



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 05:15 pm BST

PDB ID : 6NQQ  
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2), Y63(2,3,5-F3Y)  
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.  
Deposited on : 2019-01-21  
Resolution : 2.60 Å(reported)

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](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	:	2.11
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)	:	2.11

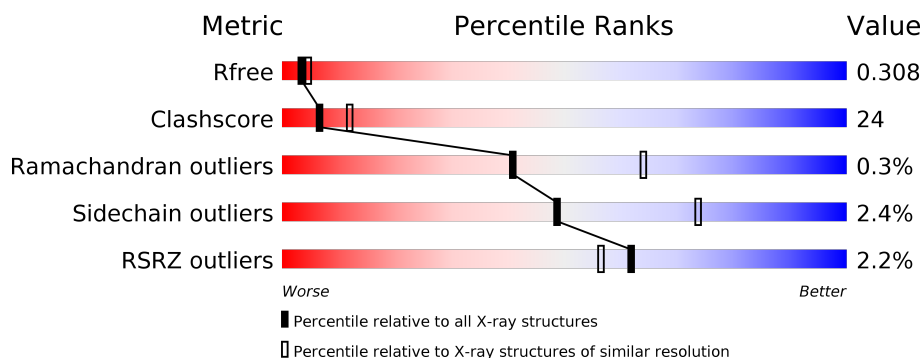
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>26%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	255	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	255	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	255	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>33%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	255	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>•</div> <div>14%</div> </div> </div>
1	F	255	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	255	<p>%</p> <p>57% 26% 15%</p>
1	H	255	<p>2%</p> <p>53% 30% 16%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	KZ1	B	63	-	-	X	-
1	KZ1	C	63	-	-	X	-
1	KZ1	D	63	-	-	X	-
1	KZ1	E	63	-	-	X	-
1	KZ1	F	63	-	-	X	-
1	KZ1	G	63	-	-	X	-
1	KZ1	H	63	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13976 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	F	N	O	S	0	1	0
			1734	1106	3	289	327	9			
1	B	216	Total	C	F	N	O	S	0	0	0
			1733	1104	3	292	325	9			
1	C	222	Total	C	F	N	O	S	0	0	0
			1756	1122	3	295	327	9			
1	D	223	Total	C	F	N	O	S	0	0	0
			1761	1121	3	296	332	9			
1	E	220	Total	C	F	N	O	S	0	0	0
			1742	1111	3	292	327	9			
1	F	220	Total	C	F	N	O	S	0	0	0
			1740	1107	3	292	329	9			
1	G	216	Total	C	F	N	O	S	0	0	0
			1707	1089	3	286	320	9			
1	H	215	Total	C	F	N	O	S	0	1	0
			1726	1100	3	289	325	9			

There are 328 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
A	63	KZ1	TYR	chromophore	UNP Q5TLG6
A	63	KZ1	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
A	224	MET	-	expression tag	UNP Q5TLG6
A	225	ASP	-	expression tag	UNP Q5TLG6
A	226	GLU	-	expression tag	UNP Q5TLG6
A	227	LEU	-	expression tag	UNP Q5TLG6
A	228	TYR	-	expression tag	UNP Q5TLG6
A	229	LYS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
B	63	KZ1	TYR	chromophore	UNP Q5TLG6
B	63	KZ1	GLY	chromophore	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	224	MET	-	expression tag	UNP Q5TLG6
B	225	ASP	-	expression tag	UNP Q5TLG6
B	226	GLU	-	expression tag	UNP Q5TLG6
B	227	LEU	-	expression tag	UNP Q5TLG6
B	228	TYR	-	expression tag	UNP Q5TLG6
B	229	LYS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
C	63	KZ1	TYR	chromophore	UNP Q5TLG6
C	63	KZ1	GLY	chromophore	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	224	MET	-	expression tag	UNP Q5TLG6
C	225	ASP	-	expression tag	UNP Q5TLG6
C	226	GLU	-	expression tag	UNP Q5TLG6
C	227	LEU	-	expression tag	UNP Q5TLG6
C	228	TYR	-	expression tag	UNP Q5TLG6
C	229	LYS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
D	63	KZ1	TYR	chromophore	UNP Q5TLG6
D	63	KZ1	GLY	chromophore	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	224	MET	-	expression tag	UNP Q5TLG6
D	225	ASP	-	expression tag	UNP Q5TLG6
D	226	GLU	-	expression tag	UNP Q5TLG6
D	227	LEU	-	expression tag	UNP Q5TLG6
D	228	TYR	-	expression tag	UNP Q5TLG6
D	229	LYS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
E	63	KZ1	TYR	chromophore	UNP Q5TLG6
E	63	KZ1	GLY	chromophore	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	224	MET	-	expression tag	UNP Q5TLG6
E	225	ASP	-	expression tag	UNP Q5TLG6
E	226	GLU	-	expression tag	UNP Q5TLG6
E	227	LEU	-	expression tag	UNP Q5TLG6
E	228	TYR	-	expression tag	UNP Q5TLG6
E	229	LYS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	KZ1	CYS	chromophore	UNP Q5TLG6
F	63	KZ1	TYR	chromophore	UNP Q5TLG6
F	63	KZ1	GLY	chromophore	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	224	MET	-	expression tag	UNP Q5TLG6
F	225	ASP	-	expression tag	UNP Q5TLG6
F	226	GLU	-	expression tag	UNP Q5TLG6
F	227	LEU	-	expression tag	UNP Q5TLG6
F	228	TYR	-	expression tag	UNP Q5TLG6
F	229	LYS	-	expression tag	UNP Q5TLG6
G	-27	GLY	-	expression tag	UNP Q5TLG6
G	-26	SER	-	expression tag	UNP Q5TLG6
G	-25	SER	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	HIS	-	expression tag	UNP Q5TLG6
G	-21	HIS	-	expression tag	UNP Q5TLG6
G	-20	HIS	-	expression tag	UNP Q5TLG6
G	-19	HIS	-	expression tag	UNP Q5TLG6
G	-18	SER	-	expression tag	UNP Q5TLG6
G	-17	SER	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	LEU	-	expression tag	UNP Q5TLG6
G	-14	VAL	-	expression tag	UNP Q5TLG6
G	-13	PRO	-	expression tag	UNP Q5TLG6
G	-12	GLY	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	SER	-	expression tag	UNP Q5TLG6
G	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
G	-1	ASN	-	expression tag	UNP Q5TLG6
G	0	ASN	-	expression tag	UNP Q5TLG6
G	1	MET	-	expression tag	UNP Q5TLG6
G	2	ALA	-	expression tag	UNP Q5TLG6
G	63	KZ1	CYS	chromophore	UNP Q5TLG6
G	63	KZ1	TYR	chromophore	UNP Q5TLG6
G	63	KZ1	GLY	chromophore	UNP Q5TLG6
G	159	THR	MET	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	engineered mutation	UNP Q5TLG6
G	224	MET	-	expression tag	UNP Q5TLG6
G	225	ASP	-	expression tag	UNP Q5TLG6
G	226	GLU	-	expression tag	UNP Q5TLG6
G	227	LEU	-	expression tag	UNP Q5TLG6
G	228	TYR	-	expression tag	UNP Q5TLG6
G	229	LYS	-	expression tag	UNP Q5TLG6
H	-27	GLY	-	expression tag	UNP Q5TLG6
H	-26	SER	-	expression tag	UNP Q5TLG6
H	-25	SER	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	HIS	-	expression tag	UNP Q5TLG6
H	-21	HIS	-	expression tag	UNP Q5TLG6
H	-20	HIS	-	expression tag	UNP Q5TLG6
H	-19	HIS	-	expression tag	UNP Q5TLG6
H	-18	SER	-	expression tag	UNP Q5TLG6
H	-17	SER	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	LEU	-	expression tag	UNP Q5TLG6
H	-14	VAL	-	expression tag	UNP Q5TLG6
H	-13	PRO	-	expression tag	UNP Q5TLG6
H	-12	GLY	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	SER	-	expression tag	UNP Q5TLG6
H	-9	HIS	-	expression tag	UNP Q5TLG6
H	-8	MET	-	expression tag	UNP Q5TLG6

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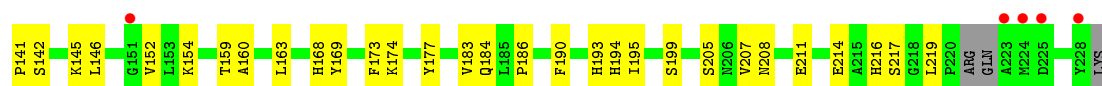
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	VAL	-	expression tag	UNP Q5TLG6
H	-6	SER	-	expression tag	UNP Q5TLG6
H	-5	LYS	-	expression tag	UNP Q5TLG6
H	-4	GLY	-	expression tag	UNP Q5TLG6
H	-3	GLU	-	expression tag	UNP Q5TLG6
H	-2	GLU	-	expression tag	UNP Q5TLG6
H	-1	ASN	-	expression tag	UNP Q5TLG6
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	KZ1	CYS	chromophore	UNP Q5TLG6
H	63	KZ1	TYR	chromophore	UNP Q5TLG6
H	63	KZ1	GLY	chromophore	UNP Q5TLG6
H	159	THR	MET	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	engineered mutation	UNP Q5TLG6
H	224	MET	-	expression tag	UNP Q5TLG6
H	225	ASP	-	expression tag	UNP Q5TLG6
H	226	GLU	-	expression tag	UNP Q5TLG6
H	227	LEU	-	expression tag	UNP Q5TLG6
H	228	TYR	-	expression tag	UNP Q5TLG6
H	229	LYS	-	expression tag	UNP Q5TLG6

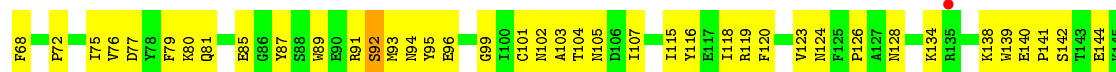
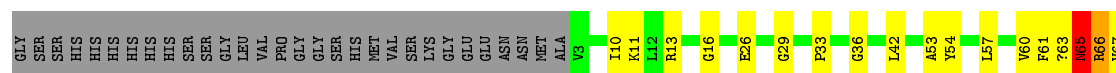
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	11	Total O 11 11	0	0
2	C	8	Total O 8 8	0	0
2	D	6	Total O 6 6	0	0
2	E	10	Total O 10 10	0	0
2	F	9	Total O 9 9	0	0
2	G	14	Total O 14 14	0	0
2	H	10	Total O 10 10	0	0

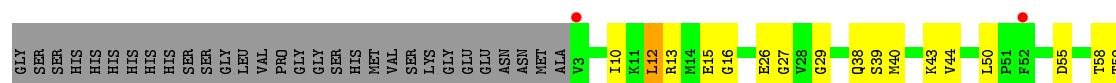




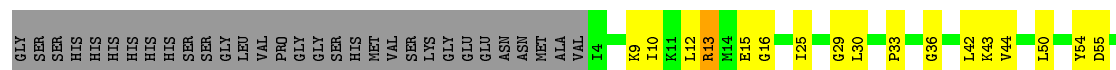
• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa

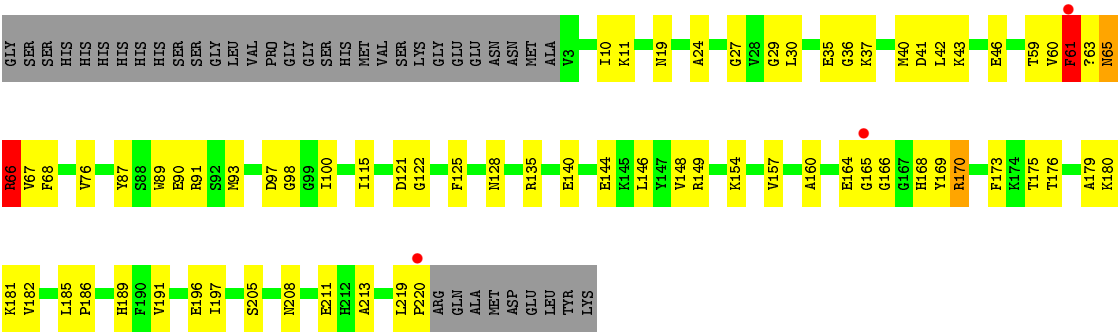


• Molecule 1: Fluorescent protein Dronpa

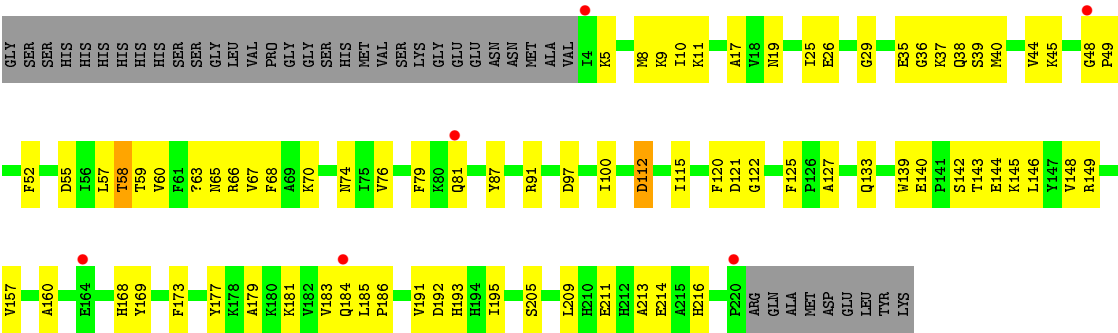


• Molecule 1: Fluorescent protein Dronpa





● Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.84Å 86.38Å 143.59Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	39.52 – 2.60 39.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.52-2.60) 83.9 (39.53-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, $R_{free}$	0.263 , 0.311 0.265 , 0.308	Depositor DCC
$R_{free}$ test set	2000 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.981	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8068e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: KZ1

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	0.56	0/1759	0.66	1/2380 (0.0%)
1	B	0.56	0/1755	0.71	1/2371 (0.0%)
1	C	0.58	0/1777	0.66	1/2404 (0.0%)
1	D	0.58	0/1782	0.68	0/2410
1	E	0.50	0/1763	0.65	0/2386
1	F	0.49	0/1761	0.65	0/2383
1	G	0.44	0/1729	0.69	2/2341 (0.1%)
1	H	0.44	0/1748	0.66	0/2364
All	All	0.52	0/14074	0.67	5/19039 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASN	N-CA-C	-7.39	91.05	111.00
1	A	65	ASN	N-CA-C	-7.18	91.60	111.00
1	C	65	ASN	N-CA-C	-7.00	92.11	111.00
1	G	65	ASN	N-CA-C	-5.56	96.00	111.00
1	G	61	PHE	N-CA-CB	5.28	120.10	110.60

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	1734	0	1622	61	0
1	B	1733	0	1632	80	1
1	C	1756	0	1640	89	0
1	D	1761	0	1634	94	0
1	E	1742	0	1619	82	1
1	F	1740	0	1605	102	1
1	G	1707	0	1580	75	1
1	H	1726	0	1613	75	0
2	A	9	0	0	1	0
2	B	11	0	0	5	0
2	C	8	0	0	1	0
2	D	6	0	0	0	0
2	E	10	0	0	4	0
2	F	9	0	0	0	0
2	G	14	0	0	2	0
2	H	10	0	0	1	0
All	All	13976	0	12945	633	2

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 24.

The worst 5 of 633 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:119:ARG:HH21	1:F:119:ARG:CZ	1.06	1.61
1:C:63:KZ1:CA1	1:C:63:KZ1:N	1.68	1.54
1:F:63:KZ1:N	1:F:63:KZ1:CA1	1.70	1.52
1:H:63:KZ1:N	1:H:63:KZ1:CA1	1.69	1.52
1:A:63:KZ1:N	1:A:63:KZ1:CA1	1.69	1.51

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	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:HIS:O	1:F:227:LEU:O[1_655]	1.85	0.35
1:E:96:GLU:OE1	1:G:149:ARG:NH1[2_646]	2.06	0.14

## 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	214/255 (84%)	208 (97%)	5 (2%)	1 (0%)	29	52
1	B	213/255 (84%)	205 (96%)	8 (4%)	0	100	100
1	C	217/255 (85%)	212 (98%)	5 (2%)	0	100	100
1	D	218/255 (86%)	207 (95%)	10 (5%)	1 (0%)	29	52
1	E	215/255 (84%)	206 (96%)	8 (4%)	1 (0%)	29	52
1	F	215/255 (84%)	205 (95%)	9 (4%)	1 (0%)	29	52
1	G	213/255 (84%)	204 (96%)	7 (3%)	2 (1%)	17	35
1	H	213/255 (84%)	209 (98%)	4 (2%)	0	100	100
All	All	1718/2040 (84%)	1656 (96%)	56 (3%)	6 (0%)	41	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	227	LEU
1	F	226	GLU
1	G	66	ARG
1	A	65	ASN
1	D	65	ASN

### 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	182/217 (84%)	177 (97%)	5 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	182/217 (84%)	178 (98%)	4 (2%)	52	76
1	C	180/217 (83%)	177 (98%)	3 (2%)	60	81
1	D	182/217 (84%)	177 (97%)	5 (3%)	44	71
1	E	180/217 (83%)	174 (97%)	6 (3%)	38	64
1	F	179/217 (82%)	174 (97%)	5 (3%)	43	69
1	G	175/217 (81%)	170 (97%)	5 (3%)	42	68
1	H	180/217 (83%)	178 (99%)	2 (1%)	73	88
All	All	1440/1736 (83%)	1405 (98%)	35 (2%)	49	74

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	SER
1	E	91	ARG
1	G	170	ARG
1	D	211	GLU
1	E	12	LEU

Some 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 ⓘ

8 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	KZ1	F	63	1	25,25,26	2.40	9 (36%)	32,36,38	3.73	12 (37%)
1	KZ1	C	63	1	25,25,26	3.46	17 (68%)	32,36,38	4.04	13 (40%)
1	KZ1	A	63	1	25,25,26	2.92	16 (64%)	32,36,38	3.57	14 (43%)
1	KZ1	G	63	1	25,25,26	2.77	14 (56%)	32,36,38	3.25	10 (31%)
1	KZ1	E	63	1	25,25,26	3.05	14 (56%)	32,36,38	4.86	18 (56%)
1	KZ1	H	63	1	25,25,26	3.00	15 (60%)	32,36,38	3.63	13 (40%)
1	KZ1	D	63	1	25,25,26	2.52	9 (36%)	32,36,38	3.43	14 (43%)
1	KZ1	B	63	1	25,25,26	3.39	18 (72%)	32,36,38	3.76	16 (50%)

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	KZ1	F	63	1	-	2/9/29/30	0/2/2/2
1	KZ1	C	63	1	-	2/9/29/30	0/2/2/2
1	KZ1	A	63	1	-	2/9/29/30	0/2/2/2
1	KZ1	G	63	1	-	0/9/29/30	0/2/2/2
1	KZ1	E	63	1	-	4/9/29/30	0/2/2/2
1	KZ1	H	63	1	-	2/9/29/30	0/2/2/2
1	KZ1	D	63	1	-	2/9/29/30	0/2/2/2
1	KZ1	B	63	1	-	2/9/29/30	0/2/2/2

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	KZ1	CG2-CD1	-6.98	1.34	1.39
1	E	63	KZ1	CA2-C2	-6.67	1.42	1.48
1	B	63	KZ1	CA2-C2	-6.66	1.42	1.48
1	C	63	KZ1	CA2-C2	-6.64	1.42	1.48
1	C	63	KZ1	CA3-C	6.49	1.71	1.49

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	KZ1	O2-C2-CA2	-16.24	121.84	130.96
1	G	63	KZ1	O-C-CA3	-12.89	87.47	126.39
1	B	63	KZ1	O-C-CA3	-12.71	88.03	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	KZ1	O-C-CA3	-12.21	89.52	126.39
1	H	63	KZ1	O-C-CA3	-11.96	90.27	126.39

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	63	KZ1	N2-CA2-CB2-CG2
1	F	63	KZ1	C2-CA2-CB2-CG2
1	A	63	KZ1	C1-CA1-CB1-SG1
1	A	63	KZ1	C-CA3-N3-C2
1	E	63	KZ1	N-CA1-CB1-SG1

There are no ring outliers.

8 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	63	KZ1	9	0
1	C	63	KZ1	9	0
1	A	63	KZ1	5	0
1	G	63	KZ1	17	0
1	E	63	KZ1	10	0
1	H	63	KZ1	18	0
1	D	63	KZ1	8	0
1	B	63	KZ1	13	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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%)	0.08	3 (1%) 75 71	42, 63, 87, 109	0
1	B	215/255 (84%)	0.26	2 (0%) 84 82	55, 73, 97, 122	0
1	C	221/255 (86%)	0.23	5 (2%) 60 54	40, 64, 88, 104	0
1	D	222/255 (87%)	0.23	3 (1%) 75 71	52, 72, 98, 131	0
1	E	219/255 (85%)	0.28	8 (3%) 41 34	44, 67, 94, 113	0
1	F	219/255 (85%)	0.30	9 (4%) 37 30	53, 71, 97, 122	0
1	G	215/255 (84%)	0.12	3 (1%) 75 71	48, 65, 89, 102	0
1	H	214/255 (83%)	0.25	6 (2%) 53 46	56, 74, 97, 111	0
All	All	1740/2040 (85%)	0.22	39 (2%) 62 56	40, 69, 95, 131	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	224	MET	4.1
1	C	151	GLY	4.0
1	H	48	GLY	3.4
1	E	3	VAL	3.1
1	B	165	GLY	3.1

### 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. 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	KZ1	H	63	24/25	0.80	0.21	58,68,75,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KZ1	F	63	24/25	0.83	0.20	58,68,75,80	0
1	KZ1	G	63	24/25	0.85	0.19	58,68,75,80	0
1	KZ1	C	63	24/25	0.85	0.24	58,68,75,80	0
1	KZ1	D	63	24/25	0.85	0.20	58,68,75,80	0
1	KZ1	B	63	24/25	0.85	0.22	58,68,75,80	0
1	KZ1	A	63	24/25	0.87	0.19	58,68,75,80	0
1	KZ1	E	63	24/25	0.91	0.15	58,68,75,80	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.