



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 10:22 PM EDT

PDB ID : 9EBX
Title : Chimeric fluorescence biosensor formed from a lactate-binding protein and GFP
Authors : Horwitz, S.M.; Ambarian, J.A.; Waidmann, L.; Davis, K.M.
Deposited on : 2024-11-13
Resolution : 2.42 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

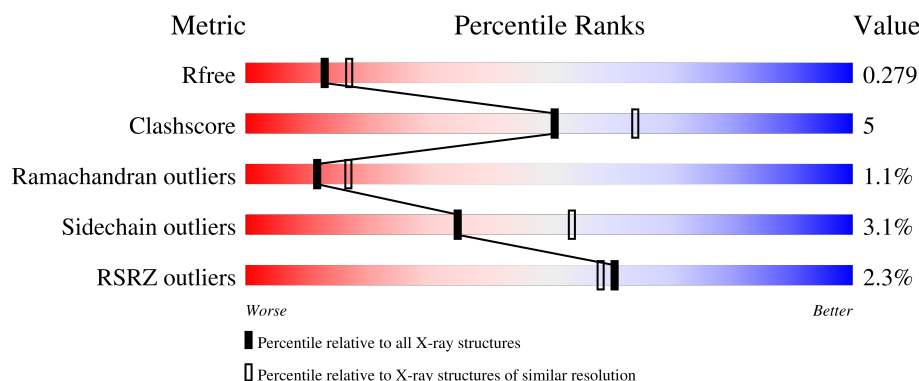
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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 $\leq 5\%$. 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	515	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3528 atoms, of which 2 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 Green fluorescent protein,Methyl-accepting chemotaxis transducer (TlpC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3517	2242	596	666	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P42212
A	2	LYS	-	expression tag	UNP P42212
A	3	HIS	-	expression tag	UNP P42212
A	4	HIS	-	expression tag	UNP P42212
A	5	HIS	-	expression tag	UNP P42212
A	6	HIS	-	expression tag	UNP P42212
A	7	HIS	-	expression tag	UNP P42212
A	8	HIS	-	expression tag	UNP P42212
A	9	HIS	-	expression tag	UNP P42212
A	10	VAL	-	expression tag	UNP P42212
A	73	LEU	PHE	conflict	UNP P42212
A	74	SWG	SER	chromophore	UNP P42212
A	74	SWG	TYR	chromophore	UNP P42212
A	74	SWG	GLY	chromophore	UNP P42212
A	79	ALA	SER	conflict	UNP P42212
A	152	SER	TYR	conflict	UNP P42212
A	153	SER	ASN	conflict	UNP P42212
A	154	GLY	-	linker	UNP P42212
A	155	ARG	-	linker	UNP P42212
A	156	THR	-	linker	UNP P42212
A	157	GLY	-	linker	UNP P42212
A	158	ILE	-	linker	UNP P42212
A	159	ASP	SER	conflict	UNP O24911
A	160	PRO	TYR	conflict	UNP O24911
A	161	PHE	LYS	conflict	UNP O24911
A	162	THR	VAL	conflict	UNP O24911

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	SER	-	linker	UNP O24911
A	423	SER	-	linker	UNP O24911
A	424	HIS	-	linker	UNP O24911
A	425	SER	-	linker	UNP O24911
A	430	THR	MET	conflict	UNP P42212
A	440	ALA	VAL	conflict	UNP P42212
A	452	GLY	SER	conflict	UNP P42212
A	483	LYS	ALA	conflict	UNP P42212
A	508	LEU	HIS	conflict	UNP P42212
A	515	GLN	LYS	conflict	UNP P42212

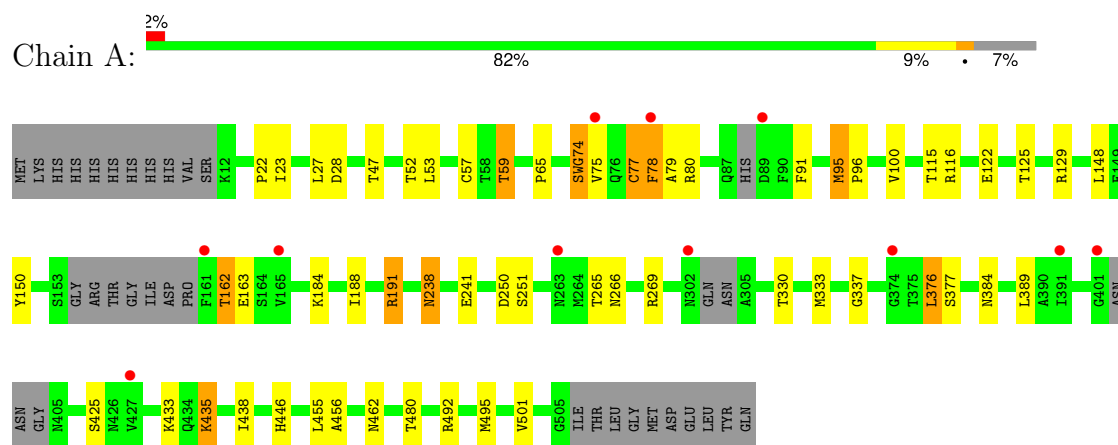
- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	9	Total	H	O	0	0
			11	2	9		

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: Green fluorescent protein, Methyl-accepting chemotaxis transducer (TlpC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	34.35Å 57.98Å 67.32Å 97.82° 91.43° 104.24°	Depositor
Resolution (Å)	46.13 – 2.42 46.13 – 2.42	Depositor EDS
% Data completeness (in resolution range)	86.9 (46.13-2.42) 86.9 (46.13-2.42)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487: 000	Depositor
R, R_{free}	0.234 , 0.280 0.234 , 0.279	Depositor DCC
R_{free} test set	17365 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3528	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% 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: SWG

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	0.32	0/3563	0.56	0/4848

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	A	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	191	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	492	ARG	Sidechain

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	3517	0	3136	34	0
2	A	9	2	0	0	0
All	All	3526	2	3136	34	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 5.

The worst 5 of 34 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:77:CYS:HA	1:A:91:PHE:HB3	1.56	0.85
1:A:74:SWG:C3	1:A:75:VAL:HG23	2.25	0.67
1:A:65:PRO:HG2	1:A:148:LEU:HD13	1.79	0.63
1:A:191:ARG:HH11	1:A:191:ARG:HB2	1.64	0.62
1:A:22:PRO:HB2	1:A:125:THR:HG22	1.84	0.59

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	468/515 (91%)	435 (93%)	28 (6%)	5 (1%)	12 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	LYS
1	A	162	THR
1	A	238	ASN
1	A	78	PHE
1	A	241	GLU

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	321/450 (71%)	311 (97%)	10 (3%)	35 54

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	435	LYS
1	A	501	VAL
1	A	115	THR
1	A	330	THR

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	76	GLN
1	A	475	ASN
1	A	481	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	SWG	A	74	1	22,25,26	1.64	6 (27%)	27,35,37	2.63	13 (48%)

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	SWG	A	74	1	-	2/8/29/30	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	SWG	C1-N3	-3.63	1.31	1.37
1	A	74	SWG	CG-CD2	2.66	1.47	1.41
1	A	74	SWG	CA2-C2	-2.54	1.45	1.48
1	A	74	SWG	CA3-N3	-2.53	1.42	1.47
1	A	74	SWG	CB2-CA2	2.27	1.37	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	SWG	C3-CA3-N3	7.17	128.75	112.43
1	A	74	SWG	CG-CB2-CA2	-4.88	121.45	130.86
1	A	74	SWG	CB2-CA2-C2	4.51	127.82	122.36
1	A	74	SWG	O3-C3-CA3	-4.41	105.60	125.47
1	A	74	SWG	C2-CA2-N2	-3.67	106.32	108.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	74	SWG	C3-CA3-N3-C2
1	A	74	SWG	N1-CA1-CB1-OG1

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	74	SWG	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	480/515 (93%)	0.27	11 (2%) 61 58	45, 67, 97, 113	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	ASN	3.8
1	A	161	PHE	3.3
1	A	75	VAL	3.1
1	A	89	ASP	2.9
1	A	427	VAL	2.6

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	SWG	A	74	23/24	0.92	0.09	42,60,67,74	0

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.