Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 05:07 am GMT

PDB ID	:	4UTS
Title	:	Room temperature crystal structure of the fast switching M159T mutant of fluorescent protein Dronpa
Authors	:	Kaucikas, M.; Fitzpatrick, A.; Bryan, E.; Struve, A.; Henning, R.; Kosheleva, I.; Srajer, V.; van Thor, J.J.
Deposited on	:	2014-07-22
Resolution	:	2.03 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 (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 (i)) were used in the production of this report:

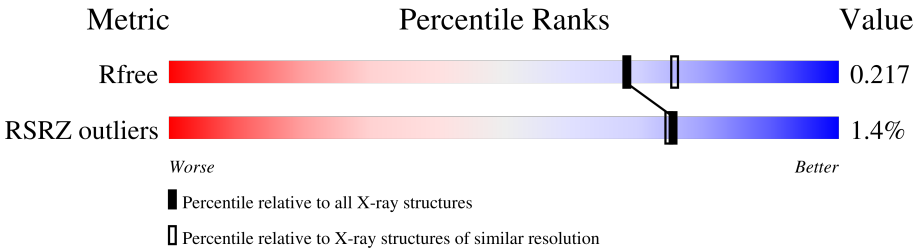
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	130704	10434 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7146 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 FLUORESCENT PROTEIN DRONPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	B	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	C	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	D	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GYC	CYS	chromophore	UNP Q5TLG6
A	63	GYC	TYR	chromophore	UNP Q5TLG6
A	63	GYC	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
B	63	GYC	CYS	chromophore	UNP Q5TLG6
B	63	GYC	TYR	chromophore	UNP Q5TLG6
B	63	GYC	GLY	chromophore	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
C	63	GYC	CYS	chromophore	UNP Q5TLG6
C	63	GYC	TYR	chromophore	UNP Q5TLG6
C	63	GYC	GLY	chromophore	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
D	63	GYC	CYS	chromophore	UNP Q5TLG6
D	63	GYC	TYR	chromophore	UNP Q5TLG6
D	63	GYC	GLY	chromophore	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	55	Total O 55 55	0	0
2	C	62	Total O 62 62	0	0
2	D	56	Total O 56 56	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.66Å 111.14Å 117.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.63 – 2.03 55.57 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.8 (55.63-2.03) 98.8 (55.57-2.03)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.213 0.181 , 0.217	Depositor DCC
R_{free} test set	3241 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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4.2 Too-close contacts

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4.3 Torsion angles

4.3.1 Protein backbone

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4.3.2 Protein sidechains

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4.3.3 RNA

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

4 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	GYC	D	63	1	22,22,23	3.94	10 (45%)	26,30,32	3.96	11 (42%)
1	GYC	C	63	1	22,22,23	2.80	5 (22%)	26,30,32	2.57	10 (38%)
1	GYC	A	63	1	22,22,23	4.35	8 (36%)	26,30,32	3.71	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GYC	B	63	1	22,22,23	2.86	9 (40%)	26,30,32	3.14	10 (38%)

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	GYC	D	63	1	-	2/9/29/30	0/2/2/2
1	GYC	C	63	1	-	3/9/29/30	0/2/2/2
1	GYC	A	63	1	-	2/9/29/30	0/2/2/2
1	GYC	B	63	1	-	2/9/29/30	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB2-CA2	15.64	1.48	1.35
1	D	63	GYC	CB2-CA2	14.06	1.46	1.35
1	B	63	GYC	CB2-CA2	9.81	1.43	1.35
1	C	63	GYC	CB2-CA2	9.14	1.42	1.35
1	A	63	GYC	CB1-CA1	-7.61	1.44	1.53
1	D	63	GYC	CA2-C2	-6.57	1.42	1.48
1	A	63	GYC	C1-N2	5.69	1.40	1.32
1	D	63	GYC	C1-N2	5.38	1.40	1.32
1	A	63	GYC	CA2-C2	-4.97	1.43	1.48
1	C	63	GYC	CA2-C2	-4.71	1.44	1.48
1	C	63	GYC	C1-N2	4.61	1.39	1.32
1	D	63	GYC	CB1-CA1	-4.11	1.48	1.53
1	C	63	GYC	CB1-CA1	-4.10	1.48	1.53
1	B	63	GYC	CA2-C2	-3.92	1.44	1.48
1	A	63	GYC	O2-C2	3.83	1.31	1.23
1	B	63	GYC	C2-N3	-3.65	1.31	1.39
1	A	63	GYC	CB1-SG1	-3.61	1.73	1.81
1	C	63	GYC	O2-C2	3.46	1.30	1.23
1	B	63	GYC	CB1-CA1	-3.43	1.49	1.53
1	D	63	GYC	O2-C2	3.32	1.30	1.23
1	D	63	GYC	CA1-C1	-3.15	1.44	1.51
1	B	63	GYC	C1-N2	3.06	1.36	1.32
1	D	63	GYC	C2-N3	-3.03	1.32	1.39
1	B	63	GYC	CA2-N2	-2.79	1.32	1.38
1	D	63	GYC	C1-N3	2.76	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CA2-N2	-2.47	1.33	1.38
1	A	63	GYC	C1-N3	2.33	1.41	1.37
1	B	63	GYC	O2-C2	2.33	1.28	1.23
1	D	63	GYC	CA2-N2	-2.22	1.33	1.38
1	B	63	GYC	CA1-C1	-2.15	1.46	1.51
1	D	63	GYC	CA1-N1	-2.08	1.38	1.48
1	B	63	GYC	CA3-N3	-2.02	1.43	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	GYC	O2-C2-CA2	-12.03	124.21	130.96
1	D	63	GYC	O2-C2-CA2	-11.70	124.39	130.96
1	D	63	GYC	CA2-C2-N3	11.61	108.86	103.37
1	A	63	GYC	CA2-C2-N3	9.66	107.94	103.37
1	B	63	GYC	O2-C2-CA2	-8.75	126.05	130.96
1	B	63	GYC	CA2-C2-N3	7.75	107.03	103.37
1	C	63	GYC	CB2-CA2-N2	-6.05	120.43	128.83
1	C	63	GYC	CB2-CA2-C2	5.95	129.38	122.28
1	A	63	GYC	N3-C1-N2	-5.81	107.43	111.45
1	B	63	GYC	CB2-CA2-C2	5.79	129.19	122.28
1	D	63	GYC	CB2-CA2-C2	5.77	129.16	122.28
1	D	63	GYC	N3-C1-N2	-5.69	107.51	111.45
1	C	63	GYC	O2-C2-CA2	-5.16	128.06	130.96
1	D	63	GYC	CB2-CA2-N2	-4.68	122.33	128.83
1	B	63	GYC	CB2-CA2-N2	-4.54	122.53	128.83
1	A	63	GYC	CB2-CA2-C2	4.19	127.28	122.28
1	A	63	GYC	CA2-N2-C1	3.97	108.69	105.77
1	C	63	GYC	CA2-C2-N3	3.94	105.23	103.37
1	A	63	GYC	CA1-C1-N3	3.48	129.38	124.85
1	C	63	GYC	N3-C1-N2	-3.12	109.29	111.45
1	A	63	GYC	CB2-CA2-N2	-3.08	124.55	128.83
1	C	63	GYC	C2-N3-C1	2.91	109.44	107.97
1	B	63	GYC	CA3-N3-C1	-2.90	123.69	127.16
1	C	63	GYC	CD1-CG2-CB2	-2.89	111.39	121.22
1	A	63	GYC	O3-C3-CA3	-2.88	117.68	126.39
1	B	63	GYC	CA1-C1-N3	2.87	128.59	124.85
1	B	63	GYC	N3-C1-N2	-2.82	109.50	111.45
1	B	63	GYC	CD2-CE2-CZ	2.74	122.88	119.88
1	D	63	GYC	O3-C3-CA3	-2.60	118.53	126.39
1	D	63	GYC	CA2-N2-C1	2.58	107.68	105.77
1	B	63	GYC	CD1-CG2-CB2	-2.48	112.77	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	GYC	CD1-CG2-CB2	-2.45	112.86	121.22
1	C	63	GYC	CD1-CE1-CZ	2.44	122.55	119.88
1	D	63	GYC	CA1-C1-N2	2.43	128.46	123.56
1	D	63	GYC	CE2-CD2-CG2	-2.39	118.13	121.25
1	C	63	GYC	CD2-CG2-CB2	2.37	129.28	121.22
1	B	63	GYC	CE2-CD2-CG2	-2.31	118.23	121.25
1	C	63	GYC	CE1-CD1-CG2	-2.19	118.39	121.25
1	D	63	GYC	CA1-CB1-SG1	2.04	118.84	114.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	GYC	C3-CA3-N3-C2
1	B	63	GYC	C3-CA3-N3-C1
1	B	63	GYC	C3-CA3-N3-C2
1	C	63	GYC	C3-CA3-N3-C2
1	D	63	GYC	C3-CA3-N3-C1
1	D	63	GYC	C3-CA3-N3-C2
1	A	63	GYC	C3-CA3-N3-C1
1	C	63	GYC	C3-CA3-N3-C1
1	C	63	GYC	N1-CA1-CB1-SG1

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	63:GYC	C3	65:ASN	N	1.79
1	A	63:GYC	C3	65:ASN	N	1.66
1	B	63:GYC	C3	65:ASN	N	1.61

5 Fit of model and data

5.1 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^{th} 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	213/214 (99%)	-0.00	4 (1%) 66 66	19, 34, 71, 126	0
1	B	213/214 (99%)	-0.12	5 (2%) 60 59	22, 39, 64, 87	0
1	C	213/214 (99%)	-0.43	0 100 100	17, 27, 46, 80	0
1	D	213/214 (99%)	-0.23	3 (1%) 75 74	17, 31, 58, 88	0
All	All	852/856 (99%)	-0.19	12 (1%) 75 74	17, 33, 63, 126	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	LEU	3.6
1	A	2	SER	3.5
1	B	212	HIS	2.9
1	A	3	VAL	2.8
1	B	2	SER	2.8
1	D	188	TYR	2.7
1	D	2	SER	2.5
1	B	3	VAL	2.4
1	D	73	GLU	2.3
1	B	4	ILE	2.2
1	A	83	PHE	2.1
1	B	194	HIS	2.1

5.2 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. The B-factors column lists the minimum, median, 95^{th} 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	GYC	A	63	21/22	0.97	0.11	22,24,29,31	0
1	GYC	B	63	21/22	0.97	0.14	29,33,37,45	0
1	GYC	C	63	21/22	0.97	0.09	17,19,24,27	0
1	GYC	D	63	21/22	0.97	0.10	20,23,29,30	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such residues in this entry.