



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:22 PM UTC

PDB ID : 6NQL / pdb_00006nql
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2), Y63(3-CIY)
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on : 2019-01-21
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

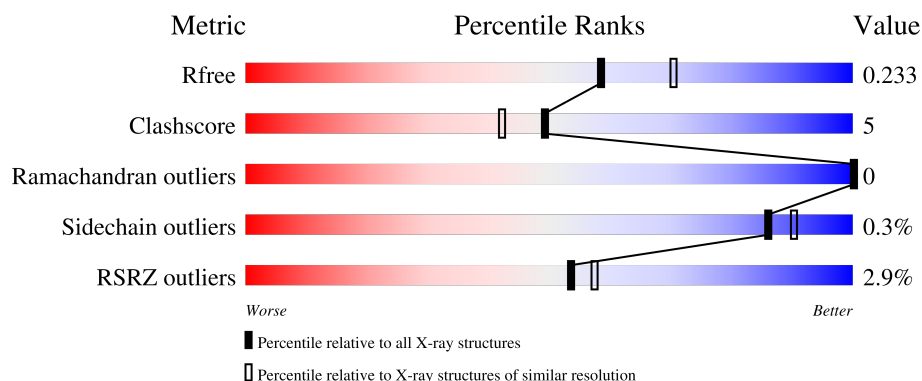
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	3% 76% 8% 15%
1	B	255	2% 76% 9% 15%
1	C	255	2% 77% 8% 15%
1	D	255	4% 75% 11% 15%
1	E	255	2% 75% 10% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	255	 3% 75% 9% 15%
1	G	255	 2% 74% 11% 15%
1	H	255	 3% 78% 7% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15594 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	217	Total	C	Cl	N	O	S	0	2	0
			1750	1117	1	295	328	9			
1	B	217	Total	C	Cl	N	O	S	0	2	0
			1758	1123	1	297	328	9			
1	C	217	Total	C	Cl	N	O	S	0	2	0
			1749	1117	1	294	328	9			
1	D	217	Total	C	Cl	N	O	S	0	0	0
			1741	1111	1	296	324	9			
1	E	216	Total	C	Cl	N	O	S	0	1	0
			1746	1115	1	294	327	9			
1	F	216	Total	C	Cl	N	O	S	0	1	0
			1742	1112	1	293	327	9			
1	G	217	Total	C	Cl	N	O	S	0	1	0
			1740	1111	1	293	326	9			
1	H	217	Total	C	Cl	N	O	S	0	1	0
			1740	1111	1	293	326	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	KZ7	CYS	chromophore	UNP Q5TLG6
A	63	KZ7	TYR	chromophore	UNP Q5TLG6
A	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
B	63	KZ7	TYR	chromophore	UNP Q5TLG6
B	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
C	63	KZ7	TYR	chromophore	UNP Q5TLG6
C	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
D	63	KZ7	TYR	chromophore	UNP Q5TLG6
D	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
E	63	KZ7	TYR	chromophore	UNP Q5TLG6
E	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
F	63	KZ7	TYR	chromophore	UNP Q5TLG6
F	63	KZ7	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...

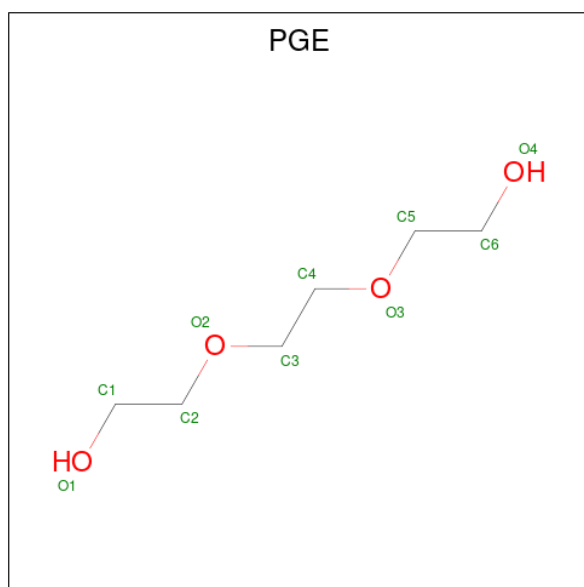
Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
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	KZ7	CYS	chromophore	UNP Q5TLG6
G	63	KZ7	TYR	chromophore	UNP Q5TLG6
G	63	KZ7	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	KZ7	CYS	chromophore	UNP Q5TLG6
H	63	KZ7	TYR	chromophore	UNP Q5TLG6
H	63	KZ7	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 TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		

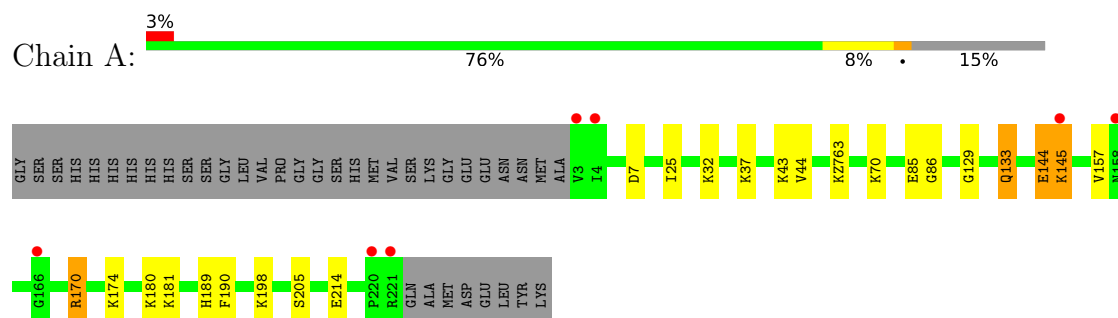
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total	O	0	0
			228	228		
3	B	190	Total	O	0	0
			190	190		
3	C	216	Total	O	0	0
			216	216		
3	D	174	Total	O	0	0
			174	174		
3	E	213	Total	O	0	0
			213	213		
3	F	187	Total	O	0	0
			187	187		
3	G	211	Total	O	0	0
			211	211		
3	H	179	Total	O	0	0
			179	179		

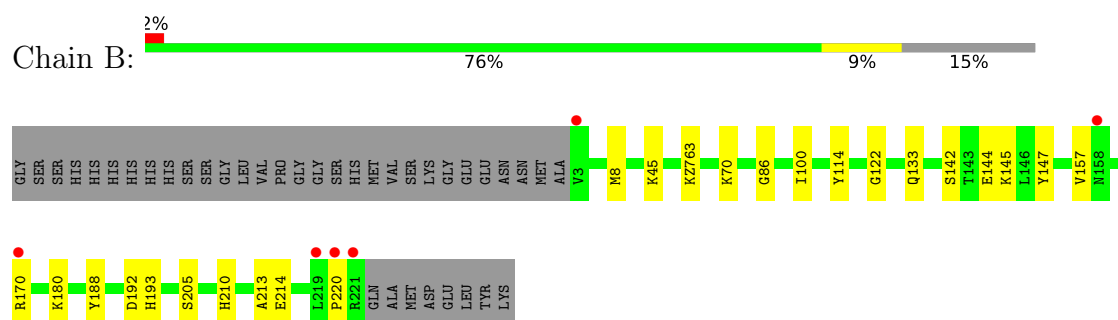
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

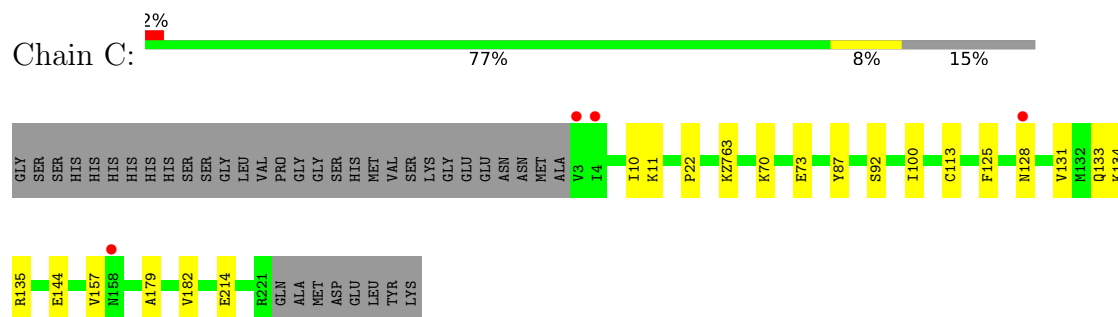
• Molecule 1: Fluorescent protein Dronpa



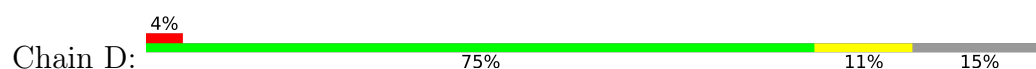
• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa

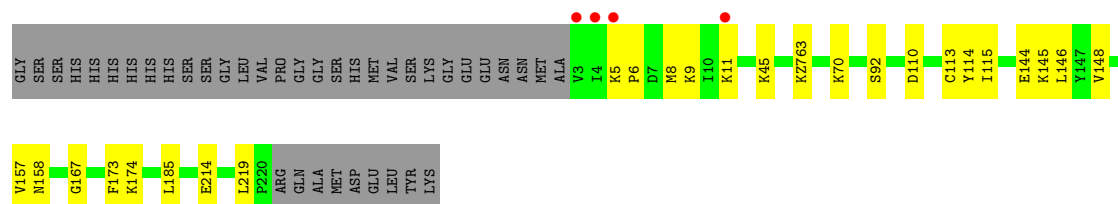
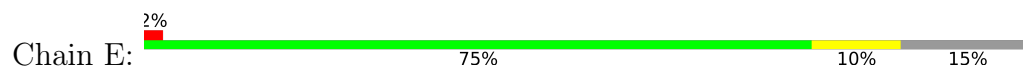


• Molecule 1: Fluorescent protein Dronpa

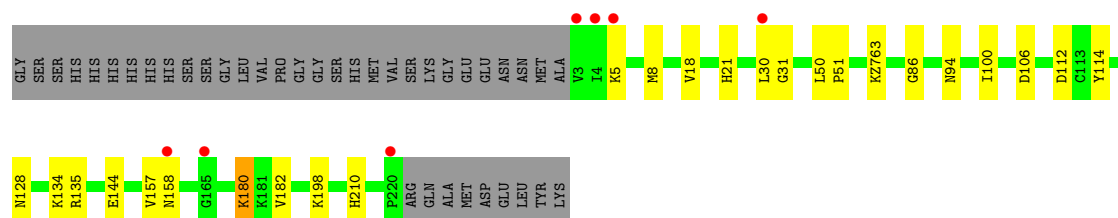
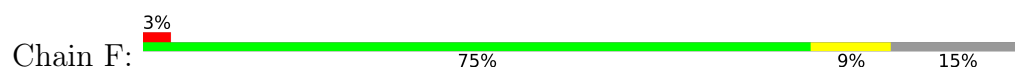




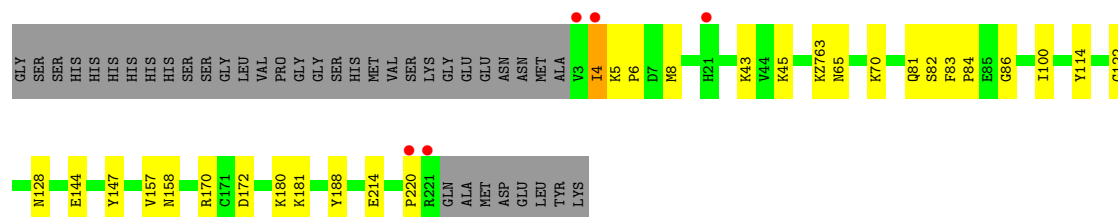
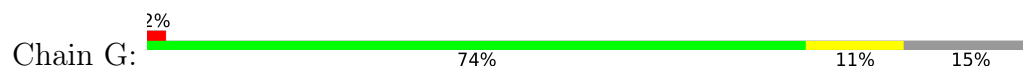
• Molecule 1: Fluorescent protein Dronpa



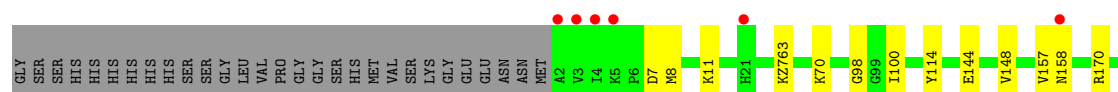
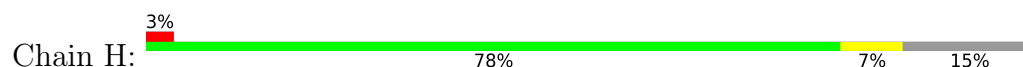
• Molecule 1: Fluorescent protein Dronpa



• 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, α , β , γ	81.70Å 86.28Å 143.35Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	39.59 – 2.15 39.59 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.59-2.15) 84.6 (39.59-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.14Å)	Xtrriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, R_{free}	0.197 , 0.234 0.198 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.457	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15594	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 49.92 % 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 6.9675e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: KZ7, PGE

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	0.41	1/1777 (0.1%)	0.62	3/2401 (0.1%)
1	B	0.33	0/1786	0.55	0/2414
1	C	0.53	3/1776 (0.2%)	0.62	2/2401 (0.1%)
1	D	0.35	0/1765	0.57	0/2385
1	E	0.35	0/1770	0.61	0/2391
1	F	0.40	2/1766 (0.1%)	0.58	1/2387 (0.0%)
1	G	0.33	0/1764	0.53	0/2386
1	H	0.30	0/1764	0.53	0/2384
All	All	0.38	6/14168 (0.0%)	0.58	6/19149 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	182	VAL	C-O	-8.15	1.16	1.24
1	C	10	ILE	C-O	-6.72	1.17	1.24
1	F	180	LYS	C-O	-6.65	1.15	1.24
1	C	73	GLU	C-O	-6.34	1.16	1.24
1	F	182	VAL	C-O	-5.42	1.18	1.24
1	A	170	ARG	C-O	-5.04	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLU	CA-C-N	-7.49	111.71	122.94
1	A	144	GLU	C-N-CA	-7.49	111.71	122.94
1	C	182	VAL	N-CA-C	5.69	116.61	108.93
1	F	31	GLY	N-CA-C	5.67	119.86	110.55
1	A	145	LYS	O-C-N	5.09	129.84	123.23
1	C	133	GLN	CB-CG-CD	-5.00	104.09	112.60

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	1750	0	1656	20	0
1	B	1758	0	1670	15	0
1	C	1749	0	1654	11	0
1	D	1741	0	1648	23	0
1	E	1746	0	1661	21	0
1	F	1742	0	1650	23	0
1	G	1740	0	1639	22	0
1	H	1740	0	1642	14	0
2	B	10	0	14	0	0
2	C	10	0	14	0	0
2	H	10	0	14	0	0
3	A	228	0	0	4	0
3	B	190	0	0	5	0
3	C	216	0	0	3	0
3	D	174	0	0	6	0
3	E	213	0	0	4	0
3	F	187	0	0	5	0
3	G	211	0	0	6	0
3	H	179	0	0	3	0
All	All	15594	0	13262	147	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 (147) 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:F:5:LYS:NZ	1:F:112:ASP:HB3	1.66	1.09
1:D:70:LYS:HB3	1:D:214:GLU:HG2	1.45	0.97
1:D:135:ARG:HA	1:D:164:GLU:OE2	1.69	0.93
1:B:220:PRO:HD3	3:B:401:HOH:O	1.70	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:O	1:D:164:GLU:HG3	1.72	0.88
1:G:70:LYS:HB3	1:G:214:GLU:HG2	1.56	0.88
1:G:5:LYS:HB3	3:G:441:HOH:O	1.76	0.84
1:G:158:ASN:HB3	1:G:170:ARG:HH12	1.42	0.84
1:F:5:LYS:HZ1	1:F:112:ASP:HB3	1.39	0.83
1:A:145:LYS:HG3	1:A:190:PHE:CD1	2.16	0.81
1:F:5:LYS:HZ2	1:F:112:ASP:HB3	1.47	0.77
1:B:210:HIS:HD2	3:B:548:HOH:O	1.68	0.76
1:G:128:ASN:ND2	3:G:302:HOH:O	2.24	0.70
1:E:158:ASN:ND2	3:E:301:HOH:O	2.24	0.68
1:F:198:LYS:HG3	1:F:210:HIS:CD2	2.29	0.67
1:H:7:ASP:OD1	3:H:401:HOH:O	2.14	0.65
1:D:135:ARG:HA	1:D:164:GLU:CD	2.22	0.64
1:G:158:ASN:HB3	1:G:170:ARG:NH1	2.10	0.64
1:H:174:LYS:HD2	3:H:455:HOH:O	1.98	0.64
1:G:220:PRO:HD3	3:G:386:HOH:O	1.98	0.64
1:F:5:LYS:NZ	1:F:112:ASP:CB	2.54	0.64
1:A:145:LYS:CD	1:A:190:PHE:HD1	2.10	0.63
1:B:133:GLN:NE2	3:B:402:HOH:O	2.26	0.62
1:C:135:ARG:NH1	3:C:403:HOH:O	2.22	0.61
1:F:86:GLY:C	1:F:180:LYS:HD2	2.24	0.61
1:D:135:ARG:C	1:D:164:GLU:HG3	2.25	0.61
1:A:145:LYS:CG	1:A:190:PHE:CD1	2.83	0.61
1:D:5:LYS:NZ	3:D:303:HOH:O	2.31	0.61
1:F:21:HIS:HB2	3:F:301:HOH:O	2.01	0.61
1:A:198:LYS:NZ	3:A:303:HOH:O	2.33	0.60
1:C:144:GLU:HA	1:C:157:VAL:HB	1.84	0.60
1:D:128:ASN:O	1:D:135:ARG:NH2	2.35	0.59
1:F:5:LYS:HB2	1:F:8:MET:SD	2.42	0.59
1:F:18:VAL:O	3:F:301:HOH:O	2.17	0.59
1:G:144:GLU:HA	1:G:157:VAL:HB	1.84	0.58
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.85	0.57
1:G:158:ASN:CB	1:G:170:ARG:HH12	2.15	0.57
1:H:144:GLU:HA	1:H:157:VAL:HB	1.85	0.57
1:E:5:LYS:HB3	1:E:6:PRO:HD2	1.86	0.57
1:B:70:LYS:HB3	1:B:214:GLU:HG2	1.87	0.57
1:F:5:LYS:CE	1:F:112:ASP:HB3	2.36	0.56
1:A:144:GLU:HA	1:A:157:VAL:HB	1.87	0.56
1:B:144:GLU:HA	1:B:157:VAL:HB	1.87	0.55
1:C:134:LYS:NZ	3:C:412:HOH:O	2.39	0.55
1:E:11:LYS:HE2	1:E:115:ILE:HG12	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:CD	1:A:190:PHE:CD1	2.90	0.54
1:E:9:LYS:NZ	3:E:306:HOH:O	2.39	0.54
1:E:144:GLU:HA	1:E:157:VAL:HB	1.90	0.54
1:D:164:GLU:OE2	3:D:301:HOH:O	2.17	0.54
1:A:145:LYS:HD2	1:A:190:PHE:CD1	2.44	0.53
1:G:6:PRO:HD2	3:G:441:HOH:O	2.07	0.53
1:A:37:LYS:NZ	3:A:305:HOH:O	2.36	0.53
1:A:145:LYS:HD2	1:A:190:PHE:HD1	1.74	0.53
1:E:167:GLY:HA2	3:E:365:HOH:O	2.09	0.53
1:F:50:LEU:O	1:F:134:LYS:NZ	2.31	0.52
1:F:5:LYS:HZ2	1:F:112:ASP:CB	2.19	0.52
1:G:8:MET:HE2	1:G:114:TYR:CZ	2.44	0.52
1:A:70:LYS:HB3	1:A:214:GLU:HG2	1.92	0.52
1:F:158:ASN:ND2	3:F:307:HOH:O	2.41	0.52
1:C:22:PRO:HD2	3:C:552:HOH:O	2.11	0.51
1:F:144:GLU:HA	1:F:157:VAL:HB	1.92	0.51
1:F:8:MET:HE2	1:F:114:TYR:CZ	2.46	0.51
1:E:158:ASN:HB3	3:E:439:HOH:O	2.11	0.50
1:H:158:ASN:HB3	1:H:170:ARG:NH2	2.26	0.50
1:D:4:ILE:HD11	1:D:83:PHE:HB2	1.94	0.50
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.92	0.50
1:D:65:ASN:N	3:D:311:HOH:O	2.45	0.50
1:C:92[A]:SER:OG	1:C:100:ILE:HD11	2.12	0.50
1:G:4:ILE:O	1:G:4:ILE:HG22	2.11	0.50
1:G:65:ASN:N	3:G:311:HOH:O	2.45	0.50
1:A:145:LYS:HG3	1:A:190:PHE:CE1	2.46	0.50
1:C:128:ASN:OD1	1:C:128:ASN:C	2.55	0.49
1:D:93:MET:O	1:D:100:ILE:HD12	2.12	0.49
1:F:30:LEU:HD12	1:F:30:LEU:C	2.37	0.49
1:H:8:MET:HE2	1:H:114:TYR:CZ	2.48	0.48
1:D:144:GLU:HA	1:D:157:VAL:HB	1.96	0.48
1:A:145:LYS:CG	1:A:190:PHE:CE1	2.97	0.47
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.96	0.47
1:E:8:MET:HE2	1:E:114:TYR:CZ	2.49	0.47
1:F:106:ASP:HB2	3:F:460:HOH:O	2.15	0.47
1:F:5:LYS:CE	1:F:112:ASP:CB	2.92	0.47
1:D:133:GLN:OE1	1:D:135:ARG:NH2	2.44	0.47
1:E:5:LYS:HB3	1:E:6:PRO:CD	2.45	0.47
1:A:129:GLY:O	1:A:133:GLN:HB2	2.15	0.46
1:G:82:SER:HA	1:G:181:LYS:HE2	1.96	0.46
1:G:45:LYS:NZ	3:G:306:HOH:O	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:SER:HB3	3:B:560:HOH:O	2.15	0.46
1:B:142:SER:OG	1:B:193:HIS:HB2	2.16	0.46
1:D:145:LYS:HG3	1:D:190:PHE:CE1	2.51	0.46
1:G:43:LYS:HE3	1:G:45:LYS:NZ	2.31	0.46
1:B:45:LYS:HE3	1:E:110:ASP:OD2	2.15	0.46
1:E:148:VAL:HG21	1:E:185:LEU:HB3	1.97	0.46
1:D:8:MET:HE2	1:D:114:TYR:CZ	2.51	0.45
1:E:146:LEU:HD12	1:E:146:LEU:N	2.31	0.45
1:E:8:MET:HE3	1:E:8:MET:HB3	1.91	0.45
1:A:43:LYS:HA	1:A:205:SER:O	2.17	0.45
1:B:8:MET:HE2	1:B:114:TYR:CZ	2.51	0.45
1:A:7:ASP:OD1	1:A:32:LYS:NZ	2.48	0.45
1:C:11:LYS:HE2	1:C:113:CYS:SG	2.57	0.45
1:D:158:ASN:ND2	3:D:313:HOH:O	2.50	0.44
1:F:94:ASN:HA	1:F:100:ILE:HD13	1.99	0.44
1:H:173:PHE:C	1:H:174:LYS:HD3	2.42	0.44
1:F:8:MET:HE3	1:F:8:MET:HB3	1.88	0.44
1:B:147:TYR:HB3	1:B:188:TYR:CD1	2.52	0.44
1:F:51:PRO:C	1:F:134:LYS:HE3	2.43	0.44
1:B:192:ASP:O	1:B:213:ALA:HA	2.18	0.44
1:G:158:ASN:CG	1:G:172:ASP:OD1	2.61	0.44
1:C:125:PHE:CE1	1:C:131:VAL:HG21	2.52	0.44
1:E:145:LYS:C	1:E:146:LEU:HD12	2.42	0.44
3:D:409:HOH:O	1:H:202:LYS:HE3	2.18	0.43
1:H:158:ASN:HB3	1:H:170:ARG:CZ	2.47	0.43
1:A:86:GLY:C	1:A:180:LYS:HD2	2.43	0.43
1:G:147:TYR:HB3	1:G:188:TYR:CD1	2.53	0.43
1:D:157:VAL:HG13	1:D:173:PHE:HB2	1.99	0.43
1:H:11:LYS:HB3	1:H:11:LYS:HE2	1.90	0.43
1:D:145:LYS:N	1:D:145:LYS:HD3	2.33	0.43
1:D:196:GLU:HB2	1:D:198:LYS:HE3	2.01	0.43
1:F:128:ASN:O	1:F:135:ARG:NH2	2.51	0.43
1:G:86:GLY:C	1:G:180:LYS:HD2	2.44	0.43
1:A:189:HIS:HA	3:A:304:HOH:O	2.19	0.43
1:H:148:VAL:HG21	1:H:185:LEU:HB3	2.01	0.43
1:A:174:LYS:HE2	3:A:492:HOH:O	2.18	0.42
1:E:11:LYS:HB2	1:E:113:CYS:SG	2.59	0.42
1:D:203:ASP:CB	3:D:450:HOH:O	2.68	0.42
1:A:25:ILE:HG12	1:A:44:VAL:HG22	2.01	0.42
1:E:173:PHE:O	1:E:174:LYS:NZ	2.48	0.42
1:B:210:HIS:CD2	3:B:548:HOH:O	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ASP:HB2	3:H:497:HOH:O	2.19	0.42
1:E:45:LYS:HA	1:E:45:LYS:HD2	1.94	0.42
1:B:100:ILE:O	1:B:122:GLY:HA2	2.20	0.41
1:F:30:LEU:CD1	3:F:309:HOH:O	2.67	0.41
1:E:174:LYS:HA	1:E:174:LYS:HD3	1.86	0.41
1:G:100:ILE:O	1:G:122:GLY:HA2	2.20	0.41
1:A:85:GLU:CD	1:A:181:LYS:HD2	2.46	0.41
1:H:198:LYS:HD2	1:H:198:LYS:HA	1.74	0.41
1:C:100:ILE:HG21	1:E:92[B]:SER:HB3	2.03	0.41
1:G:83:PHE:HB3	1:G:84:PRO:HA	2.03	0.41
1:D:139:TRP:CE2	1:D:161:LEU:HD21	2.56	0.41
1:G:81:GLN:O	1:G:181:LYS:CE	2.69	0.41
1:B:8:MET:HE3	1:B:8:MET:HB3	1.95	0.41
1:B:86:GLY:C	1:B:180:LYS:HD2	2.46	0.41
1:C:87:TYR:CB	1:C:179:ALA:HA	2.51	0.41
1:H:98:GLY:O	1:H:100:ILE:HG12	2.21	0.41
1:G:4:ILE:HD11	1:G:83:PHE:HB2	2.03	0.40
1:D:145:LYS:HG3	1:D:190:PHE:CD1	2.56	0.40
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.04	0.40
1:E:219:LEU:HD23	1:E:219:LEU:HA	1.88	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	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
1	B	214/255 (84%)	211 (99%)	3 (1%)	0	100	100
1	C	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
1	D	212/255 (83%)	210 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	212/255 (83%)	209 (99%)	3 (1%)	0	100	100
1	F	212/255 (83%)	210 (99%)	2 (1%)	0	100	100
1	G	213/255 (84%)	211 (99%)	2 (1%)	0	100	100
1	H	213/255 (84%)	211 (99%)	2 (1%)	0	100	100
All	All	1704/2040 (84%)	1686 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/217 (85%)	183 (99%)	2 (1%)	65	71
1	B	187/217 (86%)	185 (99%)	2 (1%)	65	71
1	C	185/217 (85%)	185 (100%)	0	100	100
1	D	183/217 (84%)	183 (100%)	0	100	100
1	E	186/217 (86%)	186 (100%)	0	100	100
1	F	185/217 (85%)	185 (100%)	0	100	100
1	G	183/217 (84%)	182 (100%)	1 (0%)	81	86
1	H	183/217 (84%)	183 (100%)	0	100	100
All	All	1477/1736 (85%)	1472 (100%)	5 (0%)	86	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	170	ARG
1	B	145	LYS
1	B	170	ARG
1	G	4	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	21	HIS
1	C	38	GLN
1	D	21	HIS
1	E	212	HIS
1	F	133	GLN
1	H	21	HIS
1	H	208	ASN
1	H	210	HIS

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	KZ7	D	63	1	22,23,24	2.69	6 (27%)	28,32,34	2.58	7 (25%)
1	KZ7	H	63	1	22,23,24	2.90	8 (36%)	28,32,34	2.56	9 (32%)
1	KZ7	G	63	1	22,23,24	2.78	5 (22%)	28,32,34	2.24	8 (28%)
1	KZ7	C	63	1	22,23,24	2.77	6 (27%)	28,32,34	2.43	6 (21%)
1	KZ7	A	63	1	22,23,24	2.84	8 (36%)	28,32,34	2.49	5 (17%)
1	KZ7	F	63	1	22,23,24	2.77	7 (31%)	28,32,34	2.69	8 (28%)
1	KZ7	B	63	1	22,23,24	2.84	7 (31%)	28,32,34	2.38	6 (21%)
1	KZ7	E	63	1	22,23,24	2.66	7 (31%)	28,32,34	2.49	7 (25%)

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	KZ7	D	63	1	-	3/10/29/30	0/2/2/2
1	KZ7	H	63	1	-	3/10/29/30	0/2/2/2
1	KZ7	G	63	1	-	4/10/29/30	0/2/2/2
1	KZ7	C	63	1	-	3/10/29/30	0/2/2/2
1	KZ7	A	63	1	-	3/10/29/30	0/2/2/2
1	KZ7	F	63	1	-	4/10/29/30	0/2/2/2
1	KZ7	B	63	1	-	4/10/29/30	0/2/2/2
1	KZ7	E	63	1	-	4/10/29/30	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	63	KZ7	CA2-C2	-11.00	1.36	1.48
1	A	63	KZ7	CA2-C2	-10.71	1.37	1.48
1	G	63	KZ7	CA2-C2	-10.59	1.37	1.48
1	B	63	KZ7	CA2-C2	-10.52	1.37	1.48
1	C	63	KZ7	CA2-C2	-10.24	1.37	1.48
1	F	63	KZ7	CA2-C2	-10.09	1.37	1.48
1	D	63	KZ7	CA2-C2	-9.97	1.37	1.48
1	E	63	KZ7	CA2-C2	-9.44	1.38	1.48
1	E	63	KZ7	CG2-CB2	4.27	1.54	1.46
1	B	63	KZ7	CG2-CB2	4.21	1.54	1.46
1	F	63	KZ7	CG2-CB2	4.19	1.54	1.46
1	A	63	KZ7	CG2-CB2	3.89	1.54	1.46
1	D	63	KZ7	CG2-CB2	3.80	1.53	1.46
1	H	63	KZ7	CG2-CB2	3.77	1.53	1.46
1	G	63	KZ7	CG2-CB2	3.75	1.53	1.46
1	B	63	KZ7	C2-N3	-3.63	1.31	1.40
1	C	63	KZ7	CG2-CB2	3.60	1.53	1.46
1	A	63	KZ7	C2-N3	-3.46	1.32	1.40
1	H	63	KZ7	C2-N3	-3.45	1.32	1.40
1	C	63	KZ7	CA2-N2	-3.41	1.31	1.38
1	F	63	KZ7	CA2-N2	-3.35	1.31	1.38
1	E	63	KZ7	C2-N3	-3.30	1.32	1.40
1	E	63	KZ7	CA2-N2	-3.26	1.31	1.38
1	G	63	KZ7	C2-N3	-3.21	1.32	1.40
1	C	63	KZ7	C2-N3	-3.17	1.32	1.40
1	F	63	KZ7	C2-N3	-3.17	1.32	1.40
1	D	63	KZ7	C2-N3	-3.10	1.32	1.40
1	D	63	KZ7	CA2-N2	-2.99	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	KZ7	CB2-CA2	-2.90	1.32	1.35
1	A	63	KZ7	CA2-N2	-2.81	1.32	1.38
1	B	63	KZ7	CA2-N2	-2.81	1.32	1.38
1	H	63	KZ7	CA2-N2	-2.77	1.32	1.38
1	G	63	KZ7	CA2-N2	-2.65	1.33	1.38
1	F	63	KZ7	CB2-CA2	-2.47	1.32	1.35
1	F	63	KZ7	OH-CZ	2.45	1.41	1.36
1	H	63	KZ7	CB2-CA2	-2.35	1.32	1.35
1	E	63	KZ7	OH-CZ	2.30	1.41	1.36
1	E	63	KZ7	C1-N2	2.29	1.35	1.32
1	G	63	KZ7	CB2-CA2	-2.28	1.33	1.35
1	B	63	KZ7	OH-CZ	2.27	1.40	1.36
1	D	63	KZ7	CB2-CA2	-2.24	1.33	1.35
1	A	63	KZ7	C1-N2	2.20	1.35	1.32
1	B	63	KZ7	O2-C2	-2.17	1.18	1.23
1	A	63	KZ7	O2-C2	-2.15	1.18	1.23
1	H	63	KZ7	O2-C2	-2.12	1.18	1.23
1	F	63	KZ7	O2-C2	-2.12	1.18	1.23
1	E	63	KZ7	O2-C2	-2.09	1.18	1.23
1	H	63	KZ7	OH-CZ	2.08	1.40	1.36
1	A	63	KZ7	CB2-CA2	-2.08	1.33	1.35
1	C	63	KZ7	OH-CZ	2.07	1.40	1.36
1	D	63	KZ7	C1-N2	2.06	1.35	1.32
1	H	63	KZ7	CE1-CL	2.04	1.78	1.73
1	B	63	KZ7	CZ-CE1	-2.01	1.37	1.39
1	A	63	KZ7	OH-CZ	2.01	1.40	1.36

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	KZ7	O2-C2-CA2	-9.89	124.71	131.02
1	H	63	KZ7	O2-C2-CA2	-9.59	124.90	131.02
1	F	63	KZ7	O2-C2-CA2	-9.44	125.00	131.02
1	A	63	KZ7	O2-C2-CA2	-9.43	125.00	131.02
1	C	63	KZ7	O2-C2-CA2	-8.70	125.47	131.02
1	B	63	KZ7	O2-C2-CA2	-8.28	125.73	131.02
1	E	63	KZ7	O2-C2-CA2	-8.20	125.79	131.02
1	G	63	KZ7	O2-C2-CA2	-8.06	125.88	131.02
1	E	63	KZ7	CA2-C2-N3	6.70	109.13	103.50
1	F	63	KZ7	CA2-C2-N3	6.31	108.80	103.50
1	A	63	KZ7	CA2-C2-N3	6.02	108.56	103.50
1	D	63	KZ7	CA2-C2-N3	5.97	108.51	103.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	KZ7	CA2-C2-N3	5.81	108.38	103.50
1	H	63	KZ7	CA2-C2-N3	5.76	108.33	103.50
1	C	63	KZ7	CA2-C2-N3	5.42	108.06	103.50
1	G	63	KZ7	CA2-C2-N3	4.53	107.31	103.50
1	B	63	KZ7	N3-C1-N2	-3.84	108.46	111.48
1	C	63	KZ7	N3-C1-N2	-3.83	108.47	111.48
1	G	63	KZ7	N3-C1-N2	-3.75	108.53	111.48
1	F	63	KZ7	CA1-CB1-SG1	-3.73	106.42	114.40
1	F	63	KZ7	N3-C1-N2	-3.58	108.66	111.48
1	H	63	KZ7	N3-C1-N2	-3.52	108.71	111.48
1	F	63	KZ7	CA2-N2-C1	3.47	108.51	105.80
1	A	63	KZ7	N3-C1-N2	-3.32	108.86	111.48
1	E	63	KZ7	N3-C1-N2	-3.20	108.96	111.48
1	C	63	KZ7	CA2-N2-C1	3.19	108.29	105.80
1	D	63	KZ7	N3-C1-N2	-3.16	108.99	111.48
1	E	63	KZ7	CA2-N2-C1	3.13	108.24	105.80
1	E	63	KZ7	C2-N3-C1	-2.96	106.70	108.07
1	B	63	KZ7	CA1-CB1-SG1	-2.86	108.28	114.40
1	F	63	KZ7	C2-N3-C1	-2.86	106.74	108.07
1	C	63	KZ7	CA1-CB1-SG1	-2.85	108.30	114.40
1	E	63	KZ7	C2-CA2-N2	-2.77	106.96	108.95
1	G	63	KZ7	CA1-CB1-SG1	-2.76	108.51	114.40
1	H	63	KZ7	CD1-CE1-CZ	-2.71	119.34	120.92
1	B	63	KZ7	CG2-CB2-CA2	-2.65	126.72	129.87
1	H	63	KZ7	CG2-CB2-CA2	-2.65	126.72	129.87
1	E	63	KZ7	CA1-CB1-SG1	-2.63	108.78	114.40
1	D	63	KZ7	CA2-N2-C1	2.62	107.85	105.80
1	B	63	KZ7	CA2-N2-C1	2.53	107.78	105.80
1	A	63	KZ7	CG2-CB2-CA2	-2.52	126.87	129.87
1	A	63	KZ7	CA1-CB1-SG1	-2.45	109.15	114.40
1	H	63	KZ7	CA1-CB1-SG1	-2.41	109.24	114.40
1	D	63	KZ7	CA3-N3-C2	2.38	128.89	123.67
1	F	63	KZ7	C2-CA2-N2	-2.33	107.28	108.95
1	G	63	KZ7	CA2-N2-C1	2.25	107.56	105.80
1	D	63	KZ7	C2-N3-C1	-2.24	107.03	108.07
1	G	63	KZ7	CA1-C1-N2	2.14	127.75	123.57
1	D	63	KZ7	CD1-CE1-CL	2.12	121.92	118.45
1	G	63	KZ7	CD1-CE1-CL	2.12	121.92	118.45
1	H	63	KZ7	CA3-N3-C2	2.11	128.31	123.67
1	F	63	KZ7	CA3-N3-C2	2.09	128.27	123.67
1	C	63	KZ7	CA3-N3-C2	2.04	128.15	123.67
1	H	63	KZ7	CA2-N2-C1	2.03	107.39	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	KZ7	CA1-C1-N2	2.03	127.53	123.57
1	G	63	KZ7	CG2-CB2-CA2	-2.02	127.46	129.87

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	KZ7	C3-CA3-N3-C2
1	B	63	KZ7	C3-CA3-N3-C2
1	C	63	KZ7	C3-CA3-N3-C2
1	D	63	KZ7	C3-CA3-N3-C2
1	E	63	KZ7	C3-CA3-N3-C2
1	E	63	KZ7	C2-CA2-CB2-CG2
1	F	63	KZ7	C3-CA3-N3-C2
1	G	63	KZ7	C3-CA3-N3-C2
1	H	63	KZ7	C3-CA3-N3-C2
1	D	63	KZ7	C2-CA2-CB2-CG2
1	F	63	KZ7	C2-CA2-CB2-CG2
1	E	63	KZ7	N2-CA2-CB2-CG2
1	G	63	KZ7	C2-CA2-CB2-CG2
1	D	63	KZ7	N2-CA2-CB2-CG2
1	F	63	KZ7	N2-CA2-CB2-CG2
1	G	63	KZ7	N2-CA2-CB2-CG2
1	B	63	KZ7	N2-CA2-CB2-CG2
1	C	63	KZ7	N2-CA2-CB2-CG2
1	A	63	KZ7	N2-CA2-CB2-CG2
1	H	63	KZ7	N2-CA2-CB2-CG2
1	B	63	KZ7	C2-CA2-CB2-CG2
1	B	63	KZ7	C3-CA3-N3-C1
1	C	63	KZ7	C3-CA3-N3-C1
1	E	63	KZ7	C3-CA3-N3-C1
1	G	63	KZ7	C3-CA3-N3-C1
1	A	63	KZ7	C3-CA3-N3-C1
1	F	63	KZ7	C3-CA3-N3-C1
1	H	63	KZ7	C3-CA3-N3-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z > 2$
2	PGE	B	301	-	9,9,9	0.56	0	8,8,8	0.67	0
2	PGE	H	301	-	9,9,9	0.49	0	8,8,8	0.39	0
2	PGE	C	301	-	9,9,9	0.56	0	8,8,8	0.74	0

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
2	PGE	B	301	-	-	4/7/7/7	-
2	PGE	H	301	-	-	2/7/7/7	-
2	PGE	C	301	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PGE	O2-C3-C4-O3
2	B	301	PGE	O2-C3-C4-O3
2	H	301	PGE	O2-C3-C4-O3
2	B	301	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	301	PGE	C3-C4-O3-C5
2	B	301	PGE	C4-C3-O2-C2
2	C	301	PGE	O1-C1-C2-O2
2	C	301	PGE	C6-C5-O3-C4
2	C	301	PGE	C4-C3-O2-C2
2	B	301	PGE	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	216/255 (84%)	0.08	7 (3%)	50	54	10, 26, 46, 73	2 (0%)
1	B	216/255 (84%)	0.25	6 (2%)	55	59	12, 30, 49, 67	2 (0%)
1	C	216/255 (84%)	-0.00	4 (1%)	66	70	9, 27, 47, 63	2 (0%)
1	D	216/255 (84%)	0.24	9 (4%)	40	46	21, 32, 50, 78	0
1	E	215/255 (84%)	0.02	4 (1%)	66	70	10, 26, 43, 62	1 (0%)
1	F	215/255 (84%)	0.25	7 (3%)	49	53	13, 31, 50, 72	1 (0%)
1	G	216/255 (84%)	0.06	5 (2%)	61	65	9, 28, 47, 59	1 (0%)
1	H	216/255 (84%)	0.23	8 (3%)	45	50	12, 31, 50, 67	1 (0%)
All	All	1726/2040 (84%)	0.14	50 (2%)	53	57	9, 29, 48, 78	10 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	VAL	4.4
1	F	4	ILE	4.1
1	D	3	VAL	4.1
1	B	220	PRO	3.9
1	E	3	VAL	3.7
1	H	2	ALA	3.7
1	H	220	PRO	3.6
1	G	3	VAL	3.5
1	H	4	ILE	3.5
1	G	4	ILE	3.4
1	A	3	VAL	3.4
1	A	221	ARG	3.3
1	B	221	ARG	3.1
1	E	4	ILE	3.0
1	H	21	HIS	3.0
1	B	3	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	220	PRO	2.8
1	C	3	VAL	2.8
1	H	3	VAL	2.7
1	A	158	ASN	2.7
1	D	219	LEU	2.7
1	A	220	PRO	2.7
1	G	220	PRO	2.6
1	H	5	LYS	2.6
1	B	219	LEU	2.5
1	H	219	LEU	2.5
1	D	165	GLY	2.5
1	D	221	ARG	2.5
1	C	128	ASN	2.5
1	A	4	ILE	2.4
1	D	100	ILE	2.4
1	G	21	HIS	2.4
1	G	221	ARG	2.3
1	F	5	LYS	2.3
1	H	158	ASN	2.2
1	E	5	LYS	2.2
1	F	30	LEU	2.2
1	D	164	GLU	2.2
1	D	198	LYS	2.2
1	C	4	ILE	2.1
1	A	166	GLY	2.1
1	B	158	ASN	2.1
1	C	158	ASN	2.1
1	E	11	LYS	2.1
1	F	158	ASN	2.1
1	F	220	PRO	2.1
1	F	165	GLY	2.1
1	A	145	LYS	2.1
1	D	4	ILE	2.1
1	B	170	ARG	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, 95th 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($\text{\AA}^2$)	Q<0.9
1	KZ7	D	63	22/23	0.94	0.08	20,26,31,36	0
1	KZ7	H	63	22/23	0.95	0.07	23,30,34,38	0
1	KZ7	C	63	22/23	0.96	0.07	15,24,30,31	0
1	KZ7	A	63	22/23	0.96	0.07	17,24,28,29	0
1	KZ7	E	63	22/23	0.96	0.06	12,19,25,29	0
1	KZ7	F	63	22/23	0.96	0.08	23,25,34,34	0
1	KZ7	G	63	22/23	0.96	0.07	18,23,27,35	0
1	KZ7	B	63	22/23	0.96	0.07	21,28,30,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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, 95th 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($\text{\AA}^2$)	Q<0.9
2	PGE	B	301	10/10	0.75	0.18	31,36,42,43	0
2	PGE	H	301	10/10	0.77	0.16	25,33,45,46	0
2	PGE	C	301	10/10	0.80	0.45	83,91,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.