



wwPDB X-ray Structure Validation Summary Report

Sep 14, 2023 – 02:43 AM EDT

PDB ID : 4V49
Title : Crystal Structure of a Streptomycin Dependent Ribosome from E. Coli 70S Ribosome.
Authors : Vila-Sanjurjo, A.; Ridgeway, W.K.; Seymaner, V.; Zhang, W.; Santoso, S.; Yu, K.; Cate, J.H.D.
Deposited on : 2003-06-13
Resolution : 8.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

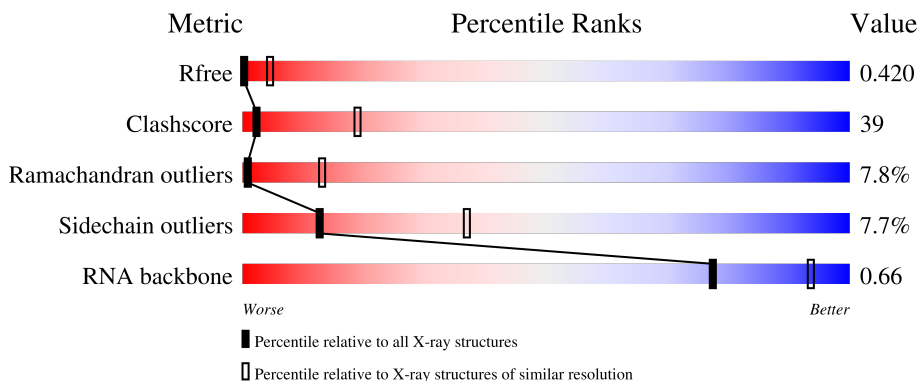
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.70 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}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RNA backbone	3102	1079 (11.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AA	1527	
2	AV	76	
2	AW	76	
3	AU	18	
4	AB	234	
5	AC	206	

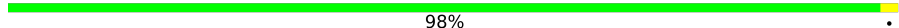
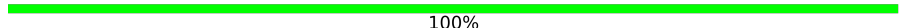
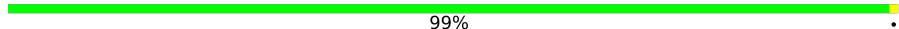
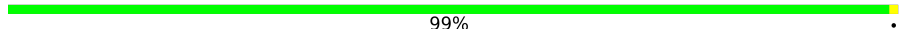
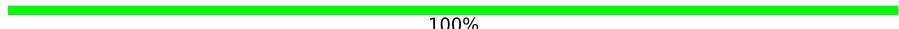
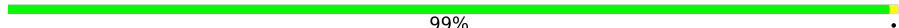
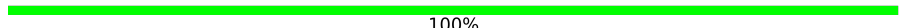
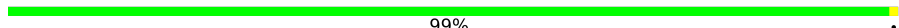
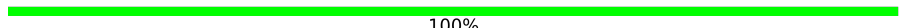
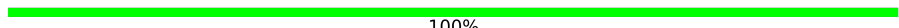
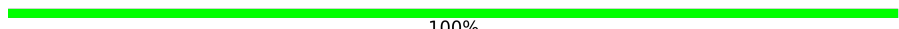
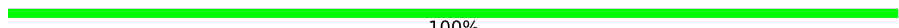
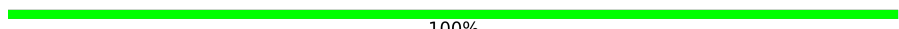
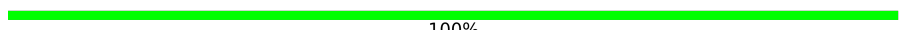
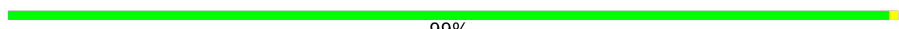
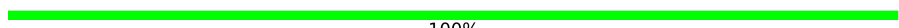
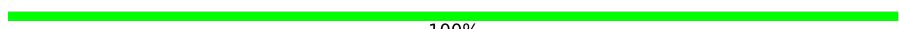
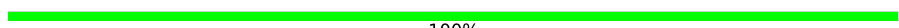
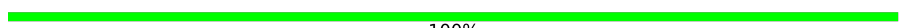
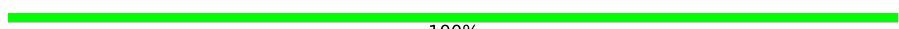
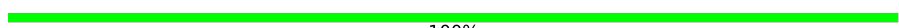

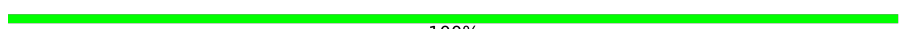


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Mol	Chain	Length	Quality of chain
6	AD	208	40% 54% 5%
7	AE	150	37% 53% 9%
8	AF	101	40% 58%
9	AG	155	42% 54%
10	AH	138	41% 50% 8%
11	AI	127	31% 60% 8%
12	AJ	98	15% 64% 19%
13	AK	119	24% 69% 7%
14	AL	124	34% 55% 11%
15	AM	125	26% 64% 10%
16	AN	60	22% 65% 13%
17	AO	88	36% 52% 11%
18	AP	83	37% 60%
19	AQ	104	38% 53% 8%
20	AR	73	32% 62% 7%
21	AS	80	22% 64% 14%
22	AT	99	27% 58% 14%
23	B0	2887	40% 47% 11%
24	B9	118	56% 41%
25	BA	270	100%
26	BB	205	100%
27	BC	197	100%
28	BD	178	98%
29	BE	177	100%
30	BF	52	100%

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Mol	Chain	Length	Quality of chain
31	BG	143	 98%
32	BH	143	 100%
33	BI	132	 99%
34	BJ	141	 99%
35	BK	124	 100%
36	BL	114	 99%
37	BM	111	 100%
38	BN	125	 99%
39	BO	117	 100%
40	BP	100	 100%
41	BQ	130	 100%
42	BR	93	 100%
43	BS	113	 100%
44	BT	173	 100%
45	BU	86	 99%
46	BV	16	 100%
47	BW	65	 100%
48	BX	55	 100%
49	BY	73	 100%
50	BZ	58	 100%
51	B1	53	 100%
52	B2	46	 100%
53	B3	63	 100%
54	B4	35	 100%
55	B5	217	 94% 6%

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 122017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1527	32819	14610	6085	10597	1527	0	0	0

- Molecule 2 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AV	76	1625	725	293	531	76	0	0	0
2	AW	76	1625	725	293	531	76	0	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AU	9	176	81	24	62	9	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AB	234	1900	1213	341	341	5	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AC	206	1612	1016	314	281	1	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AD	208	1702	1066	339	290	7	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AE	150	1146	724	217	201	4	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	AF	101	842	531	155	153	3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AG	155	1256	781	252	217	6	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AH	138	1115	705	215	192	3	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	AI	127	1010	639	198	173	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AJ	98	794	499	156	138	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AK	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AM	125	Total	C	N	O	S	0	0	0
			996	617	207	170	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AN	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	104	Total	C	N	O	S	0	0	0
			856	547	161	146	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	AR	73	596	380	118	98	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	AS	80	647	414	119	112	2	0	0	0

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	AT	99	762	469	162	129	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	B0	2825	60636	27047	11191	19573	2825	0	0	0

- Molecule 24 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	B9	118	2519	1124	464	813	118	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	BA	270	Total C 270 270	0	0	270

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BB	205	Total C 205 205	0	0	205

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	BC	197	Total C 197 197	0	0	197

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	BD	178	Total C 178 178	0	0	178

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	BE	177	Total C 177 177	0	0	177

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	BF	52	Total C 52 52	0	0	52

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	BG	143	Total C 143 143	0	0	143

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	BH	143	Total C 143 143	0	0	143

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	BI	132	Total C 132 132	0	0	132

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	BJ	141	Total C 141 141	0	0	141

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BK	124	Total C 124 124	0	0	124

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BL	114	Total C 114 114	0	0	114

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BM	111	Total C 111 111	0	0	111

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BN	125	Total C 125 125	0	0	125

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BO	117	Total C 117 117	0	0	117

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	BP	100	Total C 100 100	0	0	100

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BQ	130	Total C 130 130	0	0	130

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	BR	93	Total C 93 93	0	0	93

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	BS	113	Total C 113 113	0	0	113

- Molecule 44 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	BT	173	Total C 173 173	0	0	173

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	BU	86	Total C 86 86	0	0	86

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	BV	16	Total C 16 16	0	0	16

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	BW	65	Total C 65 65	0	0	65

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	BX	55	Total C 55 55	0	0	55

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	BY	73	Total C 73 73	0	0	73

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	BZ	58	Total C 58 58	0	0	58

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	B1	53	Total C 53 53	0	0	53

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	B2	46	Total C 46 46	0	0	46

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	B3	63	Total C 63 63	0	0	63

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	B4	35	Total C 35 35	0	0	35

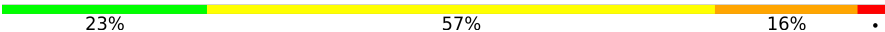
- Molecule 55 is a protein called 50S ribosomal protein L1P.

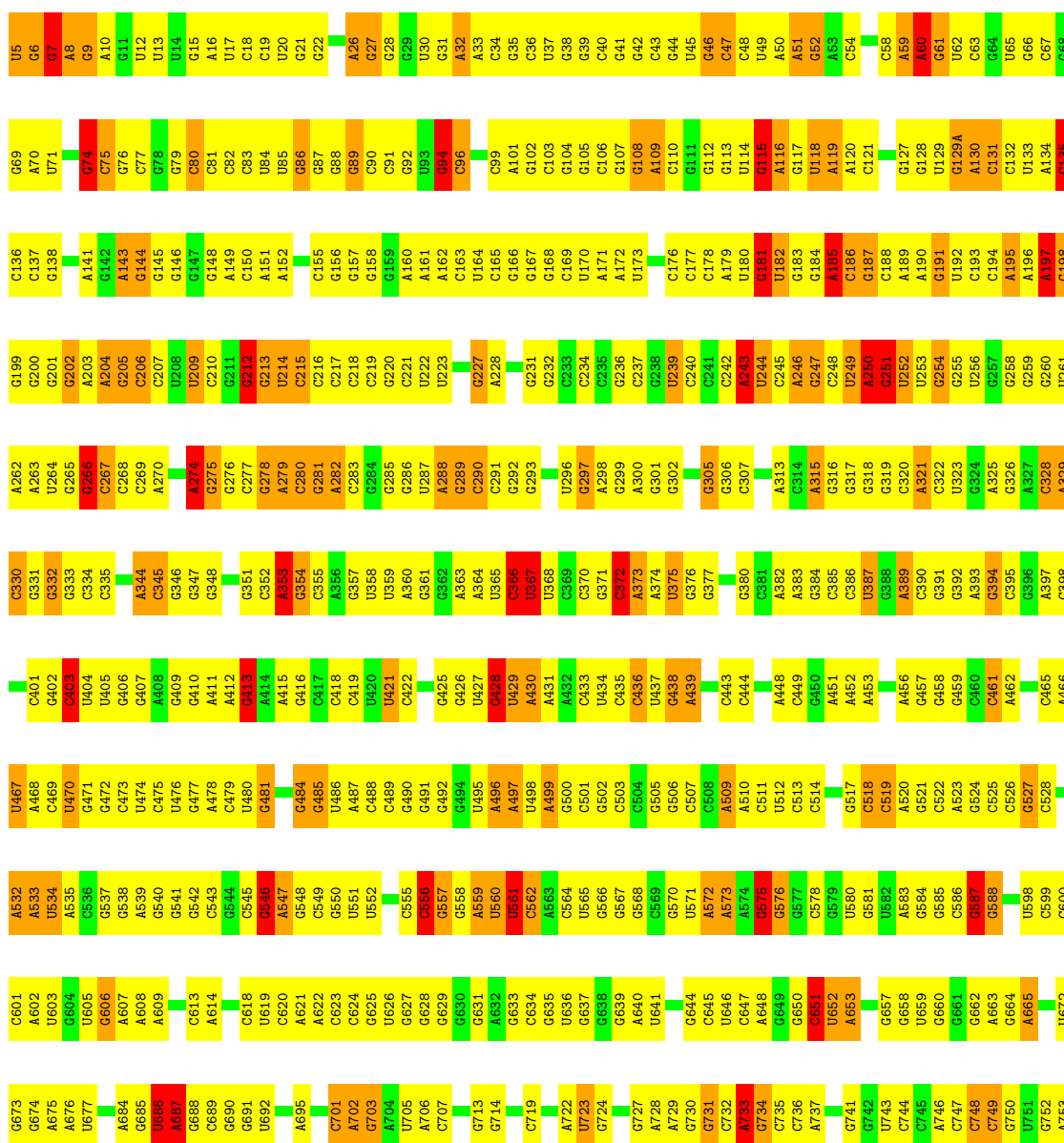
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
55	B5	217	Total 217	C 217	0	0	217

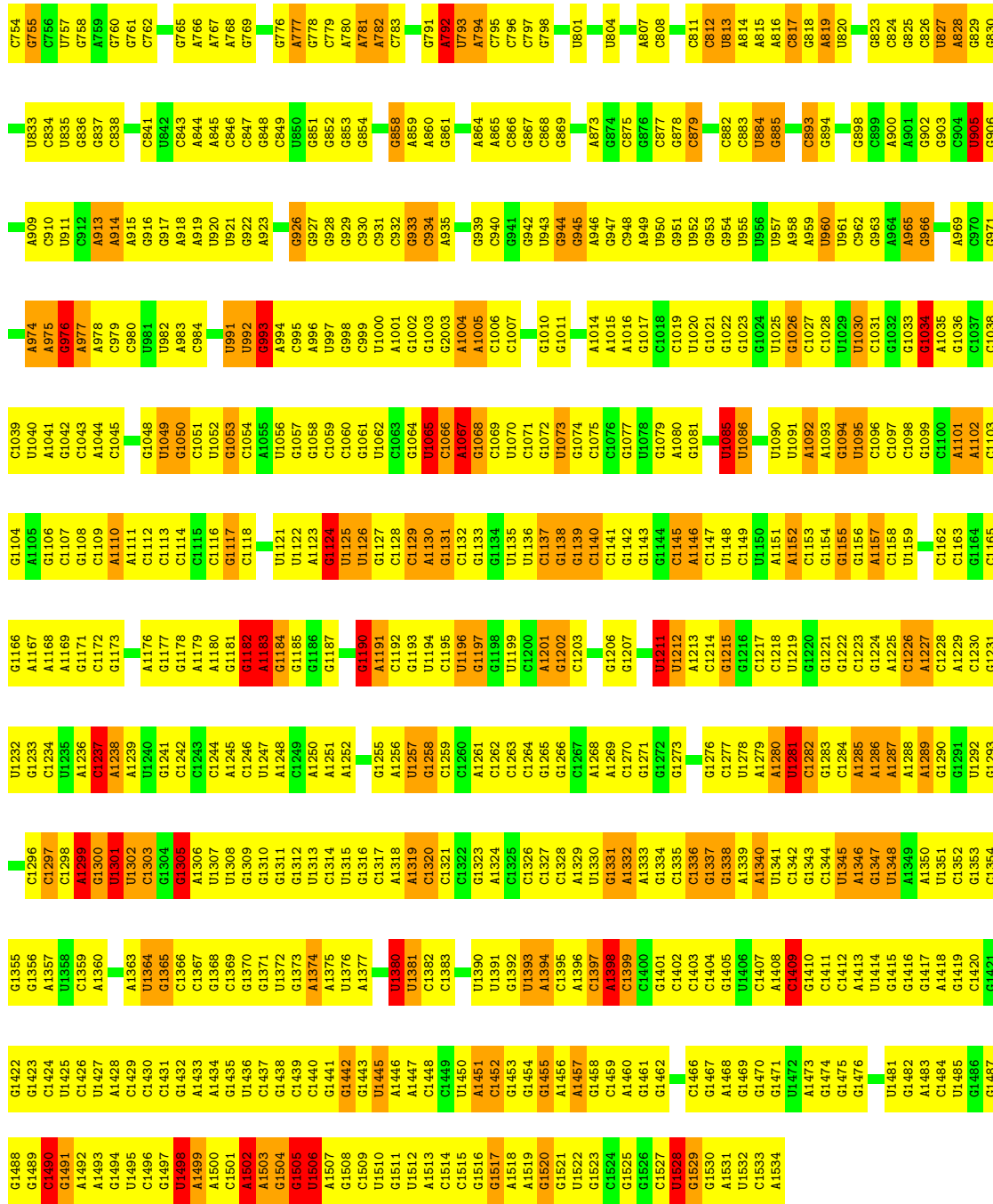
3 Residue-property plots

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

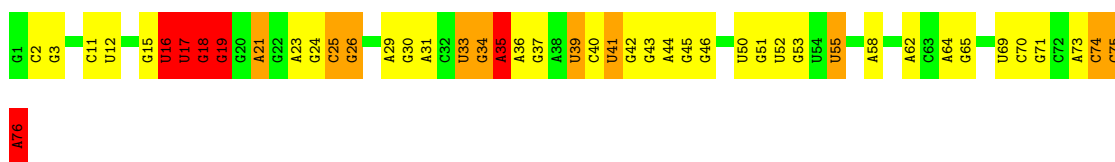
- Molecule 1: 16S RIBOSOMAL RNA

Chain AA: 





Chain AW:  39% 39% 13% 8%



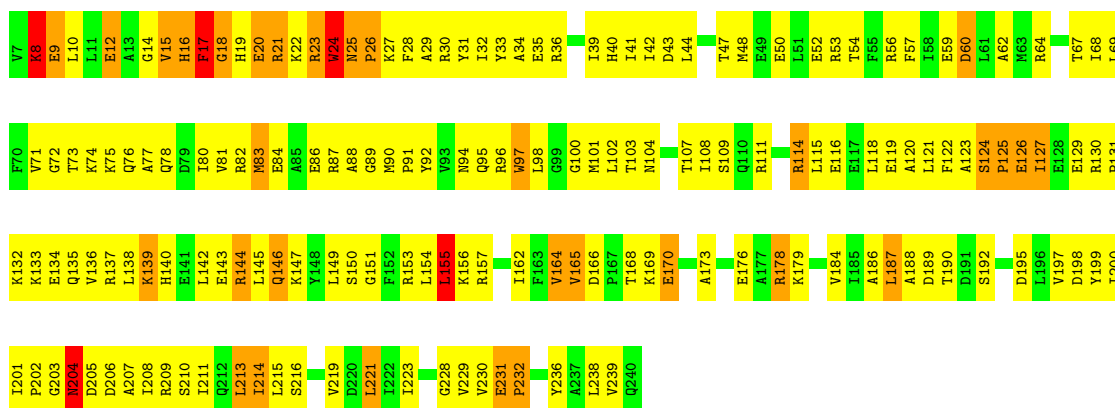
- Molecule 3: mRNA

Chain AU:  44% 6% 50%

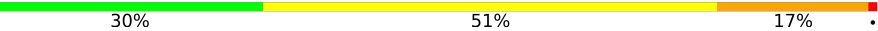


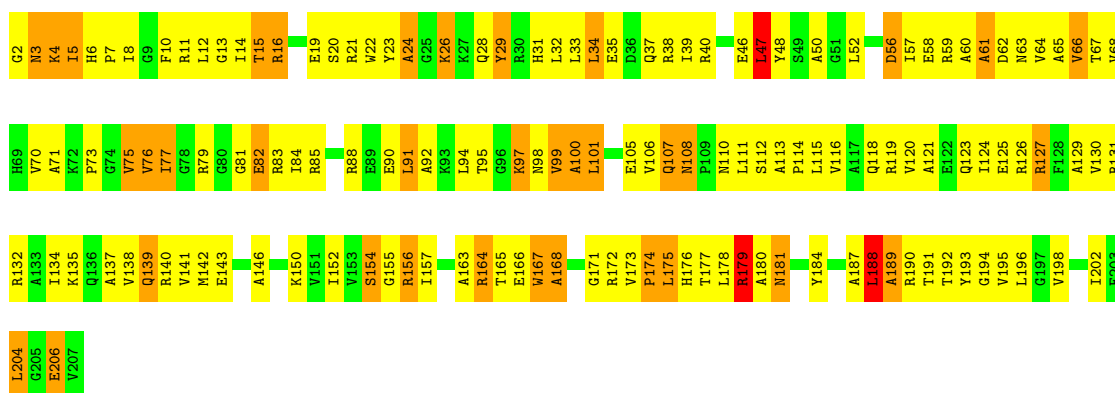
- Molecule 4: 30S ribosomal protein S2

Chain AB:  27% 57% 13% .



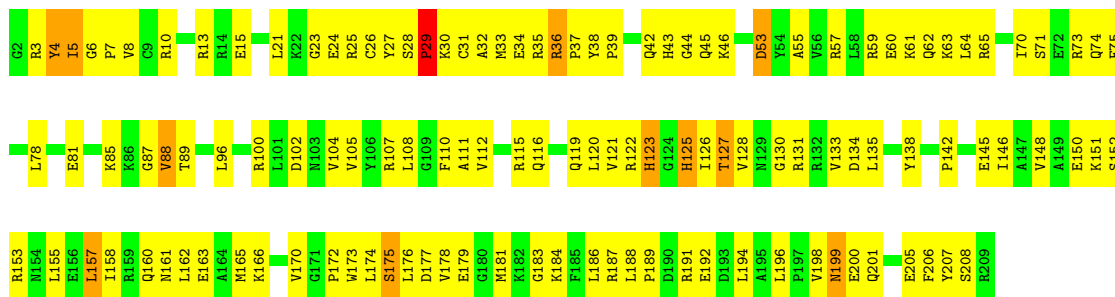
- Molecule 5: 30S ribosomal protein S3

Chain AC:  30% 51% 17% .



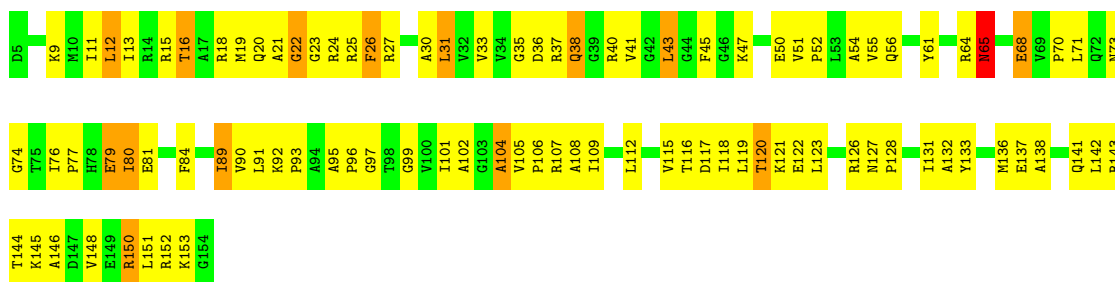
- Molecule 6: 30S ribosomal protein S4

Chain AD:  40% 54% 5%



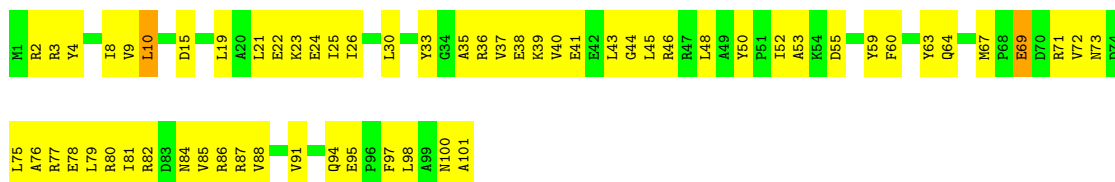
- Molecule 7: 30S ribosomal protein S5

Chain AE: 37% 53% 9%



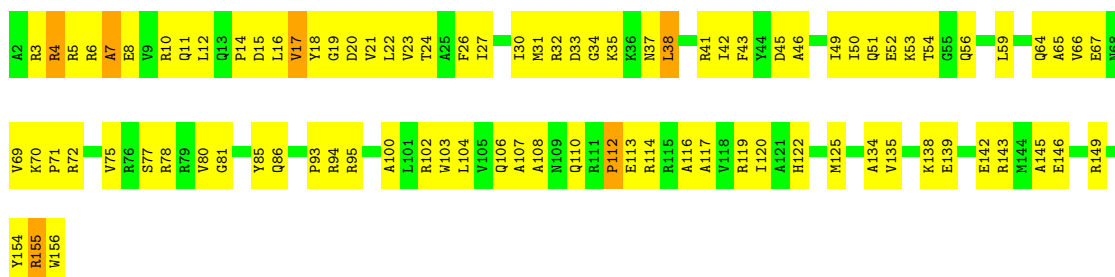
- Molecule 8: 30S ribosomal protein S6

Chain AF: 40% 58%



- Molecule 9: 30S ribosomal protein S7

Chain AG: 42% 54%

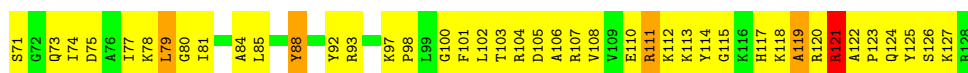
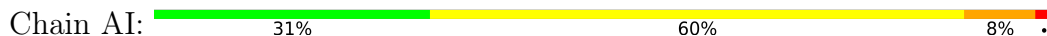


- Molecule 10: 30S ribosomal protein S8

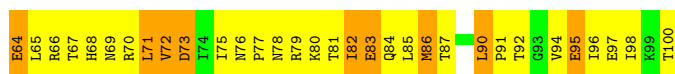
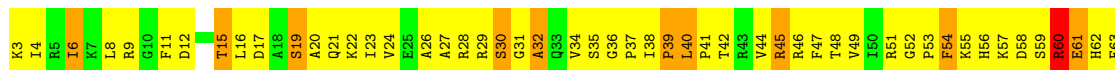
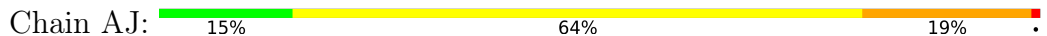
Chain AH: 41% 50% 8%



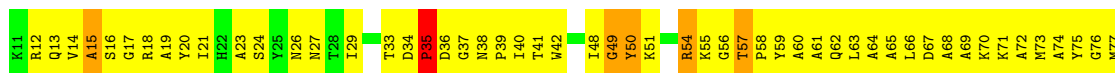
• Molecule 11: 30S ribosomal protein S9



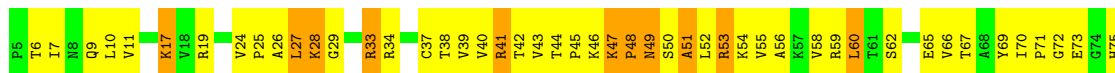
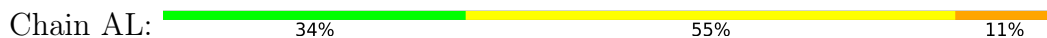
• Molecule 12: 30S ribosomal protein S10



• Molecule 13: 30S ribosomal protein S11

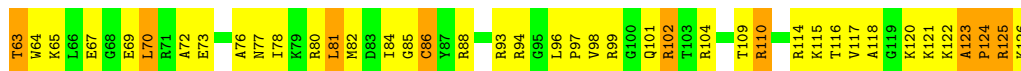
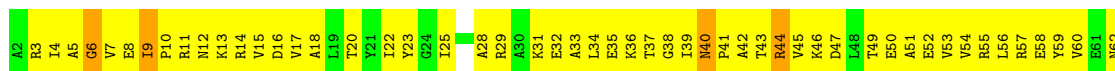


• Molecule 14: 30S ribosomal protein S12



• Molecule 15: 30S ribosomal protein S13





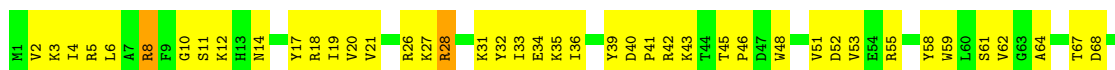
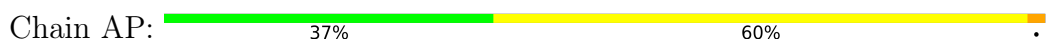
- Molecule 16: 30S ribosomal protein S14



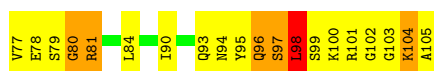
- Molecule 17: 30S ribosomal protein S15



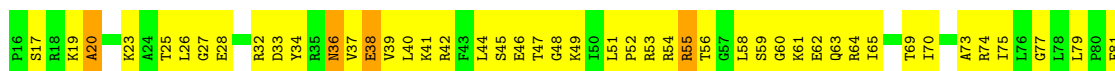
- Molecule 18: 30S ribosomal protein S16



- Molecule 19: 30S ribosomal protein S17



- Molecule 20: 30S ribosomal protein S18

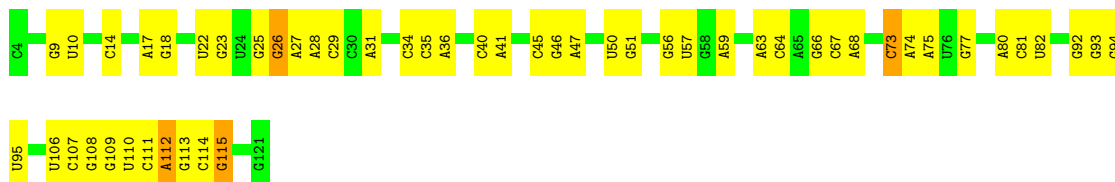


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U2959	U2764	G2662	A2456	A2372	A2297	U3199	G3156				
A2960	A2765	U2663	A2457	A2373	A2298	U3199	G3157				
C2961	C2766	G2664	A2458	A2374	A2299	U3199	G3158				
U2962	U2767	U2665	A2459	A2375	A2300	U3199	G3159				
A2963	A2768	G2666	A2460	A2376	A2301	U3199	G3160				
C2964	C2769	U2667	A2461	A2377	A2302	U3199	G3161				
U2965	U2770	G2668	A2462	A2378	A2303	U3199	G3162				
A2966	A2771	U2669	A2463	A2379	A2304	U3199	G3163				
C2967	C2772	G2669	A2464	A2380	A2305	U3199	G3164				
U2968	U2773	U2670	A2465	A2381	A2306	U3199	G3165				
A2969	A2774	G2670	A2466	A2382	A230						

- Molecule 24: 5S RIBOSOMAL RNA

Chain B9:  56% 41%



- Molecule 25: 50S ribosomal protein L2

Chain BA:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L3

Chain BB:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L4

Chain BC:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L5

Chain BD:  98%



- Molecule 29: 50S ribosomal protein L6

Chain BE:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L9

Chain BF:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L11

Chain BG:  98%



- Molecule 32: 50S ribosomal protein L13

Chain BH: 100%

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L14

Chain BI: 99%



- Molecule 34: 50S ribosomal protein L15

Chain BJ: 99%



- Molecule 35: 50S ribosomal protein L16

Chain BK: 100%

There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L17

Chain BL: 99%



- Molecule 37: 50S ribosomal protein L18

Chain BM: 100%

There are no outlier residues recorded for this chain.

- Molecule 38: 50S ribosomal protein L19

Chain BN: 99%



- Molecule 39: 50S ribosomal protein L20

Chain BO:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L21

Chain BP:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: 50S ribosomal protein L22

Chain BQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 50S ribosomal protein L23

Chain BR:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 50S ribosomal protein L24

Chain BS:  100%

There are no outlier residues recorded for this chain.

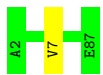
- Molecule 44: general stress protein Ctc

Chain BT:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L27

Chain BU:  99%



- Molecule 46: 50S RIBOSOMAL PROTEIN L28

Chain BV:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L29

Chain BW:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L30

Chain BX:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L31

Chain BY:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 50S ribosomal protein L32

Chain BZ:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 50S ribosomal protein L33

Chain B1:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L34

Chain B2:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 50S ribosomal protein L35

Chain B3:  100%

There are no outlier residues recorded for this chain.

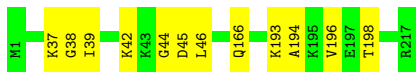
- Molecule 54: 50S ribosomal protein L36

Chain B4:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S ribosomal protein L1P

Chain B5:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	682.32Å 682.32Å 386.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 8.70 241.24 – 8.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (70.00-8.70) 93.0 (241.24-8.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 8.45Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.394 , 0.415 0.384 , 0.420	Depositor DCC
R_{free} test set	1966 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	443.4	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.30 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	122017	wwPDB-VP
Average B, all atoms (Å ²)	641.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	1.53	69/36688 (0.2%)	1.32	264/57135 (0.5%)
2	AV	2.23	23/1817 (1.3%)	1.84	42/2831 (1.5%)
2	AW	1.75	19/1816 (1.0%)	1.94	32/2827 (1.1%)
3	AU	45.18	35/188 (18.6%)	20.47	49/274 (17.9%)
4	AB	0.37	0/1935	0.68	1/2609 (0.0%)
5	AC	0.38	0/1636	0.66	0/2205
6	AD	0.37	0/1732	0.63	0/2318
7	AE	0.48	0/1162	0.79	0/1564
8	AF	0.34	0/855	0.63	0/1154
9	AG	0.35	0/1275	0.62	0/1709
10	AH	0.44	0/1135	0.74	0/1527
11	AI	0.36	0/1028	0.62	0/1378
12	AJ	0.36	0/807	0.71	0/1085
13	AK	0.39	0/899	0.70	0/1213
14	AL	0.70	1/986 (0.1%)	0.76	1/1320 (0.1%)
15	AM	0.44	1/1007 (0.1%)	1.11	3/1347 (0.2%)
16	AN	0.40	0/500	0.78	0/664
17	AO	0.36	0/744	0.63	1/992 (0.1%)
18	AP	0.43	0/716	0.76	0/963
19	AQ	0.44	0/869	0.75	0/1159
20	AR	0.36	0/602	0.63	0/799
21	AS	0.35	0/661	0.72	1/890 (0.1%)
22	AT	0.39	0/764	0.73	0/1006
23	B0	0.49	17/67885 (0.0%)	0.75	49/105852 (0.0%)
24	B9	0.68	1/2815 (0.0%)	0.76	3/4384 (0.1%)
All	All	1.97	166/130522 (0.1%)	1.25	446/199205 (0.2%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	2	40
2	AV	0	7
2	AW	0	7
23	B0	0	5
All	All	2	59

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AU	14	A	C6-N6	279.73	3.57	1.33
3	AU	13	A	C6-N6	279.69	3.57	1.33
3	AU	6	A	C6-N6	279.55	3.57	1.33
3	AU	12	A	C6-N6	279.29	3.57	1.33
3	AU	8	G	C6-O6	259.50	3.57	1.24

The worst 5 of 446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AU	8	G	C5-C6-O6	-177.72	21.96	128.60
3	AU	6	A	C5-C6-N6	-127.11	22.02	123.70
3	AU	14	A	C5-C6-N6	-127.08	22.03	123.70
3	AU	12	A	C5-C6-N6	-127.07	22.05	123.70
3	AU	13	A	C5-C6-N6	-127.04	22.07	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	181	G	C3'
1	AA	1528	U	C3'

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	187	G	Sidechain
1	AA	191	G	Sidechain
1	AA	197	A	Sidechain
1	AA	231	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32819	0	16577	3629	5
2	AV	1625	0	821	141	0
2	AW	1625	0	819	141	0
3	AU	176	0	79	11	0
4	AB	1900	0	1951	231	0
5	AC	1612	0	1676	292	0
6	AD	1702	0	1767	227	4
7	AE	1146	0	1207	233	0
8	AF	842	0	857	81	4
9	AG	1256	0	1294	119	0
10	AH	1115	0	1177	122	0
11	AI	1010	0	1043	172	0
12	AJ	794	0	838	216	0
13	AK	884	0	903	187	0
14	AL	970	0	1055	157	0
15	AM	996	0	1071	145	0
16	AN	491	0	531	160	0
17	AO	733	0	771	55	0
18	AP	700	0	720	96	0
19	AQ	856	0	926	355	0
20	AR	596	0	667	83	0
21	AS	647	0	673	129	0
22	AT	762	0	848	259	0
23	B0	60636	0	30552	1930	8
24	B9	2519	0	1287	43	0
25	BA	270	0	0	0	0
26	BB	205	0	0	0	0
27	BC	197	0	0	0	0
28	BD	178	0	0	12	0
29	BE	177	0	0	0	0
30	BF	52	0	0	0	0
31	BG	143	0	0	7	0
32	BH	143	0	0	0	0
33	BI	132	0	0	3	0
34	BJ	141	0	0	1	0
35	BK	124	0	0	0	0
36	BL	114	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BM	111	0	0	0	0
38	BN	125	0	0	1	0
39	BO	117	0	0	0	0
40	BP	100	0	0	0	0
41	BQ	130	0	0	0	0
42	BR	93	0	0	0	0
43	BS	113	0	0	0	0
44	BT	173	0	0	0	0
45	BU	86	0	0	1	0
46	BV	16	0	0	0	0
47	BW	65	0	0	0	0
48	BX	55	0	0	0	0
49	BY	73	0	0	0	0
50	BZ	58	0	0	0	0
51	B1	53	0	0	0	0
52	B2	46	0	0	0	0
53	B3	63	0	0	0	0
54	B4	35	0	0	0	0
55	B5	217	0	0	36	0
All	All	122017	0	70110	7429	12

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 39.

The worst 5 of 7429 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:AA:293:G:H4'	1:AA:609:A:C2	1.16	1.69
1:AA:675:A:H1'	13:AK:116:HIS:CD2	1.26	1.66
1:AA:21:G:C1'	1:AA:914:A:H62	1.08	1.65
6:AD:88:VAL:CA	7:AE:97:GLY:HA3	1.24	1.64
23:B0:3128:G:H4'	23:B0:3174:C:C4'	1.23	1.64

The worst 5 of 12 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)
6:AD:172:PRO:O	8:AF:15:ASP:CB[3_555]	1.18	1.02
1:AA:416:G:C4'	23:B0:3153:G:O2'[3_555]	1.79	0.41
1:AA:416:G:O2'	23:B0:3153:G:O2'[3_555]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AD:172:PRO:O	8:AF:15:ASP:CA[3_555]	1.87	0.33
6:AD:186:LEU:CD1	8:AF:15:ASP:OD2[3_555]	1.91	0.29

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	
4	AB	232/234 (99%)	174 (75%)	34 (15%)	24 (10%)	0	8
5	AC	204/206 (99%)	135 (66%)	40 (20%)	29 (14%)	0	4
6	AD	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	2	22
7	AE	148/150 (99%)	130 (88%)	13 (9%)	5 (3%)	3	26
8	AF	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	15	55
9	AG	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	16
10	AH	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	4	29
11	AI	125/127 (98%)	89 (71%)	26 (21%)	10 (8%)	1	12
12	AJ	96/98 (98%)	59 (62%)	20 (21%)	17 (18%)	0	3
13	AK	117/119 (98%)	88 (75%)	20 (17%)	9 (8%)	1	13
14	AL	122/124 (98%)	98 (80%)	15 (12%)	9 (7%)	1	14
15	AM	123/125 (98%)	88 (72%)	27 (22%)	8 (6%)	1	16
16	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	6
17	AO	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	1	18
18	AP	81/83 (98%)	65 (80%)	15 (18%)	1 (1%)	13	50
19	AQ	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	13
20	AR	71/73 (97%)	62 (87%)	7 (10%)	2 (3%)	5	30
21	AS	78/80 (98%)	48 (62%)	19 (24%)	11 (14%)	0	4
22	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2334/2372 (98%)	1792 (77%)	361 (16%)	181 (8%)	1 13

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	9	GLU
4	AB	15	VAL
4	AB	16	HIS
4	AB	17	PHE
4	AB	21	ARG

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
4	AB	202/202 (100%)	180 (89%)	22 (11%)	6 23
5	AC	160/160 (100%)	142 (89%)	18 (11%)	6 21
6	AD	180/180 (100%)	172 (96%)	8 (4%)	28 53
7	AE	115/115 (100%)	100 (87%)	15 (13%)	4 18
8	AF	90/90 (100%)	88 (98%)	2 (2%)	52 71
9	AG	126/126 (100%)	122 (97%)	4 (3%)	39 61
10	AH	119/119 (100%)	109 (92%)	10 (8%)	11 33
11	AI	98/98 (100%)	90 (92%)	8 (8%)	11 34
12	AJ	88/88 (100%)	79 (90%)	9 (10%)	7 25
13	AK	90/90 (100%)	84 (93%)	6 (7%)	16 41
14	AL	104/104 (100%)	96 (92%)	8 (8%)	13 37
15	AM	100/100 (100%)	90 (90%)	10 (10%)	7 26
16	AN	49/49 (100%)	47 (96%)	2 (4%)	30 55
17	AO	79/79 (100%)	72 (91%)	7 (9%)	9 30
18	AP	72/72 (100%)	67 (93%)	5 (7%)	15 40
19	AQ	96/96 (100%)	90 (94%)	6 (6%)	18 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AR	64/64 (100%)	61 (95%)	3 (5%)	26	51
21	AS	71/71 (100%)	68 (96%)	3 (4%)	30	54
22	AT	76/76 (100%)	69 (91%)	7 (9%)	9	29
All	All	1979/1979 (100%)	1826 (92%)	153 (8%)	13	37

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	AM	81	LEU
21	AS	10	PHE
15	AM	125	ARG
18	AP	8	ARG
22	AT	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
8	AF	73	ASN
19	AQ	93	GLN
11	AI	124	GLN
19	AQ	26	GLN
21	AS	56	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1479/1527 (96%)	217 (14%)	92 (6%)
2	AV	75/76 (98%)	13 (17%)	3 (4%)
2	AW	74/76 (97%)	13 (17%)	3 (4%)
23	B0	2802/2887 (97%)	430 (15%)	56 (1%)
24	B9	116/118 (98%)	10 (8%)	0
3	AU	8/18 (44%)	1 (12%)	0
All	All	4554/4702 (96%)	684 (15%)	154 (3%)

5 of 684 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A

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Mol	Chain	Res	Type
1	AA	9	G
1	AA	27	G
1	AA	31	G

5 of 154 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	B0	1193	G
23	B0	3171	A
23	B0	1278	A
23	B0	1807	A
23	B0	2426	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	108
23	B0	31
2	AW	4
2	AV	4

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Mol	Chain	Number of breaks
24	B9	2
3	AU	1
14	AL	1

The worst 5 of 151 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1443:G	O3'	1445:U	P	10.46
1	AA	1459:C	O3'	1460:A	P	10.16
1	AA	1458:G	O3'	1459:C	P	8.01
1	B0	1888:C	O3'	1889:G	P	6.63
1	B0	3180:U	O3'	3181:C	P	5.39

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.