



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 18, 2016 – 12:03 PM EDT

PDB ID : 5LP2
Title : Adhesin domain of the type 1 HopQ of Helicobacter pylori strain G27
Authors : Moonens, K.; Kruse, T.; Gerhard, M.; Remaut, H.
Deposited on : 2016-08-11
Resolution : 2.60 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.

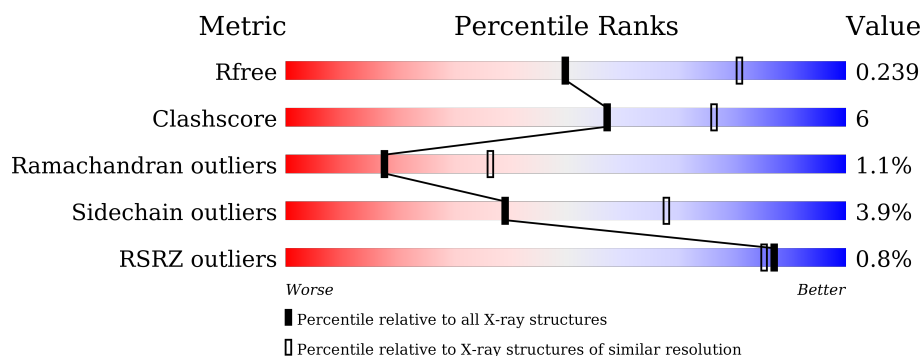
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

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X-RAY DIFFRACTION

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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	434	<div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>
1	B	434	<div> <div></div> <div>71%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>
1	C	434	<div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>
1	D	434	<div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10987 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 HopQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	360	Total	C	N	O	S	0	0	0
			2738	1679	486	563	10			
1	A	360	Total	C	N	O	S	0	0	0
			2738	1679	486	563	10			
1	C	360	Total	C	N	O	S	0	0	0
			2738	1679	486	563	10			
1	D	360	Total	C	N	O	S	0	0	0
			2738	1679	486	563	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP B5Z8H1
B	444	HIS	-	expression tag	UNP B5Z8H1
B	445	HIS	-	expression tag	UNP B5Z8H1
B	446	HIS	-	expression tag	UNP B5Z8H1
B	447	HIS	-	expression tag	UNP B5Z8H1
B	448	HIS	-	expression tag	UNP B5Z8H1
B	449	HIS	-	expression tag	UNP B5Z8H1
A	16	MET	-	initiating methionine	UNP B5Z8H1
A	444	HIS	-	expression tag	UNP B5Z8H1
A	445	HIS	-	expression tag	UNP B5Z8H1
A	446	HIS	-	expression tag	UNP B5Z8H1
A	447	HIS	-	expression tag	UNP B5Z8H1
A	448	HIS	-	expression tag	UNP B5Z8H1
A	449	HIS	-	expression tag	UNP B5Z8H1
C	16	MET	-	initiating methionine	UNP B5Z8H1
C	444	HIS	-	expression tag	UNP B5Z8H1
C	445	HIS	-	expression tag	UNP B5Z8H1
C	446	HIS	-	expression tag	UNP B5Z8H1
C	447	HIS	-	expression tag	UNP B5Z8H1
C	448	HIS	-	expression tag	UNP B5Z8H1
C	449	HIS	-	expression tag	UNP B5Z8H1

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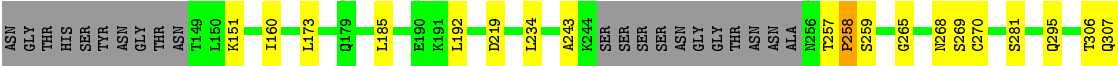
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	MET	-	initiating methionine	UNP B5Z8H1
D	444	HIS	-	expression tag	UNP B5Z8H1
D	445	HIS	-	expression tag	UNP B5Z8H1
D	446	HIS	-	expression tag	UNP B5Z8H1
D	447	HIS	-	expression tag	UNP B5Z8H1
D	448	HIS	-	expression tag	UNP B5Z8H1
D	449	HIS	-	expression tag	UNP B5Z8H1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	11	Total O 11 11	0	0
2	A	6	Total O 6 6	0	0
2	C	7	Total O 7 7	0	0
2	D	11	Total O 11 11	0	0



• Molecule 1: HopQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.70 Å 57.70 Å 285.60 Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	49.40 – 2.60 49.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.40-2.60) 99.4 (49.38-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.208 , 0.236 0.215 , 0.239	Depositor DCC
R_{free} test set	2924 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.457 for -k,-h,-l 0.449 for k,h,-l 0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10987	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.68	0/2770	0.80	0/3749
1	B	0.67	0/2770	0.80	0/3749
1	C	0.68	0/2770	0.80	0/3749
1	D	0.68	0/2770	0.80	0/3749
All	All	0.68	0/11080	0.80	0/14996

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
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	PRO	Peptide
1	B	110	PRO	Peptide
1	C	110	PRO	Peptide
1	C	263	ALA	Peptide
1	D	110	PRO	Peptide

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	2738	0	2684	35	0
1	B	2738	0	2684	35	0
1	C	2738	0	2684	35	0
1	D	2738	0	2684	31	0
2	A	6	0	0	1	0
2	B	11	0	0	1	0
2	C	7	0	0	1	0
2	D	11	0	0	0	0
All	All	10987	0	10736	130	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.

The worst 5 of 130 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:269:SER:O	1:B:270:CYS:HB2	1.67	0.94
1:D:269:SER:O	1:D:270:CYS:HB2	1.68	0.93
1:C:269:SER:O	1:C:270:CYS:HB2	1.68	0.89
1:A:269:SER:O	1:A:270:CYS:HB2	1.68	0.89
1:A:108:LYS:C	1:A:110:PRO:HD3	1.99	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	350/434 (81%)	319 (91%)	28 (8%)	3 (1%)	21	42
1	B	350/434 (81%)	320 (91%)	26 (7%)	4 (1%)	17	36
1	C	350/434 (81%)	318 (91%)	28 (8%)	4 (1%)	17	36
1	D	350/434 (81%)	319 (91%)	27 (8%)	4 (1%)	17	36
All	All	1400/1736 (81%)	1276 (91%)	109 (8%)	15 (1%)	17	36

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	SER
1	B	110	PRO
1	B	115	GLN
1	A	109	SER
1	A	110	PRO

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	302/361 (84%)	290 (96%)	12 (4%)	38	67
1	B	302/361 (84%)	290 (96%)	12 (4%)	38	67
1	C	302/361 (84%)	290 (96%)	12 (4%)	38	67
1	D	302/361 (84%)	291 (96%)	11 (4%)	42	71
All	All	1208/1444 (84%)	1161 (96%)	47 (4%)	39	68

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	GLN
1	C	91	LEU
1	D	317	SER
1	A	415	LEU
1	C	108	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	C	115	GLN
1	C	285	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](#)

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	360/434 (82%)	-0.31	3 (0%) 87 85	40, 61, 96, 128	0
1	B	360/434 (82%)	-0.27	2 (0%) 90 88	40, 61, 97, 126	0
1	C	360/434 (82%)	-0.29	4 (1%) 82 79	38, 60, 96, 124	0
1	D	360/434 (82%)	-0.27	3 (0%) 87 85	41, 61, 100, 133	0
All	All	1440/1736 (82%)	-0.29	12 (0%) 87 85	38, 61, 98, 133	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ASN	4.2
1	C	134	GLY	3.4
1	B	179	GLN	2.9
1	B	256	ASN	2.8
1	D	256	ASN	2.7

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.