wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 05:18 am GMT

PDB ID	:	4WFN
Title	:	Crystal structure of the large ribosomal subunit (50S) of Deinococcus radiodurans containing a three residue insertion in L22 in complex with erythromycin
Authors	:	Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on	:	2014-09-16
Resolution	:	3.54 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 (i) 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 (i)) were used in the production of this report:

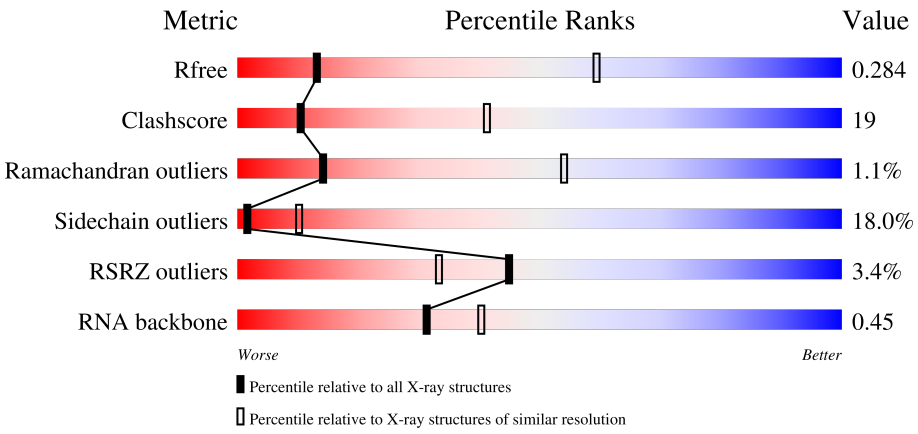
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

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 <=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	A	275	.% 40% 45% 10% 5%
2	B	211	2% 45% 43% 10% •
3	C	205	4% 42% 44% 8% 5%
4	D	180	6% 48% 46% 5% •

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Mol	Chain	Length	Quality of chain
5	E	185	2%, 52%, 35%, 5%, 8%
6	G	174	5%, 40%, 32%, 10%, 18%
7	H	134	%, 49%, 43%, 7%
8	I	156	3%, 42%, 35%, 9%, 14%
9	J	141	3%, 46%, 39%, 11%
10	K	116	43%, 45%, 9%
11	L	114	5%, 55%, 28%, 8%, 9%
12	M	165	29%, 27%, 9%, 35%
13	N	118	2%, 47%, 44%, 7%
14	O	100	4%, 42%, 45%, 7%, 6%
15	P	137	30%, 50%, 15%, 5%
16	Q	95	%, 52%, 35%, 11%
17	R	115	3%, 38%, 46%, 11%
18	S	237	8%, 51%, 19%, 26%
19	T	91	5%, 41%, 34%, 5%, 19%
20	U	81	5%, 35%, 43%, 11%, 11%
21	V	67	3%, 60%, 31%, 6%
22	W	55	51%, 44%, 5%
23	Z	60	42%, 47%, 5%, 7%
24	1	55	9%, 31%, 47%, 18%
25	2	47	2%, 26%, 53%, 17%
26	3	65	8%, 31%, 49%, 11%, 9%
27	X	2880	3%, 33%, 43%, 15%, 7%
28	Y	124	3%, 42%, 40%, 16%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	B	301	-	-	-	X
29	MG	K	202	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 84117 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1987	1235	399	350	3	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	194	1481	920	284	275	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	I	134	1011	619	206	186	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	P	130	1038	655	205	176	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	T	74	556	351	107	97	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	V	65	525	322	106	95	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	Z	56	443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	1	53	431	274	80	76	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	2	46	383	230	91	60	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	3	59	462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	X	2680	57533	25663	10626	18564	2680	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

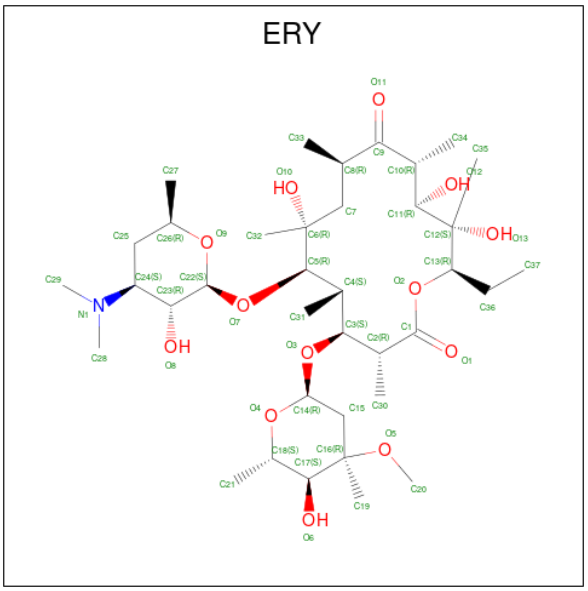
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
28	Y	122	2601	1161	476	842	122	0	0	0

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
29	A	1	1	1	0	0
29	B	1	1	1	0	0
29	K	2	2	2	0	0
29	M	2	2	2	0	0
29	X	64	64	64	0	0

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



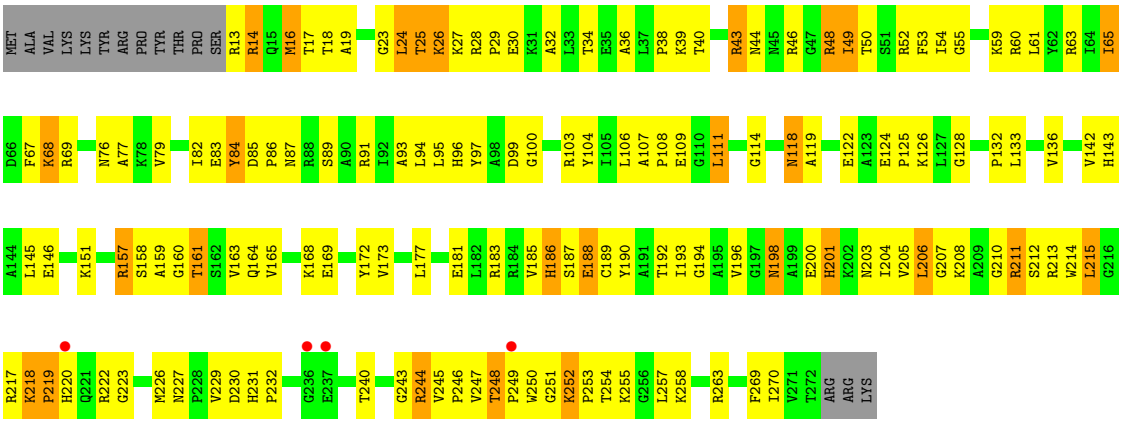
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
30	X	1	51	37	1	13	0	0

3 Residue-property plots (i)

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

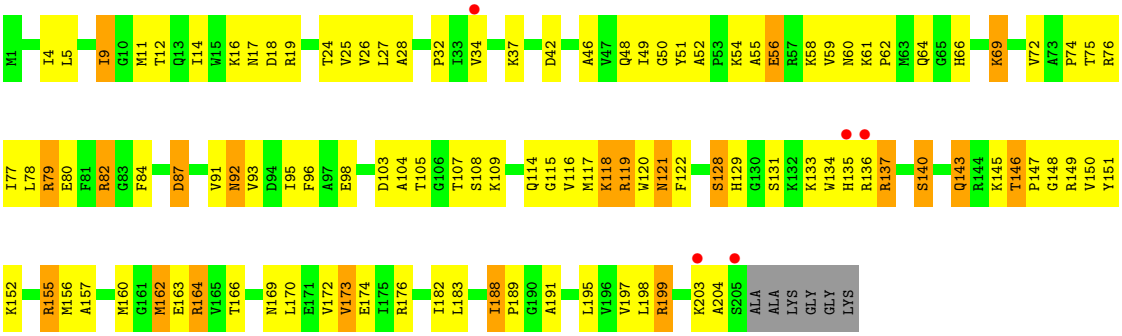
• Molecule 1: 50S ribosomal protein L2

Chain A:



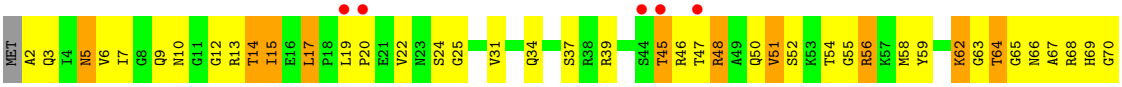
• Molecule 2: 50S ribosomal protein L3

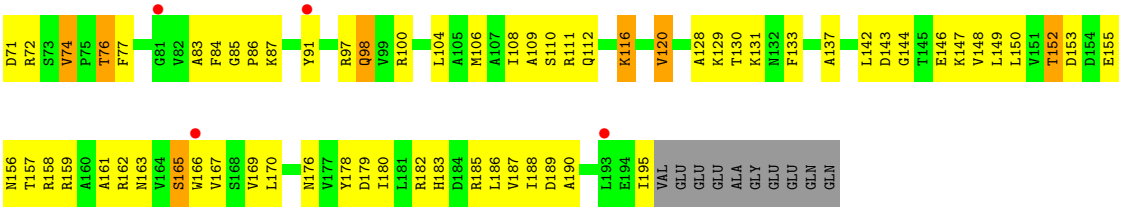
Chain B:



• Molecule 3: 50S ribosomal protein L4

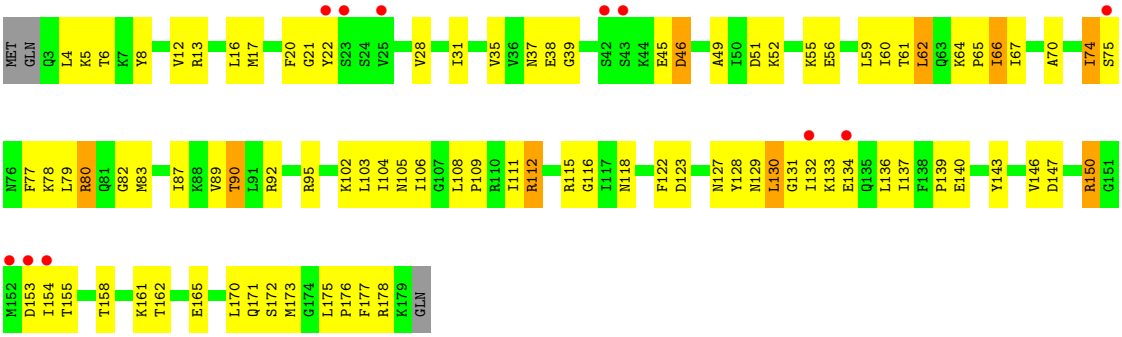
Chain C:





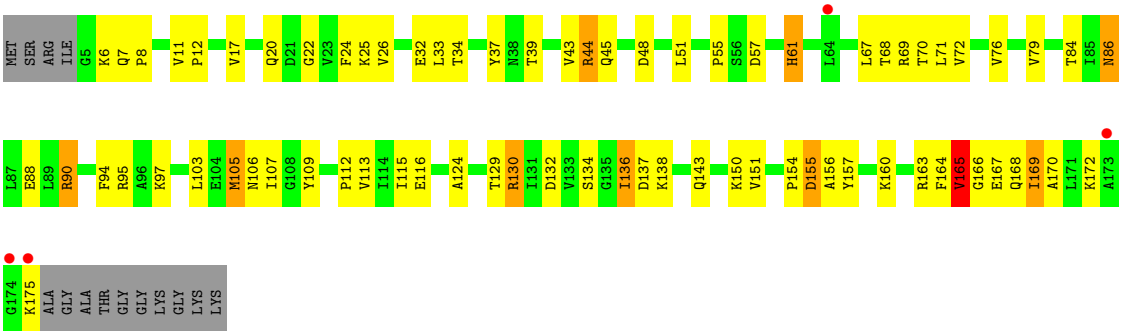
- Molecule 4: 50S ribosomal protein L5

Chain D:



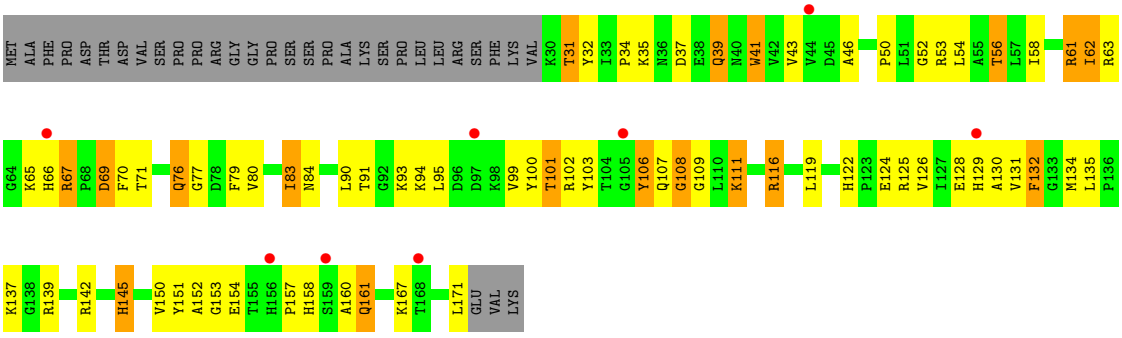
- Molecule 5: 50S ribosomal protein L6

Chain E:



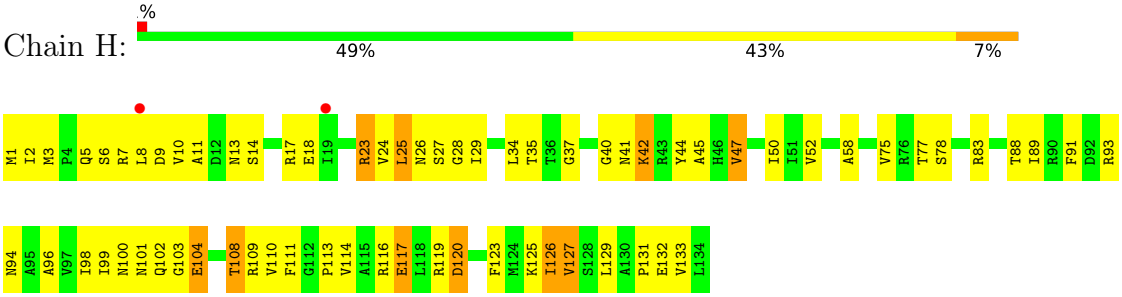
- Molecule 6: 50S ribosomal protein L13

Chain G:



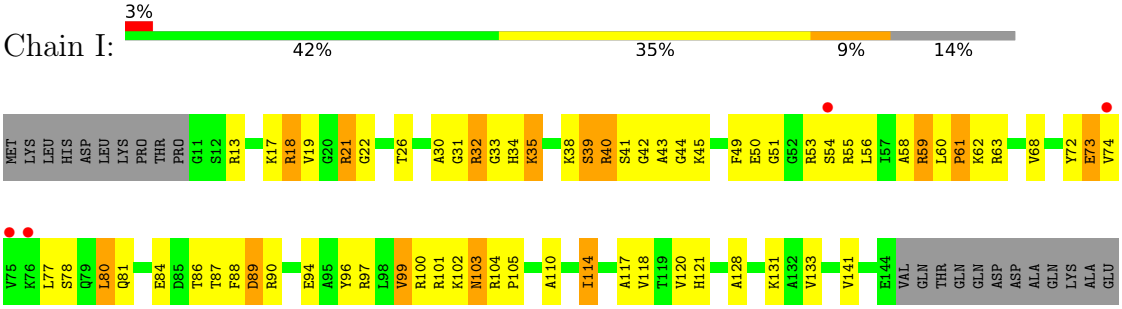
- Molecule 7: 50S ribosomal protein L14

Chain H:



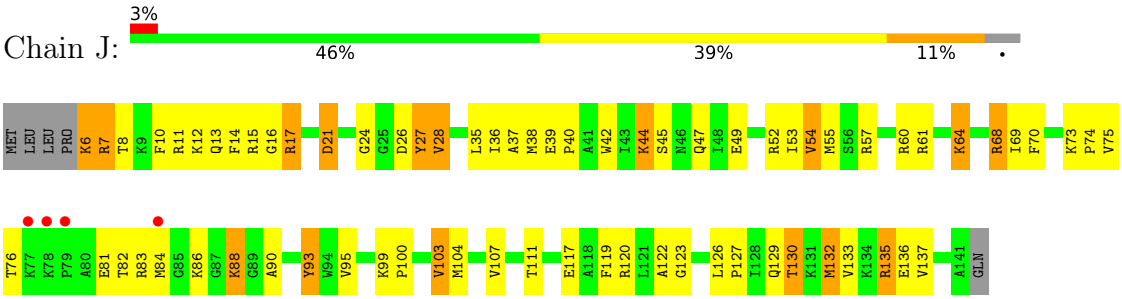
- Molecule 8: 50S ribosomal protein L15

Chain I:



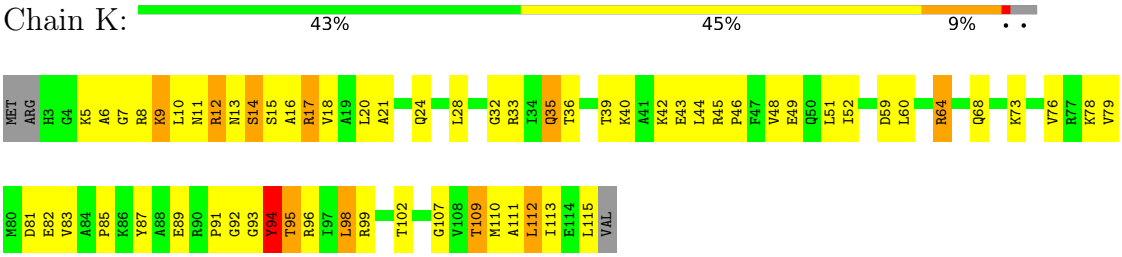
- Molecule 9: 50S ribosomal protein L16

Chain J:



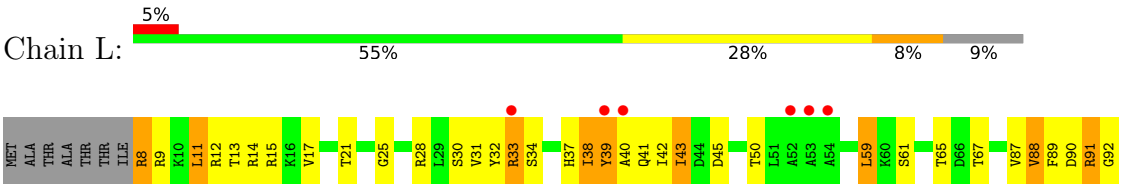
- Molecule 10: 50S ribosomal protein L17

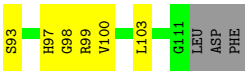
Chain K:



- Molecule 11: 50S ribosomal protein L18

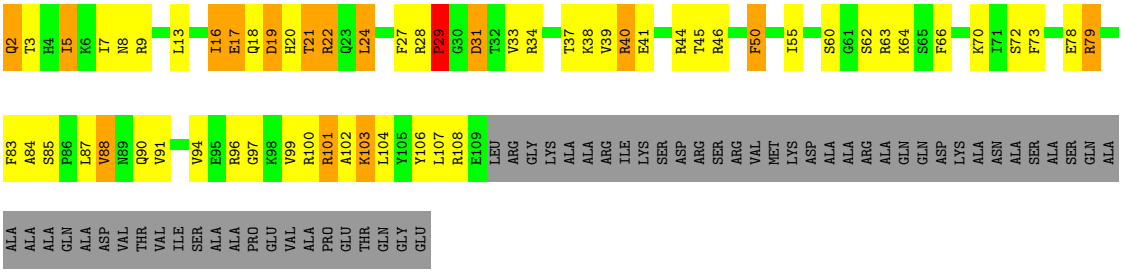
Chain L:





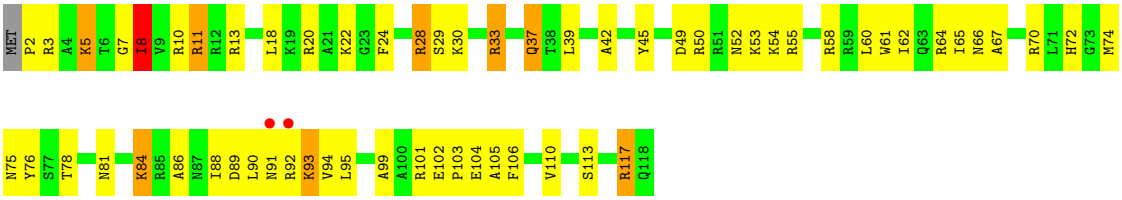
- Molecule 12: 50S ribosomal protein L19

Chain M:



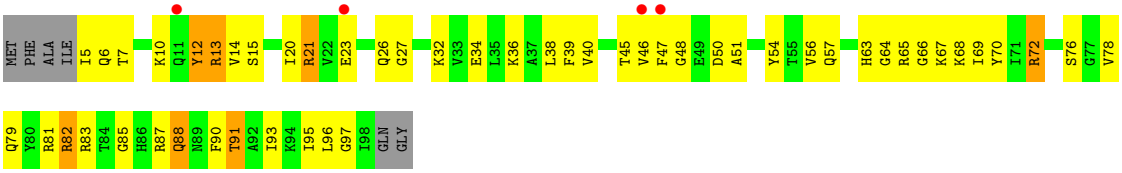
- Molecule 13: 50S ribosomal protein L20

Chain N:



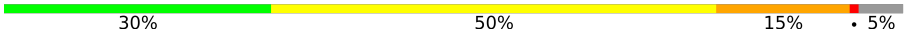
- Molecule 14: 50S ribosomal protein L21

Chain O:



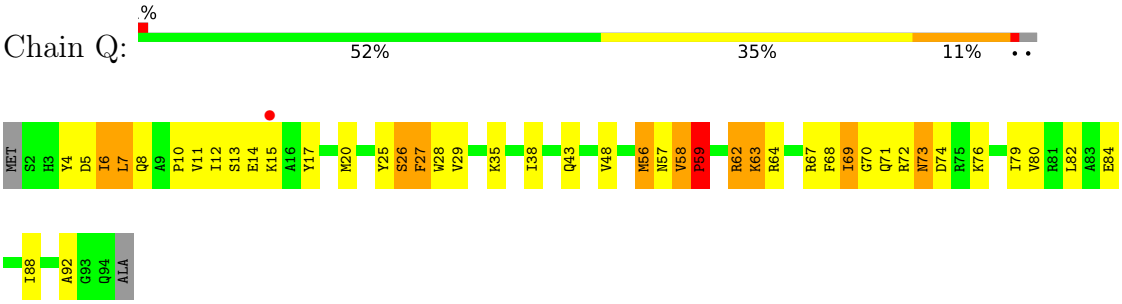
- Molecule 15: 50S ribosomal protein L22,50S ribosomal protein L22

Chain P:



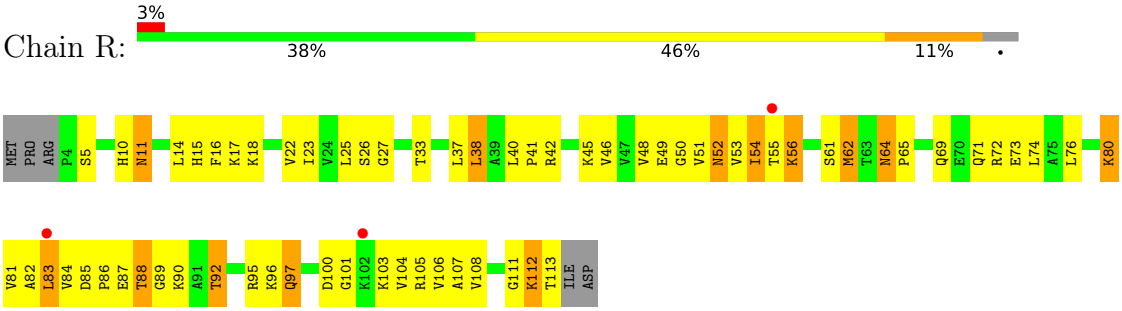
- Molecule 16: 50S ribosomal protein L23

Chain Q:



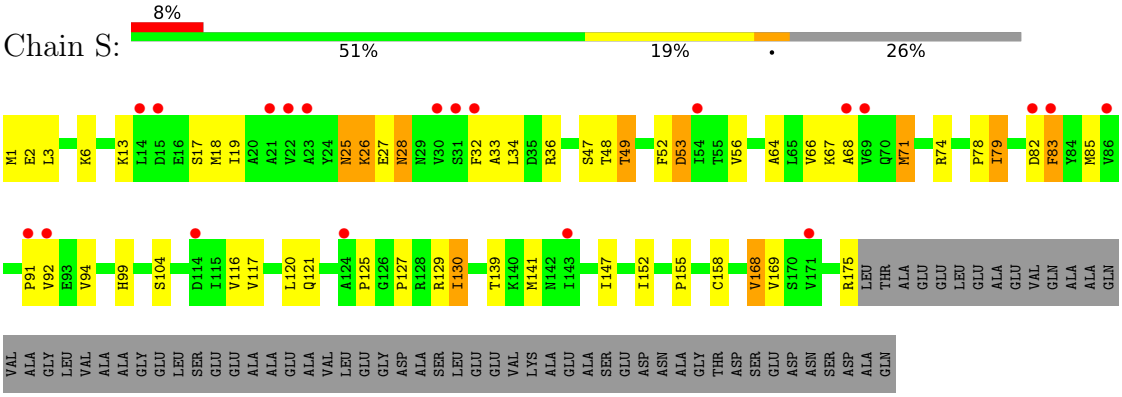
• Molecule 17: 50S ribosomal protein L24

Chain R:



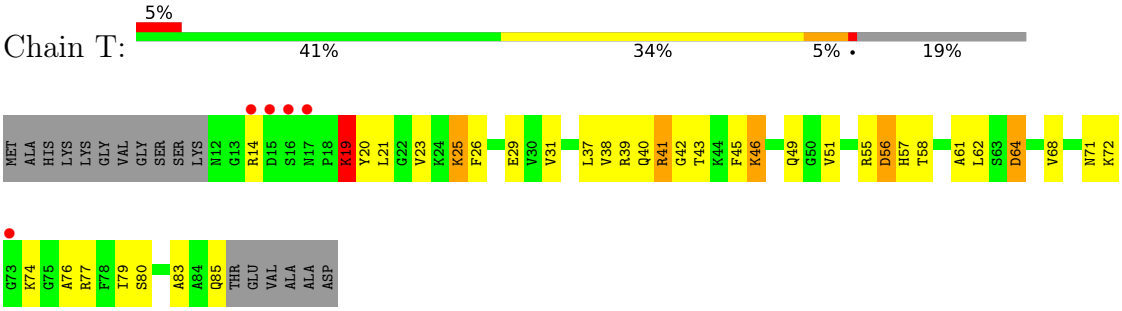
• Molecule 18: 50S ribosomal protein L25

Chain S:



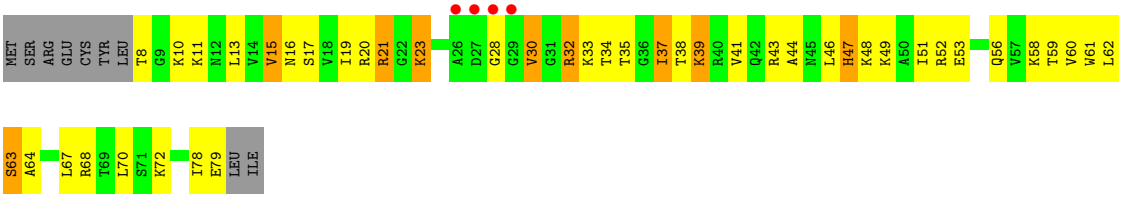
• Molecule 19: 50S ribosomal protein L27

Chain T:



• Molecule 20: 50S ribosomal protein L28

Chain U:

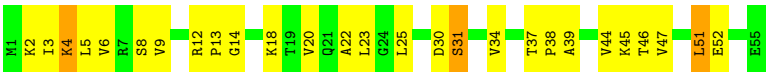


• Molecule 21: 50S ribosomal protein L29

Chain V:

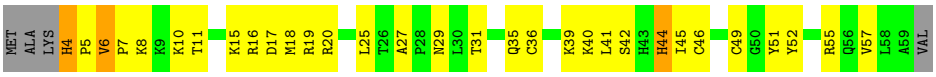
• Molecule 22: 50S ribosomal protein L30

Chain W:



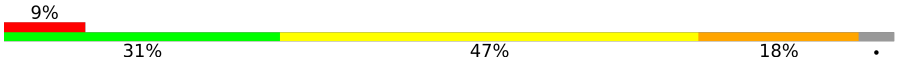
• Molecule 23: 50S ribosomal protein L32

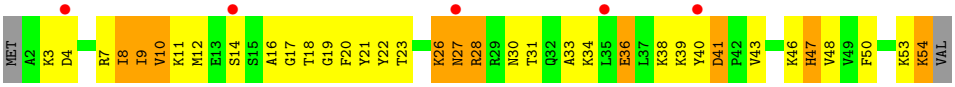
Chain Z:



• Molecule 24: 50S ribosomal protein L33

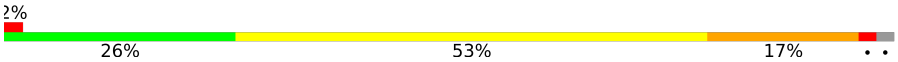
Chain 1:

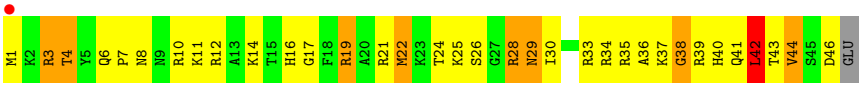




• Molecule 25: 50S ribosomal protein L34

Chain 2:



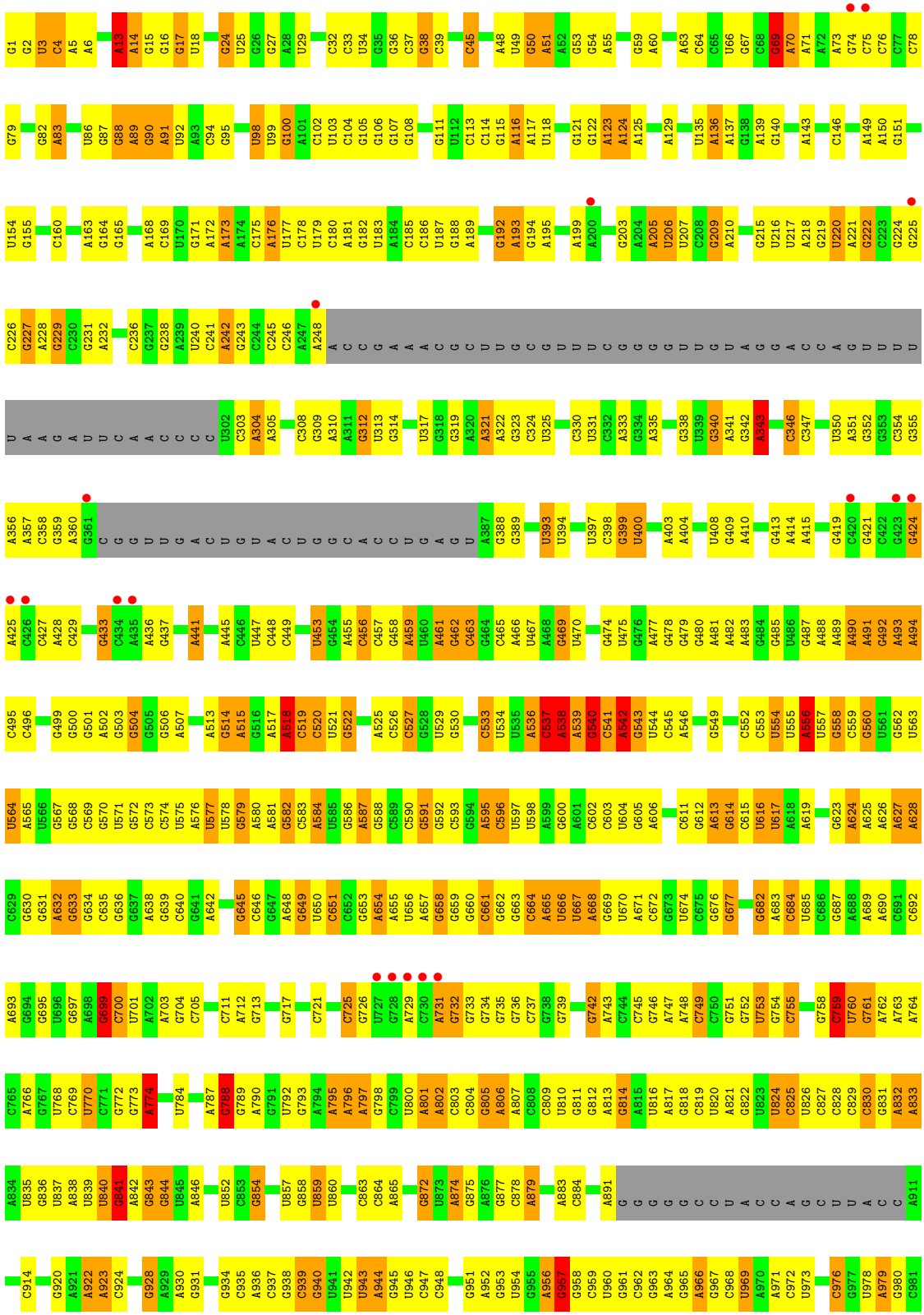


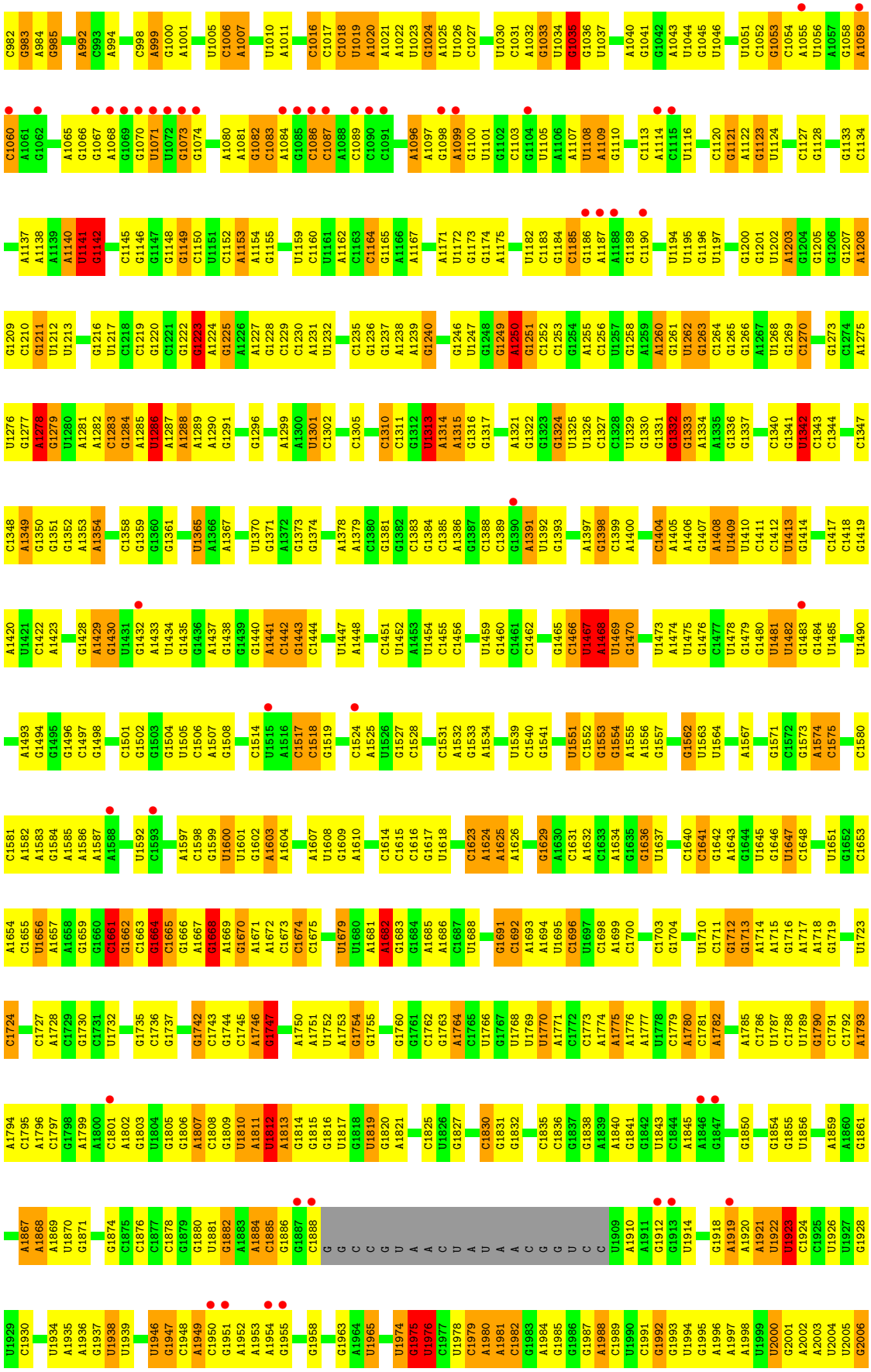
• Molecule 26: 50S ribosomal protein L35

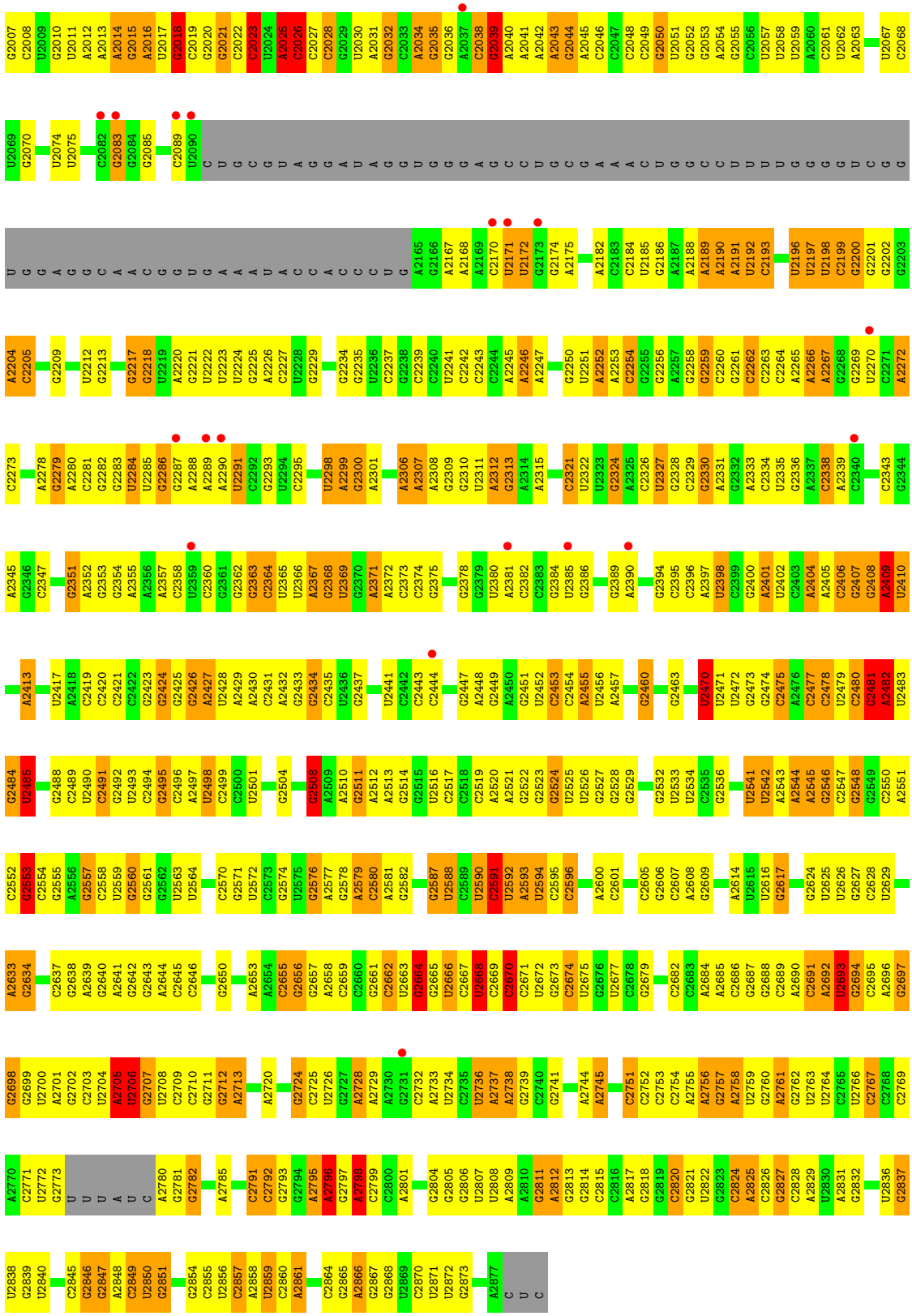
Chain 3:

- Molecule 27: 23S ribosomal RNA

Chain X: 3% 33% 43% 15% • 7%

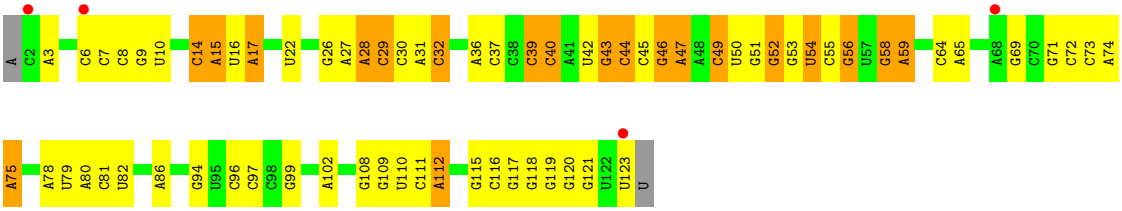






- Molecule 28: 5S ribosomal RNA

Chain Y:


A
C2
A3
C6
C7
C8
G9
U10
C14
A15
U16
A17
U22
G26
A27
A28
C29
C30
A31
C32
A36
C37
C38
C39
C40
A41
U42
G43
C44
C45
G46
A47
A48
C49
U50
G51
G52
G53
U54
C55
G56
U57
G58
A59
C64
A65
A68
G69
C70
G71
C72
C73
A74

A75
A78
U79
A80
C81
U82
A86
G94
U95
C96
C97
C98
G99
A102
G108
G109
U110
C111
A112
G115
C116
G117
G118
G119
G120
G121
U122
U123
U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.282 0.235 , 0.284	Depositor DCC
R_{free} test set	13533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	84117	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A	0.43	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.40	0/2907	0.96	1/4529 (0.0%)
All	All	0.58	3/91554 (0.0%)	1.11	433/137514 (0.3%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

The worst 5 of 433 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1344	0
28	Y	2601	0	1327	62	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84117	0	55290	2467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 2467 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)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	13 52
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	29 68
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	15 55
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	25 65
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	25 65
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100 100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	19 60
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	4 33
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100 100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	17 58
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100 100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	17 58
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	9 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	4	32
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	4	31
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	17	58
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	11	48
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	18
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	1	17
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	8	43
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	14	54

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	A	202/216 (94%)	163 (81%)	39 (19%)	1	8
2	B	155/157 (99%)	127 (82%)	28 (18%)	1	10
3	C	154/163 (94%)	131 (85%)	23 (15%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	153/156 (98%)	140 (92%)	13 (8%)	10	40
5	E	136/144 (94%)	115 (85%)	21 (15%)	2	18
6	G	118/146 (81%)	93 (79%)	25 (21%)	1	6
7	H	103/103 (100%)	88 (85%)	15 (15%)	3	19
8	I	101/121 (84%)	82 (81%)	19 (19%)	1	9
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	7
10	K	90/93 (97%)	70 (78%)	20 (22%)	1	5
11	L	74/82 (90%)	57 (77%)	17 (23%)	1	5
12	M	94/133 (71%)	71 (76%)	23 (24%)	0	4
13	N	96/97 (99%)	81 (84%)	15 (16%)	2	17
14	O	75/79 (95%)	61 (81%)	14 (19%)	1	9
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	5
16	Q	75/76 (99%)	61 (81%)	14 (19%)	1	9
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	7
18	S	149/192 (78%)	135 (91%)	14 (9%)	8	37
19	T	55/67 (82%)	44 (80%)	11 (20%)	1	8
20	U	57/66 (86%)	45 (79%)	12 (21%)	1	7
21	V	53/55 (96%)	46 (87%)	7 (13%)	4	23
22	W	48/48 (100%)	39 (81%)	9 (19%)	1	9
23	Z	50/53 (94%)	44 (88%)	6 (12%)	5	27
24	1	46/48 (96%)	32 (70%)	14 (30%)	0	3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0	3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	6
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	1	10

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	37	HIS
26	3	39	ASP
14	O	47	PHE
26	3	11	LYS
22	W	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
17	R	97	GLN
19	T	71	ASN
24	1	32	GLN
7	H	101	ASN
6	G	161	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

5 of 667 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	2204	A
27	X	2705	A
27	X	2299	A
27	X	2404	A
27	X	2756	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 71 ligands modelled in this entry, 70 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	$\#\|Z\| > 2$
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	7 (8%)

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
30	ERY	X	2902	-	-	3/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	O2-C13	2.06	1.50	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	X	2902	ERY	O8-C23-C22	-2.50	103.96	110.05
30	X	2902	ERY	C2-C3-C4	-2.46	105.94	113.05
30	X	2902	ERY	C30-C2-C1	-2.30	103.83	109.02
30	X	2902	ERY	C16-C15-C14	-2.20	111.25	115.07
30	X	2902	ERY	C34-C10-C11	-2.16	111.69	114.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C15-C14-O3-C3
30	X	2902	ERY	O4-C14-O3-C3

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Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C25-C24-N1-C28

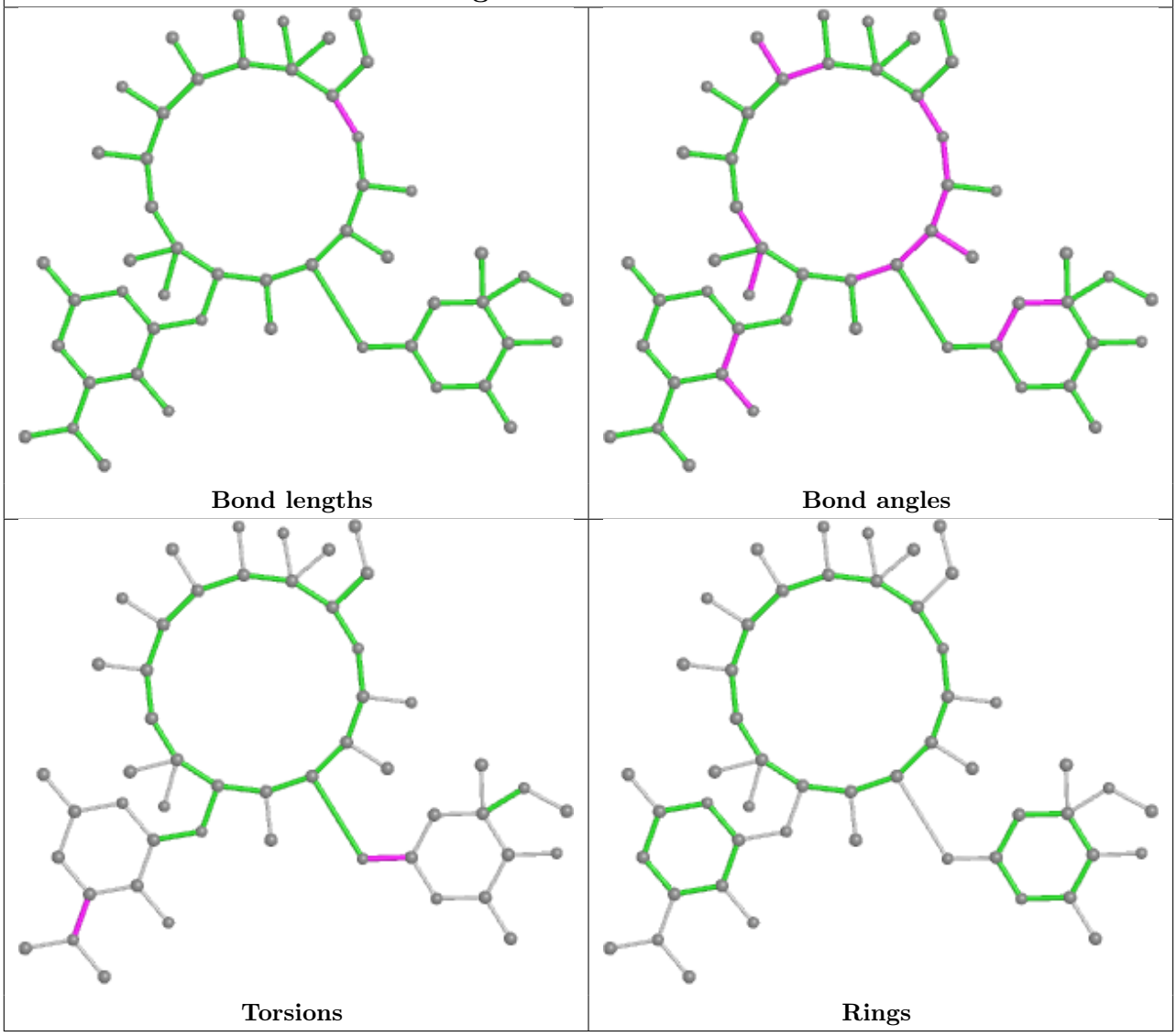
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	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 then 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.

Ligand ERY X 2902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	A	260/275 (94%)	0.01	4 (1%)	73	61	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.33	5 (2%)	59	45	27, 50, 107, 233	0
3	C	194/205 (94%)	0.02	9 (4%)	32	23	39, 102, 180, 292	0
4	D	177/180 (98%)	0.15	11 (6%)	20	15	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.28	4 (2%)	60	46	57, 131, 192, 243	0
6	G	142/174 (81%)	-0.01	8 (5%)	24	17	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.40	2 (1%)	73	61	33, 45, 87, 135	0
8	I	134/156 (85%)	0.19	4 (2%)	50	37	55, 126, 192, 315	0
9	J	136/141 (96%)	-0.00	4 (2%)	51	38	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.47	0	100	100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.08	6 (5%)	23	16	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.48	0	100	100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.20	2 (1%)	70	57	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.26	4 (4%)	35	25	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.40	0	100	100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.39	1 (1%)	80	69	49, 94, 162, 192	0
17	R	110/115 (95%)	0.02	3 (2%)	54	41	65, 100, 189, 259	0
18	S	175/237 (73%)	0.39	20 (11%)	5	5	93, 144, 224, 285	0
19	T	74/91 (81%)	0.11	5 (6%)	17	13	72, 112, 158, 228	0
20	U	72/81 (88%)	0.37	4 (5%)	24	17	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.26	2 (3%)	49	36	76, 115, 164, 208	0
22	W	55/55 (100%)	0.10	0	100	100	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.42	0	100	100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.42	5 (9%)	8	6	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
25	2	46/47 (97%)	0.11	1 (2%)	62	48	38, 67, 122, 169	0
26	3	59/65 (90%)	0.42	5 (8%)	10	9	80, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.13	84 (3%)	49	36	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.09	4 (3%)	46	34	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.10	197 (3%)	45	33	26, 89, 188, 339	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	15	ASP	7.4
27	X	1072	U	7.1
18	S	23	ALA	7.1
18	S	22	VAL	7.0
27	X	731	A	6.6

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 monosaccharides 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
29	MG	K	202	1/1	0.77	0.83	27,27,27,27	0
29	MG	B	301	1/1	0.79	0.78	34,34,34,34	0
29	MG	X	2930	1/1	0.80	0.99	29,29,29,29	0
29	MG	X	2919	1/1	0.82	0.10	62,62,62,62	0
29	MG	X	2958	1/1	0.82	0.48	44,44,44,44	0
29	MG	X	2915	1/1	0.83	0.17	63,63,63,63	0
29	MG	X	2906	1/1	0.85	0.85	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	2933	1/1	0.86	0.65	36,36,36,36	0
29	MG	K	201	1/1	0.86	0.49	27,27,27,27	0
29	MG	X	2931	1/1	0.87	0.57	46,46,46,46	0
29	MG	X	2907	1/1	0.90	0.77	28,28,28,28	0
29	MG	X	2963	1/1	0.90	0.31	56,56,56,56	0
29	MG	X	2925	1/1	0.91	1.04	31,31,31,31	0
29	MG	X	2946	1/1	0.91	0.19	46,46,46,46	0
29	MG	X	2952	1/1	0.91	0.44	29,29,29,29	0
29	MG	X	2917	1/1	0.91	0.86	40,40,40,40	0
29	MG	X	2911	1/1	0.91	0.53	56,56,56,56	0
29	MG	X	2965	1/1	0.91	0.91	43,43,43,43	0
29	MG	X	2960	1/1	0.92	0.32	61,61,61,61	0
29	MG	X	2943	1/1	0.92	0.95	42,42,42,42	0
29	MG	X	2951	1/1	0.92	0.76	32,32,32,32	0
29	MG	X	2957	1/1	0.93	0.85	52,52,52,52	0
29	MG	X	2916	1/1	0.93	0.87	41,41,41,41	0
29	MG	A	301	1/1	0.93	0.39	54,54,54,54	0
29	MG	X	2961	1/1	0.93	1.07	56,56,56,56	0
29	MG	X	2926	1/1	0.93	0.91	44,44,44,44	0
29	MG	X	2964	1/1	0.93	0.90	28,28,28,28	0
29	MG	X	2939	1/1	0.93	0.60	50,50,50,50	0
29	MG	X	2956	1/1	0.94	0.52	27,27,27,27	0
29	MG	X	2962	1/1	0.94	0.13	69,69,69,69	0
29	MG	X	2901	1/1	0.94	0.39	69,69,69,69	0
29	MG	X	2923	1/1	0.94	0.40	40,40,40,40	0
29	MG	X	2908	1/1	0.94	0.61	32,32,32,32	0
30	ERY	X	2902	51/51	0.94	0.23	31,34,36,36	0
29	MG	X	2904	1/1	0.95	0.56	32,32,32,32	0
29	MG	X	2927	1/1	0.95	0.34	29,29,29,29	0
29	MG	X	2921	1/1	0.95	0.34	28,28,28,28	0
29	MG	X	2950	1/1	0.95	0.40	32,32,32,32	0
29	MG	X	2905	1/1	0.95	0.50	31,31,31,31	0
29	MG	X	2903	1/1	0.95	0.66	30,30,30,30	0
29	MG	X	2934	1/1	0.95	0.25	29,29,29,29	0
29	MG	X	2937	1/1	0.95	0.69	44,44,44,44	0
29	MG	X	2948	1/1	0.96	0.28	34,34,34,34	0
29	MG	X	2936	1/1	0.96	0.65	45,45,45,45	0
29	MG	X	2913	1/1	0.96	0.46	43,43,43,43	0
29	MG	X	2910	1/1	0.96	0.64	56,56,56,56	0
29	MG	X	2920	1/1	0.96	0.46	52,52,52,52	0
29	MG	X	2912	1/1	0.96	0.14	27,27,27,27	0
29	MG	X	2947	1/1	0.96	0.26	34,34,34,34	0

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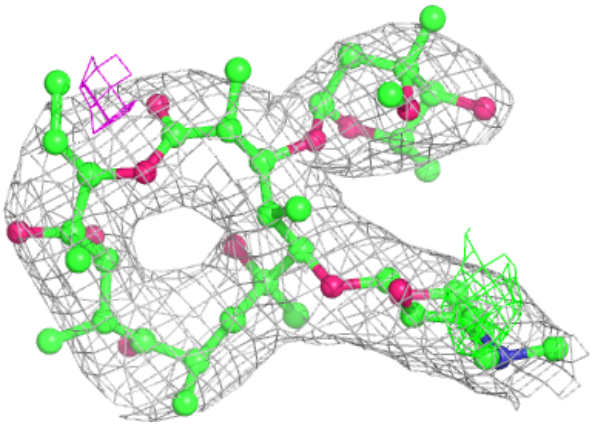
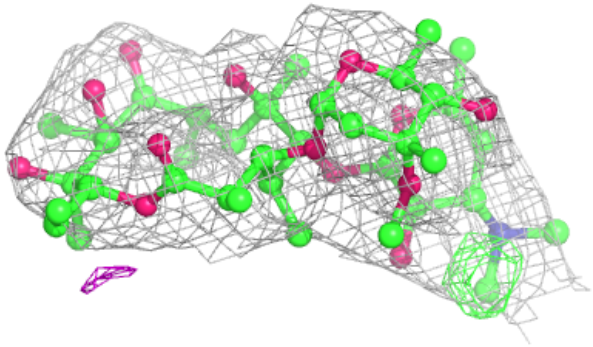
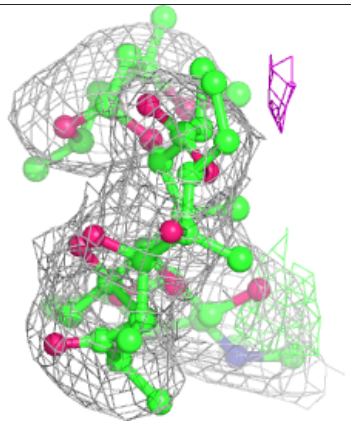
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	2955	1/1	0.97	0.48	30,30,30,30	0
29	MG	X	2922	1/1	0.97	0.34	29,29,29,29	0
29	MG	X	2944	1/1	0.97	0.41	35,35,35,35	0
29	MG	X	2945	1/1	0.97	0.14	38,38,38,38	0
29	MG	X	2959	1/1	0.97	0.64	41,41,41,41	0
29	MG	X	2935	1/1	0.97	0.47	34,34,34,34	0
29	MG	M	201	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2909	1/1	0.97	0.45	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2941	1/1	0.97	0.46	38,38,38,38	0
29	MG	X	2942	1/1	0.97	0.66	46,46,46,46	0
29	MG	X	2954	1/1	0.97	0.44	45,45,45,45	0
29	MG	X	2918	1/1	0.98	0.80	43,43,43,43	0
29	MG	X	2940	1/1	0.98	0.36	36,36,36,36	0
29	MG	X	2928	1/1	0.98	0.39	55,55,55,55	0
29	MG	X	2932	1/1	0.98	0.40	37,37,37,37	0
29	MG	X	2949	1/1	0.98	0.44	42,42,42,42	0
29	MG	X	2929	1/1	0.98	0.14	30,30,30,30	0
29	MG	X	2938	1/1	0.98	0.79	31,31,31,31	0
29	MG	X	2924	1/1	0.99	0.22	38,38,38,38	0
29	MG	X	2953	1/1	0.99	0.39	56,56,56,56	0
29	MG	X	2914	1/1	0.99	0.57	27,27,27,27	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 ERY X 2902: 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.