

wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 10:20 PM EDT

PDB ID : 4JTH

Title: Crystal structure of F114R/R117Q mutant of 3-deoxy-D-manno-octulosonate

8-phosphate synthase (KDO8PS) from Neisseria meningitidis

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Deposited on : 2013-03-23

Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

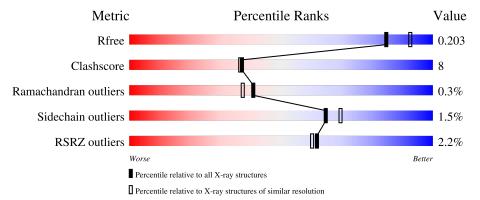
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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% 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.

Mol	Chain	Length	Quality of chain	
1	A	280	83%	6% 11%
1	В	280	% 75 %	13% • 10%
1	С	280	81%	11% • 8%
1	D	280	80%	10% • 9%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8774 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	250	Total	С	N	О	S	0	5	0
1	A	250	1953	1254	326	362	11	0	9	
1	В	251	Total	С	N	О	S	0	10	0
1	Ъ	251	1994	1280	336	366	12	0	10	
1	С	259	Total	С	N	О	S	0	6	0
1		259	2020	1296	341	372	11	0	U	
1	D	256	Total	С	N	О	S	0	6	0
1	D	250	2000	1281	341	367	11	U	U	U

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ARG	PHE	engineered mutation	UNP Q9JZ55
A	117	GLN	ARG	engineered mutation	UNP Q9JZ55
В	114	ARG	PHE	engineered mutation	UNP Q9JZ55
В	117	GLN	ARG	engineered mutation	UNP Q9JZ55
С	114	ARG	PHE	engineered mutation	UNP Q9JZ55
С	117	GLN	ARG	engineered mutation	UNP Q9JZ55
D	114	ARG	PHE	engineered mutation	UNP Q9JZ55
D	117	GLN	ARG	engineered mutation	UNP Q9JZ55

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

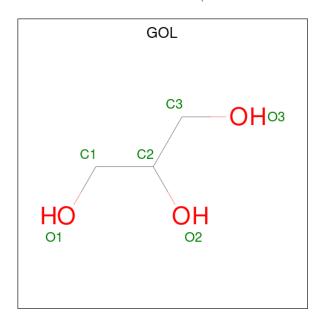
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Cl 1 1	0	0
2	С	2	Total Cl 2 2	0	0
2	D	2	Total Cl 2 2	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	Total Na 1 1	0	0

 \bullet Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 6 3 3	0	0

• Molecule 5 is water.

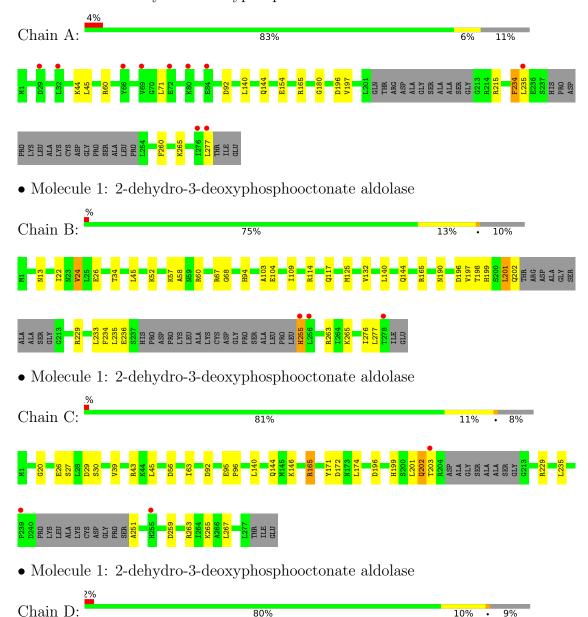
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	162	Total O 162 162	0	0
5	В	224	Total O 224 224	0	0
5	С	215	Total O 215 215	0	0
5	D	194	Total O 194 194	0	0



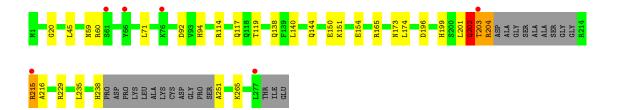
3 Residue-property plots (i)

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 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.

• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	82.15Å 85.99Å 163.11Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 - 2.00	Depositor
rtesolution (A)	45.95 - 2.00	EDS
% Data completeness	$100.0 \ (45.95 - 2.00)$	Depositor
(in resolution range)	$100.0 \ (45.95 - 2.00)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) > 1$	3.81 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.159 , 0.194	Depositor
R, R_{free}	0.167 , 0.203	DCC
R_{free} test set	3931 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 47.6	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8774	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: NA, GOL, CL

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	Boı	nd lengths	Bond angles		
WIOI		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.88	0/1987	0.88	3/2686 (0.1%)	
1	В	0.99	1/2038 (0.0%)	0.94	3/2754 (0.1%)	
1	С	0.97	2/2066 (0.1%)	0.93	5/2793~(0.2%)	
1	D	0.87	0/2049	0.89	$4/2769 \ (0.1\%)$	
All	All	0.93	3/8140 (0.0%)	0.91	15/11002 (0.1%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
1	С	26	GLU	CD-OE2	-5.94	1.19	1.25
1	В	104	GLU	CD-OE2	5.64	1.31	1.25
1	С	171	TYR	CG-CD2	-5.16	1.32	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	229	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	60	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	D	196	ASP	CB-CG-OD1	5.78	123.50	118.30
1	В	201	LEU	CB-CA-C	-5.72	99.33	110.20
1	С	92	ASP	CB-CG-OD1	5.69	123.42	118.30

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	1953	0	1993	10	0
1	В	1994	0	2048	59	0
1	С	2020	0	2078	22	0
1	D	2000	0	2055	39	0
2	В	1	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	1	0
3	С	1	0	0	0	0
4	D	6	0	8	0	0
5	A	162	0	0	2	0
5	В	224	0	0	4	0
5	С	215	0	0	5	0
5	D	194	0	0	15	0
All	All	8774	0	8182	126	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 8.

The worst 5 of 126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:C:259:ASP:HB2	5:C:601:HOH:O	1.45	1.17
1:B:199[B]:HIS:CE1	1:B:236[B]:GLU:HG3	1.91	1.05
1:D:154:GLU:HG2	5:D:585:HOH:O	1.65	0.97
1:C:146:LYS:HD2	5:C:604:HOH:O	1.65	0.97
1:B:109[B]:ILE:HD12	1:B:125[B]:MET:HG3	1.51	0.92

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	Perce	entiles
1	A	249/280 (89%)	244 (98%)	5 (2%)	0	100	100
1	В	255/280 (91%)	250 (98%)	5 (2%)	0	100	100
1	C	259/280 (92%)	252 (97%)	6 (2%)	1 (0%)	34	30
1	D	256/280 (91%)	252 (98%)	2 (1%)	2 (1%)	19	13
All	All	1019/1120 (91%)	998 (98%)	18 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	GLN
1	С	229	ARG
1	D	229	ARG

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	Percent	iles
1	A	$216/236 \ (92\%)$	213 (99%)	3 (1%)	67 7	2
1	В	223/236 (94%)	219 (98%)	4 (2%)	59 6	3
1	С	$226/236 \ (96\%)$	224 (99%)	2 (1%)	78 8	3
1	D	$224/236 \ (95\%)$	219 (98%)	5 (2%)	52 5	5
All	All	889/944 (94%)	875 (98%)	14 (2%)	65 6	7

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	165	ARG
1	С	202	GLN
1	D	215	ARG
1	D	202	GLN
1	D	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:



Mol	Chain	Res	Type
1	С	202	GLN
1	D	59	ASN
1	D	217	GLN
1	D	202	GLN
1	В	186	GLN

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)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	B	ond leng	${ m gths}$	В	ond ang	gles
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	303	-	5,5,5	0.21	0	5,5,5	0.67	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
4	GOL	D	303	-	-	2/4/4/4	-



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	250/280 (89%)	-0.11	10 (4%) 38 37	13, 27, 57, 80	1 (0%)
1	В	251/280 (89%)	-0.31	3 (1%) 79 78	12, 22, 41, 84	0
1	С	259/280 (92%)	-0.37	3 (1%) 79 78	12, 20, 41, 83	0
1	D	256/280 (91%)	-0.11	6 (2%) 60 59	13, 26, 54, 74	0
All	All	1016/1120 (90%)	-0.23	22 (2%) 62 60	12, 24, 53, 84	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	255	HIS	6.1
1	A	66	TYR	5.7
1	A	277	LEU	4.9
1	D	203	THR	3.9
1	С	239	PRO	3.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	D	303	6/6	0.81	0.29	41,49,51,54	6
3	NA	С	303	1/1	0.95	0.12	28,28,28,28	0
2	CL	D	302	1/1	0.95	0.08	47,47,47,47	0
2	CL	В	301	1/1	0.98	0.09	25,25,25,25	0
2	CL	С	301	1/1	0.99	0.06	24,24,24,24	0
2	CL	С	302	1/1	0.99	0.05	32,32,32,32	0
2	CL	D	301	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

