



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:42 AM GMT

PDB ID : 1QUF
Title : X-RAY STRUCTURE OF A COMPLEX NADP⁺-FERREDOXIN:NADP
+REDUCTASE FROM THE CYANOBACTERIUM ANABAENA PCC 7119
AT 2.25 ANGSTROMS
Authors : Serre, L.; Frey, M.; Vellieux, F.M.D.
Deposited on : 1996-09-07
Resolution : 2.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

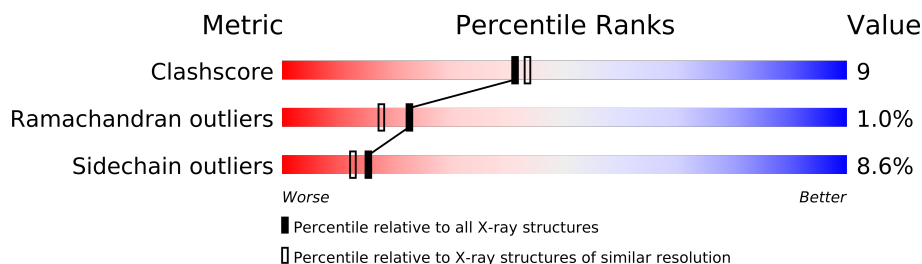
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2874 atoms, of which 4 are hydrogens and 0 are deuterium.

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.

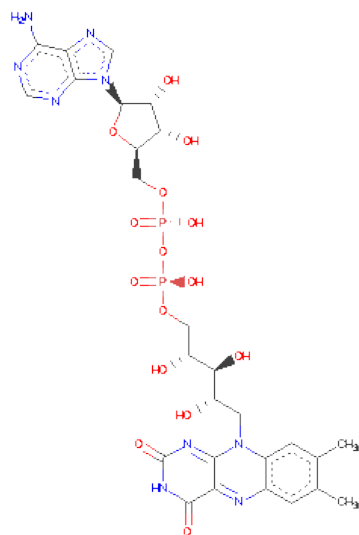
- Molecule 1 is a protein called FERREDONIN-NADP+ REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2330	1485	397	439	9	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	GLN	GLU	CONFLICT	UNP P21890
A	254	GLU	GLN	CONFLICT	UNP P21890

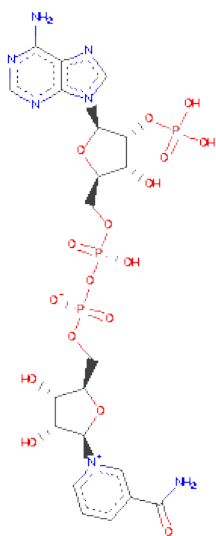
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-

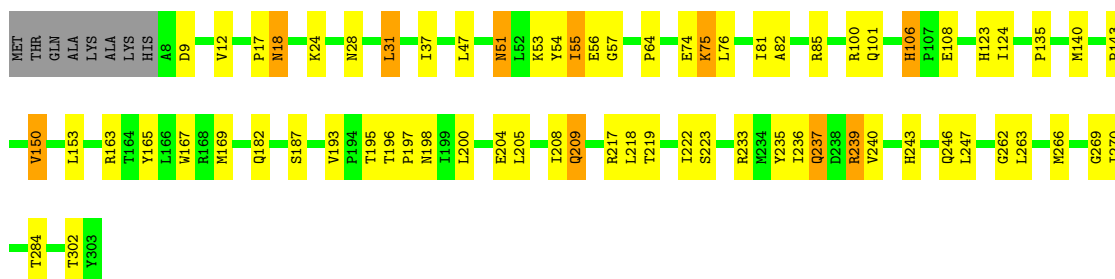
letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			52	21	4	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	439	Total	O	0	0
			439	439		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 85.84Å 97.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.25	Depositor
% Data completeness (in resolution range)	83.0 (15.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.73	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/2393	0.85	2/3245 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	HIS	N-CA-C	7.49	131.24	111.00
1	A	218	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2330	0	2293	42	0
2	A	53	0	30	0	0
3	A	48	4	19	4	0
4	A	439	0	0	5	7
All	All	2870	4	2342	44	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 44 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:ILE:HG13	4:A:658:HOH:O	1.84	0.77
1:A:153:LEU:HD13	1:A:270:ILE:HD13	1.70	0.72
1:A:165:TYR:O	1:A:169:MET:HG3	1.90	0.71
1:A:237:GLN:HE21	1:A:237:GLN:H	1.40	0.70
1:A:31:LEU:HB3	1:A:200:LEU:HD22	1.76	0.67

The worst 5 of 7 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	Distance(Å)	Clash(Å)
4:A:614:HOH:O	4:A:816:HOH:O[3_665]	0.81	1.39
4:A:629:HOH:O	4:A:810:HOH:O[3_665]	1.32	0.88
4:A:639:HOH:O	4:A:649:HOH:O[3_665]	1.44	0.76
4:A:605:HOH:O	4:A:810:HOH:O[3_665]	1.78	0.42
4:A:549:HOH:O	4:A:705:HOH:O[5_555]	2.05	0.15

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	296/304 (97%)	282 (95%)	11 (4%)	3 (1%)	22	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	9	ASP
1	A	108	GLU

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	246/256 (96%)	224 (91%)	22 (9%)	14 11

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	182	GLN
1	A	266	MET
1	A	150	VAL
1	A	167	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	299	HIS
1	A	237	GLN
1	A	51	ASN
1	A	243	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	FAD	A	304	-	58,58,58	1.33	4 (6%)	85,89,89	2.37	12 (14%)
3	NAP	A	305	-	52,52,52	2.32	14 (26%)	80,80,80	7.06	39 (48%)

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	A	304	-	1/1/9/9	0/34/50/50	0/1/6/6
3	NAP	A	305	-	1/1/12/12	1/35/67/67	0/3/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	NAP	P2B-O2B	-6.46	1.39	1.59
3	A	305	NAP	C2N-N1N	6.32	1.43	1.35
3	A	305	NAP	O4D-C1D	6.07	1.50	1.41
2	A	304	FAD	C4-C4X	5.83	1.50	1.41
3	A	305	NAP	C8A-N9A	-5.20	1.28	1.36

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	NAP	C1B-N9A-C4A	26.71	172.78	126.64
3	A	305	NAP	C8A-N9A-C4A	-23.49	88.97	106.90
3	A	305	NAP	C2N-N1N-C1D	22.36	174.74	119.33
3	A	305	NAP	C6N-N1N-C2N	-19.90	99.57	122.04
3	A	305	NAP	C6N-N1N-C1D	-17.69	75.49	119.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	304	FAD	C1B
3	A	305	NAP	C1B

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	NAP	C2D-C1D-N1N-C6N

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.