wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 07:37 pm GMT

PDB ID	:	6H2P
Title	:	Crystal Structure of Arg184Gln mutant of Human Prolidase with Mn ions and Cacodylate ligand
Authors	:	Wilk, P.; Piwowarczyk, R.; Weiss, M.S.
Deposited on	:	2018-07-14
Resolution	:	1.48 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 (i)) were used in the production of this report:

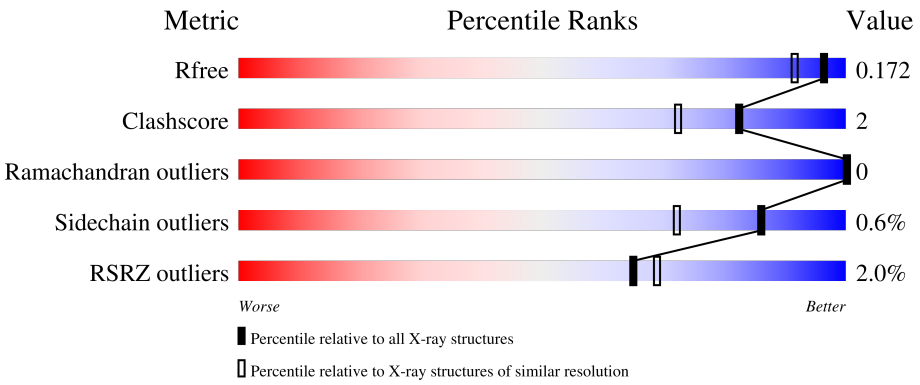
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	492	2% 91% 6% •
1	B	492	% 92% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16759 atoms, of which 7660 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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	477	7590	2420	3768	667	703	32	0	17	0
1	B	482	7764	2484	3846	672	730	32	0	28	0

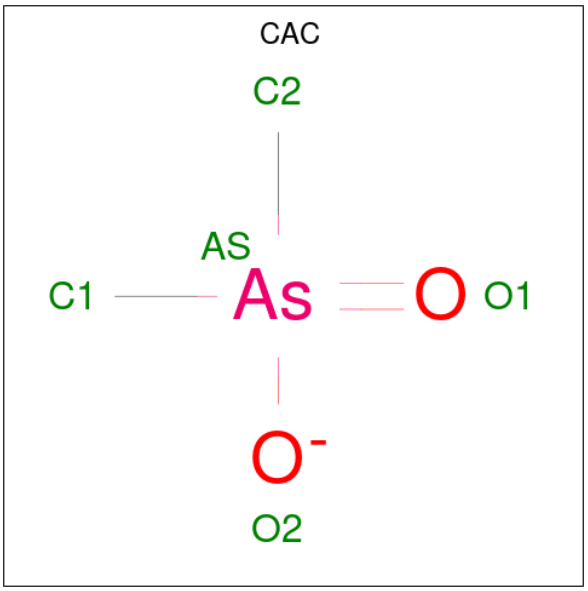
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLN	ARG	engineered mutation	UNP P12955
A	?	-	ALA	deletion	UNP P12955
B	184	GLN	ARG	engineered mutation	UNP P12955
B	?	-	ALA	deletion	UNP P12955

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

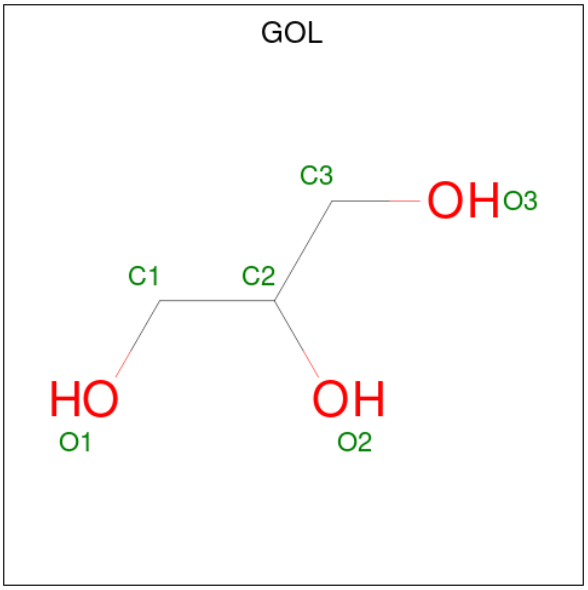
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
3	A	1	5	1	2	2	0	0
			Total	As	C	O		
3	B	1	5	1	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	26	6	14	6	0	1
			Total	C	H	O		
4	A	1	14	3	8	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	B	1	14	3	8	3	0	0
			Total	C	H	O		
4	B	1	14	3	8	3	0	0

- Molecule 5 is water.

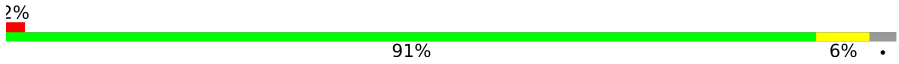
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	622	622	622	0	0
			Total	O		
5	B	687	687	687	0	0

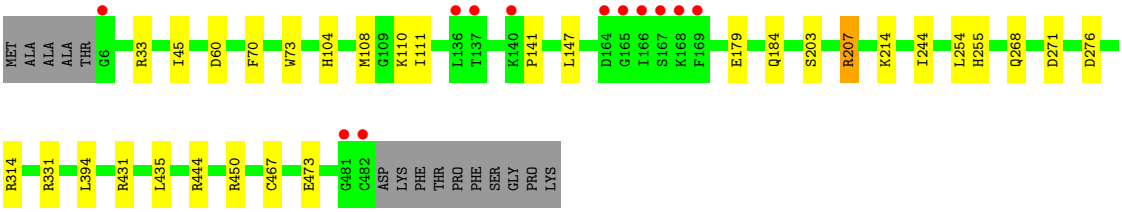
3 Residue-property plots (i)

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: Xaa-Pro dipeptidase

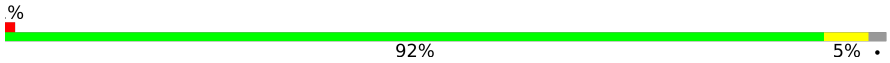
Chain A:

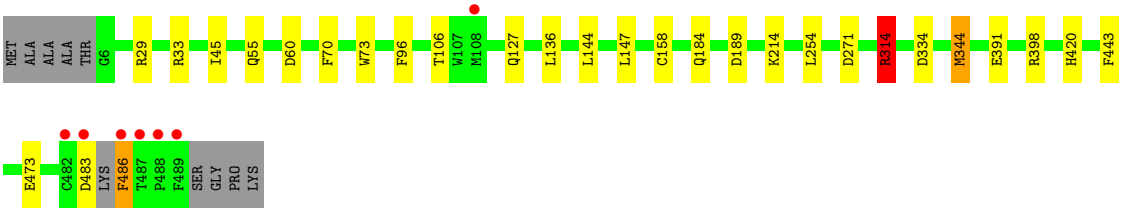




• Molecule 1: Xaa-Pro dipeptidase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	103.45Å 107.08Å 216.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 1.48 47.99 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.99-1.48) 99.8 (47.99-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.148 , 0.170 0.150 , 0.172	Depositor DCC
R_{free} test set	2101 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	16759	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: CAC, GOL, 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	0.69	1/3951 (0.0%)	0.80	7/5343 (0.1%)
1	B	0.70	2/4055 (0.0%)	0.82	10/5489 (0.2%)
All	All	0.69	3/8006 (0.0%)	0.81	17/10832 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	GLU	CG-CD	6.92	1.62	1.51
1	B	473	GLU	CG-CD	5.38	1.60	1.51
1	B	158	CYS	CB-SG	5.19	1.91	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	314	ARG	NE-CZ-NH2	9.27	124.94	120.30
1	A	444	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	444	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	207[A]	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	207[B]	ARG	NE-CZ-NH1	6.93	123.77	120.30

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	3822	3768	3770	22	0
1	B	3918	3846	3853	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	24	30	29	0	0
4	B	12	16	16	1	0
5	A	622	0	0	11	0
5	B	687	0	0	7	1
All	All	9099	7660	7668	38	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 2.

The worst 5 of 38 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:A:314[B]:ARG:NH2	5:A:601:HOH:O	1.91	1.02
1:A:314[A]:ARG:NH1	5:A:602:HOH:O	1.92	1.01
1:A:331[B]:ARG:NH2	5:A:604:HOH:O	2.01	0.92
1:A:254[B]:LEU:O	5:A:603:HOH:O	2.00	0.78
1:B:391:GLU:OE1	5:B:601:HOH:O	2.05	0.75

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)
5:B:1096:HOH:O	5:B:1123:HOH:O[5_455]	2.16	0.04

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	492/492 (100%)	482 (98%)	10 (2%)	0	100	100
1	B	506/492 (103%)	493 (97%)	13 (3%)	0	100	100
All	All	998/984 (101%)	975 (98%)	23 (2%)	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	416/410 (102%)	416 (100%)	0	100	100
1	B	428/410 (104%)	421 (98%)	7 (2%)	62	34
All	All	844/820 (103%)	837 (99%)	7 (1%)	86	64

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60[B]	ASP
1	B	314	ARG
1	B	486	PHE
1	B	483	ASP
1	B	60[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	506	-	5,5,5	0.53	0	5,5,5	0.25	0
4	GOL	A	505	-	5,5,5	0.40	0	5,5,5	0.31	0
3	CAC	B	503	2	0,4,4	-	-	0,6,6	-	-
4	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.22	0
3	CAC	A	503	2	0,4,4	-	-	0,6,6	-	-
4	GOL	B	504	-	5,5,5	0.35	0	5,5,5	0.62	0
4	GOL	A	504[A]	-	5,5,5	0.44	0	5,5,5	0.40	0
4	GOL	A	504[B]	-	5,5,5	0.34	0	5,5,5	0.45	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	A	505	-	-	0/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	A	504[A]	-	-	4/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	504[B]	-	-	0/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504[A]	GOL	O1-C1-C2-C3
4	A	506	GOL	C1-C2-C3-O3
4	B	505	GOL	O1-C1-C2-C3
4	A	504[A]	GOL	O2-C2-C3-O3
4	A	504[A]	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	CAC	1	0
4	B	504	GOL	1	0

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	477/492 (96%)	-0.18	12 (2%)	57	61	14, 21, 42, 68	0
1	B	482/492 (97%)	-0.29	7 (1%)	73	77	14, 20, 39, 110	0
All	All	959/984 (97%)	-0.23	19 (1%)	65	69	14, 21, 41, 110	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	ASP	5.8
1	A	482	CYS	5.0
1	B	482	CYS	3.7
1	B	487	THR	3.7
1	A	168	LYS	3.6

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
4	GOL	A	504[A]	6/6	0.83	0.17	39,46,63,75	12
4	GOL	A	504[B]	6/6	0.83	0.17	21,46,66,70	14
4	GOL	B	504	6/6	0.85	0.18	26,56,82,82	0
4	GOL	A	505	6/6	0.86	0.13	28,64,79,93	0
4	GOL	A	506	6/6	0.93	0.13	34,43,68,68	0
4	GOL	B	505	6/6	0.95	0.19	29,39,47,52	0
3	CAC	B	503	5/5	0.98	0.16	20,27,40,53	5
3	CAC	A	503	5/5	0.99	0.09	19,25,50,54	0
2	MN	B	502	1/1	0.99	0.12	16,16,16,16	0
2	MN	A	501	1/1	1.00	0.13	14,14,14,14	0
2	MN	A	502	1/1	1.00	0.13	13,13,13,13	0
2	MN	B	501	1/1	1.00	0.10	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.