



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2021 – 02:18 PM EDT

PDB ID : 7RRH  
Title : Crystal structure of fast switching R66M/M159T mutant of fluorescent protein Dronpa (Dronpa2)  
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.  
Deposited on : 2021-08-09  
Resolution : 1.75 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

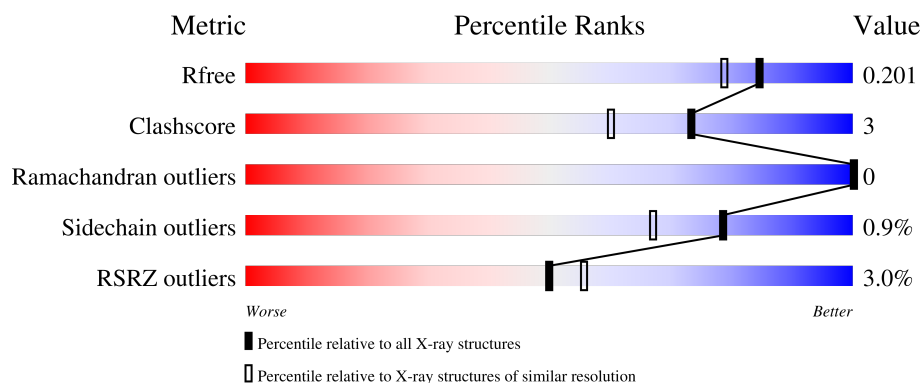
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	255	
1	B	255	
1	C	255	
1	D	255	
1	E	255	

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Mol	Chain	Length	Quality of chain
1	F	255	<div><div></div><div>6%</div><div>71%</div><div>13%</div><div>16%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11331 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	216	Total	C	N	O	S	0	7	0
			1776	1137	296	333	10			
1	B	215	Total	C	N	O	S	0	5	0
			1756	1121	293	332	10			
1	C	216	Total	C	N	O	S	0	2	0
			1744	1115	290	329	10			
1	D	216	Total	C	N	O	S	0	1	0
			1738	1111	290	327	10			
1	E	213	Total	C	N	O	S	0	4	0
			1734	1103	290	331	10			
1	F	214	Total	C	N	O	S	0	2	0
			1722	1099	287	326	10			

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP Q5TLG6
A	-26	SER	-	expression tag	UNP Q5TLG6
A	-25	SER	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	HIS	-	expression tag	UNP Q5TLG6
A	-21	HIS	-	expression tag	UNP Q5TLG6
A	-20	HIS	-	expression tag	UNP Q5TLG6
A	-19	HIS	-	expression tag	UNP Q5TLG6
A	-18	SER	-	expression tag	UNP Q5TLG6
A	-17	SER	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	LEU	-	expression tag	UNP Q5TLG6
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
A	63	GYC	CYS	chromophore	UNP Q5TLG6
A	63	GYC	TYR	chromophore	UNP Q5TLG6
A	63	GYC	GLY	chromophore	UNP Q5TLG6
A	66	MET	ARG	engineered mutation	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	conflict	UNP Q5TLG6
A	224	MET	-	insertion	UNP Q5TLG6
A	225	ASP	-	insertion	UNP Q5TLG6
A	226	GLU	-	insertion	UNP Q5TLG6
A	227	LEU	-	insertion	UNP Q5TLG6
A	228	TYR	-	insertion	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	UNP Q5TLG6
B	63	GYC	CYS	chromophore	UNP Q5TLG6
B	63	GYC	TYR	chromophore	UNP Q5TLG6
B	63	GYC	GLY	chromophore	UNP Q5TLG6
B	66	MET	ARG	engineered mutation	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	conflict	UNP Q5TLG6
B	224	MET	-	insertion	UNP Q5TLG6
B	225	ASP	-	insertion	UNP Q5TLG6
B	226	GLU	-	insertion	UNP Q5TLG6
B	227	LEU	-	insertion	UNP Q5TLG6
B	228	TYR	-	insertion	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	UNP Q5TLG6
C	63	GYC	CYS	chromophore	UNP Q5TLG6
C	63	GYC	TYR	chromophore	UNP Q5TLG6
C	63	GYC	GLY	chromophore	UNP Q5TLG6
C	66	MET	ARG	engineered mutation	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	conflict	UNP Q5TLG6
C	224	MET	-	insertion	UNP Q5TLG6
C	225	ASP	-	insertion	UNP Q5TLG6
C	226	GLU	-	insertion	UNP Q5TLG6
C	227	LEU	-	insertion	UNP Q5TLG6
C	228	TYR	-	insertion	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	UNP Q5TLG6
D	63	GYC	CYS	chromophore	UNP Q5TLG6
D	63	GYC	TYR	chromophore	UNP Q5TLG6
D	63	GYC	GLY	chromophore	UNP Q5TLG6
D	66	MET	ARG	engineered mutation	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	conflict	UNP Q5TLG6
D	224	MET	-	insertion	UNP Q5TLG6
D	225	ASP	-	insertion	UNP Q5TLG6
D	226	GLU	-	insertion	UNP Q5TLG6
D	227	LEU	-	insertion	UNP Q5TLG6
D	228	TYR	-	insertion	UNP Q5TLG6
E	-27	GLY	-	expression tag	UNP Q5TLG6
E	-26	SER	-	expression tag	UNP Q5TLG6
E	-25	SER	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	HIS	-	expression tag	UNP Q5TLG6
E	-21	HIS	-	expression tag	UNP Q5TLG6
E	-20	HIS	-	expression tag	UNP Q5TLG6
E	-19	HIS	-	expression tag	UNP Q5TLG6
E	-18	SER	-	expression tag	UNP Q5TLG6
E	-17	SER	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	LEU	-	expression tag	UNP Q5TLG6
E	-14	VAL	-	expression tag	UNP Q5TLG6
E	-13	PRO	-	expression tag	UNP Q5TLG6
E	-12	GLY	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6
E	-10	SER	-	expression tag	UNP Q5TLG6
E	-9	HIS	-	expression tag	UNP Q5TLG6
E	-8	MET	-	expression tag	UNP Q5TLG6
E	-7	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	SER	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	GLY	-	expression tag	UNP Q5TLG6
E	-3	GLU	-	expression tag	UNP Q5TLG6
E	-2	GLU	-	expression tag	UNP Q5TLG6
E	-1	ASN	-	expression tag	UNP Q5TLG6
E	0	ASN	-	expression tag	UNP Q5TLG6
E	1	MET	-	expression tag	UNP Q5TLG6
E	2	ALA	-	expression tag	UNP Q5TLG6
E	63	GYC	CYS	chromophore	UNP Q5TLG6
E	63	GYC	TYR	chromophore	UNP Q5TLG6
E	63	GYC	GLY	chromophore	UNP Q5TLG6
E	66	MET	ARG	engineered mutation	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	conflict	UNP Q5TLG6
E	224	MET	-	insertion	UNP Q5TLG6
E	225	ASP	-	insertion	UNP Q5TLG6
E	226	GLU	-	insertion	UNP Q5TLG6
E	227	LEU	-	insertion	UNP Q5TLG6
E	228	TYR	-	insertion	UNP Q5TLG6
F	-27	GLY	-	expression tag	UNP Q5TLG6
F	-26	SER	-	expression tag	UNP Q5TLG6
F	-25	SER	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	HIS	-	expression tag	UNP Q5TLG6
F	-21	HIS	-	expression tag	UNP Q5TLG6
F	-20	HIS	-	expression tag	UNP Q5TLG6
F	-19	HIS	-	expression tag	UNP Q5TLG6
F	-18	SER	-	expression tag	UNP Q5TLG6
F	-17	SER	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	LEU	-	expression tag	UNP Q5TLG6
F	-14	VAL	-	expression tag	UNP Q5TLG6
F	-13	PRO	-	expression tag	UNP Q5TLG6
F	-12	GLY	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	SER	-	expression tag	UNP Q5TLG6
F	-9	HIS	-	expression tag	UNP Q5TLG6
F	-8	MET	-	expression tag	UNP Q5TLG6
F	-7	VAL	-	expression tag	UNP Q5TLG6
F	-6	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	GLY	-	expression tag	UNP Q5TLG6
F	-3	GLU	-	expression tag	UNP Q5TLG6
F	-2	GLU	-	expression tag	UNP Q5TLG6
F	-1	ASN	-	expression tag	UNP Q5TLG6
F	0	ASN	-	expression tag	UNP Q5TLG6
F	1	MET	-	expression tag	UNP Q5TLG6
F	2	ALA	-	expression tag	UNP Q5TLG6
F	63	GYC	CYS	chromophore	UNP Q5TLG6
F	63	GYC	TYR	chromophore	UNP Q5TLG6
F	63	GYC	GLY	chromophore	UNP Q5TLG6
F	66	MET	ARG	engineered mutation	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	conflict	UNP Q5TLG6
F	224	MET	-	insertion	UNP Q5TLG6
F	225	ASP	-	insertion	UNP Q5TLG6
F	226	GLU	-	insertion	UNP Q5TLG6
F	227	LEU	-	insertion	UNP Q5TLG6
F	228	TYR	-	insertion	UNP Q5TLG6

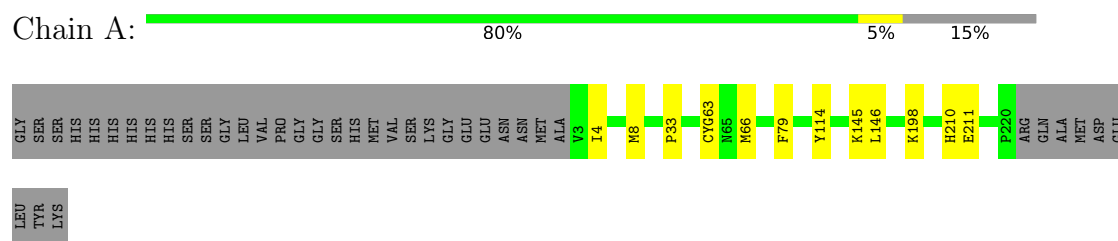
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	166	Total O 166 166	0	0
2	B	193	Total O 193 193	0	0
2	C	162	Total O 162 162	0	0
2	D	145	Total O 145 145	0	0
2	E	123	Total O 123 123	0	0
2	F	72	Total O 72 72	0	0

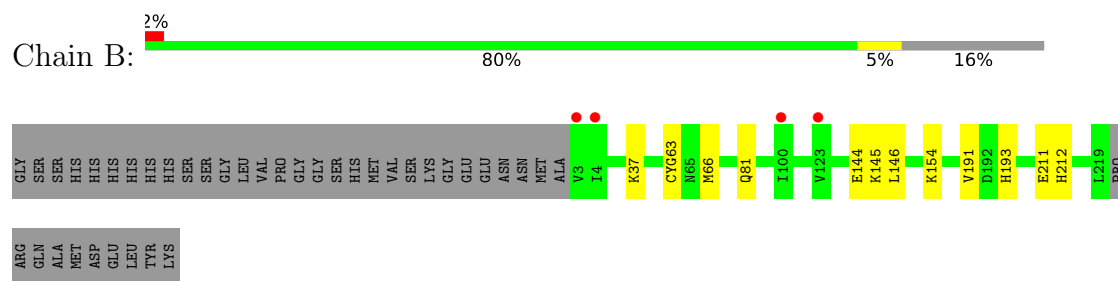
### 3 Residue-property plots [i](#)

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 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.

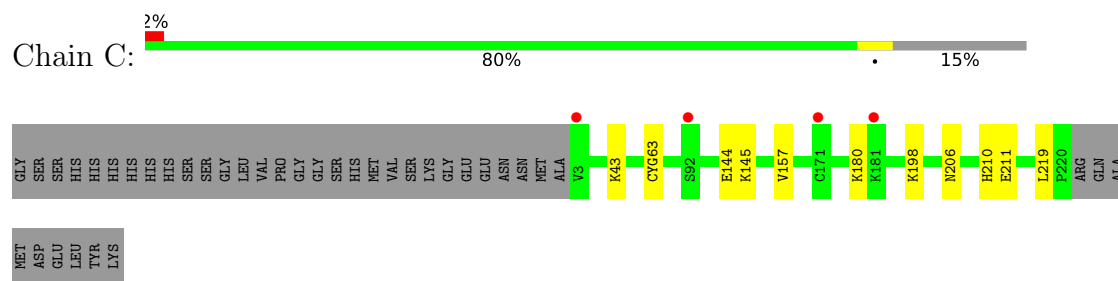
#### • Molecule 1: Fluorescent protein Dronpa



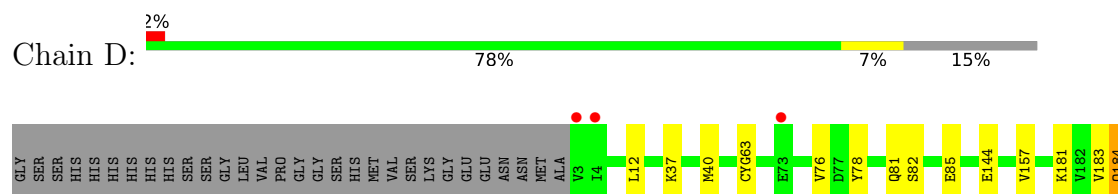
#### • Molecule 1: Fluorescent protein Dronpa



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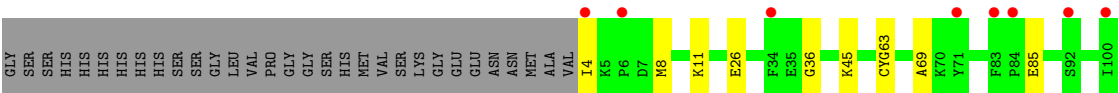
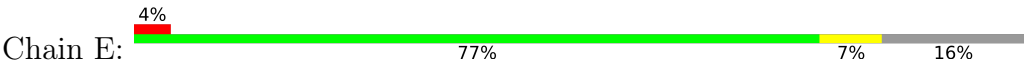


#### • Molecule 1: Fluorescent protein Dronpa

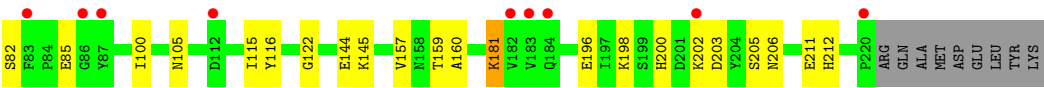
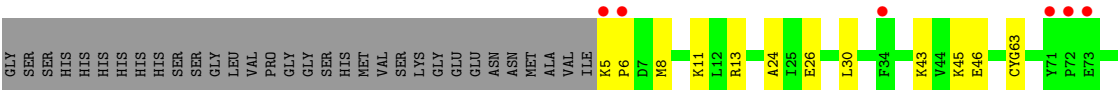




● Molecule 1: Fluorescent protein Dronpa



● Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.63Å 71.54Å 108.27Å 90.00° 110.12° 90.00°	Depositor
Resolution (Å)	37.77 – 1.75 39.41 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.8 (37.77-1.75) 89.9 (39.41-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, $R_{free}$	0.176 , 0.202 0.177 , 0.201	Depositor DCC
$R_{free}$ test set	6643 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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>1</sup>Intensities estimated from amplitudes.

<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.

## 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: GYC

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	0.48	0/1814	0.66	0/2450
1	B	0.54	0/1787	0.65	0/2414
1	C	0.55	0/1772	0.64	0/2395
1	D	0.55	0/1763	0.66	0/2383
1	E	0.46	0/1758	0.62	0/2376
1	F	0.47	0/1750	0.60	0/2366
All	All	0.51	0/10644	0.64	0/14384

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	1776	0	1710	8	0
1	B	1756	0	1672	9	0
1	C	1744	0	1664	7	0
1	D	1738	0	1658	12	0
1	E	1734	0	1632	10	0
1	F	1722	0	1632	22	0
2	A	166	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	193	0	0	1	0
2	C	162	0	0	1	0
2	D	145	0	0	1	0
2	E	123	0	0	0	0
2	F	72	0	0	0	0
All	All	11331	0	9968	68	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 3.

All (68) 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:D:12:LEU:HD21	1:D:40:MET:HE1	1.53	0.90
1:B:193:HIS:HD2	1:B:211:GLU:OE2	1.65	0.79
1:D:81:GLN:O	1:D:181:LYS:NZ	2.19	0.74
1:D:76:VAL:HG11	1:D:184:GLN:HG2	1.70	0.73
1:F:26:GLU:HG3	1:F:45:LYS:HG3	1.72	0.70
1:F:85:GLU:OE1	1:F:181:LYS:HD3	1.92	0.68
1:D:219:LEU:HD12	1:D:220:PRO:HD2	1.76	0.68
1:B:37:LYS:HE3	1:B:212[B]:HIS:CD2	2.29	0.67
1:F:24:ALA:HB3	1:F:46:GLU:HG3	1.75	0.67
1:F:85:GLU:CD	1:F:181:LYS:HD3	2.14	0.67
1:E:26:GLU:HG3	1:E:45:LYS:HG3	1.77	0.66
1:C:198:LYS:HE3	1:C:210:HIS:HB2	1.78	0.66
1:F:30:LEU:HD12	1:F:30:LEU:C	2.17	0.65
1:F:11:LYS:HG2	1:F:115:ILE:HG22	1.77	0.65
1:F:202:LYS:HG3	1:F:203:ASP:N	2.13	0.62
1:A:198:LYS:HG3	1:A:210[A]:HIS:CD2	2.36	0.61
1:B:66:MET:HE1	1:B:193:HIS:NE2	2.15	0.60
1:E:85:GLU:N	1:E:85:GLU:OE1	2.32	0.59
1:D:200:HIS:NE2	2:D:302:HOH:O	2.33	0.57
1:A:211:GLU:OE2	2:A:301:HOH:O	2.18	0.56
1:A:4:ILE:HD13	1:A:114:TYR:OH	2.06	0.56
1:A:146:LEU:HD12	1:A:146:LEU:N	2.21	0.55
1:F:202:LYS:HG3	1:F:203:ASP:H	1.73	0.53
1:A:4:ILE:HD11	1:A:33:PRO:HG2	1.88	0.53
1:F:43:LYS:HA	1:F:205:SER:O	2.10	0.52
1:D:85:GLU:OE2	1:D:181:LYS:HE3	2.08	0.52
1:F:30:LEU:HD12	1:F:30:LEU:O	2.09	0.51
1:B:66:MET:CE	1:B:193:HIS:NE2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:SER:HA	1:D:181:LYS:NZ	2.25	0.51
1:D:85:GLU:OE2	1:D:181:LYS:CE	2.60	0.50
1:F:11:LYS:O	1:F:115:ILE:HA	2.11	0.50
1:C:43:LYS:NZ	1:C:206:ASN:OD1	2.44	0.50
1:B:81:GLN:NE2	2:B:307:HOH:O	2.42	0.49
1:D:82:SER:HA	1:D:181:LYS:HZ2	1.76	0.49
1:E:4:ILE:HA	1:E:8:MET:CE	2.44	0.48
1:F:159:THR:OG1	1:F:160:ALA:N	2.45	0.48
1:B:66:MET:HE1	1:B:191:VAL:HG11	1.94	0.48
1:F:196:GLU:CD	1:F:198:LYS:HE3	2.33	0.48
1:C:198:LYS:HE3	1:C:210:HIS:CB	2.43	0.47
1:A:4:ILE:HD11	1:A:8:MET:HG3	1.95	0.47
1:F:5:LYS:N	1:F:6:PRO:HD2	2.29	0.47
1:C:211:GLU:OE2	2:C:301:HOH:O	2.21	0.47
1:F:144:GLU:HA	1:F:157:VAL:HB	1.97	0.46
1:B:193:HIS:CD2	1:B:211:GLU:OE2	2.57	0.46
1:C:144:GLU:HA	1:C:157:VAL:HB	1.98	0.45
1:F:13:ARG:NH1	1:F:26:GLU:OE1	2.42	0.45
1:E:181:LYS:HD3	1:E:181:LYS:HA	1.56	0.45
1:C:198:LYS:HD2	1:C:210:HIS:CD2	2.52	0.44
1:B:146:LEU:HD23	1:B:154:LYS:O	2.17	0.44
1:F:100:ILE:O	1:F:122:GLY:HA2	2.18	0.44
1:A:66:MET:HG2	1:A:79:PHE:CE1	2.52	0.43
1:F:196:GLU:OE1	1:F:198:LYS:HE3	2.18	0.43
1:F:211:GLU:HG2	1:F:212:HIS:H	1.84	0.43
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.89	0.43
1:F:105:ASN:OD1	1:F:116:TYR:HB3	2.20	0.42
1:E:144:GLU:HA	1:E:157:VAL:HB	2.01	0.42
1:E:11:LYS:O	1:E:115:ILE:HA	2.20	0.42
1:D:37:LYS:HD3	1:D:212:HIS:HB2	2.01	0.42
1:F:5:LYS:O	1:F:5:LYS:HG3	2.19	0.42
1:B:144:GLU:OE2	1:B:193:HIS:HE1	2.03	0.42
1:D:78:TYR:CD2	1:D:183:VAL:HG22	2.55	0.41
1:D:144:GLU:HA	1:D:157:VAL:HB	2.02	0.41
1:E:69:ALA:HA	1:E:213:ALA:O	2.21	0.41
1:A:198:LYS:HE2	1:A:210[A]:HIS:ND1	2.36	0.41
1:E:184:GLN:HA	1:E:184:GLN:OE1	2.20	0.41
1:E:4:ILE:HA	1:E:8:MET:HE1	2.03	0.41
1:F:200:HIS:HA	1:F:206:ASN:O	2.21	0.40
1:E:36:GLY:O	1:E:212:HIS:HA	2.22	0.40

There are no symmetry-related clashes.



## 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	220/255 (86%)	218 (99%)	2 (1%)	0	100	100
1	B	217/255 (85%)	216 (100%)	1 (0%)	0	100	100
1	C	215/255 (84%)	212 (99%)	3 (1%)	0	100	100
1	D	214/255 (84%)	211 (99%)	3 (1%)	0	100	100
1	E	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
1	F	213/255 (84%)	210 (99%)	3 (1%)	0	100	100
All	All	1293/1530 (84%)	1279 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	192/217 (88%)	191 (100%)	1 (0%)	88	83
1	B	188/217 (87%)	187 (100%)	1 (0%)	88	83
1	C	186/217 (86%)	184 (99%)	2 (1%)	73	59
1	D	185/217 (85%)	184 (100%)	1 (0%)	88	83
1	E	184/217 (85%)	183 (100%)	1 (0%)	88	83
1	F	183/217 (84%)	179 (98%)	4 (2%)	52	29
All	All	1118/1302 (86%)	1108 (99%)	10 (1%)	78	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	B	145	LYS
1	C	145	LYS
1	C	180	LYS
1	D	184	GLN
1	E	145	LYS
1	F	8	MET
1	F	82	SER
1	F	145	LYS
1	F	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	F	63	1	22,22,23	1.13	1 (4%)	26,30,32	2.58	7 (26%)
1	GYC	B	63	1	22,22,23	1.27	3 (13%)	26,30,32	2.60	9 (34%)
1	GYC	D	63	1	22,22,23	1.22	3 (13%)	26,30,32	2.69	9 (34%)
1	GYC	C	63	1	22,22,23	1.10	3 (13%)	26,30,32	2.43	10 (38%)
1	GYC	A	63	1	22,22,23	1.14	3 (13%)	26,30,32	2.16	9 (34%)
1	GYC	E	63	1	22,22,23	1.10	2 (9%)	26,30,32	2.44	9 (34%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	GYC	CB2-CA2	4.23	1.38	1.35
1	B	63	GYC	CB2-CA2	4.03	1.38	1.35
1	D	63	GYC	CB2-CA2	3.99	1.38	1.35
1	E	63	GYC	CB2-CA2	3.76	1.38	1.35
1	C	63	GYC	CB2-CA2	3.61	1.38	1.35
1	A	63	GYC	CB2-CA2	3.11	1.37	1.35
1	A	63	GYC	CA2-C2	-2.80	1.45	1.48
1	B	63	GYC	CA2-C2	-2.51	1.46	1.48
1	C	63	GYC	CA2-C2	-2.28	1.46	1.48
1	A	63	GYC	C2-N3	-2.27	1.34	1.39
1	B	63	GYC	C2-N3	-2.22	1.34	1.39
1	E	63	GYC	C2-N3	-2.11	1.34	1.39
1	D	63	GYC	C2-N3	-2.11	1.34	1.39
1	D	63	GYC	CA2-C2	-2.05	1.46	1.48
1	C	63	GYC	C2-N3	-2.03	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	GYC	O2-C2-CA2	-10.11	125.28	130.96
1	F	63	GYC	O2-C2-CA2	-8.50	126.19	130.96
1	B	63	GYC	O2-C2-CA2	-8.34	126.28	130.96
1	C	63	GYC	O2-C2-CA2	-8.10	126.41	130.96
1	E	63	GYC	O2-C2-CA2	-7.95	126.49	130.96
1	A	63	GYC	O2-C2-CA2	-7.29	126.86	130.96
1	B	63	GYC	CA2-C2-N3	5.51	105.97	103.37
1	F	63	GYC	CA2-N2-C1	4.59	109.15	105.77
1	F	63	GYC	C2-CA2-N2	-4.47	105.81	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	GYC	CA2-C2-N3	4.33	105.42	103.37
1	C	63	GYC	CA2-C2-N3	4.14	105.33	103.37
1	D	63	GYC	CA2-C2-N3	4.12	105.32	103.37
1	F	63	GYC	CA2-C2-N3	4.12	105.32	103.37
1	B	63	GYC	CB2-CA2-N2	3.75	134.02	128.83
1	B	63	GYC	C2-CA2-N2	-3.57	106.43	108.93
1	E	63	GYC	C2-CA2-N2	-3.55	106.45	108.93
1	F	63	GYC	CG2-CB2-CA2	-3.41	125.76	129.94
1	C	63	GYC	O-C-CA3	-3.40	116.12	126.39
1	A	63	GYC	CA2-C2-N3	3.35	104.96	103.37
1	E	63	GYC	CA2-N2-C1	3.19	108.12	105.77
1	B	63	GYC	CA2-N2-C1	3.19	108.12	105.77
1	D	63	GYC	CB2-CA2-N2	3.17	133.22	128.83
1	E	63	GYC	CG2-CB2-CA2	-3.12	126.12	129.94
1	D	63	GYC	CA2-N2-C1	2.85	107.87	105.77
1	D	63	GYC	C2-CA2-N2	-2.80	106.97	108.93
1	C	63	GYC	CB2-CA2-N2	2.80	132.71	128.83
1	C	63	GYC	C2-CA2-N2	-2.76	107.00	108.93
1	A	63	GYC	CA1-CB1-SG1	-2.76	108.50	114.44
1	E	63	GYC	O-C-CA3	-2.66	118.36	126.39
1	D	63	GYC	O2-C2-N3	2.54	129.40	124.35
1	D	63	GYC	O-C-CA3	-2.52	118.79	126.39
1	F	63	GYC	O-C-CA3	-2.50	118.83	126.39
1	C	63	GYC	CA2-N2-C1	2.48	107.60	105.77
1	A	63	GYC	O-C-CA3	-2.46	118.95	126.39
1	E	63	GYC	CA1-CB1-SG1	-2.41	109.24	114.44
1	A	63	GYC	CG2-CB2-CA2	-2.40	127.00	129.94
1	B	63	GYC	CA1-CB1-SG1	-2.40	109.27	114.44
1	A	63	GYC	CB2-CA2-N2	2.38	132.12	128.83
1	D	63	GYC	CG2-CB2-CA2	-2.34	127.07	129.94
1	E	63	GYC	CB2-CA2-N2	2.34	132.06	128.83
1	B	63	GYC	CB2-CA2-C2	-2.30	119.53	122.28
1	C	63	GYC	CA1-CB1-SG1	-2.27	109.54	114.44
1	A	63	GYC	CA2-N2-C1	2.26	107.44	105.77
1	A	63	GYC	C2-N3-C1	2.25	109.11	107.97
1	C	63	GYC	CA1-C1-N3	-2.22	121.96	124.85
1	E	63	GYC	CA1-C1-N3	-2.21	121.98	124.85
1	B	63	GYC	CG2-CB2-CA2	-2.16	127.30	129.94
1	C	63	GYC	CD2-CG2-CD1	2.15	120.82	117.64
1	B	63	GYC	O-C-CA3	-2.10	120.05	126.39
1	F	63	GYC	O2-C2-N3	2.08	128.49	124.35
1	D	63	GYC	CB2-CA2-C2	-2.07	119.81	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	C2-CA2-N2	-2.05	107.49	108.93
1	C	63	GYC	CG2-CB2-CA2	-2.01	127.48	129.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	GYC	C-CA3-N3-C2
1	A	63	GYC	N2-CA2-CB2-CG2
1	A	63	GYC	C2-CA2-CB2-CG2
1	B	63	GYC	N2-CA2-CB2-CG2
1	B	63	GYC	C2-CA2-CB2-CG2
1	C	63	GYC	C-CA3-N3-C2
1	C	63	GYC	N2-CA2-CB2-CG2
1	C	63	GYC	C2-CA2-CB2-CG2
1	D	63	GYC	N2-CA2-CB2-CG2
1	D	63	GYC	C2-CA2-CB2-CG2
1	E	63	GYC	C-CA3-N3-C2
1	E	63	GYC	N2-CA2-CB2-CG2
1	E	63	GYC	C2-CA2-CB2-CG2
1	F	63	GYC	C-CA3-N3-C2
1	F	63	GYC	N2-CA2-CB2-CG2
1	F	63	GYC	C2-CA2-CB2-CG2
1	B	63	GYC	C-CA3-N3-C2
1	D	63	GYC	C-CA3-N3-C2

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](#)

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](#)

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	215/255 (84%)	-0.28	0 100 100	26, 38, 56, 102	0
1	B	214/255 (83%)	-0.15	4 (1%) 66 73	27, 38, 60, 83	0
1	C	215/255 (84%)	-0.01	4 (1%) 66 73	30, 41, 59, 83	0
1	D	215/255 (84%)	0.00	5 (2%) 60 66	30, 46, 72, 112	0
1	E	212/255 (83%)	0.34	10 (4%) 31 36	28, 49, 78, 98	0
1	F	213/255 (83%)	0.47	15 (7%) 16 21	40, 61, 92, 117	0
All	All	1284/1530 (83%)	0.06	38 (2%) 50 56	26, 44, 79, 117	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	PHE	7.0
1	B	4	ILE	4.9
1	E	100	ILE	4.5
1	F	5	LYS	4.1
1	D	220	PRO	4.1
1	F	71	TYR	3.7
1	E	34	PHE	3.6
1	E	4	ILE	3.5
1	F	83	PHE	3.5
1	E	6	PRO	3.4
1	D	4	ILE	3.4
1	C	3	VAL	3.4
1	B	3	VAL	3.3
1	F	184	GLN	3.3
1	B	100	ILE	3.3
1	F	6	PRO	3.3
1	F	202	LYS	3.1
1	D	3	VAL	3.1
1	D	219	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	92[A]	SER	2.7
1	F	87	TYR	2.7
1	E	92[A]	SER	2.6
1	F	182	VAL	2.4
1	F	73	GLU	2.4
1	F	183	VAL	2.4
1	F	220	PRO	2.4
1	C	171	CYS	2.3
1	E	84	PRO	2.3
1	C	181	LYS	2.2
1	F	112	ASP	2.2
1	D	73	GLU	2.2
1	E	101	CYS	2.2
1	E	171	CYS	2.2
1	F	86	GLY	2.2
1	E	71	TYR	2.1
1	F	72	PRO	2.1
1	E	83	PHE	2.1
1	B	123	VAL	2.0

## 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	GYC	F	63	21/22	0.90	0.12	60,65,69,73	0
1	GYC	D	63	21/22	0.94	0.09	35,43,57,65	0
1	GYC	B	63	21/22	0.94	0.09	27,37,49,49	0
1	GYC	E	63	21/22	0.95	0.08	42,47,53,61	0
1	GYC	C	63	21/22	0.96	0.08	34,39,50,54	0
1	GYC	A	63	21/22	0.97	0.08	26,34,44,47	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.