0/1027	1.49	19/1373 (1.4%)
19	Q	0.79	0/737	1.40	15/988 (1.5%)
20	R	0.71	0/835	1.30	11/1121 (1.0%)
21	S	0.63	0/1370	1.26	20/1862 (1.1%)
22	T	0.74	0/633	1.30	9/838 (1.1%)
23	U	0.75	0/556	1.41	10/741 (1.3%)
24	V	0.60	0/537	1.25	6/714 (0.8%)
25	W	0.68	0/426	1.19	4/568 (0.7%)
26	Y	0.96	1/469 (0.2%)	1.52	15/629 (2.4%)
30	4	0.57	0/298	1.13	1/390 (0.3%)
All	All	0.63	14/90993 (0.0%)	1.08	700/136818 (0.5%)

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	X	0	228
2	Z	0	4
9	G	0	1
17	O	0	1
All	All	0	234

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2594	U	P-OP2	14.72	1.78	1.49
1	X	2594	U	P-OP1	-11.28	1.26	1.49
1	X	2592	U	P-OP2	-10.37	1.28	1.49
11	I	29	THR	CA-CB	8.62	1.68	1.53
11	I	29	THR	CA-C	6.28	1.61	1.52

The worst 5 of 700 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	28	ARG	CA-C-N	30.73	158.25	119.84
15	M	28	ARG	C-N-CA	30.73	158.25	119.84
4	B	125	GLY	CA-C-N	12.97	133.84	119.83
4	B	125	GLY	C-N-CA	12.97	133.84	119.83
1	X	2592	U	N1-C1'-C2'	12.78	133.17	114.00

There are no chirality outliers.

5 of 234 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	10	A	Sidechain
1	X	24	G	Sidechain
1	X	25	U	Sidechain
1	X	34	U	Sidechain
1	X	98	U	Sidechain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	4406	0
2	Z	2598	0	1328	214	0
3	A	1637	0	1673	483	0
4	B	1539	0	1600	376	0
5	C	1506	0	1525	414	0
6	D	1400	0	1481	458	0
7	E	1286	0	1336	346	0
8	F	504	0	530	133	0
9	G	1114	0	1144	394	0
10	H	997	0	1046	224	1
11	I	1067	0	1103	340	0
12	J	1090	0	1125	265	0
13	K	878	0	930	172	1
14	L	779	0	820	283	0
15	M	871	0	894	211	0
16	N	978	0	1020	304	0
17	O	741	0	756	244	0
18	P	1014	0	1096	198	0
19	Q	726	0	753	205	0
20	R	825	0	881	277	0
21	S	1345	0	1372	340	0
22	T	625	0	655	146	0
23	U	552	0	604	195	0
24	V	533	0	558	137	0
25	W	424	0	470	108	0
26	Y	457	0	462	88	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	329	86	0
31	M	1	0	0	0	0
31	X	30	0	0	0	0
31	Z	4	0	0	0	0
32	X	24	0	19	22	0
33	4	1	0	0	0	0
33	Y	1	0	0	0	0
All	All	83657	0	54559	10162	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 74.

The worst 5 of 10162 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)
1:X:1281:A:H1'	1:X:2592:U:C5	1.68	1.26
1:X:2198:U:H3'	1:X:2199:C:C4'	1.66	1.24
1:X:2198:U:C3'	1:X:2199:C:H4'	1.68	1.23
1:X:1781:C:OP1	3:A:219:PRO:HB2	1.41	1.20
1:X:1281:A:C1'	1:X:2592:U:H5	1.55	1.20

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)
10:H:107:GLY:O	13:K:86:LYS:NZ[8_555]	2.03	0.17

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 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	
3	A	216/274 (79%)	109 (50%)	52 (24%)	55 (26%)	0	0
4	B	203/211 (96%)	124 (61%)	47 (23%)	32 (16%)	0	2
5	C	195/205 (95%)	92 (47%)	46 (24%)	57 (29%)	0	0
6	D	175/180 (97%)	78 (45%)	54 (31%)	43 (25%)	0	0
7	E	169/185 (91%)	91 (54%)	42 (25%)	36 (21%)	0	1
8	F	68/144 (47%)	37 (54%)	21 (31%)	10 (15%)	0	3
9	G	140/174 (80%)	66 (47%)	32 (23%)	42 (30%)	0	0
10	H	132/134 (98%)	91 (69%)	26 (20%)	15 (11%)	0	5
11	I	139/156 (89%)	51 (37%)	50 (36%)	38 (27%)	0	0
12	J	134/142 (94%)	63 (47%)	46 (34%)	25 (19%)	0	1
13	K	111/116 (96%)	61 (55%)	31 (28%)	19 (17%)	0	2
14	L	102/114 (90%)	48 (47%)	25 (24%)	29 (28%)	0	0
15	M	106/166 (64%)	68 (64%)	17 (16%)	21 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	56 (49%)	30 (26%)	29 (25%)	0	0
17	O	92/100 (92%)	52 (56%)	19 (21%)	21 (23%)	0	1
18	P	125/134 (93%)	75 (60%)	35 (28%)	15 (12%)	0	4
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	63 (58%)	17 (16%)	28 (26%)	0	0
21	S	173/237 (73%)	97 (56%)	40 (23%)	36 (21%)	0	1
22	T	82/91 (90%)	51 (62%)	16 (20%)	15 (18%)	0	1
23	U	70/81 (86%)	39 (56%)	15 (21%)	16 (23%)	0	1
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	1
25	W	53/55 (96%)	22 (42%)	18 (34%)	13 (24%)	0	0
26	Y	56/60 (93%)	31 (55%)	17 (30%)	8 (14%)	0	3
30	4	35/37 (95%)	22 (63%)	11 (31%)	2 (6%)	1	13
All	All	2954/3391 (87%)	1563 (53%)	749 (25%)	642 (22%)	0	1

5 of 642 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	58	HIS
3	A	66	ASP
3	A	91	ARG
3	A	98	ALA

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	
3	A	164/215 (76%)	126 (77%)	38 (23%)	1	5
4	B	155/157 (99%)	130 (84%)	25 (16%)	2	14
5	C	157/163 (96%)	126 (80%)	31 (20%)	1	8
6	D	153/156 (98%)	136 (89%)	17 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	119 (88%)	17 (12%)	4	22
8	F	53/107 (50%)	48 (91%)	5 (9%)	8	31
9	G	118/146 (81%)	91 (77%)	27 (23%)	1	5
10	H	103/103 (100%)	79 (77%)	24 (23%)	1	5
11	I	108/121 (89%)	91 (84%)	17 (16%)	2	15
12	J	110/116 (95%)	91 (83%)	19 (17%)	2	11
13	K	90/93 (97%)	69 (77%)	21 (23%)	1	5
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	2
15	M	94/134 (70%)	79 (84%)	15 (16%)	2	14
16	N	96/97 (99%)	80 (83%)	16 (17%)	2	13
17	O	75/79 (95%)	67 (89%)	8 (11%)	6	27
18	P	109/115 (95%)	92 (84%)	17 (16%)	2	15
19	Q	75/76 (99%)	58 (77%)	17 (23%)	1	5
20	R	91/96 (95%)	73 (80%)	18 (20%)	1	7
21	S	149/192 (78%)	118 (79%)	31 (21%)	1	6
22	T	62/67 (92%)	55 (89%)	7 (11%)	5	25
23	U	57/66 (86%)	45 (79%)	12 (21%)	1	6
24	V	54/55 (98%)	45 (83%)	9 (17%)	2	13
25	W	48/48 (100%)	36 (75%)	12 (25%)	0	4
26	Y	51/53 (96%)	42 (82%)	9 (18%)	2	11
30	4	35/35 (100%)	30 (86%)	5 (14%)	3	18
All	All	2417/2716 (89%)	1977 (82%)	440 (18%)	2	10

5 of 440 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	K	64	ARG
16	N	56	ASP
30	4	23	VAL
23	U	42	GLN
13	K	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	34	ASN
20	R	32	GLN
16	N	41	ASN
18	P	16	GLN
21	S	28	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	690 (25%)	283 (10%)
2	Z	121/123 (98%)	24 (19%)	0
All	All	2801/3003 (93%)	714 (25%)	283 (10%)

5 of 714 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	14	A
1	X	27	G
1	X	34	U
1	X	35	G

5 of 283 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2324	G
1	X	2418	A
1	X	2624	G
1	X	995	A
1	X	984	A

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

Of 38 ligands modelled in this entry, 37 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
32	ZLD	X	2911	-	26,26,26	1.23	2 (7%)	36,36,36	2.77	10 (27%)

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
32	ZLD	X	2911	-	-	8/13/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2911	ZLD	O10-C7	3.30	1.40	1.35
32	X	2911	ZLD	C5-C16	2.08	1.41	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2911	ZLD	C6-C8-C9	8.84	123.40	113.38
32	X	2911	ZLD	O10-C8-C9	7.74	117.90	109.13
32	X	2911	ZLD	C2-N4-C7	-6.42	119.25	125.98
32	X	2911	ZLD	O15-C7-N4	4.35	132.83	128.80
32	X	2911	ZLD	O10-C7-N4	-4.00	106.55	109.92

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2911	ZLD	C5-C2-N4-C7

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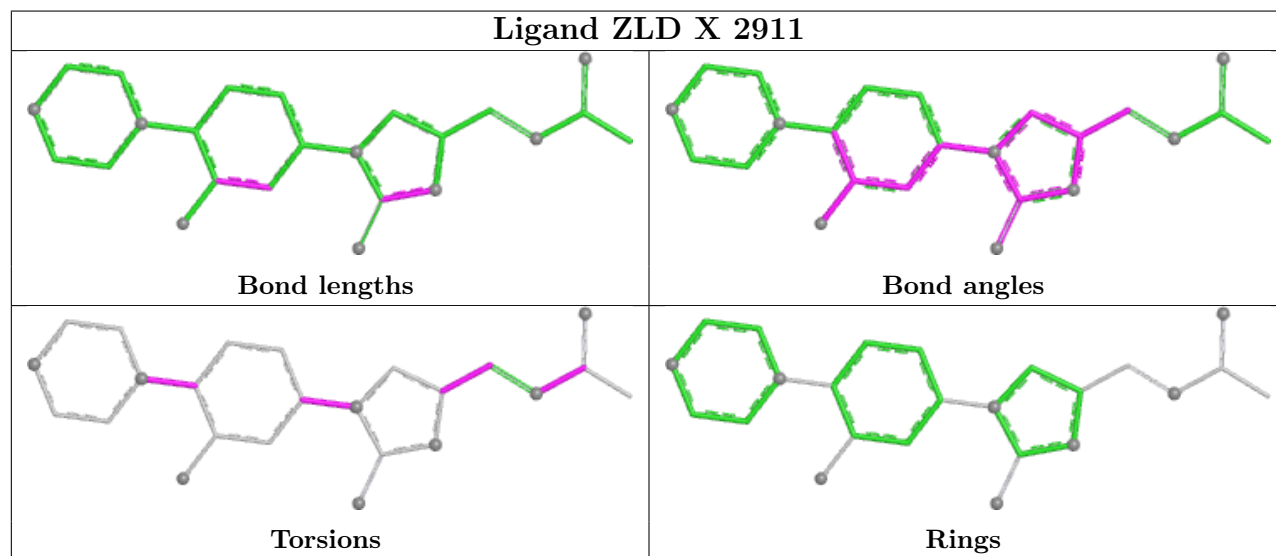
Mol	Chain	Res	Type	Atoms
32	X	2911	ZLD	C1-C2-N4-C7
32	X	2911	ZLD	C6-C8-C9-N11
32	X	2911	ZLD	O10-C8-C9-N11
32	X	2911	ZLD	C13-C12-N11-C9

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2911	ZLD	22	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	2686/2880 (93%)	1.46	676 (25%) 1 2	1, 35, 97, 115	0
2	Z	122/123 (99%)	1.99	56 (45%) 0 1	28, 74, 94, 101	0
3	A	218/274 (79%)	1.27	37 (16%) 4 4	8, 44, 57, 63	0
4	B	205/211 (97%)	0.31	8 (3%) 43 23	1, 12, 35, 53	0
5	C	197/205 (96%)	0.82	20 (10%) 12 8	2, 45, 62, 78	0
6	D	177/180 (98%)	1.27	38 (21%) 2 3	54, 65, 73, 76	0
7	E	171/185 (92%)	1.09	26 (15%) 5 5	38, 59, 72, 76	0
8	F	70/144 (48%)	2.07	29 (41%) 0 1	62, 71, 75, 76	0
9	G	142/174 (81%)	0.87	19 (13%) 7 6	19, 37, 53, 57	0
10	H	134/134 (100%)	0.32	1 (0%) 84 63	1, 8, 30, 42	0
11	I	141/156 (90%)	1.49	36 (25%) 1 2	10, 54, 69, 84	0
12	J	136/142 (95%)	0.93	19 (13%) 6 5	25, 44, 59, 66	0
13	K	113/116 (97%)	0.40	5 (4%) 39 21	1, 2, 13, 23	0
14	L	104/114 (91%)	1.18	22 (21%) 2 3	38, 54, 61, 67	0
15	M	108/166 (65%)	0.36	1 (0%) 81 58	1, 11, 40, 46	0
16	N	117/118 (99%)	0.74	10 (8%) 16 11	2, 32, 55, 64	0
17	O	94/100 (94%)	0.82	14 (14%) 5 5	13, 46, 63, 66	0
18	P	127/134 (94%)	0.33	4 (3%) 51 29	1, 10, 40, 57	0
19	Q	93/95 (97%)	0.95	14 (15%) 5 5	23, 36, 60, 63	0
20	R	110/115 (95%)	0.88	12 (10%) 10 7	32, 44, 66, 70	0
21	S	175/237 (73%)	1.16	29 (16%) 4 4	53, 62, 72, 79	0
22	T	84/91 (92%)	1.11	14 (16%) 4 4	23, 47, 66, 69	0
23	U	72/81 (88%)	1.43	21 (29%) 1 1	39, 52, 63, 64	0
24	V	66/67 (98%)	0.54	5 (7%) 20 13	34, 52, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.63	3 (5%) 30 18	32, 41, 57, 66	0
26	Y	58/60 (96%)	0.45	4 (6%) 23 14	1, 7, 32, 34	0
27	1	53/55 (96%)	13.62	53 (100%) 0 0	33, 47, 62, 65	0
28	2	46/47 (97%)	11.97	46 (100%) 0 0	1, 12, 25, 35	0
29	3	63/66 (95%)	12.77	63 (100%) 0 0	23, 34, 43, 50	0
30	4	37/37 (100%)	1.42	8 (21%) 2 3	52, 65, 72, 73	0
All	All	5974/6562 (91%)	1.50	1293 (21%) 2 3	1, 41, 84, 115	0

The worst 5 of 1293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	64	ARG	36.4
27	1	7	ARG	32.5
27	1	5	GLY	27.9
29	3	51	ALA	24.1
27	1	6	PRO	23.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

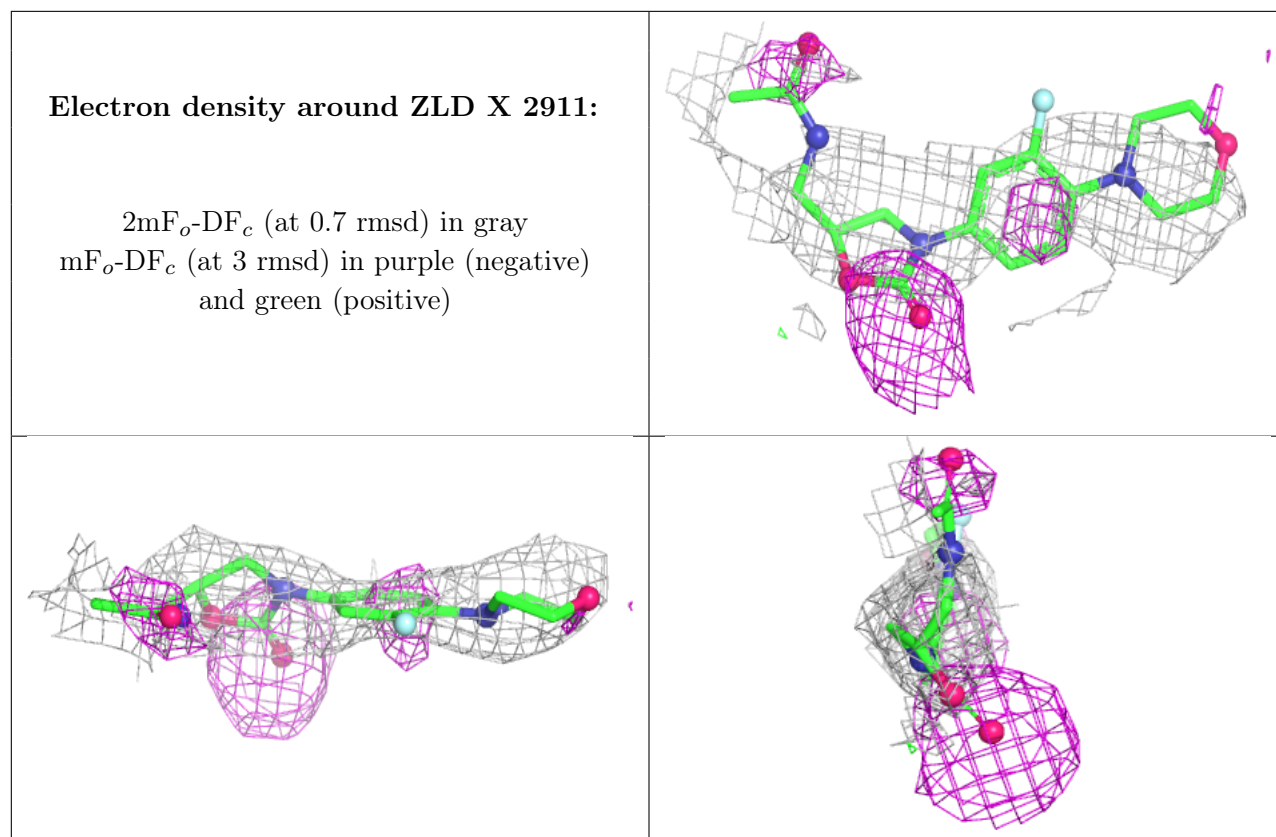
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2902	1/1	0.56	0.81	61,61,61,61	0
31	MG	X	2897	1/1	0.62	0.26	1,1,1,1	0
32	ZLD	X	2911	24/24	0.63	0.23	28,31,37,37	0
31	MG	M	167	1/1	0.67	0.56	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	2908	1/1	0.70	0.47	48,48,48,48	0
31	MG	X	2907	1/1	0.73	0.53	1,1,1,1	0
31	MG	X	2887	1/1	0.75	0.25	37,37,37,37	0
31	MG	X	2898	1/1	0.78	0.48	1,1,1,1	0
31	MG	X	2882	1/1	0.80	0.46	49,49,49,49	0
31	MG	X	2886	1/1	0.80	0.28	15,15,15,15	0
31	MG	X	2881	1/1	0.82	0.20	10,10,10,10	0
31	MG	X	2900	1/1	0.83	0.44	1,1,1,1	0
31	MG	X	2885	1/1	0.83	0.31	45,45,45,45	0
31	MG	X	2889	1/1	0.83	0.38	1,1,1,1	0
31	MG	X	2890	1/1	0.85	0.39	1,1,1,1	0
31	MG	X	2883	1/1	0.86	0.55	1,1,1,1	0
31	MG	Z	126	1/1	0.88	0.16	12,12,12,12	0
31	MG	X	2895	1/1	0.88	0.44	1,1,1,1	0
31	MG	X	2905	1/1	0.88	0.41	18,18,18,18	0
31	MG	X	2899	1/1	0.89	0.35	1,1,1,1	0
31	MG	Z	127	1/1	0.89	0.23	3,3,3,3	0
31	MG	X	2909	1/1	0.90	0.38	1,1,1,1	0
31	MG	X	2904	1/1	0.93	0.42	1,1,1,1	0
31	MG	X	2896	1/1	0.93	0.34	1,1,1,1	0
31	MG	X	2888	1/1	0.93	0.28	1,1,1,1	0
33	ZN	Y	61	1/1	0.93	0.20	89,89,89,89	0
31	MG	Z	124	1/1	0.94	0.22	11,11,11,11	0
31	MG	X	2906	1/1	0.94	0.13	40,40,40,40	0
31	MG	X	2891	1/1	0.94	0.22	23,23,23,23	0
31	MG	X	2901	1/1	0.95	0.36	1,1,1,1	0
31	MG	X	2903	1/1	0.95	0.31	1,1,1,1	0
31	MG	X	2910	1/1	0.95	0.53	14,14,14,14	0
33	ZN	4	38	1/1	0.95	0.05	78,78,78,78	0
31	MG	X	2893	1/1	0.96	0.17	3,3,3,3	0
31	MG	X	2884	1/1	0.96	0.09	19,19,19,19	0
31	MG	Z	125	1/1	0.96	0.26	1,1,1,1	0
31	MG	X	2892	1/1	0.97	0.20	1,1,1,1	0
31	MG	X	2894	1/1	0.97	0.25	2,2,2,2	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.