wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3A44
Title	:	Crystal structure of HypA in the dimeric form
Authors	:	Watanabe, S.; Arai, T.; Matsumi, R.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2009-06-30
Resolution	:	3.31 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 (i)) were used in the production of this report:

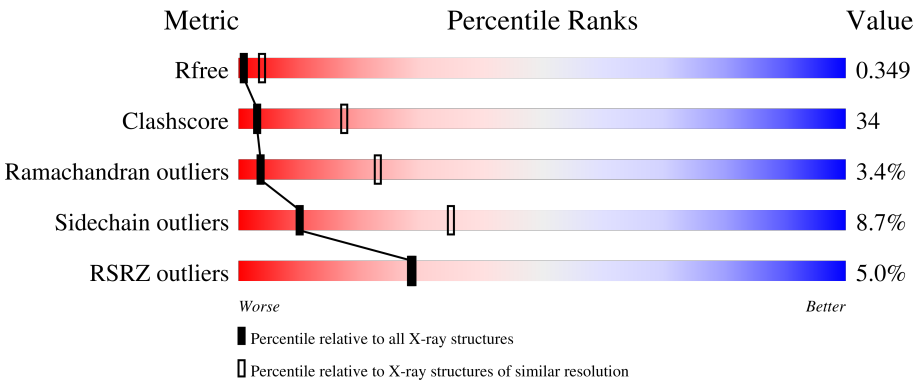
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.31 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}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	139	% 51% 41% 5% ••
1	B	139	2% 47% 41% 7% 5%
1	C	139	10% 46% 36% 6% 12%
1	D	139	6% 53% 33% 5% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	FME	B	1	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3852 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 Hydrogenase nickel incorporation protein hypA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1008	640	170	193	5	0	0	0
1	B	132	1001	637	171	187	6	0	0	0
1	C	122	899	568	154	172	5	0	0	0
1	D	127	940	599	159	177	5	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

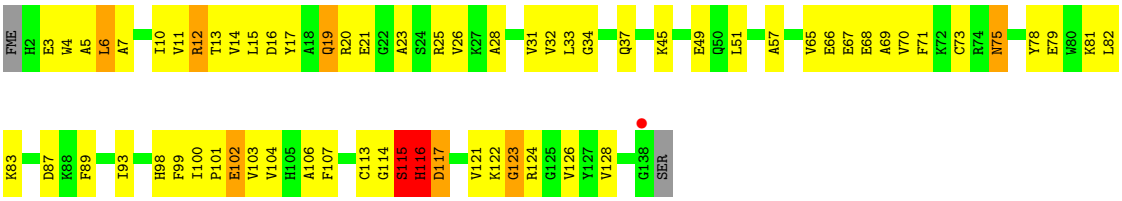
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	2	2	2	0	0

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.

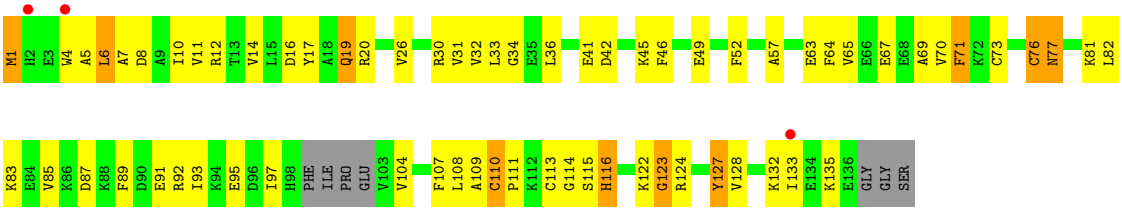
• Molecule 1: Hydrogenase nickel incorporation protein hypA

Chain A:



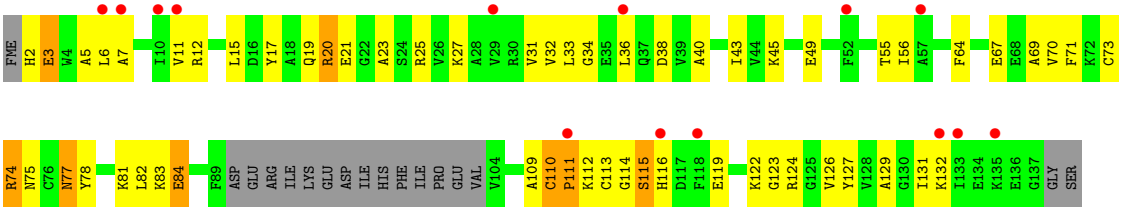
• Molecule 1: Hydrogenase nickel incorporation protein hypA

Chain B:



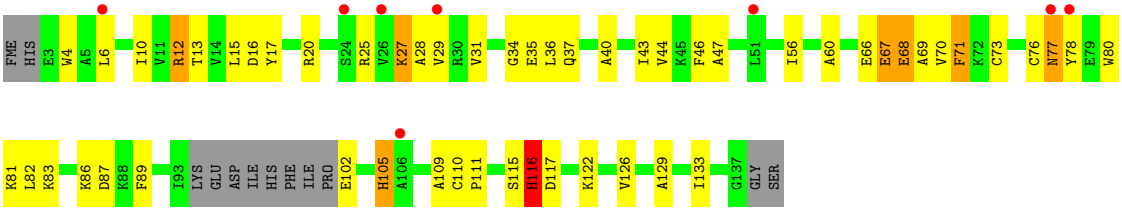
• Molecule 1: Hydrogenase nickel incorporation protein hypA

Chain C:



• Molecule 1: Hydrogenase nickel incorporation protein hypA

Chain D:


FME
HIS
E3
W4
A5
L6
I10
V11
R12
T13
V14
L15
D16
Y17
R20
S24
R25
V26
K27
A28
V29
R30
V31
G34
E35
L36
Q37
A40
I43
V44
K45
F46
A47
L51
I56
A60
E66
E67
E68
A69
V70
F71
K72
C73
C76
N77
Y78
E79
W80
K81
L82
K83
K86
D87
K88
F89
I93
LYS
GLU
ASP
ILE
HIS
PHE
ILE
PRO
E102
H105
A106
A109
C110
P111
S115
H116
D117
K122
V126
A129
I133
G137
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.83Å 97.97Å 136.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 3.31 49.16 – 3.31	Depositor EDS
% Data completeness (in resolution range)	92.1 (49.16-3.31) 92.2 (49.16-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.292 , 0.337 0.285 , 0.349	Depositor DCC
R_{free} test set	539 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	101.0	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3852	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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: ZN, FME

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	0.36	0/1022	0.59	0/1384
1	B	0.35	0/1007	0.59	0/1360
1	C	0.32	0/910	0.59	0/1229
1	D	0.37	0/954	0.63	0/1288
All	All	0.35	0/3893	0.60	0/5261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1008	0	940	79	0
1	B	1001	0	936	85	0
1	C	899	0	843	66	0
1	D	940	0	878	81	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	2	0	0	0	0
All	All	3852	0	3597	253	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 34.

The worst 5 of 253 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:D:109:ALA:HB2	1:D:116:HIS:CD2	1.77	1.19
1:A:23:ALA:HB2	1:B:133:ILE:HD12	1.23	1.07
1:D:25:ARG:HA	1:D:56:ILE:HB	1.40	1.02
1:D:109:ALA:HB2	1:D:116:HIS:NE2	1.75	1.01
1:D:109:ALA:CB	1:D:116:HIS:CD2	2.46	0.99

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	135/139 (97%)	115 (85%)	15 (11%)	5 (4%)	3 21
1	B	128/139 (92%)	108 (84%)	18 (14%)	2 (2%)	9 37
1	C	118/139 (85%)	99 (84%)	11 (9%)	8 (7%)	1 9
1	D	123/139 (88%)	110 (89%)	11 (9%)	2 (2%)	9 37
All	All	504/556 (91%)	432 (86%)	55 (11%)	17 (3%)	3 23

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	C	115	SER
1	C	116	HIS
1	D	68	GLU
1	A	4	TRP

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	94/113 (83%)	83 (88%)	11 (12%)	5 21
1	B	93/113 (82%)	86 (92%)	7 (8%)	13 41
1	C	84/113 (74%)	79 (94%)	5 (6%)	19 50
1	D	87/113 (77%)	79 (91%)	8 (9%)	9 32
All	All	358/452 (79%)	327 (91%)	31 (9%)	10 35

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	CYS
1	D	77	ASN
1	B	127	TYR
1	D	105	HIS
1	D	27	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	D	77	ASN
1	D	116	HIS
1	A	75	ASN
1	A	19	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	B	1	1	8,9,10	0.54	0	7,9,11	1.65	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	B	1	1	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	FME	C-CA-N	3.24	115.58	109.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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.

No monomer is involved in short contacts.

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	137/139 (98%)	0.11	1 (0%)	87	89	80, 120, 138, 157	0
1	B	131/139 (94%)	0.16	3 (2%)	60	59	69, 120, 152, 175	0
1	C	122/139 (87%)	0.29	14 (11%)	4	4	90, 134, 161, 174	0
1	D	127/139 (91%)	0.25	8 (6%)	20	21	86, 123, 159, 167	0
All	All	517/556 (92%)	0.20	26 (5%)	28	28	69, 124, 155, 175	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	TRP	5.2
1	D	26	VAL	4.4
1	D	78	TYR	4.3
1	C	57	ALA	3.3
1	C	111	PRO	3.2

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	B	1	10/11	0.72	0.61	125,129,132,137	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	140	1/1	0.86	0.21	140,140,140,140	0
2	ZN	C	141	1/1	0.94	0.15	128,128,128,128	0
2	ZN	A	140	1/1	0.97	0.25	142,142,142,142	0
2	ZN	C	140	1/1	0.98	0.21	112,112,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.