

Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 10:52 AM EDT

PDB ID	:	8T7P
Title	:	X-ray crystal structure of $PfA-M1(M462S)$
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Deposited on		
Resolution	:	2.00 Å(reported)

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 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:

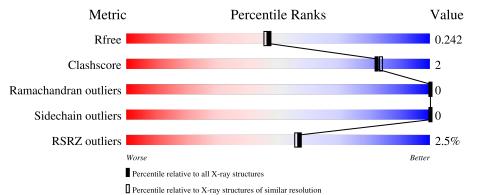
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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	А	898	^{2%} 93%	5% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7883 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	884	Total 7178	C 4630	N 1161	O 1360	S 27	0	7	0

Chain Modelled Residue Actual Comment Reference UNP 096935 А 194 MET _ initiating methionine GLN ASN UNP 096935 А 213conflict UNP 096935 Α 223GLN ASN conflict А 378 PRO HIS conflict UNP 096935 А 462 SER MET engineered mutation UNP 096935 А GLN ASN conflict UNP 096935 501 GLN ASN <u>UNP 096</u>935 А 745conflict GLN А 795 ASN conflict UNP 096935 <u>UNP</u> O96935 GLN ASN А 1069conflict А HIS UNP 096935 1086 expression tag А 1087 HIS expression tag UNP 096935 _ HIS А 1088 UNP 096935 expression tag _ UNP 096935 А 1089 HIS expression tag -Α HIS UNP 096935 1090 expression tag _ HIS UNP 096935 А 1091 _ expression tag

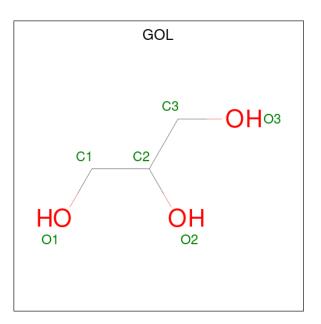
There are 15 discrepancies between the modelled and reference sequences:

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Mg 2 2	0	0

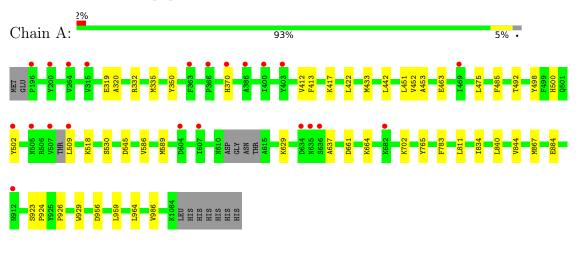
• Molecule 5 is water.

Μ	ol	Chain	Residues	Ato	ms	ZeroOcc	AltConf
Ę	5	А	672	Total 672	O 672	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: Aminopeptidase N



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	75.01Å 108.93Å 117.63Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.37 - 2.00	Depositor
Resolution (A)	30.37 - 2.00	EDS
% Data completeness	99.7 (30.37-2.00)	Depositor
(in resolution range)	99.7 (30.37 - 2.00)	EDS
R _{merge}	0.27	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.205 , 0.243	Depositor
R, R_{free}	0.207 , 0.242	DCC
R_{free} test set	3321 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.8	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 49.5	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, MG, ZN

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/7361	0.38	0/9969	

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	А	7178	0	7018	35	0
2	А	1	0	0	0	0
3	А	30	0	40	0	0
4	А	2	0	0	0	0
5	А	672	0	0	9	1
All	All	7883	0	7058	35	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.

All (35) 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:884:GLU:HG3	5:A:1201:HOH:O	1.14	1.30
1:A:702:LYS:HD3	5:A:1390:HOH:O	1.73	0.88
1:A:884:GLU:OE2	5:A:1201:HOH:O	1.90	0.88
1:A:661:ASP:OD2	1:A:664:LYS:HE2	1.75	0.87
1:A:884:GLU:CG	5:A:1201:HOH:O	1.86	0.80
1:A:485:PHE:CD1	5:A:1407:HOH:O	2.42	0.72
1:A:485:PHE:CE1	5:A:1407:HOH:O	2.47	0.67
1:A:453:ALA:HB2	1:A:475:LEU:HD23	1.84	0.60
1:A:702:LYS:CD	5:A:1390:HOH:O	2.38	0.59
1:A:702:LYS:CE	5:A:1390:HOH:O	2.51	0.58
1:A:413:PHE:HB2	1:A:452:VAL:HG22	1.87	0.55
1:A:412:VAL:HB	1:A:422:LEU:HD22	1.88	0.55
1:A:586:VAL:HA	1:A:589:MET:HE2	1.94	0.49
1:A:433:MET:HG2	1:A:498:TYR:CZ	2.49	0.48
1:A:492:THR:HG22	1:A:530:SER:OG	2.16	0.46
1:A:319:GLU:HA	1:A:320:ALA:HA	1.66	0.46
1:A:509:LEU:HD22	1:A:518:LYS:HD3	1.98	0.46
1:A:332:ARG:HG3	1:A:335:MET:HG2	1.98	0.45
1:A:956:ASP:HB3	1:A:959:LEU:HB3	1.97	0.45
1:A:661:ASP:CG	1:A:664:LYS:HE2	2.35	0.45
1:A:545:ASP:OD1	1:A:765:TYR:OH	2.31	0.45
1:A:350:TYR:O	1:A:370:HIS:NE2	2.50	0.44
1:A:661:ASP:OD1	1:A:664:LYS:HG2	2.17	0.44
1:A:964:LEU:HD21	1:A:986:VAL:HG11	1.99	0.44
1:A:811:LEU:HB3	1:A:867:MET:SD	2.58	0.44
1:A:923:SER:HA	1:A:924:PRO:HD3	1.92	0.42
1:A:412:VAL:HG12	1:A:451:LEU:HB2	2.00	0.42
1:A:661:ASP:OD2	1:A:664:LYS:CE	2.58	0.42
1:A:417:LYS:NZ	5:A:1266:HOH:O	2.53	0.42
1:A:783:PHE:HB3	1:A:844:VAL:HG13	2.02	0.42
1:A:442:LEU:HD22	1:A:502:TYR:CE2	2.55	0.41
1:A:629:LYS:NZ	1:A:637:ALA:O	2.38	0.41
1:A:834:ILE:HG13	1:A:840:LEU:HD22	2.02	0.41
1:A:463:GLU:HG3	1:A:500:HIS:HB3	2.02	0.41
1:A:926:PRO:HA	1:A:929:TRP:CE2	2.56	0.41

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:A:1390:HOH:O	5:A:1782:HOH:O[2_554]	2.07	0.13



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		
1	А	885/898~(99%)	870 (98%)	15 (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	А	788/830~(95%)	788 (100%)	0	100 1	00	

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	А	882	ASN

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	Trune	Chain	Dec	s Link Bond lengths			Bond angles			
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	GOL	А	1103	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.28	0
3	GOL	А	1105	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.26	0
3	GOL	А	1102	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.21	0
3	GOL	А	1106	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.28	0
3	GOL	А	1104	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.26	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
3	GOL	А	1103	-	-	3/4/4/4	-
3	GOL	А	1105	-	-	1/4/4/4	-
3	GOL	А	1102	-	-	0/4/4/4	-
3	GOL	А	1106	-	-	2/4/4/4	-
3	GOL	А	1104	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1106	GOL	O1-C1-C2-C3

Continued on next page...

Mol	Chain	Res	Type	Atoms
3	А	1103	GOL	O2-C2-C3-O3
3	А	1103	GOL	O1-C1-C2-C3
3	А	1103	GOL	C1-C2-C3-O3
3	А	1106	GOL	O1-C1-C2-O2
3	А	1105	GOL	O1-C1-C2-O2

Continued from previous page...

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>2		$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9	
1	А	884/898~(98%)	0.16	22 (2%)	57	56	12, 22, 41, 79	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	196	PRO	5.4
1	А	635	ASN	3.7
1	А	912	ASN	3.4
1	А	403	TYR	3.1
1	А	366	PRO	2.9
1	А	200	TYR	2.8
1	А	502	TYR	2.8
1	А	469	ILE	2.7
1	А	509	LEU	2.6
1	А	607	ILE	2.5
1	А	370	HIS	2.5
1	А	636	SER	2.4
1	А	682	LYS	2.4
1	А	634	ASP	2.4
1	А	315	VAL	2.3
1	А	604	ASP	2.3
1	А	507	VAL	2.2
1	А	363	PHE	2.2
1	А	386	ALA	2.2
1	А	264	VAL	2.1
1	А	505	ASN	2.1
1	А	400	ILE	2.0

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.

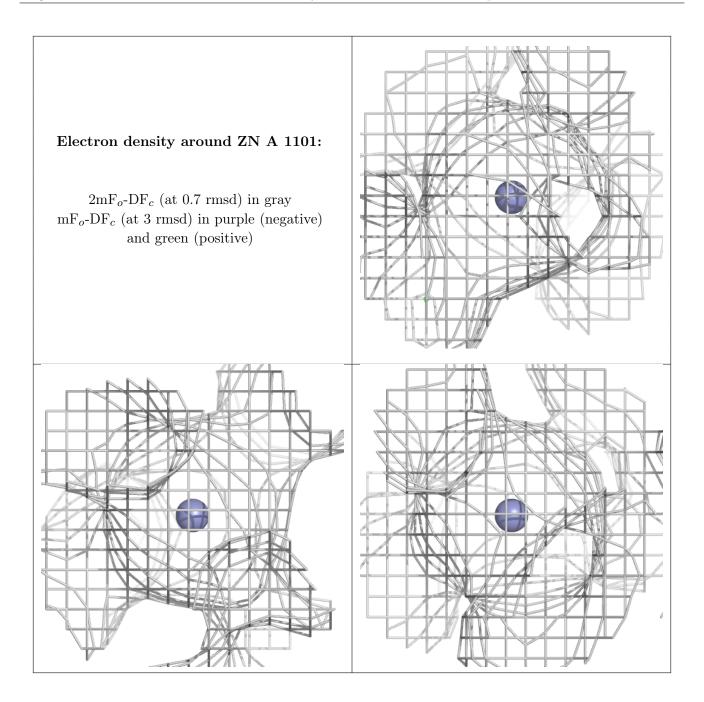
6.4 Ligands (i)

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	B-factors(Å ²)	Q < 0.9
3	GOL	А	1106	6/6	0.66	0.27	52,53,53,53	0
3	GOL	А	1105	6/6	0.70	0.38	56,57,57,57	0
3	GOL	А	1103	6/6	0.81	0.21	28,28,29,29	0
3	GOL	А	1104	6/6	0.81	0.23	51,52,52,53	0
4	MG	А	1108	1/1	0.81	0.09	39,39,39,39	0
3	GOL	А	1102	6/6	0.94	0.13	18,18,20,21	0
4	MG	А	1107	1/1	0.97	0.06	27,27,27,27	0
2	ZN	А	1101	1/1	1.00	0.07	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

