wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 08:48 PM EST

PDB ID	:	1D8I
Title	:	X-RAY CRYSTAL STRUCTURE OF YEAST RNA TRIPHOSPHATASE IN COMPLEX WITH A SULFATE ION.
Authors	:	Lima, C.D.; Wang, L.K.; Shuman, S.
Deposited on	:	1999-10-24
Resolution	:	2.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

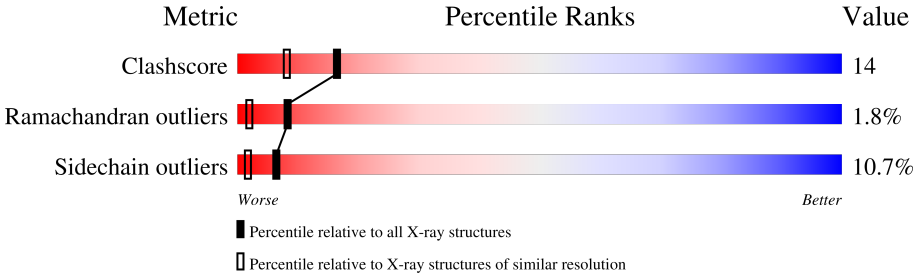
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	49% 29% 12% • 7%
1	B	311	50% 30% 10% • 7%
1	C	311	49% 31% 10% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

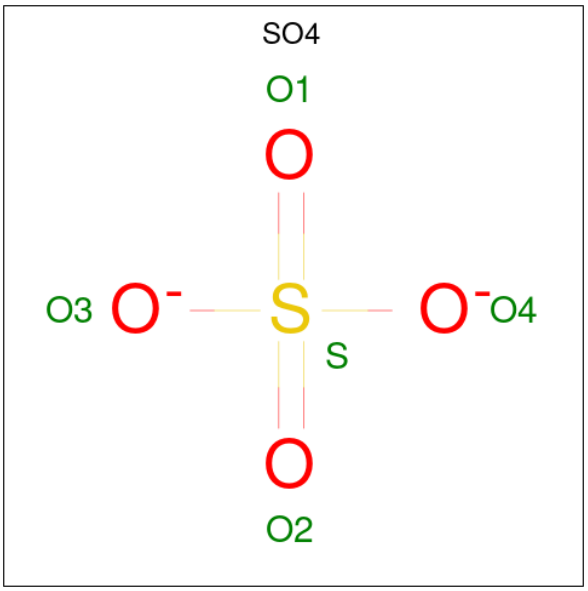
- Molecule 1 is a protein called MRNA TRIPHOSPHATASE CET1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2295	1457	393	440	5	0	0	0
1	B	288	2295	1457	393	440	5	0	0	0
1	C	288	2295	1457	393	440	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	conflict	UNP O13297
B	242	ARG	LYS	conflict	UNP O13297
C	242	ARG	LYS	conflict	UNP O13297

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	121	Total O 121 121	0	0
3	B	134	Total O 134 134	0	0
3	C	159	Total O 159 159	0	0

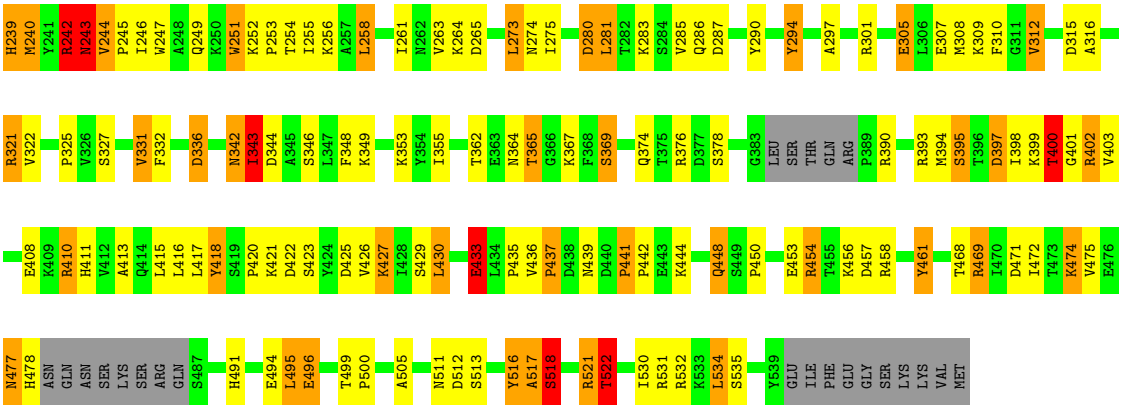
3 Residue-property plots (i)

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

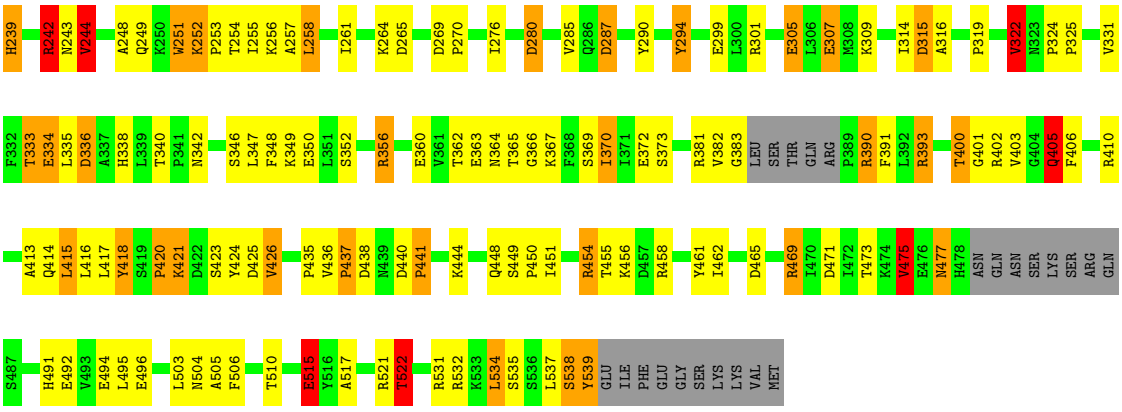
• Molecule 1: MRNA TRIPHOSPHATASE CET1

Chain A: 49% 29% 12% • 7%



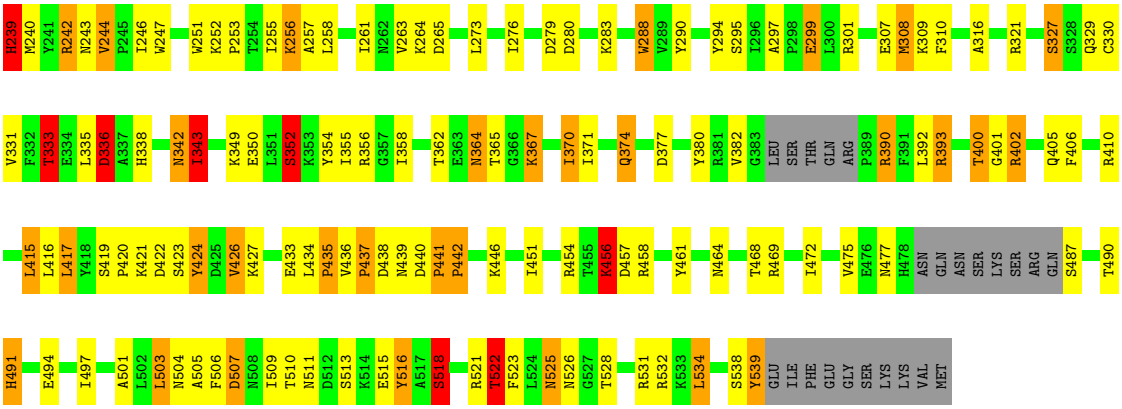
• Molecule 1: MRNA TRIPHOSPHATASE CET1

Chain B: 50% 30% 10% • 7%



• Molecule 1: MRNA TRIPHOSPHATASE CET1

Chain C: 49% 31% 10% • 7%


H239 M240 Y241 R242 N243 V244 P245 I246 W247 W251 K252 P253 T254 I255 K256 A257 L258 I261 N262 V263 K264 D265 L273 I276 D279 D280 K283 W288 V289 Y290 Y294 S295 I296 A297 P298 E299 L300 R301 E307 M308 K309 F310 A316 R321 S327 S328 Q329 C330
V331 F332 T333 E334 L335 D336 A337 H338 N342 I343 K349 E350 L351 S352 K353 Y354 I355 R356 G357 I358 T362 E363 N364 T365 G366 K367 I370 I371 Q374 D377 Y380 R381 V382 G383 LEU SER THR GLN ARG P389 R390 F391 L392 R393 T400 G401 R402 Q405 F406 R410
L415 L416 L417 Y418 S419 P420 K421 D422 S423 Y424 D425 V426 K427 E433 L434 P435 V436 P437 D438 N439 D440 P441 P442 K446 I451 R454 T455 K456 D457 R458 Y461 N464 T468 R469 I472 V475 E476 N477 H478 ASN GLN ASN SER LYS SER ARG GLN S487 T490
H491 E494 I497 A501 L502 L503 N504 A505 F506 D507 N508 I509 T510 N511 D512 S513 K514 E515 Y516 A517 S518 R521 T522 F523 L524 N525 N526 G527 T528 R531 R532 K533 L534 S538 Y539 GLU ILE PHE GLU GLY SER LYS LYS VAL MET

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.36Å 116.09Å 82.31Å 90.00° 110.25° 90.00°	Depositor
Resolution (Å)	25.00 – 2.05	Depositor
% Data completeness (in resolution range)	82.2 (25.00-2.05)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7329	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.99	2/2342 (0.1%)	2.17	84/3178 (2.6%)
1	B	0.93	1/2342 (0.0%)	2.00	72/3178 (2.3%)
1	C	1.00	6/2342 (0.3%)	2.08	85/3178 (2.7%)
All	All	0.98	9/7026 (0.1%)	2.08	241/9534 (2.5%)

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	A	0	18
1	B	0	15
1	C	0	19
All	All	0	52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	PHE	N-CA	-10.36	1.25	1.46
1	C	330	CYS	CB-SG	-9.36	1.66	1.82
1	C	247	TRP	NE1-CE2	-6.76	1.28	1.37
1	C	295	SER	CB-OG	6.32	1.50	1.42
1	C	419	SER	CB-OG	5.82	1.49	1.42

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH1	-20.80	109.90	120.30
1	B	531	ARG	NE-CZ-NH2	18.95	129.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	521	ARG	NE-CZ-NH1	-17.89	111.35	120.30
1	A	321	ARG	NE-CZ-NH2	17.59	129.10	120.30
1	A	458	ARG	NE-CZ-NH1	-16.57	112.02	120.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	MET	Mainchain
1	A	242	ARG	Mainchain
1	A	243	ASN	Mainchain
1	A	273	LEU	Mainchain
1	A	294	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2295	0	2274	74	0
1	B	2295	0	2273	66	0
1	C	2295	0	2274	60	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	121	0	0	18	0
3	B	134	0	0	16	1
3	C	159	0	0	8	1
All	All	7329	0	6821	197	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 14.

The worst 5 of 197 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:A:441:PRO:HB2	1:A:442:PRO:HD3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:PRO:HB2	1:C:442:PRO:HD3	1.51	0.91
1:C:441:PRO:HB2	1:C:442:PRO:CD	2.04	0.86
1:C:538:SER:O	1:C:539:TYR:HB3	1.74	0.85
1:A:263:VAL:HA	3:A:701:HOH:O	1.77	0.84

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)
3:B:723:HOH:O	3:C:662:HOH:O[2_657]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	282/311 (91%)	260 (92%)	18 (6%)	4 (1%)	11 3
1	B	282/311 (91%)	264 (94%)	13 (5%)	5 (2%)	8 2
1	C	282/311 (91%)	260 (92%)	16 (6%)	6 (2%)	7 1
All	All	846/933 (91%)	784 (93%)	47 (6%)	15 (2%)	8 2

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	GLY
1	A	437	PRO
1	B	401	GLY
1	B	437	PRO
1	C	401	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	259/291 (89%)	232 (90%)	27 (10%)	7 2
1	B	259/291 (89%)	230 (89%)	29 (11%)	6 1
1	C	259/291 (89%)	232 (90%)	27 (10%)	7 2
All	All	777/873 (89%)	694 (89%)	83 (11%)	6 2

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	246	ILE
1	C	446	LYS
1	C	258	LEU
1	C	367	LYS
1	C	475	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	342	ASN
1	C	508	ASN
1	C	405	GLN
1	B	342	ASN
1	C	243	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	B	602	-	4,4,4	0.63	0	6,6,6	0.26	0
2	SO4	A	601	-	4,4,4	0.63	0	6,6,6	0.24	0
2	SO4	A	604	-	4,4,4	0.64	0	6,6,6	1.03	0
2	SO4	B	605	-	4,4,4	0.95	0	6,6,6	1.28	1 (16%)
2	SO4	C	603	-	4,4,4	0.57	0	6,6,6	0.47	0
2	SO4	C	606	-	4,4,4	0.39	0	6,6,6	0.61	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	605	SO4	O4-S-O2	2.42	121.92	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.