wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:47 AM GMT

PDB ID	:	3PIP
Title	:	Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit
Authors	:	Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Kinashi, H.; Rozenberg, H.; Yonath, A.
Deposited on	:	2010-11-07
Resolution	:	3.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

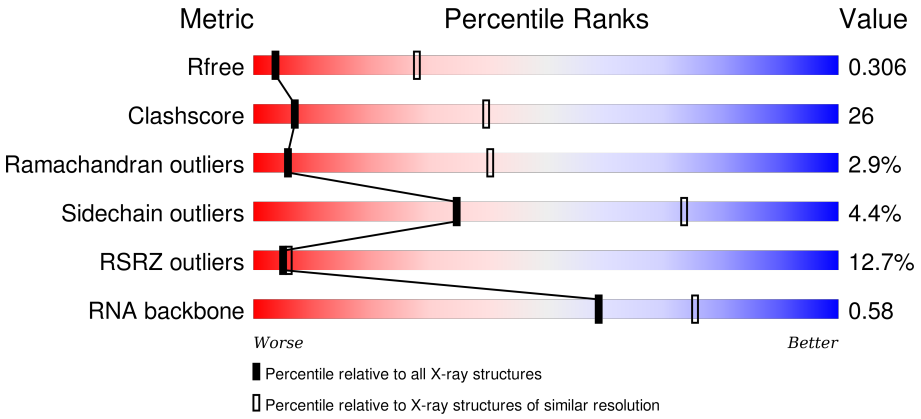
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.45 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}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)
RNA backbone	2183	1045 (4.10-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 25% 38% 24% • 8%
2	Y	123	2% 33% 50% 14% • •
3	A	274	20% 40% 45% 8% 8%
4	B	211	4% 48% 43% 5% • •

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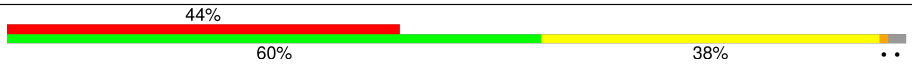
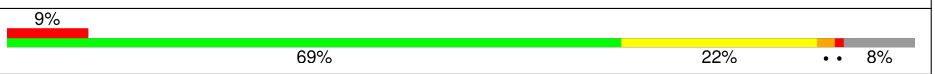
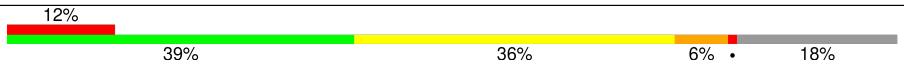
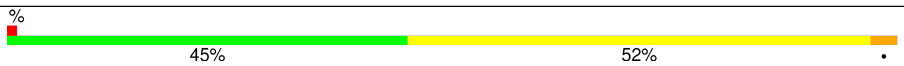
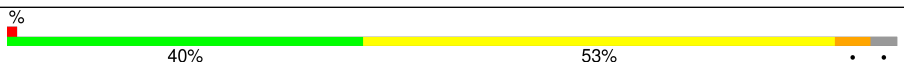
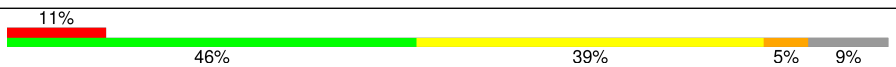
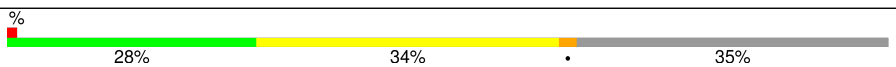
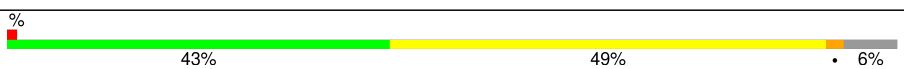
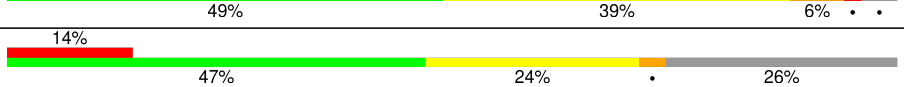
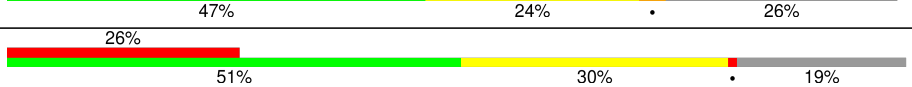
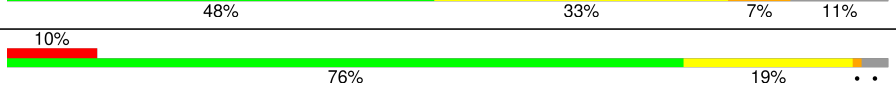
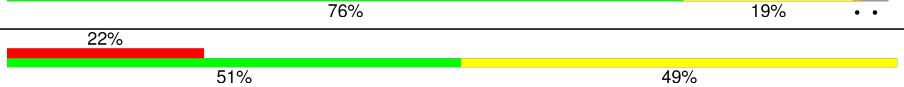
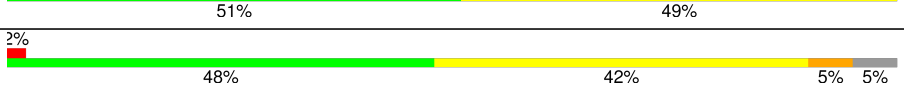
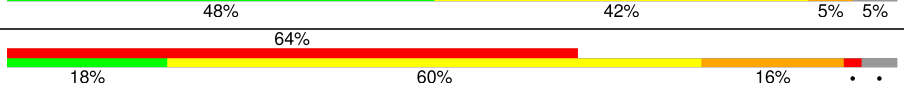
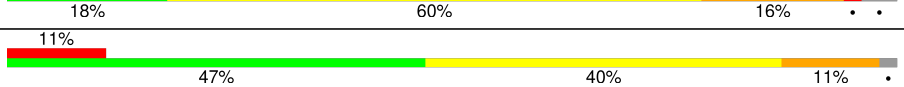
Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	

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	LC2	X	2881	-	-	-	X
32	LMA	X	2882	-	-	X	X
33	MG	X	2884	-	-	-	X
33	MG	X	2886	-	-	-	X
33	MG	X	2887	-	-	-	X
33	MG	X	2890	-	-	-	X
33	MG	X	2891	-	-	-	X
33	MG	X	2892	-	-	-	X
33	MG	X	2899	-	-	-	X
33	MG	X	2900	-	-	-	X
33	MG	X	2901	-	-	-	X
33	MG	X	2905	-	-	-	X
33	MG	X	2908	-	-	-	X
33	MG	X	2918	-	-	-	X
33	MG	X	2919	-	-	-	X
33	MG	X	2922	-	-	-	X
33	MG	X	2926	-	-	-	X
33	MG	X	2932	-	-	-	X
33	MG	X	2934	-	-	-	X
33	MG	X	2937	-	-	-	X
33	MG	X	2940	-	-	-	X
33	MG	X	2948	-	-	-	X
33	MG	X	2950	-	-	-	X
33	MG	X	2951	-	-	-	X
35	NA	X	2958	-	-	-	X
35	NA	X	2961	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83963 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 RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2644	56750	25314	10473	18320	2643	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	120	2561	1143	471	827	120	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	253	1920	1196	382	340	2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	177	1394	889	244	254	7	0	0	0

- 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	63	Total	C	N	O	S	0	0	0
			451	280	82	86	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	134	Total	C	N	O	0	0	0
			1005	616	203	186			

- 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			

- 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 779	C 476	N 161	O 142	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total 1004	C 633	N 197	O 172	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total 714	C 452	N 130	O 130	S 2	0	0	0

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

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

- 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	74	Total	C	N	O	S	0	0	0
			556	351	107	97	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	0	0	0
			537	334	110	93			

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

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

- 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	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

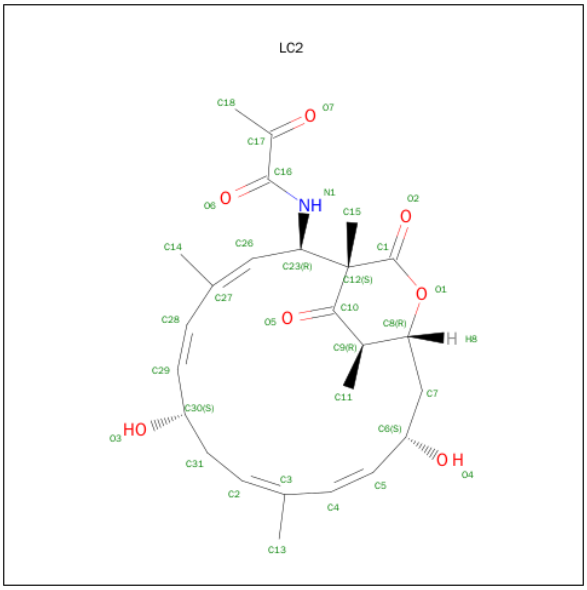
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

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

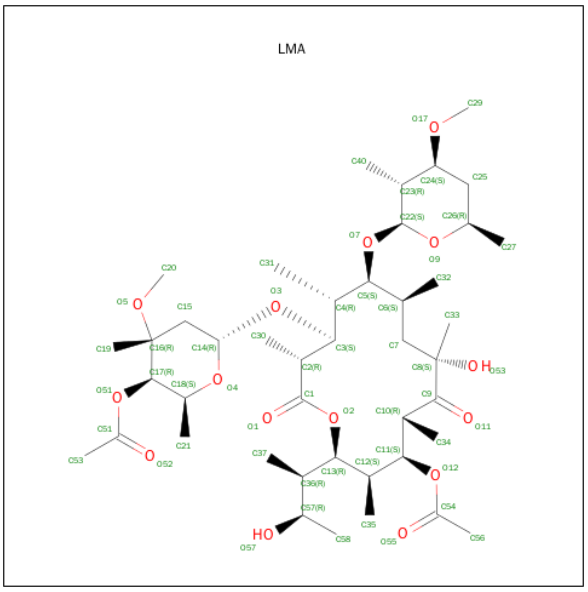
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-DIHYDROXY-1,4,10,19-TETRAMETHYL-17,18-DIOXO-16-OXABICYCLO[13.2.2]NONADECA-3,5,9,11-TETRAEN-2-YL]-2-OXOPROPANAMIDE (three-letter code: LC2) (formula: $C_{25}H_{33}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	X	1	Total	C	N	O	0	0
			33	25	1	7		

- Molecule 32 is LANKAMYCIN (three-letter code: LMA) (formula: $C_{43}H_{74}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 58 43 15	0	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	71	Total Mg 71 71	0	0
33	I	1	Total Mg 1 1	0	0
33	U	1	Total Mg 1 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	X	4	Total K 4 4	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

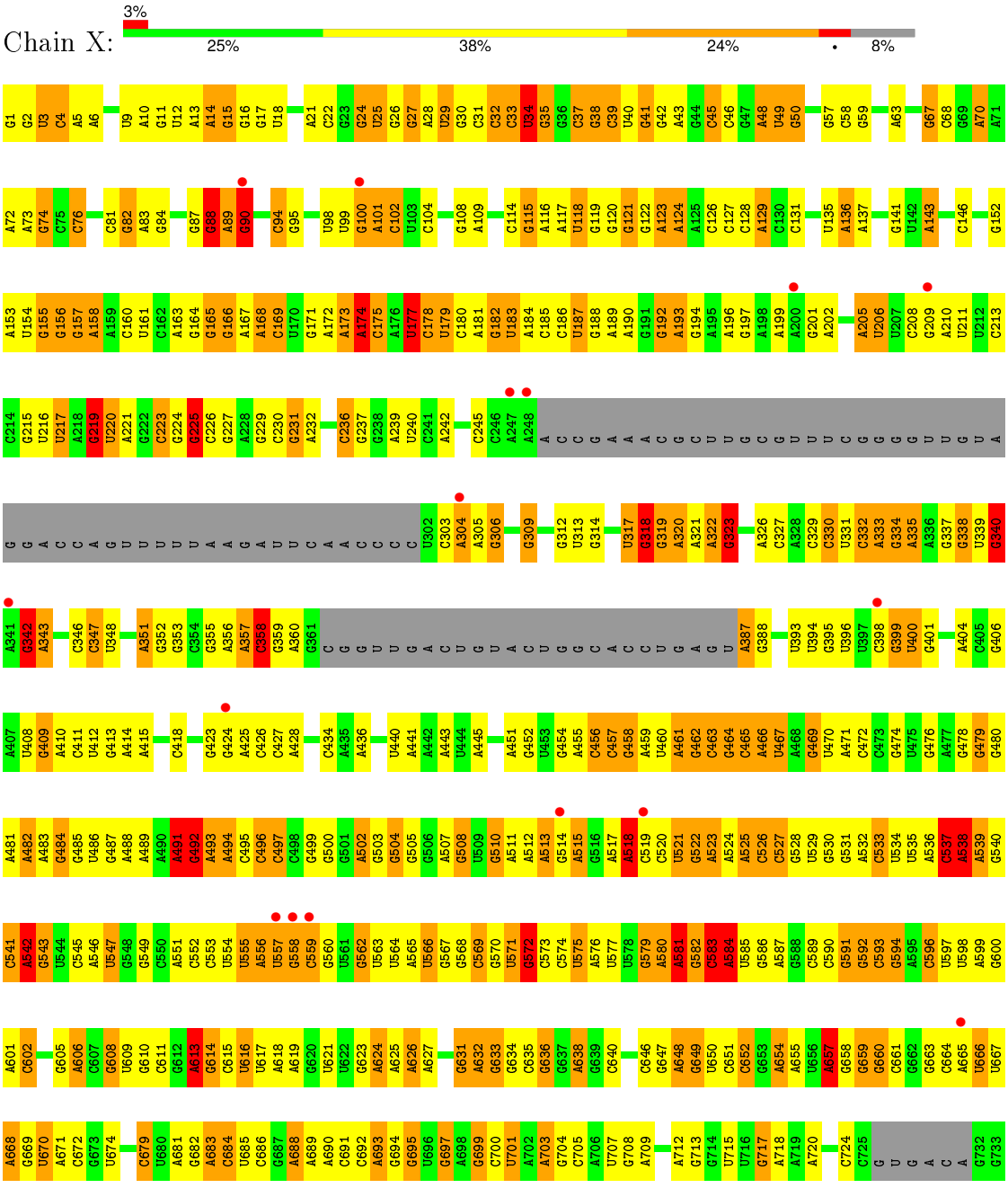
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	X	5	Total Na 5 5	0	0

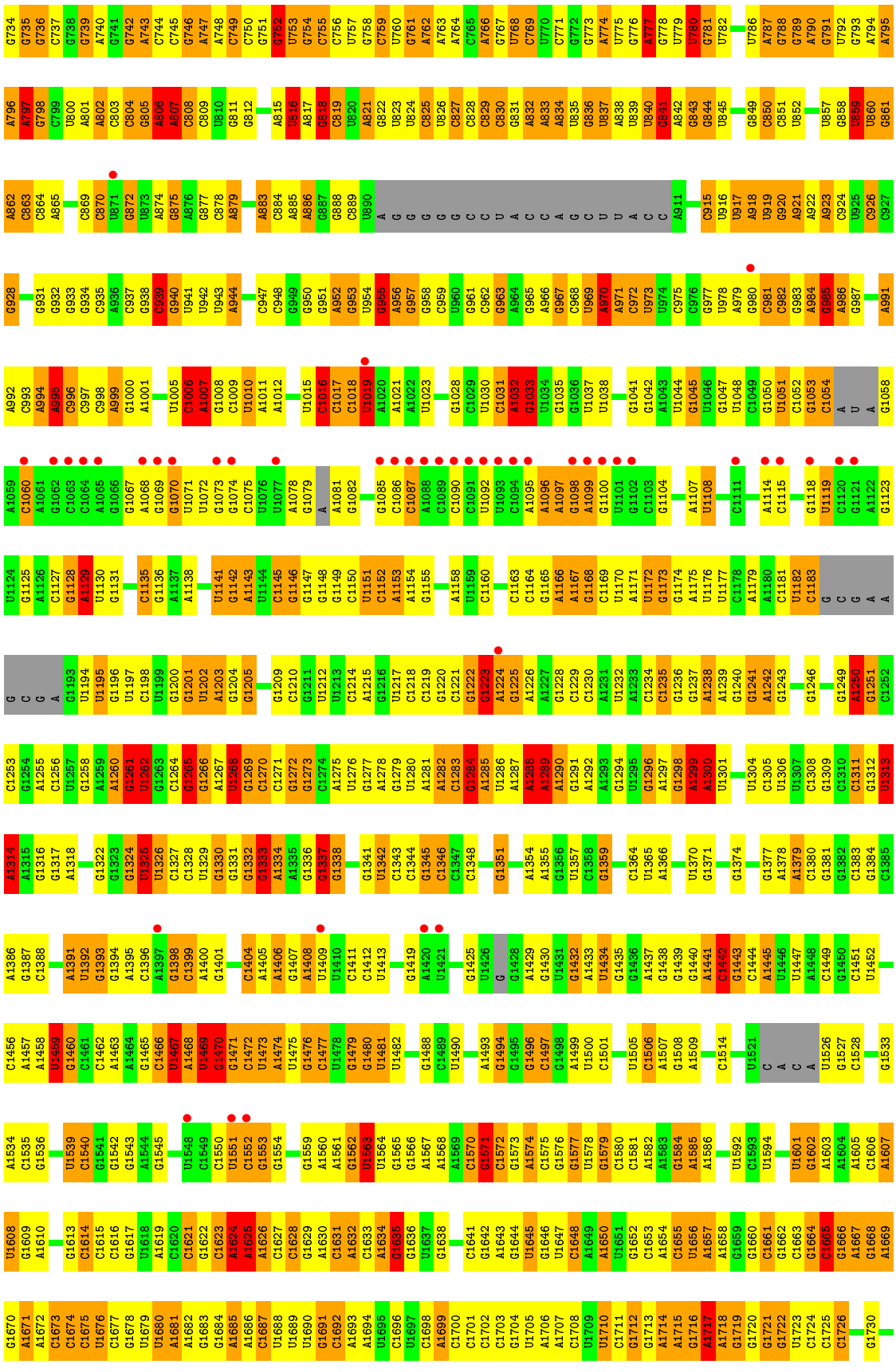
3 Residue-property plots (i)

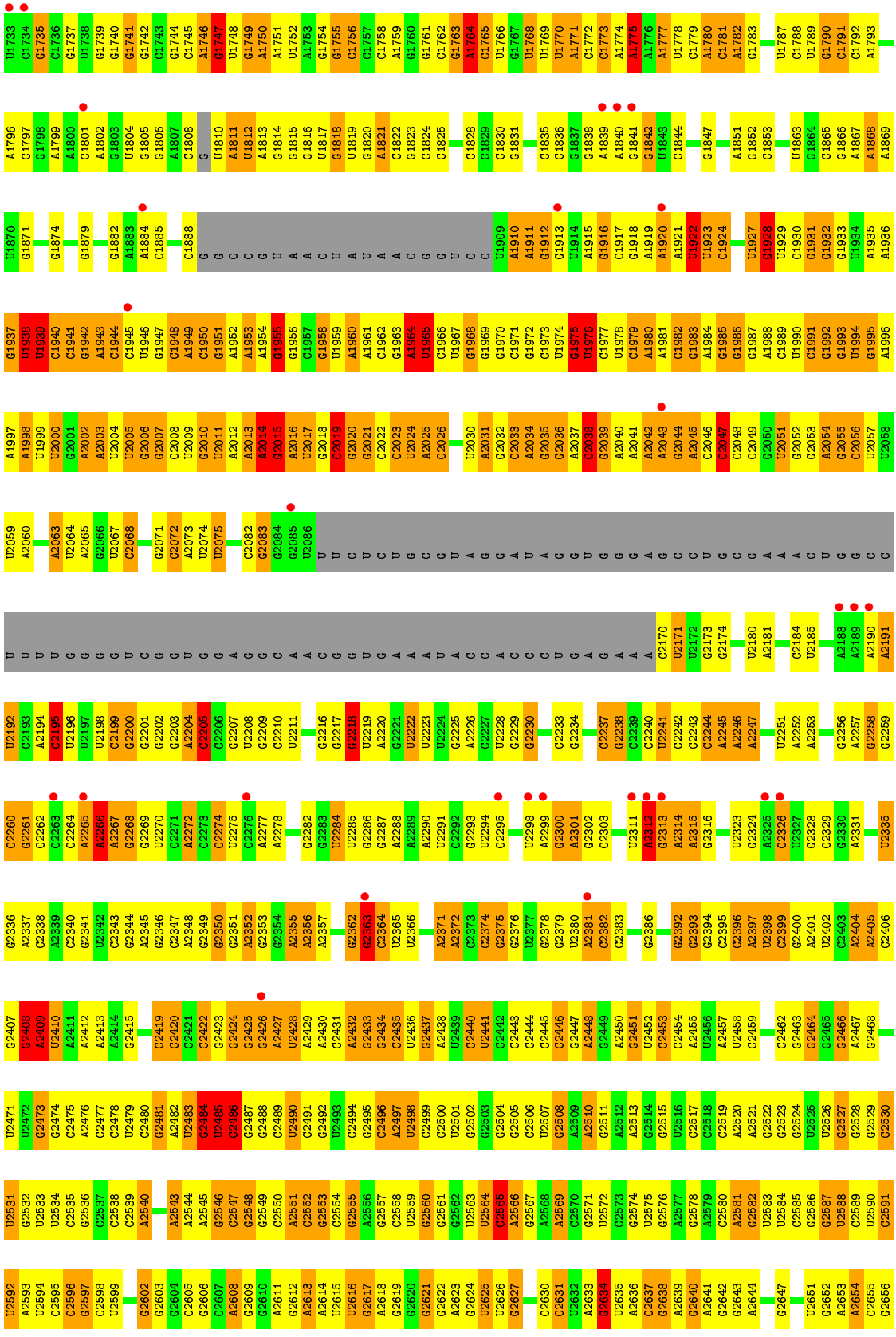
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

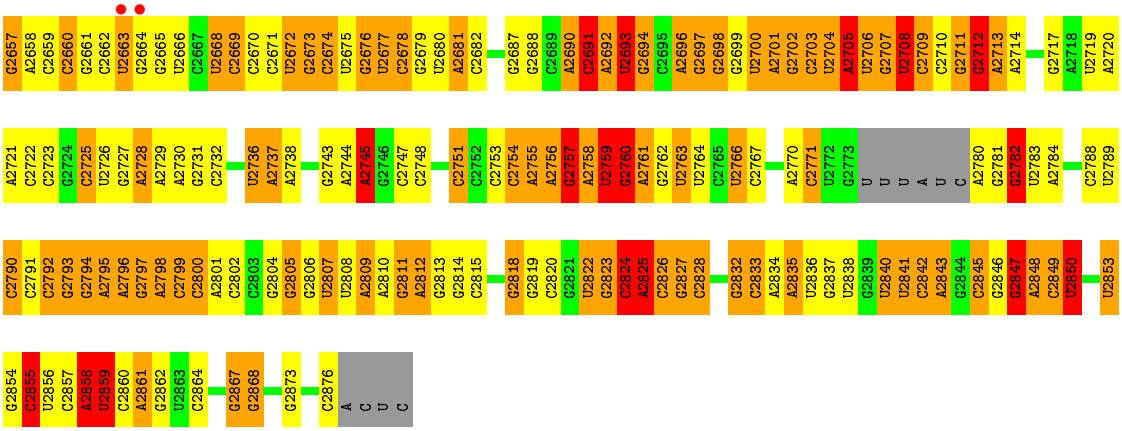
- Molecule 1: RIBOSOMAL 23S RNA

Chain X:



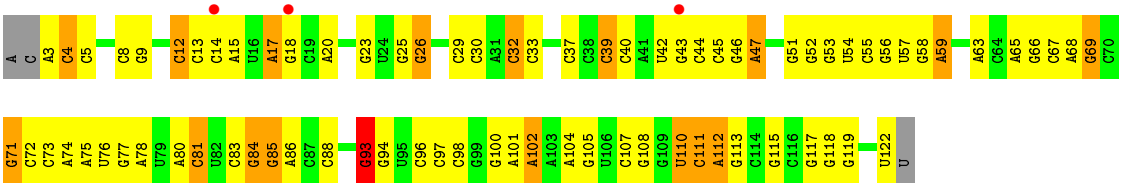






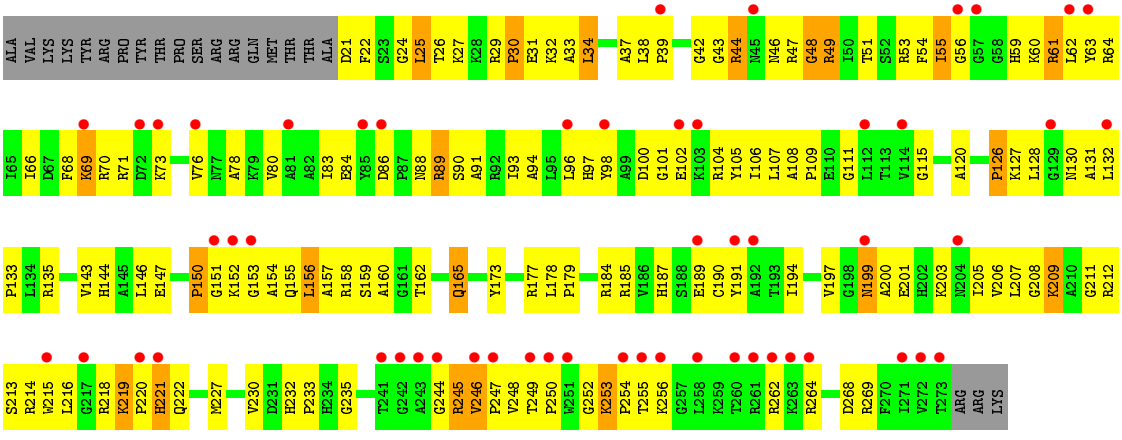
• Molecule 2: 5S ribosomal RNA

Chain Y:



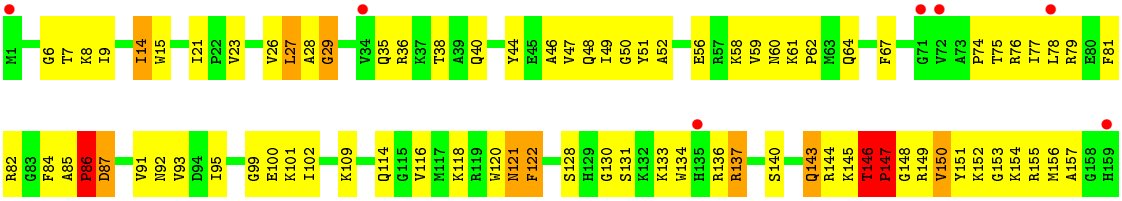
• Molecule 3: 50S ribosomal protein L2

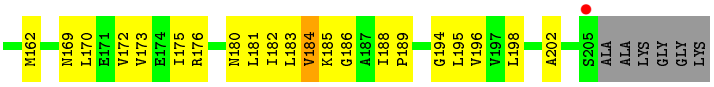
Chain A:



• Molecule 4: 50S ribosomal protein L3

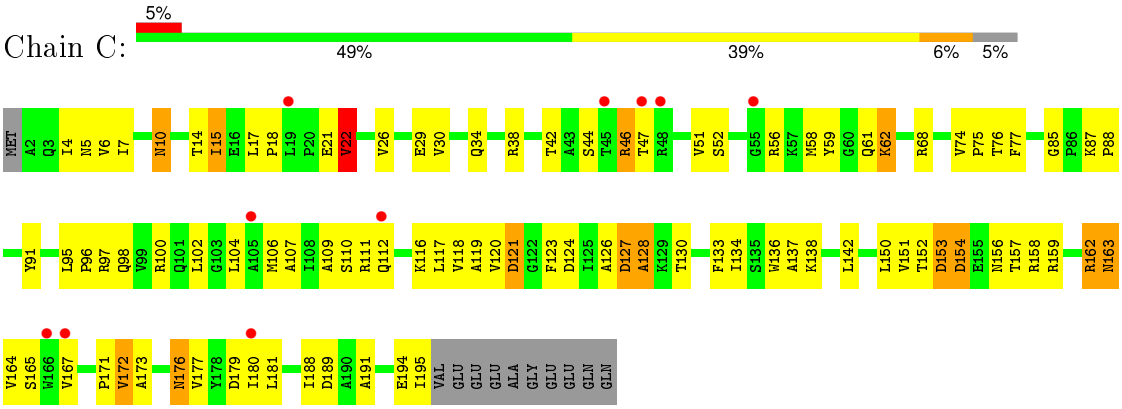
Chain B:





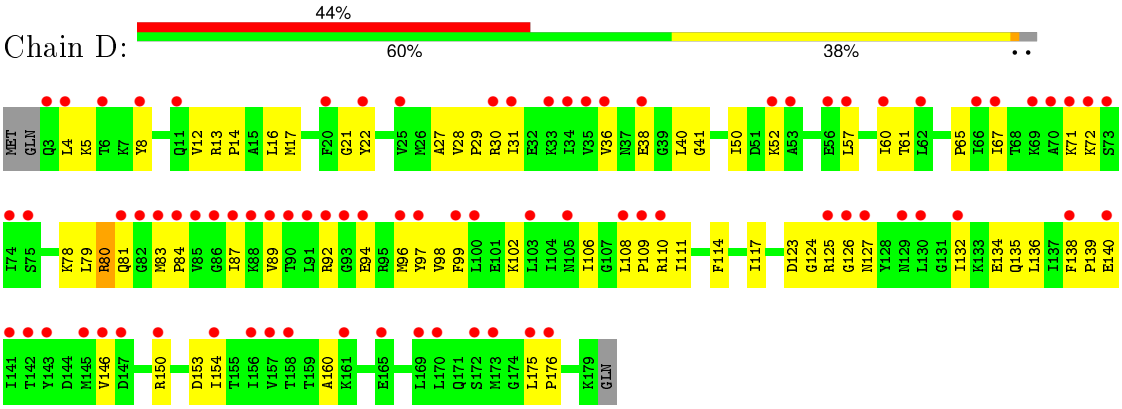
- Molecule 5: 50S ribosomal protein L4

Chain C:



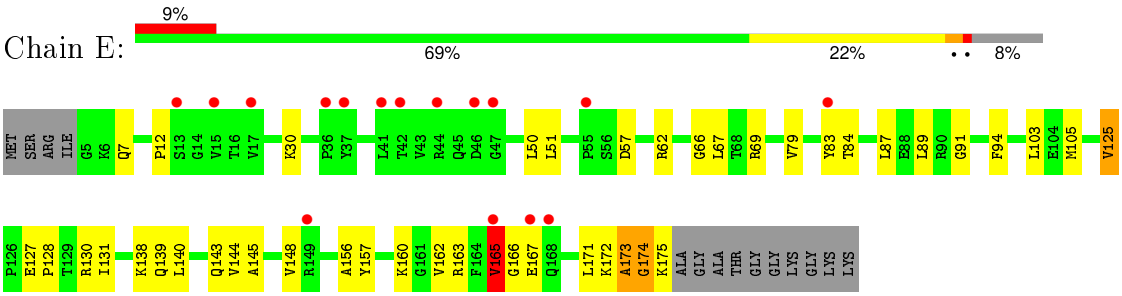
- Molecule 6: 50S ribosomal protein L5

Chain D:



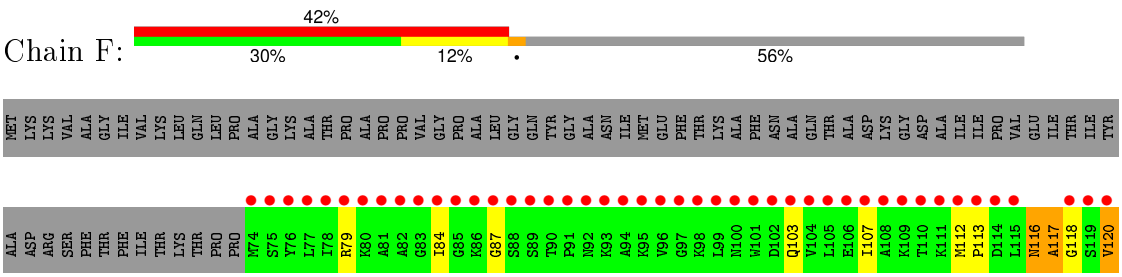
- Molecule 7: 50S ribosomal protein L6

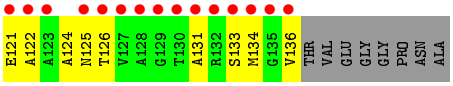
Chain E:



- Molecule 8: 50S ribosomal protein L11

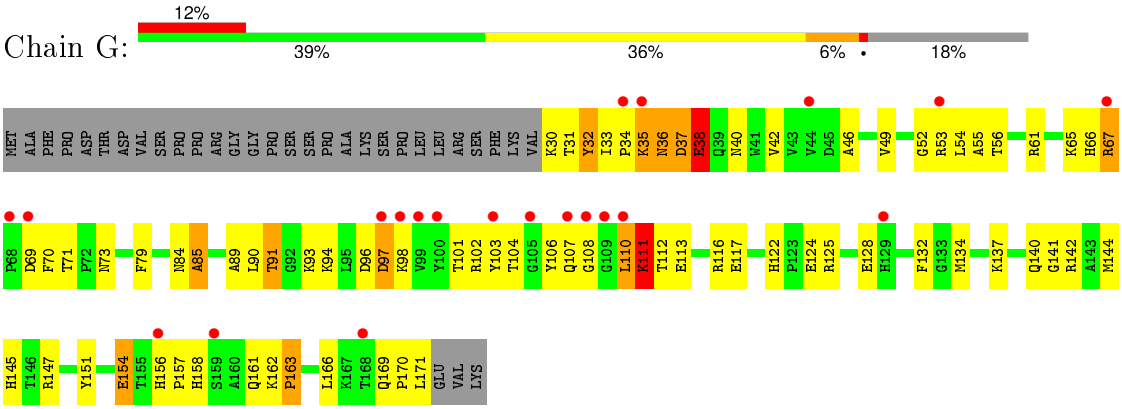
Chain F:





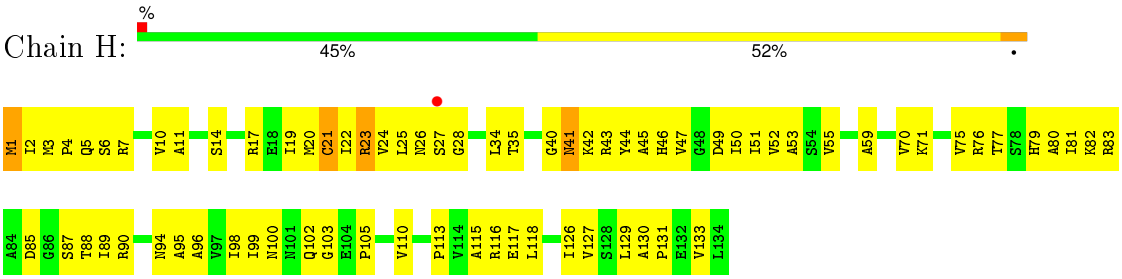
• Molecule 9: 50S ribosomal protein L13

Chain G:



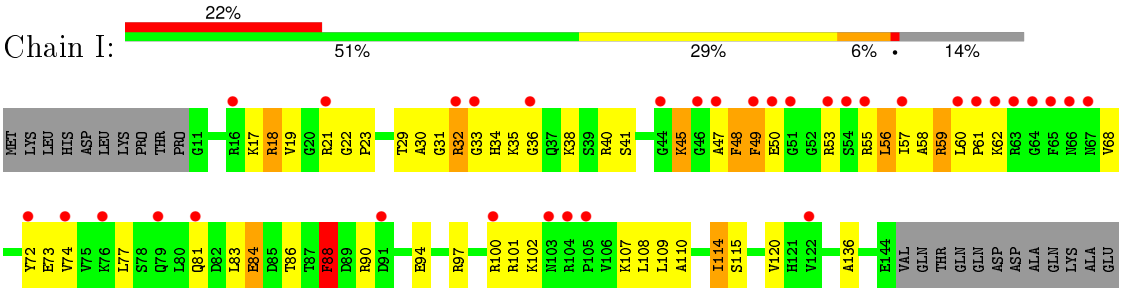
• Molecule 10: 50S ribosomal protein L14

Chain H:



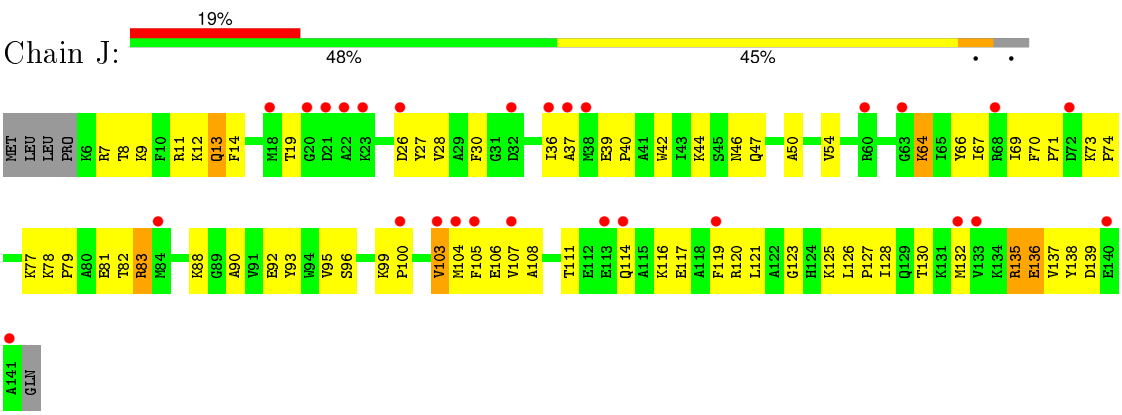
• Molecule 11: 50S ribosomal protein L15

Chain I:



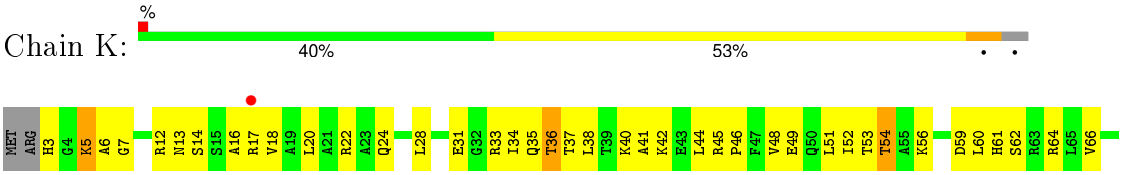
• Molecule 12: 50S ribosomal protein L16

Chain J:



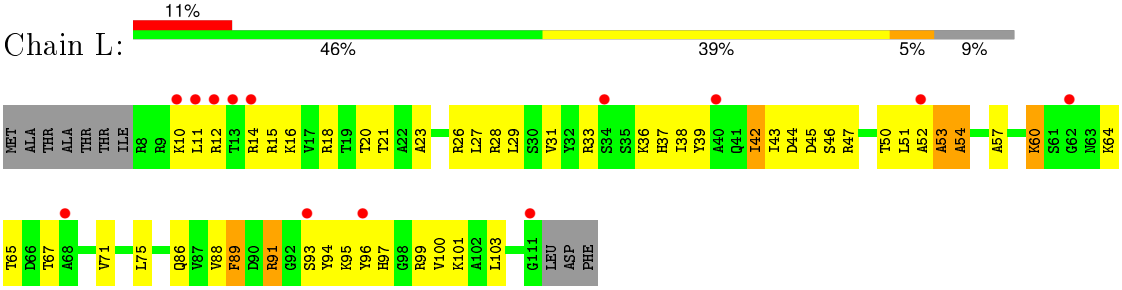
- Molecule 13: 50S ribosomal protein L17

Chain K:



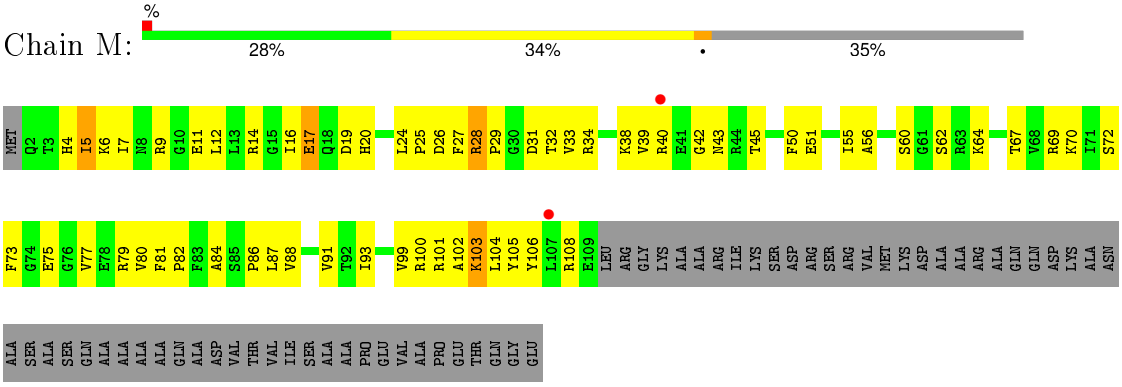
- Molecule 14: 50S ribosomal protein L18

Chain L:



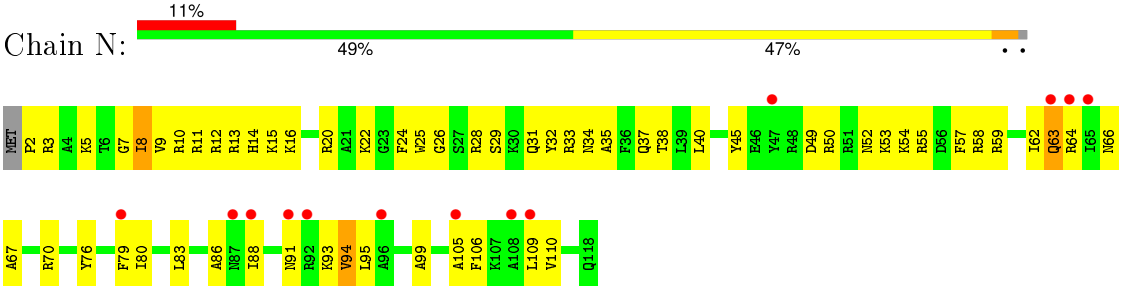
- Molecule 15: 50S ribosomal protein L19

Chain M:



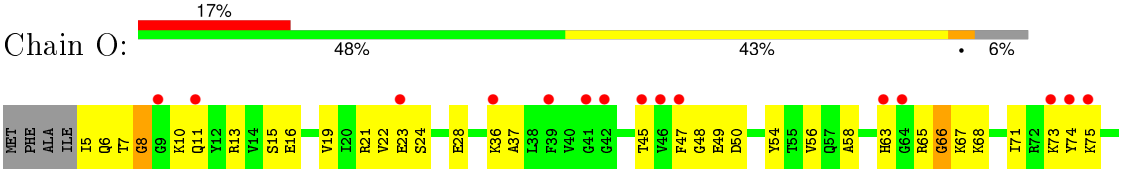
- Molecule 16: 50S ribosomal protein L20

Chain N:



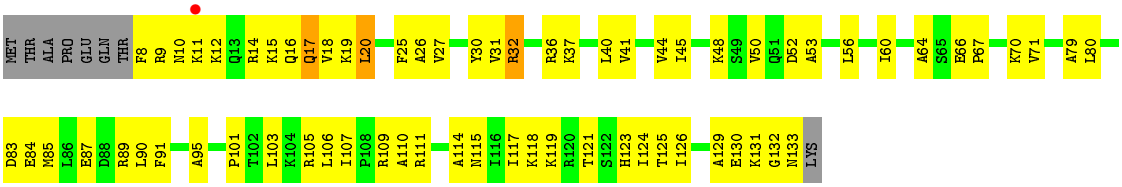
- Molecule 17: 50S ribosomal protein L21

Chain O:



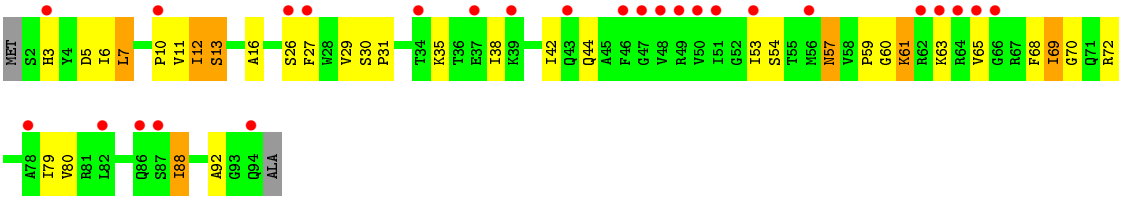
- Molecule 18: 50S ribosomal protein L22

Chain P:



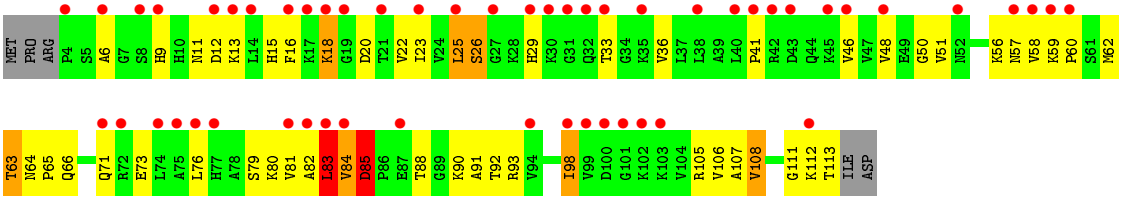
- Molecule 19: 50S ribosomal protein L23

Chain Q:



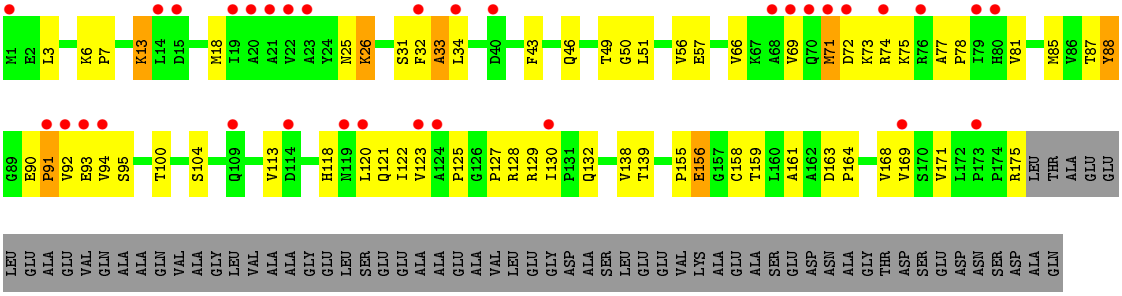
- Molecule 20: 50S ribosomal protein L24

Chain R:



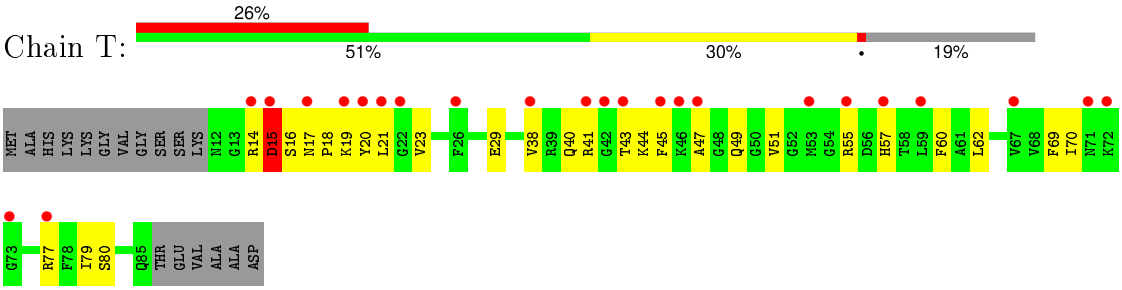
- Molecule 21: 50S ribosomal protein L25

Chain S:



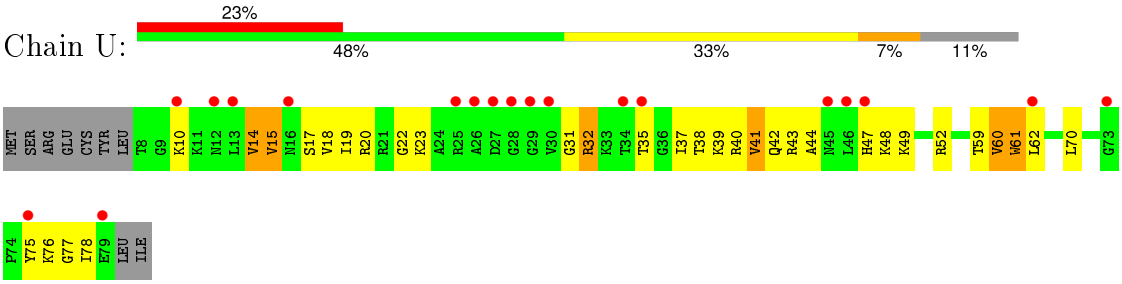
- Molecule 22: 50S ribosomal protein L27

Chain T:



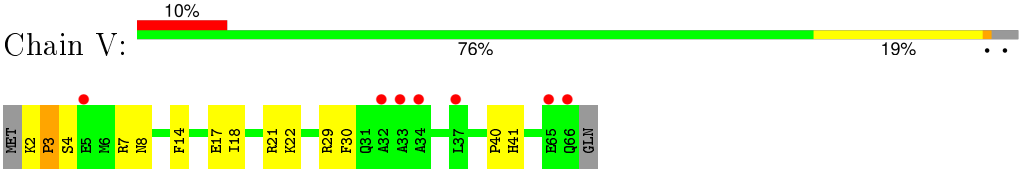
- Molecule 23: 50S ribosomal protein L28

Chain U:



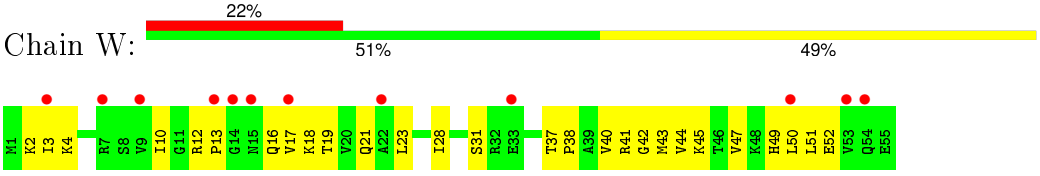
- Molecule 24: 50S ribosomal protein L29

Chain V:



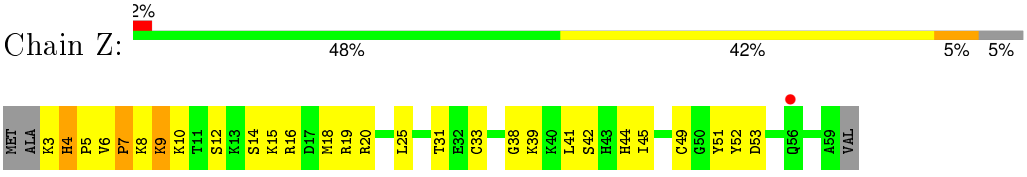
- Molecule 25: 50S ribosomal protein L30

Chain W:



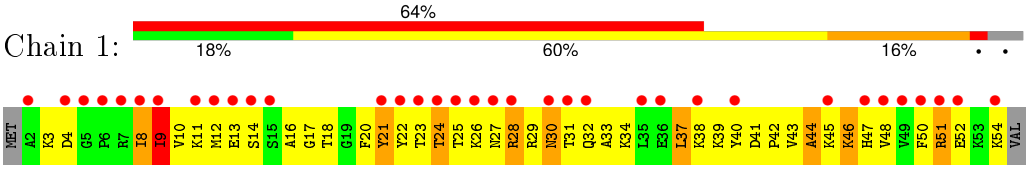
- Molecule 26: 50S ribosomal protein L32

Chain Z:



- Molecule 27: 50S ribosomal protein L33

Chain 1:

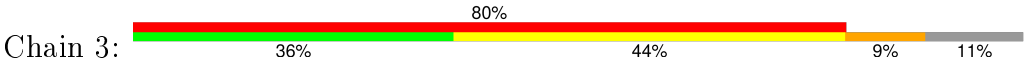


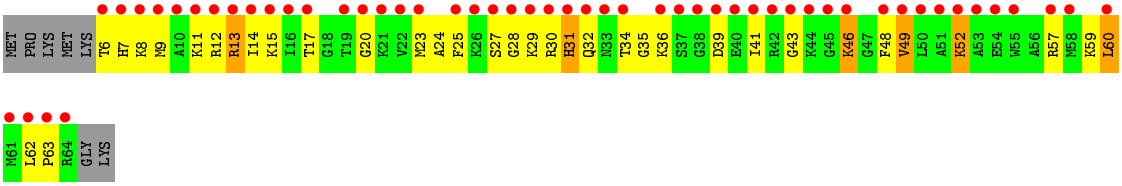
- Molecule 28: 50S ribosomal protein L34

Chain 2:

• Molecule 29: 50S ribosomal protein L35

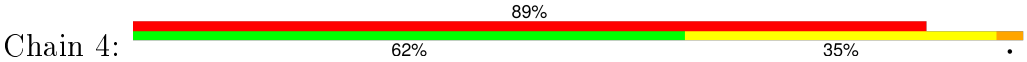
Chain 3:

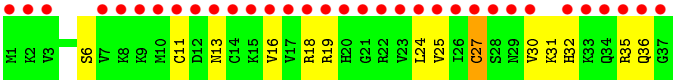




• Molecule 30: 50S ribosomal protein L36

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.72Å 408.56Å 693.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 93.01 – 3.44	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-3.45) 82.4 (93.01-3.44)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.257 , 0.301 0.265 , 0.306	Depositor DCC
R_{free} test set	2643 reflections (1.03%)	DCC
Wilson B-factor (Å^2)	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 76.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 262327 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, K, LC2, MG, LMA

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	1.17	260/63542 (0.4%)	1.58	1813/99100 (1.8%)
2	Y	0.80	1/2863 (0.0%)	1.13	21/4461 (0.5%)
3	A	0.65	0/1958	0.83	2/2638 (0.1%)
4	B	0.85	0/1567	0.93	2/2105 (0.1%)
5	C	0.84	0/1504	0.84	1/2036 (0.0%)
6	D	0.46	0/1413	0.56	0/1896
7	E	0.57	0/1308	0.60	0/1771
8	F	0.37	0/455	0.45	0/611
9	G	0.75	0/1138	0.82	0/1539
10	H	0.94	0/1007	0.99	0/1352
11	I	0.62	0/1016	0.71	0/1359
12	J	0.80	0/1113	0.80	0/1486
13	K	0.93	1/886 (0.1%)	1.01	0/1188
14	L	0.72	0/785	0.93	1/1048 (0.1%)
15	M	0.99	0/884	1.07	1/1186 (0.1%)
16	N	0.93	0/994	0.85	0/1323
17	O	0.77	0/750	0.81	0/1000
18	P	1.01	2/1017 (0.2%)	0.97	1/1362 (0.1%)
19	Q	0.66	0/725	0.69	0/974
20	R	0.66	0/835	0.72	1/1121 (0.1%)
21	S	0.51	0/1370	0.60	1/1862 (0.1%)
22	T	0.74	0/563	0.77	0/747
23	U	0.57	0/541	0.70	1/723 (0.1%)
24	V	0.67	0/529	0.63	0/704
25	W	0.60	0/426	0.71	0/568
26	Z	0.89	0/464	0.94	1/622 (0.2%)
27	1	0.32	0/438	0.60	0/583
28	2	0.57	0/387	0.54	0/509
29	3	0.22	0/468	0.38	0/614
30	4	0.69	1/298 (0.3%)	0.58	0/390
All	All	1.06	265/91244 (0.3%)	1.42	1846/136878 (1.3%)

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
7	E	0	4
8	F	0	3
9	G	0	8
10	H	0	2
11	I	0	1
12	J	0	1
All	All	0	19

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	616	U	C3'-C2'	-13.53	1.37	1.52
1	X	1775	A	O3'-P	-11.52	1.47	1.61
1	X	1299	A	N9-C4	-11.34	1.31	1.37
1	X	1260	A	N9-C4	-11.21	1.31	1.37
1	X	2669	C	N1-C6	-10.57	1.30	1.37

The worst 5 of 1846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	29	ARG	C-N-CD	-19.10	78.58	120.60
1	X	1678	G	N1-C6-O6	-18.90	108.56	119.90
1	X	2486	C	C5-C6-N1	17.23	129.62	121.00
1	X	2815	C	C6-N1-C2	17.04	127.12	120.30
14	L	54	ALA	CB-CA-C	16.51	134.87	110.10

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	125	VAL	Peptide
7	E	130	ARG	Sidechain
7	E	165	VAL	Peptide
7	E	174	GLY	Peptide
8	F	116	ASN	Peptide

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	X	56750	0	28598	2022	3
2	Y	2561	0	1306	67	0
3	A	1920	0	1974	255	0
4	B	1539	0	1600	168	0
5	C	1481	0	1504	122	0
6	D	1394	0	1470	73	0
7	E	1286	0	1336	30	0
8	F	451	0	474	21	0
9	G	1114	0	1144	113	0
10	H	997	0	1046	97	0
11	I	1005	0	1036	117	0
12	J	1090	0	1125	97	0
13	K	878	0	930	93	0
14	L	779	0	820	77	0
15	M	871	0	894	85	3
16	N	978	0	1020	107	0
17	O	741	0	756	66	0
18	P	1004	0	1083	70	0
19	Q	714	0	731	35	0
20	R	825	0	881	78	0
21	S	1345	0	1372	56	0
22	T	556	0	579	30	0
23	U	537	0	580	40	0
24	V	525	0	546	20	0
25	W	424	0	470	24	0
26	Z	452	0	457	39	0
27	1	431	0	456	91	0
28	2	383	0	414	51	0
29	3	462	0	506	78	0
30	4	297	0	330	18	0
31	X	33	0	33	18	0
32	X	58	0	69	43	0
33	I	1	0	0	0	0
33	U	1	0	0	0	0
33	X	71	0	0	0	0
34	X	4	0	0	0	0
35	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	83963	0	55540	3669	3

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 26.

The worst 5 of 3669 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:699:G:N2	28:2:5:TYR:CE1	1.89	1.36
27:1:28:ARG:HB2	27:1:30:ASN:OD1	1.24	1.34
1:X:699:G:N2	28:2:5:TYR:HE1	1.25	1.28
1:X:775:U:H5'	1:X:776:G:N2	1.49	1.26
1:X:699:G:N7	28:2:11:LYS:HG3	1.51	1.26

All (3) 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)
1:X:1552:C:O2	15:M:43:ASN:ND2[8_455]	0.99	1.21
1:X:1552:C:O2	15:M:43:ASN:CG[8_455]	1.93	0.27
1:X:1552:C:C2	15:M:43:ASN:ND2[8_455]	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	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	5 38
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	5 37
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	3 28
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	17 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	7 45
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	12 53
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	6 40
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100 100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	2 23
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	13 54
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	21 67
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	19 64
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	6 41
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	11 52
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	5 37
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	12 53
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	2 23
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	2 22
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	6 40
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	3 31
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	1 16
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	12 53
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	11 51
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	1 9
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100 100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	4 36
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	6 40

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
4	B	86	PRO
4	B	122	PHE
4	B	137	ARG
4	B	147	PRO

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
3	A	194/215 (90%)	180 (93%)	14 (7%)	18 57
4	B	155/157 (99%)	147 (95%)	8 (5%)	29 68
5	C	154/163 (94%)	146 (95%)	8 (5%)	29 68
6	D	152/156 (97%)	151 (99%)	1 (1%)	88 95
7	E	136/144 (94%)	135 (99%)	1 (1%)	88 95
8	F	46/107 (43%)	46 (100%)	0	100 100
9	G	118/146 (81%)	111 (94%)	7 (6%)	24 64
10	H	103/103 (100%)	100 (97%)	3 (3%)	50 82
11	I	100/121 (83%)	93 (93%)	7 (7%)	19 58
12	J	110/115 (96%)	106 (96%)	4 (4%)	42 77
13	K	90/93 (97%)	85 (94%)	5 (6%)	26 66
14	L	74/82 (90%)	70 (95%)	4 (5%)	27 66
15	M	94/134 (70%)	90 (96%)	4 (4%)	35 74
16	N	96/97 (99%)	94 (98%)	2 (2%)	61 86
17	O	75/79 (95%)	73 (97%)	2 (3%)	52 83
18	P	108/115 (94%)	107 (99%)	1 (1%)	84 94
19	Q	73/76 (96%)	69 (94%)	4 (6%)	27 66
20	R	91/96 (95%)	83 (91%)	8 (9%)	12 47
21	S	149/192 (78%)	146 (98%)	3 (2%)	63 86
22	T	55/67 (82%)	54 (98%)	1 (2%)	66 88
23	U	54/66 (82%)	51 (94%)	3 (6%)	26 66
24	V	53/55 (96%)	53 (100%)	0	100 100
25	W	48/48 (100%)	48 (100%)	0	100 100
26	Z	51/53 (96%)	50 (98%)	1 (2%)	63 86
27	1	46/48 (96%)	36 (78%)	10 (22%)	1 6
28	2	39/40 (98%)	34 (87%)	5 (13%)	5 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	3	46/52 (88%)	41 (89%)	5 (11%)	8 35
30	4	35/35 (100%)	35 (100%)	0	100 100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	35 73

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	103	VAL
15	M	5	ILE
28	2	9	ASN
12	J	135	ARG
13	K	54	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
9	G	169	GLN
10	H	46	HIS
21	S	118	HIS
7	E	111	HIS
9	G	73	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2630/2880 (91%)	470 (17%)	73 (2%)
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	73 (2%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1324	G
1	X	1496	G
1	X	2736	U
1	X	1441	A
1	X	1607	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 84 ligands modelled in this entry, 82 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
31	LC2	X	2881	-	28,34,34	1.77	5 (17%)	20,49,49	0.88	0
32	LMA	X	2882	-	59,60,60	4.61	26 (44%)	76,90,90	1.29	6 (7%)

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
31	LC2	X	2881	-	-	0/31/61/61	0/0/2/2
32	LMA	X	2882	-	-	0/80/115/115	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2882	LMA	C30-C2	-18.36	1.10	1.53
32	X	2882	LMA	C2-C1	-16.05	1.13	1.51
32	X	2882	LMA	O53-C8	-9.80	1.25	1.43
32	X	2882	LMA	C33-C8	-7.77	1.41	1.52
32	X	2882	LMA	C35-C12	-7.60	1.36	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	2882	LMA	C3-C2-C1	-2.80	104.39	109.86
32	X	2882	LMA	C25-C24-C23	-2.47	106.52	113.55
32	X	2882	LMA	C13-C12-C11	-2.01	108.54	113.05
32	X	2882	LMA	O7-C5-C4	3.75	112.91	108.19
32	X	2882	LMA	O51-C51-C53	4.41	119.42	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LC2	18	0
32	X	2882	LMA	43	0

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

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, 95^{th} 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	2644/2880 (91%)	0.13	91 (3%) 49 42	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.12	3 (2%) 61 54	108, 183, 252, 342	0
3	A	253/274 (92%)	1.05	54 (21%) 1 1	66, 158, 225, 423	0
4	B	205/211 (97%)	0.28	8 (3%) 43 37	35, 85, 159, 249	0
5	C	194/205 (94%)	0.02	10 (5%) 31 27	61, 142, 250, 381	0
6	D	177/180 (98%)	2.09	80 (45%) 0 0	174, 255, 358, 427	0
7	E	171/185 (92%)	0.35	16 (9%) 11 11	87, 183, 269, 354	0
8	F	63/144 (43%)	5.33	60 (95%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.68	21 (14%) 3 3	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.17	1 (0%) 89 84	39, 71, 135, 248	0
11	I	134/156 (85%)	0.92	34 (25%) 1 1	75, 168, 261, 375	0
12	J	136/141 (96%)	0.93	27 (19%) 1 2	76, 135, 223, 388	0
13	K	113/116 (97%)	0.03	1 (0%) 85 79	32, 61, 101, 128	0
14	L	104/114 (91%)	0.33	13 (12%) 5 6	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.05	2 (1%) 70 63	32, 73, 138, 298	0
16	N	117/118 (99%)	0.51	13 (11%) 7 8	57, 116, 177, 328	0
17	O	94/100 (94%)	0.78	17 (18%) 2 2	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.17	1 (0%) 87 81	33, 84, 149, 226	0
19	Q	93/95 (97%)	1.41	26 (27%) 1 1	86, 134, 245, 329	0
20	R	110/115 (95%)	2.35	53 (48%) 0 0	93, 166, 332, 423	0
21	S	175/237 (73%)	0.84	33 (18%) 2 2	130, 202, 285, 326	0
22	T	74/91 (81%)	1.68	24 (32%) 1 0	112, 141, 201, 284	0
23	U	72/81 (88%)	1.56	19 (26%) 1 1	119, 188, 304, 349	0
24	V	65/67 (97%)	0.42	7 (10%) 8 8	116, 175, 235, 292	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	0.97	12 (21%) 1 1	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.21	1 (1%) 71 64	44, 79, 182, 234	0
27	1	53/55 (96%)	3.21	35 (66%) 0 0	126, 192, 295, 403	0
28	2	46/47 (97%)	0.71	5 (10%) 7 8	72, 123, 258, 308	0
29	3	59/66 (89%)	4.40	53 (89%) 0 0	139, 213, 356, 435	0
30	4	37/37 (100%)	7.35	33 (89%) 0 0	152, 219, 307, 382	0
All	All	5931/6561 (90%)	0.58	753 (12%) 5 6	32, 131, 276, 575	0

The worst 5 of 753 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	23.8
8	F	113	PRO	16.0
30	4	28	SER	14.6
30	4	1	MET	14.2
30	4	24	LEU	14.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
33	MG	X	2886	1/1	0.76	1.10	89.31	54,54,54,54	0
33	MG	X	2905	1/1	0.91	0.68	47.64	50,50,50,50	0
33	MG	X	2884	1/1	0.93	1.00	29.40	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	X	2948	1/1	0.82	0.83	29.14	110,110,110,110	0
33	MG	X	2899	1/1	0.97	0.54	18.41	41,41,41,41	0
33	MG	X	2951	1/1	0.90	0.47	17.09	142,142,142,142	0
33	MG	X	2908	1/1	0.92	0.67	13.35	80,80,80,80	0
33	MG	X	2918	1/1	0.93	0.53	12.77	84,84,84,84	0
33	MG	X	2934	1/1	0.94	0.41	10.28	56,56,56,56	0
35	NA	X	2958	1/1	0.91	0.47	8.97	48,48,48,48	0
35	NA	X	2961	1/1	0.92	0.43	7.99	75,75,75,75	0
33	MG	X	2937	1/1	0.94	0.36	7.71	109,109,109,109	0
33	MG	X	2922	1/1	0.92	0.36	7.64	53,53,53,53	0
32	LMA	X	2882	58/58	0.80	0.38	5.85	120,120,120,120	0
33	MG	X	2887	1/1	0.95	0.41	5.38	35,35,35,35	0
33	MG	X	2891	1/1	0.89	0.33	5.36	50,50,50,50	0
33	MG	X	2950	1/1	0.88	0.30	4.71	36,36,36,36	0
33	MG	X	2900	1/1	0.94	0.64	4.61	42,42,42,42	0
33	MG	X	2932	1/1	0.94	0.35	4.43	62,62,62,62	0
33	MG	X	2901	1/1	0.92	0.39	4.14	19,19,19,19	0
33	MG	X	2926	1/1	0.79	0.46	3.05	67,67,67,67	0
33	MG	X	2919	1/1	0.94	0.34	3.05	65,65,65,65	0
31	LC2	X	2881	33/33	0.83	0.33	2.67	49,106,118,122	0
33	MG	X	2890	1/1	0.96	0.40	2.35	59,59,59,59	0
33	MG	X	2940	1/1	0.82	0.31	2.34	71,71,71,71	0
33	MG	X	2892	1/1	0.95	0.30	2.20	71,71,71,71	0
33	MG	X	2928	1/1	0.87	0.34	1.35	29,29,29,29	0
33	MG	X	2896	1/1	0.95	0.26	0.27	24,24,24,24	0
34	K	X	2954	1/1	0.96	0.24	0.09	70,70,70,70	0
33	MG	X	2916	1/1	0.90	0.20	-0.14	44,44,44,44	0
33	MG	X	2897	1/1	0.96	0.15	-2.75	79,79,79,79	0
33	MG	X	2943	1/1	0.95	0.20	-	43,43,43,43	0
33	MG	X	2917	1/1	0.74	0.32	-	104,104,104,104	0
33	MG	X	2942	1/1	0.81	0.63	-	77,77,77,77	0
33	MG	X	2925	1/1	0.88	0.57	-	80,80,80,80	0
33	MG	X	2883	1/1	0.92	0.54	-	23,23,23,23	0
33	MG	X	2938	1/1	0.91	0.62	-	62,62,62,62	0
33	MG	X	2902	1/1	0.81	0.17	-	89,89,89,89	0
33	MG	X	2893	1/1	0.84	0.41	-	66,66,66,66	0
33	MG	X	2944	1/1	0.85	0.29	-	77,77,77,77	0
33	MG	X	2927	1/1	0.95	0.74	-	65,65,65,65	0
33	MG	X	2911	1/1	0.28	0.63	-	124,124,124,124	0
33	MG	X	2903	1/1	0.90	0.54	-	65,65,65,65	0
33	MG	X	2907	1/1	0.94	0.36	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	X	2894	1/1	0.82	0.47	-	65,65,65,65	0
33	MG	I	157	1/1	0.74	0.47	-	67,67,67,67	0
33	MG	X	2915	1/1	0.87	0.57	-	67,67,67,67	0
33	MG	X	2933	1/1	0.95	0.37	-	83,83,83,83	0
33	MG	X	2904	1/1	0.88	0.43	-	64,64,64,64	0
33	MG	X	2952	1/1	0.95	0.35	-	59,59,59,59	0
34	K	X	2955	1/1	0.93	0.14	-	113,113,113,113	0
33	MG	X	2941	1/1	0.89	0.23	-	71,71,71,71	0
33	MG	X	2920	1/1	0.85	0.37	-	100,100,100,100	0
33	MG	X	2931	1/1	0.84	0.69	-	72,72,72,72	0
33	MG	X	2946	1/1	0.94	0.16	-	123,123,123,123	0
34	K	X	2956	1/1	0.83	0.38	-	146,146,146,146	0
33	MG	X	2935	1/1	0.94	0.22	-	36,36,36,36	0
33	MG	X	2888	1/1	0.96	0.49	-	51,51,51,51	0
33	MG	X	2930	1/1	0.97	0.21	-	77,77,77,77	0
33	MG	X	2895	1/1	0.90	0.29	-	26,26,26,26	0
33	MG	X	2906	1/1	0.97	0.39	-	52,52,52,52	0
33	MG	U	82	1/1	0.67	0.38	-	72,72,72,72	0
33	MG	X	2945	1/1	0.95	0.17	-	67,67,67,67	0
33	MG	X	2949	1/1	0.93	0.56	-	83,83,83,83	0
33	MG	X	2913	1/1	0.97	0.40	-	63,63,63,63	0
33	MG	X	2924	1/1	0.92	0.13	-	51,51,51,51	0
33	MG	X	2885	1/1	0.88	0.47	-	68,68,68,68	0
35	NA	X	2960	1/1	0.85	0.47	-	86,86,86,86	0
35	NA	X	2962	1/1	0.79	1.12	-	98,98,98,98	0
33	MG	X	2912	1/1	0.67	0.20	-	62,62,62,62	0
33	MG	X	2936	1/1	0.94	0.25	-	55,55,55,55	0
33	MG	X	2889	1/1	0.98	0.24	-	61,61,61,61	0
34	K	X	2957	1/1	0.89	0.57	-	82,82,82,82	0
33	MG	X	2947	1/1	0.98	0.13	-	56,56,56,56	0
33	MG	X	2909	1/1	0.80	0.17	-	58,58,58,58	0
33	MG	X	2923	1/1	0.93	0.15	-	97,97,97,97	0
33	MG	X	2910	1/1	0.90	0.36	-	44,44,44,44	0
33	MG	X	2939	1/1	0.97	0.49	-	54,54,54,54	0
35	NA	X	2959	1/1	0.91	0.26	-	60,60,60,60	0
33	MG	X	2898	1/1	0.98	0.38	-	19,19,19,19	0
33	MG	X	2953	1/1	0.97	0.38	-	53,53,53,53	0
33	MG	X	2914	1/1	0.87	0.52	-	74,74,74,74	0
33	MG	X	2929	1/1	0.92	0.82	-	61,61,61,61	0
33	MG	X	2921	1/1	0.91	0.18	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.