



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:20 PM GMT

PDB ID : 1X6L
Title : Crystal structure of *S. marcescens* chitinase A mutant W167A
Authors : Aronson Jr., N.N.; Halloran, B.A.; Alexyev, M.F.; Zhou, X.E.; Wang, Y.;
Meehan, E.J.; Chen, L.
Deposited on : 2004-08-11
Resolution : 1.90 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
<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

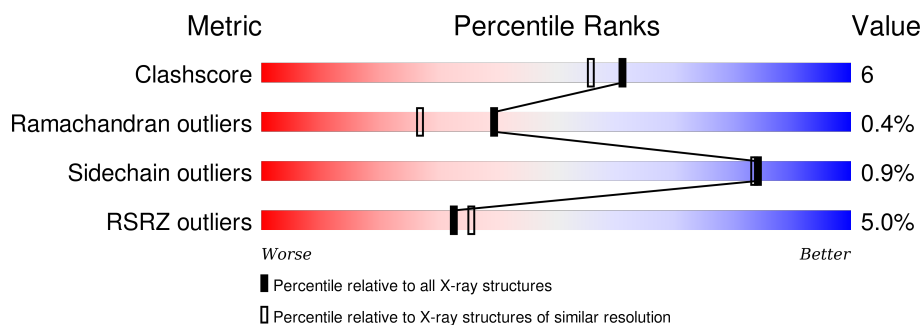
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	563	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4502 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 Chitinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4119	2619	694	792	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	PRO	ALA	SEE REMARK 999	UNP P07254
A	144	SER	PRO	SEE REMARK 999	UNP P07254
A	167	ALA	TRP	ENGINEERED	UNP P07254
A	226	ILE	VAL	SEE REMARK 999	UNP P07254
A	395	ALA	PRO	SEE REMARK 999	UNP P07254
A	437	ILE	VAL	SEE REMARK 999	UNP P07254
A	473	GLU	LYS	SEE REMARK 999	UNP P07254
A	484	SER	GLY	SEE REMARK 999	UNP P07254

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	383	Total	O	0	0
			383	383		

- Molecule 1: Chitinase A



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.51Å 132.71Å 192.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 38.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.9 (19.94-1.90) 93.7 (38.97-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.233 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 76660 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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](#)

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	0.30	0/4218	0.54	0/5723

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	A	4119	0	3998	45	0
2	A	383	0	0	5	0
All	All	4502	0	3998	45	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 6.

All (45) 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:43:VAL:HG22	1:A:54:VAL:HG12	1.49	0.95
1:A:191:PHE:HA	1:A:271:SER:O	1.87	0.75
1:A:528:VAL:HG13	1:A:533:LEU:HB2	1.72	0.70
1:A:54:VAL:HG11	1:A:304:TRP:CH2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG11	1:A:304:TRP:CZ2	2.34	0.61
1:A:421:VAL:HG12	1:A:425:ASN:ND2	2.18	0.58
1:A:166:GLU:H	1:A:190:GLY:HA3	1.68	0.58
1:A:244:ALA:HB3	1:A:247:ASP:CG	2.24	0.58
1:A:421:VAL:HG12	1:A:425:ASN:HD21	1.69	0.56
1:A:340:LYS:HG3	2:A:841:HOH:O	2.05	0.55
1:A:365:ALA:HA	1:A:387:LEU:HD11	1.90	0.54
1:A:164:PHE:CD2	1:A:179:ILE:HD11	2.43	0.54
1:A:163:TYR:CZ	1:A:188:LEU:HD22	2.44	0.53
1:A:407:LEU:O	1:A:421:VAL:HG23	2.11	0.51
1:A:316:PHE:CD1	1:A:364:SER:HB2	2.46	0.51
1:A:207:ILE:HD11	1:A:276:THR:HG21	1.91	0.51
1:A:540:GLU:HG3	1:A:542:ASP:OD1	2.11	0.51
1:A:45:GLN:HG3	2:A:834:HOH:O	2.12	0.49
1:A:172:ARG:HD3	1:A:542:ASP:OD2	2.12	0.49
1:A:275:TRP:HA	1:A:315:GLU:HG2	1.92	0.49
1:A:524:LYS:O	1:A:528:VAL:HG23	2.13	0.49
1:A:165:VAL:HG22	2:A:573:HOH:O	2.11	0.49
1:A:244:ALA:O	1:A:250:LYS:HE2	2.14	0.48
1:A:379:GLN:NE2	1:A:432:VAL:HA	2.28	0.48
1:A:165:VAL:HG23	1:A:168:GLY:HA3	1.96	0.47
1:A:281:PHE:O	1:A:284:MET:HB2	2.15	0.46
1:A:153:LYS:HE2	1:A:561:GLY:HA2	1.97	0.46
1:A:439:VAL:HB	1:A:536:LEU:HD23	1.98	0.45
1:A:316:PHE:CD1	1:A:316:PHE:N	2.84	0.45
1:A:110:MET:C	1:A:110:MET:SD	2.94	0.45
1:A:164:PHE:O	1:A:190:GLY:N	2.50	0.45
1:A:273:GLY:O	1:A:277:LEU:HB2	2.17	0.44
1:A:410:PRO:HD3	2:A:720:HOH:O	2.18	0.43
1:A:358:GLU:HA	1:A:383:ASP:OD2	2.19	0.43
1:A:250:LYS:HE3	2:A:834:HOH:O	2.17	0.43
1:A:192:ILE:HG23	1:A:227:SER:O	2.19	0.43
1:A:499:ALA:O	1:A:500:GLU:HB2	2.18	0.43
1:A:364:SER:OG	1:A:369:LYS:HD2	2.19	0.43
1:A:298:LYS:O	1:A:302:GLN:HG3	2.20	0.42
1:A:361:SER:HB3	1:A:382:MET:CE	2.50	0.42
1:A:477:VAL:HG23	1:A:482:ILE:HD11	2.01	0.41
1:A:223:ASP:O	1:A:224:PHE:HB2	2.20	0.41
1:A:211:PHE:O	1:A:215:GLN:HG2	2.21	0.41
1:A:456:ASN:O	1:A:458:ILE:HG12	2.21	0.41
1:A:29:PRO:HG2	1:A:123:SER:HB3	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	Percentiles
1	A	537/563 (95%)	515 (96%)	20 (4%)	2 (0%)	39 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	A	316	PHE

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	428/447 (96%)	424 (99%)	4 (1%)	84 83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	284	MET
1	A	315	GLU
1	A	316	PHE

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	52	ASN
1	A	330	GLN
1	A	425	ASN
1	A	485	GLN
1	A	532	GLN

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](#)

There are no ligands in this entry.

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	539/563 (95%)	0.34	27 (5%)	32 35	25, 36, 48, 67	21 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	562	VAL	9.1
1	A	493	TYR	8.8
1	A	188	LEU	8.0
1	A	190	GLY	5.1
1	A	388	MET	4.7
1	A	235	LEU	4.1
1	A	455	GLN	3.6
1	A	316	PHE	3.6
1	A	70	ASN	3.2
1	A	58	ASN	3.1
1	A	191	PHE	3.1
1	A	69	TRP	3.1
1	A	399	LYS	3.0
1	A	84	LYS	2.8
1	A	487	MET	2.8
1	A	508	SER	2.6
1	A	313	ASP	2.6
1	A	561	GLY	2.6
1	A	189	TYR	2.5
1	A	458	ILE	2.3
1	A	187	LEU	2.2
1	A	330	GLN	2.2
1	A	415	ASP	2.1
1	A	417	ALA	2.1
1	A	539	TRP	2.1
1	A	315	GLU	2.1
1	A	271	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.