



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8DHR / pdb_00008dhr
Title : An ester mutant of SfGFP
Authors : Reddi, R.; Valiyaveetil, F.I.
Deposited on : 2022-06-28
Resolution : 1.75 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

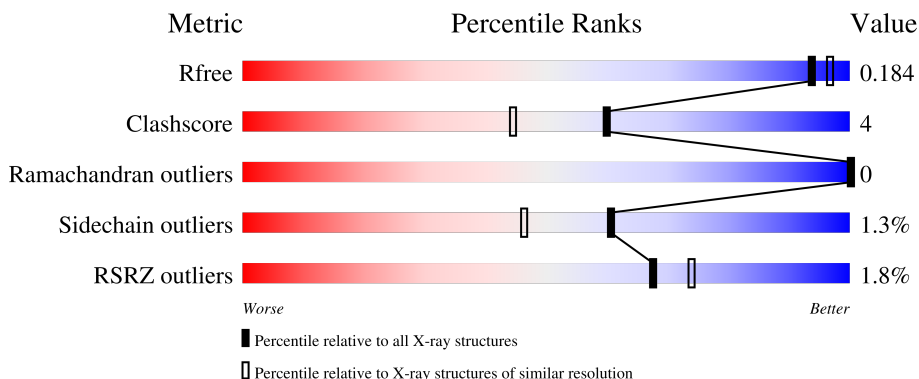
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	244	 2% 83% 9% 7%
1	B	244	 2% 88% 5% 7%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4053 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1789	1132	306	346	5	0	0	0
1	B	226	1785	1129	305	346	5	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	SER	engineered mutation	UNP P42212
A	39	ASN	TYR	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	105	THR	ASN	engineered mutation	UNP P42212
A	145	PHE	TYR	engineered mutation	UNP P42212
A	151	TYF	TYR	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	206	VAL	ALA	engineered mutation	UNP P42212
A	239	GLY	-	expression tag	UNP P42212
A	240	SER	-	expression tag	UNP P42212
A	241	HIS	-	expression tag	UNP P42212
A	242	HIS	-	expression tag	UNP P42212
A	243	HIS	-	expression tag	UNP P42212
A	244	HIS	-	expression tag	UNP P42212
A	245	HIS	-	expression tag	UNP P42212
A	246	HIS	-	expression tag	UNP P42212
B	30	ARG	SER	engineered mutation	UNP P42212
B	39	ASN	TYR	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	105	THR	ASN	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	151	TYF	TYR	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	206	VAL	ALA	engineered mutation	UNP P42212
B	239	GLY	-	expression tag	UNP P42212
B	240	SER	-	expression tag	UNP P42212
B	241	HIS	-	expression tag	UNP P42212
B	242	HIS	-	expression tag	UNP P42212
B	243	HIS	-	expression tag	UNP P42212
B	244	HIS	-	expression tag	UNP P42212
B	245	HIS	-	expression tag	UNP P42212
B	246	HIS	-	expression tag	UNP P42212

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	227	Total O 227 227	0	0
2	B	252	Total O 252 252	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.92Å 37.49Å 91.85Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	44.08 – 1.75 44.08 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.2 (44.08-1.75) 92.4 (44.08-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.67Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.181 , 0.188 0.179 , 0.184	Depositor DCC
R_{free} test set	1343 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4053	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5080e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/1792	0.51	0/2425
1	B	0.29	0/1788	0.51	0/2421
All	All	0.29	0/3580	0.51	0/4846

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 [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	1789	0	1715	18	0
1	B	1785	0	1704	13	0
2	A	227	0	0	0	0
2	B	252	0	0	2	0
All	All	4053	0	3419	30	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 4.

The worst 5 of 30 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:66:CRO:C3	1:B:68:VAL:N	2.42	0.83
1:B:64:LEU:O	1:B:66:CRO:N1	2.19	0.75
1:B:17:GLU:OE1	1:B:122:ARG:NH1	2.24	0.70
1:A:206:VAL:HG13	1:B:206:VAL:HG13	1.79	0.65
1:A:64:LEU:O	1:A:66:CRO:N1	2.31	0.63

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	219/244 (90%)	216 (99%)	3 (1%)	0	100	100
1	B	219/244 (90%)	216 (99%)	3 (1%)	0	100	100
All	All	438/488 (90%)	432 (99%)	6 (1%)	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	192/212 (91%)	188 (98%)	4 (2%)	47	27
1	B	191/212 (90%)	190 (100%)	1 (0%)	81	75
All	All	383/424 (90%)	378 (99%)	5 (1%)	61	46

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	123	ILE
1	A	133	ASP
1	A	230	THR
1	B	230	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	HIS
1	B	184	GLN
1	A	169	HIS
1	B	121	ASN
1	B	135	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](#)

2 non-standard protein/DNA/RNA residues are 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	66	-	22,23,24	2.45	7 (31%)	30,32,34	2.11	10 (33%)
1	CRO	B	66	-	22,23,24	2.37	8 (36%)	30,32,34	3.14	9 (30%)

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	66	-	-	2/12/31/32	0/2/2/2
1	CRO	B	66	-	-	2/12/31/32	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	C1-N2	6.96	1.42	1.32
1	A	66	CRO	C1-N2	6.08	1.41	1.32
1	A	66	CRO	CA2-C2	5.48	1.54	1.48
1	B	66	CRO	C1-N3	4.77	1.45	1.37
1	A	66	CRO	C1-N3	4.08	1.44	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	C3-CA3-N3	9.81	134.75	112.43
1	B	66	CRO	C2-N3-C1	-8.55	104.11	108.07
1	A	66	CRO	O2-C2-CA2	-6.09	127.13	131.02
1	B	66	CRO	CA2-C2-N3	6.03	108.56	103.50
1	B	66	CRO	O2-C2-CA2	-4.23	128.32	131.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C1
1	A	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C3-CA3-N3-C1

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	7	0
1	B	66	CRO	5	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	64:LEU	C	66:CRO	N1	2.79
1	B	64:LEU	C	66:CRO	N1	2.69
1	A	66:CRO	C3	68:VAL	N	2.67
1	B	66:CRO	C3	68:VAL	N	2.42

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	224/244 (91%)	-0.20	4 (1%) 67 74	5, 13, 31, 51	0
1	B	224/244 (91%)	-0.25	4 (1%) 67 74	5, 12, 29, 49	0
All	All	448/488 (91%)	-0.23	8 (1%) 67 74	5, 13, 30, 51	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	3.9
1	B	230	THR	3.8
1	B	133	ASP	2.8
1	B	156	LYS	2.4
1	A	182	TYR	2.3

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	B	66	22/23	0.91	0.08	3,5,15,31	0
1	CRO	A	66	22/23	0.95	0.06	3,5,10,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.