



# Full wwPDB X-ray Structure Validation Report

Jun 12, 2014 – 08:36 PM EDT

PDB ID : 4OGS  
Title : Crystal structure of GFP S205A/T203V at 2.2 Å resolution  
Authors : Remington, S.J.; Saif, M.  
Deposited on : 2014-01-16  
Resolution : 2.21 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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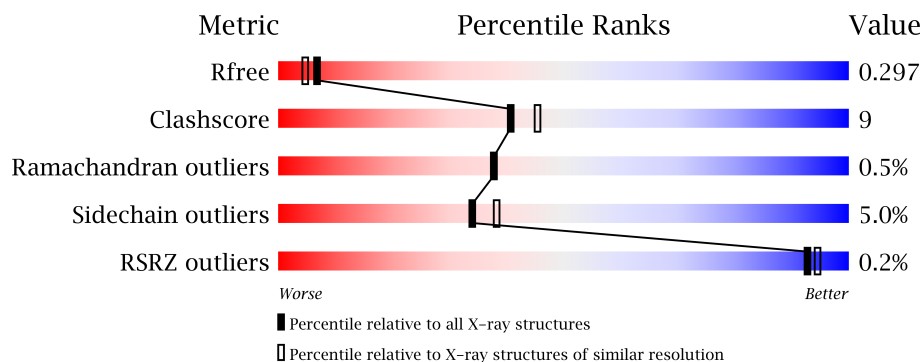
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance



The reported resolution of this entry is 2.21 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))
$R_{free}$	66092	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	
1	B	236	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3678 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	226	Total	C	N	O	S	0	1	0
			1770	1129	297	338	6			
1	B	226	Total	C	N	O	S	0	0	0
			1752	1119	294	333	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	203	VAL	THR	ENGINEERED MUTATION	UNP P42212
A	205	ALA	SER	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	203	VAL	THR	ENGINEERED MUTATION	UNP P42212
B	205	ALA	SER	ENGINEERED MUTATION	UNP P42212

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		

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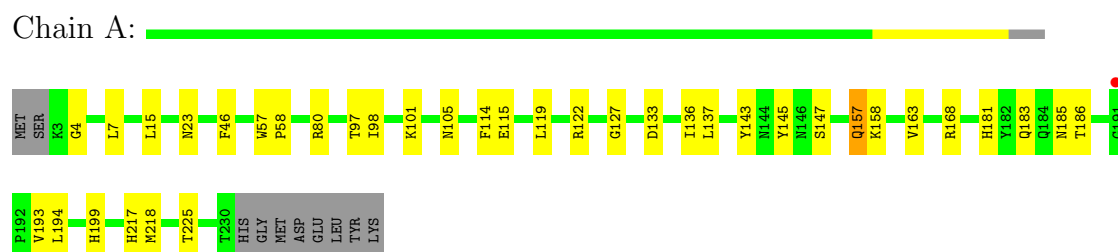
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	66	Total	O	0	0
			66	66		

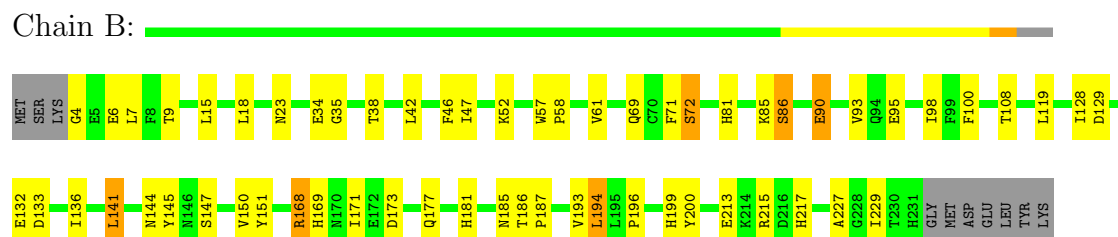
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



- Molecule 1: Green fluorescent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.61Å 86.61Å 119.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.21 14.98 – 2.22	Depositor EDS
% Data completeness (in resolution range)	65.5 (15.00-2.21) 66.0 (14.98-2.22)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.181 , 0.306 0.183 , 0.297	Depositor DCC
$R_{free}$ test set	773 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15202 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRO, 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	0.71	0/1793	0.86	0/2431
1	B	0.74	1/1772 (0.1%)	0.80	1/2404 (0.0%)
All	All	0.72	1/3565 (0.0%)	0.83	1/4835 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	GLU	CB-CG	16.16	1.82	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1645	26	1
1	B	1752	0	1632	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	2	0
3	A	89	0	0	9	2
3	B	66	0	0	3	1
All	All	3678	0	3277	63	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:90:GLU:CB	1:B:90:GLU:CG	1.82	1.54
1:B:168:ARG:NH1	2:B:301:CL:CL	2.44	0.86
1:A:4:GLY:HA2	1:A:7:LEU:HD13	1.62	0.81
1:A:157:GLN:CG	3:A:331:HOH:O	2.29	0.80
1:A:80:ARG:HG2	3:A:334:HOH:O	1.88	0.74
1:B:52:LYS:HB3	3:B:426:HOH:O	1.88	0.72
1:A:199:HIS:CD2	3:A:328:HOH:O	2.44	0.70
1:A:157:GLN:HG2	3:A:331:HOH:O	1.92	0.69
1:B:23:ASN:OD1	1:B:128:ILE:HD12	1.93	0.67
1:B:128:ILE:O	1:B:129:ASP:HB2	1.97	0.64
1:B:58:PRO:HA	1:B:61:VAL:HG23	1.81	0.62
1:B:47:ILE:CB	3:B:458:HOH:O	2.48	0.60
1:A:158:LYS:HG3	3:A:330:HOH:O	1.99	0.60
1:A:157:GLN:HG3	3:A:331:HOH:O	2.00	0.58
1:A:168:ARG:NH1	2:B:301:CL:CL	2.74	0.58
1:B:199:HIS:HB2	1:B:227:ALA:O	2.05	0.56
1:A:23:ASN:ND2	1:A:137:LEU:HD11	2.20	0.56
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.88	0.55
1:B:147:SER:O	1:B:168:ARG:NH2	2.38	0.54
1:B:132:GLU:CB	3:B:424:HOH:O	2.57	0.52
1:A:57:TRP:N	1:A:58:PRO:CD	2.73	0.52
1:A:7:LEU:HD23	1:A:114:PHE:CE2	2.46	0.51
1:B:150:VAL:O	1:B:200:TYR:HB2	2.10	0.50
1:B:90:GLU:H	1:B:90:GLU:CG	2.25	0.49
1:A:46:PHE:O	1:A:217:HIS:HA	2.13	0.49
1:A:119:LEU:C	1:A:119:LEU:HD13	2.33	0.49
1:B:187:PRO:HG3	1:B:193:VAL:HG11	1.94	0.49
1:A:158:LYS:CD	3:A:330:HOH:O	2.61	0.48
1:A:163:VAL:HB	1:A:183:GLN:HB3	1.96	0.48
1:B:69:GLN:O	1:B:72:SER:OG	2.31	0.48
1:A:7:LEU:HD23	1:A:114:PHE:CD2	2.47	0.48
1:B:100:PHE:CD2	1:B:136:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:LYS:CG	3:A:330:HOH:O	2.60	0.48
1:A:80:ARG:HA	1:A:194:LEU:HD21	1.94	0.48
1:B:151:TYR:CD1	1:B:200:TYR:HB3	2.49	0.48
1:A:133:ASP:HA	3:A:320:HOH:O	2.13	0.48
1:A:136:ILE:HD12	1:A:136:ILE:N	2.30	0.47
1:B:81:HIS:O	1:B:196:PRO:HB3	2.14	0.47
1:B:119:LEU:C	1:B:119:LEU:HD13	2.36	0.45
1:B:86:SER:HB3	1:B:194:LEU:HD22	1.99	0.45
1:B:199:HIS:HB3	1:B:229:ILE:HD12	1.98	0.45
1:A:143:TYR:OH	1:A:218:MET:HG3	2.16	0.45
1:B:90:GLU:CG	1:B:90:GLU:CA	2.84	0.45
1:B:35:GLY:HA3	1:B:71:PHE:CD1	2.53	0.44
1:B:85:LYS:O	1:B:86:SER:C	2.56	0.44
1:B:93:VAL:O	1:B:185:ASN:HA	2.18	0.43
1:A:105:ASN:O	1:A:127:GLY:HA2	2.18	0.43
1:B:133:ASP:OD1	1:B:133:ASP:N	2.52	0.42
1:B:213:GLU:OE2	1:B:215:ARG:HB2	2.19	0.42
1:B:46:PHE:O	1:B:217:HIS:HA	2.19	0.42
1:A:4:GLY:O	1:A:7:LEU:HB2	2.20	0.42
1:A:147:SER:OG	1:B:144:ASN:HB2	2.19	0.42
1:B:18:LEU:HD23	1:B:18:LEU:O	2.20	0.42
1:B:95:GLU:HA	1:B:108:THR:O	2.20	0.41
1:B:57:TRP:N	1:B:58:PRO:CD	2.83	0.41
1:B:42:LEU:HD21	1:B:71:PHE:CB	2.51	0.41
1:B:4:GLY:O	1:B:7:LEU:HB2	2.20	0.41
1:B:141:LEU:CD1	1:B:169:HIS:HB3	2.50	0.41
1:B:98:ILE:HG23	1:B:181:HIS:CE1	2.56	0.41
1:B:42:LEU:HD21	1:B:71:PHE:CG	2.56	0.41
1:A:98:ILE:HG12	1:A:181:HIS:CD2	2.55	0.40
1:B:90:GLU:N	1:B:90:GLU:CG	2.85	0.40
1:A:115:GLU:OE1	1:A:122:ARG:NH2	2.53	0.40

All (2) 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	Distance(Å)	Clash(Å)
3:A:305:HOH:O	3:B:425:HOH:O[6_555]	2.06	0.14
1:A:101:LYS:CG	3:A:318:HOH:O[7_555]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	222/236 (94%)	211 (95%)	10 (4%)	1 (0%)	38	38
1	B	221/236 (94%)	205 (93%)	15 (7%)	1 (0%)	38	38
All	All	443/472 (94%)	416 (94%)	25 (6%)	2 (0%)	38	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL
1	B	86	SER

### 5.3.2 Protein sidechains ⓘ

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	180/205 (88%)	173 (96%)	7 (4%)	43	52
1	B	179/205 (87%)	168 (94%)	11 (6%)	26	28
All	All	359/410 (88%)	341 (95%)	18 (5%)	34	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	97	THR
1	A	145	TYR
1	A	157	GLN
1	A	185	ASN
1	A	186	THR
1	A	225	THR

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Mol	Chain	Res	Type
1	B	6	GLU
1	B	9	THR
1	B	15	LEU
1	B	34	GLU
1	B	38	THR
1	B	72	SER
1	B	141	LEU
1	B	145	TYR
1	B	173	ASP
1	B	186	THR
1	B	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	170	ASN
1	B	170	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/236 (95%)	-0.49	1 (0%) 90 92	39, 54, 82, 117	0
1	B	226/236 (95%)	-0.32	0 100 100	42, 63, 87, 116	0
All	All	452/472 (95%)	-0.41	1 (0%) 93 94	39, 57, 87, 117	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	2.1

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

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRO	A	66	21/23	0.08	-0.70	41,45,48,53	0
1	CRO	B	66	21/23	0.08	-1.11	48,53,59,62	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	B	301	1/1	0.02	-8.37	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.