



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 08:08 AM GMT

PDB ID : 2WIU
Title : Mercury-modified bacterial persistence regulator hipBA
Authors : Evdokimov, A.; Voznesensky, I.; Fennell, K.; Anderson, M.; Smith, J.F.;
Fisher, D.A.
Deposited on : 2009-05-17
Resolution : 2.35 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>

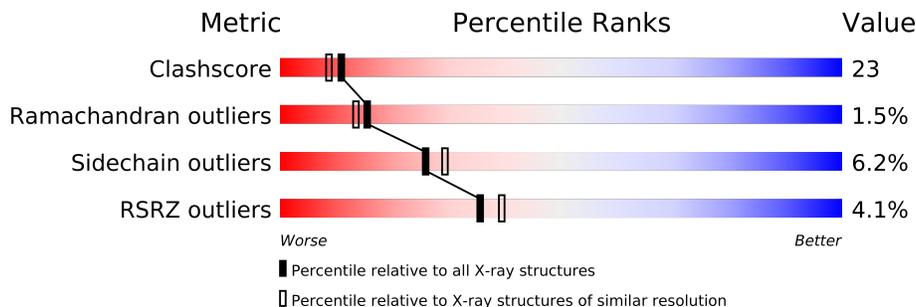
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	446	
1	C	446	
2	B	88	
2	D	88	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CL	B	1088	-	X
4	CL	D	1089	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8029 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 PROTEIN HIPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3397	2171	593	620	13	0	0	0
1	C	401	3190	2043	557	576	14	0	3	0

- Molecule 2 is a protein called HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	71	576	366	96	111	3	0	1	0
2	D	71	571	362	95	111	3	0	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Hg 1	0	0
3	A	2	Total 2	Hg 2	0	0
3	D	1	Total 1	Hg 1	0	0
3	C	3	Total 3	Hg 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Cl 2	0	0
4	A	3	Total 3	Cl 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Cl	0	0
			2	2		
4	C	3	Total	Cl	0	0
			3	3		

- Molecule 5 is water.

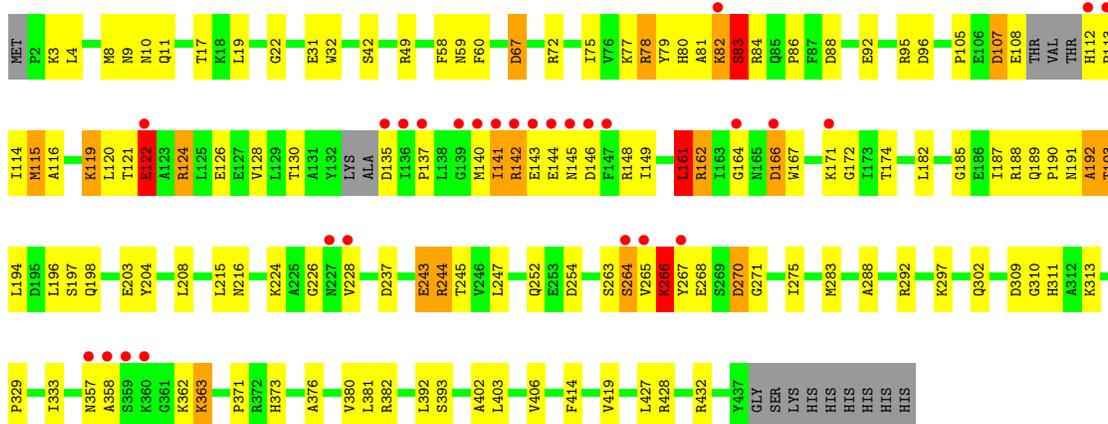
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	18	Total	O	0	0
			18	18		
5	C	135	Total	O	0	0
			135	135		
5	D	17	Total	O	0	0
			17	17		

3 Residue-property plots

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 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.

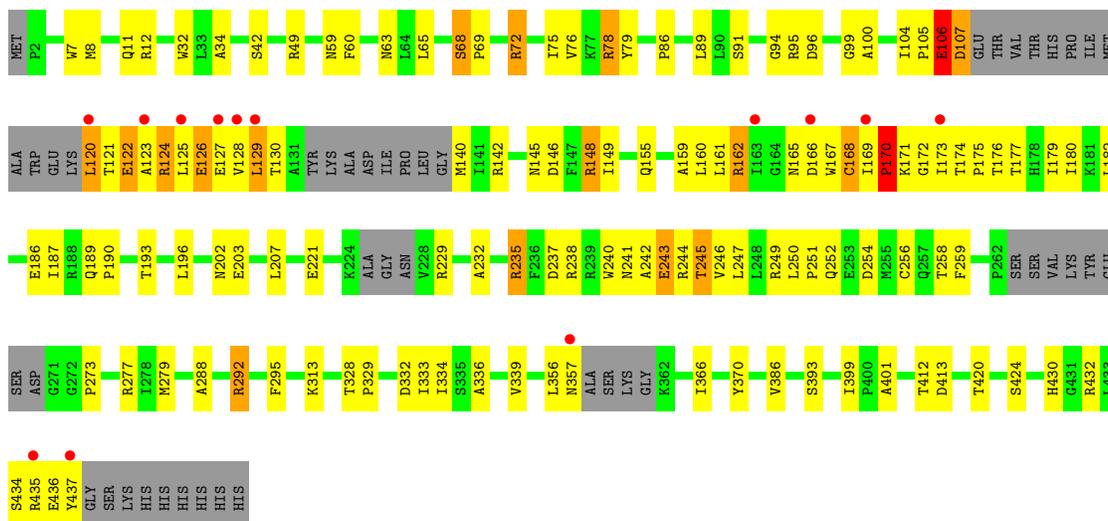
- Molecule 1: PROTEIN HIPA

Chain A: 



- Molecule 1: PROTEIN HIPA

Chain C: 



- Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB

Chain B: 



- Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.93Å 166.93Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.67 – 2.35 49.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (166.67-2.35) 82.3 (49.92-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.264 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.2	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	4 of 100078 reflections (0.004%)	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.31 % 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 2.2508e-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

Bond lengths and bond angles in the following residue types are not validated in this section: HG, CL

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	0.87	1/3470 (0.0%)	1.01	10/4701 (0.2%)
1	C	0.85	0/3264	0.97	4/4418 (0.1%)
2	B	0.98	2/587 (0.3%)	0.86	0/790
2	D	1.01	0/579	0.92	1/780 (0.1%)
All	All	0.88	3/7900 (0.0%)	0.98	15/10689 (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	4
1	C	0	4
2	B	0	1
2	D	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LEU	C-N	-18.74	0.91	1.34
2	B	33	LYS	CD-CE	5.79	1.65	1.51
2	B	33	LYS	CG-CD	5.71	1.71	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	O-C-N	-11.79	103.83	122.70
1	A	161	LEU	C-N-CA	9.29	144.93	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ARG	O-C-N	-9.12	108.11	122.70
1	A	432	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	A	161	LEU	CA-C-N	7.85	134.48	117.20

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASP	Peptide
1	A	164	GLY	Peptide
1	A	270	ASP	Peptide
1	A	358	ALA	Peptide
2	B	71	CYS	Peptide

5.2 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 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	3397	0	3426	141	2
1	C	3190	0	3237	162	0
2	B	576	0	586	28	0
2	D	571	0	575	26	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	1	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
5	A	108	0	0	3	0
5	B	18	0	0	1	0
5	C	135	0	0	5	0
5	D	17	0	0	0	0
All	All	8029	0	7824	352	2

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 23.

The worst 5 of 352 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:THR:HG22	1:C:124:ARG:NH1	1.21	1.48
1:A:263:SER:O	1:A:266:LYS:HG2	1.16	1.28
1:C:63:ASN:ND2	1:C:256[B]:CYS:SG	2.08	1.27
1:C:121:THR:CG2	1:C:124:ARG:NH1	1.99	1.23
1:C:121:THR:CG2	1:C:124:ARG:HH12	1.53	1.19

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:LYS:NZ	1:A:135:ASP:OD1[7_554]	1.63	0.57
1:A:22:GLY:O	1:A:190:PRO:O[7_554]	2.10	0.10

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	425/446 (95%)	387 (91%)	31 (7%)	7 (2%)	14	13
1	C	392/446 (88%)	365 (93%)	21 (5%)	6 (2%)	15	13
2	B	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
2	D	67/88 (76%)	62 (92%)	4 (6%)	1 (2%)	15	13
All	All	952/1068 (89%)	877 (92%)	61 (6%)	14 (2%)	15	13

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	83	SER
1	A	141	ILE
1	C	106	GLU
2	D	25	GLY

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	365/380 (96%)	343 (94%)	22 (6%)	27	32
1	C	346/380 (91%)	325 (94%)	21 (6%)	26	31
2	B	66/80 (82%)	63 (96%)	3 (4%)	38	48
2	D	65/80 (81%)	58 (89%)	7 (11%)	9	9
All	All	842/920 (92%)	789 (94%)	53 (6%)	26	29

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	43	SER
1	C	106	GLU
2	D	34	LYS
2	B	65	GLU
1	C	68	SER

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	357	ASN
1	C	241	ASN
2	D	23	GLN

5.3.3 RNA [i](#)

There are no RNA chains 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 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	431/446 (96%)	-0.02	28 (6%) 18 21	25, 44, 87, 115	0
1	C	401/446 (89%)	-0.19	13 (3%) 45 49	24, 43, 87, 114	0
2	B	71/88 (80%)	-0.40	0 100 100	29, 43, 67, 83	0
2	D	71/88 (80%)	-0.26	0 100 100	30, 45, 72, 82	0
All	All	974/1068 (91%)	-0.13	41 (4%) 35 38	24, 43, 85, 115	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	8.1
1	A	143	GLU	5.8
1	A	360	LYS	5.8
1	A	359	SER	5.5
1	A	144	GLU	5.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CL	D	1089	1/1	0.23	26.00	63,63,63,63	0
4	CL	B	1088	1/1	0.22	13.00	53,53,53,53	0
4	CL	C	1441	1/1	0.17	0.98	57,57,57,57	0
4	CL	B	1089	1/1	0.14	0.62	73,73,73,73	0
3	HG	C	1440	1/1	0.12	0.47	40,40,40,40	1
4	CL	C	1442	1/1	0.13	0.24	66,66,66,66	0
4	CL	D	1088	1/1	0.12	0.17	66,66,66,66	0
4	CL	A	1442	1/1	0.13	0.15	58,58,58,58	0
4	CL	C	1443	1/1	0.11	-0.34	72,72,72,72	0
3	HG	A	1439	1/1	0.13	-0.42	45,45,45,45	1
4	CL	A	1441	1/1	0.14	-0.94	70,70,70,70	0
3	HG	A	1438	1/1	0.09	-1.26	78,78,78,78	1
3	HG	B	1087	1/1	0.06	-1.36	77,77,77,77	1
3	HG	D	1087	1/1	0.07	-1.41	69,69,69,69	1
3	HG	C	1438	1/1	0.06	-1.71	78,78,78,78	1
4	CL	A	1440	1/1	0.08	-2.79	68,68,68,68	0
3	HG	C	1439	1/1	0.14	-	55,55,55,55	1

6.5 Other polymers (i)

There are no such residues in this entry.