

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 4, 2023 - 07:21 am GMT

PDB ID	:	1H42
Title	:	FERREDOXIN:NADP+ REDUCTASE MUTANT WITH THR 155 RE-
		PLACED BY GLY, ALA 160 REPLACED BY THR AND LEU 263 RE-
		PLACED BY PRO (T155G-A160T-L263P)
Authors	:	Hermoso, J.A.; Mayoral, T.; Medina, M.; Sanz-Aparicio, J.; Gomez-Moreno,
		С.
Deposited on	:	2002-09-26
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
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:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.15 Å.

141614

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	Percent	ile Ranks Value
Clashscore		2
Worse	2	Better
Perc	centile relative to all X-ray structures	
Pero	centile relative to X-ray structures of sir	nilar resolution
Metric	Whole archive	Similar resolution
Metric	(# Entries)	$(\# \text{Entries, resolution range}(\text{\AA}))$

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 $\leq =5\%$

1585(2.16-2.16)

Note EDS was not executed.

Clashscore

Mol	Chain	Length	Quality of chain				
1	А	304	94%	•	•		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2695 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.

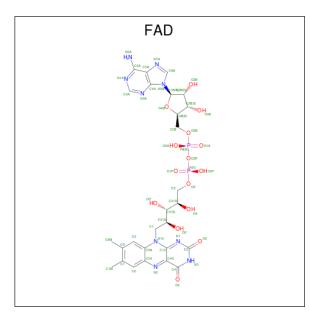
• Molecule 1 is a protein called FERREDOXIN–NADP+ REDUCTASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	295	Total 2336	C 1486	N 399	0 442	${ m S} 9$	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	155	GLY	THR	engineered mutation	UNP P21890
А	160	THR	ALA	engineered mutation	UNP P21890
А	263	PRO	LEU	engineered mutation	UNP P21890

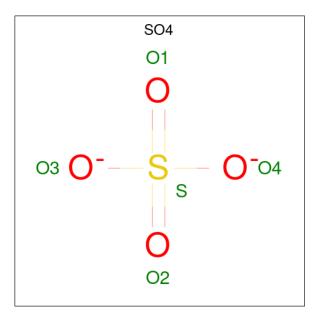
• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	Λ	1	Total	С	Ν	Ο	Р	0	1
	Z A	1	75	37	14	21	3	0	1



• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	А	279	Total 279	О 279	0	0

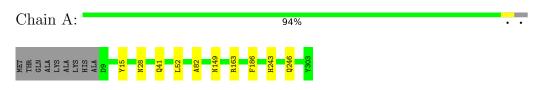


# 3 Residue-property plots (i)

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: FERREDOXIN–NADP+ REDUCTASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants	85.81Å 85.81Å 96.13Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	14.86 - 2.15	Depositor
% Data completeness	98.8 (14.86-2.15)	Depositor
(in resolution range)	50.0 (14.00-2.15)	Depositor
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
$R, R_{free}$	0.200 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2695	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	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, FAD

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		
IVIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.62	0/2393	0.60	0/3242	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	А	2336	0	2308	6	0
2	А	75	0	24	3	0
3	А	5	0	0	0	0
4	А	279	0	0	0	0
All	All	2695	0	2332	9	0

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 2.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1304[B]:FAD:C4B	2:A:1304[B]:FAD:O4B	1.73	1.31
2:A:1304[B]:FAD:O4B	2:A:1304[B]:FAD:C5B	2.18	0.91
2:A:1304[B]:FAD:O4B	2:A:1304[B]:FAD:H52A	1.93	0.67
1:A:149:ASN:HD22	1:A:186:PHE:H	1.48	0.61
1:A:243:HIS:HD2	1:A:246:GLN:HE22	1.55	0.53
1:A:28:ASN:ND2	1:A:41:GLN:HE21	2.11	0.49
1:A:15:TYR:HD2	1:A:52:LEU:HD23	1.78	0.48
1:A:82:ALA:O	1:A:163:ARG:HD3	2.18	0.44
1:A:243:HIS:HD2	1:A:246:GLN:NE2	2.18	0.40

There are no symmetry-related clashes.

## 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)

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)

3 ligands are modelled in this entry.



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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	Turne	Chain	Pog Link		ain Res Link Bond lengths				B	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
2	FAD	А	1304[B]	-	$53,\!58,\!58$	2.29	9 (16%)	68,89,89	2.26	12 (17%)	
2	FAD	А	1304[A]	-	$53,\!58,\!58$	1.64	9 (16%)	68,89,89	1.66	10 (14%)	
3	SO4	А	1305	-	4,4,4	0.52	0	$6,\!6,\!6$	0.04	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	А	1304[B]	-	-	5/30/50/50	0/6/6/6
2	FAD	А	1304[A]	-	-	4/30/50/50	0/6/6/6

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	А	1304[B]	FAD	O4B-C4B	12.54	1.73	1.45
2	А	1304[A]	FAD	C6-C7	-4.96	1.32	1.39
2	А	1304[B]	FAD	C6-C7	-4.96	1.32	1.39
2	А	1304[A]	FAD	O4B-C1B	4.17	1.46	1.41
2	А	1304[A]	FAD	C5'-C4'	-3.89	1.46	1.51
2	А	1304[B]	FAD	C5'-C4'	-3.89	1.46	1.51
2	А	1304[A]	FAD	C5X-N5	-3.41	1.32	1.39
2	А	1304[B]	FAD	C5X-N5	-3.41	1.32	1.39
2	А	1304[A]	FAD	C2B-C1B	2.95	1.58	1.53
2	А	1304[A]	FAD	C9-C8	-2.74	1.35	1.39
2	А	1304[B]	FAD	C9-C8	-2.74	1.35	1.39
2	А	1304[B]	FAD	C2A-N3A	2.68	1.36	1.32
2	А	1304[A]	FAD	C2A-N3A	2.66	1.36	1.32
2	А	1304[A]	FAD	P-O2P	-2.51	1.43	1.55
2	А	1304[B]	FAD	P-O2P	-2.51	1.43	1.55
2	А	1304[A]	FAD	PA-O5B	-2.18	1.50	1.59
2	А	1304[B]	FAD	PA-O5B	-2.18	1.50	1.59
2	А	1304[B]	FAD	O4B-C1B	2.12	1.44	1.41

All (18) bond length outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1304[B]	FAD	O4B-C4B-C3B	-11.31	82.74	105.11
2	А	1304[B]	FAD	O4B-C4B-C5B	-7.24	85.56	109.37
2	А	1304[B]	FAD	C5A-C6A-N6A	4.86	127.74	120.35
2	А	1304[A]	FAD	C5A-C6A-N6A	4.83	127.70	120.35
2	А	1304[A]	FAD	O4B-C1B-C2B	-4.18	100.81	106.93
2	А	1304[A]	FAD	C10-N1-C2	4.08	125.07	116.90
2	А	1304[B]	FAD	C10-N1-C2	4.08	125.07	116.90
2	А	1304[A]	FAD	O2'-C2'-C3'	-3.93	99.55	109.10
2	А	1304[B]	FAD	O2'-C2'-C3'	-3.93	99.55	109.10
2	А	1304[A]	FAD	O3'-C3'-C4'	-3.21	101.06	108.81
2	А	1304[B]	FAD	O3'-C3'-C4'	-3.21	101.06	108.81
2	А	1304[A]	FAD	C4X-C10-N1	-2.37	119.24	124.73
2	А	1304[B]	FAD	C4X-C10-N1	-2.37	119.24	124.73
2	А	1304[A]	FAD	C1'-C2'-C3'	2.32	116.27	109.79
2	А	1304[B]	FAD	C1'-C2'-C3'	2.32	116.27	109.79
2	А	1304[B]	FAD	O4B-C1B-C2B	-2.19	103.72	106.93
2	А	1304[A]	FAD	C4X-C10-N10	2.17	119.66	116.48
2	А	1304[B]	FAD	C4X-C10-N10	2.17	119.66	116.48
2	А	1304[A]	FAD	C1'-N10-C9A	-2.12	116.97	120.51
2	А	1304[B]	FAD	C1'-N10-C9A	-2.12	116.97	120.51
2	А	1304[A]	FAD	O2A-PA-O1A	2.12	122.70	112.24
2	А	1304[B]	FAD	O2A-PA-O1A	2.12	122.70	112.24

All (22) bond angle outliers are listed below:

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1304[B]	FAD	O4B-C4B-C5B-O5B
2	А	1304[A]	FAD	C5B-O5B-PA-O3P
2	А	1304[B]	FAD	C5B-O5B-PA-O3P
2	А	1304[A]	FAD	PA-O3P-P-O1P
2	А	1304[B]	FAD	PA-O3P-P-O1P
2	А	1304[A]	FAD	C4B-C5B-O5B-PA
2	А	1304[B]	FAD	C4B-C5B-O5B-PA
2	А	1304[A]	FAD	PA-O3P-P-O2P
2	А	1304[B]	FAD	PA-O3P-P-O2P

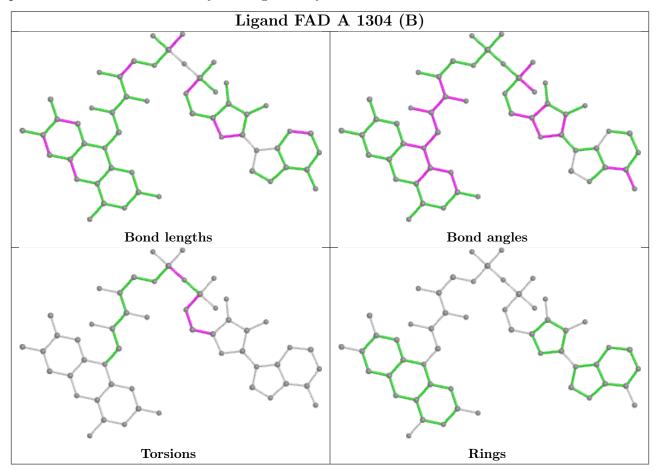
There are no ring outliers.

1 monomer is involved in 3 short contacts:

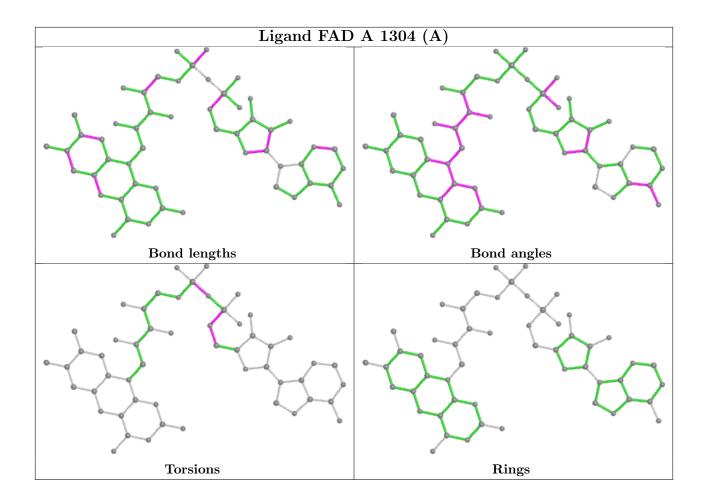


Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
2	А	1304[B]	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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.

