



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:31 PM BST

PDB ID : 4V89
Title : Crystal Structure of Release Factor RF3 Trapped in the GTP State on a Rotated Conformation of the Ribosome (without viomycin)
Authors : Zhou, J.; Lancaster, L.; Trakhanov, S.; Noller, H.F.
Deposited on : 2011-11-17
Resolution : 3.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

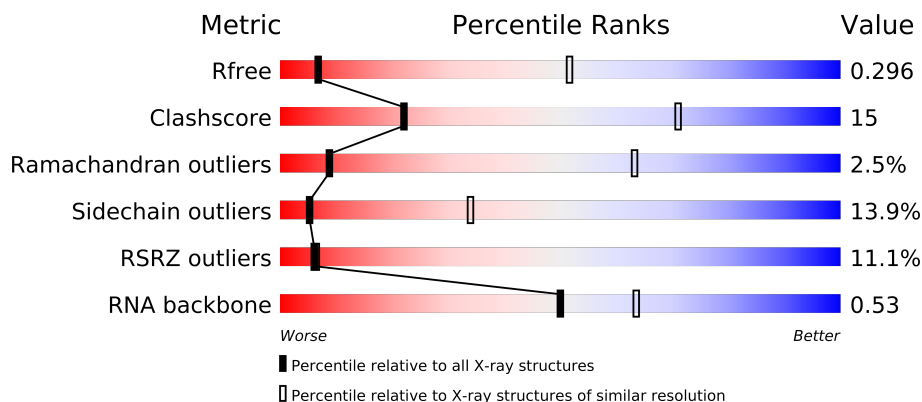
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.70 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}	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1533	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	


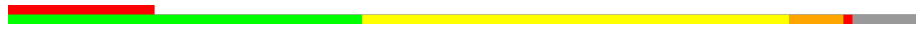


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Mol	Chain	Length	Quality of chain
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	27	
23	AW	534	
24	B0	85	
25	B1	78	
26	B2	63	
27	B3	59	
28	B4	57	
29	B5	55	
30	B6	46	
31	B7	65	
32	B8	38	
33	BA	2903	
34	BB	118	
35	BC	273	
36	BD	209	
37	BE	201	
38	BF	179	
39	BG	177	
40	BH	165	
41	BI	142	
42	BJ	121	
42	BK	121	
42	BL	121	
42	BM	121	
43	BN	142	
44	BO	123	
45	BP	144	
46	BQ	136	
47	BR	127	
48	BS	117	
49	BT	115	
50	BU	118	
51	BV	103	

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Mol	Chain	Length	Quality of chain
52	BW	110	
53	BX	100	
54	BY	104	
55	BZ	94	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146665 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AW	530	HIS	-	EXPRESSION TAG	UNP P0A7I4
AW	531	HIS	-	EXPRESSION TAG	UNP P0A7I4
AW	532	HIS	-	EXPRESSION TAG	UNP P0A7I4
AW	533	HIS	-	EXPRESSION TAG	UNP P0A7I4
AW	534	HIS	-	EXPRESSION TAG	UNP P0A7I4

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B0	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B1	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B2	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B3	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B4	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	B5	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B6	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B7	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B8	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	2853	Total	C	N	O	P	0	0	0
			61252	27324	11274	19801	2853			

- Molecule 34 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 36 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 37 is a protein called 50S ribosomal protein L4.

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

- Molecule 38 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 39 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 40 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	163	Total	C	N	O	S	0	0	0
			1230	775	219	229	7			

- Molecule 41 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 42 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BK	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BL	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BM	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BN	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BO	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BP	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BQ	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BR	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BS	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BT	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BU	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BV	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BX	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

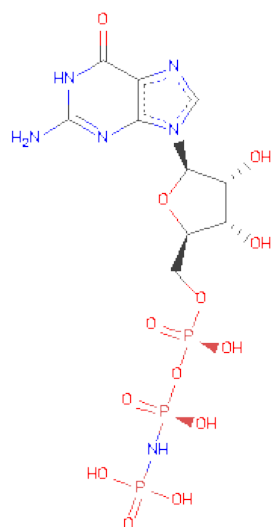
- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BY	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BZ	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 56 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	AW	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

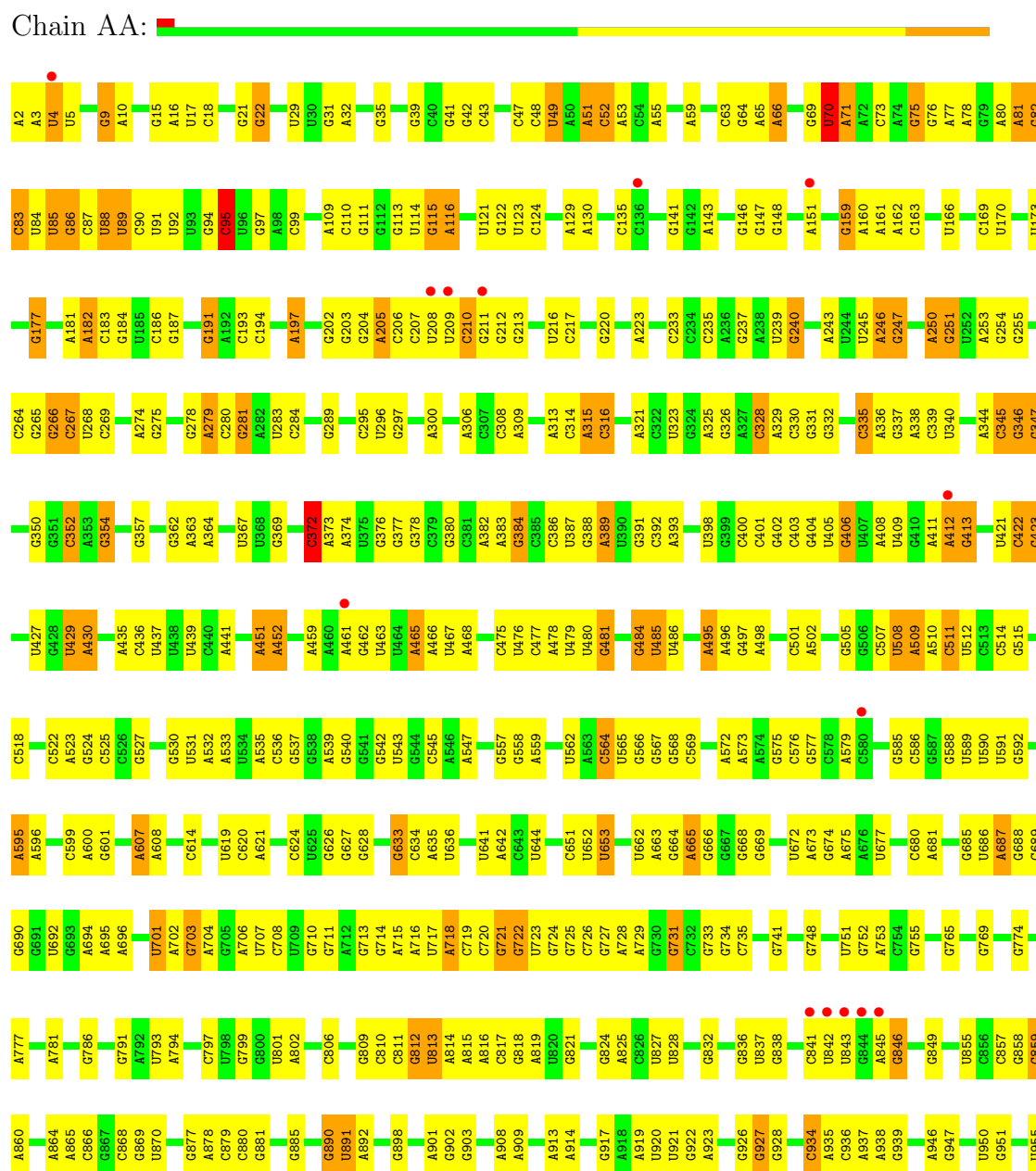
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

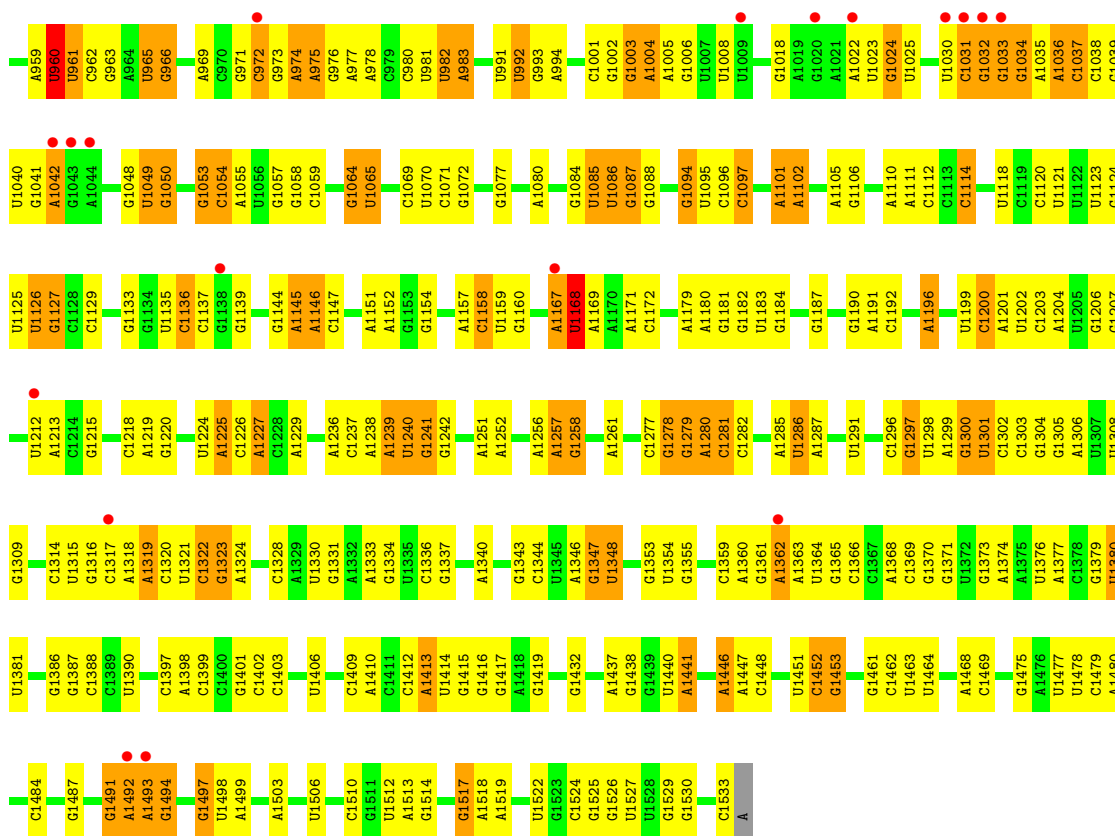
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AW	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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.

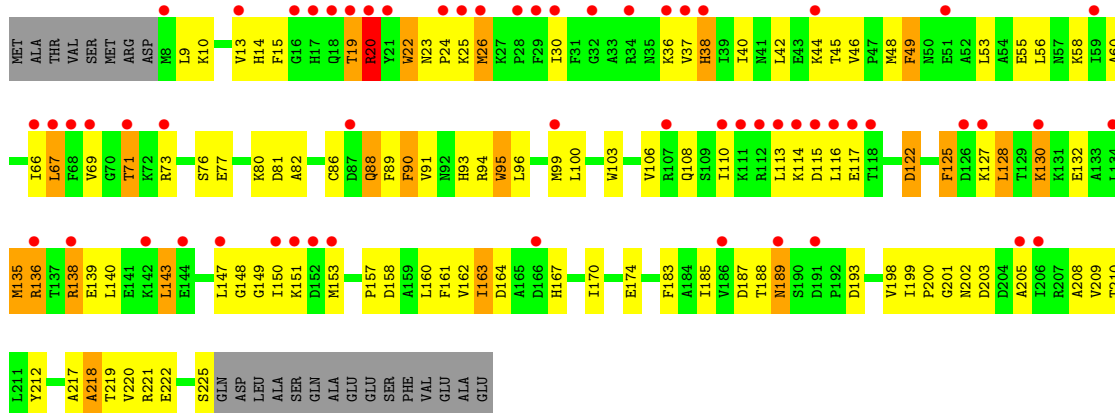
• Molecule 1: 16S rRNA





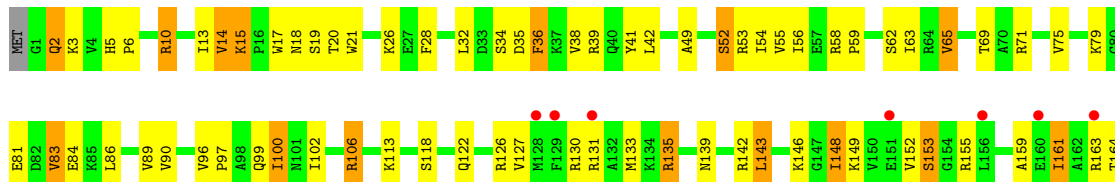
- Molecule 2: 30S ribosomal protein S2

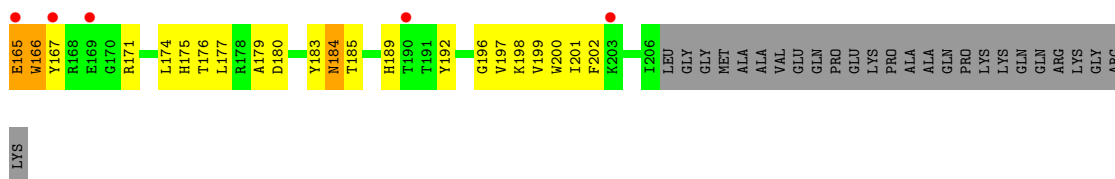
Chain AB:



- Molecule 3: 30S ribosomal protein S3

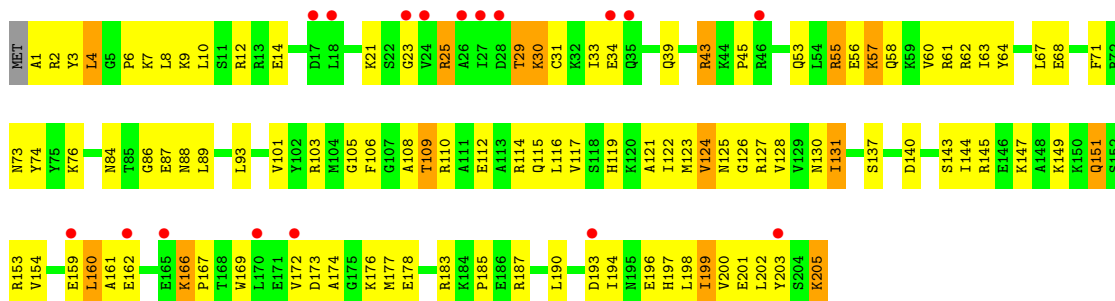
Chain AC:





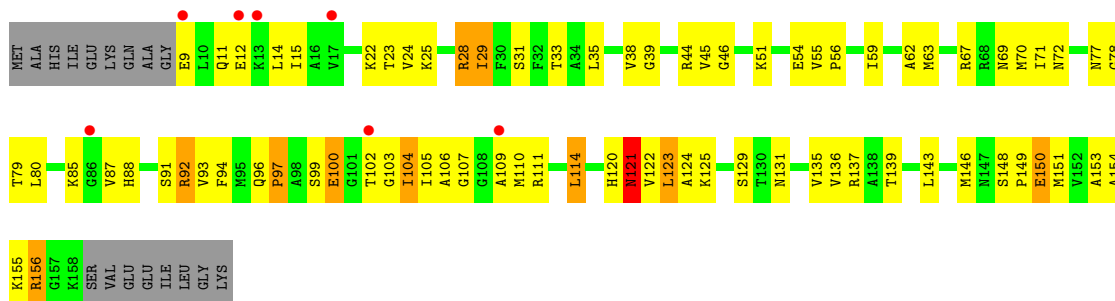
• Molecule 4: 30S ribosomal protein S4

Chain AD:



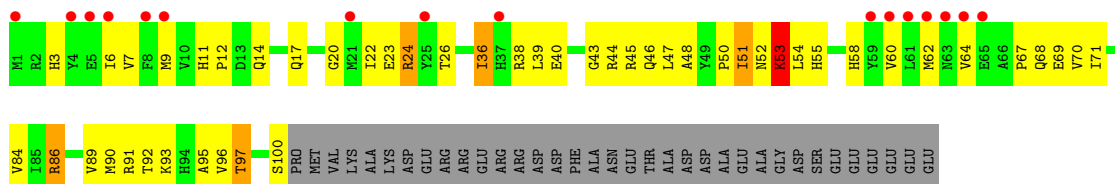
• Molecule 5: 30S ribosomal protein S5

Chain AE:



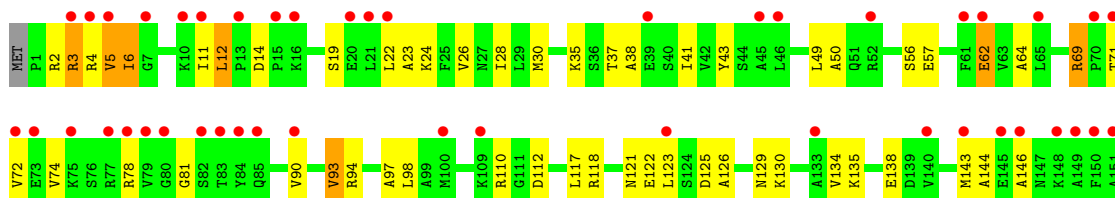
• Molecule 6: 30S ribosomal protein S6

Chain AF:



• Molecule 7: 30S ribosomal protein S7

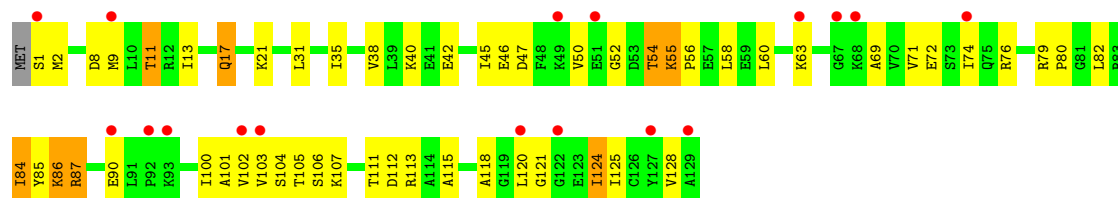
Chain AG:



HIS
TYR
ARG
TRP
LEU
SER
LEU
ARG
SER
PHE
SER
HIS
GLN
ALA
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LYS
GLN
PRO
ALA
LEU
GLY
TYR
LEU
ASN

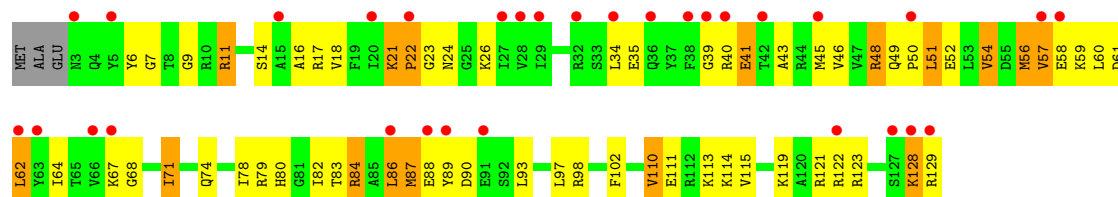
• Molecule 8: 30S ribosomal protein S8

Chain AH:



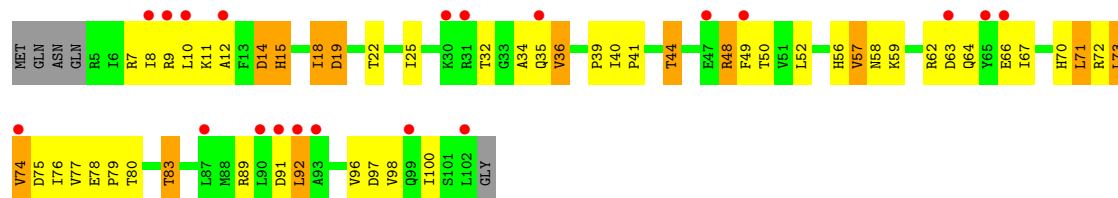
• Molecule 9: 30S ribosomal protein S9

Chain AI:



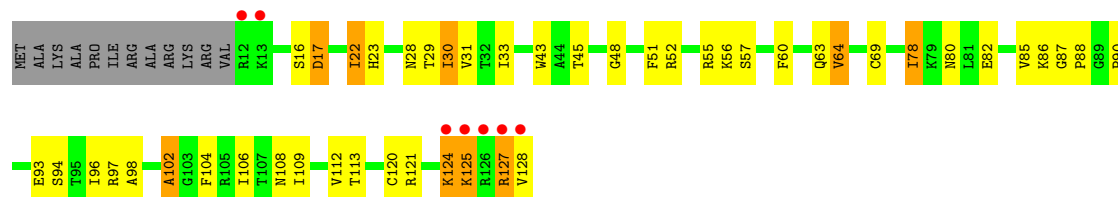
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



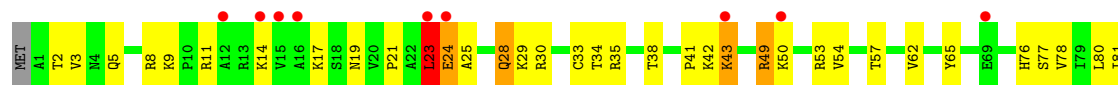
• Molecule 11: 30S ribosomal protein S11

Chain AK:



• Molecule 12: 30S ribosomal protein S12

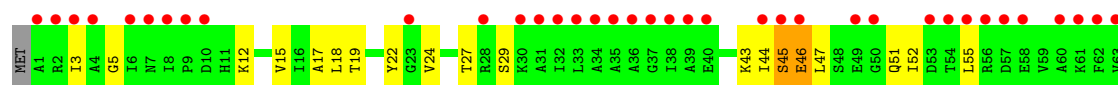
Chain AL:





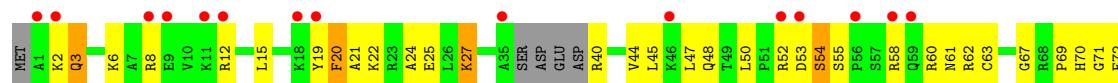
- Molecule 13: 30S ribosomal protein S13

Chain AM:



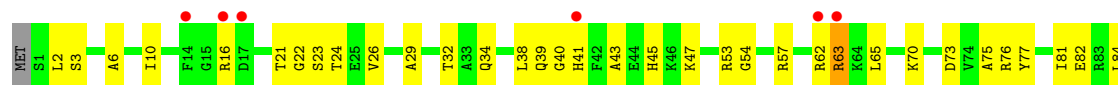
- Molecule 14: 30S ribosomal protein S14

Chain AN:



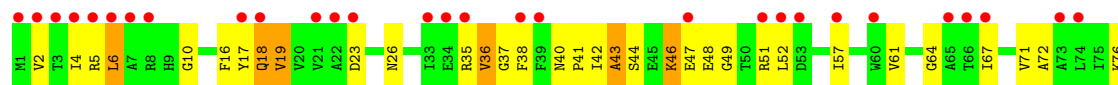
- Molecule 15: 30S ribosomal protein S15

Chain AO:



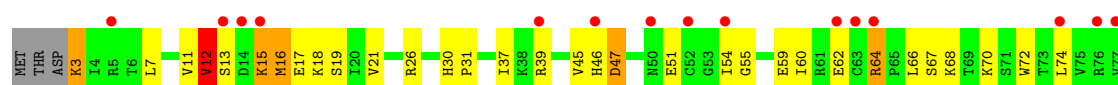
- Molecule 16: 30S ribosomal protein S16

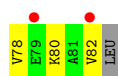
Chain AP:



- Molecule 17: 30S ribosomal protein S17

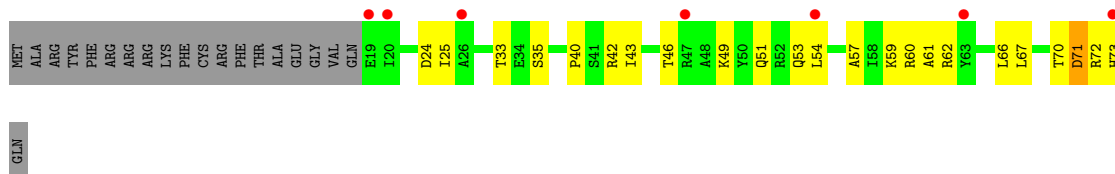
Chain AQ:





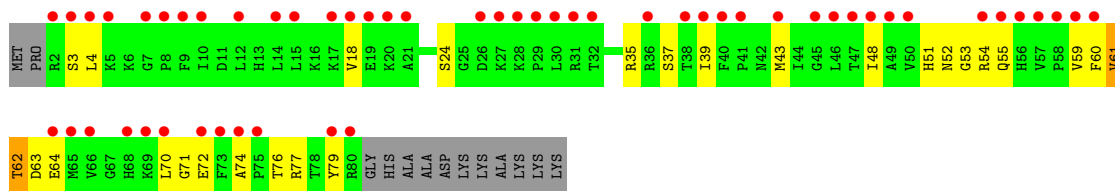
- Molecule 18: 30S ribosomal protein S18

Chain AR:



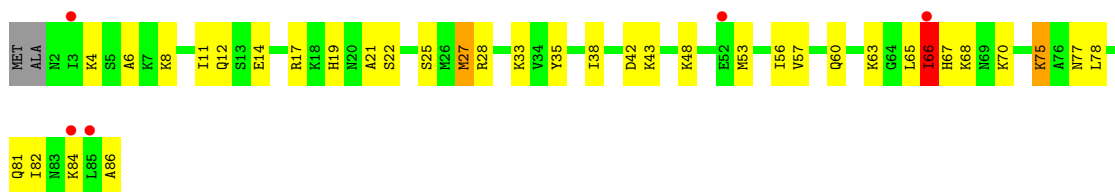
- Molecule 19: 30S ribosomal protein S19

Chain AS:



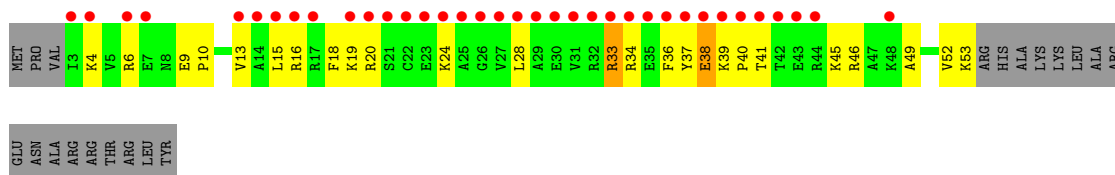
- Molecule 20: 30S ribosomal protein S20

Chain AT:



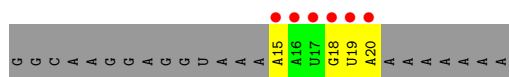
- Molecule 21: 30S ribosomal protein S21

Chain AU:



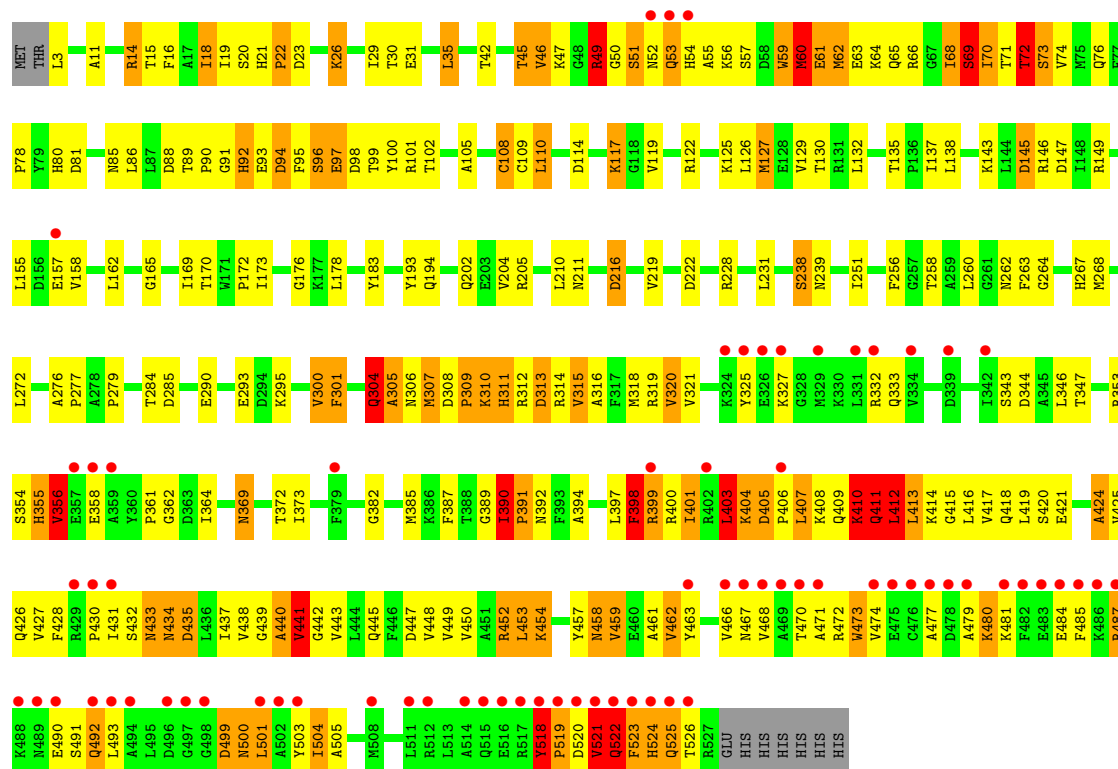
- Molecule 22: messenger RNA

Chain AV:

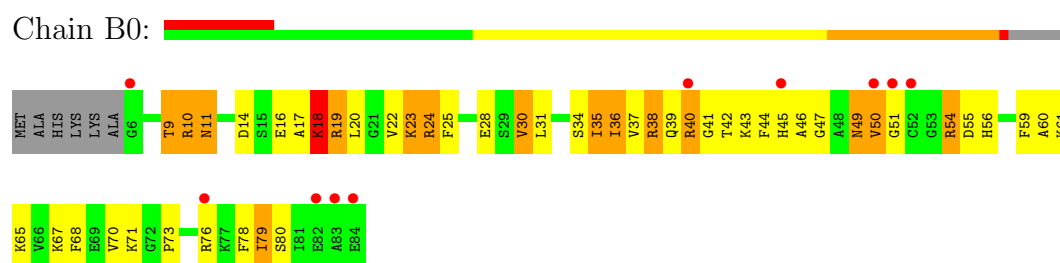


- Molecule 23: Peptide chain release factor 3

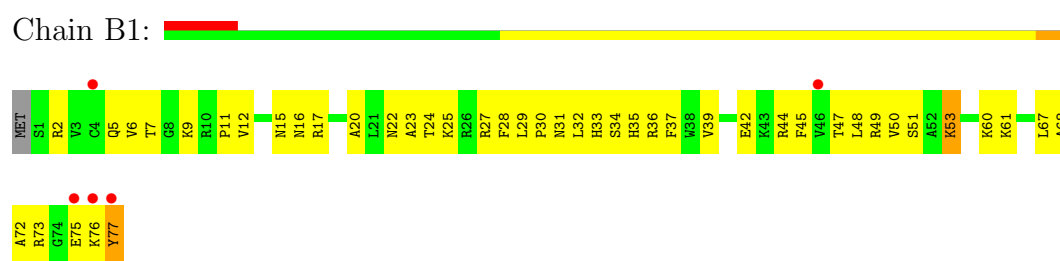
Chain AW:



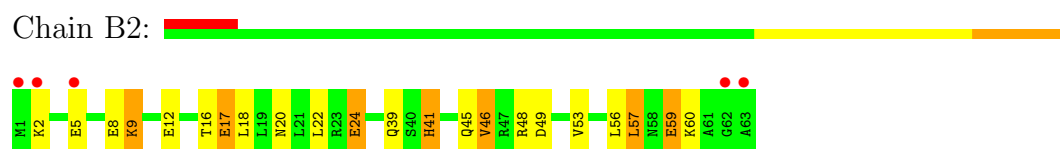
• Molecule 24: 50S ribosomal protein L27



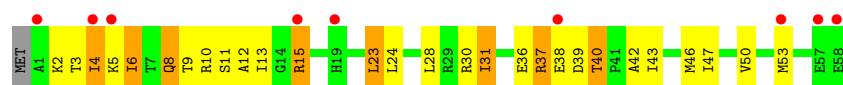
• Molecule 25: 50S ribosomal protein L28



• Molecule 26: 50S ribosomal protein L29



Chain B3: 



- Molecule 28: 50S ribosomal protein L32

Chain B4: 



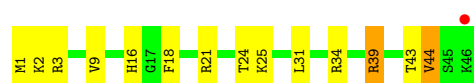
- Molecule 29: 50S ribosomal protein L33

Chain B5: 



- Molecule 30: 50S ribosomal protein L34

Chain B6: 



- Molecule 31: 50S ribosomal protein L35

Chain B7: 



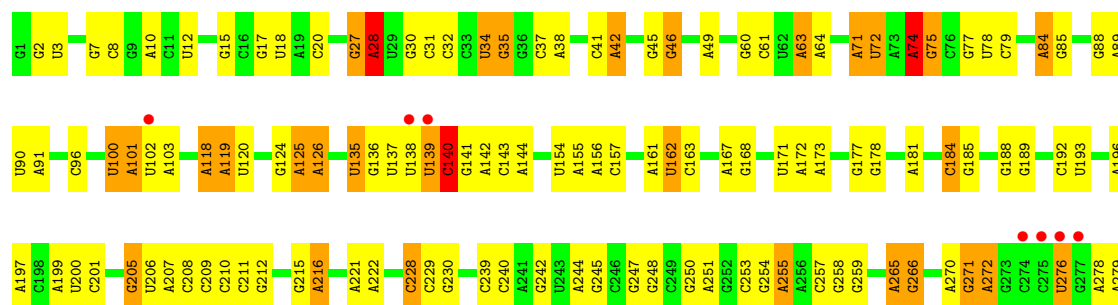
- Molecule 32: 50S ribosomal protein L36

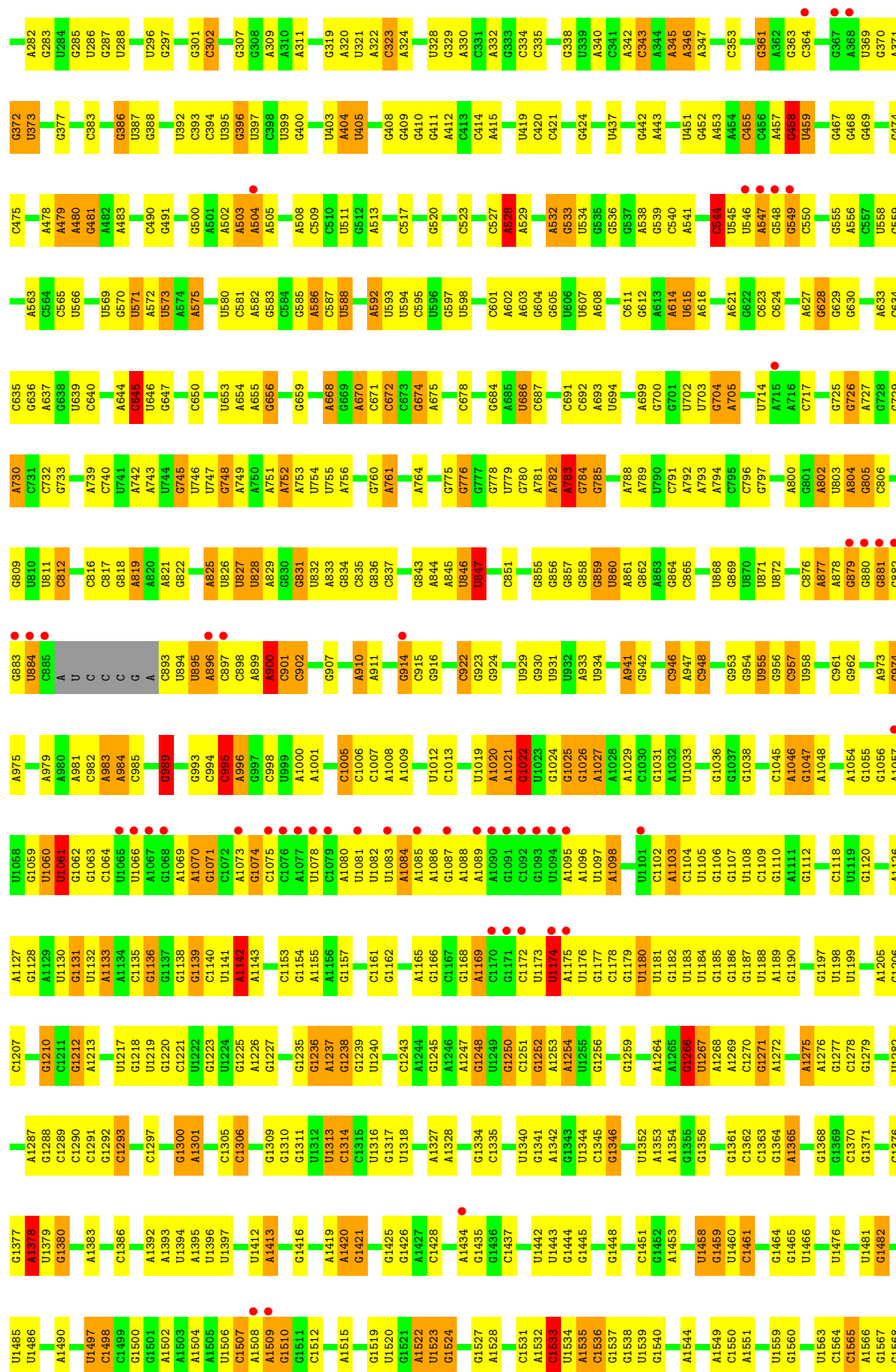
Chain B8: 



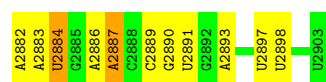
- Molecule 33: 23S rRNA

Chain BA: 



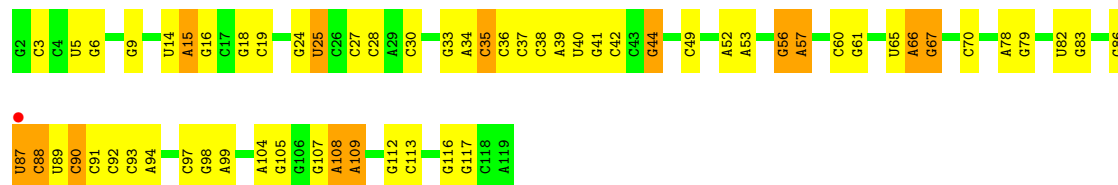






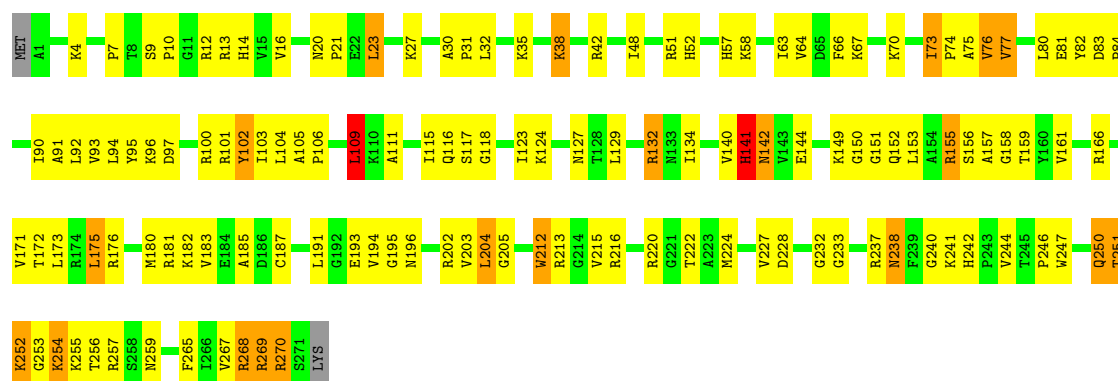
• Molecule 34: 5S rRNA

Chain BB:



• Molecule 35: 50S ribosomal protein L2

Chain BC:



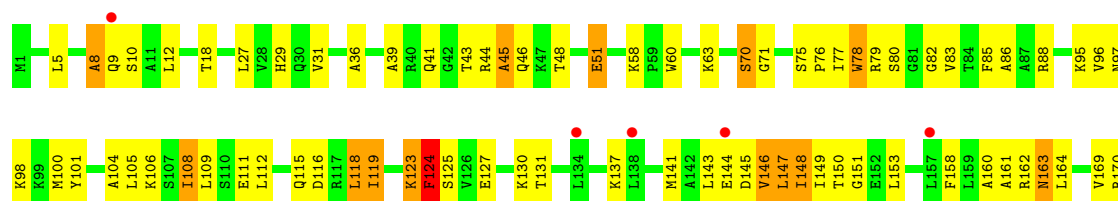
• Molecule 36: 50S ribosomal protein L3

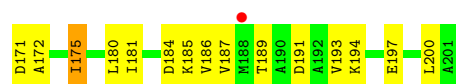
Chain BD:



• Molecule 37: 50S ribosomal protein L4

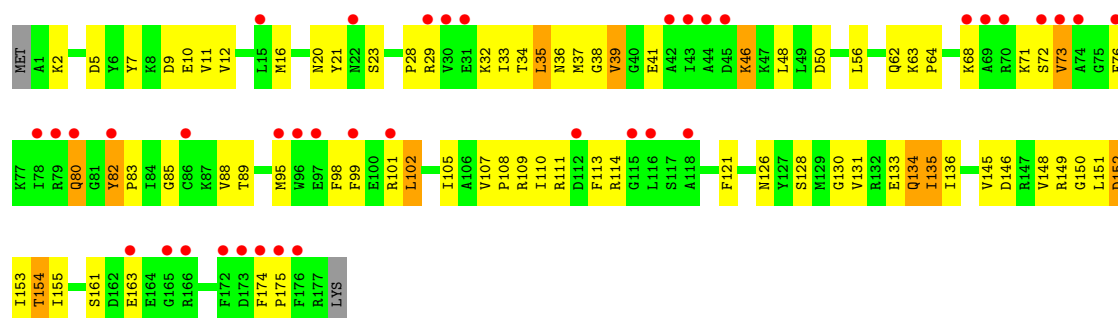
Chain BE:





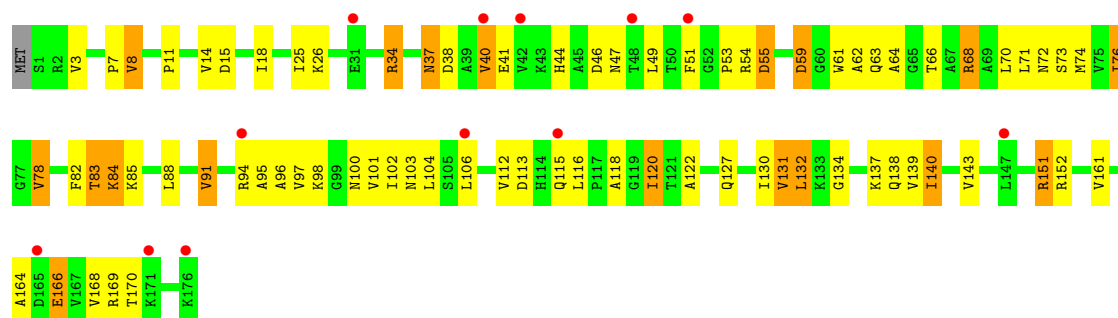
• Molecule 38: 50S ribosomal protein L5

Chain BF:



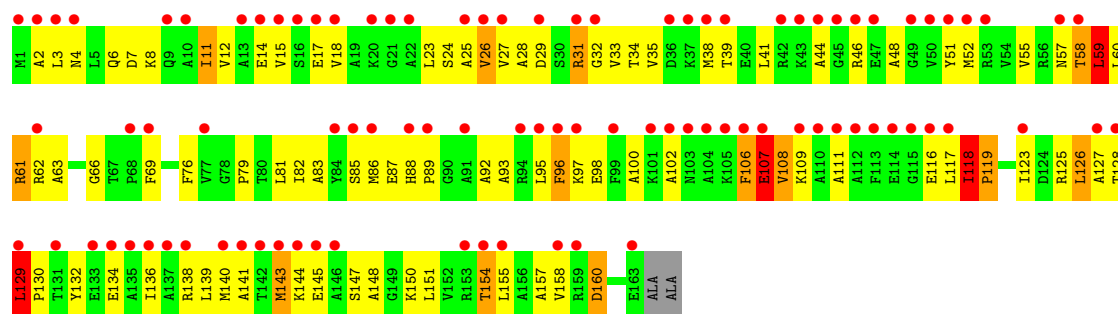
• Molecule 39: 50S ribosomal protein L6

Chain BG:



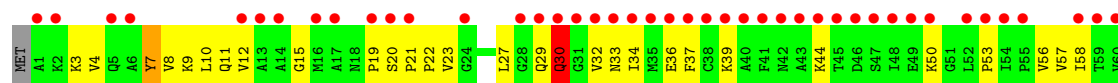
• Molecule 40: 50S ribosomal protein L10

Chain BH:



• Molecule 41: 50S ribosomal protein L11

Chain BI:

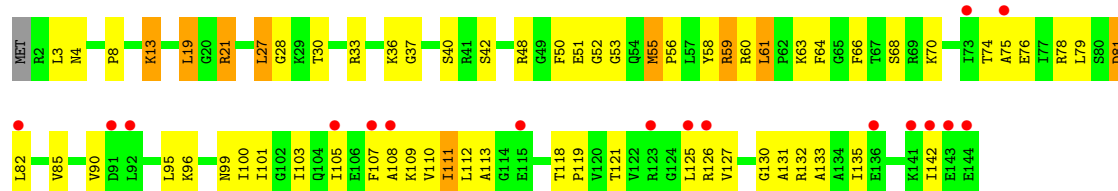


L140	D141	I142
K68	R69	V73
T3	F4	T5
A6	K7	P8
V11	H12	R13
D14	M15	V16
V17	O18	D19
A20	T21	G22
K23	T24	L25
G26	A29	T30
E31	R34	R35
L36	K39	H40
K41	A42	E43
E44	T45	P46
H47	V48	D49
T50	G51	S52
B53	L54	V55
V56	L57	N58
A59	P60	K61
V64	T65	V73

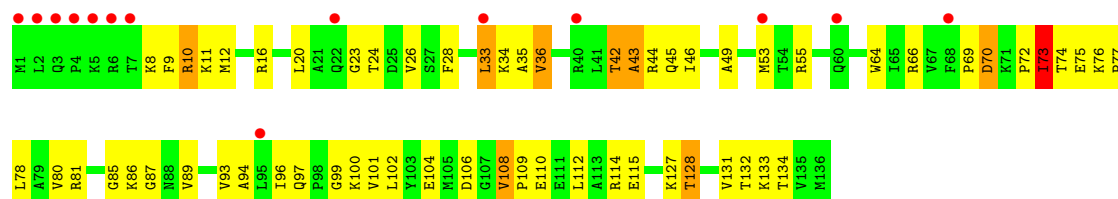
- Chain BO:



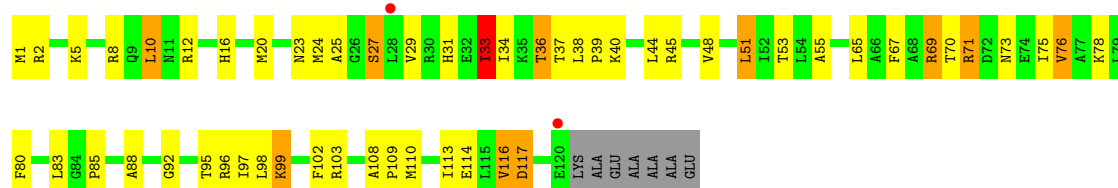
- Chain BP:



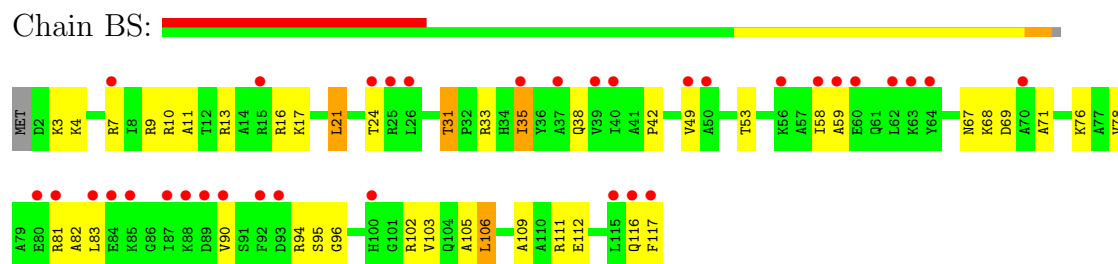
- Chain BQ:



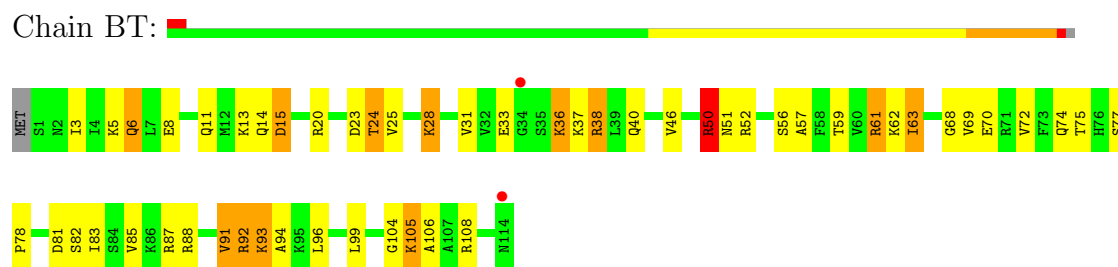
- Chain BR:



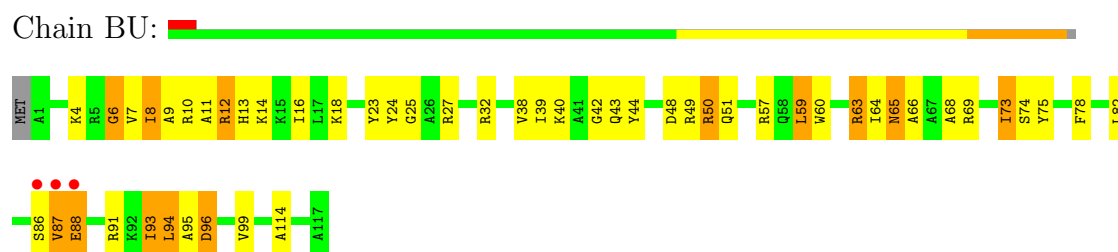
- Molecule 48: 50S ribosomal protein L18



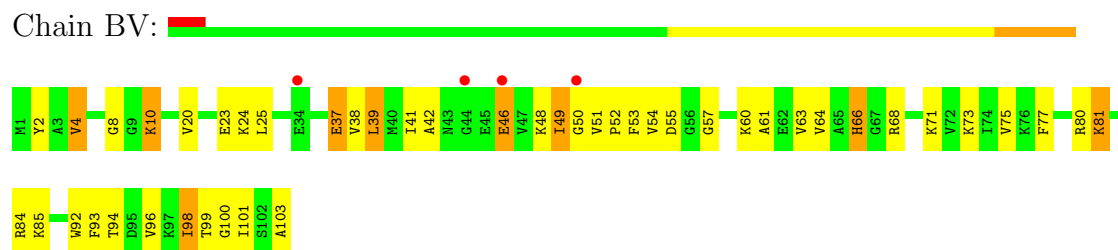
- Molecule 49: 50S ribosomal protein L19



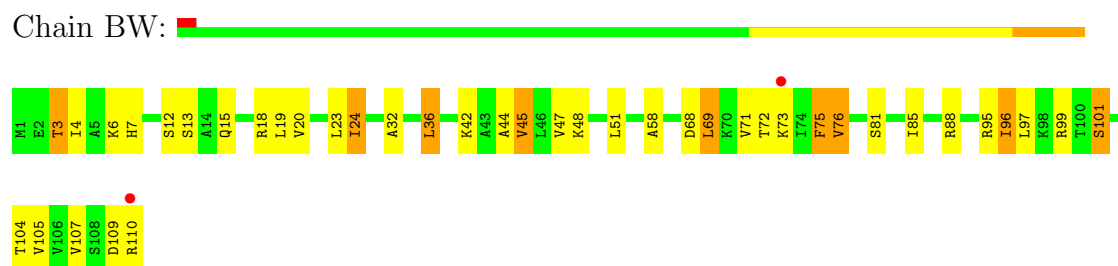
- Molecule 50: 50S ribosomal protein L20



- Molecule 51: 50S ribosomal protein L21

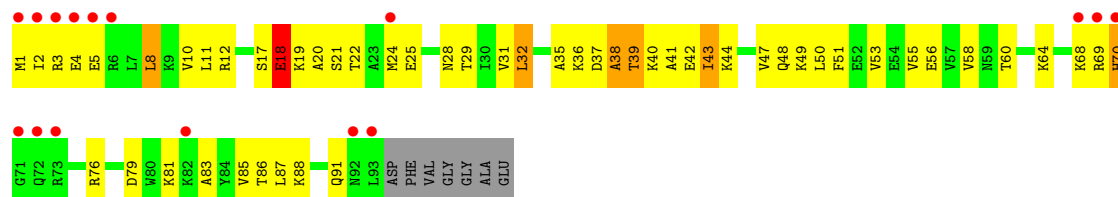


- Molecule 52: 50S ribosomal protein L22



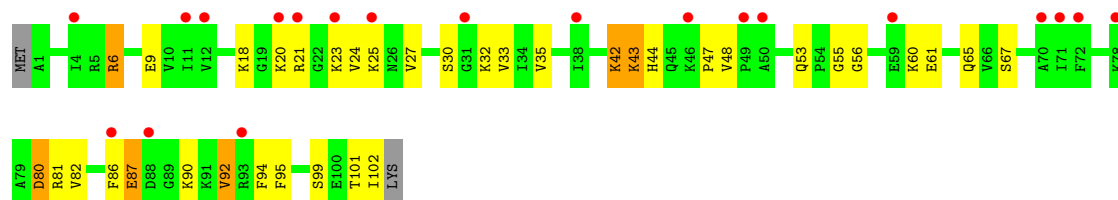
- Molecule 53: 50S ribosomal protein L23

Chain BX:



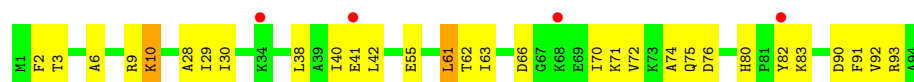
- Molecule 54: 50S ribosomal protein L24

Chain BY:



- Molecule 55: 50S ribosomal protein L25

Chain BZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	258.00Å 312.00Å 333.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 59.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.70) 98.1 (59.67-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2, phenix	Depositor
R, R_{free}	0.240 , 0.290 0.253 , 0.296	Depositor DCC
R_{free} test set	16644 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	7 of 329524 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	146665	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.41	0/36809	0.84	55/57423 (0.1%)
2	AB	0.32	0/1735	0.65	0/2338
3	AC	0.35	0/1651	0.57	0/2225
4	AD	0.35	0/1665	0.58	0/2227
5	AE	0.38	0/1118	0.69	0/1504
6	AF	0.36	0/835	0.60	0/1128
7	AG	0.29	0/1195	0.52	0/1602
8	AH	0.31	0/989	0.53	0/1326
9	AI	0.32	0/1034	0.61	0/1375
10	AJ	0.33	0/796	0.59	0/1077
11	AK	0.35	0/893	0.61	0/1205
12	AL	0.36	0/969	0.70	1/1300 (0.1%)
13	AM	0.29	0/892	0.58	0/1193
14	AN	0.31	0/785	0.66	0/1043
15	AO	0.34	0/722	0.60	0/964
16	AP	0.35	0/659	0.61	0/884
17	AQ	0.36	0/657	0.66	0/881
18	AR	0.41	0/462	0.61	0/621
19	AS	0.28	0/652	0.49	0/877
20	AT	0.41	0/671	0.68	0/888
21	AU	0.34	0/430	0.69	0/570
22	AV	0.45	0/144	0.93	0/222
23	AW	0.48	4/4221 (0.1%)	0.72	4/5702 (0.1%)
24	B0	0.48	0/603	0.82	0/797
25	B1	0.37	0/635	0.69	0/848
26	B2	0.41	0/510	0.75	1/677 (0.1%)
27	B3	0.39	0/453	0.68	0/605
28	B4	0.41	0/450	0.66	0/599
29	B5	0.40	0/416	0.55	0/554
30	B6	0.43	0/380	0.67	0/498
31	B7	0.39	0/513	0.70	1/676 (0.1%)
32	B8	0.36	0/303	0.64	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BA	0.50	3/68601 (0.0%)	0.94	135/107017 (0.1%)
34	BB	0.41	0/2828	0.83	0/4410
35	BC	0.43	0/2121	0.76	1/2852 (0.0%)
36	BD	0.49	0/1586	0.80	0/2134
37	BE	0.40	0/1571	0.72	1/2113 (0.0%)
38	BF	0.33	0/1434	0.55	0/1926
39	BG	0.40	0/1343	0.65	0/1816
40	BH	0.36	0/1244	0.74	2/1675 (0.1%)
41	BI	0.29	0/1046	0.60	0/1410
42	BJ	0.35	0/227	0.65	0/304
42	BK	0.31	0/227	0.51	0/304
42	BL	0.30	0/227	0.51	0/304
42	BM	0.36	0/227	0.58	0/304
43	BN	0.49	0/1152	0.78	0/1551
44	BO	0.44	0/947	0.71	0/1268
45	BP	0.40	0/1054	0.77	1/1403 (0.1%)
46	BQ	0.39	0/1093	0.63	0/1460
47	BR	0.45	0/973	0.75	1/1301 (0.1%)
48	BS	0.34	0/902	0.57	0/1209
49	BT	0.46	0/929	0.75	0/1242
50	BU	0.54	0/960	0.73	0/1278
51	BV	0.37	0/829	0.71	0/1107
52	BW	0.48	0/864	0.77	0/1156
53	BX	0.45	0/744	0.78	0/994
54	BY	0.40	0/787	0.73	0/1051
55	BZ	0.35	0/766	0.59	0/1025
All	All	0.44	7/158929 (0.0%)	0.84	203/236840 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
3	AC	0	1
5	AE	0	2
6	AF	0	1
11	AK	0	1
13	AM	0	1
14	AN	0	2
23	AW	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	B0	0	1
37	BE	0	1
39	BG	0	1
40	BH	0	3
41	BI	0	2
43	BN	0	1
45	BP	0	1
47	BR	0	1
50	BU	0	1
53	BX	0	1
54	BY	0	1
All	All	0	28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1914	C	O3'-P	-15.87	1.42	1.61
23	AW	22	PRO	C-N	9.22	1.55	1.34
33	BA	2104	C	O3'-P	-8.83	1.50	1.61
23	AW	72	THR	C-O	5.98	1.34	1.23
23	AW	73	SER	CB-OG	5.42	1.49	1.42

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1914	C	OP2-P-O3'	13.60	135.11	105.20
33	BA	1914	C	P-O3'-C3'	-12.52	104.68	119.70
33	BA	140	C	C2-N1-C1'	9.97	129.77	118.80
33	BA	645	C	C2-N1-C1'	9.86	129.65	118.80
35	BC	109	LEU	CA-CB-CG	9.67	137.53	115.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	135	MET	Peptide
2	AB	20	ARG	Peptide
2	AB	218	ALA	Peptide
3	AC	153	SER	Peptide
5	AE	78	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32873	0	16542	561	1
2	AB	1704	0	1732	81	0
3	AC	1624	0	1699	67	4
4	AD	1643	0	1710	70	1
5	AE	1105	0	1148	46	0
6	AF	817	0	808	33	0
7	AG	1181	0	1240	34	0
8	AH	979	0	1034	35	0
9	AI	1022	0	1070	53	0
10	AJ	786	0	828	43	0
11	AK	877	0	887	37	0
12	AL	955	0	1019	63	0
13	AM	883	0	944	38	0
14	AN	774	0	827	41	0
15	AO	714	0	737	21	0
16	AP	649	0	666	23	0
17	AQ	648	0	691	26	0
18	AR	455	0	478	14	0
19	AS	637	0	665	17	1
20	AT	665	0	714	24	0
21	AU	425	0	449	22	0
22	AV	129	0	65	2	0
23	AW	4144	0	4127	307	0
24	B0	596	0	610	71	0
25	B1	625	0	655	36	0
26	B2	509	0	543	15	0
27	B3	449	0	491	21	0
28	B4	444	0	461	14	0
29	B5	409	0	440	6	0
30	B6	377	0	418	8	0
31	B7	504	0	574	16	0
32	B8	302	0	340	21	0
33	BA	61252	0	30808	1107	4
34	BB	2529	0	1281	45	0
35	BC	2082	0	2157	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BD	1565	0	1616	102	0
37	BE	1552	0	1619	65	0
38	BF	1410	0	1447	62	0
39	BG	1323	0	1374	58	0
40	BH	1230	0	1282	91	0
41	BI	1032	0	1088	42	0
42	BJ	227	0	237	13	0
42	BK	227	0	237	5	0
42	BL	227	0	237	8	0
42	BM	227	0	237	14	0
43	BN	1129	0	1162	67	0
44	BO	938	0	1012	38	0
45	BP	1045	0	1117	49	0
46	BQ	1074	0	1157	46	0
47	BR	960	0	1000	41	0
48	BS	892	0	923	26	0
49	BT	917	0	965	44	0
50	BU	947	0	1022	55	0
51	BV	816	0	839	49	0
52	BW	857	0	922	24	0
53	BX	738	0	807	40	0
54	BY	779	0	834	26	0
55	BZ	753	0	780	19	1
56	AW	32	0	13	7	0
57	AW	1	0	0	0	0
All	All	146665	0	100785	3630	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 3630 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:497:G:OP2	23:AW:480:LYS:HE3	1.11	1.25
1:AA:497:G:OP2	23:AW:480:LYS:CE	1.83	1.25
12:AL:101:LEU:HG	23:AW:409:GLN:NE2	1.53	1.21
33:BA:974:G:C8	33:BA:989:G:C2	2.31	1.18
40:BH:25:ALA:HB3	40:BH:85:SER:OG	1.38	1.18

The worst 5 of 6 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	Distance(Å)	Clash(Å)
3:AC:131:ARG:NH2	33:BA:2156:G:O2'[4_445]	1.71	0.49
3:AC:135:ARG:CG	33:BA:2157:G:OP2[4_445]	1.99	0.21
3:AC:131:ARG:CB	33:BA:2157:G:OP1[4_445]	2.11	0.09
1:AA:205:A:OP2	19:AS:24:SER:OG[2_355]	2.12	0.08
3:AC:131:ARG:NE	33:BA:2157:G:O5'[4_445]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	175 (81%)	40 (18%)	1 (0%)	38	88
3	AC	204/233 (88%)	178 (87%)	24 (12%)	2 (1%)	22	81
4	AD	203/206 (98%)	170 (84%)	29 (14%)	4 (2%)	11	68
5	AE	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	8	62
6	AF	98/135 (73%)	77 (79%)	20 (20%)	1 (1%)	22	81
7	AG	149/179 (83%)	124 (83%)	25 (17%)	0	100	100
8	AH	127/130 (98%)	113 (89%)	13 (10%)	1 (1%)	27	83
9	AI	125/130 (96%)	109 (87%)	12 (10%)	4 (3%)	6	58
10	AJ	96/103 (93%)	77 (80%)	16 (17%)	3 (3%)	7	59
11	AK	115/129 (89%)	100 (87%)	15 (13%)	0	100	100
12	AL	121/124 (98%)	107 (88%)	12 (10%)	2 (2%)	14	71
13	AM	112/118 (95%)	96 (86%)	14 (12%)	2 (2%)	13	70
14	AN	92/101 (91%)	73 (79%)	19 (21%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	18	76
17	AQ	78/84 (93%)	65 (83%)	12 (15%)	1 (1%)	18	76
18	AR	53/75 (71%)	46 (87%)	7 (13%)	0	100	100
19	AS	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
20	AT	83/87 (95%)	73 (88%)	9 (11%)	1 (1%)	19	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AU	49/71 (69%)	36 (74%)	12 (24%)	1 (2%)	11	68
23	AW	523/534 (98%)	382 (73%)	82 (16%)	59 (11%)	1	16
24	B0	77/85 (91%)	49 (64%)	24 (31%)	4 (5%)	3	42
25	B1	75/78 (96%)	65 (87%)	10 (13%)	0	100	100
26	B2	61/63 (97%)	47 (77%)	12 (20%)	2 (3%)	6	57
27	B3	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
28	B4	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	12	69
29	B5	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	11	67
30	B6	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	10	65
31	B7	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	14	72
32	B8	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	8	61
35	BC	269/273 (98%)	234 (87%)	29 (11%)	6 (2%)	10	66
36	BD	207/209 (99%)	176 (85%)	26 (13%)	5 (2%)	9	64
37	BE	199/201 (99%)	170 (85%)	23 (12%)	6 (3%)	7	59
38	BF	175/179 (98%)	145 (83%)	27 (15%)	3 (2%)	14	71
39	BG	174/177 (98%)	141 (81%)	32 (18%)	1 (1%)	33	86
40	BH	161/165 (98%)	123 (76%)	31 (19%)	7 (4%)	4	48
41	BI	139/142 (98%)	113 (81%)	26 (19%)	0	100	100
42	BJ	28/121 (23%)	20 (71%)	8 (29%)	0	100	100
42	BK	28/121 (23%)	23 (82%)	5 (18%)	0	100	100
42	BL	28/121 (23%)	22 (79%)	6 (21%)	0	100	100
42	BM	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	2	32
43	BN	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	16	74
44	BO	120/123 (98%)	97 (81%)	19 (16%)	4 (3%)	6	57
45	BP	141/144 (98%)	118 (84%)	22 (16%)	1 (1%)	30	85
46	BQ	134/136 (98%)	112 (84%)	18 (13%)	4 (3%)	7	59
47	BR	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	27	83
48	BS	114/117 (97%)	99 (87%)	14 (12%)	1 (1%)	25	82
49	BT	112/115 (97%)	93 (83%)	16 (14%)	3 (3%)	8	62
50	BU	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	14	71
51	BV	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	11	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BW	108/110 (98%)	97 (90%)	10 (9%)	1 (1%)	25	82
53	BX	91/100 (91%)	62 (68%)	25 (28%)	4 (4%)	4	48
54	BY	100/104 (96%)	78 (78%)	21 (21%)	1 (1%)	22	81
55	BZ	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
All	All	6270/7019 (89%)	5201 (83%)	915 (15%)	154 (2%)	9	63

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	14	VAL
4	AD	30	LYS
4	AD	125	ASN
13	AM	46	GLU
17	AQ	12	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	149 (83%)	31 (17%)	3	21
3	AC	170/190 (90%)	145 (85%)	25 (15%)	4	30
4	AD	172/173 (99%)	148 (86%)	24 (14%)	5	33
5	AE	113/126 (90%)	93 (82%)	20 (18%)	3	20
6	AF	87/116 (75%)	74 (85%)	13 (15%)	4	30
7	AG	124/147 (84%)	114 (92%)	10 (8%)	17	64
8	AH	104/105 (99%)	89 (86%)	15 (14%)	5	31
9	AI	105/107 (98%)	87 (83%)	18 (17%)	3	22
10	AJ	86/90 (96%)	70 (81%)	16 (19%)	2	16
11	AK	90/99 (91%)	77 (86%)	13 (14%)	5	31
12	AL	103/104 (99%)	88 (85%)	15 (15%)	5	31
13	AM	92/96 (96%)	87 (95%)	5 (5%)	31	79
14	AN	79/84 (94%)	71 (90%)	8 (10%)	11	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	76/77 (99%)	69 (91%)	7 (9%)	13	57
16	AP	65/65 (100%)	58 (89%)	7 (11%)	9	48
17	AQ	74/78 (95%)	62 (84%)	12 (16%)	3	25
18	AR	48/65 (74%)	44 (92%)	4 (8%)	16	62
19	AS	70/79 (89%)	65 (93%)	5 (7%)	21	70
20	AT	65/66 (98%)	58 (89%)	7 (11%)	9	48
21	AU	44/61 (72%)	38 (86%)	6 (14%)	5	35
23	AW	447/458 (98%)	380 (85%)	67 (15%)	4	30
24	B0	59/63 (94%)	44 (75%)	15 (25%)	1	7
25	B1	67/68 (98%)	61 (91%)	6 (9%)	14	58
26	B2	55/55 (100%)	48 (87%)	7 (13%)	6	38
27	B3	48/49 (98%)	39 (81%)	9 (19%)	2	16
28	B4	47/48 (98%)	44 (94%)	3 (6%)	25	74
29	B5	45/49 (92%)	40 (89%)	5 (11%)	9	46
30	B6	38/38 (100%)	34 (90%)	4 (10%)	10	49
31	B7	51/52 (98%)	49 (96%)	2 (4%)	43	85
32	B8	34/34 (100%)	31 (91%)	3 (9%)	14	60
35	BC	216/218 (99%)	184 (85%)	32 (15%)	4	30
36	BD	164/164 (100%)	145 (88%)	19 (12%)	8	43
37	BE	165/165 (100%)	144 (87%)	21 (13%)	6	38
38	BF	148/150 (99%)	134 (90%)	14 (10%)	12	55
39	BG	137/138 (99%)	115 (84%)	22 (16%)	3	26
40	BH	123/123 (100%)	105 (85%)	18 (15%)	5	31
41	BI	109/110 (99%)	94 (86%)	15 (14%)	5	34
42	BJ	26/85 (31%)	23 (88%)	3 (12%)	8	44
42	BK	26/85 (31%)	25 (96%)	1 (4%)	44	86
42	BL	26/85 (31%)	25 (96%)	1 (4%)	44	86
42	BM	26/85 (31%)	23 (88%)	3 (12%)	8	44
43	BN	116/116 (100%)	90 (78%)	26 (22%)	1	10
44	BO	103/104 (99%)	83 (81%)	20 (19%)	2	14
45	BP	102/103 (99%)	89 (87%)	13 (13%)	6	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BQ	109/109 (100%)	91 (84%)	18 (16%)	3	24
47	BR	100/103 (97%)	85 (85%)	15 (15%)	4	30
48	BS	86/87 (99%)	72 (84%)	14 (16%)	3	25
49	BT	99/100 (99%)	82 (83%)	17 (17%)	3	21
50	BU	89/90 (99%)	75 (84%)	14 (16%)	4	27
51	BV	84/84 (100%)	73 (87%)	11 (13%)	6	37
52	BW	93/93 (100%)	76 (82%)	17 (18%)	2	17
53	BX	80/84 (95%)	69 (86%)	11 (14%)	5	34
54	BY	83/85 (98%)	69 (83%)	14 (17%)	3	23
55	BZ	78/78 (100%)	73 (94%)	5 (6%)	25	74
All	All	5226/5685 (92%)	4500 (86%)	726 (14%)	5	34

5 of 726 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	B0	9	THR
35	BC	250	GLN
51	BV	37	GLU
24	B0	49	ASN
29	B5	4	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
23	AW	21	HIS
23	AW	409	GLN
51	BV	66	HIS
23	AW	76	GLN
23	AW	306	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1531/1533 (99%)	278 (18%)	29 (1%)
22	AV	5/27 (18%)	3 (60%)	0
33	BA	2849/2903 (98%)	501 (17%)	53 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	BB	117/118 (99%)	20 (17%)	3 (2%)
All	All	4502/4581 (98%)	802 (17%)	85 (1%)

5 of 802 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	BA	404	A
33	BA	704	G
33	BA	2726	A
33	BA	442	G
33	BA	504	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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
56	GNP	AW	601	57	34,34,34	2.44	9 (26%)	48,54,54	5.28	11 (22%)

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
56	GNP	AW	601	57	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AW	601	GNP	PB-N3B	-6.81	1.58	1.64
56	AW	601	GNP	PG-N3B	-6.67	1.58	1.64
56	AW	601	GNP	PB-O3A	-5.68	1.52	1.59
56	AW	601	GNP	PA-O3A	-4.43	1.52	1.59
56	AW	601	GNP	PG-O1G	4.28	1.51	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AW	601	GNP	C6-C5-N7	-33.78	129.59	134.14
56	AW	601	GNP	C6-N1-C2	8.14	124.80	120.20
56	AW	601	GNP	PB-N3B-PG	-4.98	121.69	130.07
56	AW	601	GNP	O2B-PB-O1B	4.16	118.69	109.90
56	AW	601	GNP	PA-O3A-PB	-3.73	119.27	132.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1532/1533 (99%)	0.09	32 (2%) 60 38	72, 119, 232, 344	0
2	AB	218/241 (90%)	1.42	59 (27%) 1 2	124, 181, 235, 328	0
3	AC	206/233 (88%)	0.71	12 (5%) 22 15	88, 129, 167, 218	0
4	AD	205/206 (99%)	0.78	17 (8%) 11 9	88, 120, 177, 250	0
5	AE	150/167 (89%)	0.64	7 (4%) 30 20	88, 123, 176, 253	0
6	AF	100/135 (74%)	0.97	16 (16%) 3 3	106, 153, 182, 204	0
7	AG	151/179 (84%)	1.48	45 (29%) 1 2	132, 178, 218, 300	0
8	AH	129/130 (99%)	0.96	17 (13%) 4 4	108, 137, 177, 228	0
9	AI	127/130 (97%)	1.39	31 (24%) 1 2	102, 145, 212, 252	0
10	AJ	98/103 (95%)	1.16	20 (20%) 1 2	95, 124, 243, 282	0
11	AK	117/129 (90%)	0.36	7 (5%) 21 15	81, 116, 155, 200	0
12	AL	123/124 (99%)	0.72	10 (8%) 12 10	83, 103, 188, 250	0
13	AM	114/118 (96%)	1.93	48 (42%) 1 1	137, 194, 233, 273	0
14	AN	96/101 (95%)	1.12	15 (15%) 3 4	93, 161, 212, 250	0
15	AO	88/89 (98%)	0.83	8 (9%) 9 8	100, 137, 190, 275	0
16	AP	82/82 (100%)	1.78	31 (37%) 1 1	78, 105, 160, 252	0
17	AQ	80/84 (95%)	1.27	17 (21%) 1 2	96, 139, 204, 301	0
18	AR	55/75 (73%)	1.02	7 (12%) 4 5	91, 119, 176, 247	0
19	AS	79/92 (85%)	2.91	54 (68%) 0 1	158, 201, 238, 282	0
20	AT	85/87 (97%)	0.68	5 (5%) 22 15	96, 126, 172, 184	0
21	AU	51/71 (71%)	3.55	36 (70%) 0 1	158, 215, 255, 264	0
22	AV	6/27 (22%)	9.94	6 (100%) 0 0	221, 256, 294, 306	0
23	AW	525/534 (98%)	0.93	72 (13%) 4 4	35, 99, 188, 267	0
24	B0	79/85 (92%)	0.99	10 (12%) 4 5	61, 105, 177, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	B1	77/78 (98%)	1.09	6 (7%)	13 10	68, 83, 132, 154	0
26	B2	63/63 (100%)	0.57	5 (7%)	13 10	72, 100, 145, 187	0
27	B3	58/59 (98%)	1.10	9 (15%)	3 4	67, 92, 143, 174	0
28	B4	56/57 (98%)	0.31	1 (1%)	65 43	44, 65, 108, 150	0
29	B5	50/55 (90%)	2.60	30 (60%)	0 1	133, 176, 209, 228	0
30	B6	46/46 (100%)	0.40	1 (2%)	59 37	48, 60, 84, 197	0
31	B7	64/65 (98%)	0.80	4 (6%)	19 13	63, 85, 109, 128	0
32	B8	38/38 (100%)	1.16	3 (7%)	13 10	82, 104, 135, 178	0
33	BA	2853/2903 (98%)	0.01	109 (3%)	38 25	28, 79, 260, 445	0
34	BB	118/118 (100%)	-0.16	1 (0%)	83 63	71, 127, 173, 221	0
35	BC	271/273 (99%)	0.27	0	100 100	47, 77, 100, 151	0
36	BD	209/209 (100%)	0.22	1 (0%)	88 73	48, 64, 108, 162	0
37	BE	201/201 (100%)	0.44	6 (2%)	48 29	45, 94, 146, 200	0
38	BF	177/179 (98%)	1.21	38 (21%)	1 2	117, 157, 214, 286	0
39	BG	176/177 (99%)	0.78	12 (6%)	17 12	71, 108, 162, 189	0
40	BH	163/165 (98%)	2.73	93 (57%)	0 1	135, 263, 334, 394	0
41	BI	141/142 (99%)	3.32	95 (67%)	0 1	185, 276, 378, 452	0
42	BJ	30/121 (24%)	3.14	22 (73%)	0 1	222, 260, 328, 407	0
42	BK	30/121 (24%)	4.91	25 (83%)	0 1	222, 263, 318, 343	0
42	BL	30/121 (24%)	3.12	22 (73%)	0 1	187, 275, 348, 365	0
42	BM	30/121 (24%)	2.86	21 (70%)	0 1	206, 255, 324, 352	0
43	BN	142/142 (100%)	0.77	6 (4%)	35 22	56, 72, 105, 173	0
44	BO	122/123 (99%)	0.63	3 (2%)	54 34	48, 75, 107, 196	0
45	BP	143/144 (99%)	0.97	17 (11%)	5 6	55, 100, 149, 201	0
46	BQ	136/136 (100%)	0.99	14 (10%)	7 7	65, 92, 133, 188	0
47	BR	120/127 (94%)	0.38	2 (1%)	67 44	39, 64, 85, 233	0
48	BS	116/117 (99%)	1.54	34 (29%)	1 2	91, 125, 157, 180	0
49	BT	114/115 (99%)	0.28	2 (1%)	65 43	61, 83, 133, 164	0
50	BU	117/118 (99%)	0.10	3 (2%)	53 33	44, 69, 116, 219	0
51	BV	103/103 (100%)	0.48	4 (3%)	37 24	51, 93, 151, 334	0
52	BW	110/110 (100%)	0.39	2 (1%)	65 43	42, 61, 101, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
53	BX	93/100 (93%)	0.92	16 (17%) 2 3	52, 88, 150, 197	0
54	BY	102/104 (98%)	1.16	20 (19%) 2 2	68, 95, 169, 203	0
55	BZ	94/94 (100%)	0.54	4 (4%) 34 22	83, 112, 151, 177	0
All	All	10889/11600 (93%)	0.64	1213 (11%) 6 6	28, 105, 249, 452	0

The worst 5 of 1213 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	88	HIS	20.2
33	BA	2157	G	17.8
33	BA	885	C	16.2
22	AV	19	U	14.8
42	BK	11	VAL	13.9

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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	GNP	AW	601	32/32	0.22	0.30	81,97,115,121	0
57	MG	AW	602	1/1	0.19	-0.97	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.