



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:53 PM EDT

PDB ID : 5V3S
Title : Crystal structure of IP-1A from *Alcaligenes faecalis* at 1.8Å resolution
Authors : Yalpani, N.; Altier, D.; Guan, R.; Montelione, G.
Deposited on : 2017-03-08
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

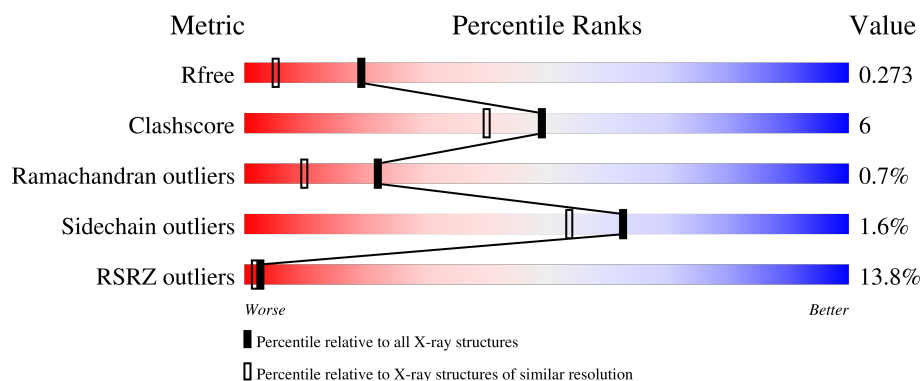
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	154	
1	B	154	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2525 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 Two-component insecticidal protein 16 kDa unit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	Se	0	1	0
			1162	734	196	228	2	2			
1	B	140	Total	C	N	O	S	Se	0	0	0
			1096	695	177	220	2	2			

There are 20 discrepancies between the modelled and reference sequences:

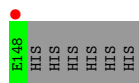
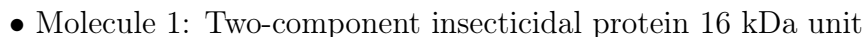
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MSE	ILE	conflict	UNP A0A0U4HUZ5
A	135	MSE	THR	conflict	UNP A0A0U4HUZ5
A	147	LEU	-	expression tag	UNP A0A0U4HUZ5
A	148	GLU	-	expression tag	UNP A0A0U4HUZ5
A	149	HIS	-	expression tag	UNP A0A0U4HUZ5
A	150	HIS	-	expression tag	UNP A0A0U4HUZ5
A	151	HIS	-	expression tag	UNP A0A0U4HUZ5
A	152	HIS	-	expression tag	UNP A0A0U4HUZ5
A	153	HIS	-	expression tag	UNP A0A0U4HUZ5
A	154	HIS	-	expression tag	UNP A0A0U4HUZ5
B	20	MSE	ILE	conflict	UNP A0A0U4HUZ5
B	135	MSE	THR	conflict	UNP A0A0U4HUZ5
B	147	LEU	-	expression tag	UNP A0A0U4HUZ5
B	148	GLU	-	expression tag	UNP A0A0U4HUZ5
B	149	HIS	-	expression tag	UNP A0A0U4HUZ5
B	150	HIS	-	expression tag	UNP A0A0U4HUZ5
B	151	HIS	-	expression tag	UNP A0A0U4HUZ5
B	152	HIS	-	expression tag	UNP A0A0U4HUZ5
B	153	HIS	-	expression tag	UNP A0A0U4HUZ5
B	154	HIS	-	expression tag	UNP A0A0U4HUZ5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total 154	O 154	0	0
2	B	113	Total 113	O 113	0	0

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- Molecule 1: Two-component insecticidal protein 16 kDa unit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.29Å 34.42Å 71.44Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	27.99 – 1.80 30.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (27.99-1.80) 96.8 (30.97-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.216 , 0.270 0.223 , 0.273	Depositor DCC
R_{free} test set	1339 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.49% 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	1.07	1/1194 (0.1%)	1.04	3/1607 (0.2%)
1	B	0.94	0/1119	0.95	1/1506 (0.1%)
All	All	1.01	1/2313 (0.0%)	0.99	4/3113 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CD-OE2	-6.02	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD1	8.57	126.01	118.30
1	B	65	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	39	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	111	ASP	CB-CG-OD2	-5.44	113.41	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	GLU	Peptide

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	1162	0	1097	13	0
1	B	1096	0	1049	13	0
2	A	154	0	0	7	2
2	B	113	0	0	5	0
All	All	2525	0	2146	26	2

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 6.

All (26) 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:B:77:GLU:OE1	1:B:77:GLU:N	1.99	0.95
1:B:32:LYS:HD3	1:B:34:GLU:OE2	1.78	0.82
1:A:21:GLU:OE1	2:A:201:HOH:O	2.04	0.73
1:A:77:GLU:HG2	2:A:245:HOH:O	1.93	0.67
1:B:21:GLU:OE1	2:B:201:HOH:O	2.15	0.63
1:A:136:GLY:CA	2:A:208:HOH:O	2.49	0.59
1:B:94:LYS:CE	1:B:117:ASP:HB2	2.41	0.51
1:A:48:ASP:OD2	1:A:51:LYS:HD2	2.11	0.51
1:B:34:GLU:OE1	2:B:202:HOH:O	2.20	0.51
1:B:147:LEU:HD22	2:B:252:HOH:O	2.10	0.51
1:B:67:ASP:HB3	2:B:253:HOH:O	2.11	0.49
1:A:34:GLU:OE1	2:A:202:HOH:O	2.19	0.48
1:B:94:LYS:HE3	1:B:117:ASP:HB2	1.96	0.47
1:B:9:GLU:N	1:B:11:SER:HG	2.14	0.46
1:A:27:VAL:O	1:A:28[B]:ASN:HB2	2.16	0.46
1:A:111:ASP:CG	1:A:129:GLY:H	2.19	0.45
1:B:34:GLU:HB2	1:B:90:TYR:CE1	2.52	0.45
1:A:34:GLU:HB2	1:A:90:TYR:CE1	2.51	0.45
1:A:136:GLY:HA3	2:A:208:HOH:O	2.15	0.44
1:A:12:LYS:O	1:A:13:ILE:C	2.56	0.43
1:A:14:ARG:HG3	1:A:105:TRP:CH2	2.53	0.43
1:B:86:GLY:HA2	1:B:101:TRP:CZ3	2.54	0.43
1:B:67:ASP:CB	2:B:253:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:O	1:B:145:LYS:HD2	2.20	0.42
1:A:154:HIS:C	2:A:218:HOH:O	2.59	0.41
1:A:50:ASP:HB2	2:A:207:HOH:O	2.20	0.41

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	Interatomic distance (Å)	Clash overlap (Å)
2:A:343:HOH:O	2:A:350:HOH:O[2_646]	2.14	0.06
2:A:205:HOH:O	2:A:224:HOH:O[2_746]	2.15	0.05

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	145/154 (94%)	138 (95%)	5 (3%)	2 (1%)	11	3
1	B	138/154 (90%)	133 (96%)	5 (4%)	0	100	100
All	All	283/308 (92%)	271 (96%)	10 (4%)	2 (1%)	22	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ALA
1	A	81	SER

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	126/128 (98%)	125 (99%)	1 (1%)	81	78
1	B	119/128 (93%)	116 (98%)	3 (2%)	47	34
All	All	245/256 (96%)	241 (98%)	4 (2%)	62	54

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	MSE
1	B	81	SER
1	B	93	ASP
1	B	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	153	HIS

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	144/154 (93%)	0.64	16 (11%)	5 4	9, 17, 48, 82	0
1	B	138/154 (89%)	0.74	23 (16%)	1 1	13, 21, 49, 64	0
All	All	282/308 (91%)	0.69	39 (13%)	2 2	9, 19, 49, 82	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	SER	7.5
1	A	105	TRP	6.7
1	A	81	SER	5.6
1	B	10	GLU	5.3
1	B	105	TRP	5.1
1	A	80	SER	5.1
1	B	11	SER	5.0
1	A	10	GLU	4.9
1	A	13	ILE	4.8
1	A	79	ALA	4.7
1	B	106	SER	4.6
1	B	78	ASN	4.5
1	B	133	GLY	4.5
1	B	107	GLY	4.3
1	B	108	SER	4.2
1	A	133	GLY	4.0
1	B	79	ALA	4.0
1	B	81	SER	3.9
1	B	13	ILE	3.8
1	A	106	SER	3.6
1	B	132	SER	3.5
1	A	9	GLU	3.5
1	B	147	LEU	3.5
1	A	132	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLU	3.4
1	B	131	PRO	2.8
1	A	134	ALA	2.7
1	A	78	ASN	2.5
1	B	129	GLY	2.5
1	B	109	ASN	2.5
1	B	80	SER	2.5
1	A	14	ARG	2.4
1	B	134	ALA	2.4
1	B	93	ASP	2.4
1	A	129	GLY	2.3
1	B	77	GLU	2.3
1	B	14	ARG	2.3
1	A	130	SER	2.2
1	B	130	SER	2.1

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.