

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 16, 2023 – 09:30 PM EDT

96A Q183R
J.; Tainer, J.A.; Get-

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 (i) 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 (1)) were used in the production of this report:

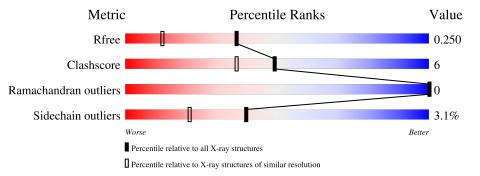
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	228	82%	15%	••



#### 2AWM

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2102 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		
1	А	225	Total 1792	C 1137	N 303	0 347	${ m S}{ m 5}$	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	ALA	-	expression tag	UNP P42212
А	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
А	66	CRO	TYR	chromophore	UNP P42212
А	66	CRO	GLY	chromophore	UNP P42212
А	96	ALA	ARG	engineered mutation	UNP P42212
А	99	SER	PHE	engineered mutation	UNP P42212
А	153	THR	MET	engineered mutation	UNP P42212
А	163	ALA	VAL	engineered mutation	UNP P42212
А	183	ARG	GLN	engineered mutation	UNP P42212

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

M	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
2		А	2	Total Mg 2 2	0	0

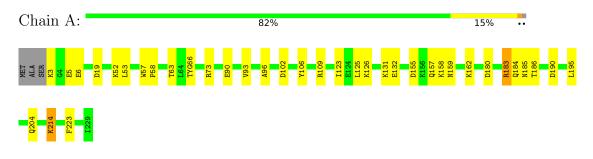
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	А	308	Total ( 308 3	O 08	0	0



# 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.



 $\bullet$  Molecule 1: green fluorescent protein



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	51.51Å 62.34Å 71.26Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.70	Depositor
Resolution (A)	30.93 - 1.70	EDS
% Data completeness	91.1 (50.00-1.70)	Depositor
(in resolution range)	91.1 (30.93 - 1.70)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.06	Depositor
$< I/\sigma(I) > 1$	$7.20 (at 1.70 \text{\AA})$	Xtriage
Refinement program	SHELXL-97	Depositor
B B.	0.164 , $0.223$	Depositor
$R, R_{free}$	0.228 , $0.250$	DCC
$R_{free}$ test set	1145 reflections $(4.84\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	1.4	Xtriage
Anisotropy	2.280	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 71.0	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.30, \langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2102	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, MG

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).

Mal	Chain	Bond lengths		Bo	ond angles
Mol Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.41	0/1809	1.03	4/2444~(0.2%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	А	183	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	А	109	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	А	106	TYR	CB-CG-CD1	6.29	124.78	121.00
1	А	73	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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	А	1792	0	1739	21	0
2	А	2	0	0	0	0
3	А	308	0	0	6	3
All	All	2102	0	1739	21	3

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 6.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:102:ASP:O	1:A:131:LYS:NZ	1.95	0.97	
1:A:180:ASP:OD1	3:A:1277:HOH:O	1.95	0.85	
1:A:132:GLU:O	3:A:1232:HOH:O	1.97	0.81	
1:A:19:ASP:OD2	3:A:1037:HOH:O	2.05	0.74	
1:A:162:LYS:HD2	3:A:1223:HOH:O	2.06	0.54	

The worst 5 of 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

All (3) 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)
3:A:1263:HOH:O	3:A:1309:HOH:O[4_555]	1.78	0.42
3:A:1197:HOH:O	3:A:1296:HOH:O[3_645]	1.87	0.33
3:A:1040:HOH:O	3:A:1286:HOH:O[2_665]	2.13	0.07

## 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	А	220/228~(96%)	218 (99%)	2(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	А	194/196~(99%)	188~(97%)	6 (3%)	40 21	

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	157	GLN
1	А	190	ASP
1	А	214	LYS
1	А	52	LYS
1	А	5	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	А	164	ASN
1	А	204	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 Ch	Chain	n Res	Res Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
1	CRO	А	66	1	23,23,24	2.15	6 (26%)	30,32,34	1.86	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	А	66	1	-	0/12/31/32	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	66	CRO	CA2-C2	-7.42	1.41	1.48
1	А	66	CRO	CB2-CA2	3.85	1.38	1.35
1	А	66	CRO	CG2-CB2	-2.48	1.42	1.46
1	А	66	CRO	CE1-CD1	2.46	1.43	1.38
1	А	66	CRO	CA3-N3	-2.28	1.42	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	66	CRO	CG2-CB2-CA2	4.03	134.88	129.94
1	А	66	CRO	CB2-CA2-N2	-3.91	123.40	128.83
1	А	66	CRO	CB2-CA2-C2	3.17	126.06	122.28
1	А	66	CRO	O3-C3-CA3	-3.15	116.87	126.39
1	А	66	CRO	CD1-CE1-CZ	-2.60	117.03	119.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

