wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 07:03 am BST

PDB ID	:	5HNO
Title	:	The structure of the kdo-capped saccharide binding subunit of the O-12 specific ABC transporter, Wzt
Authors	:	Mallette, E.; Mann, E.; Whitfield, C.; Kimber, M.S.
Deposited on	:	2016-01-18
Resolution	:	1.70 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 following versions of software and data (see references (1)) were used in the production of this report:

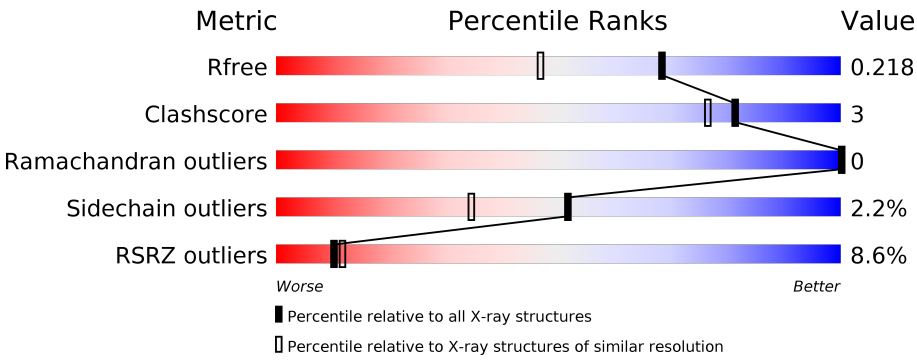
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	190	4%, 78%, 7%, •, 14%
1	B	190	14%, 82%, 6%, •, 12%
1	C	190	5%, 83%, •, 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8052 atoms, of which 3926 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 ABC type transport system putative ATP binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	164	2599	811	1314	222	247	5	0	4	0
1	B	168	2601	808	1312	225	251	5	0	2	0
1	C	166	2574	800	1300	222	247	5	0	1	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	MET	-	initiating methionine	UNP Q6U8B1
A	255	HIS	-	expression tag	UNP Q6U8B1
A	256	HIS	-	expression tag	UNP Q6U8B1
A	257	HIS	-	expression tag	UNP Q6U8B1
A	258	HIS	-	expression tag	UNP Q6U8B1
A	259	HIS	-	expression tag	UNP Q6U8B1
A	260	HIS	-	expression tag	UNP Q6U8B1
A	261	GLU	-	expression tag	UNP Q6U8B1
A	262	ASN	-	expression tag	UNP Q6U8B1
A	263	LEU	-	expression tag	UNP Q6U8B1
A	264	TYR	-	expression tag	UNP Q6U8B1
A	265	PHE	-	expression tag	UNP Q6U8B1
A	266	GLN	-	expression tag	UNP Q6U8B1
A	267	GLY	-	expression tag	UNP Q6U8B1
A	351	MET	CYS	conflict	UNP Q6U8B1
A	352	SER	ARG	conflict	UNP Q6U8B1
A	354	ALA	ARG	conflict	UNP Q6U8B1
A	355	GLN	ARG	conflict	UNP Q6U8B1
A	357	GLY	ALA	conflict	UNP Q6U8B1
A	358	ASP	ILE	conflict	UNP Q6U8B1
A	359	ILE	SER	conflict	UNP Q6U8B1
A	360	TRP	GLY	conflict	UNP Q6U8B1
A	361	GLY	GLU	conflict	UNP Q6U8B1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ASP	THR	conflict	UNP Q6U8B1
A	363	SER	ARG	conflict	UNP Q6U8B1
A	443	SER	-	expression tag	UNP Q6U8B1
B	254	MET	-	initiating methionine	UNP Q6U8B1
B	255	HIS	-	expression tag	UNP Q6U8B1
B	256	HIS	-	expression tag	UNP Q6U8B1
B	257	HIS	-	expression tag	UNP Q6U8B1
B	258	HIS	-	expression tag	UNP Q6U8B1
B	259	HIS	-	expression tag	UNP Q6U8B1
B	260	HIS	-	expression tag	UNP Q6U8B1
B	261	GLU	-	expression tag	UNP Q6U8B1
B	262	ASN	-	expression tag	UNP Q6U8B1
B	263	LEU	-	expression tag	UNP Q6U8B1
B	264	TYR	-	expression tag	UNP Q6U8B1
B	265	PHE	-	expression tag	UNP Q6U8B1
B	266	GLN	-	expression tag	UNP Q6U8B1
B	267	GLY	-	expression tag	UNP Q6U8B1
B	351	MET	CYS	conflict	UNP Q6U8B1
B	352	SER	ARG	conflict	UNP Q6U8B1
B	354	ALA	ARG	conflict	UNP Q6U8B1
B	355	GLN	ARG	conflict	UNP Q6U8B1
B	357	GLY	ALA	conflict	UNP Q6U8B1
B	358	ASP	ILE	conflict	UNP Q6U8B1
B	359	ILE	SER	conflict	UNP Q6U8B1
B	360	TRP	GLY	conflict	UNP Q6U8B1
B	361	GLY	GLU	conflict	UNP Q6U8B1
B	362	ASP	THR	conflict	UNP Q6U8B1
B	363	SER	ARG	conflict	UNP Q6U8B1
B	443	SER	-	expression tag	UNP Q6U8B1
C	254	MET	-	initiating methionine	UNP Q6U8B1
C	255	HIS	-	expression tag	UNP Q6U8B1
C	256	HIS	-	expression tag	UNP Q6U8B1
C	257	HIS	-	expression tag	UNP Q6U8B1
C	258	HIS	-	expression tag	UNP Q6U8B1
C	259	HIS	-	expression tag	UNP Q6U8B1
C	260	HIS	-	expression tag	UNP Q6U8B1
C	261	GLU	-	expression tag	UNP Q6U8B1
C	262	ASN	-	expression tag	UNP Q6U8B1
C	263	LEU	-	expression tag	UNP Q6U8B1
C	264	TYR	-	expression tag	UNP Q6U8B1
C	265	PHE	-	expression tag	UNP Q6U8B1
C	266	GLN	-	expression tag	UNP Q6U8B1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	267	GLY	-	expression tag	UNP Q6U8B1
C	351	MET	CYS	conflict	UNP Q6U8B1
C	352	SER	ARG	conflict	UNP Q6U8B1
C	354	ALA	ARG	conflict	UNP Q6U8B1
C	355	GLN	ARG	conflict	UNP Q6U8B1
C	357	GLY	ALA	conflict	UNP Q6U8B1
C	358	ASP	ILE	conflict	UNP Q6U8B1
C	359	ILE	SER	conflict	UNP Q6U8B1
C	360	TRP	GLY	conflict	UNP Q6U8B1
C	361	GLY	GLU	conflict	UNP Q6U8B1
C	362	ASP	THR	conflict	UNP Q6U8B1
C	363	SER	ARG	conflict	UNP Q6U8B1
C	443	SER	-	expression tag	UNP Q6U8B1

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

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

- Molecule 3 is water.

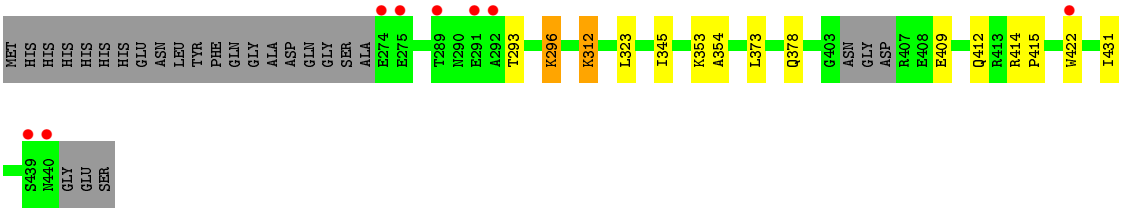
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	74	Total O 74 74	0	0
3	C	96	Total O 96 96	0	0

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 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.

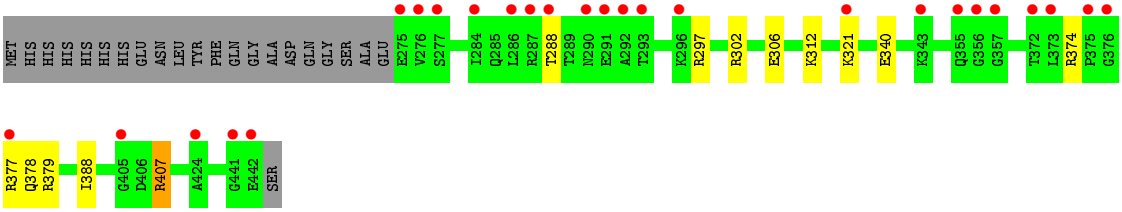
- Molecule 1: ABC type transport system putative ATP binding protein

Chain A:



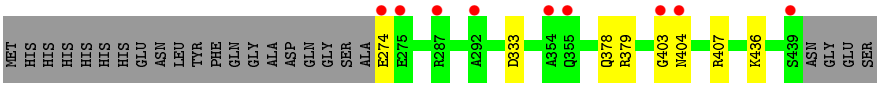
- Molecule 1: ABC type transport system putative ATP binding protein

Chain B:



- Molecule 1: ABC type transport system putative ATP binding protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.75Å 53.55Å 87.47Å 90.00° 125.77° 90.00°	Depositor
Resolution (Å)	35.49 – 1.70 36.13 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.49-1.70) 93.5 (36.13-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.215 0.186 , 0.218	Depositor DCC
R_{free} test set	4153 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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	0.27	0/1312	0.50	0/1765
1	B	0.25	0/1312	0.47	0/1765
1	C	0.26	0/1294	0.52	0/1741
All	All	0.26	0/3918	0.50	0/5271

There are no bond length outliers.

There are no bond angle outliers.

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	1285	1314	1314	9	0
1	B	1289	1312	1316	9	0
1	C	1274	1300	1302	3	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	106	0	0	4	1
3	B	74	0	0	3	0
3	C	96	0	0	1	1
All	All	4126	3926	3932	20	1

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 20 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:436:LYS:NZ	3:C:601:HOH:O	1.90	1.02
1:B:407:ARG:NH2	3:B:501:HOH:O	2.00	0.91
1:C:333:ASP:OD2	1:C:379:ARG:NH2	2.21	0.73
1:A:354:ALA:O	3:A:601:HOH:O	2.06	0.72
1:A:312:LYS:NZ	3:A:603:HOH:O	2.22	0.65

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:691:HOH:O	3:C:676:HOH:O[3_555]	2.12	0.08

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	164/190 (86%)	161 (98%)	3 (2%)	0	100	100
1	B	168/190 (88%)	162 (96%)	6 (4%)	0	100	100
1	C	165/190 (87%)	161 (98%)	4 (2%)	0	100	100
All	All	497/570 (87%)	484 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	138/154 (90%)	134 (97%)	4 (3%)	42	23
1	B	138/154 (90%)	136 (99%)	2 (1%)	67	53
1	C	136/154 (88%)	133 (98%)	3 (2%)	52	34
All	All	412/462 (89%)	403 (98%)	9 (2%)	52	34

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	379	ARG
1	C	407	ARG
1	C	274	GLU
1	A	378	GLN
1	B	407	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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	164/190 (86%)	0.31	8 (4%) 29 33	23, 35, 64, 103	0
1	B	168/190 (88%)	0.72	26 (15%) 2 2	24, 52, 85, 107	0
1	C	166/190 (87%)	0.24	9 (5%) 25 28	22, 36, 64, 92	0
All	All	498/570 (87%)	0.42	43 (8%) 10 12	22, 39, 77, 107	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	ALA	6.4
1	B	276	VAL	6.3
1	B	293	THR	6.3
1	B	424	ALA	5.5
1	B	442	GLU	5.5

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 carbohydrates 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	C	501	1/1	0.98	0.10	40,40,40,40	0
2	CL	A	501	1/1	0.99	0.06	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.