

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 2I6R

Title : Crystal structure of E. coli HypE, a hydrogenase maturation protein

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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

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

henix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

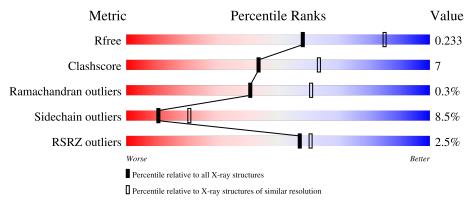
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	75% 179	%	• 5%	6
1	В	334	79%	L4%	• 69	~
1	С	334	75%	1%		-
1	D	334	79%	16%		-



2 Entry composition (i)

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	Λ	316	Total	С	N	О	S	0	0	0
1	A	310	2322	1468	404	438	12	U	0	
1	В	315	Total	С	N	О	S	0	0	0
1	Б	319	2318	1467	404	435	12	U	U	
1	С	321	Total	С	N	О	S	0	0	0
1		321	2361	1492	411	446	12	U	U	
1	D	322	Total	С	N	О	S	0	0	0
1	ש	322	2366	1494	412	448	12	0		

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
В	-11	MET	-	expression tag	UNP Q7ABB2
В	-10	GLY	-	expression tag	UNP Q7ABB2
В	-9	SER	-	expression tag	UNP Q7ABB2
В	-8	SER	-	expression tag	UNP Q7ABB2
В	-7	HIS	-	expression tag	UNP Q7ABB2
В	-6	HIS	-	expression tag	UNP Q7ABB2
В	-5	HIS	-	expression tag	UNP Q7ABB2
В	-4	HIS	-	expression tag	UNP Q7ABB2
В	-3	HIS	-	expression tag	UNP Q7ABB2

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-2	HIS	-	expression tag	UNP Q7ABB2
В	-1	GLY	-	expression tag	UNP Q7ABB2
В	0	SER	-	expression tag	UNP Q7ABB2
С	-11	MET	-	expression tag	UNP Q7ABB2
С	-10	GLY	-	expression tag	UNP Q7ABB2
С	-9	SER	-	expression tag	UNP Q7ABB2
С	-8	SER	-	expression tag	UNP Q7ABB2
С	-7	HIS	-	expression tag	UNP Q7ABB2
С	-6	HIS	-	expression tag	UNP Q7ABB2
С	-5	HIS	-	expression tag	UNP Q7ABB2
С	-4	HIS	-	expression tag	UNP Q7ABB2
С	-3	HIS	-	expression tag	UNP Q7ABB2
С	-2	HIS	-	expression tag	UNP Q7ABB2
С	-1	GLY	-	expression tag	UNP Q7ABB2
С	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.

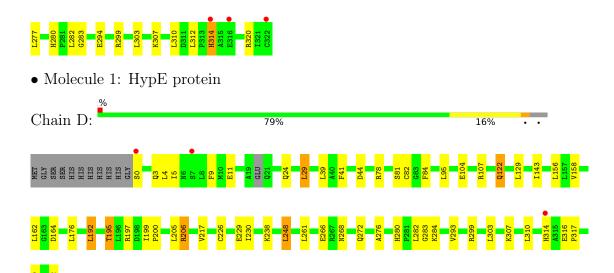
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	В	103	Total O 103 103	0	0
2	С	78	Total O 78 78	0	0
2	D	142	Total O 142 142	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HypE protein Chain A: • Molecule 1: HypE protein Chain B: 79% 14% • Molecule 1: HypE protein Chain C: 75% 19%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	254.76Å 71.78Å 113.03Å	Depositor
a, b, c, α , β , γ	90.00° 115.12° 90.00°	Depositor
Resolution (Å)	43.73 - 2.51	Depositor
resolution (A)	43.73 - 2.51	EDS
% Data completeness	99.1 (43.73-2.51)	Depositor
(in resolution range)	99.1 (43.73-2.51)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.82 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.240	Depositor
it, it free	0.189 , 0.233	DCC
R_{free} test set	3190 reflections (5.05%)	wwPDB-VP
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
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h-2*l,-k,l	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.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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		
MIOI	Wioi Chain		RMSZ # Z > 5		# Z > 5	
1	A	0.44	0/2353	0.63	0/3194	
1	В	0.50	0/2351	0.65	1/3195 (0.0%)	
1	С	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	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
1	В	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	В	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2322	0	2381	40	0
1	В	2318	0	2377	31	0
1	С	2361	0	2415	40	0
1	D	2366	0	2418	34	0
2	A	74	0	0	1	0
2	В	103	0	0	2	0
2	С	78	0	0	2	0
2	D	142	0	0	0	0
All	All	9764	0	9591	126	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} (\mathring{\rm A}) \end{array}$	Clash overlap (Å)
1:C:146:GLY:O	1:C:149:THR:HG22	1.64	0.95
1:A:210:ARG:HH11	1:A:210:ARG:HG3	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	Perce	ntiles
1	A	308/334~(92%)	294 (96%)	13 (4%)	1 (0%)	41	61
1	В	309/334~(92%)	296 (96%)	11 (4%)	2 (1%)	25	43
1	C	317/334~(95%)	302 (95%)	14 (4%)	1 (0%)	41	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
1	D	318/334 (95%)	306 (96%)	12 (4%)	0	100	100
All	All	1252/1336 (94%)	1198 (96%)	50 (4%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	314	HIS
1	В	186	CYS
1	С	209	THR
1	A	186	CYS

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	242/256~(94%)	221 (91%)	21 (9%)	10 20
1	В	241/256 (94%)	225 (93%)	16 (7%)	16 32
1	\mathbf{C}	245/256~(96%)	221 (90%)	24 (10%)	8 15
1	D	246/256~(96%)	224 (91%)	22 (9%)	9 19
All	All	974/1024 (95%)	891 (92%)	83 (8%)	10 21

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

Mol	Chain	Res	Type
1	С	307	LYS
1	D	192	LEU
1	С	312	LEU
1	D	44	ASP
1	D	266	GLU

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



Mol	Chain	Res	Type
1	С	268	ASN
1	С	278	HIS
1	D	314	HIS
1	D	122	GLN
1	D	268	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 monosaccharides 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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	316/334 (94%)	0.25	10 (3%) 47 51	30, 40, 50, 61	0
1	В	315/334 (94%)	-0.04	11 (3%) 44 47	32, 39, 51, 63	0
1	С	321/334 (96%)	0.01	8 (2%) 57 61	32, 40, 49, 60	0
1	D	322/334 (96%)	-0.01	3 (0%) 84 86	32, 39, 49, 64	0
All	All	1274/1336 (95%)	0.05	32 (2%) 57 61	30, 39, 50, 64	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	SER	3.9
1	С	1	MET	3.8
1	D	314	HIS	3.7
1	В	314	HIS	3.2
1	В	3	GLN	3.1

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 monosaccharides 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.

