

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 05:29 am BST

PDB ID 2W38

> Title : Crystal structure of the pseudaminidase from Pseudomonas aeruginosa

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2008-11-07 Deposited on

1.90 Å(reported) Resolution

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 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

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

Xtriage (Phenix) 1.13 EDS 2.11

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

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

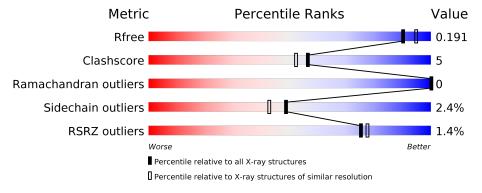
Validation Pipeline (wwPDB-VP) 2.11

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 1.90 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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		
			<mark>%</mark>		
1	A	438	87%	9%	• •



2 Entry composition (i)

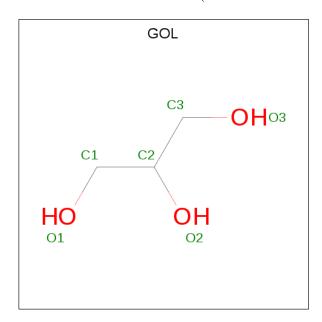
There are 3 unique types of molecules in this entry. The entry contains 3725 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIALIDASE.

\mathbf{Mol}	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	432	Total 3285	C 2081	N 564	O 636	S 4	0	0	0

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0

• Molecule 3 is water.

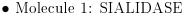


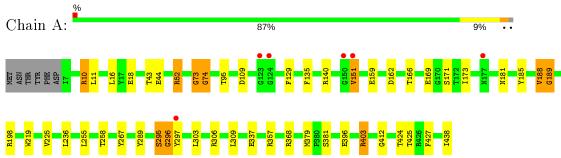
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	416	Total O 416 416	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants	126.20Å 126.20Å 126.20Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.74 - 1.90	Depositor
Resolution (A)	33.73 - 1.90	EDS
% Data completeness	94.4 (33.74-1.90)	Depositor
(in resolution range)	94.4 (33.73-1.90)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.68 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
D.D.	0.175 , 0.198	Depositor
R, R_{free}	0.170 , 0.191	DCC
R_{free} test set	2543 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35\;,45.4$	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3725	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% 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: GOL

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	В	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.79	$2/3371 \ (0.1\%)$	0.90	$23/4591 \ (0.5\%)$

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	A	109	ASP	C-N	-19.13	0.90	1.34
1	A	297	TYR	C-N	5.50	1.46	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	306	ARG	NE-CZ-NH2	-16.41	112.09	120.30
1	A	403	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	A	306	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	403	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	297	TYR	O-C-N	10.46	139.44	122.70
1	A	296	GLY	N-CA-C	8.77	135.03	113.10
1	A	297	TYR	CA-C-N	-8.33	98.88	117.20
1	A	296	GLY	CA-C-O	-8.20	105.83	120.60
1	A	52	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	296	GLY	CA-C-N	6.85	132.27	117.20
1	A	295	SER	C-N-CA	6.53	136.00	122.30



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-	110116	predidus	puyc

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	188	VAL	O-C-N	-6.35	112.40	123.20
1	A	10	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	188	VAL	CA-C-N	5.79	127.77	116.20
1	A	52	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	357	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	295	SER	CA-C-N	5.30	126.81	116.20
1	A	295	SER	O-C-N	-5.28	114.23	123.20
1	A	74	GLY	N-CA-C	-5.14	100.26	113.10
1	A	109	ASP	C-N-CA	5.12	134.51	121.70
1	A	73	GLY	N-CA-C	-5.08	100.40	113.10
1	A	306	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	189	GLY	N-CA-C	5.05	125.73	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	VAL	Peptide
1	A	295	SER	Peptide

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	3285	0	3130	30	0
2	A	24	0	32	4	0
3	A	416	0	0	13	0
All	All	3725	0	3162	32	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.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:438:ILE:C	3:A:2412:HOH:O	1.65	1.30



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Continued from prec		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:A:162:ASP:OD2	1:A:166:THR:HG22	1.57	1.04
2:A:1442:GOL:H31	3:A:2303:HOH:O	1.80	0.80
1:A:189:GLY:HA2	3:A:2186:HOH:O	1.82	0.79
1:A:18:GLU:HG2	3:A:2015:HOH:O	1.92	0.69
1:A:189:GLY:CA	3:A:2186:HOH:O	2.42	0.64
1:A:74:GLY:HA3	3:A:2068:HOH:O	1.98	0.63
1:A:151:VAL:HG22	3:A:2171:HOH:O	1.99	0.62
1:A:396:GLU:OE2	1:A:403:ARG:HD2	2.04	0.57
1:A:74:GLY:CA	3:A:2068:HOH:O	2.50	0.57
1:A:396:GLU:OE2	1:A:403:ARG:CD	2.55	0.55
1:A:10:ARG:NH2	3:A:2004:HOH:O	2.17	0.53
1:A:52:ARG:HD2	3:A:2043:HOH:O	2.07	0.53
1:A:424:THR:HG22	1:A:424:THR:O	2.09	0.52
2:A:1442:GOL:C3	3:A:2303:HOH:O	2.51	0.51
1:A:173:ILE:HG13	1:A:219:TRP:CE2	2.46	0.51
1:A:379:MET:HG2	3:A:2046:HOH:O	2.14	0.47
1:A:337:GLU:CG	3:A:2322:HOH:O	2.65	0.45
1:A:16:LEU:C	1:A:16:LEU:HD23	2.37	0.45
1:A:135:PHE:CE1	1:A:185:TYR:HB2	2.52	0.44
1:A:412:GLY:HA3	1:A:425:THR:O	2.18	0.44
1:A:258:THR:HG21	1:A:296:GLY:H	1.83	0.43
1:A:140:ARG:HD2	1:A:159:GLU:OE1	2.19	0.43
1:A:181:ASN:OD1	1:A:198:ARG:HD3	2.20	0.42
1:A:95:THR:OG1	1:A:129:PHE:HA	2.20	0.42
1:A:255:LEU:O	1:A:267:TYR:HA	2.20	0.42
1:A:73:GLY:HA2	1:A:74:GLY:HA2	1.78	0.41
1:A:225:VAL:O	2:A:1441:GOL:H32	2.21	0.41
1:A:396:GLU:OE2	1:A:403:ARG:HD3	2.21	0.41
1:A:368:ARG:HD3	1:A:427:PHE:CZ	2.57	0.40
1:A:11:LEU:HD12	1:A:309:LEU:HB3	2.03	0.40
1:A:43:THR:HB	2:A:1442:GOL:H2	2.03	0.40

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	\mathbf{ntiles}
1	A	430/438 (98%)	413 (96%)	17 (4%)	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.

M	ol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1		A	339/345 (98%)	331 (98%)	8 (2%)	49 43	

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	151	VAL
1	A	169	GLU
1	A	171	SER
1	A	236	LEU
1	A	289	TYR
1	A	303	LEU
1	A	381	SER

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)

4 ligands are modelled in this entry.

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	Tuno	Chain	Res	Link	В	ond leng	gths	Е	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1439	-	5,5,5	0.39	0	5,5,5	0.77	0
2	GOL	A	1440	-	5,5,5	0.36	0	5,5,5	0.82	0
2	GOL	A	1441	-	5,5,5	0.40	0	5,5,5	0.42	0
2	GOL	A	1442	-	5,5,5	0.53	0	5,5,5	0.52	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
2	GOL	A	1439	-	-	2/4/4/4	-
2	GOL	A	1440	_	1	2/4/4/4	-
2	GOL	A	1441	-	-	0/4/4/4	_
2	GOL	A	1442	-	=	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

N	Iol	Chain	Res	Type	Atoms
	2	A	1440	GOL	O1-C1-C2-C3
	2	A	1439	GOL	C1-C2-C3-O3



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Mol	Chain	Res	Type	Atoms
2	A	1440	GOL	O1-C1-C2-O2
2	A	1439	GOL	O2-C2-C3-O3
2	A	1442	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1441	GOL	1	0
2	A	1442	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

\mathbf{Model}	Chain	Residue-1	Atom-1	Residue-2	Atom-2	${f Distance} \; ({f A})$
1	A	109:ASP	С	110:SER	N	0.90



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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
1	A	432/438 (98%)	-0.09	6 (1%) 75 77	13, 20, 36, 48	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	4.9
1	A	123	GLY	3.3
1	A	150	GLY	3.2
1	A	297	TYR	2.3
1	A	124	GLY	2.2
1	A	177	ASN	2.2

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, 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	${f B-factors}({f \AA}^2)$	Q < 0.9
2	GOL	A	1441	6/6	0.89	0.13	24,26,29,30	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	GOL	A	1439	6/6	0.94	0.12	19,23,29,35	0
2	GOL	A	1442	6/6	0.95	0.38	26,29,30,31	0
2	GOL	A	1440	6/6	0.97	0.08	23,25,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

