Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:06 PM GMT

PDB ID	:	1NHS
Title	:	AN L40C MUTATION CONVERTS THE CYSTEINE-SULFENIC ACID REDOX CENTRE IN ENTEROCOCCAL NADH PEROXIDASE TO A DISULFIDE
Authors	:	Mande, S.S.; Claiborne, A.; Hol, W.G.J.
Deposited on	:	1994-12-09
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

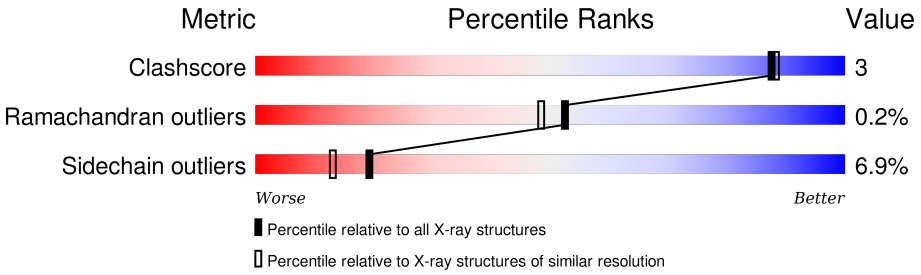
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	447	86% 11% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3803 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.

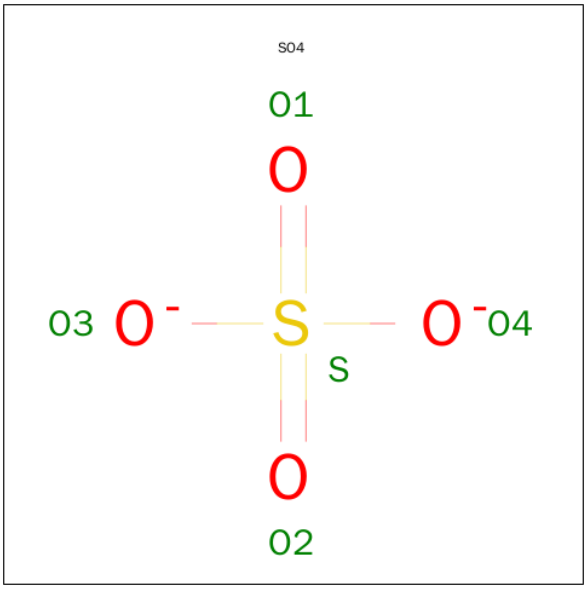
- Molecule 1 is a protein called NADH PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3493	2225	573	682	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

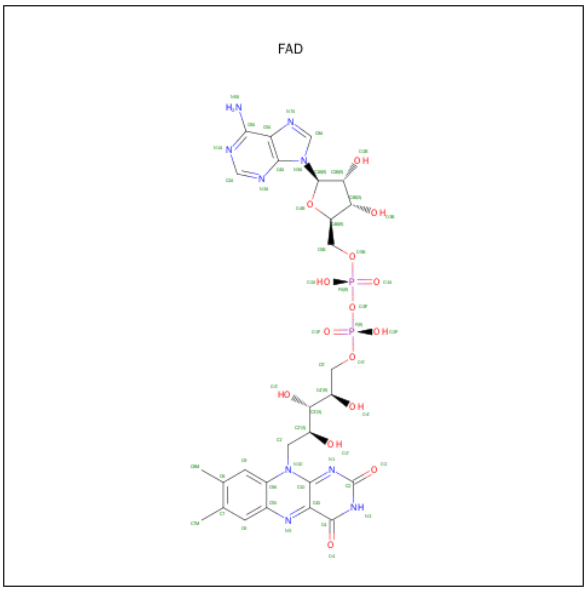
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	SER	ENGINEERED MUTATION	UNP P37062

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



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	252	Total	O	0	0
			252	252		

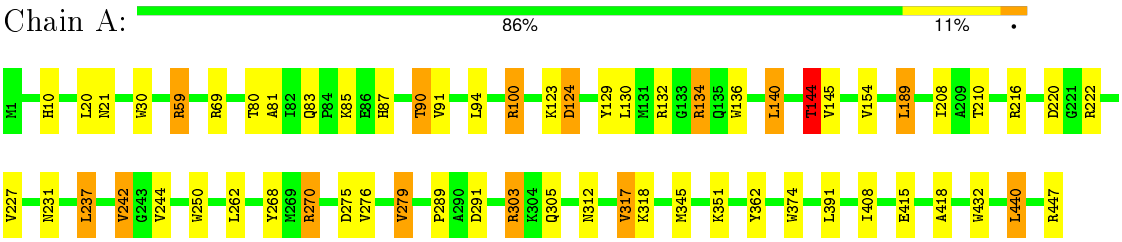
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: NADH PEROXIDASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.30Å 134.80Å 145.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3803	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: OCS, 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	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.70	0/3547	1.32	40/4807 (0.8%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	59	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	A	59	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	132	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	134	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	374	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	A	374	TRP	CE2-CD2-CG	-8.49	100.51	107.30
1	A	432	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	A	30	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	A	303	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	432	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	136	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	250	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	136	TRP	CD1-CG-CD2	7.29	112.14	106.30
1	A	250	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	374	TRP	CB-CG-CD1	-7.03	117.86	127.00
1	A	134	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	345	MET	CG-SD-CE	-6.95	89.08	100.20
1	A	362	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	A	374	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	A	30	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	136	TRP	CG-CD2-CE3	6.04	139.34	133.90
1	A	100	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	391	LEU	CA-CB-CG	5.64	128.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	A	124	ASP	CA-C-N	-5.51	105.08	117.20
1	A	242	VAL	CA-CB-CG2	-5.50	102.65	110.90
1	A	279	VAL	N-CA-CB	-5.45	99.51	111.50
1	A	237	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	432	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	136	TRP	CB-CG-CD1	-5.38	120.01	127.00
1	A	189	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	432	TRP	CG-CD1-NE1	-5.25	104.84	110.10
1	A	30	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	270	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	374	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	144	THR	N-CA-CB	-5.12	100.58	110.30
1	A	270	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	80	THR	N-CA-CB	-5.04	100.72	110.30
1	A	69	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	A	3493	0	3489	18	0
2	A	5	0	0	0	0
3	A	53	0	31	0	0
4	A	252	0	0	0	0
All	All	3803	0	3520	18	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 3.

All (18) 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:279:VAL:HG22	1:A:305:GLN:HB3	1.74	0.69
1:A:312:ASN:HD21	1:A:318:LYS:H	1.46	0.64
1:A:312:ASN:ND2	1:A:317:VAL:H	2.01	0.58
1:A:312:ASN:HD22	1:A:317:VAL:H	1.51	0.57
1:A:268:TYR:HB2	1:A:270:ARG:HD2	1.87	0.55
1:A:418:ALA:HB1	1:A:440:LEU:HD13	1.89	0.53
1:A:81:ALA:HB3	1:A:90:THR:HG23	1.92	0.50
1:A:83:GLN:HE22	1:A:90:THR:HG22	1.77	0.49
1:A:289:PRO:HG3	1:A:408:ILE:HG21	1.94	0.49
1:A:312:ASN:HD21	1:A:318:LYS:N	2.11	0.47
1:A:87:HIS:HE1	1:A:275:ASP:OD2	1.97	0.47
1:A:216:ARG:HG2	1:A:227:VAL:HG22	1.98	0.46
1:A:144:THR:HG22	1:A:145:VAL:HG13	2.00	0.42
1:A:91:VAL:HG22	1:A:100:ARG:HG2	2.01	0.42
1:A:85:LYS:O	1:A:87:HIS:HD2	2.03	0.41
1:A:208:ILE:HG22	1:A:210:THR:HG23	2.01	0.41
1:A:129:TYR:HD2	1:A:140:LEU:HD13	1.86	0.41
1:A:10:HIS:ND1	1:A:303:ARG:HD2	2.36	0.40

There are no symmetry-related clashes.

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	444/447 (99%)	431 (97%)	12 (3%)	1 (0%)	52 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LYS

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	375/375 (100%)	349 (93%)	26 (7%)	19 13

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	21	ASN
1	A	59	ARG
1	A	90	THR
1	A	94	LEU
1	A	124	ASP
1	A	130	LEU
1	A	134	ARG
1	A	140	LEU
1	A	144	THR
1	A	154	VAL
1	A	189	LEU
1	A	220	ASP
1	A	222	ARG
1	A	231	ASN
1	A	237	LEU
1	A	242	VAL
1	A	244	VAL
1	A	262	LEU
1	A	276	VAL
1	A	291	ASP
1	A	317	VAL
1	A	351	LYS
1	A	415	GLU
1	A	440	LEU
1	A	447	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	87	HIS
1	A	288	ASN
1	A	312	ASN
1	A	385	GLN
1	A	402	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	OCS	A	42	1	7,8,9	2.17	3 (42%)	7,11,13	1.98	2 (28%)

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
1	OCS	A	42	1	-	0/4/7/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	OCS	OD2-SG	-4.10	1.35	1.46
1	A	42	OCS	OD3-SG	-2.02	1.39	1.45
1	A	42	OCS	CB-SG	2.86	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	OCS	OD1-SG-CB	-3.47	104.01	106.94
1	A	42	OCS	O-C-CA	-2.62	118.67	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	FAD	A	448	-	48,58,58	1.11	4 (8%)	54,89,89	2.36	8 (14%)
2	SO4	A	449	-	4,4,4	1.52	0	6,6,6	0.32	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
3	FAD	A	448	-	-	0/30/50/50	0/6/6/6
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	448	FAD	C10-N10	2.25	1.41	1.39
3	A	448	FAD	C4-N3	2.87	1.38	1.33
3	A	448	FAD	C9A-N10	2.93	1.42	1.38
3	A	448	FAD	O4B-C1B	3.57	1.45	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	448	FAD	N3A-C2A-N1A	-12.43	119.37	128.89
3	A	448	FAD	C4X-C10-N10	-3.86	118.25	120.52
3	A	448	FAD	C4X-C4-N3	-3.39	118.96	123.59
3	A	448	FAD	C1'-N10-C9A	2.08	121.19	118.86
3	A	448	FAD	P-O3P-PA	3.14	141.55	132.73
3	A	448	FAD	C4A-C5A-N7A	3.41	112.61	109.48
3	A	448	FAD	C4X-N5-C5X	4.55	122.00	116.76
3	A	448	FAD	C4-N3-C2	5.78	120.25	115.25

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

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.