



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1RRX / pdb_00001rrx
Title : Crystallographic Evidence for Isomeric Chromophores in 3-Fluorotyrosyl-Green Fluorescent Protein
Authors : Bae, J.H.; Paramita Pal, P.; Moroder, L.; Huber, R.; Budisa, N.
Deposited on : 2003-12-09
Resolution : 2.10 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 ⓘ 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

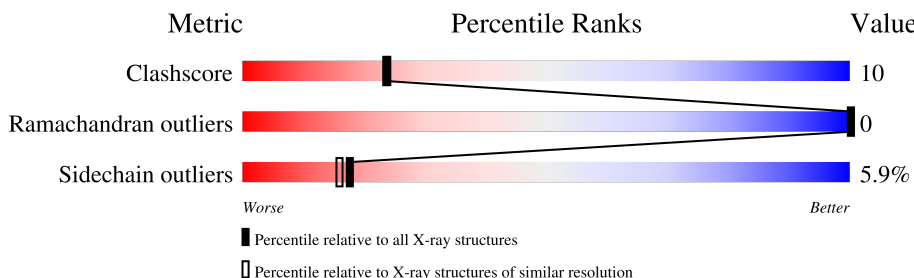
1 Overall quality at a glance

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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	226	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1881 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 SIGF1-GFP fusion protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	F	N	O	S	0	0	0
			1820	1151	10	305	348	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	MFC	THR	chromophore	UNP P42212
A	66	MFC	TYR	chromophore	UNP P42212
A	66	MFC	GLY	chromophore	UNP P42212

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		

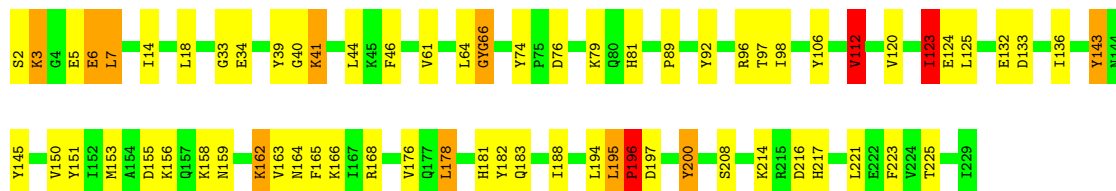
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: SIGF1-GFP fusion protein

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.00Å 62.43Å 70.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.41 – 2.10	Depositor
% Data completeness (in resolution range)	94.9 (41.41-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1881	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.78	2/1702 (0.1%)	1.16	16/2278 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	LEU	C-O	8.64	1.40	1.23
1	A	112	VAL	CA-CB	5.63	1.61	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	LEU	CA-C-O	-9.39	104.83	120.80
1	A	197	ASP	N-CA-C	-8.96	98.97	110.53
1	A	97	THR	N-CA-C	-6.82	97.23	108.76
1	A	41	LYS	N-CA-C	6.66	120.10	109.24
1	A	196	PRO	N-CA-C	6.10	120.57	111.41
1	A	123	ILE	N-CA-C	6.03	117.16	108.48
1	A	64	LEU	N-CA-C	-5.85	94.63	111.00
1	A	195	LEU	CA-C-N	5.62	125.59	120.03
1	A	195	LEU	C-N-CA	5.62	125.59	120.03
1	A	176	VAL	N-CA-C	5.43	116.49	108.45
1	A	123	ILE	CB-CA-C	-5.41	102.56	110.62
1	A	61	VAL	N-CA-C	5.40	116.03	110.36
1	A	162	LYS	N-CA-C	-5.38	100.93	109.59
1	A	216	ASP	N-CA-C	-5.14	102.45	110.10
1	A	221	LEU	N-CA-C	-5.08	100.00	108.34
1	A	188	ILE	N-CA-C	-5.03	106.25	111.58

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	1820	0	1736	36	0
2	A	61	0	0	4	0
All	All	1881	0	1736	36	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 10.

All (36) 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:168:ARG:NH2	1:A:168:ARG:HB2	2.07	0.69
1:A:163:VAL:HB	1:A:183:GLN:HB3	1.80	0.64
1:A:2:SER:HB3	1:A:5:GLU:HB2	1.81	0.61
1:A:41:LYS:HD2	1:A:223:PHE:CE1	2.38	0.58
1:A:168:ARG:HB2	1:A:168:ARG:HH21	1.70	0.56
1:A:6:GLU:H	1:A:6:GLU:CD	2.13	0.55
1:A:18:LEU:C	1:A:18:LEU:HD23	2.32	0.55
1:A:76:ASP:O	1:A:79:LYS:HG2	2.12	0.50
1:A:153:MET:HE2	2:A:241:HOH:O	2.12	0.50
1:A:41:LYS:HD2	1:A:223:PHE:HE1	1.78	0.48
1:A:112:VAL:HA	1:A:120:VAL:O	2.14	0.48
1:A:133:ASP:OD2	1:A:133:ASP:N	2.47	0.48
1:A:143:YOF:OH	1:A:208:SER:O	2.32	0.47
1:A:155:ASP:HB2	1:A:162:LYS:HG3	1.97	0.46
1:A:2:SER:N	2:A:276:HOH:O	2.48	0.46
1:A:14:ILE:HD12	1:A:34:GLU:C	2.41	0.46
1:A:123:ILE:HG22	1:A:124:GLU:N	2.31	0.46
1:A:166:LYS:HD3	1:A:178:LEU:HD21	1.97	0.45
1:A:7:LEU:HD21	1:A:89:PRO:HB3	1.98	0.45
1:A:33:GLY:HA3	1:A:44:LEU:HD13	1.98	0.45
1:A:158:LYS:O	1:A:159:ASN:HB3	2.17	0.44
1:A:164:ASN:ND2	2:A:241:HOH:O	2.51	0.44
1:A:81:HIS:O	1:A:196:PRO:HB3	2.18	0.43
1:A:46:PHE:O	1:A:217:HIS:HB2	2.18	0.43
1:A:156:LYS:HG2	1:A:195:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HD2	2:A:249:HOH:O	2.18	0.43
1:A:150:VAL:HG13	1:A:165:PHE:CD1	2.53	0.43
1:A:2:SER:HB3	1:A:5:GLU:CB	2.50	0.42
1:A:66:MFC:N2	1:A:66:MFC:HD1	2.35	0.42
1:A:3:LYS:HB2	1:A:3:LYS:NZ	2.35	0.41
1:A:125:LEU:C	1:A:125:LEU:HD23	2.45	0.41
1:A:98:ILE:HG12	1:A:181:HIS:CD2	2.55	0.41
1:A:136:ILE:HD12	1:A:136:ILE:N	2.35	0.41
1:A:6:GLU:CD	1:A:6:GLU:N	2.79	0.41
1:A:150:VAL:O	1:A:200:YOF:HA	2.20	0.41
1:A:40:GLY:O	1:A:223:PHE:HA	2.21	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	212/226 (94%)	208 (98%)	4 (2%)	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	188/188 (100%)	177 (94%)	11 (6%)	18	16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	GLU
1	A	7	LEU
1	A	112	VAL
1	A	123	ILE
1	A	132	GLU
1	A	178	LEU
1	A	194	LEU
1	A	196	PRO
1	A	214	LYS
1	A	225	THR

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	135	ASN
1	A	146	ASN
1	A	159	ASN
1	A	164	ASN
1	A	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	YOF	A	106	1	12,13,14	1.33	1 (8%)	10,17,19	1.75	2 (20%)
1	YOF	A	74	1	12,13,14	1.52	2 (16%)	10,17,19	1.71	3 (30%)
1	YOF	A	151	1	12,13,14	0.87	0	10,17,19	1.27	1 (10%)
1	MFC	A	66	1	23,24,25	3.87	13 (56%)	30,34,36	2.71	9 (30%)
1	YOF	A	92	1	12,13,14	1.55	2 (16%)	10,17,19	1.32	1 (10%)
1	YOF	A	200	1	12,13,14	1.01	0	10,17,19	1.11	1 (10%)
1	YOF	A	145	1	12,13,14	1.13	2 (16%)	10,17,19	0.88	0
1	YOF	A	143	1	12,13,14	1.52	2 (16%)	10,17,19	1.45	2 (20%)
1	YOF	A	182	1	12,13,14	1.06	0	10,17,19	1.14	1 (10%)
1	YOF	A	39	1	12,13,14	2.87	1 (8%)	10,17,19	1.00	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
1	YOF	A	106	1	-	2/5/6/8	0/1/1/1
1	YOF	A	74	1	-	2/5/6/8	0/1/1/1
1	YOF	A	151	1	-	0/5/6/8	0/1/1/1
1	MFC	A	66	1	-	1/12/31/32	0/2/2/2
1	YOF	A	92	1	-	0/5/6/8	0/1/1/1
1	YOF	A	200	1	-	0/5/6/8	0/1/1/1
1	YOF	A	145	1	-	2/5/6/8	0/1/1/1
1	YOF	A	143	1	-	0/5/6/8	0/1/1/1
1	YOF	A	182	1	-	0/5/6/8	0/1/1/1
1	YOF	A	39	1	-	1/5/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	YOF	CB-CA	9.62	1.73	1.53
1	A	66	MFC	CB2-CA2	8.45	1.43	1.35
1	A	66	MFC	CD2-CG2	7.15	1.52	1.39
1	A	66	MFC	CE1-CZ	7.13	1.51	1.39
1	A	66	MFC	C1-N2	5.91	1.40	1.32
1	A	66	MFC	CE1-CD1	5.60	1.47	1.38
1	A	66	MFC	CD2-CE2	4.40	1.45	1.37
1	A	66	MFC	O2-C2	-3.95	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	MFC	CA2-C2	-3.89	1.44	1.48
1	A	66	MFC	OH-CZ	-3.82	1.28	1.36
1	A	74	YOF	CE2-CD2	3.75	1.44	1.38
1	A	143	YOF	CD1-CE1	3.33	1.43	1.37
1	A	66	MFC	CZ-CE2	3.23	1.41	1.39
1	A	92	YOF	CD1-CE1	3.05	1.42	1.37
1	A	143	YOF	CE2-CD2	3.03	1.43	1.38
1	A	66	MFC	CA3-C3	-2.93	1.38	1.49
1	A	66	MFC	O3-C3	2.72	1.35	1.20
1	A	66	MFC	CD1-CG2	2.61	1.44	1.39
1	A	106	YOF	CZ-CE1	-2.46	1.37	1.39
1	A	74	YOF	CD1-CE1	2.42	1.41	1.37
1	A	145	YOF	F-CE1	-2.39	1.29	1.35
1	A	92	YOF	CZ-CE1	2.23	1.41	1.39
1	A	145	YOF	CZ-CE1	2.07	1.40	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	MFC	C2-N3-C1	8.10	111.81	108.07
1	A	66	MFC	N3-C1-N2	-5.45	107.19	111.48
1	A	66	MFC	O2-C2-CA2	-5.34	127.61	131.02
1	A	66	MFC	C3-CA3-N3	4.62	122.95	112.43
1	A	106	YOF	CG-CD1-CE1	4.57	122.36	119.37
1	A	66	MFC	C1-CA1-N1	-3.84	102.91	109.78
1	A	143	YOF	CG-CD1-CE1	3.69	121.78	119.37
1	A	66	MFC	CG2-CD2-CE2	3.61	122.08	119.27
1	A	92	YOF	CG-CD1-CE1	3.57	121.71	119.37
1	A	151	YOF	CG-CD1-CE1	3.49	121.66	119.37
1	A	66	MFC	CA1-C1-N3	3.17	128.44	124.69
1	A	182	YOF	CG-CD1-CE1	3.15	121.44	119.37
1	A	66	MFC	CA2-N2-C1	3.09	108.22	105.80
1	A	74	YOF	CG-CD1-CE1	3.07	121.38	119.37
1	A	74	YOF	CD2-CE2-CZ	-2.96	117.54	120.50
1	A	200	YOF	CG-CD1-CE1	2.81	121.21	119.37
1	A	66	MFC	CB2-CA2-C2	2.51	125.40	122.36
1	A	74	YOF	F-CE1-CZ	2.46	122.76	118.34
1	A	143	YOF	F-CE1-CZ	2.25	122.39	118.34
1	A	106	YOF	CD2-CE2-CZ	-2.13	118.36	120.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	39	YOF	O-C-CA-CB
1	A	74	YOF	C-CA-CB-CG
1	A	145	YOF	N-CA-CB-CG
1	A	145	YOF	C-CA-CB-CG
1	A	106	YOF	CA-CB-CG-CD1
1	A	106	YOF	CA-CB-CG-CD2
1	A	74	YOF	N-CA-CB-CG
1	A	66	MFC	N3-C1-CA1-CB1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	MFC	1	0
1	A	200	YOF	1	0
1	A	143	YOF	1	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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	66:MFC	C3	68:VAL	N	1.62

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.