



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 04:41 pm GMT

PDB ID : 5GGY
Title : X-ray crystal structure of Periplasmic Desferal binding protein FhuD from *Vibrio cholerae*
Authors : Agarwal, S.; Dey, S.; Ghosh, B.; Dasgupta, J.
Deposited on : 2016-06-16
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc29047
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc29047

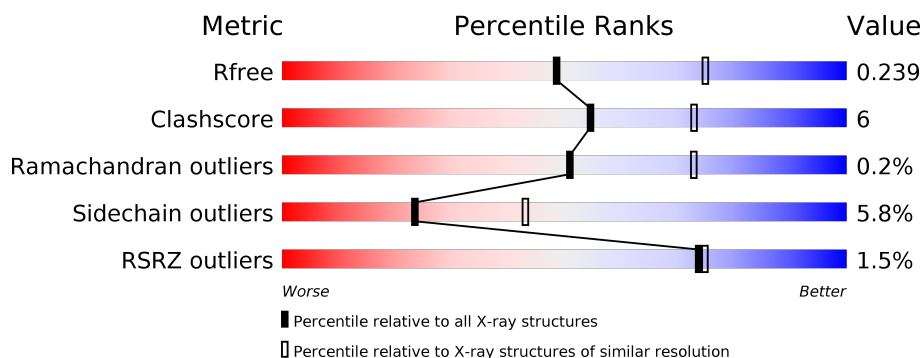
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	282	<div> <div style="display: flex; justify-content: space-between;"> % </div> <div style="display: flex; align-items: center;"> <div style="width: 76%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 17%; height: 10px; background: grey;"></div> <div style="width: 5%; height: 10px; background: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 17% • 5% </div> </div>
1	N	282	<div> <div style="display: flex; justify-content: space-between;"> % </div> <div style="display: flex; align-items: center;"> <div style="width: 77%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 17%; height: 10px; background: grey;"></div> <div style="width: 6%; height: 10px; background: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 77% 17% • 6% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4324 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 Iron(III) ABC transporter, periplasmic iron-compound-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2081	1345	347	385	4			
1	N	266	Total	C	N	O	S	0	0	0
			2071	1340	345	382	4			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	HIS	-	expression tag	UNP A0A0H3AJ03
A	39	HIS	-	expression tag	UNP A0A0H3AJ03
A	40	HIS	-	expression tag	UNP A0A0H3AJ03
A	41	HIS	-	expression tag	UNP A0A0H3AJ03
A	42	HIS	-	expression tag	UNP A0A0H3AJ03
A	43	HIS	-	expression tag	UNP A0A0H3AJ03
A	44	SER	-	expression tag	UNP A0A0H3AJ03
A	45	SER	-	expression tag	UNP A0A0H3AJ03
A	46	GLY	-	expression tag	UNP A0A0H3AJ03
A	47	LEU	-	expression tag	UNP A0A0H3AJ03
A	48	VAL	-	expression tag	UNP A0A0H3AJ03
A	49	PRO	-	expression tag	UNP A0A0H3AJ03
A	50	ARG	-	expression tag	UNP A0A0H3AJ03
A	51	GLY	-	expression tag	UNP A0A0H3AJ03
A	52	SER	-	expression tag	UNP A0A0H3AJ03
A	53	HIS	-	expression tag	UNP A0A0H3AJ03
A	54	MET	-	expression tag	UNP A0A0H3AJ03
N	38	HIS	-	expression tag	UNP A0A0H3AJ03
N	39	HIS	-	expression tag	UNP A0A0H3AJ03
N	40	HIS	-	expression tag	UNP A0A0H3AJ03
N	41	HIS	-	expression tag	UNP A0A0H3AJ03
N	42	HIS	-	expression tag	UNP A0A0H3AJ03
N	43	HIS	-	expression tag	UNP A0A0H3AJ03
N	44	SER	-	expression tag	UNP A0A0H3AJ03

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Chain	Residue	Modelled	Actual	Comment	Reference
N	45	SER	-	expression tag	UNP A0A0H3AJ03
N	46	GLY	-	expression tag	UNP A0A0H3AJ03
N	47	LEU	-	expression tag	UNP A0A0H3AJ03
N	48	VAL	-	expression tag	UNP A0A0H3AJ03
N	49	PRO	-	expression tag	UNP A0A0H3AJ03
N	50	ARG	-	expression tag	UNP A0A0H3AJ03
N	51	GLY	-	expression tag	UNP A0A0H3AJ03
N	52	SER	-	expression tag	UNP A0A0H3AJ03
N	53	HIS	-	expression tag	UNP A0A0H3AJ03
N	54	MET	-	expression tag	UNP A0A0H3AJ03

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	N	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	N	88	Total O 88 88	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.25Å 71.75Å 125.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.50 47.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.32-2.50) 92.3 (47.32-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.190 , 0.240 0.186 , 0.239	Depositor DCC
R_{free} test set	887 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	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	4324	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.23	0/2131	0.41	0/2910
1	N	0.23	0/2121	0.41	0/2897
All	All	0.23	0/4252	0.41	0/5807

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

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	2081	0	2101	26	0
1	N	2071	0	2090	25	0
2	A	1	0	0	1	0
2	N	1	0	0	1	0
3	A	82	0	0	0	0
3	N	88	0	0	0	0
All	All	4324	0	4191	50	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 (50) 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:177:MET:HG3	1:A:302:ARG:HB2	1.78	0.66
1:A:158:LYS:NZ	1:N:91:GLU:OE2	2.30	0.63
1:N:177:MET:HG3	1:N:302:ARG:HB2	1.83	0.60
1:A:55:ARG:NH1	1:A:113:LEU:O	2.35	0.58
1:A:268:LYS:HA	1:A:271:LYS:HE2	1.85	0.58
1:A:143:PHE:HB3	1:A:239:TRP:HA	1.86	0.58
1:N:54:MET:HB3	1:N:116:ASP:HB2	1.87	0.57
1:N:77:ALA:HB3	1:N:80:LEU:HD21	1.88	0.56
1:N:234:GLN:HG2	1:N:242:VAL:HG11	1.87	0.56
1:A:245:ARG:NH2	1:A:248:GLU:OE2	2.40	0.54
1:N:143:PHE:HB3	1:N:239:TRP:HA	1.90	0.53
1:A:201:THR:HG23	1:A:213:TYR:HB2	1.91	0.52
1:N:61:TRP:HB2	2:N:401:CL:CL	2.46	0.52
1:N:234:GLN:HG3	1:N:235:PRO:HD2	1.91	0.51
1:N:148:ASN:OD1	1:N:149:ALA:N	2.43	0.51
1:A:205:ALA:HB3	1:A:209:SER:HB3	1.93	0.51
1:A:145:GLU:CD	1:A:145:GLU:H	2.14	0.50
1:N:258:LEU:HD11	1:N:312:LEU:HG	1.93	0.50
1:A:57:VAL:HG23	1:A:115:PRO:HB3	1.94	0.49
1:A:61:TRP:HB2	2:A:401:CL:CL	2.49	0.49
1:A:180:ARG:NE	1:A:306:GLU:OE2	2.45	0.49
1:A:79:GLU:HG3	1:A:101:THR:HA	1.95	0.49
1:A:77:ALA:HB3	1:A:80:LEU:HD21	1.96	0.48
1:N:214:THR:HG22	1:N:234:GLN:HB3	1.95	0.47
1:A:62:ASP:O	1:A:66:GLN:HG2	2.14	0.47
1:N:150:ALA:HB2	1:N:221:TYR:CD1	2.49	0.47
1:N:58:VAL:HG12	1:N:119:LEU:HB2	1.97	0.47
1:N:246:LEU:HD12	1:N:249:LEU:HD12	1.97	0.47
1:N:79:GLU:HG3	1:N:101:THR:HA	1.96	0.46
1:N:88:VAL:HG12	1:N:89:GLN:HG3	1.98	0.46
1:N:148:ASN:HD21	1:N:217:SER:HA	1.80	0.46
1:N:144:SER:C	1:N:146:GLN:H	2.20	0.45
1:A:270:GLN:HA	1:A:275:TRP:CD1	2.52	0.45
1:A:314:ALA:O	1:A:315:VAL:HG22	2.16	0.44
1:N:247:SER:O	1:N:250:GLN:NE2	2.46	0.44
1:N:221:TYR:CE2	1:N:301:LEU:HD13	2.53	0.43
1:A:69:GLU:OE2	1:A:173:LYS:NZ	2.42	0.43
1:A:58:VAL:HG11	1:A:64:LEU:HB2	2.00	0.42
1:A:142:ASN:OD1	1:A:143:PHE:N	2.45	0.42
1:A:254:GLN:H	1:A:254:GLN:HG2	1.66	0.42
1:N:259:TYR:OH	1:N:266:GLU:OE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:VAL:HG21	1:N:312:LEU:HD11	2.00	0.42
1:N:263:PHE:CZ	1:N:265:GLU:HB2	2.55	0.42
1:A:194:ASP:OD2	1:A:194:ASP:N	2.54	0.41
1:A:271:LYS:HB2	1:A:271:LYS:HE3	1.77	0.41
1:N:87:VAL:O	1:N:89:GLN:N	2.52	0.41
1:A:201:THR:HG21	1:A:219:PRO:HB2	2.03	0.41
1:A:125:GLN:HA	1:A:128:LEU:HG	2.02	0.40
1:N:147:ASP:OD2	1:N:150:ALA:HB3	2.21	0.40
1:A:218:THR:OG1	1:A:219:PRO:HD3	2.21	0.40

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	265/282 (94%)	257 (97%)	7 (3%)	1 (0%)	38	59
1	N	264/282 (94%)	253 (96%)	11 (4%)	0	100	100
All	All	529/564 (94%)	510 (96%)	18 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	VAL

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	225/239 (94%)	209 (93%)	16 (7%)	17	32
1	N	223/239 (93%)	213 (96%)	10 (4%)	32	56
All	All	448/478 (94%)	422 (94%)	26 (6%)	23	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	82	SER
1	A	103	THR
1	A	104	GLU
1	A	117	VAL
1	A	144	SER
1	A	145	GLU
1	A	169	VAL
1	A	172	GLN
1	A	190	HIS
1	A	194	ASP
1	A	201	THR
1	A	202	LEU
1	A	210	VAL
1	A	265	GLU
1	A	276	ARG
1	N	67	VAL
1	N	89	GLN
1	N	91	GLU
1	N	187	SER
1	N	200	VAL
1	N	201	THR
1	N	202	LEU
1	N	245	ARG
1	N	286	VAL
1	N	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	267/282 (94%)	-0.19	4 (1%) 74 75	16, 30, 54, 100	0
1	N	266/282 (94%)	-0.24	4 (1%) 74 75	17, 29, 52, 156	0
All	All	533/564 (94%)	-0.22	8 (1%) 74 75	16, 29, 54, 156	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	150	ALA	10.2
1	N	148	ASN	4.9
1	A	195	THR	4.7
1	N	151	GLN	4.1
1	A	254	GLN	3.4
1	N	254	GLN	2.7
1	A	315	VAL	2.5
1	A	145	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
2	CL	N	401	1/1	0.98	0.05	-2.65	33,33,33,33	0
2	CL	A	401	1/1	0.97	0.07	-3.52	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.