



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:41 AM GMT

PDB ID : 2I6R
Title : Crystal structure of E. coli HypE, a hydrogenase maturation protein
Authors : Rangarajan, E.S.; Proteau, A.; Iannuzzi, P.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2006-08-29
Resolution : 2.51 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

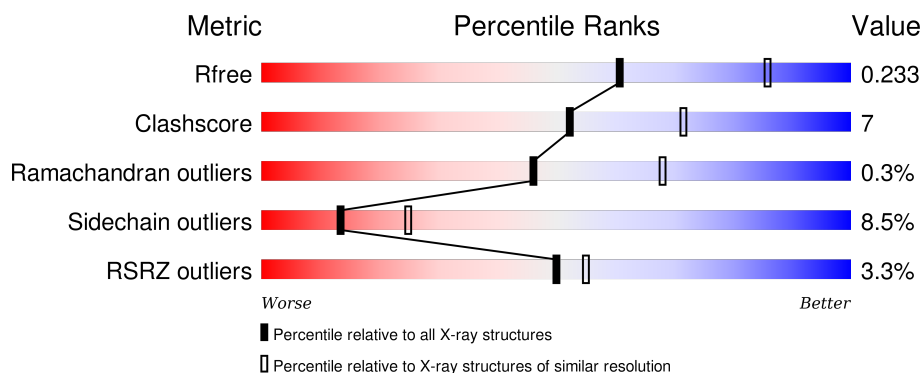
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	334	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	334	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	C	334	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	334	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9764 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 HypE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2322	1468	404	438	12			
1	B	315	Total	C	N	O	S	0	0	0
			2318	1467	404	435	12			
1	C	321	Total	C	N	O	S	0	0	0
			2361	1492	411	446	12			
1	D	322	Total	C	N	O	S	0	0	0
			2366	1494	412	448	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q7ABB2
A	-10	GLY	-	EXPRESSION TAG	UNP Q7ABB2
A	-9	SER	-	EXPRESSION TAG	UNP Q7ABB2
A	-8	SER	-	EXPRESSION TAG	UNP Q7ABB2
A	-7	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-6	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-5	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-4	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-3	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-2	HIS	-	EXPRESSION TAG	UNP Q7ABB2
A	-1	GLY	-	EXPRESSION TAG	UNP Q7ABB2
A	0	SER	-	EXPRESSION TAG	UNP Q7ABB2
B	-11	MET	-	EXPRESSION TAG	UNP Q7ABB2
B	-10	GLY	-	EXPRESSION TAG	UNP Q7ABB2
B	-9	SER	-	EXPRESSION TAG	UNP Q7ABB2
B	-8	SER	-	EXPRESSION TAG	UNP Q7ABB2
B	-7	HIS	-	EXPRESSION TAG	UNP Q7ABB2
B	-6	HIS	-	EXPRESSION TAG	UNP Q7ABB2
B	-5	HIS	-	EXPRESSION TAG	UNP Q7ABB2
B	-4	HIS	-	EXPRESSION TAG	UNP Q7ABB2
B	-3	HIS	-	EXPRESSION TAG	UNP Q7ABB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q7ABB2
B	-1	GLY	-	EXPRESSION TAG	UNP Q7ABB2
B	0	SER	-	EXPRESSION TAG	UNP Q7ABB2
C	-11	MET	-	EXPRESSION TAG	UNP Q7ABB2
C	-10	GLY	-	EXPRESSION TAG	UNP Q7ABB2
C	-9	SER	-	EXPRESSION TAG	UNP Q7ABB2
C	-8	SER	-	EXPRESSION TAG	UNP Q7ABB2
C	-7	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-6	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-5	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-4	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-3	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-2	HIS	-	EXPRESSION TAG	UNP Q7ABB2
C	-1	GLY	-	EXPRESSION TAG	UNP Q7ABB2
C	0	SER	-	EXPRESSION TAG	UNP Q7ABB2
D	-11	MET	-	EXPRESSION TAG	UNP Q7ABB2
D	-10	GLY	-	EXPRESSION TAG	UNP Q7ABB2
D	-9	SER	-	EXPRESSION TAG	UNP Q7ABB2
D	-8	SER	-	EXPRESSION TAG	UNP Q7ABB2
D	-7	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-6	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-5	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-4	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-3	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-2	HIS	-	EXPRESSION TAG	UNP Q7ABB2
D	-1	GLY	-	EXPRESSION TAG	UNP Q7ABB2
D	0	SER	-	EXPRESSION TAG	UNP Q7ABB2

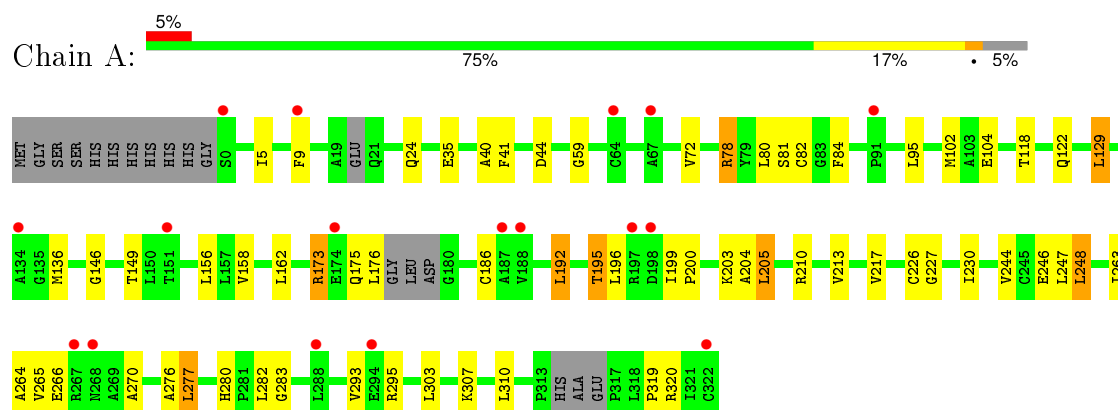
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	103	Total O 103 103	0	0
2	C	78	Total O 78 78	0	0
2	D	142	Total O 142 142	0	0

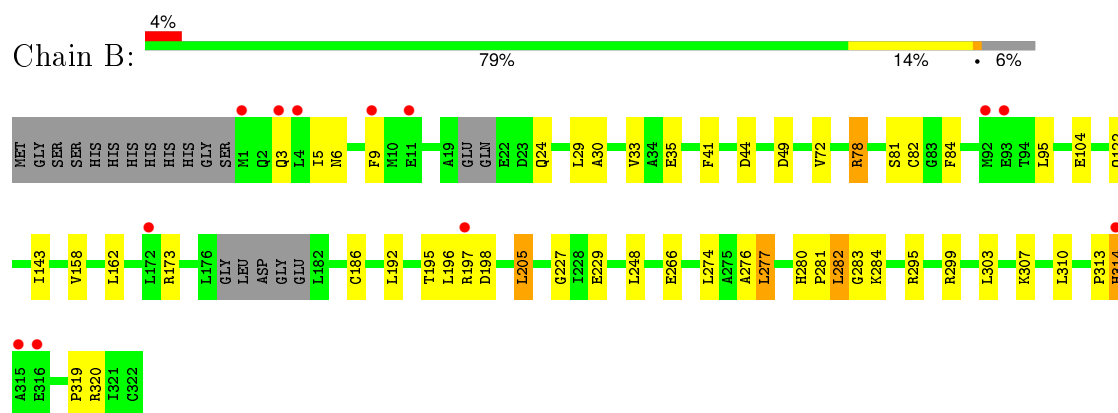
3 Residue-property plots [i](#)

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 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.

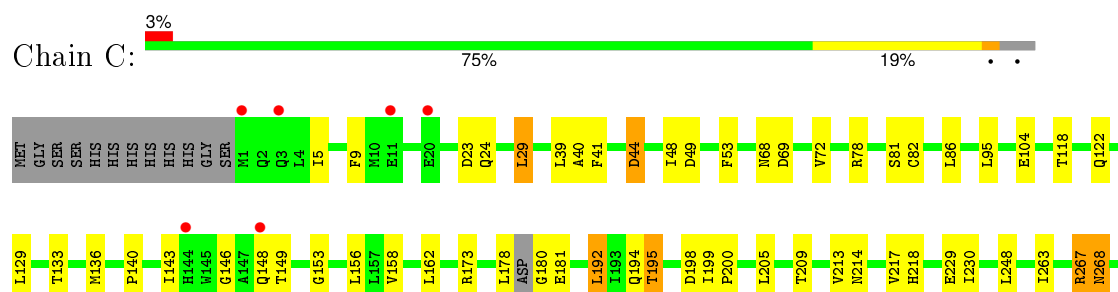
• Molecule 1: HypE protein

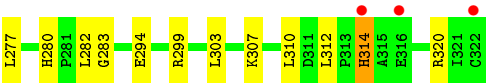


• Molecule 1: HypE protein

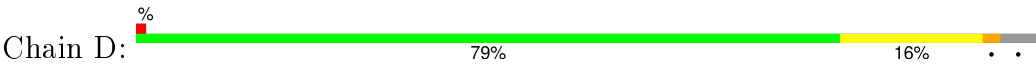


• Molecule 1: HypE protein





● Molecule 1: HypE protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.76 Å 71.78 Å 113.03 Å 90.00° 115.12° 90.00°	Depositor
Resolution (Å)	43.73 – 2.51 43.73 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.73-2.51) 99.1 (43.73-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.240 0.189 , 0.233	Depositor DCC
R_{free} test set	3189 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
Estimated twinning fraction	0.012 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63144 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9764	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.44	0/2353	0.63	0/3194
1	B	0.50	0/2351	0.65	1/3195 (0.0%)
1	C	0.46	0/2395	0.64	0/3255
1	D	0.52	0/2400	0.66	0/3262
All	All	0.48	0/9499	0.64	1/12906 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	282	LEU	N-CA-C	5.16	124.92	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	313	PRO	Peptide

5.2 Too-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 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	2322	0	2381	40	0
1	B	2318	0	2377	31	0
1	C	2361	0	2415	40	0
1	D	2366	0	2418	34	0
2	A	74	0	0	1	0
2	B	103	0	0	2	0
2	C	78	0	0	2	0
2	D	142	0	0	0	0
All	All	9764	0	9591	126	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 7.

The worst 5 of 126 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:C:146:GLY:O	1:C:149:THR:HG22	1.64	0.95
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.43	0.84
1:A:146:GLY:O	1:A:149:THR:HG22	1.77	0.83
1:C:314:HIS:H	1:C:314:HIS:CD2	1.95	0.79
1:D:158:VAL:HG21	1:D:162:LEU:HD21	1.64	0.79

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	308/334 (92%)	294 (96%)	13 (4%)	1 (0%)	46 68
1	B	309/334 (92%)	296 (96%)	11 (4%)	2 (1%)	30 50
1	C	317/334 (95%)	302 (95%)	14 (4%)	1 (0%)	46 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	318/334 (95%)	306 (96%)	12 (4%)	0	100	100
All	All	1252/1336 (94%)	1198 (96%)	50 (4%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	HIS
1	B	186	CYS
1	C	209	THR
1	A	186	CYS

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	242/256 (94%)	221 (91%)	21 (9%)	13	24
1	B	241/256 (94%)	225 (93%)	16 (7%)	21	38
1	C	245/256 (96%)	221 (90%)	24 (10%)	10	19
1	D	246/256 (96%)	224 (91%)	22 (9%)	12	23
All	All	974/1024 (95%)	891 (92%)	83 (8%)	13	25

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	24	GLN
1	C	178	LEU
1	D	268	ASN
1	C	29	LEU
1	C	95	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	218	HIS
1	C	268	ASN
1	D	122	GLN
1	C	122	GLN
1	D	21	GLN

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	316/334 (94%)	0.32	17 (5%)	29 33	30, 40, 50, 61	0
1	B	315/334 (94%)	0.01	12 (3%)	44 49	32, 39, 51, 63	0
1	C	321/334 (96%)	0.07	9 (2%)	56 61	32, 40, 49, 60	0
1	D	322/334 (96%)	0.05	4 (1%)	81 83	32, 39, 49, 64	0
All	All	1274/1336 (95%)	0.11	42 (3%)	50 55	30, 39, 50, 64	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.0
1	A	0	SER	4.0
1	D	314	HIS	3.9
1	B	314	HIS	3.3
1	B	3	GLN	3.3

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.