



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2019 – 02:13 PM EDT

PDB ID : 6NQS  
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2)- Y63(3-OMeY)  
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.  
Deposited on : 2019-01-21  
Resolution : 2.50 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

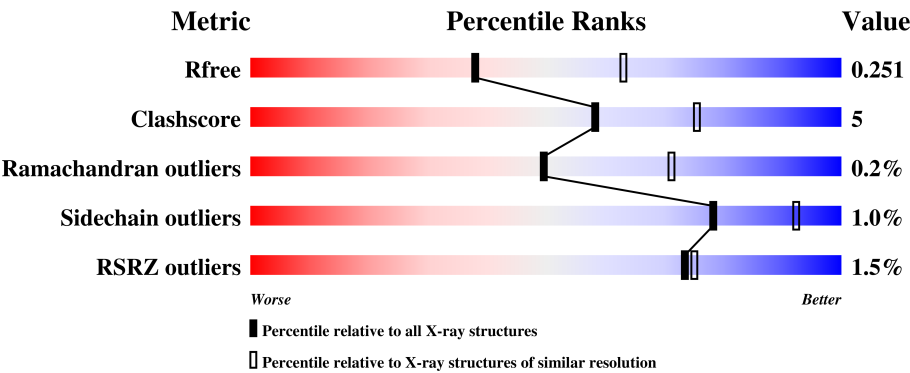
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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 <sub>free</sub>	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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>%</div><div><div></div><div>76%</div><div>11%</div><div>13%</div></div></div>
1	B	255	<div><div>%</div><div><div></div><div>77%</div><div>11%</div><div>12%</div></div></div>
1	C	255	<div><div></div><div><div></div><div>78%</div><div>6%</div><div>16%</div></div></div>
1	D	255	<div><div></div><div><div></div><div>73%</div><div>11%</div><div>16%</div></div></div>
1	E	255	<div><div></div><div><div></div><div>75%</div><div>10%</div><div>15%</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	255	 % 75% 10% 15%
1	G	255	 4% 76% 10% 13%
1	H	255	 3% 78% 9% 13%

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	KXV	E	63	X	-	-	-
1	KXV	F	63	X	-	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14760 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	222	Total	C	N	O	S	0	3	0
			1790	1143	301	337	9			
1	B	224	Total	C	N	O	S	0	4	0
			1814	1159	304	341	10			
1	C	214	Total	C	N	O	S	0	5	0
			1737	1108	291	329	9			
1	D	215	Total	C	N	O	S	0	4	0
			1755	1121	297	328	9			
1	E	216	Total	C	N	O	S	0	4	0
			1751	1119	294	329	9			
1	F	216	Total	C	N	O	S	0	4	0
			1755	1122	295	329	9			
1	G	222	Total	C	N	O	S	0	1	0
			1770	1132	298	331	9			
1	H	223	Total	C	N	O	S	0	2	0
			1785	1139	302	335	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
A	63	KXV	TYR	chromophore	UNP Q5TLG6
A	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
B	63	KXV	TYR	chromophore	UNP Q5TLG6
B	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
C	63	KXV	TYR	chromophore	UNP Q5TLG6
C	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
D	63	KXV	TYR	chromophore	UNP Q5TLG6
D	63	KXV	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

*Continued on next page...*



*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
E	63	KXV	TYR	chromophore	UNP Q5TLG6
E	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
F	63	KXV	TYR	chromophore	UNP Q5TLG6
F	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
G	63	KXV	TYR	chromophore	UNP Q5TLG6
G	63	KXV	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

*Continued on next page...*

*Continued from previous page...*

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	KXV	CYS	chromophore	UNP Q5TLG6
H	63	KXV	TYR	chromophore	UNP Q5TLG6
H	63	KXV	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

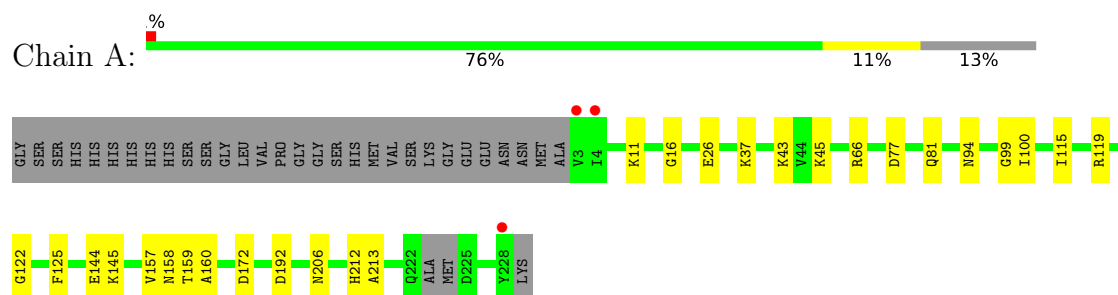
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	78	Total O 78 78	0	0
2	B	82	Total O 82 82	0	0
2	C	69	Total O 69 69	0	0
2	D	72	Total O 72 72	0	0
2	E	72	Total O 72 72	0	0
2	F	85	Total O 85 85	0	0
2	G	71	Total O 71 71	0	0
2	H	74	Total O 74 74	0	0

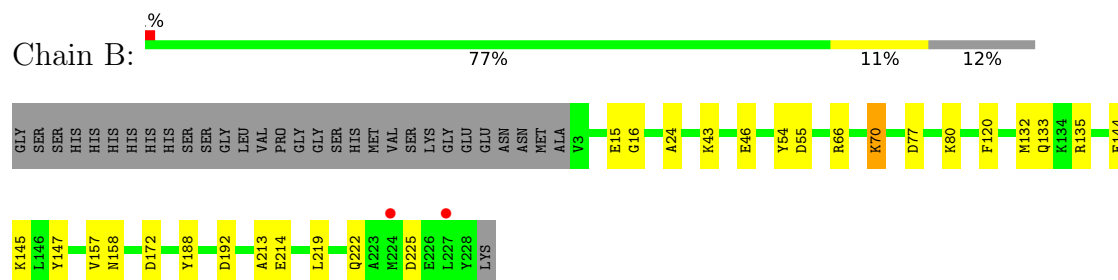
### 3 Residue-property plots [i](#)

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.

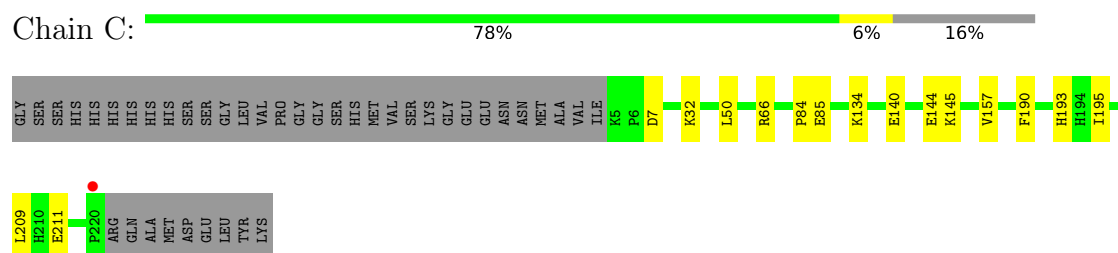
#### • Molecule 1: Fluorescent protein Dronpa



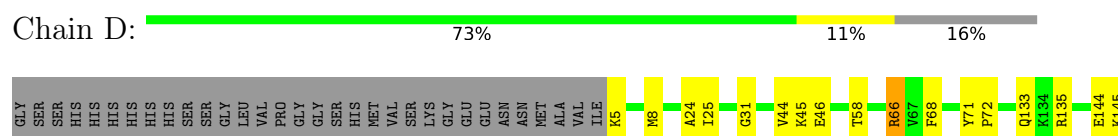
#### • Molecule 1: Fluorescent protein Dronpa



#### • Molecule 1: Fluorescent protein Dronpa

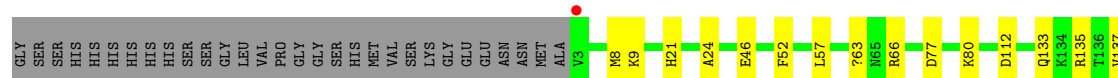
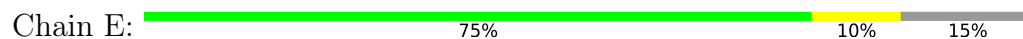


#### • Molecule 1: Fluorescent protein Dronpa

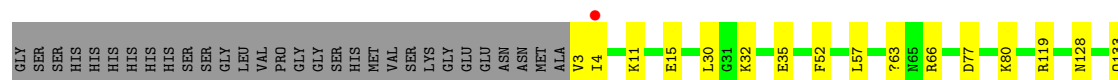
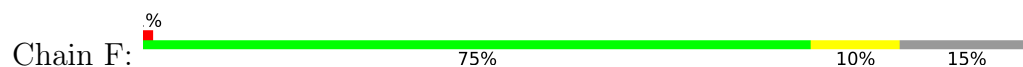




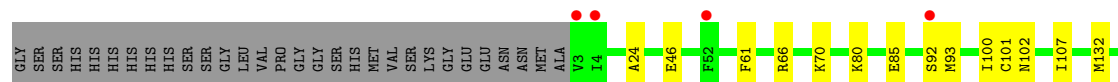
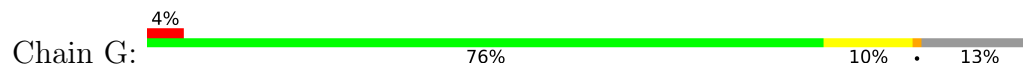
- Molecule 1: Fluorescent protein Dronpa



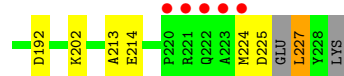
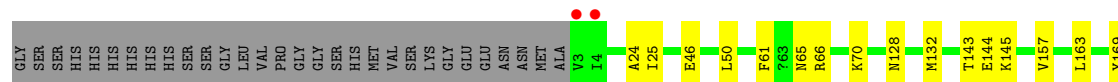
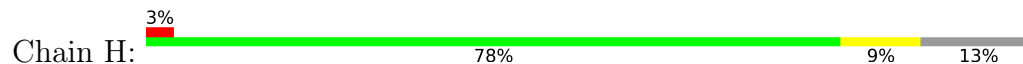
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.40Å 86.49Å 144.08Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	39.87 – 2.50 39.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.87-2.50) 88.3 (39.87-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, $R_{free}$	0.214 , 0.251 0.217 , 0.251	Depositor DCC
$R_{free}$ test set	2007 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.754	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.11 % 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 4.4159e-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

### 5.1 Standard geometry

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

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	0.36	0/1819	0.60	0/2458
1	B	0.41	0/1850	0.60	0/2499
1	C	0.39	0/1773	0.59	0/2400
1	D	0.41	0/1791	0.59	0/2419
1	E	0.51	0/1784	0.65	0/2413
1	F	0.49	0/1788	0.60	0/2419
1	G	0.46	0/1796	0.64	0/2427
1	H	0.39	0/1811	0.61	1/2446 (0.0%)
All	All	0.43	0/14412	0.61	1/19481 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	0
1	F	1	0
1	G	0	1
1	H	0	1
All	All	2	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	65	ASN	N-CA-C	-5.61	95.85	111.00

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	E	63	KXV	CA1
1	F	63	KXV	CA1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	61	PHE	Mainchain
1	H	61	PHE	Mainchain

## 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	1790	0	1679	15	0
1	B	1814	0	1715	18	0
1	C	1737	0	1618	10	0
1	D	1755	0	1662	24	0
1	E	1751	0	1642	22	0
1	F	1755	0	1659	19	0
1	G	1770	0	1658	22	0
1	H	1785	0	1674	13	0
2	A	78	0	0	1	0
2	B	82	0	0	8	0
2	C	69	0	0	2	0
2	D	72	0	0	4	0
2	E	72	0	0	8	0
2	F	85	0	0	3	0
2	G	71	0	0	5	0
2	H	74	0	0	3	0
All	All	14760	0	13307	142	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 5.

All (142) 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:E:63:KXV:CA1	1:E:63:KXV:N	1.69	1.56
1:F:63:KXV:N	1:F:63:KXV:CA1	1.68	1.51
1:G:219:LEU:CB	1:G:220:PRO:HD3	1.34	1.39
1:G:219:LEU:CB	1:G:220:PRO:CD	2.00	1.30
1:D:198:LYS:HE2	1:D:210:HIS:CD2	2.02	0.95
1:D:198:LYS:HE2	1:D:210:HIS:CG	2.08	0.88
1:D:133[B]:GLN:OE1	1:D:135:ARG:NH1	2.11	0.84
1:B:158:ASN:ND2	1:B:172:ASP:OD1	2.13	0.81
1:E:168:HIS:O	1:G:227:LEU:O	1.99	0.80
1:G:93:MET:O	1:G:100:ILE:HG23	1.82	0.80
1:G:219:LEU:CB	1:G:220:PRO:HD2	2.12	0.78
1:G:92:SER:HB2	1:G:102:ASN:OD1	1.85	0.76
1:A:145:LYS:NZ	2:A:301:HOH:O	2.18	0.76
1:E:133[A]:GLN:OE1	1:E:135:ARG:NH1	2.20	0.74
1:G:70:LYS:NZ	2:G:301:HOH:O	2.22	0.72
1:A:77:ASP:O	1:A:81:GLN:NE2	2.18	0.67
1:B:219:LEU:HD23	1:B:219:LEU:H	1.60	0.65
1:F:144:GLU:HA	1:F:157:VAL:HB	1.79	0.65
1:E:77:ASP:OD1	2:E:301:HOH:O	2.14	0.65
1:F:133[B]:GLN:OE1	1:F:135:ARG:NH1	2.30	0.64
1:F:4:ILE:HD12	2:F:383:HOH:O	1.98	0.64
1:F:11:LYS:NZ	2:F:305:HOH:O	2.29	0.63
1:F:4:ILE:HD13	1:F:80:LYS:HG2	1.80	0.63
1:D:198:LYS:CE	1:D:210:HIS:CE1	2.82	0.63
1:E:21[A]:HIS:ND1	2:E:308:HOH:O	2.31	0.63
1:G:227:LEU:HD23	1:G:227:LEU:N	2.15	0.61
1:C:144:GLU:HA	1:C:157:VAL:HB	1.83	0.60
1:G:144:GLU:HA	1:G:157:VAL:HB	1.83	0.60
1:G:138:LYS:HB2	2:G:335:HOH:O	2.04	0.58
1:D:144:GLU:HA	1:D:157:VAL:HB	1.86	0.58
1:E:144:GLU:HA	1:E:157:VAL:HB	1.87	0.57
1:D:66:ARG:HD3	2:D:326:HOH:O	2.04	0.56
1:C:85:GLU:OE2	1:C:85:GLU:N	2.39	0.56
1:E:157:VAL:HG13	1:E:173:PHE:HB2	1.88	0.56
1:B:133[B]:GLN:OE1	1:B:135:ARG:NH1	2.38	0.56
1:C:193:HIS:ND1	1:C:211:GLU:OE2	2.39	0.55
1:D:198:LYS:HE2	1:D:210:HIS:CE1	2.42	0.54
1:B:70:LYS:HE2	2:B:303:HOH:O	2.07	0.54
1:B:70:LYS:HB3	1:B:214:GLU:HG2	1.90	0.54
1:D:193:HIS:ND1	1:D:211:GLU:OE1	2.42	0.53
1:E:80:LYS:NZ	2:E:301:HOH:O	2.40	0.53
1:H:227:LEU:CD1	1:H:227:LEU:N	2.72	0.53

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:ND2	1:A:172:ASP:OD1	2.42	0.53
1:E:24:ALA:HB3	1:E:46:GLU:HB2	1.91	0.53
1:H:227:LEU:HD13	1:H:227:LEU:N	2.24	0.53
1:G:198:LYS:HG3	1:G:210:HIS:ND1	2.24	0.52
1:E:199:SER:HA	2:E:309:HOH:O	2.10	0.52
1:G:93:MET:HB3	1:G:171:CYS:SG	2.50	0.51
1:H:144:GLU:HA	1:H:157:VAL:HB	1.92	0.51
1:E:137:VAL:HG22	1:E:164:GLU:HG2	1.91	0.51
1:D:198:LYS:HE2	1:D:210:HIS:NE2	2.24	0.51
1:F:3:VAL:HG22	1:F:4:ILE:HG13	1.92	0.51
1:B:54:TYR:N	2:B:306:HOH:O	2.44	0.51
1:E:80:LYS:HD2	2:E:302:HOH:O	2.10	0.51
1:B:144:GLU:HA	1:B:157:VAL:HB	1.92	0.51
1:B:145:LYS:NZ	2:B:309:HOH:O	2.38	0.51
1:E:63:KXV:C1	1:E:63:KXV:N	2.63	0.50
1:A:26:GLU:HB2	1:A:45:LYS:HE3	1.94	0.50
1:H:143:THR:OG1	2:H:301:HOH:O	2.20	0.49
1:A:144:GLU:HA	1:A:157:VAL:HB	1.94	0.49
1:A:43:LYS:HE3	1:A:206:ASN:HD21	1.77	0.49
1:B:222:GLN:NE2	2:B:311:HOH:O	2.45	0.49
1:G:80:LYS:NZ	2:G:307:HOH:O	2.46	0.49
1:D:5:LYS:HB2	1:D:8:MET:SD	2.53	0.49
1:C:140:GLU:OE1	2:C:301:HOH:O	2.20	0.48
1:F:63:KXV:C1	1:F:63:KXV:N	2.64	0.48
1:F:77:ASP:OD1	1:F:80:LYS:HD2	2.14	0.48
1:C:50:LEU:O	1:C:134:LYS:NZ	2.42	0.48
1:E:46:GLU:HA	2:E:349:HOH:O	2.13	0.48
1:G:85:GLU:OE1	1:G:85:GLU:N	2.43	0.48
1:B:15:GLU:OE1	2:B:301:HOH:O	2.20	0.47
1:D:58:THR:HG23	1:D:209:LEU:HD11	1.97	0.47
1:E:200:HIS:N	2:E:309:HOH:O	2.31	0.47
1:A:11:LYS:HB3	1:A:115:ILE:HD13	1.96	0.47
1:C:195:ILE:HD11	1:C:209:LEU:HD21	1.97	0.47
1:E:145:LYS:O	1:E:155:GLY:HA2	2.14	0.47
1:F:198:LYS:HG3	1:F:210:HIS:CD2	2.49	0.47
1:C:140:GLU:OE2	2:C:302:HOH:O	2.20	0.47
1:B:132:MET:HG2	2:B:317:HOH:O	2.14	0.47
1:F:128:ASN:HA	1:F:133[B]:GLN:HE21	1.79	0.47
1:B:192:ASP:O	1:B:213:ALA:HA	2.14	0.46
1:G:93:MET:N	1:G:101:CYS:O	2.47	0.46
1:G:192:ASP:O	1:G:213:ALA:HA	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:LEU:HD21	1:H:169:TYR:HB2	1.97	0.46
1:D:66:ARG:HA	2:D:326:HOH:O	2.15	0.46
1:A:100:ILE:O	1:A:122:GLY:HA2	2.15	0.46
1:E:148:VAL:HG21	1:E:185:LEU:HB3	1.97	0.45
1:G:24:ALA:HB3	1:G:46:GLU:HB2	1.98	0.45
1:D:158:ASN:HB3	2:D:336:HOH:O	2.17	0.45
1:G:92:SER:HA	1:G:102:ASN:HA	1.96	0.45
1:F:32:LYS:HB3	1:F:35[B]:GLU:HG3	1.99	0.45
1:B:147:TYR:HB3	1:B:188:TYR:CD1	2.52	0.45
1:F:147:TYR:OH	2:F:301:HOH:O	2.21	0.45
1:F:147:TYR:N	1:F:147:TYR:CD1	2.84	0.45
1:D:148:VAL:HG21	1:D:185:LEU:HB3	1.99	0.44
1:D:31:GLY:HA3	1:D:68:PHE:CE1	2.53	0.44
1:G:226:GLU:O	1:G:227:LEU:HB2	2.18	0.44
1:A:16:GLY:HA2	1:A:119:ARG:CZ	2.47	0.44
1:D:192:ASP:O	1:D:213:ALA:HA	2.18	0.44
1:E:52:PHE:HE1	1:E:57:LEU:HD11	1.83	0.43
1:F:148:VAL:HG21	1:F:185:LEU:HB3	2.00	0.43
1:D:45:LYS:NZ	2:D:306:HOH:O	2.34	0.43
1:C:7[A]:ASP:OD1	1:C:32:LYS:HE2	2.18	0.43
1:H:192:ASP:O	1:H:213:ALA:HA	2.19	0.43
1:D:25:ILE:HG12	1:D:44:VAL:HG22	2.01	0.43
1:D:156:ASP:OD2	1:D:174:LYS:HA	2.19	0.42
1:D:198:LYS:HE2	1:D:210:HIS:ND1	2.32	0.42
1:D:24:ALA:HB3	1:D:46:GLU:HB2	2.01	0.42
1:E:9:LYS:HE3	1:E:112:ASP:OD2	2.20	0.42
1:G:107:ILE:O	1:G:180:LYS:NZ	2.52	0.42
1:B:43:LYS:NZ	2:B:314:HOH:O	2.48	0.42
1:H:24:ALA:HB3	1:H:46:GLU:HB2	2.00	0.42
1:G:132:MET:HG2	2:G:322:HOH:O	2.18	0.42
1:H:202:LYS:NZ	2:H:309:HOH:O	2.35	0.42
1:H:128:ASN:OD1	1:H:128:ASN:N	2.46	0.41
1:B:77:ASP:OD1	1:B:80:LYS:HD2	2.20	0.41
1:E:77:ASP:OD1	2:E:302:HOH:O	2.22	0.41
1:F:15:GLU:O	1:F:119:ARG:HA	2.21	0.41
1:H:132:MET:HG2	2:H:326:HOH:O	2.21	0.41
1:A:16:GLY:HA2	1:A:119:ARG:NH2	2.36	0.41
1:D:198:LYS:CE	1:D:210:HIS:NE2	2.83	0.41
1:H:224:MET:O	1:H:225:ASP:C	2.58	0.41
1:A:37:LYS:HE2	1:A:212:HIS:CE1	2.55	0.41
1:C:84:PRO:HD2	1:C:85:GLU:OE2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:MET:HE3	1:E:112:ASP:O	2.20	0.41
1:E:63:KXV:CB1	1:E:63:KXV:N	2.69	0.41
1:H:70:LYS:HB3	1:H:214:GLU:HG3	2.03	0.41
1:F:147:TYR:O	1:F:153:LEU:HD12	2.20	0.41
1:H:25:ILE:HD11	1:H:50:LEU:HD11	2.03	0.41
1:B:55:ASP:N	2:B:306:HOH:O	2.29	0.41
1:C:145:LYS:HD2	1:C:190:PHE:CD1	2.56	0.41
1:F:52:PHE:HE1	1:F:57:LEU:HD11	1.86	0.41
1:G:201:ASP:HB2	2:G:362:HOH:O	2.21	0.41
1:A:159:THR:OG1	1:A:160:ALA:N	2.52	0.41
1:A:99:GLY:HA3	1:A:125:PHE:CE1	2.55	0.40
1:B:16:GLY:HA3	1:B:120:PHE:O	2.21	0.40
1:D:58:THR:HG23	1:D:209:LEU:HD21	2.03	0.40
1:A:94:ASN:HB3	1:A:172:ASP:HB2	2.04	0.40
1:A:192:ASP:O	1:A:213:ALA:HA	2.22	0.40
1:B:24:ALA:HB3	1:B:46:GLU:HB2	2.04	0.40
1:D:71:TYR:HA	1:D:72:PRO:HD3	1.96	0.40
1:F:4:ILE:HD11	1:F:80:LYS:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/255 (86%)	215 (98%)	5 (2%)	0	100	100
1	B	225/255 (88%)	219 (97%)	5 (2%)	1 (0%)	36	57
1	C	216/255 (85%)	212 (98%)	4 (2%)	0	100	100
1	D	216/255 (85%)	213 (99%)	3 (1%)	0	100	100
1	E	217/255 (85%)	213 (98%)	4 (2%)	0	100	100
1	F	217/255 (85%)	212 (98%)	5 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	218/255 (86%)	211 (97%)	5 (2%)	2 (1%)	19	34
1	H	220/255 (86%)	216 (98%)	4 (2%)	0	100	100
All	All	1749/2040 (86%)	1711 (98%)	35 (2%)	3 (0%)	49	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	219	LEU
1	B	225	ASP
1	G	220	PRO

### 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	187/217 (86%)	186 (100%)	1 (0%)	90	97
1	B	191/217 (88%)	189 (99%)	2 (1%)	78	92
1	C	182/217 (84%)	181 (100%)	1 (0%)	90	97
1	D	185/217 (85%)	183 (99%)	2 (1%)	76	91
1	E	183/217 (84%)	182 (100%)	1 (0%)	90	97
1	F	186/217 (86%)	184 (99%)	2 (1%)	76	91
1	G	183/217 (84%)	180 (98%)	3 (2%)	65	86
1	H	186/217 (86%)	183 (98%)	3 (2%)	65	86
All	All	1483/1736 (85%)	1468 (99%)	15 (1%)	78	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	B	66	ARG
1	B	70	LYS
1	C	66	ARG

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	D	66	ARG
1	D	145	LYS
1	E	66	ARG
1	F	30	LEU
1	F	66	ARG
1	G	66	ARG
1	G	145	LYS
1	G	227	LEU
1	H	66	ARG
1	H	145	LYS
1	H	227	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	KXV	A	63	1	24,24,25	3.05	7 (29%)	31,33,35	3.47	10 (32%)
1	KXV	B	63	1	24,24,25	2.25	7 (29%)	31,33,35	3.30	10 (32%)
1	KXV	C	63	1	24,24,25	2.90	5 (20%)	31,33,35	2.99	10 (32%)
1	KXV	D	63	1	24,24,25	2.83	6 (25%)	31,33,35	2.97	8 (25%)
1	KXV	E	63	1	24,24,25	2.40	10 (41%)	31,33,35	3.05	13 (41%)
1	KXV	F	63	1	24,24,25	2.28	10 (41%)	31,33,35	3.03	13 (41%)
1	KXV	G	63	1	24,24,25	2.34	8 (33%)	31,33,35	3.51	12 (38%)
1	KXV	H	63	1	24,24,25	2.53	9 (37%)	31,33,35	3.50	10 (32%)

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	KXV	A	63	1	-	0/11/31/32	0/2/2/2
1	KXV	B	63	1	-	0/11/31/32	0/2/2/2
1	KXV	C	63	1	-	0/11/31/32	0/2/2/2
1	KXV	D	63	1	-	0/11/31/32	0/2/2/2
1	KXV	E	63	1	1/1/5/7	0/11/31/32	0/2/2/2
1	KXV	F	63	1	1/1/5/7	0/11/31/32	0/2/2/2
1	KXV	G	63	1	-	0/11/31/32	0/2/2/2
1	KXV	H	63	1	-	0/11/31/32	0/2/2/2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	KXV	CA2-C2	-12.57	1.36	1.48
1	C	63	KXV	CA2-C2	-11.82	1.36	1.48
1	D	63	KXV	CA2-C2	-11.53	1.37	1.48
1	B	63	KXV	CA2-C2	-5.45	1.43	1.48
1	H	63	KXV	CA2-C2	-5.44	1.43	1.48
1	E	63	KXV	C1-N2	-5.24	1.24	1.32
1	G	63	KXV	CA2-C2	-4.78	1.43	1.48
1	F	63	KXV	C1-N2	-4.78	1.25	1.32
1	H	63	KXV	C2-N3	-3.97	1.30	1.39
1	B	63	KXV	C2-N3	-3.84	1.30	1.39
1	G	63	KXV	C2-N3	-3.81	1.30	1.39
1	F	63	KXV	C2-N3	-3.66	1.31	1.39
1	E	63	KXV	CA2-C2	-3.58	1.45	1.48
1	F	63	KXV	CA2-C2	-3.55	1.45	1.48
1	F	63	KXV	CA2-N2	-3.51	1.31	1.38
1	A	63	KXV	C2-N3	-3.51	1.31	1.39
1	E	63	KXV	CA2-N2	-3.47	1.31	1.38
1	C	63	KXV	CB2-CA2	-3.44	1.32	1.35
1	C	63	KXV	C2-N3	-3.42	1.31	1.39
1	E	63	KXV	C2-N3	-3.40	1.31	1.39
1	H	63	KXV	CZ-CE1	-3.37	1.34	1.40
1	D	63	KXV	C2-N3	-3.30	1.32	1.39
1	E	63	KXV	CZ-CE1	-3.01	1.34	1.40
1	A	63	KXV	CB2-CA2	-2.96	1.32	1.35
1	H	63	KXV	C1-N3	-2.94	1.32	1.37
1	C	63	KXV	CA2-N2	-2.94	1.32	1.38
1	A	63	KXV	CA2-N2	-2.91	1.32	1.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	KXV	CD1-CE1	-2.79	1.33	1.38
1	F	63	KXV	CD1-CE1	-2.79	1.33	1.38
1	G	63	KXV	CZ-CE1	-2.73	1.35	1.40
1	F	63	KXV	CD2-CE2	-2.71	1.33	1.38
1	D	63	KXV	CA2-N2	-2.67	1.32	1.38
1	H	63	KXV	CD2-CE2	-2.67	1.33	1.38
1	E	63	KXV	CA1-C1	-2.66	1.47	1.51
1	B	63	KXV	C1-N2	-2.63	1.28	1.32
1	E	63	KXV	CD2-CE2	-2.60	1.34	1.38
1	H	63	KXV	C1-N2	-2.57	1.28	1.32
1	F	63	KXV	O4-CE1	-2.57	1.33	1.37
1	F	63	KXV	CA1-C1	-2.56	1.47	1.51
1	D	63	KXV	CB2-CA2	-2.55	1.32	1.35
1	E	63	KXV	O4-CE1	-2.52	1.33	1.37
1	B	63	KXV	CZ-CE1	-2.47	1.35	1.40
1	B	63	KXV	O2-C2	-2.32	1.18	1.23
1	A	63	KXV	O2-C2	-2.30	1.18	1.23
1	H	63	KXV	O2-C2	-2.24	1.18	1.23
1	G	63	KXV	C1-N3	-2.15	1.33	1.37
1	F	63	KXV	CZ-CE1	-2.10	1.36	1.40
1	G	63	KXV	C1-N2	-2.10	1.29	1.32
1	G	63	KXV	CD1-CE1	-2.03	1.35	1.38
1	B	63	KXV	CD2-CE2	-2.03	1.35	1.38
1	A	63	KXV	C1-N2	2.02	1.35	1.32
1	D	63	KXV	OH-CZ	2.09	1.40	1.36
1	C	63	KXV	CG2-CB2	3.31	1.53	1.46
1	G	63	KXV	CB2-CA2	3.36	1.38	1.35
1	A	63	KXV	CG2-CB2	3.45	1.53	1.46
1	H	63	KXV	CB2-CA2	3.58	1.38	1.35
1	F	63	KXV	CA1-N	3.65	1.68	1.49
1	D	63	KXV	CG2-CB2	3.75	1.54	1.46
1	E	63	KXV	CA1-N	3.81	1.69	1.49
1	G	63	KXV	CA3-C	5.64	1.68	1.49
1	B	63	KXV	CA3-C	5.66	1.68	1.49
1	H	63	KXV	CA3-C	5.84	1.69	1.49

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	KXV	O2-C2-CA2	-11.58	124.47	130.96
1	G	63	KXV	O-C-CA3	-11.37	92.07	126.39
1	B	63	KXV	O-C-CA3	-10.89	93.50	126.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	KXV	O-C-CA3	-10.47	94.80	126.39
1	C	63	KXV	O2-C2-CA2	-9.02	125.90	130.96
1	D	63	KXV	O2-C2-CA2	-8.61	126.13	130.96
1	H	63	KXV	C2-CA2-N2	-7.69	103.53	108.92
1	G	63	KXV	C2-CA2-N2	-7.04	103.99	108.92
1	H	63	KXV	O2-C2-CA2	-7.03	127.02	130.96
1	B	63	KXV	O2-C2-CA2	-6.57	127.27	130.96
1	G	63	KXV	O2-C2-CA2	-6.20	127.48	130.96
1	F	63	KXV	O2-C2-CA2	-5.70	127.76	130.96
1	B	63	KXV	C2-CA2-N2	-5.58	105.01	108.92
1	E	63	KXV	C2-CA2-N2	-5.28	105.22	108.92
1	D	63	KXV	N3-C1-N2	-4.87	108.08	111.45
1	E	63	KXV	O2-C2-CA2	-4.55	128.41	130.96
1	C	63	KXV	N3-C1-N2	-4.54	108.31	111.45
1	D	63	KXV	CF-O4-CE1	-4.31	111.15	117.53
1	F	63	KXV	CA1-C1-N2	-4.27	114.95	123.56
1	A	63	KXV	N3-C1-N2	-4.02	108.67	111.45
1	A	63	KXV	CF-O4-CE1	-3.78	111.93	117.53
1	E	63	KXV	O-C-CA3	-3.65	115.36	126.39
1	E	63	KXV	CA1-C1-N2	-3.55	116.40	123.56
1	F	63	KXV	C2-CA2-N2	-3.45	106.50	108.92
1	C	63	KXV	CF-O4-CE1	-3.36	112.57	117.53
1	F	63	KXV	O-C-CA3	-3.26	116.53	126.39
1	A	63	KXV	CA1-CB1-SG1	-3.11	107.42	114.42
1	C	63	KXV	O-C-CA3	-3.09	117.05	126.39
1	C	63	KXV	O4-CE1-CD1	-3.08	118.88	124.14
1	G	63	KXV	CB1-CA1-C1	-3.01	104.25	110.54
1	F	63	KXV	C2-N3-C1	-2.98	106.42	107.97
1	F	63	KXV	O4-CE1-CD1	-2.91	119.17	124.14
1	D	63	KXV	O-C-CA3	-2.90	117.62	126.39
1	B	63	KXV	CB1-CA1-C1	-2.84	104.61	110.54
1	C	63	KXV	CA1-CB1-SG1	-2.82	108.06	114.42
1	E	63	KXV	O4-CE1-CD1	-2.81	119.34	124.14
1	D	63	KXV	O4-CE1-CD1	-2.80	119.37	124.14
1	H	63	KXV	CF-O4-CE1	-2.76	113.44	117.53
1	E	63	KXV	CB2-CA2-N2	-2.75	124.91	128.83
1	B	63	KXV	CF-O4-CE1	-2.58	113.71	117.53
1	G	63	KXV	CF-O4-CE1	-2.52	113.80	117.53
1	E	63	KXV	CF-O4-CE1	-2.43	113.93	117.53
1	A	63	KXV	O-C-CA3	-2.41	119.11	126.39
1	C	63	KXV	CA3-N3-C1	-2.36	124.43	127.20
1	G	63	KXV	N3-C1-N2	-2.36	109.82	111.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	KXV	O4-CE1-CD1	-2.23	120.33	124.14
1	A	63	KXV	C2-CA2-N2	-2.04	107.49	108.92
1	B	63	KXV	CA3-N3-C1	2.02	129.57	127.20
1	H	63	KXV	C2-N3-C1	2.28	109.15	107.97
1	A	63	KXV	CA2-N2-C1	2.36	107.52	105.77
1	G	63	KXV	C2-N3-C1	2.45	109.24	107.97
1	C	63	KXV	CA2-N2-C1	2.47	107.59	105.77
1	G	63	KXV	O4-CE1-CZ	2.51	118.20	114.58
1	H	63	KXV	O4-CE1-CZ	2.58	118.29	114.58
1	H	63	KXV	C1-CA1-N	2.85	119.76	109.01
1	D	63	KXV	CA2-N2-C1	2.91	107.92	105.77
1	E	63	KXV	CB1-CA1-C1	2.96	116.72	110.54
1	G	63	KXV	C1-CA1-N	3.14	120.88	109.01
1	B	63	KXV	O4-CE1-CZ	3.33	119.36	114.58
1	E	63	KXV	CA2-C2-N3	3.42	104.99	103.35
1	H	63	KXV	CB2-CA2-N2	3.67	134.06	128.83
1	B	63	KXV	CB2-CA2-N2	3.77	134.20	128.83
1	F	63	KXV	CA3-N3-C1	3.85	131.71	127.20
1	F	63	KXV	CB2-CA2-C2	4.09	127.22	122.28
1	A	63	KXV	O4-CE1-CZ	4.09	120.47	114.58
1	G	63	KXV	CB2-CA2-N2	4.34	135.02	128.83
1	D	63	KXV	O4-CE1-CZ	4.54	121.11	114.58
1	F	63	KXV	CA2-C2-N3	4.68	105.59	103.35
1	F	63	KXV	CB1-CA1-C1	4.76	120.49	110.54
1	B	63	KXV	CA2-N2-C1	4.93	109.41	105.77
1	C	63	KXV	O4-CE1-CZ	4.99	121.75	114.58
1	E	63	KXV	O4-CE1-CZ	5.15	121.98	114.58
1	F	63	KXV	CA2-N2-C1	5.17	109.58	105.77
1	F	63	KXV	O4-CE1-CZ	5.25	122.12	114.58
1	H	63	KXV	CA2-N2-C1	5.65	109.94	105.77
1	E	63	KXV	CA1-C1-N3	5.76	132.36	124.85
1	G	63	KXV	CA2-N2-C1	5.76	110.02	105.77
1	E	63	KXV	CB2-CA2-C2	6.28	129.87	122.28
1	F	63	KXV	CA1-C1-N3	6.31	133.08	124.85
1	E	63	KXV	CA2-N2-C1	7.09	111.00	105.77
1	B	63	KXV	CA2-C2-N3	7.29	106.84	103.35
1	G	63	KXV	CA2-C2-N3	7.46	106.92	103.35
1	H	63	KXV	CA2-C2-N3	8.01	107.18	103.35
1	C	63	KXV	CA2-C2-N3	9.25	107.78	103.35
1	D	63	KXV	CA2-C2-N3	9.63	107.96	103.35
1	A	63	KXV	CA2-C2-N3	12.07	109.13	103.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	63	KXV	CA1
1	E	63	KXV	CA1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	63	KXV	3	0
1	F	63	KXV	2	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	221/255 (86%)	-0.10	3 (1%) 75 77	33, 40, 59, 83	0
1	B	223/255 (87%)	-0.16	2 (0%) 84 85	28, 36, 56, 73	0
1	C	213/255 (83%)	-0.21	1 (0%) 90 91	34, 40, 50, 69	0
1	D	214/255 (83%)	-0.31	1 (0%) 90 91	27, 36, 49, 72	0
1	E	215/255 (84%)	-0.21	1 (0%) 90 91	33, 39, 55, 91	0
1	F	215/255 (84%)	-0.25	2 (0%) 84 85	28, 36, 50, 89	0
1	G	221/255 (86%)	-0.04	9 (4%) 37 40	35, 41, 60, 84	0
1	H	222/255 (87%)	-0.16	7 (3%) 47 51	30, 38, 62, 75	0
All	All	1744/2040 (85%)	-0.18	26 (1%) 73 75	27, 39, 55, 91	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	224	MET	5.1
1	H	223	ALA	4.9
1	H	222	GLN	4.5
1	G	222	GLN	4.3
1	G	228	TYR	4.1
1	F	4	ILE	3.8
1	A	4	ILE	3.8
1	G	3	VAL	3.7
1	H	3	VAL	3.5
1	G	158	ASN	3.4
1	G	227	LEU	3.4
1	H	4	ILE	3.2
1	H	220	PRO	3.1
1	A	3	VAL	3.1
1	G	219	LEU	3.0
1	B	224	MET	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	221	ARG	2.7
1	A	228	TYR	2.7
1	H	221	ARG	2.7
1	F	165	GLY	2.5
1	C	220	PRO	2.4
1	E	3	VAL	2.4
1	B	227	LEU	2.2
1	G	92	SER	2.2
1	G	4	ILE	2.2
1	G	52	PHE	2.2

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

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	KXV	B	63	23/24	0.87	0.17	27,32,36,37	0
1	KXV	F	63	23/24	0.89	0.15	27,29,33,35	0
1	KXV	G	63	23/24	0.92	0.14	33,36,39,40	0
1	KXV	H	63	23/24	0.92	0.15	26,34,36,36	0
1	KXV	A	63	23/24	0.93	0.15	31,33,37,38	0
1	KXV	C	63	23/24	0.94	0.14	33,33,36,39	0
1	KXV	E	63	23/24	0.94	0.13	33,33,34,38	0
1	KXV	D	63	23/24	0.95	0.13	25,31,34,35	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.