



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 4A5Q
EMDB ID: : EMD-1978
Title : Crystal structure of the chitinase Chi1 fitted into the 3D structure of the Yersinia entomophaga toxin complex
Authors : Busby, J.N.; Landsberg, M.J.; Simpson, R.M.; Jones, S.A.; Hankamer, B.; Hurst, M.R.H.; Lott, J.S.
Deposited on : 2011-10-27
Resolution : 17.00 Å(reported)
Based on PDB ID : 3OA5

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

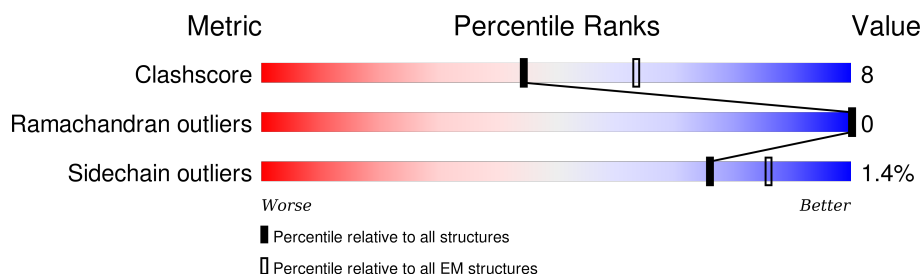
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	546	87% 6% .. 6%
1	B	546	86% 7% • 6%
1	C	546	87% 6% .. 6%
1	D	546	87% 6% .. 6%
1	E	546	86% 7% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20005 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CHI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total 4001	C 2541	N 662	O 788	S 10	0	0
1	B	515	Total 4001	C 2541	N 662	O 788	S 10	0	0
1	C	515	Total 4001	C 2541	N 662	O 788	S 10	0	0
1	D	515	Total 4001	C 2541	N 662	O 788	S 10	0	0
1	E	515	Total 4001	C 2541	N 662	O 788	S 10	0	0

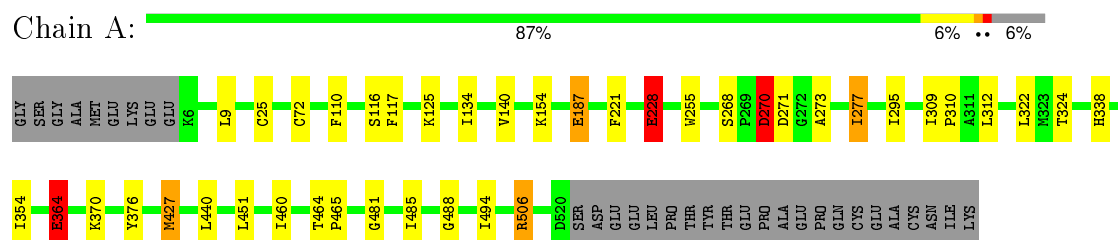
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP B6A876
A	-2	SER	-	EXPRESSION TAG	UNP B6A876
A	-1	GLY	-	EXPRESSION TAG	UNP B6A876
A	0	ALA	-	EXPRESSION TAG	UNP B6A876
B	-3	GLY	-	EXPRESSION TAG	UNP B6A876
B	-2	SER	-	EXPRESSION TAG	UNP B6A876
B	-1	GLY	-	EXPRESSION TAG	UNP B6A876
B	0	ALA	-	EXPRESSION TAG	UNP B6A876
C	-3	GLY	-	EXPRESSION TAG	UNP B6A876
C	-2	SER	-	EXPRESSION TAG	UNP B6A876
C	-1	GLY	-	EXPRESSION TAG	UNP B6A876
C	0	ALA	-	EXPRESSION TAG	UNP B6A876
D	-3	GLY	-	EXPRESSION TAG	UNP B6A876
D	-2	SER	-	EXPRESSION TAG	UNP B6A876
D	-1	GLY	-	EXPRESSION TAG	UNP B6A876
D	0	ALA	-	EXPRESSION TAG	UNP B6A876
E	-3	GLY	-	EXPRESSION TAG	UNP B6A876
E	-2	SER	-	EXPRESSION TAG	UNP B6A876
E	-1	GLY	-	EXPRESSION TAG	UNP B6A876
E	0	ALA	-	EXPRESSION TAG	UNP B6A876

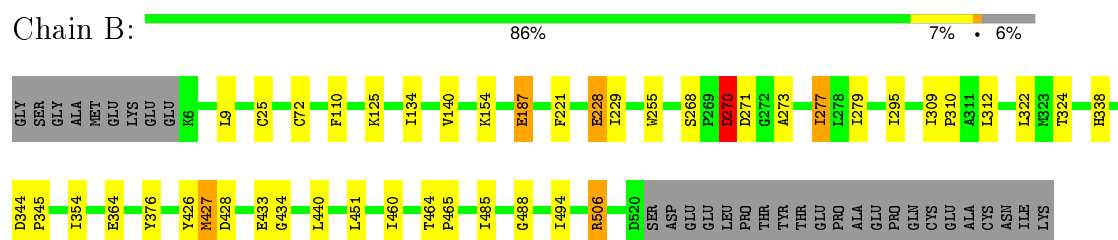
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

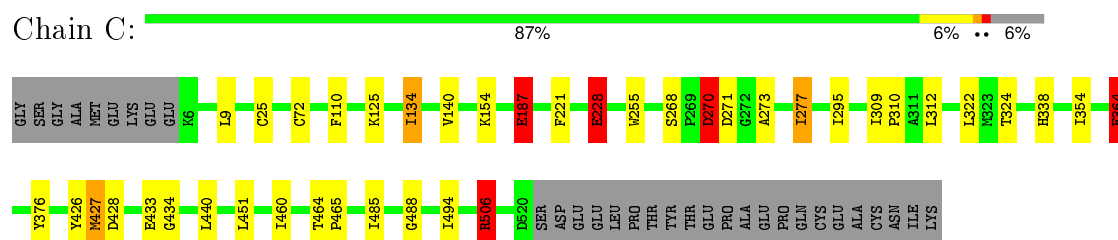
- Molecule 1: CHI1



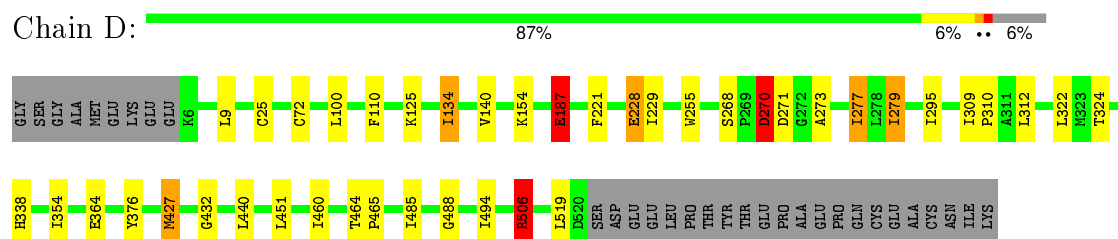
- Molecule 1: CHI1




- Molecule 1: CHI1

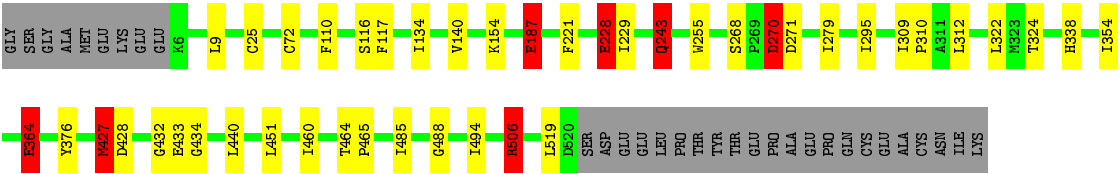


- Molecule 1: CHI1



- Molecule 1: CHI1

Chain E:  86% 7% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	950	Depositor
Magnification	59000	Depositor
Image detector	GATAN USC 4000 (MODEL 895)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	9.27	18/4093 (0.4%)	2.59	26/5555 (0.5%)
1	B	9.00	15/4093 (0.4%)	2.18	22/5555 (0.4%)
1	C	5.59	14/4093 (0.3%)	4.42	18/5555 (0.3%)
1	D	3.15	16/4093 (0.4%)	1.63	20/5555 (0.4%)
1	E	9.94	17/4093 (0.4%)	2.97	34/5555 (0.6%)
All	All	7.83	80/20465 (0.4%)	2.91	120/27775 (0.4%)

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	3
1	B	0	2
1	C	0	5
1	D	0	4
1	E	0	6
All	All	0	20

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	187	GLU	CD-OE2	442.53	6.12	1.25
1	B	187	GLU	CD-OE2	442.52	6.12	1.25
1	A	187	GLU	CD-OE2	442.51	6.12	1.25
1	E	364	GLU	CD-OE1	337.57	4.96	1.25
1	A	187	GLU	CD-OE1	314.34	4.71	1.25

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	506	ARG	NE-CZ-NH1	-212.40	14.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	506	ARG	NE-CZ-NH2	-203.54	18.53	120.30
1	E	506	ARG	NE-CZ-NH2	-160.14	40.23	120.30
1	A	187	GLU	OE1-CD-OE2	-87.70	18.07	123.30
1	B	187	GLU	OE1-CD-OE2	-87.70	18.07	123.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	GLU	Sidechain
1	A	270	ASP	Sidechain
1	A	364	GLU	Sidechain
1	B	228	GLU	Sidechain
1	B	270	ASP	Sidechain

5.2 Too-close contacts ⓘ

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	4001	0	3799	65	0
1	B	4001	0	3799	68	0
1	C	4001	0	3799	69	0
1	D	4001	0	3799	47	0
1	E	4001	0	3799	73	0
All	All	20005	0	18995	322	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 8.

The worst 5 of 322 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:E:427:MET:HE2	1:E:427:MET:CA	1.23	1.66
1:B:187:GLU:CB	1:B:187:GLU:CA	1.77	1.60
1:B:427:MET:CE	1:B:427:MET:HA	1.30	1.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:MET:HA	1:E:427:MET:CE	1.30	1.60
1:C:427:MET:HA	1:C:427:MET:CE	1.31	1.59

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 PDB entries followed by that with respect to all EM entries.

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	513/546 (94%)	496 (97%)	17 (3%)	0	100	100
1	B	513/546 (94%)	496 (97%)	17 (3%)	0	100	100
1	C	513/546 (94%)	496 (97%)	17 (3%)	0	100	100
1	D	513/546 (94%)	496 (97%)	17 (3%)	0	100	100
1	E	513/546 (94%)	496 (97%)	17 (3%)	0	100	100
All	All	2565/2730 (94%)	2480 (97%)	85 (3%)	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 PDB entries followed by that with respect to all EM entries.

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	413/456 (91%)	408 (99%)	5 (1%)	78	90
1	B	413/456 (91%)	408 (99%)	5 (1%)	78	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	413/456 (91%)	404 (98%)	9 (2%)	60	83
1	D	413/456 (91%)	407 (98%)	6 (2%)	72	88
1	E	413/456 (91%)	410 (99%)	3 (1%)	88	94
All	All	2065/2280 (91%)	2037 (99%)	28 (1%)	76	89

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	228	GLU
1	C	338	HIS
1	E	338	HIS
1	C	270	ASP
1	C	277	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no chain breaks in this entry.