wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 02:18 PM EDT

PDB ID	:	4JTI
Title	:	Crystal structure of F114R/R117Q/F139G mutant of 3-deoxy-D-manno-octu losonate 8-phosphate synthase (KDO8PS) from Neisseria meningitidis
Authors	:	Allison, T.M.; Cochrane, F.C.; Jameson, G.B.; Parker, E.J.
Deposited on	:	2013-03-23
Resolution	:	1.75 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:

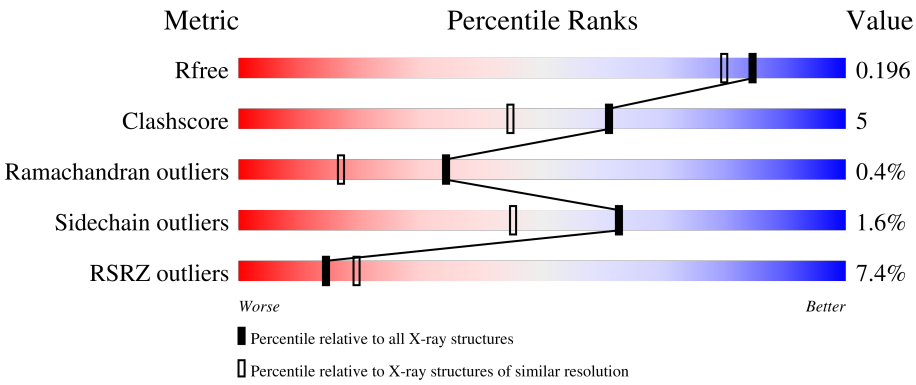
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.75 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))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	9% 80% 10% • 10%
1	B	280	5% 84% 8% 8%
1	C	280	6% 82% 9% • 8%
1	D	280	7% 81% 10% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8642 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
			Total	C	N	O	S			
1	A	253	1943	1241	331	360	11	0	1	0
1	B	257	2006	1283	343	369	11	0	6	0
1	C	258	1986	1271	341	363	11	0	2	0
1	D	258	1986	1269	339	367	11	0	2	0

There are 12 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
A	139	GLY	PHE	engineered mutation	UNP Q9JZ55
B	114	ARG	PHE	engineered mutation	UNP Q9JZ55
B	117	GLN	ARG	engineered mutation	UNP Q9JZ55
B	139	GLY	PHE	engineered mutation	UNP Q9JZ55
C	114	ARG	PHE	engineered mutation	UNP Q9JZ55
C	117	GLN	ARG	engineered mutation	UNP Q9JZ55
C	139	GLY	PHE	engineered mutation	UNP Q9JZ55
D	114	ARG	PHE	engineered mutation	UNP Q9JZ55
D	117	GLN	ARG	engineered mutation	UNP Q9JZ55
D	139	GLY	PHE	engineered mutation	UNP Q9JZ55

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	B	1	1	1	0	0
2	C	3	3	3	0	0

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

- Molecule 3 is water.

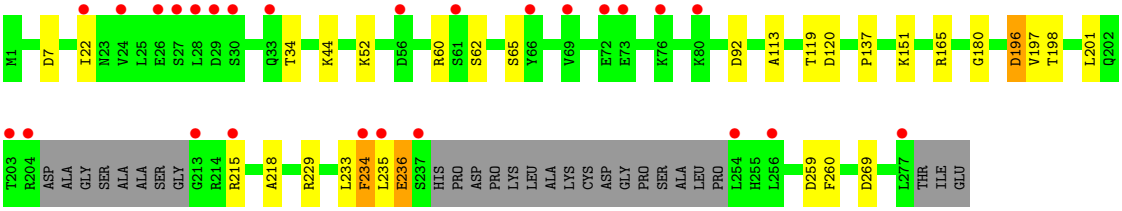
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	170	170	170	0	0
			Total	O		
3	B	193	193	193	0	0
			Total	O		
3	C	179	179	179	0	0
			Total	O		
3	D	174	174	174	0	0

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.

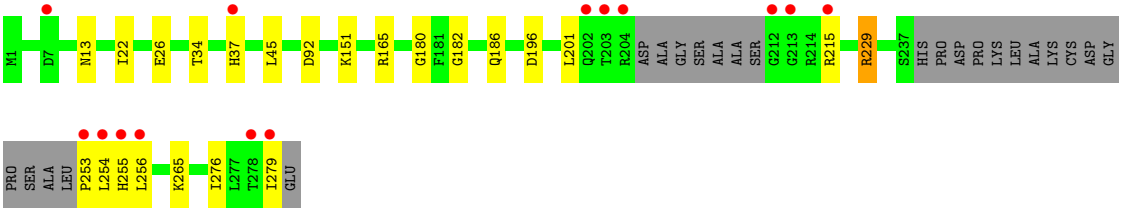
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain A:



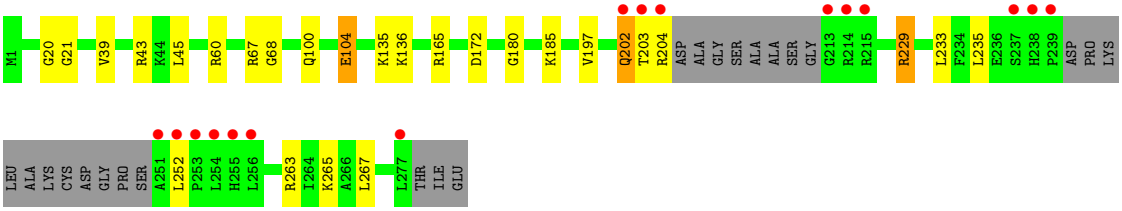
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain B:



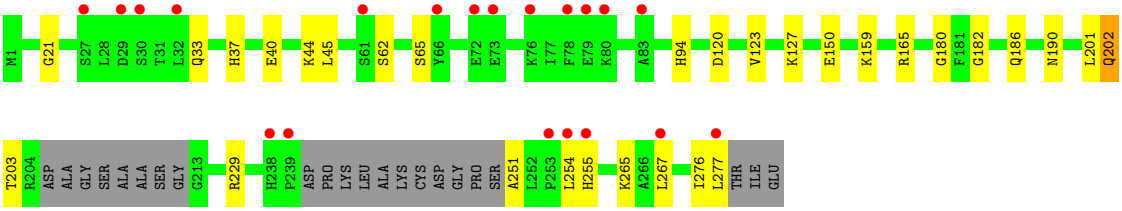
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain C:



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

Chain D:


M1
G21
S27
L28
D29
S30
T31
L32
Q33
H37
E40
K44
L45
S61
S62
S65
Y66
E72
E73
K76
I77
F78
E79
K80
A83
H94
D120
V123
K127
E150
K159
R165
G180
F181
G182
Q186
N190
L201
Q202
T203
R204
ASP
ALA
GLY
SER
ALA
ALA
SER
GLY
G213
R229
H238
P239
ASP
PRO
LYS
LEU
ALA
LYS
CYS
ASP
GLY
PRO
SER
A251
L252
P253
L254
H255
K265
A266
L267
I276
L277
THR
ILE
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.67Å 85.20Å 162.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.82 – 1.75 40.84 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.82-1.75) 99.9 (40.84-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.159 , 0.188 0.171 , 0.196	Depositor DCC
R_{free} test set	5751 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8642	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 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.95	0/1976	0.95	5/2669 (0.2%)
1	B	1.00	0/2052	0.97	5/2771 (0.2%)
1	C	1.01	3/2025 (0.1%)	0.99	5/2738 (0.2%)
1	D	0.92	1/2022 (0.0%)	0.92	2/2734 (0.1%)
All	All	0.97	4/8075 (0.0%)	0.96	17/10912 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	21	GLY	N-CA	-5.95	1.37	1.46
1	C	104	GLU	CD-OE2	-5.69	1.19	1.25
1	C	68	GLY	N-CA	-5.25	1.38	1.46
1	C	21	GLY	N-CA	-5.08	1.38	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	PHE	CB-CA-C	-5.94	98.53	110.40
1	C	252	LEU	CA-CB-CG	5.91	128.89	115.30
1	C	229	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	136	LYS	CD-CE-NZ	5.62	124.64	111.70
1	B	201	LEU	CA-CB-CG	5.60	128.17	115.30

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	1943	0	1991	20	0
1	B	2006	0	2075	15	0
1	C	1986	0	2044	22	0
1	D	1986	0	2032	22	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	170	0	0	6	0
3	B	193	0	0	3	0
3	C	179	0	0	4	0
3	D	174	0	0	9	0
All	All	8642	0	8142	73	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 5.

The worst 5 of 73 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:B:253:PRO:HA	1:B:256:LEU:HB2	1.41	1.01
1:C:202:GLN:NE2	1:C:203:THR:HG23	1.82	0.94
1:D:94:HIS:HD2	3:D:505:HOH:O	1.54	0.91
1:D:251:ALA:HB2	3:D:491:HOH:O	1.74	0.86
1:B:13:ASN:HD21	1:B:229:ARG:HH21	1.23	0.84

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	248/280 (89%)	243 (98%)	4 (2%)	1 (0%)	34	17
1	B	257/280 (92%)	251 (98%)	5 (2%)	1 (0%)	34	17
1	C	254/280 (91%)	250 (98%)	3 (1%)	1 (0%)	34	17
1	D	254/280 (91%)	251 (99%)	2 (1%)	1 (0%)	34	17
All	All	1013/1120 (90%)	995 (98%)	14 (1%)	4 (0%)	34	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	229	ARG
1	B	229	ARG
1	C	229	ARG
1	A	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	Percentiles	
1	A	215/235 (92%)	211 (98%)	4 (2%)	57	37
1	B	224/235 (95%)	221 (99%)	3 (1%)	69	54
1	C	220/235 (94%)	218 (99%)	2 (1%)	78	67
1	D	220/235 (94%)	215 (98%)	5 (2%)	50	28
All	All	879/940 (94%)	865 (98%)	14 (2%)	62	45

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

Mol	Chain	Res	Type
1	C	60	ARG
1	C	202	GLN
1	D	255	HIS
1	D	165	ARG

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Mol	Chain	Res	Type
1	D	202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	138	GLN
1	D	202	GLN
1	D	186	GLN
1	B	147	ASN
1	C	118	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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 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 (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, 95th 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>2			OWAB(Å^2)	Q<0.9
1	A	253/280 (90%)	0.33	26 (10%)	6	9	12, 27, 56, 73	1 (0%)
1	B	257/280 (91%)	-0.01	14 (5%)	25	32	13, 21, 43, 74	0
1	C	258/280 (92%)	0.05	16 (6%)	20	26	14, 23, 46, 73	0
1	D	258/280 (92%)	0.35	20 (7%)	13	17	14, 26, 57, 72	0
All	All	1026/1120 (91%)	0.18	76 (7%)	14	19	12, 24, 55, 74	1 (0%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254	LEU	11.1
1	D	277	LEU	7.5
1	B	279	ILE	7.3
1	C	239	PRO	7.2
1	B	253	PRO	6.7

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, 95th 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	B-factors(Å^2)	Q<0.9
2	CL	D	301	1/1	0.95	0.08	37,37,37,37	0
2	CL	C	302	1/1	0.97	0.05	29,29,29,29	0
2	CL	C	303	1/1	0.98	0.04	42,42,42,42	0
2	CL	C	301	1/1	0.98	0.04	28,28,28,28	0
2	CL	B	301	1/1	0.99	0.08	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.