



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2019 – 03:15 PM EDT

PDB ID : 6NQO  
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2), Y63(3-IY)  
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.  
Deposited on : 2019-01-21  
Resolution : 2.10 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

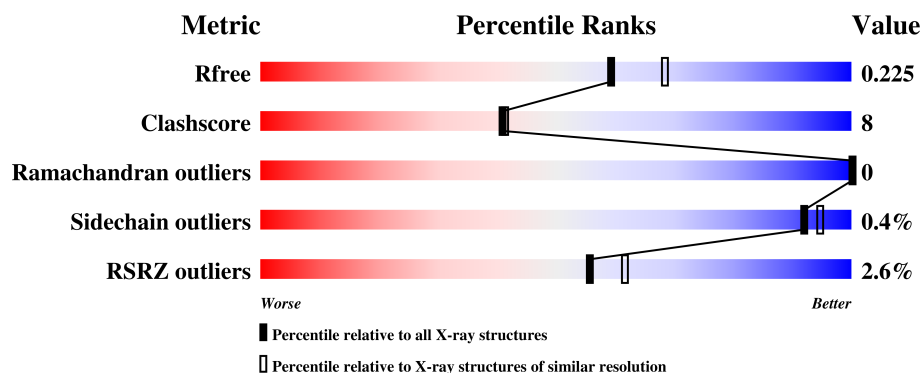
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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. 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>2%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>13%</div> </div> </div>
1	B	255	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	255	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>
1	D	255	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>15%</div> </div> </div>
1	E	255	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	255	<div> <div></div> <div>2%</div> <div>76%</div> <div>11%</div> <div>13%</div> </div>
1	G	255	<div> <div></div> <div>3%</div> <div>75%</div> <div>12%</div> <div>13%</div> </div>
1	H	255	<div> <div></div> <div>2%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15212 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	221	Total	C	I	N	O	S	0	2	0
			1776	1135	1	299	332	9			
1	B	217	Total	C	I	N	O	S	0	4	0
			1772	1130	1	302	330	9			
1	C	217	Total	C	I	N	O	S	0	5	0
			1768	1130	1	299	329	9			
1	D	216	Total	C	I	N	O	S	0	3	0
			1753	1121	1	296	326	9			
1	E	219	Total	C	I	N	O	S	0	2	0
			1770	1130	1	298	332	9			
1	F	221	Total	C	I	N	O	S	0	3	0
			1782	1139	1	299	334	9			
1	G	221	Total	C	I	N	O	S	0	2	0
			1770	1129	1	298	333	9			
1	H	217	Total	C	I	N	O	S	0	3	0
			1752	1120	1	294	328	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	KZG	CYS	chromophore	UNP Q5TLG6
A	63	KZG	TYR	chromophore	UNP Q5TLG6
A	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
B	63	KZG	TYR	chromophore	UNP Q5TLG6
B	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
C	63	KZG	TYR	chromophore	UNP Q5TLG6
C	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
D	63	KZG	TYR	chromophore	UNP Q5TLG6
D	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
E	63	KZG	TYR	chromophore	UNP Q5TLG6
E	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
F	63	KZG	TYR	chromophore	UNP Q5TLG6
F	63	KZG	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	KZG	CYS	chromophore	UNP Q5TLG6
G	63	KZG	TYR	chromophore	UNP Q5TLG6
G	63	KZG	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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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	KZG	CYS	chromophore	UNP Q5TLG6
H	63	KZG	TYR	chromophore	UNP Q5TLG6
H	63	KZG	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

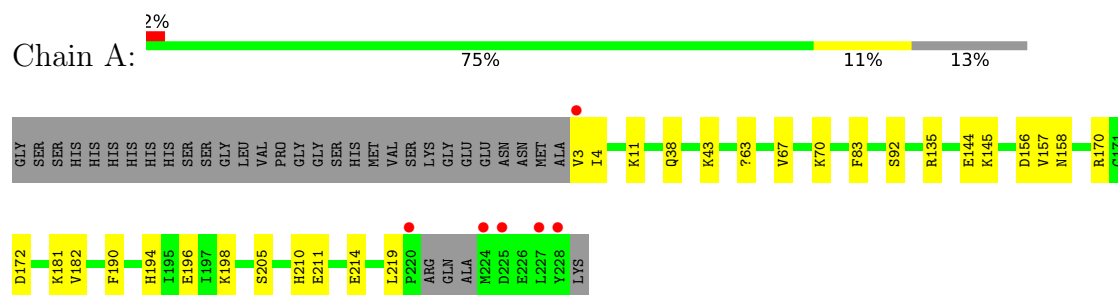
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	137	Total	O	0	0
			137	137		
2	B	142	Total	O	0	0
			142	142		
2	C	146	Total	O	0	0
			146	146		
2	D	139	Total	O	0	0
			139	139		
2	E	132	Total	O	0	0
			132	132		
2	F	138	Total	O	0	0
			138	138		
2	G	130	Total	O	0	0
			130	130		
2	H	105	Total	O	0	0
			105	105		

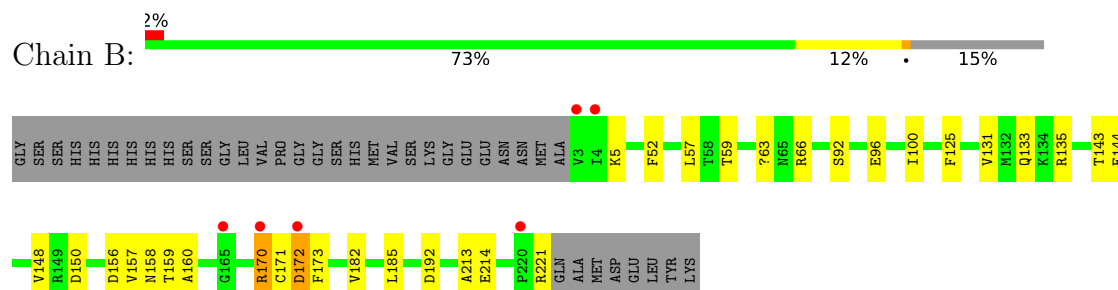
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

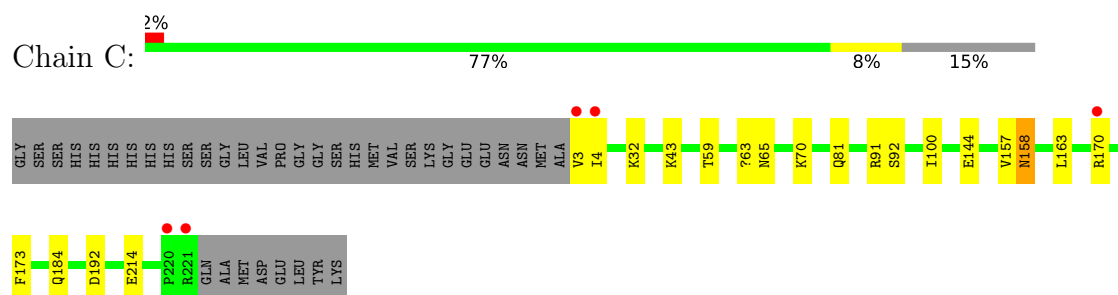
#### • Molecule 1: Fluorescent protein Dronpa



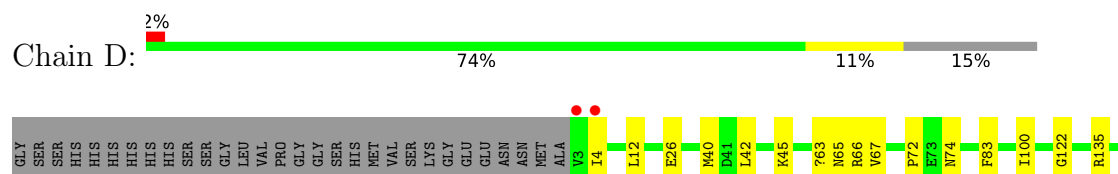
#### • Molecule 1: Fluorescent protein Dronpa

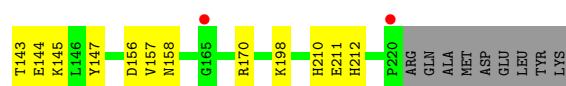


#### • Molecule 1: Fluorescent protein Dronpa

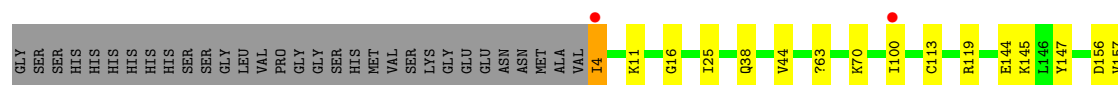
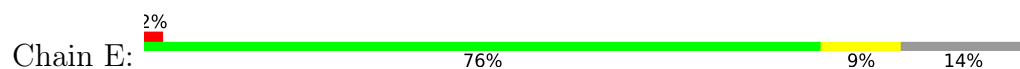


#### • Molecule 1: Fluorescent protein Dronpa

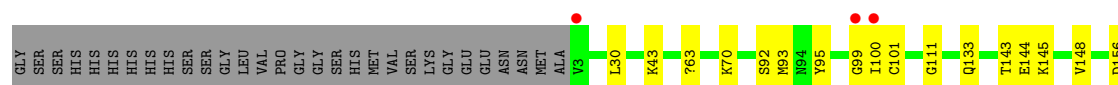
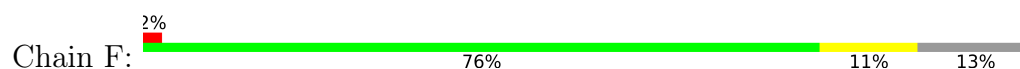




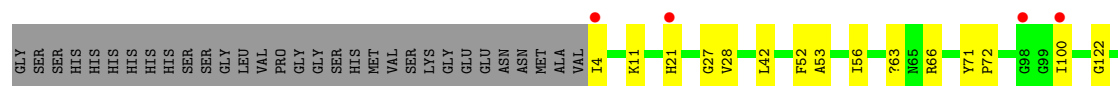
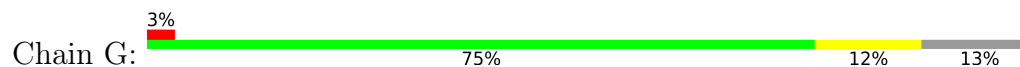
- Molecule 1: Fluorescent protein Dronpa



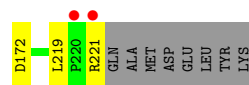
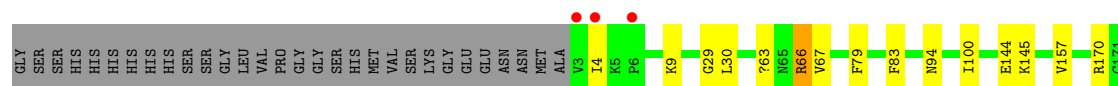
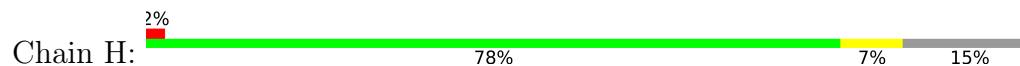
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.38Å 79.31Å 85.57Å 89.99° 87.62° 84.97°	Depositor
Resolution (Å)	37.54 – 2.10 39.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.7 (37.54-2.10) 81.2 (39.50-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, $R_{free}$	0.182 , 0.228 0.183 , 0.225	Depositor DCC
$R_{free}$ test set	1990 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.136 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KZG

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	0.33	0/1805	0.56	0/2436
1	B	0.50	0/1805	0.72	6/2437 (0.2%)
1	C	0.46	0/1805	0.63	1/2441 (0.0%)
1	D	0.37	0/1784	0.55	0/2411
1	E	0.43	0/1797	0.58	0/2427
1	F	0.42	0/1811	0.60	0/2444
1	G	0.46	0/1797	0.59	0/2429
1	H	0.36	0/1783	0.54	0/2413
All	All	0.42	0/14387	0.60	7/19438 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172[A]	ASP	CA-C-O	6.82	134.41	120.10
1	B	172[B]	ASP	CA-C-O	6.82	134.41	120.10
1	B	170[A]	ARG	CA-C-O	6.08	132.86	120.10
1	B	170[B]	ARG	CA-C-O	6.08	132.86	120.10
1	B	172[A]	ASP	CA-C-N	-5.75	104.55	117.20
1	B	172[B]	ASP	CA-C-N	-5.75	104.55	117.20
1	C	65	ASN	N-CA-C	-5.30	96.69	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1689	32	0
1	B	1772	0	1684	43	0
1	C	1768	0	1682	40	0
1	D	1753	0	1671	29	0
1	E	1770	0	1672	34	0
1	F	1782	0	1686	31	0
1	G	1770	0	1659	23	0
1	H	1752	0	1648	29	0
2	A	137	0	0	4	0
2	B	142	0	0	2	0
2	C	146	0	0	5	1
2	D	139	0	0	2	0
2	E	132	0	0	1	0
2	F	138	0	0	4	0
2	G	130	0	0	8	1
2	H	105	0	0	1	0
All	All	15212	0	13391	212	1

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 8.

All (212) 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:C:63:KZG:N	1:C:63:KZG:CA1	1.70	1.49
1:C:170[B]:ARG:HD2	1:E:145:LYS:NZ	1.57	1.19
1:H:9:LYS:HD2	1:H:30:LEU:HD22	1.23	1.14
1:A:158:ASN:ND2	1:B:158:ASN:OD1	1.82	1.11
1:C:158:ASN:OD1	1:E:158:ASN:OD1	1.72	1.06
1:C:158:ASN:OD1	1:E:158:ASN:CG	1.95	1.06
1:C:158:ASN:HB3	1:C:170[B]:ARG:NH2	1.73	1.04
1:C:170[B]:ARG:CD	1:E:145:LYS:NZ	2.28	0.96
1:H:9:LYS:HD2	1:H:30:LEU:CD2	1.97	0.93
1:C:170[B]:ARG:HD2	1:E:145:LYS:HZ3	1.24	0.92
1:H:66:ARG:HG2	1:H:79:PHE:CE1	2.04	0.92
1:H:29:GLY:O	1:H:30:LEU:HD23	1.71	0.90
1:C:170[B]:ARG:CD	1:E:145:LYS:HZ3	1.82	0.89
1:C:158:ASN:CB	1:C:170[B]:ARG:NH2	2.40	0.84
1:B:158:ASN:HB3	1:B:170[B]:ARG:NH1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.58	0.82
1:C:170[B]:ARG:HD2	1:E:145:LYS:CE	2.10	0.81
1:B:96:GLU:OE2	1:B:170[A]:ARG:HG2	1.84	0.78
1:H:66:ARG:HE	1:H:66:ARG:HA	1.51	0.75
1:C:158:ASN:HB3	1:C:170[B]:ARG:HH22	1.53	0.73
1:D:145:LYS:NZ	1:F:145[B]:LYS:NZ	2.35	0.73
1:C:158:ASN:HB2	1:C:170[B]:ARG:CZ	2.19	0.72
1:A:70:LYS:HB3	1:A:214:GLU:HG2	1.70	0.72
1:E:4:ILE:O	1:E:4:ILE:HG13	1.89	0.72
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.72	0.71
1:B:150:ASP:OD1	2:B:301:HOH:O	2.09	0.71
1:B:158:ASN:HB3	1:B:170[B]:ARG:CZ	2.22	0.70
1:H:66:ARG:HA	1:H:66:ARG:NE	2.06	0.69
1:F:92[A]:SER:OG	1:F:100:ILE:HD11	1.92	0.69
1:C:170[B]:ARG:NE	1:E:145:LYS:HZ3	1.91	0.69
1:F:95:TYR:HD1	1:F:99:GLY:O	1.76	0.68
1:A:156:ASP:OD1	1:B:170[B]:ARG:CD	2.42	0.68
1:C:170[B]:ARG:HD2	1:E:145:LYS:HZ1	1.58	0.68
1:C:170[B]:ARG:CD	1:E:145:LYS:HZ1	2.06	0.67
1:G:163:LEU:HD11	1:G:169:TYR:HB2	1.77	0.67
1:C:170[B]:ARG:NE	1:E:145:LYS:NZ	2.43	0.67
1:A:11:LYS:NZ	2:A:302:HOH:O	2.24	0.66
1:F:70:LYS:HB3	1:F:214:GLU:HG2	1.77	0.66
1:F:111:GLY:O	2:F:301:HOH:O	2.13	0.66
1:H:63:KZG:CA2	1:H:66:ARG:HH22	2.09	0.66
1:C:158:ASN:O	1:E:145:LYS:HD3	1.96	0.65
1:H:9:LYS:CD	1:H:30:LEU:HD22	2.14	0.65
1:G:226:GLU:OE2	2:G:301:HOH:O	2.15	0.65
1:B:182:VAL:HG12	1:F:184:GLN:HG3	1.79	0.64
1:A:144:GLU:HA	1:A:157:VAL:HB	1.80	0.64
1:G:4:ILE:HG13	1:G:4:ILE:O	1.97	0.64
1:C:158:ASN:CB	1:C:170[B]:ARG:CZ	2.76	0.63
1:F:133:GLN:NE2	2:F:304:HOH:O	2.32	0.62
1:B:170[B]:ARG:HH21	1:B:170[B]:ARG:HG2	1.64	0.62
1:E:158:ASN:HB3	1:E:170:ARG:NH1	2.14	0.62
1:D:145:LYS:NZ	1:F:145[B]:LYS:HZ2	1.97	0.62
1:C:3:VAL:HG13	1:C:4:ILE:HD12	1.82	0.61
1:D:144:GLU:HA	1:D:157:VAL:HB	1.83	0.61
1:H:63:KZG:CB2	1:H:66:ARG:HH22	2.14	0.61
1:A:170:ARG:HH21	1:B:156:ASP:HB3	1.67	0.60
1:B:158:ASN:HB3	1:B:170[B]:ARG:HH12	1.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ARG:HG2	1:H:79:PHE:CZ	2.36	0.60
1:B:144:GLU:HA	1:B:157:VAL:HB	1.83	0.60
1:C:170[A]:ARG:NH1	2:C:306:HOH:O	2.34	0.60
1:A:145:LYS:HZ1	1:B:143:THR:H	1.51	0.59
1:D:145:LYS:NZ	1:F:145[B]:LYS:HZ1	1.99	0.59
1:G:144:GLU:HA	1:G:157:VAL:HB	1.85	0.59
1:E:144:GLU:HA	1:E:157:VAL:HB	1.85	0.59
1:H:66:ARG:HB3	1:H:79:PHE:CG	2.37	0.58
1:H:144:GLU:HA	1:H:157:VAL:HB	1.85	0.58
1:B:96:GLU:CD	1:B:170[A]:ARG:HG2	2.23	0.58
1:E:145:LYS:HD2	1:E:188:TYR:OH	2.04	0.58
1:C:59[B]:THR:HG22	2:C:326:HOH:O	2.03	0.58
1:A:67:VAL:HG11	1:A:83:PHE:HE2	1.69	0.57
1:D:158:ASN:HB3	1:D:170:ARG:NH2	2.20	0.57
1:F:143:THR:O	1:F:145[B]:LYS:HE2	2.04	0.57
1:C:63:KZG:N	1:C:63:KZG:CB1	2.61	0.57
1:A:194:HIS:HE1	1:B:221:ARG:HG3	1.70	0.56
1:G:174:LYS:HD3	2:G:425:HOH:O	2.05	0.56
1:G:194:HIS:CE1	1:H:221:ARG:HA	2.40	0.56
1:A:67:VAL:HG11	1:A:83:PHE:CE2	2.40	0.56
1:D:145:LYS:HZ1	1:F:145[B]:LYS:HZ2	1.54	0.56
1:E:63:KZG:I	1:E:157:VAL:HG11	2.75	0.55
1:A:145:LYS:HG2	1:A:190:PHE:CD1	2.42	0.55
1:D:147:TYR:OH	1:F:170:ARG:HD3	2.06	0.55
1:D:4:ILE:HD11	1:D:83:PHE:HB2	1.89	0.55
1:A:170:ARG:NH1	1:A:172:ASP:OD2	2.39	0.55
1:D:67:VAL:HG11	1:D:83:PHE:HE2	1.72	0.55
1:D:170:ARG:NE	1:F:156:ASP:OD1	2.37	0.55
1:G:21[A]:HIS:HE2	1:G:52:PHE:HD2	1.54	0.54
1:B:158:ASN:HB3	1:B:170[B]:ARG:NH2	2.22	0.54
1:D:143:THR:H	1:F:145[A]:LYS:HZ1	1.55	0.54
1:A:158:ASN:ND2	1:B:158:ASN:CG	2.58	0.54
1:A:156:ASP:OD1	1:B:170[B]:ARG:HD2	2.07	0.54
1:H:63:KZG:C2	1:H:66:ARG:HH22	2.20	0.54
1:C:92[A]:SER:OG	1:C:100:ILE:HD11	2.09	0.53
2:G:383:HOH:O	1:H:145:LYS:HE2	2.08	0.53
1:B:159:THR:OG1	1:B:160:ALA:N	2.40	0.53
1:C:32:LYS:HB3	2:C:333:HOH:O	2.08	0.53
1:A:194:HIS:CE1	1:B:221:ARG:HG3	2.43	0.53
1:D:26:GLU:HB2	1:D:45:LYS:HE2	1.91	0.53
1:C:170[B]:ARG:HD3	1:E:156:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:VAL:HG21	1:H:83:PHE:CE2	2.44	0.52
1:B:159:THR:O	1:B:170[B]:ARG:NH2	2.43	0.52
1:D:211:GLU:HG2	1:D:212:HIS:N	2.24	0.52
1:A:3:VAL:HG12	1:A:4:ILE:HG13	1.92	0.52
1:E:158:ASN:ND2	1:E:170:ARG:HH12	2.07	0.52
1:D:12:LEU:HD21	1:D:40:MET:HE1	1.92	0.52
1:G:158:ASN:CB	1:G:170:ARG:HH22	2.23	0.52
1:C:144:GLU:HA	1:C:157:VAL:HB	1.92	0.51
1:H:66:ARG:HB3	1:H:79:PHE:CD1	2.46	0.51
1:F:30:LEU:HB2	2:F:307:HOH:O	2.11	0.51
1:F:95:TYR:CD1	1:F:99:GLY:O	2.61	0.51
1:H:66:ARG:NE	1:H:66:ARG:CA	2.73	0.51
1:D:12:LEU:HD21	1:D:40:MET:CE	2.40	0.50
1:D:65:ASN:OD1	1:D:67:VAL:HG13	2.12	0.50
1:B:5:LYS:CD	1:B:5:LYS:N	2.73	0.50
1:H:4:ILE:HD11	1:H:83:PHE:HB2	1.92	0.50
1:G:156:ASP:OD1	1:H:170:ARG:NE	2.41	0.49
1:D:158:ASN:OD1	1:F:158:ASN:ND2	2.45	0.49
1:G:156:ASP:OD2	2:G:302:HOH:O	2.20	0.49
1:C:43:LYS:NZ	2:C:311:HOH:O	2.45	0.49
1:D:67:VAL:HG11	1:D:83:PHE:CE2	2.47	0.49
1:H:67:VAL:HG21	1:H:83:PHE:HE2	1.76	0.49
1:E:158:ASN:HB3	1:E:170:ARG:CZ	2.42	0.49
1:C:63:KZG:N	1:C:63:KZG:C1	2.64	0.49
1:F:144:GLU:HA	1:F:157:VAL:HB	1.94	0.48
1:D:156:ASP:OD1	1:F:170:ARG:HD2	2.13	0.48
1:G:63:KZG:I	1:G:157:VAL:HG11	2.83	0.48
1:D:135:ARG:NH2	2:D:310:HOH:O	2.45	0.48
1:C:170[A]:ARG:HD3	1:E:147:TYR:OH	2.12	0.48
1:A:63:KZG:I	1:A:157:VAL:HG11	2.84	0.48
1:A:219:LEU:HD21	1:B:214:GLU:HG3	1.95	0.48
1:A:38:GLN:NE2	1:A:211:GLU:OE1	2.47	0.47
1:C:59[B]:THR:HG23	1:C:91:ARG:NH1	2.28	0.47
1:E:181:LYS:HB2	2:E:408:HOH:O	2.14	0.47
1:H:94:ASN:HA	1:H:100:ILE:HD13	1.95	0.47
1:A:83:PHE:O	1:A:181:LYS:NZ	2.48	0.47
1:B:158:ASN:CB	1:B:170[B]:ARG:HH12	2.26	0.47
1:B:52:PHE:CE1	1:B:57:LEU:HD21	2.49	0.47
1:F:100:ILE:HG13	1:F:101:CYS:H	1.79	0.47
1:B:172[A]:ASP:OD1	2:B:302:HOH:O	2.20	0.47
1:D:72:PRO:HB2	1:D:74:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:CYS:SG	1:B:173:PHE:HE1	2.37	0.47
1:A:145:LYS:HG3	2:A:324:HOH:O	2.14	0.47
1:G:4:ILE:HD11	2:G:429:HOH:O	2.15	0.47
1:B:92[A]:SER:OG	1:B:100:ILE:HD11	2.15	0.46
1:D:63:KZG:I	1:D:157:VAL:HG11	2.85	0.46
1:H:219:LEU:HA	1:H:219:LEU:HD23	1.79	0.46
1:G:71:TYR:HA	1:G:72:PRO:HD2	1.44	0.46
1:C:158:ASN:C	1:E:145:LYS:HZ2	2.18	0.46
1:G:133:GLN:NE2	2:G:308:HOH:O	2.41	0.46
1:E:38:GLN:NE2	1:E:211:GLU:OE1	2.48	0.46
1:A:170:ARG:NH2	1:B:156:ASP:HB3	2.30	0.46
1:A:158:ASN:CG	1:B:158:ASN:HD21	2.18	0.46
1:H:66:ARG:CG	1:H:79:PHE:CE1	2.89	0.46
1:B:170[B]:ARG:HG2	1:B:170[B]:ARG:NH2	2.30	0.46
1:C:59[B]:THR:HG23	1:C:91:ARG:HH11	1.81	0.45
1:A:135:ARG:NH1	2:A:313:HOH:O	2.50	0.45
1:A:198:LYS:HG3	1:A:210:HIS:CD2	2.51	0.45
1:G:194:HIS:HE1	1:H:221:ARG:HA	1.80	0.44
1:G:100:ILE:O	1:G:122:GLY:HA2	2.17	0.44
1:C:163:LEU:HD11	1:F:227:LEU:HD13	1.99	0.44
1:F:100:ILE:CG1	1:F:101:CYS:N	2.81	0.44
1:C:81:GLN:OE1	1:C:184:GLN:HB3	2.17	0.44
1:D:40:MET:HE2	1:D:42:LEU:HD21	2.00	0.44
1:D:100:ILE:O	1:D:122:GLY:HA2	2.18	0.44
1:G:200:HIS:NE2	2:G:307:HOH:O	2.36	0.44
1:B:157:VAL:O	1:B:173:PHE:HB2	2.17	0.44
1:E:16:GLY:HA2	1:E:119:ARG:CZ	2.48	0.43
1:F:145[B]:LYS:HG2	1:F:156:ASP:O	2.18	0.43
2:C:308:HOH:O	1:E:174:LYS:NZ	2.51	0.43
1:B:171:CYS:HG	1:B:173:PHE:HE1	1.54	0.43
1:F:93:MET:O	1:F:100:ILE:HG13	2.18	0.43
1:E:11:LYS:HB2	1:E:113:CYS:SG	2.58	0.43
1:H:172:ASP:OD2	2:H:301:HOH:O	2.21	0.43
1:A:196:GLU:OE2	1:B:221:ARG:HG2	2.18	0.43
1:G:66:ARG:NH1	2:G:309:HOH:O	2.43	0.43
1:A:181:LYS:HG2	1:A:182:VAL:N	2.34	0.42
1:D:135:ARG:NE	2:D:312:HOH:O	2.46	0.42
1:B:148:VAL:HG21	1:B:185:LEU:HB3	2.00	0.42
1:D:198:LYS:HG3	1:D:210:HIS:ND1	2.34	0.42
1:G:27:GLY:HA3	1:G:42:LEU:HD23	1.99	0.42
1:C:63:KZG:I	1:C:157:VAL:HG11	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:KZG:I	1:F:157:VAL:HG11	2.90	0.42
1:A:219:LEU:HG	1:B:192:ASP:HB3	2.02	0.42
1:D:145:LYS:HZ1	1:F:145[B]:LYS:NZ	2.14	0.42
1:A:158:ASN:CG	1:B:158:ASN:ND2	2.73	0.42
1:C:59[B]:THR:HG21	1:C:173:PHE:CE2	2.54	0.42
1:A:92[A]:SER:HB3	1:E:100:ILE:HG21	2.02	0.42
1:E:25:ILE:HG12	1:E:44:VAL:HG22	2.00	0.42
1:H:66:ARG:O	1:H:67:VAL:C	2.58	0.42
1:B:158:ASN:C	1:B:170[B]:ARG:HH22	2.23	0.42
1:E:158:ASN:HB3	1:E:170:ARG:HH12	1.84	0.42
1:H:63:KZG:I	1:H:157:VAL:HG11	2.90	0.42
1:C:158:ASN:OD1	1:E:158:ASN:ND2	2.50	0.42
1:B:171:CYS:SG	1:B:173:PHE:CE1	3.08	0.41
1:D:145:LYS:HZ3	1:F:145[B]:LYS:NZ	2.13	0.41
1:F:157:VAL:HG13	1:F:173:PHE:HB2	2.03	0.41
1:G:142:SER:OG	1:G:193:HIS:HB2	2.21	0.41
1:A:145:LYS:HE3	2:A:324:HOH:O	2.20	0.41
1:B:133:GLN:HG3	1:B:135[B]:ARG:NH2	2.36	0.41
1:F:195:ILE:HG22	2:F:325:HOH:O	2.19	0.41
1:G:53:ALA:O	1:G:56:ILE:HG12	2.20	0.41
1:B:125:PHE:CE1	1:B:131:VAL:HG21	2.56	0.41
1:D:158:ASN:HB3	1:D:170:ARG:CZ	2.51	0.41
1:H:63:KZG:CB2	1:H:66:ARG:NH2	2.83	0.41
1:C:192:ASP:HB3	1:E:219:LEU:HG	2.03	0.40
1:F:148:VAL:HG21	1:F:185:LEU:HB3	2.02	0.40
1:G:11:LYS:HG2	1:G:28:VAL:HG12	2.04	0.40
1:A:43:LYS:HA	1:A:205:SER:O	2.20	0.40
1:C:170[A]:ARG:HD3	1:E:147:TYR:CZ	2.56	0.40
1:B:192:ASP:O	1:B:213:ALA:HA	2.22	0.40
1:B:59:THR:O	1:B:63:KZG:C2	2.69	0.40
1:B:159:THR:O	1:B:170[B]:ARG:HG2	2.20	0.40
1:F:43:LYS:HA	1:F:205:SER:O	2.21	0.40

All (1) 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)
2:C:440:HOH:O	2:G:423:HOH:O[1_554]	2.17	0.03

## 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	218/255 (86%)	215 (99%)	3 (1%)	0	100	100
1	B	218/255 (86%)	214 (98%)	4 (2%)	0	100	100
1	C	219/255 (86%)	215 (98%)	4 (2%)	0	100	100
1	D	216/255 (85%)	212 (98%)	4 (2%)	0	100	100
1	E	216/255 (85%)	213 (99%)	3 (1%)	0	100	100
1	F	219/255 (86%)	216 (99%)	3 (1%)	0	100	100
1	G	218/255 (86%)	213 (98%)	5 (2%)	0	100	100
1	H	217/255 (85%)	210 (97%)	7 (3%)	0	100	100
All	All	1741/2040 (85%)	1708 (98%)	33 (2%)	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	188/217 (87%)	188 (100%)	0	100	100
1	B	187/217 (86%)	186 (100%)	1 (0%)	90	93
1	C	188/217 (87%)	187 (100%)	1 (0%)	90	93
1	D	187/217 (86%)	186 (100%)	1 (0%)	90	93
1	E	187/217 (86%)	186 (100%)	1 (0%)	90	93
1	F	187/217 (86%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	185/217 (85%)	184 (100%)	1 (0%)	90	93
1	H	184/217 (85%)	183 (100%)	1 (0%)	90	93
All	All	1493/1736 (86%)	1487 (100%)	6 (0%)	92	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	66	ARG
1	C	158	ASN
1	D	66	ARG
1	E	4	ILE
1	G	187	ASP
1	H	66	ARG

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	KZG	A	63	1	23,23,24	1.05	2 (8%)	30,32,34	2.28	6 (20%)
1	KZG	B	63	1	23,23,24	1.05	1 (4%)	30,32,34	2.26	6 (20%)
1	KZG	C	63	1	23,23,24	2.30	11 (47%)	30,32,34	3.21	13 (43%)
1	KZG	D	63	1	23,23,24	0.98	1 (4%)	30,32,34	2.16	7 (23%)
1	KZG	E	63	1	23,23,24	1.03	1 (4%)	30,32,34	2.47	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KZG	F	63	1	23,23,24	0.99	1 (4%)	30,32,34	2.21	7 (23%)
1	KZG	G	63	1	23,23,24	1.05	1 (4%)	30,32,34	2.27	6 (20%)
1	KZG	H	63	1	23,23,24	1.06	1 (4%)	30,32,34	2.33	7 (23%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	KZG	C1-N2	-5.27	1.24	1.32
1	C	63	KZG	CA2-C2	-4.87	1.43	1.48
1	C	63	KZG	C2-N3	-2.97	1.32	1.39
1	C	63	KZG	CA2-N2	-2.94	1.32	1.38
1	C	63	KZG	O2-C2	-2.59	1.17	1.23
1	C	63	KZG	CD1-CG2	-2.25	1.36	1.39
1	C	63	KZG	CA1-C1	-2.20	1.48	1.51
1	C	63	KZG	CD1-CE1	-2.10	1.34	1.39
1	C	63	KZG	C1-N3	-2.07	1.33	1.37
1	C	63	KZG	OH-CZ	-2.03	1.32	1.36
1	A	63	KZG	C2-N3	-2.00	1.35	1.39
1	F	63	KZG	CB2-CA2	3.62	1.38	1.35
1	A	63	KZG	CB2-CA2	3.72	1.38	1.35
1	D	63	KZG	CB2-CA2	3.74	1.38	1.35
1	E	63	KZG	CB2-CA2	3.75	1.38	1.35
1	C	63	KZG	CA1-N	3.98	1.70	1.49
1	B	63	KZG	CB2-CA2	3.99	1.38	1.35
1	G	63	KZG	CB2-CA2	4.06	1.38	1.35
1	H	63	KZG	CB2-CA2	4.18	1.38	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	KZG	O2-C2-CA2	-9.37	125.70	130.96
1	A	63	KZG	O2-C2-CA2	-7.94	126.50	130.96
1	G	63	KZG	O2-C2-CA2	-7.84	126.56	130.96
1	H	63	KZG	O2-C2-CA2	-7.65	126.67	130.96
1	F	63	KZG	O2-C2-CA2	-7.49	126.75	130.96
1	D	63	KZG	O2-C2-CA2	-7.23	126.90	130.96
1	B	63	KZG	O2-C2-CA2	-7.19	126.92	130.96
1	C	63	KZG	O2-C2-CA2	-6.49	127.32	130.96
1	C	63	KZG	C2-CA2-N2	-5.83	104.84	108.92
1	H	63	KZG	C2-CA2-N2	-4.77	105.58	108.92
1	B	63	KZG	C2-CA2-N2	-4.69	105.63	108.92
1	G	63	KZG	C2-CA2-N2	-4.59	105.70	108.92
1	A	63	KZG	C2-CA2-N2	-4.46	105.79	108.92
1	F	63	KZG	C2-CA2-N2	-4.44	105.81	108.92
1	E	63	KZG	C2-CA2-N2	-4.43	105.82	108.92
1	C	63	KZG	O-C-CA3	-4.31	113.39	126.39
1	D	63	KZG	C2-CA2-N2	-4.06	106.08	108.92
1	C	63	KZG	CG2-CB2-CA2	-3.56	125.65	130.01
1	C	63	KZG	CA1-CB1-SG1	-3.42	106.73	114.42
1	C	63	KZG	C2-N3-C1	-3.22	106.30	107.97
1	B	63	KZG	CA1-CB1-SG1	-2.95	107.79	114.42
1	B	63	KZG	O-C-CA3	-2.74	118.13	126.39
1	D	63	KZG	O-C-CA3	-2.63	118.46	126.39
1	H	63	KZG	O-C-CA3	-2.59	118.56	126.39
1	A	63	KZG	O-C-CA3	-2.56	118.65	126.39
1	H	63	KZG	CA1-CB1-SG1	-2.55	108.67	114.42
1	H	63	KZG	CG2-CB2-CA2	-2.51	126.94	130.01
1	C	63	KZG	CE2-CD2-CG2	-2.49	117.99	121.26
1	D	63	KZG	CA1-CB1-SG1	-2.41	109.00	114.42
1	D	63	KZG	CG2-CB2-CA2	-2.40	127.08	130.01
1	A	63	KZG	CA1-CB1-SG1	-2.27	109.32	114.42
1	C	63	KZG	CD1-CE1-CZ	-2.23	117.99	120.62
1	F	63	KZG	CG2-CB2-CA2	-2.21	127.31	130.01
1	E	63	KZG	O-C-CA3	-2.21	119.72	126.39
1	G	63	KZG	CA1-CB1-SG1	-2.20	109.47	114.42
1	F	63	KZG	CA1-CB1-SG1	-2.18	109.51	114.42
1	G	63	KZG	O-C-CA3	-2.13	119.96	126.39
1	F	63	KZG	O-C-CA3	-2.09	120.09	126.39
1	E	63	KZG	O2-C2-N3	2.14	128.66	124.31
1	C	63	KZG	CG2-CD1-CE1	2.28	123.47	120.00
1	D	63	KZG	CA2-C2-N3	3.83	105.18	103.35
1	C	63	KZG	CB2-CA2-C2	3.95	127.05	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	KZG	CA2-N2-C1	4.04	108.75	105.77
1	A	63	KZG	CA2-N2-C1	4.25	108.91	105.77
1	G	63	KZG	CA2-N2-C1	4.25	108.91	105.77
1	F	63	KZG	CA2-N2-C1	4.27	108.92	105.77
1	B	63	KZG	CA2-N2-C1	4.41	109.02	105.77
1	H	63	KZG	CA2-N2-C1	4.54	109.12	105.77
1	H	63	KZG	CA2-C2-N3	4.68	105.59	103.35
1	F	63	KZG	CA2-C2-N3	4.73	105.61	103.35
1	E	63	KZG	CA2-C2-N3	4.77	105.63	103.35
1	E	63	KZG	CA2-N2-C1	4.77	109.29	105.77
1	B	63	KZG	CA2-C2-N3	4.80	105.65	103.35
1	G	63	KZG	CA2-C2-N3	5.05	105.77	103.35
1	A	63	KZG	CA2-C2-N3	5.21	105.84	103.35
1	C	63	KZG	CA2-C2-N3	5.77	106.11	103.35
1	C	63	KZG	CA2-N2-C1	6.10	110.27	105.77
1	C	63	KZG	CB1-CA1-C1	7.41	126.02	110.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	KZG	1	0
1	B	63	KZG	1	0
1	C	63	KZG	4	0
1	D	63	KZG	1	0
1	E	63	KZG	1	0
1	F	63	KZG	1	0
1	G	63	KZG	1	0
1	H	63	KZG	5	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 [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	220/255 (86%)	0.10	6 (2%)	54	61	25, 34, 54, 79	0
1	B	216/255 (84%)	0.03	6 (2%)	53	59	24, 33, 52, 71	0
1	C	216/255 (84%)	-0.01	5 (2%)	60	65	23, 34, 53, 76	0
1	D	215/255 (84%)	-0.05	4 (1%)	66	71	24, 33, 51, 68	0
1	E	218/255 (85%)	0.01	6 (2%)	53	59	24, 35, 57, 74	0
1	F	220/255 (86%)	0.03	6 (2%)	54	61	25, 34, 53, 87	0
1	G	220/255 (86%)	0.08	8 (3%)	42	49	26, 38, 59, 82	0
1	H	216/255 (84%)	0.09	5 (2%)	60	65	26, 38, 56, 79	0
All	All	1741/2040 (85%)	0.04	46 (2%)	56	62	23, 35, 55, 87	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170[A]	ARG	4.5
1	E	4	ILE	4.2
1	G	228	TYR	4.1
1	A	227	LEU	3.8
1	A	3	VAL	3.7
1	F	224	MET	3.2
1	H	4	ILE	3.2
1	H	3	VAL	3.2
1	C	170[A]	ARG	3.2
1	G	227	LEU	3.2
1	F	100	ILE	3.1
1	B	4	ILE	3.1
1	F	3	VAL	3.1
1	C	4	ILE	2.9
1	E	227	LEU	2.7
1	C	3	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	221	ARG	2.7
1	D	4	ILE	2.7
1	D	165	GLY	2.7
1	G	220	PRO	2.7
1	B	3	VAL	2.6
1	F	99	GLY	2.6
1	A	228	TYR	2.6
1	D	3	VAL	2.6
1	C	221	ARG	2.6
1	G	223	ALA	2.6
1	D	220	PRO	2.6
1	B	165	GLY	2.6
1	G	100	ILE	2.4
1	F	172[A]	ASP	2.4
1	H	220	PRO	2.4
1	E	228	TYR	2.4
1	A	225	ASP	2.4
1	G	98	GLY	2.3
1	E	165	GLY	2.3
1	E	225	ASP	2.3
1	A	224	MET	2.3
1	H	6	PRO	2.3
1	B	220	PRO	2.2
1	E	100	ILE	2.2
1	G	4	ILE	2.1
1	C	220	PRO	2.1
1	A	220	PRO	2.1
1	B	172[A]	ASP	2.1
1	F	220	PRO	2.0
1	G	21[A]	HIS	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	KZG	C	63	22/23	0.99	0.09	23,29,36,36	0
1	KZG	A	63	22/23	0.99	0.10	21,26,34,40	0
1	KZG	G	63	22/23	0.99	0.10	26,33,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KZG	E	63	22/23	0.99	0.10	20,26,30,35	0
1	KZG	D	63	22/23	0.99	0.09	22,27,32,36	0
1	KZG	B	63	22/23	0.99	0.10	21,27,34,39	0
1	KZG	H	63	22/23	0.99	0.09	25,31,37,39	0
1	KZG	F	63	22/23	0.99	0.11	23,29,33,35	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.