



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 08:25 PM UTC

PDB ID : 9V85 / pdb_00009v85
Title : Superfolder GFP fused gp38 receptor binding domain of bacteriophage PP01
Authors : Kanamaru, S.; Otsuka, Y.
Deposited on : 2025-05-29
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

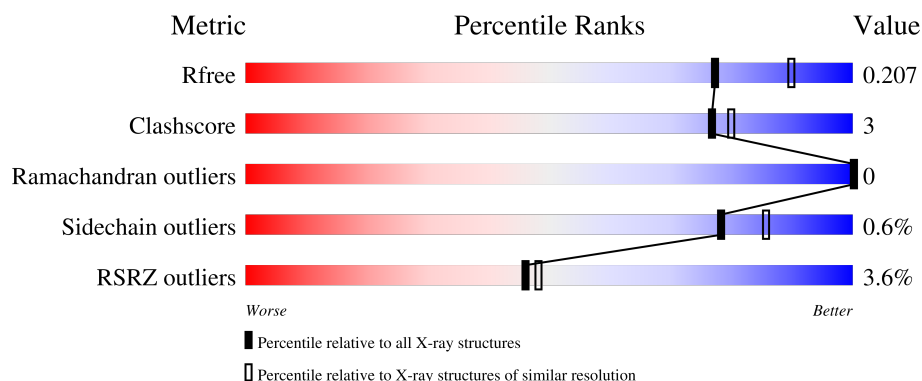
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

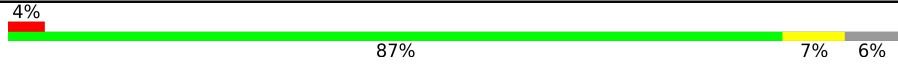
The reported resolution of this entry is 2.10 Å.

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	472	
1	C	472	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5496 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 Green fluorescent protein, Receptor-recognizing protein gp38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3343	2094	593	646	10			
1	C	222	Total	C	N	O	S	0	0	0
			1560	966	287	302	5			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP A0A059PIQ0
A	30	ARG	SER	conflict	UNP A0A059PIQ0
A	65	CRO	THR	chromophore	UNP A0A059PIQ0
A	65	CRO	TYR	chromophore	UNP A0A059PIQ0
A	65	CRO	GLY	chromophore	UNP A0A059PIQ0
A	70	SER	ALA	conflict	UNP A0A059PIQ0
A	78	ARG	GLN	conflict	UNP A0A059PIQ0
A	204	VAL	ALA	conflict	UNP A0A059PIQ0
A	228I	GLU	-	linker	UNP A0A059PIQ0
A	228J	SER	-	linker	UNP A0A059PIQ0
A	228K	ASN	-	linker	UNP A0A059PIQ0
A	228L	SER	-	linker	UNP A0A059PIQ0
A	446	SER	-	expression tag	UNP A0A2Z5WK79
A	447	LYS	-	expression tag	UNP A0A2Z5WK79
A	448	LEU	-	expression tag	UNP A0A2Z5WK79
A	449	ALA	-	expression tag	UNP A0A2Z5WK79
A	450	ALA	-	expression tag	UNP A0A2Z5WK79
A	451	ALA	-	expression tag	UNP A0A2Z5WK79
A	452	LEU	-	expression tag	UNP A0A2Z5WK79
A	453	GLU	-	expression tag	UNP A0A2Z5WK79
A	454	HIS	-	expression tag	UNP A0A2Z5WK79
A	455	HIS	-	expression tag	UNP A0A2Z5WK79
A	456	HIS	-	expression tag	UNP A0A2Z5WK79
A	457	HIS	-	expression tag	UNP A0A2Z5WK79
A	458	HIS	-	expression tag	UNP A0A2Z5WK79

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	HIS	-	expression tag	UNP A0A2Z5WK79
C	-198	SER	-	expression tag	UNP A0A059PIQ0
C	-170	ARG	SER	conflict	UNP A0A059PIQ0
C	-135	CRO	THR	chromophore	UNP A0A059PIQ0
C	-135	CRO	TYR	chromophore	UNP A0A059PIQ0
C	-135	CRO	GLY	chromophore	UNP A0A059PIQ0
C	-130	SER	ALA	conflict	UNP A0A059PIQ0
C	-122	ARG	GLN	conflict	UNP A0A059PIQ0
C	4	VAL	ALA	conflict	UNP A0A059PIQ0
C	37	GLU	-	linker	UNP A0A059PIQ0
C	38	SER	-	linker	UNP A0A059PIQ0
C	39	ASN	-	linker	UNP A0A059PIQ0
C	40	SER	-	linker	UNP A0A059PIQ0
C	260	SER	-	expression tag	UNP A0A2Z5WK79
C	261	LYS	-	expression tag	UNP A0A2Z5WK79
C	262	LEU	-	expression tag	UNP A0A2Z5WK79
C	263	ALA	-	expression tag	UNP A0A2Z5WK79
C	264	ALA	-	expression tag	UNP A0A2Z5WK79
C	265	ALA	-	expression tag	UNP A0A2Z5WK79
C	266	LEU	-	expression tag	UNP A0A2Z5WK79
C	267	GLU	-	expression tag	UNP A0A2Z5WK79
C	268	HIS	-	expression tag	UNP A0A2Z5WK79
C	269	HIS	-	expression tag	UNP A0A2Z5WK79
C	270	HIS	-	expression tag	UNP A0A2Z5WK79
C	271	HIS	-	expression tag	UNP A0A2Z5WK79
C	272	HIS	-	expression tag	UNP A0A2Z5WK79
C	273	HIS	-	expression tag	UNP A0A2Z5WK79

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	342	Total O 342 342	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	249	Total 249	O 249	0	0

- Molecule 1: Green fluorescent protein, Receptor-recognizing protein gp38



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.22Å 172.22Å 79.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 2.10 37.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.88-2.10) 100.0 (37.88-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.175 , 0.208 0.176 , 0.207	Depositor DCC
R_{free} test set	2130 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	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	0.96	EDS
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: CA, CRO

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	0.55	0/3401	0.83	2/4608 (0.0%)
1	C	0.59	0/1602	0.70	0/2177
All	All	0.56	0/5003	0.79	2/6785 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	195	ASP	N-CA-C	-5.62	103.28	110.53
1	A	194	PRO	N-CA-C	5.44	119.56	111.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	GLY	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	3343	0	3171	24	1
1	C	1560	0	1438	4	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	342	0	0	1	0
3	C	249	0	0	0	0
All	All	5496	0	4609	28	1

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 3.

The worst 5 of 28 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:73:PRO:HD2	1:A:76:MET:HE3	1.53	0.89
1:A:5:GLU:OE2	1:A:77:LYS:HD3	1.92	0.70
1:A:73:PRO:HD2	1:A:76:MET:CE	2.27	0.62
1:C:119:TRP:CG	1:C:232:THR:HG1	2.20	0.60
1:C:261:LYS:N	1:C:261:LYS:HD2	2.16	0.59

All (1) 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)
1:A:50:THR:O	1:C:163:ASN:ND2[8_666]	2.14	0.06

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	438/472 (93%)	429 (98%)	9 (2%)	0	100	100
1	C	220/472 (47%)	212 (96%)	8 (4%)	0	100	100
All	All	658/944 (70%)	641 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	339/361 (94%)	337 (99%)	2 (1%)	78	86
1	C	143/361 (40%)	142 (99%)	1 (1%)	76	83
All	All	482/722 (67%)	479 (99%)	3 (1%)	78	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	A	272	ARG
1	C	86	ARG

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	119	ASN
1	A	182	GLN
1	A	347	GLN
1	C	161	GLN
1	C	250	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	CRO	A	65	1	22,23,24	0.55	0	30,32,34	1.14	4 (13%)

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	CRO	A	65	1	-	2/12/31/32	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	CRO	C2-N3-C1	3.10	109.50	108.07
1	A	65	CRO	O2-C2-CA2	-2.79	129.24	131.02
1	A	65	CRO	O3-C3-CA3	-2.29	115.17	125.47
1	A	65	CRO	C2-CA2-N2	-2.15	107.41	108.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRO	C3-CA3-N3-C2
1	A	65	CRO	N3-C1-CA1-CB1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	CRO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	444/472 (94%)	0.26	20 (4%) 38 40	26, 43, 65, 90	0
1	C	222/472 (47%)	-0.49	4 (1%) 67 70	24, 31, 46, 85	0
All	All	666/944 (70%)	0.01	24 (3%) 46 48	24, 38, 63, 90	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	ALA	6.1
1	A	280	TYR	3.8
1	A	230	VAL	3.5
1	A	149	TYR	3.4
1	C	264	ALA	3.3

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	CRO	A	65	22/23	0.96	0.08	34,40,50,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CA	A	501	1/1	0.99	0.08	38,38,38,38	0
2	CA	C	301	1/1	0.99	0.15	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.