



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:43 PM GMT

PDB ID : 4FWD
Title : Crystal structure of the Lon-like protease MtaLonC in complex with bortezomib
Authors : Chang, C.I.; Kuo, C.I.; Huang, K.F.
Deposited on : 2012-06-30
Resolution : 2.03 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

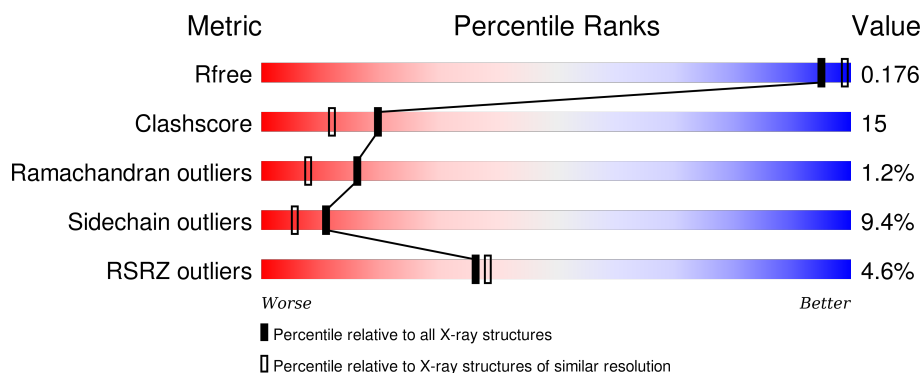
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.03 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}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	732	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4942 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.

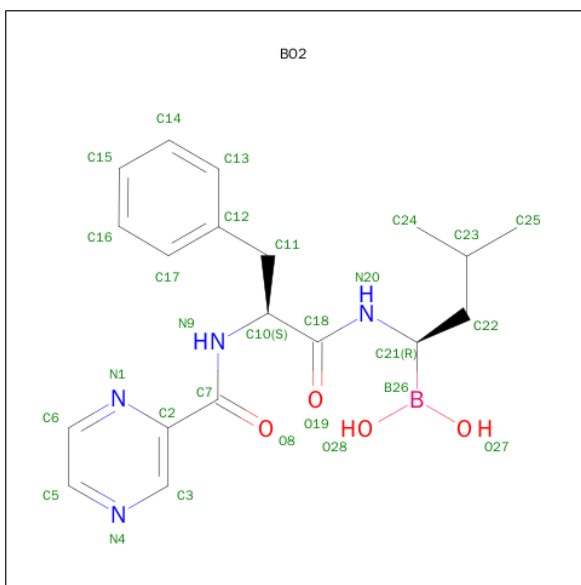
- Molecule 1 is a protein called TTC1975 peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	2	0
			4514	2865	799	842	8			

There are 13 discrepancies between the modelled and reference sequences:

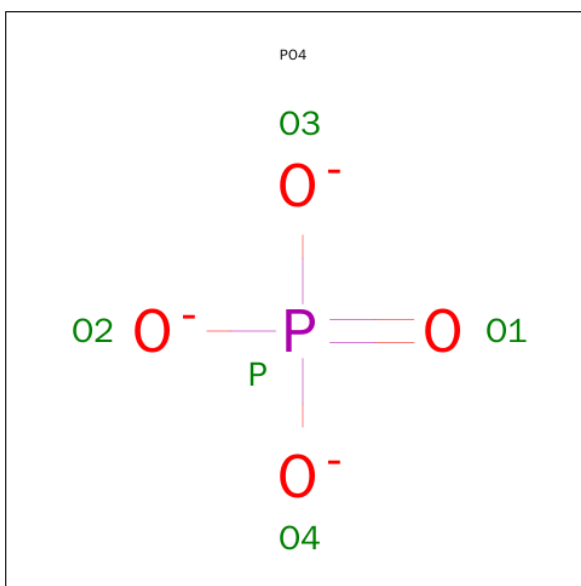
Chain	Residue	Modelled	Actual	Comment	Reference
A	720	LYS	-	EXPRESSION TAG	UNP C9DRU9
A	721	LEU	-	EXPRESSION TAG	UNP C9DRU9
A	722	ALA	-	EXPRESSION TAG	UNP C9DRU9
A	723	ALA	-	EXPRESSION TAG	UNP C9DRU9
A	724	ALA	-	EXPRESSION TAG	UNP C9DRU9
A	725	LEU	-	EXPRESSION TAG	UNP C9DRU9
A	726	GLU	-	EXPRESSION TAG	UNP C9DRU9
A	727	HIS	-	EXPRESSION TAG	UNP C9DRU9
A	728	HIS	-	EXPRESSION TAG	UNP C9DRU9
A	729	HIS	-	EXPRESSION TAG	UNP C9DRU9
A	730	HIS	-	EXPRESSION TAG	UNP C9DRU9
A	731	HIS	-	EXPRESSION TAG	UNP C9DRU9
A	732	HIS	-	EXPRESSION TAG	UNP C9DRU9

- Molecule 2 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O P	0	0
			5	4 1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	395	Total 395	O 395	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	115.92Å 115.92Å 135.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.03 47.08 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.03) 97.0 (47.08-2.02)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.195 0.151 , 0.176	Depositor DCC
R_{free} test set	3287 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
Estimated twinning fraction	0.582 for H, K, L 0.418 for K, H, -L 0.407 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.582 for H, K, L 0.418 for K, H, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 65525 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, BO2

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	1.45	27/4608 (0.6%)	1.42	44/6256 (0.7%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	651	LEU	N-CA	7.25	1.60	1.46
1	A	452	GLY	N-CA	6.58	1.55	1.46
1	A	432	ARG	CD-NE	-6.38	1.35	1.46
1	A	469	HIS	C-O	6.35	1.35	1.23
1	A	691	GLY	N-CA	6.34	1.55	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	ARG	NE-CZ-NH2	-18.43	111.09	120.30
1	A	554	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	A	436	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	373	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	432	ARG	NE-CZ-NH1	9.66	125.13	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	LEU	Peptide
1	A	343	ALA	Peptide
1	A	691	GLY	Peptide
1	A	692	PHE	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	4514	0	4531	136	0
2	A	28	0	25	5	0
3	A	5	0	0	0	0
4	A	395	0	0	11	0
All	All	4942	0	4556	136	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 15.

The worst 5 of 136 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:229:GLU:CB	1:A:230:ALA:HA	1.78	1.13
1:A:229:GLU:HB2	1:A:230:ALA:CA	1.75	1.12
1:A:492:THR:HG22	4:A:1083:HOH:O	1.51	1.09
1:A:503:VAL:HG12	2:A:801:BO2:C24	1.82	1.09
1:A:692:PHE:HZ	1:A:696:GLN:HB3	1.20	1.06

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	575/732 (79%)	545 (95%)	23 (4%)	7 (1%)	16 8

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PHE
1	A	225	ARG
1	A	344	PRO
1	A	692	PHE
1	A	294	VAL

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	461/578 (80%)	418 (91%)	43 (9%)	11 6

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ARG
1	A	292	THR
1	A	617	LEU
1	A	253	ASN
1	A	259	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	253	ASN
1	A	303	HIS
1	A	527	HIS

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Mol	Chain	Res	Type
1	A	597	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BO2	A	801	1	28,29,29	1.81	4 (14%)	31,38,38	2.12	8 (25%)
3	PO4	A	802	-	4,4,4	0.73	0	6,6,6	0.38	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	BO2	A	801	1	-	0/22/28/28	0/2/2/2
3	PO4	A	802	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BO2	C11-C12	-5.94	1.36	1.51
2	A	801	BO2	C2-C7	-5.72	1.37	1.50
2	A	801	BO2	C11-C10	-2.76	1.47	1.54
2	A	801	BO2	C5-N4	2.09	1.40	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BO2	C3-C2-C7	-4.34	115.11	119.55
2	A	801	BO2	C2-C3-N4	-3.96	117.92	122.11
2	A	801	BO2	C5-C6-N1	-3.26	118.20	122.25
2	A	801	BO2	C6-C5-N4	-2.44	118.64	121.94
2	A	801	BO2	C12-C11-C10	-2.12	107.23	113.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BO2	5	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	587/732 (80%)	-0.01	27 (4%) 36 38	20, 32, 85, 112	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	7.9
1	A	290	TRP	6.3
1	A	223	GLN	5.8
1	A	285	VAL	4.3
1	A	224	ALA	4.2

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. 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(Å ²)	Q<0.9
2	BO2	A	801	28/28	0.92	0.12	0.11	27,44,82,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	A	802	5/5	0.99	0.12	0.02	29,29,31,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.