



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:52 PM UTC

PDB ID : 1NKW / pdb_00001nkw
Title : Crystal Structure Of The Large Ribosomal Subunit From Deinococcus Radiodurans
Authors : Harms, J.M.; Schlutzen, F.; Zarivach, R.; Bashan, A.; Gat, S.; Agmon, I.; Bartels, H.; Franceschi, F.; Yonath, A.
Deposited on : 2003-01-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

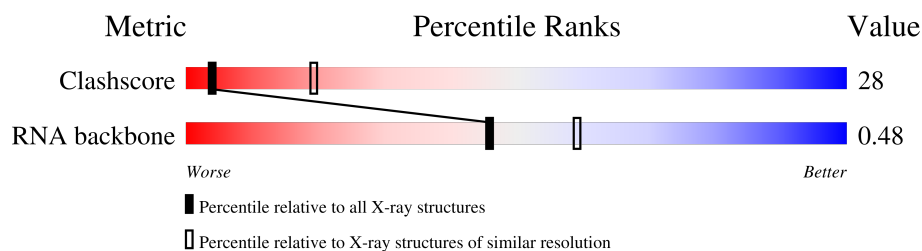
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

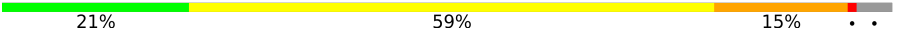
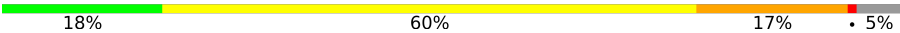
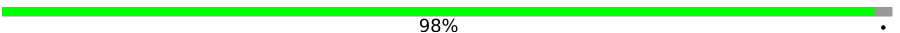
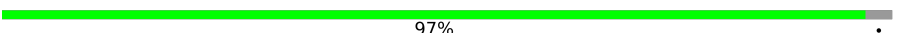
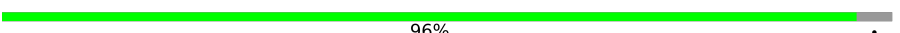
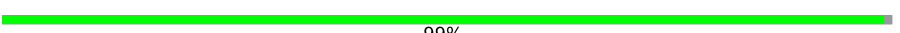
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

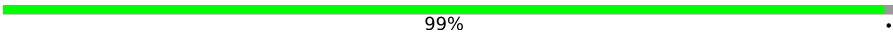
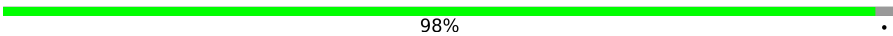
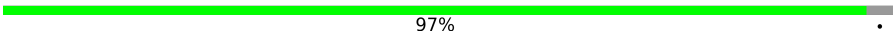
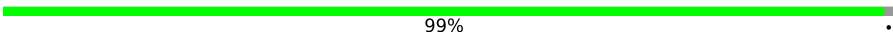
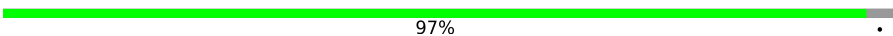
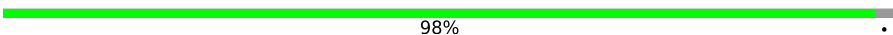
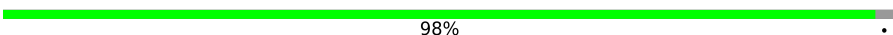
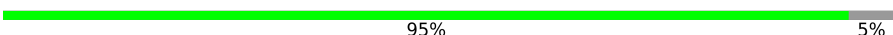
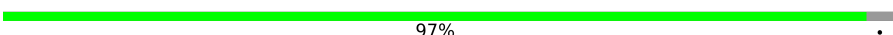
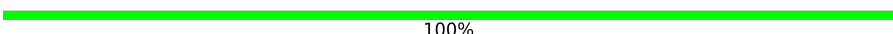
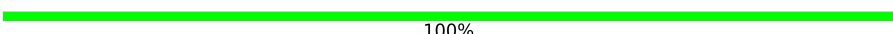
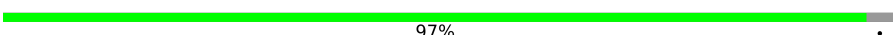
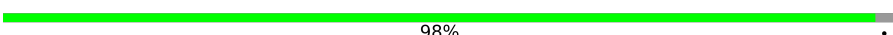
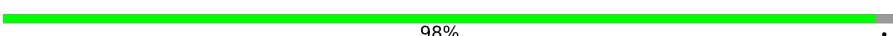
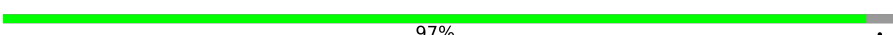
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	 21% 59% 15% . .
2	9	124	 18% 60% 17% . 5%
3	A	275	 98% .
4	B	211	 97% .
5	C	205	 96% .
6	D	180	 99% .
7	E	212	 83% 17%
8	F	146	 34% . 64%
9	G	144	 99% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	H	174	 82% 18%
11	I	134	 99% .
12	J	156	 90% 10%
13	K	142	 87% . 13%
14	L	116	 98% .
15	M	114	 97% .
16	N	166	 74% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	95	 98% .
21	S	115	 98% .
22	T	253	 88% 12%
23	U	91	 95% 5%
24	W	67	 97% .
25	X	55	 100%
26	Y	73	 100%
27	Z	60	 97% .
28	1	82	 65% 35%
29	2	47	 98% .
30	3	64	 98% .
31	4	36	 97% .

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 65300 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	205	Total	C	0	0	205
			205	205			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	E	177	Total	C	0	0	177
			177	177			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	F	52	Total	C	0	0	52
			52	52			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	G	143	Total	C	0	0	143
			143	143			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	143	Total	C	0	0	143
			143	143			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	132	Total	C	0	0	132
			132	132			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	141	Total	C	0	0	141
			141	141			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	K	124	Total	C	0	0	124
			124	124			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	114	Total C 114 114	0	0	114

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	111	Total C 111 111	8	0	111

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	125	Total C 125 125	0	0	125

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	117	Total C 117 117	16	0	117

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	100	Total C 100 100	0	0	100

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	130	Total C 130 130	0	0	130

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	93	Total C 93 93	0	0	93

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called general stress protein CTC.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	43	0	223

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	4	0	55

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Z	58	Total C 58 58	0	0	58

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	1	53	Total C 53 53	0	0	53

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	2	46	Total C 46 46	0	0	46

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	3	63	Total C 63 63	0	0	63

- Molecule 31 is a protein called 50S ribosomal protein L36.

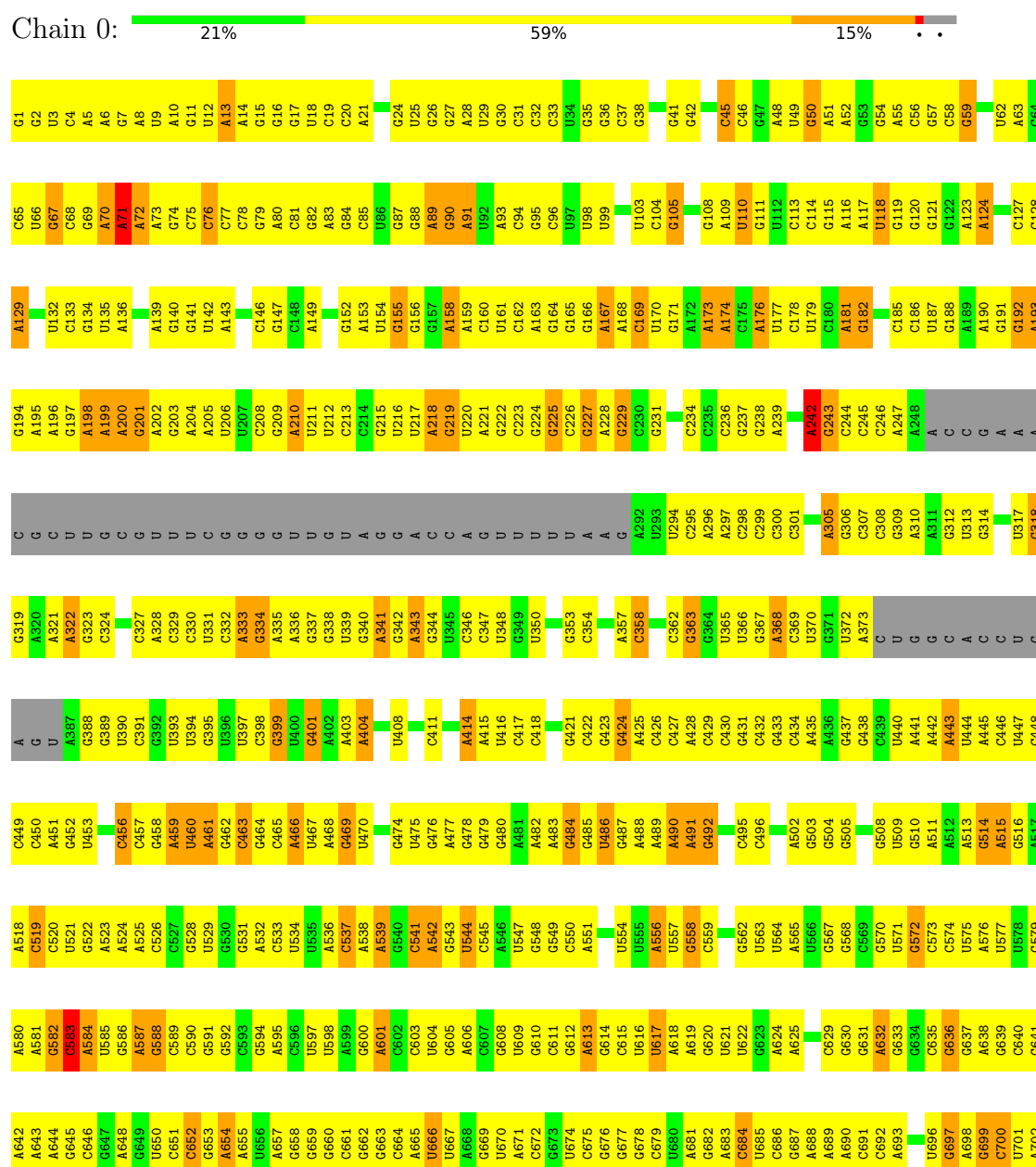
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	4	35	Total C 35 35	0	0	35

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.

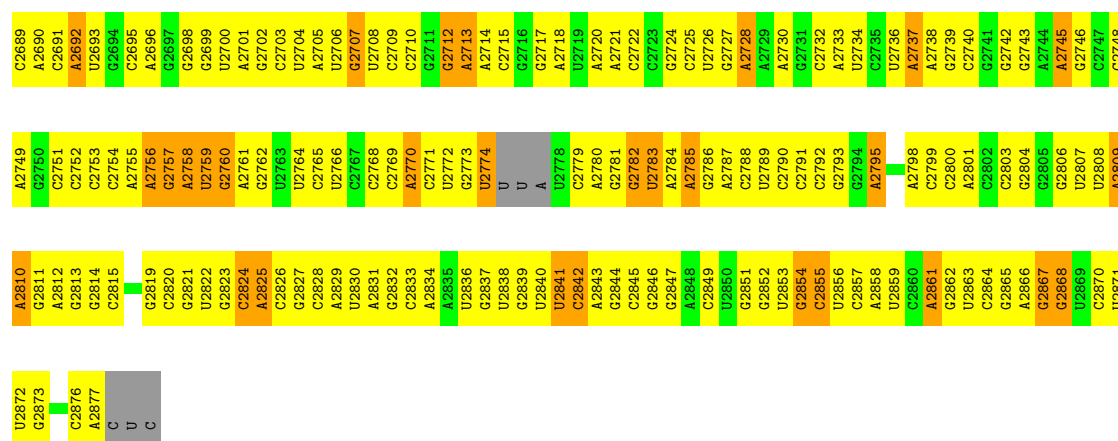
Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA



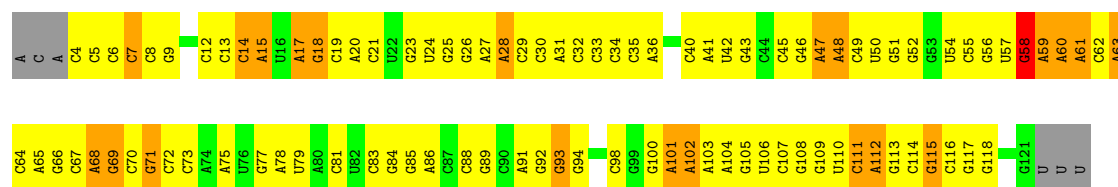






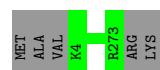
• Molecule 2: 5S ribosomal RNA

Chain 9: 18% 60% 17% 5%



• Molecule 3: 50S ribosomal protein L2

Chain A: 98%



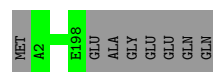
• Molecule 4: 50S ribosomal protein L3

Chain B: 97%



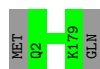
• Molecule 5: 50S ribosomal protein L4

Chain C: 96%



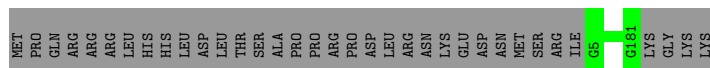
• Molecule 6: 50S ribosomal protein L5

Chain D: 99%



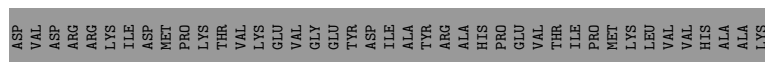
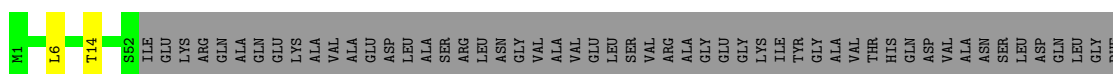
- Molecule 7: 50S ribosomal protein L6

Chain E: 83% 17%



- Molecule 8: 50S ribosomal protein L9

Chain F: 34% . 64%



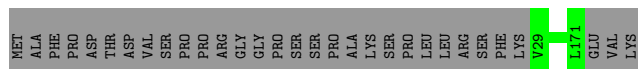
- Molecule 9: 50S ribosomal protein L11

Chain G: 99% .



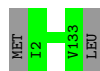
- Molecule 10: 50S ribosomal protein L13

Chain H: 82% 18%



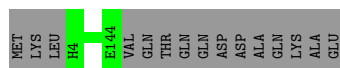
- Molecule 11: 50S ribosomal protein L14

Chain I: 99% .



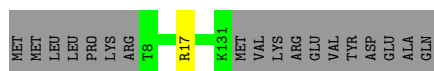
- Molecule 12: 50S ribosomal protein L15

Chain J: 90% 10%

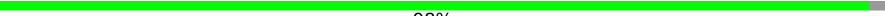


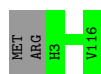
- Molecule 13: 50S ribosomal protein L16

Chain K:  87% 13%



- Molecule 14: 50S ribosomal protein L17

Chain L:  98%



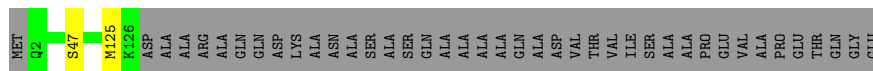
- Molecule 15: 50S ribosomal protein L18

Chain M:  97%



- Molecule 16: 50S ribosomal protein L19

Chain N:  74% 25%



- Molecule 17: 50S ribosomal protein L20

Chain O:  99%

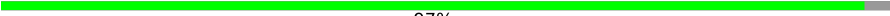


- Molecule 18: 50S ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

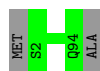
- Molecule 19: 50S ribosomal protein L22

Chain Q:  97%



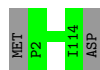
- Molecule 20: 50S ribosomal protein L23

Chain R:  98%



- Molecule 21: 50S ribosomal protein L24

Chain S: 98% .



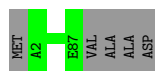
- Molecule 22: general stress protein CTC

Chain T: 88% 12%



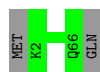
- Molecule 23: 50S ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: 50S ribosomal protein L29

Chain W: 97% .



- Molecule 25: 50S ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

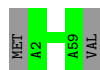
- Molecule 26: 50S ribosomal protein L31

Chain Y: 100%

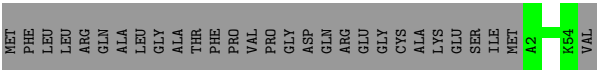
There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain Z: 97% .



- Molecule 28: 50S ribosomal protein L33



● Molecule 29: 50S ribosomal protein L34



● Molecule 30: 50S ribosomal protein L35



● Molecule 31: 50S ribosomal protein L36



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.00Å 410.00Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65300	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0	0.27	0/66467	0.65	34/103673 (0.0%)
2	9	0.45	0/2816	0.80	1/4388 (0.0%)
All	All	0.28	0/69283	0.66	35/108061 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	5

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	843	G	C2'-C3'-O3'	8.60	122.40	109.50
1	0	2668	U	C4'-C3'-O3'	-7.75	101.37	113.00
1	0	2018	G	C2'-C3'-O3'	6.84	119.76	109.50
1	0	2428	U	N1-C1'-C2'	6.69	122.04	112.00
1	0	242	A	C2'-C3'-O3'	6.69	119.53	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1264	C	Sidechain
1	0	1342	U	Sidechain
1	0	2251	U	Sidechain
1	0	2668	U	Sidechain
1	0	788	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	0	59359	0	29917	2551	1
2	9	2519	0	1285	146	0
3	A	270	0	0	0	0
4	B	205	0	0	0	0
5	C	197	0	0	0	0
6	D	178	0	0	0	0
7	E	177	0	0	0	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	0	0
15	M	111	0	0	0	0
16	N	125	0	0	1	1
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0
27	Z	58	0	0	0	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
All	All	65300	0	31202	2692	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 2692 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)
1:0:1679:U:H2'	1:0:1680:U:H5''	1.22	1.12
1:0:362:C:H2'	1:0:363:G:H4'	1.34	1.10
1:0:918:A:H2'	1:0:919:U:H5''	1.29	1.10
1:0:2548:G:H2'	1:0:2549:G:H5''	1.10	1.09
1:0:2058:U:H1'	1:0:2576:G:H21	1.08	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:C:OP1	16:N:47:SER:CA[8_455]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	523 (18%)	34 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	546 (18%)	35 (1%)

5 of 546 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2426	G
1	0	2437	G
1	0	2759	U
1	0	1410	U
1	0	1354	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.