



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 04:50 PM GMT

PDB ID : 2I2L
Title : X-ray Crystal Structure of Protein yopX from Bacillus subtilis. Northeast Structural Genomics Consortium Target SR411.
Authors : Vorobiev, S.M.; Zhou, W.; Seetharaman, J.; Forouhar, F.; Kuzin, A.A.; Ho, C.K.; Janjua, H.; Cunningham, K.; Ma, L.C.; Xiao, R.; Liu, J.; Acton, T.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-08-16
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

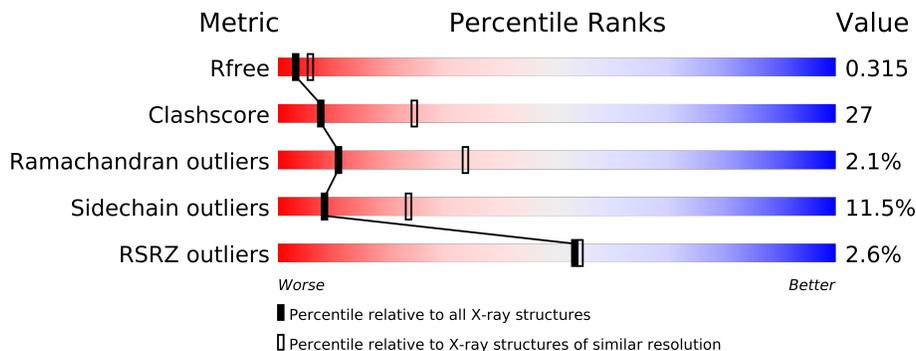
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	142	
1	B	142	
1	C	142	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3102 atoms, of which 0 are hydrogen and 0 are deuterium.

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 YopX protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	130	981	626	162	189	1	3	0	0	0
1	B	133	995	635	165	192	1	2	0	0	0
1	C	128	992	633	163	192	1	3	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O34401
A	13	MSE	MET	MODIFIED RESIDUE	UNP O34401
A	55	MSE	MET	MODIFIED RESIDUE	UNP O34401
A	135	LEU	-	CLONING ARTIFACT	UNP O34401
A	136	GLU	-	CLONING ARTIFACT	UNP O34401
A	137	HIS	-	CLONING ARTIFACT	UNP O34401
A	138	HIS	-	CLONING ARTIFACT	UNP O34401
A	139	HIS	-	CLONING ARTIFACT	UNP O34401
A	140	HIS	-	CLONING ARTIFACT	UNP O34401
A	141	HIS	-	CLONING ARTIFACT	UNP O34401
A	142	HIS	-	CLONING ARTIFACT	UNP O34401
B	1	MSE	MET	MODIFIED RESIDUE	UNP O34401
B	13	MSE	MET	MODIFIED RESIDUE	UNP O34401
B	55	MSE	MET	MODIFIED RESIDUE	UNP O34401
B	135	LEU	-	CLONING ARTIFACT	UNP O34401
B	136	GLU	-	CLONING ARTIFACT	UNP O34401
B	137	HIS	-	CLONING ARTIFACT	UNP O34401
B	138	HIS	-	CLONING ARTIFACT	UNP O34401
B	139	HIS	-	CLONING ARTIFACT	UNP O34401
B	140	HIS	-	CLONING ARTIFACT	UNP O34401
B	141	HIS	-	CLONING ARTIFACT	UNP O34401
B	142	HIS	-	CLONING ARTIFACT	UNP O34401
C	1	MSE	MET	MODIFIED RESIDUE	UNP O34401

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	MSE	MET	MODIFIED RESIDUE	UNP O34401
C	55	MSE	MET	MODIFIED RESIDUE	UNP O34401
C	135	LEU	-	CLONING ARTIFACT	UNP O34401
C	136	GLU	-	CLONING ARTIFACT	UNP O34401
C	137	HIS	-	CLONING ARTIFACT	UNP O34401
C	138	HIS	-	CLONING ARTIFACT	UNP O34401
C	139	HIS	-	CLONING ARTIFACT	UNP O34401
C	140	HIS	-	CLONING ARTIFACT	UNP O34401
C	141	HIS	-	CLONING ARTIFACT	UNP O34401
C	142	HIS	-	CLONING ARTIFACT	UNP O34401

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	48	Total O 48 48	0	0
2	C	45	Total O 45 45	0	0

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.52Å 99.52Å 87.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.73 – 2.80 28.73 – 2.79	Depositor EDS
% Data completeness (in resolution range)	83.3 (28.73-2.80) 97.5 (28.73-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.286 0.260 , 0.315	Depositor DCC
R_{free} test set	495 reflections (3.99%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.0	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	6 of 23938 reflections (0.025%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3102	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2011e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.43	0/999	0.73	2/1360 (0.1%)
1	B	0.45	0/1013	0.83	3/1382 (0.2%)
1	C	0.42	0/1010	0.65	0/1371
All	All	0.43	0/3022	0.74	5/4113 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	CA-CB-CG	14.02	147.55	115.30
1	B	132	GLY	N-CA-C	-6.30	97.35	113.10
1	A	78	LYS	N-CA-C	-5.59	95.91	111.00
1	B	133	VAL	C-N-CA	-5.53	107.87	121.70
1	A	69	SER	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	981	0	896	58	0
1	B	995	0	893	66	0
1	C	992	0	933	41	0
2	A	41	0	0	2	0
2	B	48	0	0	1	0
2	C	45	0	0	3	0
All	All	3102	0	2722	156	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 156 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:ARG:HH21	1:A:55:MSE:HE2	1.32	0.94
1:A:70:ILE:HG22	1:A:119:VAL:HA	1.54	0.89
1:B:131:GLU:O	1:B:132:GLY:O	1.94	0.86
1:B:68:ARG:HB2	1:B:121:GLY:O	1.77	0.85
1:B:130:LEU:C	1:B:131:GLU:OE2	2.15	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

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	126/142 (89%)	104 (82%)	20 (16%)	2 (2%)	14	44
1	B	129/142 (91%)	110 (85%)	16 (12%)	3 (2%)	10	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	124/142 (87%)	106 (86%)	15 (12%)	3 (2%)	9	29
All	All	379/426 (89%)	320 (84%)	51 (14%)	8 (2%)	11	33

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	B	132	GLY
1	C	16	TRP
1	C	47	SER
1	B	98	SER

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	97/123 (79%)	89 (92%)	8 (8%)	17	43
1	B	95/123 (77%)	81 (85%)	14 (15%)	4	13
1	C	103/123 (84%)	91 (88%)	12 (12%)	8	22
All	All	295/369 (80%)	261 (88%)	34 (12%)	8	23

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	LEU
1	B	68	ARG
1	C	92	VAL
1	B	54	LEU
1	A	128	GLU

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	12	GLN
1	A	51	ASN

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Mol	Chain	Res	Type
1	B	2	ASN
1	B	12	GLN
1	B	28	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	130/142 (91%)	-0.00	4 (3%) 47 47	23, 44, 71, 82	0
1	B	133/142 (93%)	-0.02	5 (3%) 38 38	14, 45, 70, 85	0
1	C	128/142 (90%)	-0.07	1 (0%) 83 83	23, 42, 65, 83	0
All	All	391/426 (91%)	-0.03	10 (2%) 53 54	14, 44, 70, 85	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	SER	4.4
1	B	37	TYR	3.5
1	A	63	LYS	3.0
1	C	77	ASP	2.9
1	B	42	VAL	2.6

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.