



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 11:46 PM EDT

PDB ID : 6HNN
Title : Crystal structure of wild-type IdmH, a putative polyketide cyclase from *Streptomyces antibioticus*
Authors : Drulyte, I.; Obajdin, J.; Trinh, C.; Hemsworth, G.R.; Berry, A.
Deposited on : 2018-09-16
Resolution : 2.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

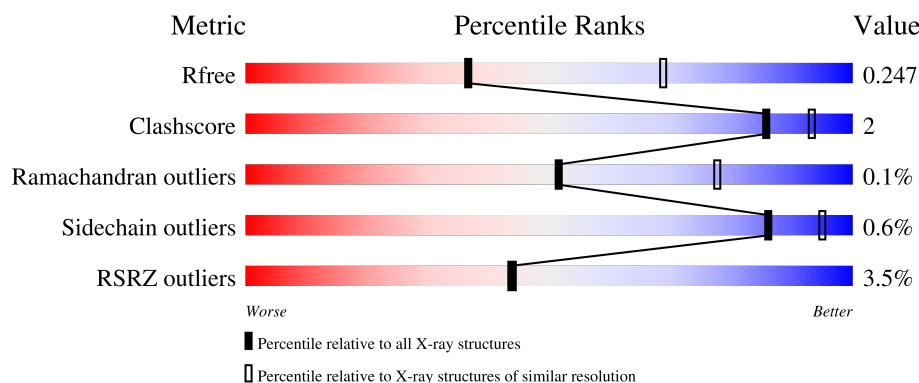
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	148	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	148	<div> <div></div> <div>89%</div> <div>7%</div> </div>
1	C	148	<div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div>
1	D	148	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	E	148	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	148	<div><div></div><div>89%</div><div><div></div><div></div><div></div></div><div>8%</div></div>
1	G	148	<div><div>3%</div><div></div><div>89%</div><div><div></div><div></div><div></div></div><div>7%</div></div>
1	H	148	<div><div>%</div><div></div><div>88%</div><div><div></div><div></div><div></div></div><div>6%</div><div>6%</div></div>
1	I	148	<div><div>8%</div><div></div><div>88%</div><div><div></div><div></div><div></div></div><div>6%</div><div>6%</div></div>
1	J	148	<div><div>16%</div><div></div><div>86%</div><div><div></div><div></div><div></div></div><div>7%</div><div>7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10274 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 Putative polyketide cyclase IdmH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1061	667	186	201	7			
1	B	138	Total	C	N	O	S	0	0	0
			1030	650	181	192	7			
1	C	138	Total	C	N	O	S	0	0	0
			1020	643	177	193	7			
1	D	139	Total	C	N	O	S	0	0	0
			1044	658	182	197	7			
1	E	138	Total	C	N	O	S	0	0	0
			1020	646	179	188	7			
1	F	136	Total	C	N	O	S	0	0	0
			1015	642	175	191	7			
1	G	138	Total	C	N	O	S	0	0	0
			1024	647	178	192	7			
1	H	139	Total	C	N	O	S	0	0	0
			1039	655	182	195	7			
1	I	139	Total	C	N	O	S	0	0	0
			1014	640	175	192	7			
1	J	138	Total	C	N	O	S	0	0	0
			998	630	176	186	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP C5HV10
A	2	SER	-	expression tag	UNP C5HV10
A	3	HIS	-	expression tag	UNP C5HV10
B	1	GLY	-	expression tag	UNP C5HV10
B	2	SER	-	expression tag	UNP C5HV10
B	3	HIS	-	expression tag	UNP C5HV10
C	1	GLY	-	expression tag	UNP C5HV10
C	2	SER	-	expression tag	UNP C5HV10
C	3	HIS	-	expression tag	UNP C5HV10

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP C5HV10
D	2	SER	-	expression tag	UNP C5HV10
D	3	HIS	-	expression tag	UNP C5HV10
E	1	GLY	-	expression tag	UNP C5HV10
E	2	SER	-	expression tag	UNP C5HV10
E	3	HIS	-	expression tag	UNP C5HV10
F	1	GLY	-	expression tag	UNP C5HV10
F	2	SER	-	expression tag	UNP C5HV10
F	3	HIS	-	expression tag	UNP C5HV10
G	1	GLY	-	expression tag	UNP C5HV10
G	2	SER	-	expression tag	UNP C5HV10
G	3	HIS	-	expression tag	UNP C5HV10
H	1	GLY	-	expression tag	UNP C5HV10
H	2	SER	-	expression tag	UNP C5HV10
H	3	HIS	-	expression tag	UNP C5HV10
I	1	GLY	-	expression tag	UNP C5HV10
I	2	SER	-	expression tag	UNP C5HV10
I	3	HIS	-	expression tag	UNP C5HV10
J	1	GLY	-	expression tag	UNP C5HV10
J	2	SER	-	expression tag	UNP C5HV10
J	3	HIS	-	expression tag	UNP C5HV10

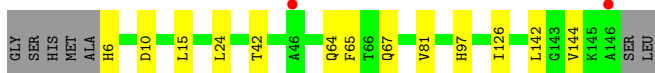
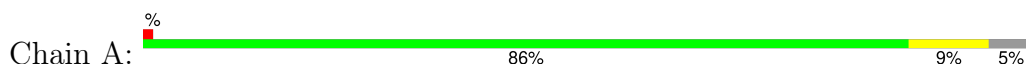
- Molecule 2 is water.

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

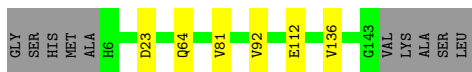
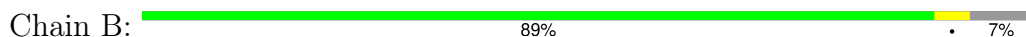
3 Residue-property plots [i](#)

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.

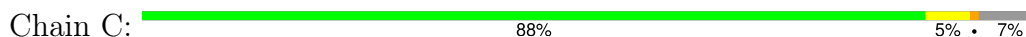
- Molecule 1: Putative polyketide cyclase IdmH



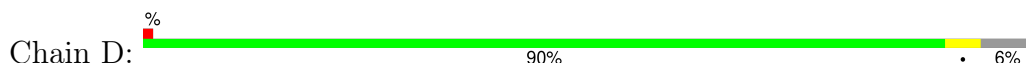
- Molecule 1: Putative polyketide cyclase IdmH



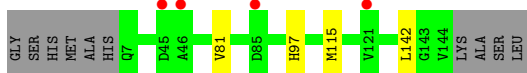
- Molecule 1: Putative polyketide cyclase IdmH



- Molecule 1: Putative polyketide cyclase IdmH

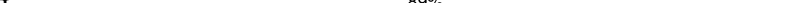


- Molecule 1: Putative polyketide cyclase IdmH

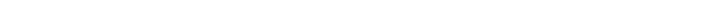


- Molecule 1: Putative polyketide cyclase IdmH

GLY SER HIS MET ALA HIS Q7 L24 R54 Q64 V81 R94 L142 GLY VAL LYS ALA SER LEU

- Chain G:  3% 89% 7%

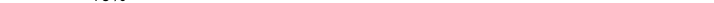
GLY
 SER
 HIS
 MET
 ALA
 HIS
 Q7
 T11
 I12
 Y16
 L27
 T42
 F65
 V77
 V81
 R94
 H97
 L142
 G143
 V144
 LYS
 ALA
 SER
 LEU

- Chain H:  88% 6% 6%

Amino Acid	Count
GLY	0
SER	0
HIS	0
MET	0
ALA	0
H6	1
A46	1
P49	1
V81	1
V92	1
I99	1
E112	1
R122	1
V136	1
L142	1
G143	1
V144	1
LYS	0
ALA	0
SER	0
LEU	0

- Chain I:

GLY	SER	HIS	MET	ALA	H6	D10	T11	I12	A13	G14	L15	Y16	F19	D23	R28	E29	R54	F69	V81	A88	C91	I99	V121	R122	D123	G124	R125	V136	V144	LYS	ALA	SER	LEU
					●		●	●	●	●	●	●	●	●							●	●		●	●	●	●			●			

- Chain J:  16% 86% 7% 7%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.68Å 103.52Å 99.58Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	51.76 – 2.70 51.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.76-2.70) 99.6 (51.76-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.211 , 0.244 0.215 , 0.247	Depositor DCC
R_{free} test set	1832 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k 0.000 for -h,l,k 0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10274	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.67	0/1088	0.83	2/1488 (0.1%)
1	B	0.63	0/1056	0.81	1/1445 (0.1%)
1	C	0.60	0/1046	0.84	5/1433 (0.3%)
1	D	0.63	0/1070	0.81	0/1464
1	E	0.57	0/1046	0.78	1/1433 (0.1%)
1	F	0.60	0/1041	0.79	2/1426 (0.1%)
1	G	0.58	0/1050	0.76	1/1438 (0.1%)
1	H	0.59	0/1065	0.80	1/1457 (0.1%)
1	I	0.57	0/1040	0.80	3/1426 (0.2%)
1	J	0.55	0/1024	0.72	1/1405 (0.1%)
All	All	0.60	0/10526	0.79	17/14415 (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	H	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	GLN	CA-CB-CG	6.63	127.99	113.40
1	F	54	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	I	28	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	I	54	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	C	125	ARG	CG-CD-NE	6.13	124.68	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	142	LEU	Peptide,Mainchain

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	1061	0	1005	6	0
1	B	1030	0	981	4	0
1	C	1020	0	957	4	0
1	D	1044	0	996	3	0
1	E	1020	0	972	2	0
1	F	1015	0	963	2	0
1	G	1024	0	970	5	0
1	H	1039	0	987	10	0
1	I	1014	0	939	12	0
1	J	998	0	920	17	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
All	All	10274	0	9690	44	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 2.

The worst 5 of 44 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:81:VAL:HG12	1:D:81:VAL:HG12	1.35	1.03
1:G:81:VAL:HG12	1:H:81:VAL:HG12	1.44	0.98
1:I:81:VAL:HG12	1:J:81:VAL:HG12	1.44	0.97
1:A:81:VAL:HG12	1:B:81:VAL:HG12	1.49	0.94
1:J:129:HIS:NE2	1:J:131:THR:CG2	2.47	0.77

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	139/148 (94%)	138 (99%)	0	1 (1%)	22	46
1	B	136/148 (92%)	136 (100%)	0	0	100	100
1	C	136/148 (92%)	136 (100%)	0	0	100	100
1	D	137/148 (93%)	136 (99%)	1 (1%)	0	100	100
1	E	136/148 (92%)	135 (99%)	1 (1%)	0	100	100
1	F	134/148 (90%)	134 (100%)	0	0	100	100
1	G	136/148 (92%)	135 (99%)	1 (1%)	0	100	100
1	H	137/148 (93%)	136 (99%)	1 (1%)	0	100	100
1	I	137/148 (93%)	136 (99%)	1 (1%)	0	100	100
1	J	136/148 (92%)	135 (99%)	1 (1%)	0	100	100
All	All	1364/1480 (92%)	1357 (100%)	6 (0%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	VAL

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	110/121 (91%)	108 (98%)	2 (2%)	59	83
1	B	106/121 (88%)	105 (99%)	1 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	104/121 (86%)	104 (100%)	0	100	100
1	D	109/121 (90%)	107 (98%)	2 (2%)	59	83
1	E	104/121 (86%)	104 (100%)	0	100	100
1	F	105/121 (87%)	104 (99%)	1 (1%)	76	91
1	G	105/121 (87%)	105 (100%)	0	100	100
1	H	107/121 (88%)	107 (100%)	0	100	100
1	I	101/121 (84%)	101 (100%)	0	100	100
1	J	97/121 (80%)	97 (100%)	0	100	100
All	All	1048/1210 (87%)	1042 (99%)	6 (1%)	86	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	118	MET
1	D	144	VAL
1	F	64	GLN
1	A	65	PHE
1	A	6	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	B	64	GLN
1	D	78	GLN
1	F	64	GLN
1	J	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	141/148 (95%)	0.00	2 (1%) 75 77	36, 56, 93, 109	0
1	B	138/148 (93%)	-0.07	0 100 100	38, 57, 76, 88	0
1	C	138/148 (93%)	-0.01	0 100 100	40, 60, 90, 116	0
1	D	139/148 (93%)	-0.01	1 (0%) 87 89	42, 63, 93, 121	0
1	E	138/148 (93%)	0.03	4 (2%) 51 52	45, 74, 109, 132	0
1	F	136/148 (91%)	-0.04	0 100 100	44, 71, 95, 104	0
1	G	138/148 (93%)	0.30	5 (3%) 42 42	47, 82, 115, 131	0
1	H	139/148 (93%)	0.18	1 (0%) 87 89	44, 71, 99, 126	0
1	I	139/148 (93%)	0.56	12 (8%) 10 8	54, 93, 115, 129	0
1	J	138/148 (93%)	0.78	23 (16%) 1 1	47, 101, 133, 149	0
All	All	1384/1480 (93%)	0.17	48 (3%) 44 44	36, 69, 112, 149	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	12	ILE	5.2
1	J	36	VAL	4.3
1	H	6	HIS	3.9
1	I	121	VAL	3.9
1	J	121	VAL	3.8

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.