W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2024 – 06:03 PM EDT

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PDB ID	:	4UCG
Title	:	NmeDAH7PS R126S variant
Authors	:	Cross, P.J.; Heyes, L.C.; Zhang, S.; Nazmi, A.R.; Parker, E.J.
Deposited on	:	2014-12-03
Resolution	:	2.00 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 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
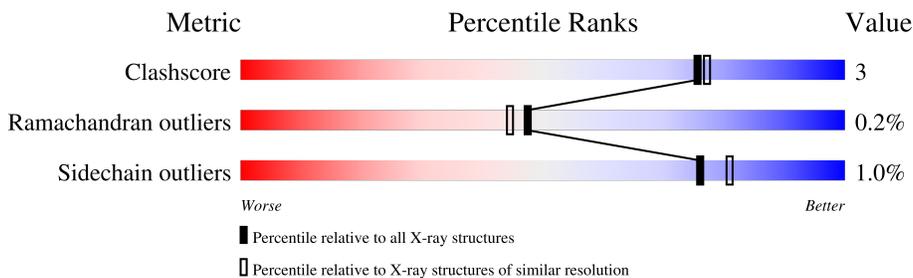
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	351	91% · ·
1	B	351	91% · 5%
1	C	351	91% · 5%
1	D	351	91% · 5%

2 Entry composition ⓘ

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 AL-DOLASE.

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

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).
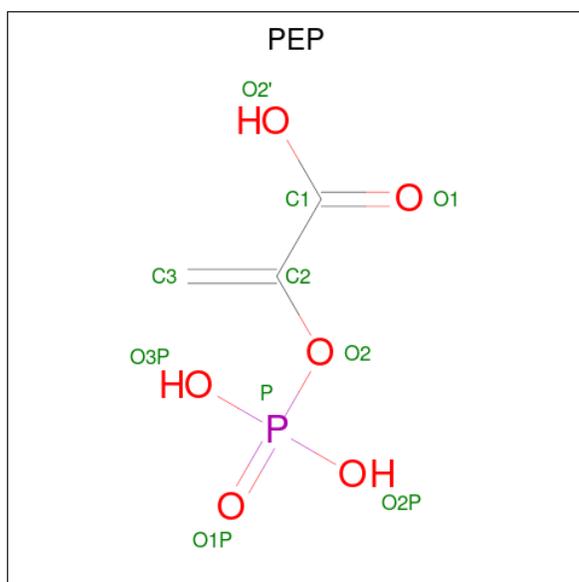
PEP

O2'
HO

C1 ⹀ O O1

C3 — C2

O3P O2
HO P

O1P
O O2P OH

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1
O

O3 O^- — S — O^- O4
S

O
O2
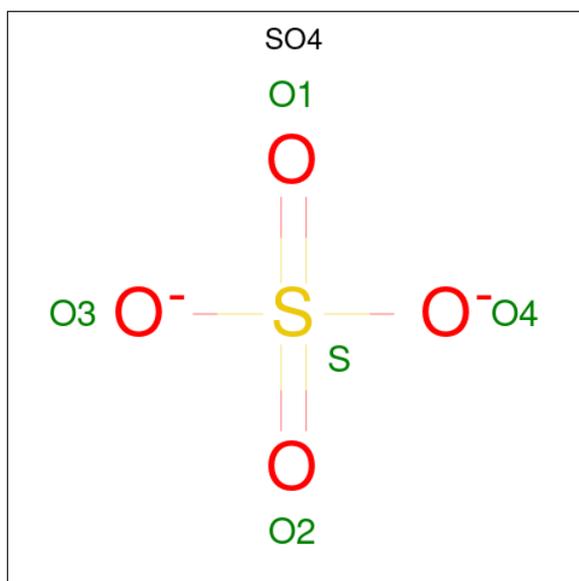
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
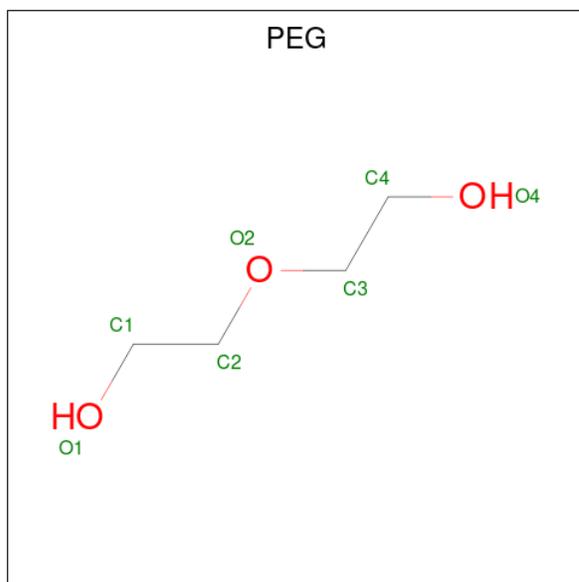
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 7	C 4	O 3	0	0
5	B	1	Total 7	C 4	O 3	0	0

- Molecule 6 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	118	Total 118	O 118	0	0

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 failed to run properly.

• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:

• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain B:

• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain C:

• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain D:

4 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, α, β, γ	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
$<I/\sigma(I)>$ [1]	1.59 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.180 , 0.220	Depositor
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.172	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11040	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, PEP, MN

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(^{o})	Ideal(^{o})
1	B	94	ARG	NE-CZ-NH1	6.68	123.64	120.30

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	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.

The worst 5 of 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

There are no symmetry-related clashes.

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	336/351 (96%)	330 (98%)	6 (2%)	0	100	100
1	B	336/351 (96%)	329 (98%)	6 (2%)	1 (0%)	41	37
1	C	336/351 (96%)	328 (98%)	8 (2%)	0	100	100
1	D	333/351 (95%)	326 (98%)	6 (2%)	1 (0%)	41	37
All	All	1341/1404 (96%)	1313 (98%)	26 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	ASP
1	B	294	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	269/289 (93%)	267 (99%)	2 (1%)	84	88
1	B	267/289 (92%)	265 (99%)	2 (1%)	84	88
1	C	263/289 (91%)	260 (99%)	3 (1%)	73	78
1	D	263/289 (91%)	260 (99%)	3 (1%)	73	78
All	All	1062/1156 (92%)	1052 (99%)	10 (1%)	76	83

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	236	ARG
1	D	269	SER
1	D	306	HIS
1	B	306	HIS
1	C	236	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	B	189	ASN
1	C	189	ASN
1	D	189	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 ⓘ

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.

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 failed to run properly - this section is therefore empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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