



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2016 – 12:56 PM EDT

PDB ID : 5JGF
Title : Crystal structure of mApe1
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Deposited on : 2016-04-20
Resolution : 1.83 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

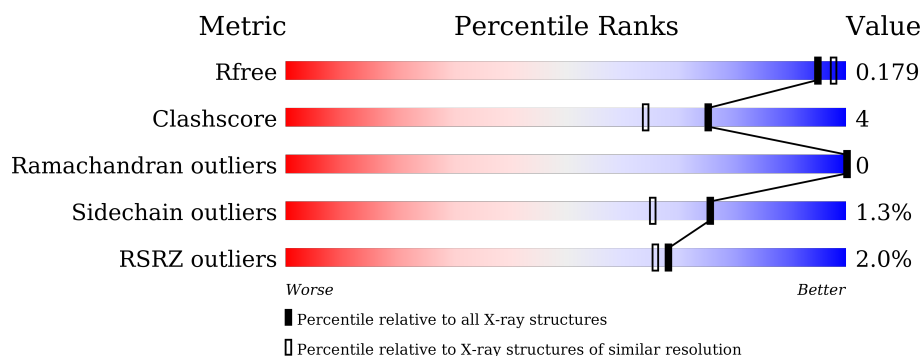
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

Mol	Chain	Length	Quality of chain	
1	A	473	<div><div style="width: 88%;"></div><div style="width: 10%; background-color: yellow;"></div><div style="width: 2%; background-color: gray;"></div></div> <div>%88%10%</div>	.
1	B	473	<div><div style="width: 88%;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 3%; background-color: gray;"></div></div> <div>3% %88%8%</div>	..
1	C	473	<div><div style="width: 88%;"></div><div style="width: 9%; background-color: yellow;"></div><div style="width: 2%; background-color: gray;"></div></div> <div>2% %88%9%</div>	.
1	D	473	<div><div style="width: 88%;"></div><div style="width: 9%; background-color: yellow;"></div><div style="width: 2%; background-color: gray;"></div></div> <div>2% %88%9%</div>	.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16586 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 Vacuolar aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3529	2260	595	666	8			
1	B	460	Total	C	N	O	S	0	0	0
			3540	2266	597	669	8			
1	C	460	Total	C	N	O	S	0	0	0
			3544	2268	597	671	8			
1	D	462	Total	C	N	O	S	0	0	0
			3564	2280	602	674	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP P14904
A	43	PRO	-	expression tag	UNP P14904
A	44	HIS	-	expression tag	UNP P14904
A	45	MET	-	expression tag	UNP P14904
B	42	GLY	-	expression tag	UNP P14904
B	43	PRO	-	expression tag	UNP P14904
B	44	HIS	-	expression tag	UNP P14904
B	45	MET	-	expression tag	UNP P14904
C	42	GLY	-	expression tag	UNP P14904
C	43	PRO	-	expression tag	UNP P14904
C	44	HIS	-	expression tag	UNP P14904
C	45	MET	-	expression tag	UNP P14904
D	42	GLY	-	expression tag	UNP P14904
D	43	PRO	-	expression tag	UNP P14904
D	44	HIS	-	expression tag	UNP P14904
D	45	MET	-	expression tag	UNP P14904

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	594	Total 594	O 594	0	0
3	B	569	Total 569	O 569	0	0
3	C	614	Total 614	O 614	0	0
3	D	624	Total 624	O 624	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	140.97Å 140.97Å 348.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.49 – 1.83 38.49 – 1.83	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.49-1.83) 96.7 (38.49-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.83Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.162 , 0.179 0.162 , 0.179	Depositor DCC
R_{free} test set	22019 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for $-1/3^*h+1/3^*k+1/3^*l, -k, 8/3^*h+4/3^*k+1/3^*l$ 0.007 for $-2/3^*h-1/3^*k-1/3^*l, -1/3^*h-2/3^*k+1/3^*l, -4/3^*h+4/3^*k+1/3^*l$ 0.006 for $-h, 1/3^*h-1/3^*k-1/3^*l, -4/3^*h-8/3^*k+1/3^*l$ 0.006 for $-h, 2/3^*h+1/3^*k+1/3^*l, 4/3^*h+8/3^*k-1/3^*l$ 0.007 for $1/3^*h+2/3^*k-1/3^*l, -k, -8/3^*h-4/3^*k-1/3^*l$ 0.007 for $-1/3^*h-2/3^*k+1/3^*l, -2/3^*h-1/3^*k-1/3^*l, 4/3^*h-4/3^*k-1/3^*l$ 0.019 for $-h-k, k, -l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16586	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 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: 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	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/3613	0.64	0/4908
1	B	0.33	1/3624 (0.0%)	0.64	0/4921
1	C	0.32	0/3628	0.64	0/4926
1	D	0.32	0/3648	0.64	0/4951
All	All	0.32	1/14513 (0.0%)	0.64	0/19706

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	CYS	CB-SG	-6.40	1.71	1.82

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	3529	0	3441	26	0
1	B	3540	0	3456	26	0
1	C	3544	0	3460	28	0
1	D	3564	0	3488	31	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	594	0	0	2	0
3	B	569	0	0	6	0
3	C	614	0	0	4	0
3	D	624	0	0	7	0
All	All	16586	0	13845	109	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 4.

The worst 5 of 109 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:502:LYS:HG3	1:C:503:HIS:CE1	2.31	0.65
1:D:265:LYS:HD3	3:D:1100:HOH:O	1.96	0.65
1:B:417:ASN:HD21	1:D:161:GLY:H	1.45	0.65
1:D:437:ASN:HB2	3:D:1054:HOH:O	1.97	0.64
1:C:323:ASN:ND2	1:C:326:GLU:HG3	2.13	0.63

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	456/473 (96%)	448 (98%)	8 (2%)	0	100	100
1	B	456/473 (96%)	449 (98%)	7 (2%)	0	100	100
1	C	456/473 (96%)	449 (98%)	7 (2%)	0	100	100
1	D	458/473 (97%)	452 (99%)	6 (1%)	0	100	100
All	All	1826/1892 (96%)	1798 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	375/398 (94%)	369 (98%)	6 (2%)	70	57
1	B	377/398 (95%)	373 (99%)	4 (1%)	80	72
1	C	378/398 (95%)	372 (98%)	6 (2%)	70	57
1	D	381/398 (96%)	377 (99%)	4 (1%)	82	75
All	All	1511/1592 (95%)	1491 (99%)	20 (1%)	76	65

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	488	LYS
1	C	121	ARG
1	D	193	LEU
1	B	330	PHE
1	B	451	ARG

Some 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	338	ASN
1	C	347	GLN
1	D	338	ASN
1	C	81	ASN
1	C	323	ASN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 8 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	460/473 (97%)	-0.43	7 (1%) 76 74	12, 18, 35, 48	0
1	B	460/473 (97%)	-0.43	12 (2%) 59 56	12, 18, 35, 50	0
1	C	460/473 (97%)	-0.48	8 (1%) 73 71	11, 16, 32, 47	0
1	D	462/473 (97%)	-0.42	9 (1%) 70 67	11, 17, 34, 46	0
All	All	1842/1892 (97%)	-0.44	36 (1%) 68 66	11, 17, 34, 50	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	ASN	4.7
1	A	48	ASN	4.0
1	D	235	ASP	4.0
1	A	234	PRO	3.6
1	D	241	PRO	3.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	601	1/1	1.00	0.04	-1.64	19,19,19,19	0
2	ZN	B	602	1/1	1.00	0.04	-1.73	18,18,18,18	0
2	ZN	D	602	1/1	1.00	0.03	-5.09	16,16,16,16	0
2	ZN	D	601	1/1	1.00	0.02	-5.23	15,15,15,15	0
2	ZN	C	601	1/1	1.00	0.01	-5.54	14,14,14,14	0
2	ZN	A	601	1/1	1.00	0.02	-6.02	17,17,17,17	0
2	ZN	C	602	1/1	1.00	0.01	-9.31	15,15,15,15	0
2	ZN	A	602	1/1	1.00	0.02	-12.17	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.