Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 06:46 PM EDT

PDB ID	:	2GZS
Title	:	Enterobactin Hydolase IroE Complex with DFP
Authors	:	Larsen, N.A.; Walsh, C.T.
Deposited on	:	2006-05-12
Resolution	:	1.40 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 (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:

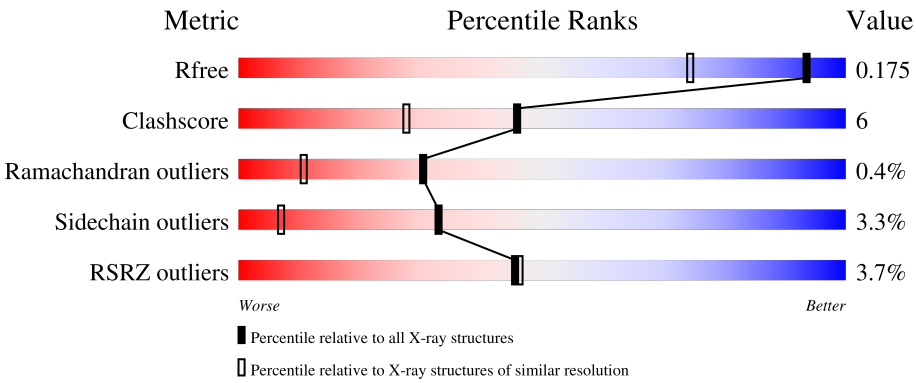
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.40 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}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	278	3% 70% 17% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2161 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.

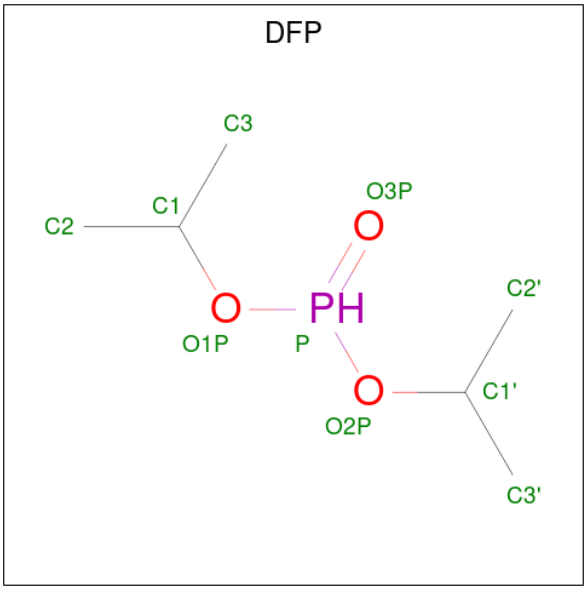
- Molecule 1 is a protein called IroE protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	249	1954	1243	340	366	1	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MSE	MET	modified residue	UNP Q6KD95
A	95	MSE	MET	modified residue	UNP Q6KD95
A	242	MSE	MET	modified residue	UNP Q6KD95
A	290	MSE	MET	modified residue	UNP Q6KD95

- Molecule 2 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: $C_6H_{15}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	10	6	3	1	0	0

- Molecule 3 is water.

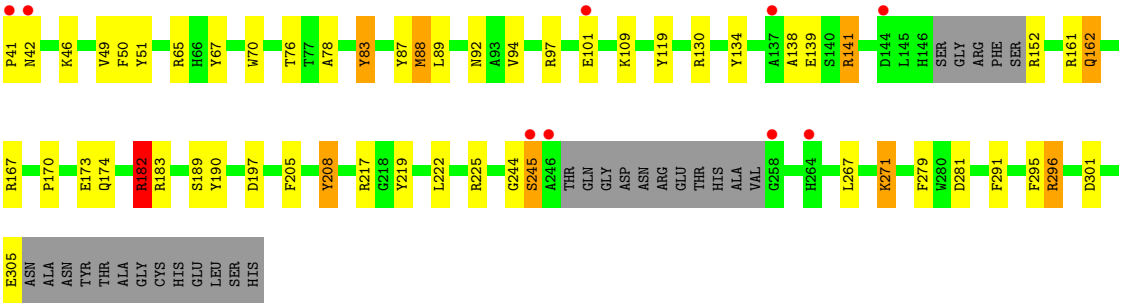
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	197	197	197	0	0

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: IroE protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	36.30Å 38.36Å 44.63Å 113.10° 93.99° 98.08°	Depositor
Resolution (Å)	20.00 – 1.40 20.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.40) 92.7 (20.00-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 1.40Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.174 , 0.186 0.164 , 0.175	Depositor DCC
R_{free} test set	1992 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2161	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.83% 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: DFP

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	0.83	1/1999 (0.1%)	1.80	57/2705 (2.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	SER	CB-OG	6.05	1.50	1.42

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	ARG	NE-CZ-NH1	-15.43	112.59	120.30
1	A	161	ARG	NE-CZ-NH1	-14.03	113.29	120.30
1	A	161	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	A	183	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	217	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	130	ARG	NE-CZ-NH2	10.83	125.71	120.30
1	A	244	GLY	O-C-N	10.77	139.93	122.70
1	A	225	ARG	CD-NE-CZ	10.13	137.78	123.60
1	A	182	ARG	CD-NE-CZ	9.93	137.50	123.60
1	A	88	MSE	CG-SE-CE	-9.69	77.59	98.90
1	A	296	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	83	TYR	CB-CG-CD2	-9.36	115.38	121.00
1	A	167	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	217	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	225	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	97	ARG	CD-NE-CZ	7.98	134.77	123.60
1	A	152	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	301	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	296	ARG	NH1-CZ-NH2	7.24	127.37	119.40
1	A	219	TYR	CB-CG-CD2	7.09	125.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	A	219	TYR	CB-CG-CD1	-6.86	116.89	121.00
1	A	87	TYR	CG-CD2-CE2	-6.78	115.88	121.30
1	A	167	ARG	NH1-CZ-NH2	6.66	126.72	119.40
1	A	65	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	281	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	134	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	A	83	TYR	CD1-CG-CD2	6.42	124.96	117.90
1	A	296	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	139	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	A	197	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	183	ARG	NH1-CZ-NH2	-6.17	112.62	119.40
1	A	244	GLY	CA-C-O	-6.10	109.62	120.60
1	A	130	ARG	CD-NE-CZ	6.06	132.08	123.60
1	A	173	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	190	TYR	CG-CD1-CE1	-5.76	116.69	121.30
1	A	67	TYR	CD1-CE1-CZ	-5.64	114.72	119.80
1	A	51	TYR	CG-CD1-CE1	5.63	125.80	121.30
1	A	167	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	244	GLY	N-CA-C	-5.52	99.31	113.10
1	A	134	TYR	CB-CG-CD1	5.46	124.28	121.00
1	A	83	TYR	CD1-CE1-CZ	-5.45	114.90	119.80
1	A	161	ARG	CD-NE-CZ	5.42	131.18	123.60
1	A	83	TYR	CE1-CZ-CE2	5.41	128.45	119.80
1	A	87	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
1	A	182	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	42	ASN	CA-C-O	-5.28	109.01	120.10
1	A	89	LEU	CB-CG-CD2	5.27	119.95	111.00
1	A	50	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	A	83	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	A	67	TYR	CB-CG-CD2	-5.17	117.89	121.00
1	A	279	PHE	CB-CG-CD1	-5.17	117.18	120.80
1	A	190	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	291	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	A	87	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	101	GLU	CB-CG-CD	5.01	127.72	114.20
1	A	219	TYR	CA-CB-CG	5.01	122.92	113.40

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	1954	0	1904	22	0
2	A	10	0	14	0	0
3	A	197	0	0	6	0
All	All	2161	0	1918	22	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 6.

All (22) 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:A:92:ASN:HD21	1:A:119:TYR:H	1.15	0.87
1:A:141:ARG:HA	1:A:141:ARG:HH11	1.45	0.81
1:A:267:LEU:HB3	1:A:271:LYS:HE2	1.63	0.80
1:A:49:VAL:HG22	3:A:1273:HOH:O	1.82	0.77
1:A:88:MSE:HE1	1:A:94:VAL:HG11	1.68	0.73
1:A:88:MSE:CE	1:A:94:VAL:HG11	2.26	0.65
1:A:170:PRO:O	1:A:174:GLN:HG3	1.97	0.64
1:A:109:LYS:HE2	1:A:305:GLU:HA	1.85	0.58
1:A:41:PRO:HB3	1:A:70:TRP:CZ2	2.40	0.57
1:A:141:ARG:HH11	1:A:141:ARG:CA	2.19	0.54
1:A:76:THR:HA	3:A:1269:HOH:O	2.12	0.49
1:A:78:ALA:HB2	1:A:83:TYR:CZ	2.49	0.48
1:A:141:ARG:HA	1:A:141:ARG:NH1	2.21	0.48
1:A:271:LYS:NZ	3:A:1282:HOH:O	2.49	0.45
1:A:296:ARG:NH1	3:A:1220:HOH:O	2.48	0.45
1:A:205:PHE:HB2	1:A:208:TYR:CZ	2.51	0.45
1:A:162:GLN:HE21	1:A:162:GLN:HB2	1.53	0.45
1:A:267:LEU:O	1:A:271:LYS:HD3	2.18	0.44
1:A:182:ARG:HD2	3:A:1362:HOH:O	2.18	0.43
1:A:138:ALA:HA	1:A:141:ARG:HG3	1.99	0.43
1:A:88:MSE:HB2	1:A:88:MSE:HE3	1.46	0.41
1:A:245:SER:HA	3:A:1298:HOH:O	2.20	0.41

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	243/278 (87%)	236 (97%)	6 (2%)	1 (0%)	30 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	SER

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	210/229 (92%)	203 (97%)	7 (3%)	33 7

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	141	ARG
1	A	162	GLN
1	A	182	ARG
1	A	222	LEU
1	A	271	LYS
1	A	295	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	162	GLN
1	A	284	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
2	DFP	A	1189	1	6,9,9	1.31	1 (16%)	6,11,11	0.74	0

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
2	DFP	A	1189	1	-	0/4/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1189	DFP	O2P-C1'	-2.61	1.41	1.45

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	245/278 (88%)	0.12	9 (3%) 45 46	8, 16, 35, 101	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	PRO	10.4
1	A	246	ALA	5.2
1	A	245	SER	4.9
1	A	258	GLY	4.1
1	A	42	ASN	3.4
1	A	144	ASP	2.6
1	A	101	GLU	2.4
1	A	264	HIS	2.3
1	A	137	ALA	2.0

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)

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	DFP	A	1189	10/10	0.97	0.10	12,18,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.