



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:59 pm GMT

PDB ID : 3OHN
Title : Crystal structure of the FimD translocation domain
Authors : Wang, T.; Li, H.
Deposited on : 2010-08-17
Resolution : 3.01 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

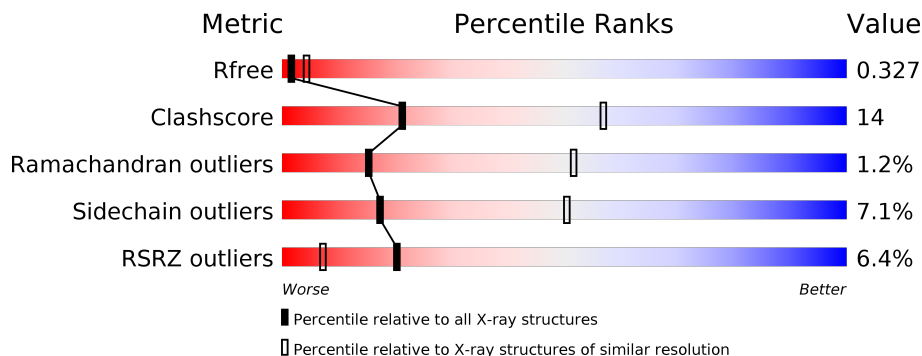
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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	558	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>14%</div> <div>••</div> <div>16%</div> </div> </div>
1	B	558	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7246 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 Outer membrane usher protein FimD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3636	2271	640	719	6			
1	B	463	Total	C	N	O	S	0	0	0
			3610	2259	634	711	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	664	GLY	-	EXPRESSION TAG	UNP C8U0R5
A	665	GLY	-	EXPRESSION TAG	UNP C8U0R5
A	666	PRO	-	EXPRESSION TAG	UNP C8U0R5
A	667	VAL	-	EXPRESSION TAG	UNP C8U0R5
A	668	ALA	-	EXPRESSION TAG	UNP C8U0R5
A	669	THR	-	EXPRESSION TAG	UNP C8U0R5
A	670	LEU	-	EXPRESSION TAG	UNP C8U0R5
A	671	VAL	-	EXPRESSION TAG	UNP C8U0R5
A	672	PRO	-	EXPRESSION TAG	UNP C8U0R5
A	673	ARG	-	EXPRESSION TAG	UNP C8U0R5
A	674	GLY	-	EXPRESSION TAG	UNP C8U0R5
A	675	SER	-	EXPRESSION TAG	UNP C8U0R5
A	676	HIS	-	EXPRESSION TAG	UNP C8U0R5
A	677	HIS	-	EXPRESSION TAG	UNP C8U0R5
A	678	HIS	-	EXPRESSION TAG	UNP C8U0R5
A	679	HIS	-	EXPRESSION TAG	UNP C8U0R5
A	680	HIS	-	EXPRESSION TAG	UNP C8U0R5
A	681	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	664	GLY	-	EXPRESSION TAG	UNP C8U0R5
B	665	GLY	-	EXPRESSION TAG	UNP C8U0R5
B	666	PRO	-	EXPRESSION TAG	UNP C8U0R5
B	667	VAL	-	EXPRESSION TAG	UNP C8U0R5
B	668	ALA	-	EXPRESSION TAG	UNP C8U0R5
B	669	THR	-	EXPRESSION TAG	UNP C8U0R5
B	670	LEU	-	EXPRESSION TAG	UNP C8U0R5

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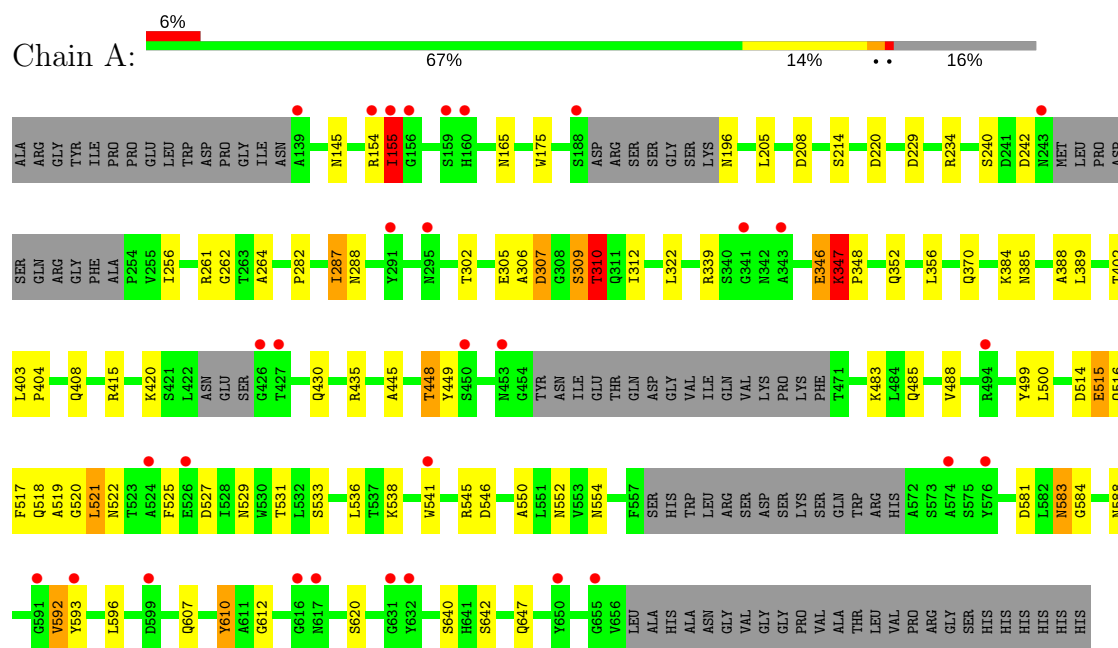
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Chain	Residue	Modelled	Actual	Comment	Reference
B	671	VAL	-	EXPRESSION TAG	UNP C8U0R5
B	672	PRO	-	EXPRESSION TAG	UNP C8U0R5
B	673	ARG	-	EXPRESSION TAG	UNP C8U0R5
B	674	GLY	-	EXPRESSION TAG	UNP C8U0R5
B	675	SER	-	EXPRESSION TAG	UNP C8U0R5
B	676	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	677	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	678	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	679	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	680	HIS	-	EXPRESSION TAG	UNP C8U0R5
B	681	HIS	-	EXPRESSION TAG	UNP C8U0R5

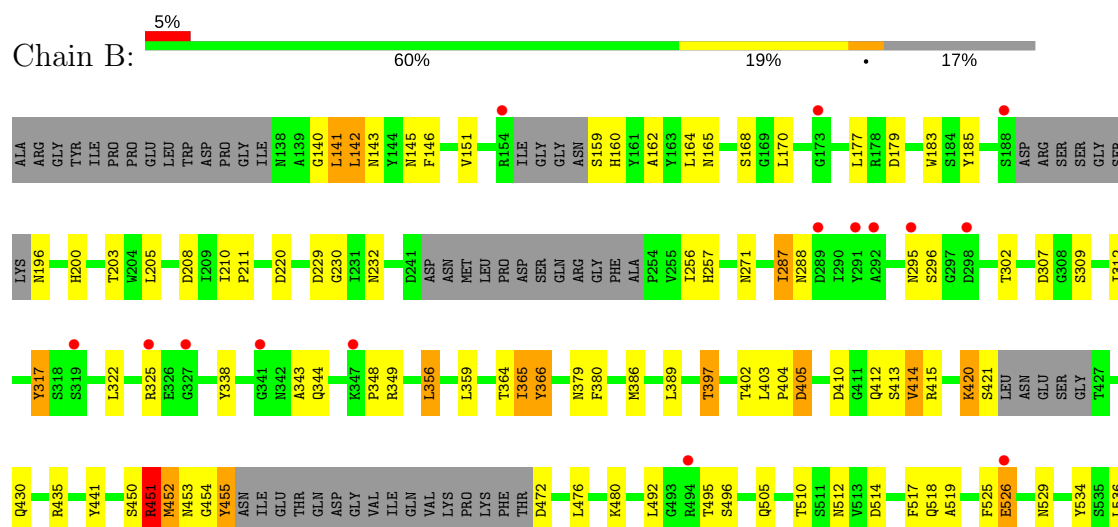
3 Residue-property plots [i](#)

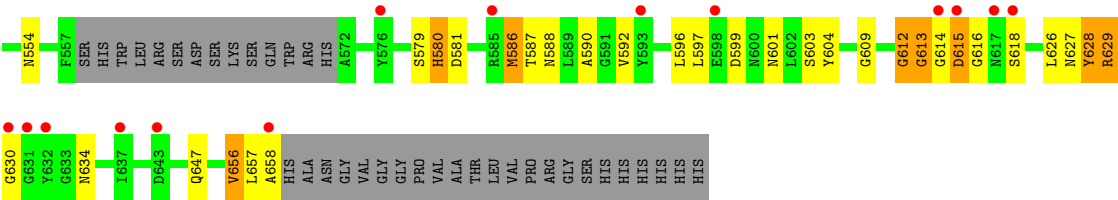
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Outer membrane usher protein FimD



• Molecule 1: Outer membrane usher protein FimD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 87.13Å 95.88Å 63.92° 88.43° 76.94°	Depositor
Resolution (Å)	28.89 – 3.01 28.89 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.89-3.01) 82.9 (28.89-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.230 , 0.305 0.315 , 0.327	Depositor DCC
R_{free} test set	1371 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7246	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3715	0.57	3/5038 (0.1%)
1	B	0.80	5/3689 (0.1%)	0.64	4/5002 (0.1%)
All	All	0.67	5/7404 (0.1%)	0.60	7/10040 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	414	VAL	CB-CG1	-7.25	1.37	1.52
1	B	366	TYR	CD2-CE2	-5.90	1.30	1.39
1	B	366	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	366	TYR	CE2-CZ	-5.42	1.31	1.38
1	B	366	TYR	CD1-CE1	-5.32	1.31	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	612	GLY	N-CA-C	-8.56	91.71	113.10
1	A	310	THR	N-CA-C	6.87	129.55	111.00
1	B	140	GLY	N-CA-C	-6.76	96.19	113.10
1	A	347	LYS	C-N-CD	-6.38	106.56	120.60
1	B	613	GLY	N-CA-C	-6.24	97.51	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3636	0	3426	63	0
1	B	3610	0	3402	130	0
All	All	7246	0	6828	192	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 14.

The worst 5 of 192 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:B:628:TYR:CE2	1:B:630:GLY:N	1.87	1.38
1:B:142:LEU:HD12	1:B:143:ASN:N	1.39	1.36
1:B:141:LEU:HD12	1:B:142:LEU:N	1.43	1.30
1:B:365:ILE:O	1:B:365:ILE:HD12	1.35	1.24
1:B:141:LEU:C	1:B:141:LEU:HD12	1.53	1.21

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	456/558 (82%)	422 (92%)	29 (6%)	5 (1%)	17	54
1	B	449/558 (80%)	409 (91%)	34 (8%)	6 (1%)	14	49
All	All	905/1116 (81%)	831 (92%)	63 (7%)	11 (1%)	15	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	A	592	VAL
1	B	451	ARG

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Mol	Chain	Res	Type
1	A	348	PRO
1	A	541	TRP

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	381/457 (83%)	360 (94%)	21 (6%)	25	61
1	B	378/457 (83%)	345 (91%)	33 (9%)	12	40
All	All	759/914 (83%)	705 (93%)	54 (7%)	17	50

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	205	LEU
1	B	317	TYR
1	B	596	LEU
1	B	208	ASP
1	B	256	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	ASN
1	B	165	ASN
1	B	491	GLN
1	A	627	ASN
1	B	504	HIS

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](#)

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 [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	468/558 (83%)	0.40	31 (6%) 19 7	20, 58, 96, 124	0
1	B	463/558 (82%)	0.41	29 (6%) 21 7	22, 62, 105, 128	0
All	All	931/1116 (83%)	0.41	60 (6%) 20 7	20, 60, 101, 128	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	4.7
1	B	188	SER	4.7
1	A	617	ASN	4.7
1	B	289	ASP	4.6
1	B	615	ASP	4.4

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.