



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:06 am GMT

PDB ID : 4UCG  
Title : NmeDAH7PS R126S variant  
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Deposited on : 2014-12-03  
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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
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

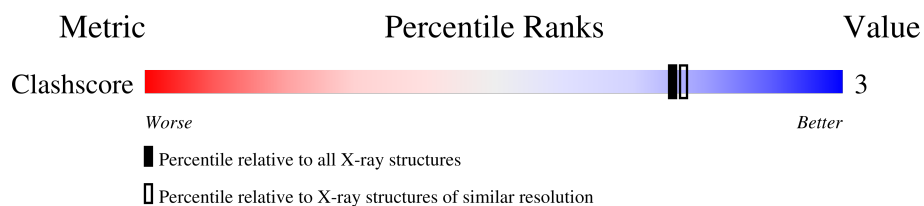
# 1 Overall quality at a glance

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	141614	9178 (2.00-2.00)

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11040 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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2572	1608	462	488	14	0	2	0
1	B	334	2570	1610	457	489	14	0	4	0
1	C	335	2549	1596	455	484	14	0	3	0
1	D	334	2533	1586	453	480	14	0	1	0

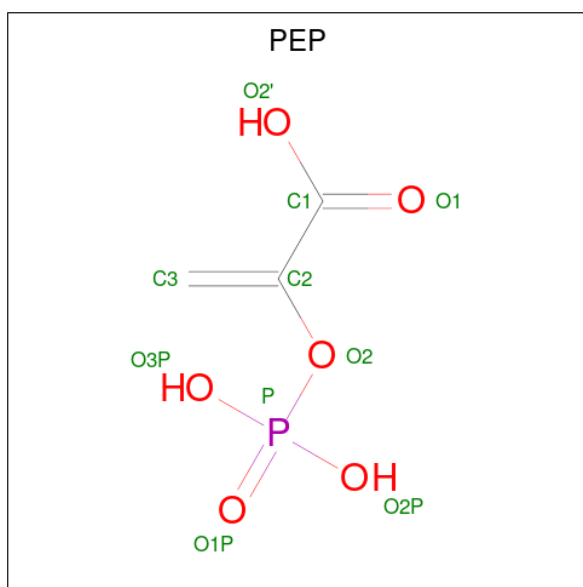
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	SER	ARG	engineered mutation	UNP Q9K169
B	126	SER	ARG	engineered mutation	UNP Q9K169
C	126	SER	ARG	engineered mutation	UNP Q9K169
D	126	SER	ARG	engineered mutation	UNP Q9K169

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C<sub>3</sub>H<sub>5</sub>O<sub>6</sub>P).



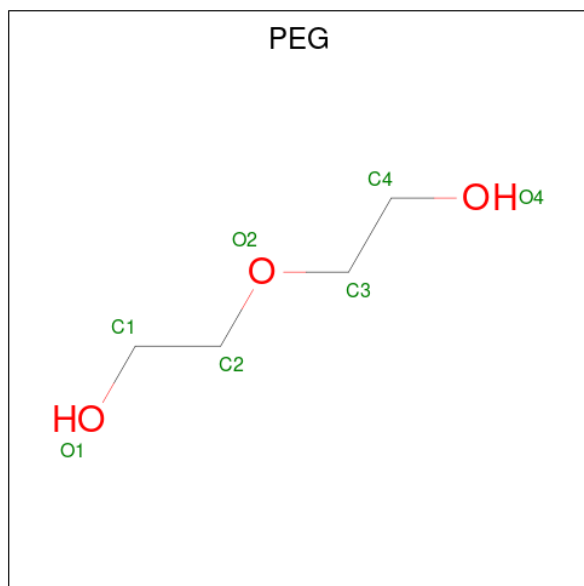
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	255	Total O 255 255	0	0
6	B	181	Total O 181 181	0	0
6	C	181	Total O 181 181	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	D	118	Total 118	O 118	0	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.95Å 132.66Å 147.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.70 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (98.70-2.00)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.180 , 0.220	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtrriage
Anisotropy	0.172	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEP, MN, PEG, 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	0.53	0/2624	0.69	0/3554
1	B	0.50	0/2620	0.68	1/3552 (0.0%)
1	C	0.50	0/2602	0.66	0/3530
1	D	0.49	0/2585	0.64	0/3505
All	All	0.51	0/10431	0.67	1/14141 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH1	6.68	123.64	120.30

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	2572	0	2529	25	0
1	B	2570	0	2506	16	0
1	C	2549	0	2475	21	0
1	D	2533	0	2478	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	0	0
3	D	10	0	2	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	8	0	10	2	0
5	B	14	0	20	0	0
6	A	255	0	0	3	0
6	B	181	0	0	0	0
6	C	181	0	0	1	0
6	D	118	0	0	0	0
All	All	11040	0	10026	62	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 (62) 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:C:219[A]:HIS:CD2	1:D:219[A]:HIS:CE1	2.16	1.33
1:C:219[A]:HIS:CD2	1:D:219[A]:HIS:ND1	2.05	1.25
1:C:219[A]:HIS:NE2	1:D:219[A]:HIS:CE1	2.14	1.14
1:A:219[B]:HIS:NE2	1:D:219[B]:HIS:ND1	2.01	1.07
1:A:219[A]:HIS:ND1	1:D:219[A]:HIS:NE2	2.03	1.06
1:B:219[B]:HIS:NE2	1:C:219[B]:HIS:ND1	2.03	1.04
1:A:219[B]:HIS:CE1	1:D:219[B]:HIS:ND1	2.29	1.00
1:C:219[A]:HIS:NE2	1:D:219[A]:HIS:HE1	1.57	0.97
1:A:219[A]:HIS:ND1	1:D:219[A]:HIS:CE1	2.38	0.92
1:C:219[A]:HIS:HD2	1:D:219[A]:HIS:ND1	1.56	0.89
1:A:219[A]:HIS:CG	1:D:219[A]:HIS:HE2	1.96	0.83
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:HE2	2.03	0.77
1:C:219[A]:HIS:HD2	1:D:219[A]:HIS:CE1	1.81	0.73
1:A:219[B]:HIS:NE2	1:D:219[B]:HIS:CE1	2.57	0.72
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:NE2	2.59	0.69
1:A:23:ALA:HB1	5:A:1354:PEG:H21	1.77	0.67
1:A:210:HIS:ND1	6:A:2173:HOH:O	2.28	0.66
1:B:219[A]:HIS:ND1	1:C:219[A]:HIS:CE1	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:CE1	2.88	0.61
1:A:219[B]:HIS:CE1	1:D:219[B]:HIS:CE1	2.88	0.61
1:B:219[B]:HIS:CE1	1:C:219[B]:HIS:HD1	2.17	0.59
1:B:219[B]:HIS:NE2	1:C:219[B]:HIS:CE1	2.69	0.59
1:A:15:VAL:CB	6:A:2001:HOH:O	2.51	0.59
1:C:210:HIS:ND1	6:C:2136:HOH:O	2.32	0.58
1:B:26[B]:TYR:CD2	1:D:19:LEU:HD21	2.39	0.57
1:C:172[A]:GLN:NE2	1:C:172[A]:GLN:HA	2.22	0.53
1:A:219[B]:HIS:NE2	1:D:219[B]:HIS:CG	2.78	0.52
1:A:189:ASN:ND2	1:A:242:ASN:HD21	2.09	0.51
1:B:219[A]:HIS:ND1	1:C:219[A]:HIS:HE1	2.09	0.50
1:A:23:ALA:HB1	5:A:1354:PEG:C2	2.41	0.50
1:C:219[A]:HIS:CD2	1:D:219[A]:HIS:HE1	1.90	0.50
1:C:189:ASN:HD21	1:C:236:ARG:H	1.59	0.50
1:A:189:ASN:HD21	1:A:236:ARG:H	1.61	0.48
1:A:189:ASN:ND2	1:A:236:ARG:H	2.12	0.48
1:B:189:ASN:ND2	1:B:236:ARG:H	2.11	0.47
1:B:189:ASN:HD21	1:B:236:ARG:H	1.61	0.47
1:C:295:GLY:O	1:C:346:ARG:NH1	2.44	0.47
1:B:26[B]:TYR:CD1	1:B:26[B]:TYR:N	2.82	0.46
1:D:189:ASN:HD21	1:D:236:ARG:H	1.62	0.46
1:B:219[A]:HIS:CG	1:C:219[A]:HIS:HE1	2.34	0.45
1:A:267:ASP:HA	1:A:302:MET:HB3	1.98	0.45
1:C:151:THR:N	1:C:152:PRO:CD	2.80	0.45
1:B:267:ASP:HA	1:B:302:MET:HB3	1.98	0.45
1:D:111:ASN:O	1:D:119:PHE:HA	2.17	0.44
1:A:26:TYR:CD1	1:A:26:TYR:N	2.86	0.43
1:A:219[A]:HIS:CG	1:D:219[A]:HIS:NE2	2.73	0.43
1:C:109:LEU:O	1:C:109:LEU:HD13	2.17	0.43
1:C:189:ASN:ND2	1:C:242:ASN:HD21	2.17	0.43
1:A:189:ASN:HD21	1:A:242:ASN:HD21	1.66	0.43
1:D:285:GLN:HG3	1:D:338:LEU:HD21	2.00	0.43
1:B:82:ARG:HA	1:B:91:ILE:HD12	2.01	0.42
1:A:77:ARG:HB3	1:A:329:TRP:CZ2	2.54	0.42
1:D:77:ARG:HB3	1:D:329:TRP:CZ2	2.55	0.42
1:D:151:THR:N	1:D:152:PRO:CD	2.82	0.42
1:B:151:THR:N	1:B:152:PRO:CD	2.82	0.42
1:A:152:PRO:HG3	6:A:2080:HOH:O	2.19	0.41
1:B:185:VAL:O	1:B:231:CYS:HA	2.21	0.41
1:C:312:GLN:O	1:C:322:ILE:HA	2.19	0.41
1:B:26[B]:TYR:OH	1:D:17:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASN:ND2	1:B:242:ASN:HD21	2.19	0.40
1:A:185:VAL:O	1:A:231:CYS:HA	2.22	0.40
1:D:189:ASN:ND2	1:D:236:ARG:H	2.18	0.40

There are no symmetry-related clashes.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

#### 4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers

There are no such residues in this entry.

#### 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.