WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 12:17 AM EDT

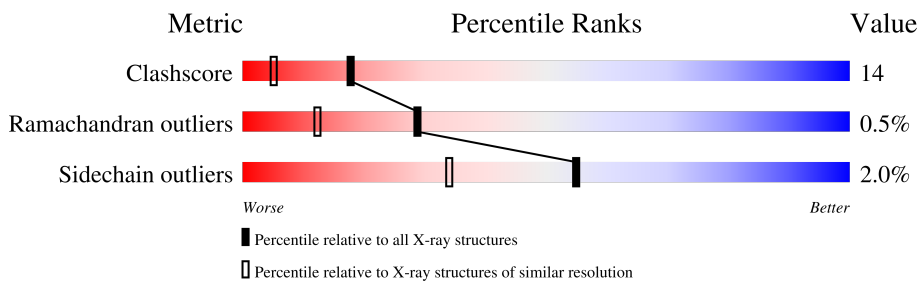|		
PDB ID	:	1L1L
Title	:	CRYSTAL STRUCTURE OF B-12 DEPENDENT (CLASS II) RIBONU-CLEOTIDE REDUCTASE
Authors	:	Sintchak, M.D.; Arjara, G.; Kellogg, B.A.; Stubbe, J.; Drennan, C.L.
Deposited on	:	2002-02-18
Resolution	:	1.75 Å(reported)

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 1.75 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.5%
Sidechain outliers		2.0%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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	739	70% 26% · ·
1	B	739	80% 17% · ·
1	C	739	75% 21% · ·
1	D	739	68% 28% · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 25227 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 RIBONUCLEOSIDE TRIPHOSPHATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5588	3526	956	1089	17			
1	B	717	Total	C	N	O	S	0	0	0
			5588	3526	956	1089	17			
1	C	717	Total	C	N	O	S	0	0	0
			5588	3526	956	1089	17			
1	D	717	Total	C	N	O	S	0	0	0
			5588	3526	956	1089	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	PHE	CYS	SEE REMARK 999	UNP Q59490
B	152	PHE	CYS	SEE REMARK 999	UNP Q59490
C	152	PHE	CYS	SEE REMARK 999	UNP Q59490
D	152	PHE	CYS	SEE REMARK 999	UNP Q59490

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	652	Total	O	0	0
			652	652		
2	B	960	Total	O	0	0
			960	960		
2	C	684	Total	O	0	0
			684	684		
2	D	579	Total	O	0	0
			579	579		

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: RIBONUCLEOSIDE TRIPHOSPHATE REDUCTASE

Chain A:

• Molecule 1: RIBONUCLEOSIDE TRIPHOSPHATE REDUCTASE

Chain B:

VAL ASP GLN THR ASP CYS GLU GLY GLY ALA CYS PRO ILE LYS

● Molecule 1: RIBONUCLEOSIDE TRIPHOSPHATE REDUCTASE

Chain C:

75%   21%

MET SER GLU E4 E10 F11 I12 K20 L26 G27 W28 V29 K32 R33 R37 K53 K75 T79 E83 R84 G91 L92 T95 R99 W102 I103 D107 Y108 Q109 R110 D114 N118 C119 W120 R125 P126 Q127 K128 D131 Y138 L139

G140 K141 Q142 M148 F154 D155 M158 K159 G160 G161 D183 D189 E190 T191 Y195 V199 K206 L209 D212 A213 D214 L220 R224 E225 L237 P244 K249 L250 I251 L254 H265 N290 K291 A292 R295 N316 VAL ARG ARG SER

A321 E322 L323 K342 L343 H346 R347 D357 S358 A359 F360 A367 R371 E372 N373 G374 E375 K385 G388 R389 I390 Q395 A396 G397 I398 D399 V402 E403 P407 E410 I411 N415 P418 L421 F422 E423 V424 F425 P426 L427 I428 A429 E430 E431 D435

E438 Y455 I459 S460 R461 I470 S475 D519 K523 I542 K543 H544 T545 K548 G551 T552 V553 A554 K555 L556 A557 E561 G562 M563 H564 L571 I572 D581 P582 R593 T594 E595 Y599 C605 P609 I610 I628 T640 N645

S648 C649 T650 I651 T652 F653 G658 E662 R666 T672 T675 S676 L677 L678 P679 G683 S684 L685 Q686 Q687 A688 P692 I693 E696 K700 R701 E704 I705 E710 Q715 L716 N717 L723 E724 LEU VAL ASP GLN THR ASP CYS GLU GLY GLY ALA CYS PRO

ILE LYS

● Molecule 1: RIBONUCLEOSIDE TRIPHOSPHATE REDUCTASE

Chain D:

68%   28%

MET SER GLU E4 E10 F11 I12 D13 R14 V15 K16 A17 S18 H22 L26 G27 W28 V29 K32 A36 R37 W38 L39 P40 E41 K42 G43 R44 V52 K53 E57 P64 R65 L66 S69 P70 S71 K75 Q76 S77 L78 T79 E80 R84 L85 Y86 G91 L92

R99 N100 R110 D114 N118 C119 W120 F121 R125 P126 Q127 K128 D131 S132 K133 P136 S137 Y138 L139 G140 K141 M148 F154 M158 G164 R177 L186 Y195 D196 A197 S198 V199 K200 A203 E208 Q211 S215 L220 R246

K249 L250 I251 L252 D253 L254 H265 G266 M275 P276 L277 I278 L281 E286 R295 D300 A314 G315 N316 VAL ARG ARG SER A321 E322 L323 A324 F333 M336 L343 H346 R347 W348 N351 N352 D357 S358 A359 G362 P365 I366 A367 R371

E375 P376 G377 I378 V379 N380 L381 D382 K385 G388 R389 I390 V391 D392 G393 Y394 I398 D399 V402 E403 E410 P418 C419 E423 V424 F425 P426 L427 I428 A429 E430 L436 F440 Y446 Y455 I459 S460 R461 Q465 S475 V489 D496 F497

V507 A514 I515 K516 M517 V518 D519 Q520 K523 V526 Q530 L536 I542 K543 H544 T545 K548 T552 V553 A554 K555 L556 A557 E561 H664 Y567 G568 A569 Y570 L571 I572 Q573 F577 Q578 D579 S580 D581 P582 L583 L584 P585 A586 L587 Y592 R593 T594 E595

A596 D597 I598 Y599 T603 T604 C605 V606 E607 I610 K611 A612 V613 G614 A615 Q639 T640 Y641 N645 C649 D655 D659 E662 R666 R669 F670 I671 T675 F681 L685 Q686 Q687 A688 P689 P692 I693 D694 K695 E696 T697 R701 I705 T706 G707

N708 E711 V712 F713 S714 Q715 L716 N717 L723 E724 LEU VAL ASP GLN THR ASP CYS GLU GLY GLY ALA CYS PRO ILE LYS

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.50Å 114.70Å 121.30Å 90.00° 110.20° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25227	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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	A	0.35	0/5702	0.60	1/7731 (0.0%)
1	B	0.46	0/5702	0.68	3/7731 (0.0%)
1	C	0.35	0/5702	0.61	2/7731 (0.0%)
1	D	0.34	0/5702	0.60	1/7731 (0.0%)
All	All	0.38	0/22808	0.63	7/30924 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	GLY	N-CA-C	-7.18	95.15	113.10
1	B	388	GLY	N-CA-C	-7.03	95.52	113.10
1	C	388	GLY	N-CA-C	-6.42	97.06	113.10
1	D	388	GLY	N-CA-C	-6.33	97.29	113.10
1	C	435	ASP	N-CA-C	-5.31	96.67	111.00

There are no chirality outliers.

There are no planarity outliers.

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	A	5588	0	5456	186	0
1	B	5588	0	5456	111	0
1	C	5588	0	5456	127	0
1	D	5588	0	5456	180	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	652	0	0	64	0
2	B	960	0	0	54	1
2	C	684	0	0	45	1
2	D	579	0	0	72	0
All	All	25227	0	21824	601	2

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 601 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:D:706:THR:HG22	2:D:1110:HOH:O	1.26	1.33
1:C:190:GLU:HG2	2:C:1386:HOH:O	1.29	1.30
1:D:158:MET:HE1	2:D:1285:HOH:O	1.28	1.30
1:B:534:LYS:HE3	2:B:1454:HOH:O	1.15	1.26
1:C:563:MET:HE2	2:C:1422:HOH:O	1.34	1.25

All (2) 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:D:715:GLN:CG	2:B:1694:HOH:O[2_545]	1.97	0.23
2:C:907:HOH:O	2:C:1175:HOH:O[2_756]	2.15	0.05

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	
1	A	713/739 (96%)	672 (94%)	36 (5%)	5 (1%)	22	8
1	B	713/739 (96%)	688 (96%)	24 (3%)	1 (0%)	51	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	713/739 (96%)	674 (94%)	36 (5%)	3 (0%)	34	17
1	D	713/739 (96%)	670 (94%)	38 (5%)	5 (1%)	22	8
All	All	2852/2956 (96%)	2704 (95%)	134 (5%)	14 (0%)	29	12

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	684	SER
1	B	684	SER
1	A	550	SER
1	C	360	PHE
1	D	579	ASP

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	
1	A	598/623 (96%)	585 (98%)	13 (2%)	52	29
1	B	598/623 (96%)	588 (98%)	10 (2%)	60	42
1	C	598/623 (96%)	586 (98%)	12 (2%)	55	34
1	D	598/623 (96%)	584 (98%)	14 (2%)	50	28
All	All	2392/2492 (96%)	2343 (98%)	49 (2%)	55	34

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	148	MET
1	D	10	GLU
1	C	154	PHE
1	C	675	THR
1	D	119	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	118	ASN
1	D	211	GLN
1	D	703	GLN
1	B	364	GLN
1	B	118	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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.