



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:58 AM UTC

PDB ID : 7RRI / pdb_00007rri
Title : Crystal structure of fast switching S142A/M159T mutant of fluorescent protein Dronpa (Dronpa2)
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on : 2021-08-09
Resolution : 2.64 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:

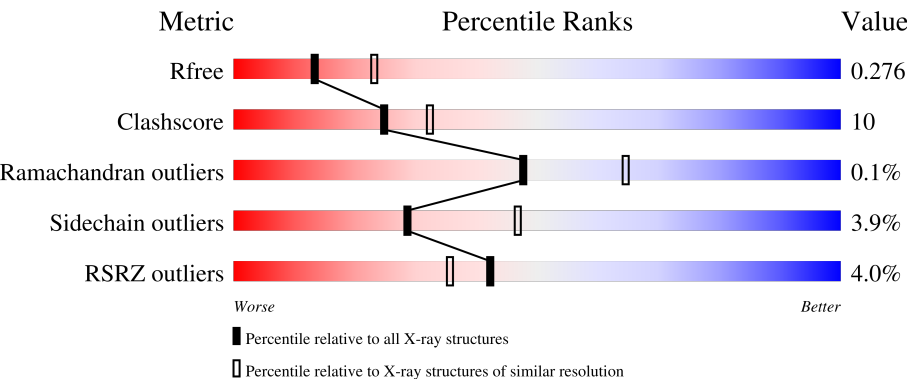
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	4% 64% 18% • 15%
1	B	255	2% 64% 18% • 15%
1	C	255	5% 63% 20% • 13%
1	D	255	4% 64% 20% •• 14%
1	E	255	4% 64% 20% • 14%

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Mol	Chain	Length	Quality of chain
1	F	255	3%64%18%•14%
1	G	255	3%65%18%••15%
1	H	255	2%60%23%•15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14128 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1726	1105	292	320	9			
1	B	216	Total	C	N	O	S	0	0	0
			1730	1108	293	320	9			
1	C	221	Total	C	N	O	S	0	0	0
			1743	1116	295	323	9			
1	D	220	Total	C	N	O	S	0	0	0
			1741	1113	293	326	9			
1	E	219	Total	C	N	O	S	0	1	0
			1745	1117	298	321	9			
1	F	219	Total	C	N	O	S	0	0	0
			1756	1124	296	327	9			
1	G	216	Total	C	N	O	S	0	0	0
			1720	1101	288	322	9			
1	H	216	Total	C	N	O	S	0	0	0
			1710	1093	288	320	9			

There are 328 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
A	63	GYC	CYS	chromophore	UNP Q5TLG6
A	63	GYC	TYR	chromophore	UNP Q5TLG6
A	63	GYC	GLY	chromophore	UNP Q5TLG6
A	142	ALA	SER	engineered mutation	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	conflict	UNP Q5TLG6
A	224	MET	-	insertion	UNP Q5TLG6
A	225	ASP	-	insertion	UNP Q5TLG6
A	226	GLU	-	insertion	UNP Q5TLG6
A	227	LEU	-	insertion	UNP Q5TLG6
A	228	TYR	-	insertion	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	UNP Q5TLG6
B	63	GYC	CYS	chromophore	UNP Q5TLG6
B	63	GYC	TYR	chromophore	UNP Q5TLG6
B	63	GYC	GLY	chromophore	UNP Q5TLG6
B	142	ALA	SER	engineered mutation	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	conflict	UNP Q5TLG6
B	224	MET	-	insertion	UNP Q5TLG6
B	225	ASP	-	insertion	UNP Q5TLG6
B	226	GLU	-	insertion	UNP Q5TLG6
B	227	LEU	-	insertion	UNP Q5TLG6
B	228	TYR	-	insertion	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	UNP Q5TLG6
C	63	GYC	CYS	chromophore	UNP Q5TLG6
C	63	GYC	TYR	chromophore	UNP Q5TLG6
C	63	GYC	GLY	chromophore	UNP Q5TLG6
C	142	ALA	SER	engineered mutation	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	conflict	UNP Q5TLG6
C	224	MET	-	insertion	UNP Q5TLG6
C	225	ASP	-	insertion	UNP Q5TLG6
C	226	GLU	-	insertion	UNP Q5TLG6
C	227	LEU	-	insertion	UNP Q5TLG6
C	228	TYR	-	insertion	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	UNP Q5TLG6
D	63	GYC	CYS	chromophore	UNP Q5TLG6
D	63	GYC	TYR	chromophore	UNP Q5TLG6
D	63	GYC	GLY	chromophore	UNP Q5TLG6
D	142	ALA	SER	engineered mutation	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	conflict	UNP Q5TLG6
D	224	MET	-	insertion	UNP Q5TLG6
D	225	ASP	-	insertion	UNP Q5TLG6
D	226	GLU	-	insertion	UNP Q5TLG6
D	227	LEU	-	insertion	UNP Q5TLG6
D	228	TYR	-	insertion	UNP Q5TLG6
E	-27	GLY	-	expression tag	UNP Q5TLG6
E	-26	SER	-	expression tag	UNP Q5TLG6
E	-25	SER	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	HIS	-	expression tag	UNP Q5TLG6
E	-21	HIS	-	expression tag	UNP Q5TLG6
E	-20	HIS	-	expression tag	UNP Q5TLG6
E	-19	HIS	-	expression tag	UNP Q5TLG6
E	-18	SER	-	expression tag	UNP Q5TLG6
E	-17	SER	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	LEU	-	expression tag	UNP Q5TLG6
E	-14	VAL	-	expression tag	UNP Q5TLG6
E	-13	PRO	-	expression tag	UNP Q5TLG6
E	-12	GLY	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	expression tag	UNP Q5TLG6
E	-9	HIS	-	expression tag	UNP Q5TLG6
E	-8	MET	-	expression tag	UNP Q5TLG6
E	-7	VAL	-	expression tag	UNP Q5TLG6
E	-6	SER	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	GLY	-	expression tag	UNP Q5TLG6
E	-3	GLU	-	expression tag	UNP Q5TLG6
E	-2	GLU	-	expression tag	UNP Q5TLG6
E	-1	ASN	-	expression tag	UNP Q5TLG6
E	0	ASN	-	expression tag	UNP Q5TLG6
E	1	MET	-	expression tag	UNP Q5TLG6
E	2	ALA	-	expression tag	UNP Q5TLG6
E	63	GYC	CYS	chromophore	UNP Q5TLG6
E	63	GYC	TYR	chromophore	UNP Q5TLG6
E	63	GYC	GLY	chromophore	UNP Q5TLG6
E	142	ALA	SER	engineered mutation	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	conflict	UNP Q5TLG6
E	224	MET	-	insertion	UNP Q5TLG6
E	225	ASP	-	insertion	UNP Q5TLG6
E	226	GLU	-	insertion	UNP Q5TLG6
E	227	LEU	-	insertion	UNP Q5TLG6
E	228	TYR	-	insertion	UNP Q5TLG6
F	-27	GLY	-	expression tag	UNP Q5TLG6
F	-26	SER	-	expression tag	UNP Q5TLG6
F	-25	SER	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	HIS	-	expression tag	UNP Q5TLG6
F	-21	HIS	-	expression tag	UNP Q5TLG6
F	-20	HIS	-	expression tag	UNP Q5TLG6
F	-19	HIS	-	expression tag	UNP Q5TLG6
F	-18	SER	-	expression tag	UNP Q5TLG6
F	-17	SER	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	LEU	-	expression tag	UNP Q5TLG6
F	-14	VAL	-	expression tag	UNP Q5TLG6
F	-13	PRO	-	expression tag	UNP Q5TLG6
F	-12	GLY	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q5TLG6
F	-8	MET	-	expression tag	UNP Q5TLG6
F	-7	VAL	-	expression tag	UNP Q5TLG6
F	-6	SER	-	expression tag	UNP Q5TLG6
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	GLY	-	expression tag	UNP Q5TLG6
F	-3	GLU	-	expression tag	UNP Q5TLG6
F	-2	GLU	-	expression tag	UNP Q5TLG6
F	-1	ASN	-	expression tag	UNP Q5TLG6
F	0	ASN	-	expression tag	UNP Q5TLG6
F	1	MET	-	expression tag	UNP Q5TLG6
F	2	ALA	-	expression tag	UNP Q5TLG6
F	63	GYC	CYS	chromophore	UNP Q5TLG6
F	63	GYC	TYR	chromophore	UNP Q5TLG6
F	63	GYC	GLY	chromophore	UNP Q5TLG6
F	142	ALA	SER	engineered mutation	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	conflict	UNP Q5TLG6
F	224	MET	-	insertion	UNP Q5TLG6
F	225	ASP	-	insertion	UNP Q5TLG6
F	226	GLU	-	insertion	UNP Q5TLG6
F	227	LEU	-	insertion	UNP Q5TLG6
F	228	TYR	-	insertion	UNP Q5TLG6
G	-27	GLY	-	expression tag	UNP Q5TLG6
G	-26	SER	-	expression tag	UNP Q5TLG6
G	-25	SER	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	HIS	-	expression tag	UNP Q5TLG6
G	-21	HIS	-	expression tag	UNP Q5TLG6
G	-20	HIS	-	expression tag	UNP Q5TLG6
G	-19	HIS	-	expression tag	UNP Q5TLG6
G	-18	SER	-	expression tag	UNP Q5TLG6
G	-17	SER	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	LEU	-	expression tag	UNP Q5TLG6
G	-14	VAL	-	expression tag	UNP Q5TLG6
G	-13	PRO	-	expression tag	UNP Q5TLG6
G	-12	GLY	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	SER	-	expression tag	UNP Q5TLG6
G	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
G	-1	ASN	-	expression tag	UNP Q5TLG6
G	0	ASN	-	expression tag	UNP Q5TLG6
G	1	MET	-	expression tag	UNP Q5TLG6
G	2	ALA	-	expression tag	UNP Q5TLG6
G	63	GYC	CYS	chromophore	UNP Q5TLG6
G	63	GYC	TYR	chromophore	UNP Q5TLG6
G	63	GYC	GLY	chromophore	UNP Q5TLG6
G	142	ALA	SER	engineered mutation	UNP Q5TLG6
G	159	THR	MET	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	conflict	UNP Q5TLG6
G	224	MET	-	insertion	UNP Q5TLG6
G	225	ASP	-	insertion	UNP Q5TLG6
G	226	GLU	-	insertion	UNP Q5TLG6
G	227	LEU	-	insertion	UNP Q5TLG6
G	228	TYR	-	insertion	UNP Q5TLG6
H	-27	GLY	-	expression tag	UNP Q5TLG6
H	-26	SER	-	expression tag	UNP Q5TLG6
H	-25	SER	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	HIS	-	expression tag	UNP Q5TLG6
H	-21	HIS	-	expression tag	UNP Q5TLG6
H	-20	HIS	-	expression tag	UNP Q5TLG6
H	-19	HIS	-	expression tag	UNP Q5TLG6
H	-18	SER	-	expression tag	UNP Q5TLG6
H	-17	SER	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	LEU	-	expression tag	UNP Q5TLG6
H	-14	VAL	-	expression tag	UNP Q5TLG6
H	-13	PRO	-	expression tag	UNP Q5TLG6
H	-12	GLY	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	SER	-	expression tag	UNP Q5TLG6
H	-9	HIS	-	expression tag	UNP Q5TLG6
H	-8	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	VAL	-	expression tag	UNP Q5TLG6
H	-6	SER	-	expression tag	UNP Q5TLG6
H	-5	LYS	-	expression tag	UNP Q5TLG6
H	-4	GLY	-	expression tag	UNP Q5TLG6
H	-3	GLU	-	expression tag	UNP Q5TLG6
H	-2	GLU	-	expression tag	UNP Q5TLG6
H	-1	ASN	-	expression tag	UNP Q5TLG6
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	GYC	CYS	chromophore	UNP Q5TLG6
H	63	GYC	TYR	chromophore	UNP Q5TLG6
H	63	GYC	GLY	chromophore	UNP Q5TLG6
H	142	ALA	SER	engineered mutation	UNP Q5TLG6
H	159	THR	MET	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	conflict	UNP Q5TLG6
H	224	MET	-	insertion	UNP Q5TLG6
H	225	ASP	-	insertion	UNP Q5TLG6
H	226	GLU	-	insertion	UNP Q5TLG6
H	227	LEU	-	insertion	UNP Q5TLG6
H	228	TYR	-	insertion	UNP Q5TLG6

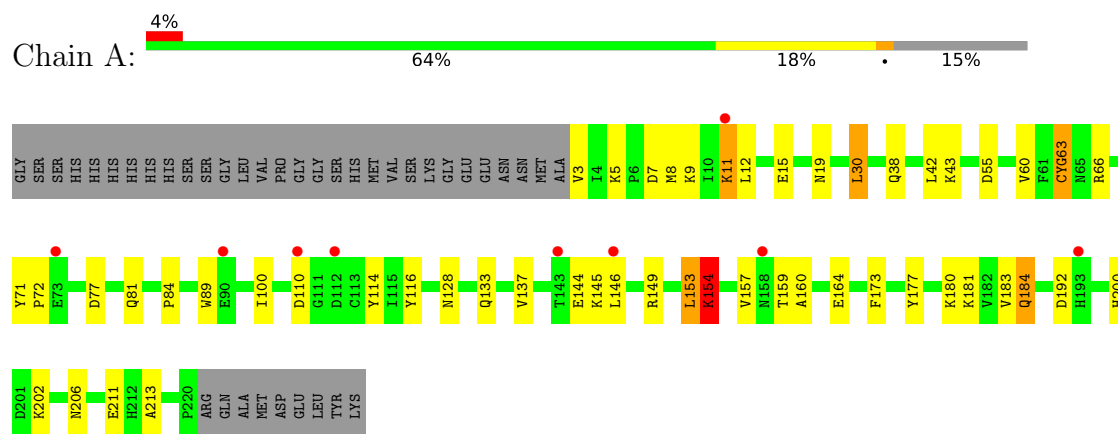
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	38	Total O 38 38	0	0
2	B	37	Total O 37 37	0	0
2	C	25	Total O 25 25	0	0
2	D	31	Total O 31 31	0	0
2	E	29	Total O 29 29	0	0
2	F	31	Total O 31 31	0	0
2	G	30	Total O 30 30	0	0
2	H	36	Total O 36 36	0	0

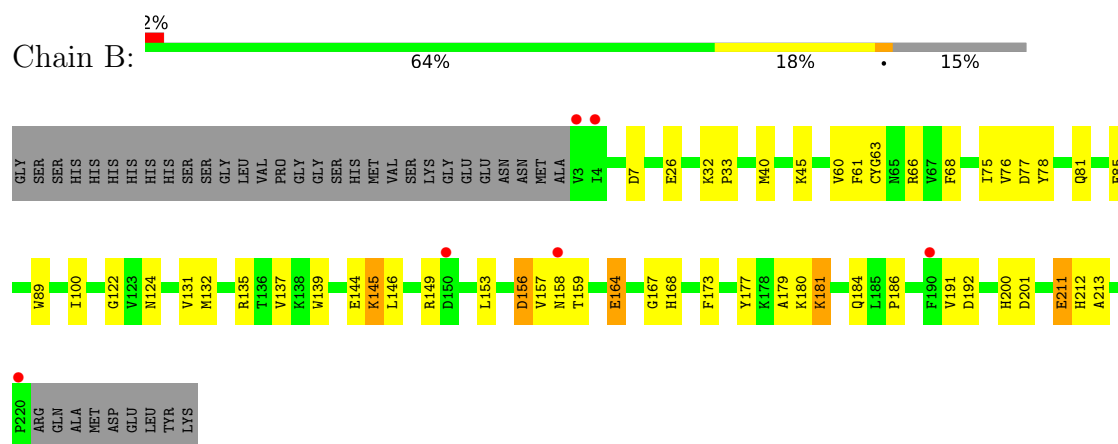
3 Residue-property plots [i](#)

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

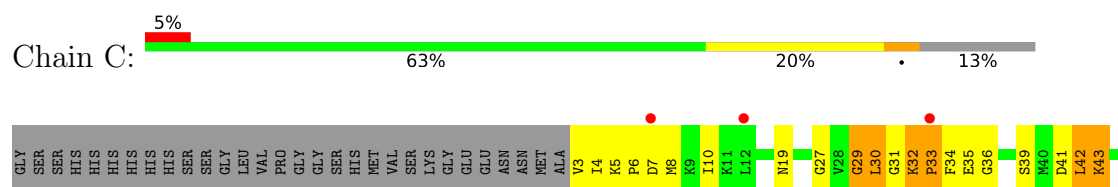
• Molecule 1: Fluorescent protein Dronpa

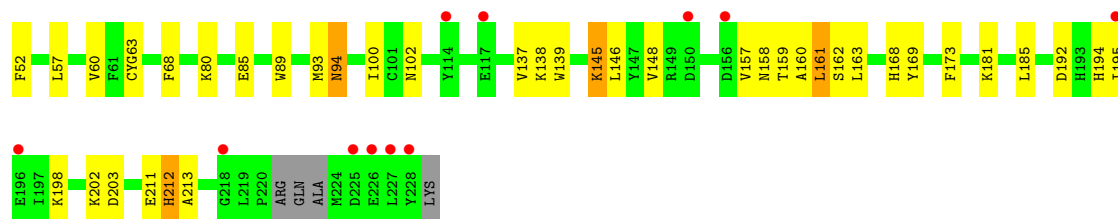


• Molecule 1: Fluorescent protein Dronpa

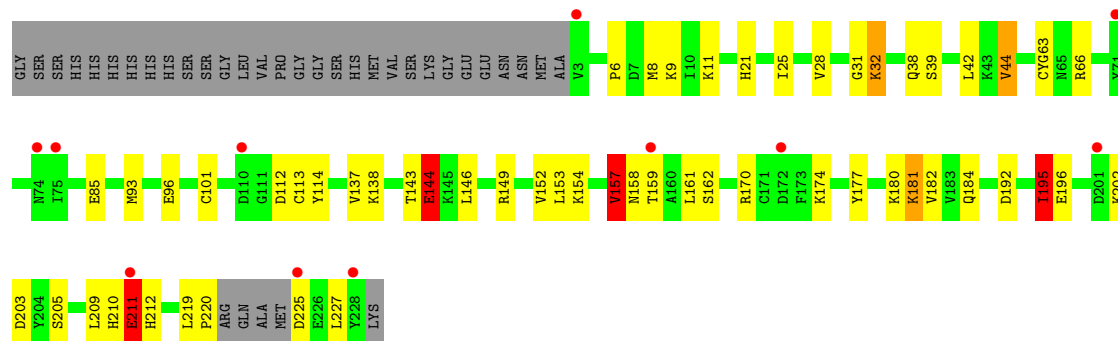


• Molecule 1: Fluorescent protein Dronpa

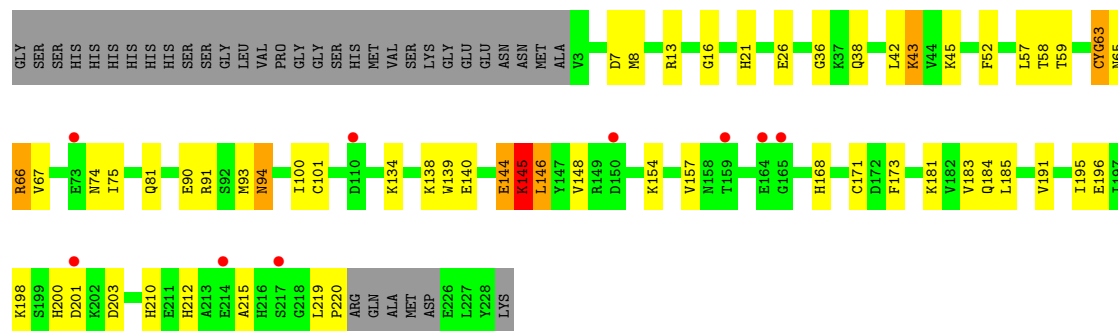




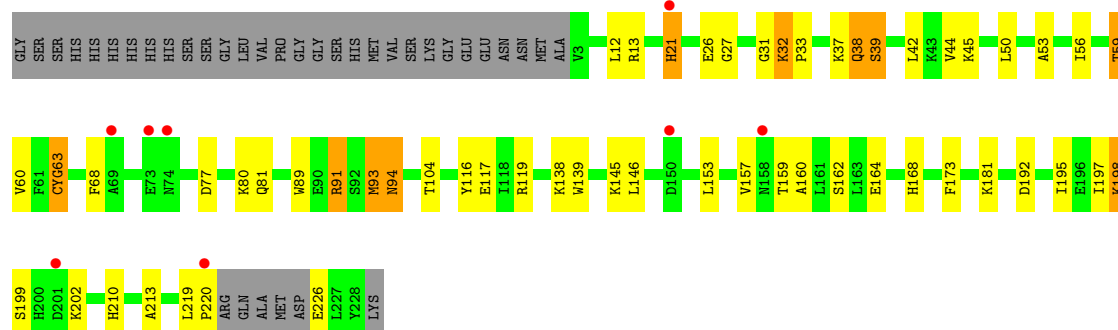
• Molecule 1: Fluorescent protein Dronpa



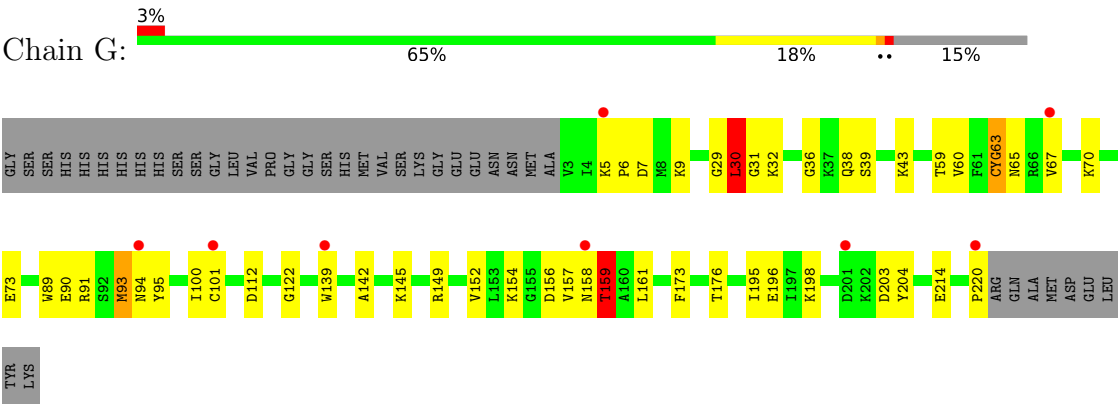
• Molecule 1: Fluorescent protein Dronpa



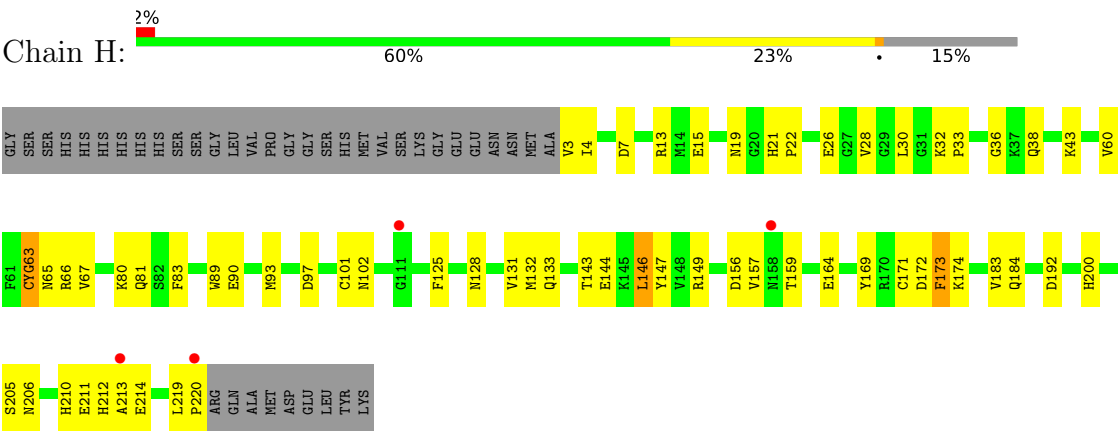
• Molecule 1: Fluorescent protein Dronpa



● 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	79.41Å 85.81Å 143.17Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	37.29 – 2.64 37.29 – 2.64	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.29-2.64) 82.7 (37.29-2.64)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, R_{free}	0.226 , 0.284 0.227 , 0.276	Depositor DCC
R_{free} test set	2674 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14128	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.98 % 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 7.9617e-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: GYC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	10/1751 (0.6%)	0.70	0/2368
1	B	0.87	12/1755 (0.7%)	0.69	0/2372
1	C	0.84	9/1767 (0.5%)	0.77	4/2391 (0.2%)
1	D	0.92	15/1765 (0.8%)	0.78	7/2389 (0.3%)
1	E	0.95	12/1769 (0.7%)	0.78	2/2390 (0.1%)
1	F	0.83	9/1780 (0.5%)	0.72	4/2403 (0.2%)
1	G	0.85	8/1745 (0.5%)	0.80	5/2362 (0.2%)
1	H	0.97	16/1735 (0.9%)	0.71	2/2352 (0.1%)
All	All	0.89	91/14067 (0.6%)	0.75	24/19027 (0.1%)

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	32	LYS	C-O	-8.60	1.18	1.25
1	D	212	HIS	C-O	-8.41	1.14	1.23
1	C	145	LYS	C-O	-8.01	1.14	1.24
1	H	32	LYS	C-O	-7.76	1.17	1.24
1	B	212	HIS	C-O	-7.70	1.15	1.23
1	H	26	GLU	C-O	-7.51	1.14	1.23
1	C	212	HIS	C-O	-7.38	1.15	1.23
1	C	158	ASN	C-O	-7.34	1.15	1.23
1	E	145	LYS	C-O	-7.26	1.15	1.24
1	F	37	LYS	C-O	-7.24	1.15	1.23
1	A	211	GLU	C-O	-7.17	1.15	1.23
1	D	32	LYS	C-O	-7.17	1.16	1.24
1	C	43	LYS	C-O	-7.15	1.15	1.24
1	B	156	ASP	C-O	-7.12	1.15	1.24
1	E	7	ASP	C-O	-7.09	1.16	1.23
1	H	174	LYS	C-O	-6.99	1.15	1.24
1	E	146	LEU	C-O	-6.95	1.15	1.24
1	E	75	ILE	C-O	-6.94	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	LYS	C-O	-6.80	1.15	1.24
1	D	144	GLU	C-O	-6.79	1.15	1.24
1	E	38	GLN	C-O	-6.78	1.15	1.23
1	H	32	LYS	N-CA	-6.76	1.39	1.46
1	H	159	THR	C-O	-6.75	1.17	1.24
1	H	131	VAL	C-O	-6.73	1.15	1.24
1	B	144	GLU	C-O	-6.67	1.15	1.23
1	D	157	VAL	C-O	-6.66	1.17	1.24
1	D	44	VAL	C-O	-6.64	1.16	1.24
1	H	172	ASP	C-O	-6.60	1.16	1.24
1	C	93	MET	C-O	-6.60	1.16	1.24
1	A	55	ASP	C-O	-6.59	1.15	1.24
1	C	211	GLU	C-O	-6.56	1.15	1.23
1	E	43	LYS	C-O	-6.53	1.16	1.24
1	E	42	LEU	C-O	-6.45	1.16	1.24
1	A	19	ASN	C-O	-6.44	1.14	1.23
1	E	8	MET	C-O	-6.37	1.16	1.23
1	D	182	VAL	C-O	-6.34	1.17	1.24
1	H	171	CYS	C-O	-6.30	1.16	1.23
1	F	38	GLN	C-O	-6.30	1.16	1.23
1	F	39	SER	C-O	-6.29	1.16	1.23
1	B	168	HIS	C-O	-6.24	1.16	1.24
1	G	30	LEU	C-O	-6.21	1.16	1.23
1	E	144	GLU	C-O	-6.20	1.16	1.24
1	H	33	PRO	C-O	-6.17	1.16	1.24
1	F	199	SER	C-O	-6.14	1.16	1.23
1	B	179	ALA	C-O	-6.12	1.16	1.23
1	H	173	PHE	C-O	-6.12	1.16	1.23
1	A	153	LEU	C-O	-6.10	1.16	1.24
1	B	167	GLY	C-O	-6.10	1.18	1.23
1	C	41	ASP	C-O	-6.08	1.16	1.24
1	B	145	LYS	C-O	-6.03	1.16	1.24
1	F	94	ASN	C-O	-5.93	1.17	1.24
1	G	95	TYR	C-O	-5.92	1.16	1.23
1	G	93	MET	C-O	-5.92	1.17	1.24
1	H	146	LEU	C-O	-5.92	1.16	1.24
1	C	198	LYS	C-O	-5.91	1.16	1.24
1	D	42	LEU	C-O	-5.91	1.16	1.24
1	H	164	GLU	C-O	-5.87	1.16	1.24
1	A	200	HIS	C-O	-5.87	1.17	1.23
1	D	159	THR	C-O	-5.85	1.15	1.23
1	D	38	GLN	C-O	-5.84	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	ARG	C-O	-5.82	1.15	1.24
1	B	211	GLU	C-O	-5.78	1.17	1.23
1	G	29	GLY	C-O	-5.70	1.17	1.23
1	B	131	VAL	C-O	-5.67	1.16	1.23
1	F	59	THR	C-O	-5.63	1.16	1.24
1	D	195	ILE	C-O	-5.62	1.18	1.24
1	F	13	ARG	C-O	-5.59	1.17	1.23
1	B	75	ILE	C-O	-5.56	1.18	1.24
1	F	197	ILE	C-O	-5.55	1.18	1.24
1	A	11	LYS	C-O	-5.51	1.17	1.24
1	H	156	ASP	C-O	-5.51	1.17	1.24
1	A	184	GLN	C-O	-5.46	1.17	1.23
1	D	31	GLY	C-O	-5.45	1.17	1.23
1	G	36	GLY	C-O	-5.43	1.17	1.24
1	H	90	GLU	C-O	-5.43	1.17	1.23
1	H	210	HIS	C-O	-5.41	1.17	1.24
1	G	31	GLY	C-O	-5.36	1.18	1.23
1	E	42	LEU	CA-C	-5.33	1.46	1.52
1	G	159	THR	C-O	-5.24	1.17	1.24
1	E	21	HIS	C-O	-5.23	1.17	1.24
1	D	196	GLU	C-O	-5.22	1.17	1.23
1	A	154	LYS	C-O	-5.21	1.17	1.23
1	A	15	GLU	C-O	-5.18	1.18	1.24
1	E	16	GLY	C-O	-5.16	1.18	1.23
1	D	31	GLY	CA-C	-5.15	1.45	1.51
1	B	164	GLU	C-O	-5.13	1.18	1.23
1	D	180	LYS	C-O	-5.09	1.17	1.24
1	F	31	GLY	C-O	-5.08	1.18	1.23
1	D	182	VAL	CA-C	-5.06	1.47	1.52
1	H	159	THR	N-CA	-5.02	1.39	1.46
1	C	203	ASP	N-CA	-5.01	1.40	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	7	ASP	N-CA-C	7.51	121.39	108.02
1	F	32	LYS	CA-C-N	7.02	127.00	119.28
1	F	32	LYS	C-N-CA	7.02	127.00	119.28
1	C	29	GLY	N-CA-C	6.43	122.02	111.27
1	D	202	LYS	N-CA-C	6.42	118.36	111.36
1	D	211	GLU	N-CA-C	6.16	118.66	108.99
1	C	202	LYS	N-CA-C	-6.10	105.50	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	GLN	CB-CG-CD	-6.04	102.34	112.60
1	G	73	GLU	CB-CG-CD	-6.03	102.34	112.60
1	D	42	LEU	N-CA-C	5.99	119.24	109.59
1	F	21	HIS	CA-C-N	-5.93	114.49	120.31
1	F	21	HIS	C-N-CA	-5.93	114.49	120.31
1	C	32	LYS	CA-C-N	5.67	126.92	119.84
1	C	32	LYS	C-N-CA	5.67	126.92	119.84
1	D	159	THR	N-CA-C	5.59	118.36	109.65
1	D	32	LYS	CA-C-N	5.49	125.32	119.28
1	D	32	LYS	C-N-CA	5.49	125.32	119.28
1	G	5	LYS	CB-CA-C	-5.40	100.91	110.47
1	G	204	TYR	N-CA-C	5.31	119.03	112.24
1	G	6	PRO	N-CA-C	-5.22	107.61	114.03
1	E	21	HIS	N-CA-C	5.18	116.44	109.24
1	H	7	ASP	N-CA-CB	-5.14	102.49	110.87
1	D	21	HIS	CB-CA-C	5.12	115.68	109.85
1	H	159	THR	N-CA-CB	-5.03	101.86	110.86

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	1726	0	1646	29	0
1	B	1730	0	1657	27	0
1	C	1743	0	1641	44	0
1	D	1741	0	1634	31	0
1	E	1745	0	1660	43	0
1	F	1756	0	1680	33	0
1	G	1720	0	1628	34	0
1	H	1710	0	1602	45	0
2	A	38	0	0	4	0
2	B	37	0	0	2	0
2	C	25	0	0	0	0
2	D	31	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	29	0	0	2	0
2	F	31	0	0	2	0
2	G	30	0	0	2	0
2	H	36	0	0	2	0
All	All	14128	0	13148	264	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 10.

All (264) 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:H:144:GLU:HG3	1:H:157:VAL:HG23	1.32	1.09
1:C:31:GLY:HA3	1:C:68:PHE:CE1	1.88	1.07
1:H:144:GLU:HG3	1:H:157:VAL:CG2	1.91	0.98
1:E:157:VAL:HG22	1:E:173:PHE:HB2	1.55	0.88
1:E:58:THR:O	1:E:63:GYC:HB11	1.74	0.87
1:E:138:LYS:HE3	1:E:139:TRP:O	1.76	0.85
1:E:138:LYS:HG2	1:E:139:TRP:N	1.90	0.85
1:G:94:ASN:OD1	1:G:100:ILE:HD13	1.77	0.84
1:A:9:LYS:HD3	1:A:30:LEU:HB3	1.57	0.84
1:H:19:ASN:HD21	1:H:125:PHE:HB2	1.44	0.83
1:G:139:TRP:CD1	1:G:161:LEU:HD21	2.14	0.82
1:G:139:TRP:NE1	1:G:161:LEU:HD21	1.95	0.79
1:G:59:THR:HG21	1:G:173:PHE:HE1	1.51	0.75
1:C:27:GLY:HA3	1:C:42:LEU:HD12	1.66	0.75
1:E:168:HIS:ND1	2:E:301:HOH:O	2.21	0.73
1:C:168:HIS:O	1:G:149:ARG:NH2	2.22	0.72
1:B:157:VAL:HB	1:B:173:PHE:HB2	1.71	0.71
1:F:159:THR:HG22	1:F:160:ALA:H	1.56	0.71
1:H:67:VAL:HG11	1:H:83:PHE:HE2	1.56	0.70
1:C:33:PRO:O	1:C:80:LYS:CE	2.42	0.67
1:D:11:LYS:HG3	1:D:28:VAL:HG12	1.77	0.67
1:C:148:VAL:HG21	1:C:185:LEU:HB3	1.77	0.67
1:A:3:VAL:N	2:A:302:HOH:O	2.27	0.67
1:A:5:LYS:HB2	1:A:8:MET:SD	2.35	0.67
1:C:5:LYS:HG2	1:C:7:ASP:H	1.61	0.66
1:B:76:VAL:HG11	1:B:184:GLN:HG2	1.77	0.66
1:D:195:ILE:HD11	1:D:209:LEU:HD21	1.77	0.65
1:E:52:PHE:HE1	1:E:57:LEU:HD11	1.59	0.65
1:E:144:GLU:HB2	1:E:157:VAL:HG12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD12	1:C:30:LEU:O	1.96	0.65
1:E:66:ARG:HG2	1:E:66:ARG:HH11	1.62	0.64
1:E:157:VAL:HG22	1:E:173:PHE:CB	2.27	0.64
1:G:157:VAL:HB	1:G:173:PHE:HB2	1.80	0.64
1:A:149:ARG:NH2	1:E:168:HIS:O	2.31	0.63
1:B:100:ILE:HG22	1:H:102:ASN:HD21	1.62	0.63
1:B:145:LYS:HG2	1:B:156:ASP:HB2	1.80	0.63
1:H:3:VAL:HG13	1:H:4:ILE:HG13	1.81	0.63
1:G:154:LYS:NZ	1:G:176:THR:OG1	2.27	0.62
1:H:67:VAL:O	1:H:80:LYS:NZ	2.32	0.62
1:E:59:THR:O	1:E:91:ARG:NH2	2.32	0.62
1:H:144:GLU:CG	1:H:157:VAL:CG2	2.73	0.62
1:C:33:PRO:O	1:C:80:LYS:NZ	2.33	0.60
1:E:26:GLU:HG3	1:E:45:LYS:HD2	1.84	0.60
1:F:26:GLU:HB2	1:F:45:LYS:HE3	1.84	0.60
1:B:149:ARG:NH2	1:F:168:HIS:O	2.35	0.59
1:F:59:THR:HG21	1:F:173:PHE:CE2	2.37	0.59
1:B:77:ASP:O	1:B:81:GLN:HG3	2.03	0.59
1:C:31:GLY:HA3	1:C:68:PHE:CZ	2.36	0.59
1:D:219:LEU:HD21	1:H:214:GLU:HG3	1.85	0.59
1:G:203:ASP:OD1	1:G:203:ASP:N	2.28	0.59
1:C:139:TRP:HB2	1:C:195:ILE:CG2	2.32	0.59
1:G:93:MET:HB2	1:G:101:CYS:HB2	1.84	0.59
1:H:219:LEU:N	1:H:219:LEU:HD12	2.18	0.58
1:B:158:ASN:O	1:F:145:LYS:CD	2.52	0.58
1:C:139:TRP:CD2	1:C:161:LEU:HD13	2.39	0.58
1:E:144:GLU:CB	1:E:157:VAL:HG12	2.34	0.57
1:B:26:GLU:OE2	1:B:45:LYS:HE2	2.05	0.57
1:D:195:ILE:HG22	2:D:304:HOH:O	2.04	0.57
1:C:30:LEU:HD12	1:C:39:SER:HB3	1.87	0.57
1:F:44:VAL:HG21	1:F:50:LEU:HD21	1.87	0.56
1:G:139:TRP:CD1	1:G:161:LEU:CD2	2.88	0.56
1:C:60:VAL:HG13	1:C:89:TRP:HH2	1.69	0.56
1:E:144:GLU:HB2	1:E:157:VAL:CG1	2.35	0.56
1:D:192:ASP:HB3	1:H:219:LEU:HD11	1.87	0.56
1:F:12:LEU:HB2	1:F:116:TYR:HB2	1.87	0.56
1:E:157:VAL:HG22	1:E:173:PHE:CG	2.40	0.56
1:G:70:LYS:HB3	1:G:214:GLU:HG2	1.88	0.55
1:C:31:GLY:HA3	1:C:68:PHE:HE1	1.63	0.55
1:B:124:ASN:HB3	2:B:316:HOH:O	2.06	0.55
1:H:65:ASN:CG	1:H:67:VAL:HG22	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:NH1	1:H:147:TYR:OH	2.40	0.55
1:G:94:ASN:OD1	1:G:100:ILE:CD1	2.54	0.55
1:B:200:HIS:ND1	1:B:201:ASP:O	2.40	0.55
1:C:27:GLY:HA3	1:C:42:LEU:CD1	2.36	0.55
1:B:200:HIS:NE2	2:B:304:HOH:O	2.33	0.55
1:E:200:HIS:ND1	1:E:201:ASP:O	2.39	0.55
1:G:59:THR:HG22	1:G:91:ARG:HH12	1.73	0.55
1:D:9:LYS:HE3	1:D:112:ASP:OD2	2.06	0.54
1:E:146:LEU:N	1:E:146:LEU:HD12	2.21	0.54
1:C:85:GLU:HG2	1:C:181:LYS:HE2	1.88	0.54
1:B:7:ASP:OD1	1:B:32:LYS:NZ	2.40	0.54
1:H:67:VAL:HG11	1:H:83:PHE:CE2	2.40	0.54
1:A:154:LYS:HG2	2:A:333:HOH:O	2.07	0.54
1:D:195:ILE:HD12	1:D:211:GLU:HG3	1.89	0.54
1:H:144:GLU:CB	1:H:157:VAL:HG22	2.37	0.54
1:B:60:VAL:HG13	1:B:89:TRP:HH2	1.72	0.54
1:D:143:THR:HB	1:H:143:THR:HG21	1.90	0.54
1:F:60:VAL:HG13	1:F:89:TRP:HH2	1.73	0.54
1:H:144:GLU:HB2	1:H:157:VAL:HG22	1.90	0.54
1:B:40:MET:HE1	1:B:61:PHE:HB3	1.89	0.53
1:D:96:GLU:CD	1:H:149:ARG:HH22	2.16	0.53
1:C:159:THR:HG22	1:C:160:ALA:H	1.73	0.53
1:A:63:GYC:O3	1:A:89:TRP:NE1	2.36	0.53
1:A:157:VAL:HB	1:A:173:PHE:HB2	1.91	0.53
1:C:30:LEU:CD1	1:C:39:SER:HB3	2.39	0.53
1:E:91:ARG:HG2	1:E:93:MET:HE2	1.91	0.53
1:G:139:TRP:CE2	1:G:161:LEU:HG	2.44	0.53
1:D:66:ARG:NH2	1:D:177:TYR:OH	2.39	0.53
1:B:192:ASP:O	1:B:213:ALA:HA	2.08	0.53
1:H:60:VAL:HG13	1:H:89:TRP:HH2	1.74	0.53
1:C:19:ASN:HA	1:E:90:GLU:OE1	2.10	0.52
1:H:43:LYS:HA	1:H:205:SER:O	2.09	0.52
1:C:146:LEU:N	1:C:146:LEU:HD12	2.24	0.52
1:D:137:VAL:HB	1:D:162:SER:OG	2.10	0.52
1:F:77:ASP:O	1:F:81:GLN:HG3	2.09	0.52
1:C:10:ILE:N	1:C:29:GLY:O	2.38	0.52
1:A:128:ASN:HA	1:A:133:GLN:HE21	1.75	0.52
1:G:30:LEU:HD23	1:G:30:LEU:N	2.24	0.52
1:H:219:LEU:N	1:H:219:LEU:CD1	2.73	0.52
1:A:159:THR:HA	2:A:317:HOH:O	2.11	0.51
1:C:137:VAL:HB	1:C:162:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:GLU:N	2:F:307:HOH:O	2.43	0.51
1:E:94[A]:ASN:ND2	2:E:306:HOH:O	2.43	0.51
1:C:157:VAL:HB	1:C:173:PHE:HB2	1.92	0.51
1:A:60:VAL:HG13	1:A:89:TRP:HH2	1.75	0.50
1:D:144:GLU:HB2	1:D:157:VAL:HG22	1.92	0.50
1:F:104:THR:HG22	1:F:119:ARG:HB3	1.92	0.50
1:B:158:ASN:O	1:F:145:LYS:HD3	2.11	0.50
1:C:160:ALA:HB1	1:C:168:HIS:HB3	1.93	0.50
1:D:8:MET:HG3	1:D:114:TYR:HE2	1.77	0.49
1:C:27:GLY:CA	1:C:42:LEU:HD12	2.39	0.49
1:A:43:LYS:NZ	2:A:307:HOH:O	2.44	0.49
1:C:36:GLY:O	1:C:212:HIS:HA	2.13	0.49
1:G:139:TRP:CZ2	1:G:161:LEU:HD11	2.48	0.49
1:H:183:VAL:O	2:H:301:HOH:O	2.20	0.49
1:E:144:GLU:HA	1:E:157:VAL:HG12	1.94	0.49
1:C:194:HIS:CG	1:G:220:PRO:HG3	2.47	0.49
1:B:66:ARG:HD2	1:B:191:VAL:HG11	1.95	0.49
1:F:63:GYC:HB11	1:F:195:ILE:HD12	1.95	0.49
1:A:100:ILE:HD12	2:G:325:HOH:O	2.12	0.49
1:E:148:VAL:HG21	1:E:185:LEU:HB3	1.95	0.48
1:G:90:GLU:HG2	1:G:176:THR:HB	1.95	0.48
1:H:81:GLN:HB3	1:H:183:VAL:CG1	2.44	0.48
1:E:13:ARG:NH1	1:E:26:GLU:OE2	2.47	0.48
1:E:171:CYS:HG	1:E:173:PHE:HE1	1.57	0.48
1:C:5:LYS:HG3	1:C:6:PRO:HD2	1.96	0.47
1:E:203:ASP:OD2	1:E:203:ASP:N	2.42	0.47
1:D:138:LYS:O	1:D:161:LEU:HD23	2.14	0.47
1:D:219:LEU:HD12	1:D:220:PRO:HD2	1.95	0.47
1:B:137:VAL:HG23	1:B:164:GLU:N	2.30	0.47
1:C:31:GLY:CA	1:C:68:PHE:CE1	2.80	0.47
1:H:183:VAL:HG12	1:H:184:GLN:N	2.29	0.47
1:F:104:THR:HG23	2:F:305:HOH:O	2.15	0.47
1:H:4:ILE:HB	2:H:309:HOH:O	2.14	0.47
1:B:85:GLU:CD	1:B:181:LYS:HD2	2.40	0.47
1:C:163:LEU:HD11	1:C:169:TYR:HB2	1.96	0.47
1:C:194:HIS:CD2	1:G:220:PRO:HG3	2.50	0.47
1:E:66:ARG:HG2	1:E:66:ARG:NH1	2.29	0.47
1:H:192:ASP:O	1:H:213:ALA:HA	2.15	0.46
1:G:139:TRP:CD2	1:G:161:LEU:HG	2.50	0.46
1:A:3:VAL:HG21	1:A:84:PRO:HB3	1.97	0.46
1:C:3:VAL:HG13	1:C:4:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:HG2	1:F:93:MET:HE2	1.98	0.46
1:G:156:ASP:OD2	2:G:302:HOH:O	2.21	0.46
1:E:59:THR:HG22	1:E:63:GYC:CE2	2.46	0.46
1:G:60:VAL:HG13	1:G:89:TRP:HH2	1.81	0.46
1:G:9:LYS:HE2	1:G:112:ASP:OD2	2.16	0.45
1:H:13:ARG:NH2	1:H:15:GLU:OE1	2.40	0.45
1:D:146:LEU:HB3	1:D:153:LEU:HD11	1.99	0.45
1:D:174:LYS:HG3	2:D:309:HOH:O	2.16	0.45
1:E:191:VAL:HA	1:E:215:ALA:HA	1.98	0.45
1:F:198:LYS:HD3	1:F:210:HIS:CD2	2.52	0.45
1:H:63:GYC:HB2	1:H:66:ARG:NH2	2.30	0.45
1:C:102:ASN:HD21	1:E:100:ILE:HG22	1.81	0.45
1:D:9:LYS:O	1:D:113:CYS:HA	2.16	0.45
1:D:149:ARG:O	1:D:152:VAL:HG22	2.16	0.45
1:A:146:LEU:HA	1:A:154:LYS:O	2.16	0.45
1:D:25:ILE:HG12	1:D:44:VAL:HG22	1.98	0.45
1:G:196:GLU:OE1	1:G:198:LYS:HE2	2.17	0.45
1:F:89:TRP:CZ3	1:F:91:ARG:HB3	2.52	0.45
1:G:100:ILE:O	1:G:122:GLY:HA2	2.17	0.44
1:A:153:LEU:HB3	1:A:177:TYR:HB2	1.99	0.44
1:E:81:GLN:HG2	1:E:183:VAL:HG12	1.99	0.44
1:A:43:LYS:HD2	1:A:206:ASN:OD1	2.16	0.44
1:G:158:ASN:N	1:G:158:ASN:OD1	2.50	0.44
1:B:146:LEU:HB3	1:B:153:LEU:HD11	2.00	0.44
1:D:170:ARG:NH2	1:H:149:ARG:HH12	2.16	0.44
1:E:145:LYS:HB2	1:E:145:LYS:HE3	1.54	0.44
1:G:90:GLU:CG	1:G:176:THR:HB	2.47	0.44
1:H:144:GLU:HB2	1:H:157:VAL:CG2	2.47	0.44
1:F:93:MET:HE3	1:F:93:MET:HB2	1.90	0.44
1:H:144:GLU:CB	1:H:157:VAL:CG2	2.96	0.44
1:C:33:PRO:O	1:C:80:LYS:HE2	2.15	0.44
1:D:225:ASP:C	1:D:227:LEU:H	2.25	0.44
1:E:63:GYC:HB12	1:E:195:ILE:HD12	1.99	0.44
1:G:65:ASN:CG	1:G:67:VAL:HG12	2.43	0.44
1:F:91:ARG:CG	1:F:93:MET:HE2	2.49	0.43
1:D:146:LEU:HA	1:D:154:LYS:O	2.17	0.43
1:E:93:MET:HB2	1:E:101:CYS:HB2	2.00	0.43
1:F:146:LEU:HD13	1:F:153:LEU:HD21	2.00	0.43
1:A:8:MET:HE3	1:A:114:TYR:CZ	2.53	0.43
1:E:140:GLU:OE2	1:E:168:HIS:NE2	2.34	0.43
1:G:139:TRP:CE2	1:G:161:LEU:CG	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:MET:HB2	1:H:101:CYS:HB2	2.00	0.43
1:H:219:LEU:HA	1:H:220:PRO:HD3	1.88	0.43
1:A:137:VAL:HG22	1:A:164:GLU:HG2	2.00	0.43
1:H:97:ASP:OD1	1:H:169:TYR:OH	2.31	0.43
1:E:65:ASN:CG	1:E:67:VAL:HG12	2.42	0.43
1:F:77:ASP:OD1	1:F:80:LYS:HD2	2.19	0.43
1:H:36:GLY:O	1:H:212:HIS:HA	2.19	0.43
1:A:71:TYR:HA	1:A:72:PRO:HD3	1.86	0.43
1:E:94[A]:ASN:OD1	1:E:94[A]:ASN:N	2.52	0.43
1:H:21:HIS:HA	1:H:22:PRO:HD3	1.92	0.43
1:C:138:LYS:HB2	1:C:138:LYS:HE3	1.90	0.43
1:F:138:LYS:NZ	1:F:139:TRP:O	2.52	0.43
1:H:200:HIS:HA	1:H:206:ASN:O	2.19	0.43
1:D:93:MET:HB2	1:D:101:CYS:HB2	2.00	0.43
1:D:192:ASP:HB3	1:H:219:LEU:CD1	2.48	0.43
1:E:144:GLU:CA	1:E:157:VAL:HG12	2.49	0.43
1:G:63:GYC:HB11	1:G:195:ILE:HD12	2.00	0.43
1:B:158:ASN:O	1:F:145:LYS:HD2	2.19	0.42
1:A:81:GLN:HB3	1:A:183:VAL:HG13	2.01	0.42
1:A:192:ASP:O	1:A:213:ALA:HA	2.19	0.42
1:C:192:ASP:O	1:C:213:ALA:HA	2.18	0.42
1:H:81:GLN:HB3	1:H:183:VAL:HG11	2.01	0.42
1:D:39:SER:HB2	1:D:210:HIS:CE1	2.54	0.42
1:F:192:ASP:O	1:F:213:ALA:HA	2.19	0.42
1:G:145:LYS:HB2	1:G:145:LYS:HE2	1.83	0.42
1:F:157:VAL:HB	1:F:173:PHE:CD2	2.54	0.42
1:C:4:ILE:HA	1:C:8:MET:HE2	2.00	0.42
1:F:145:LYS:HE2	1:F:145:LYS:HB2	1.78	0.42
1:H:183:VAL:HG12	1:H:184:GLN:H	1.85	0.42
1:A:77:ASP:O	1:A:81:GLN:HB2	2.19	0.42
1:E:219:LEU:HA	1:E:220:PRO:HD3	1.78	0.42
1:G:142:ALA:HB2	1:G:159:THR:HG21	2.01	0.42
1:C:52:PHE:HE1	1:C:57:LEU:HD11	1.84	0.42
1:D:96:GLU:OE1	1:H:149:ARG:NH2	2.47	0.42
1:E:198:LYS:HG3	1:E:210:HIS:CD2	2.55	0.42
1:F:27:GLY:HA3	1:F:42:LEU:HD23	2.01	0.42
1:A:159:THR:OG1	1:A:160:ALA:N	2.53	0.42
1:D:85:GLU:HB2	1:D:181:LYS:HD3	2.02	0.42
1:A:63:GYC:HB2	1:A:66:ARG:HH22	1.83	0.41
1:E:63:GYC:CB1	1:E:195:ILE:HD12	2.50	0.41
1:H:157:VAL:HB	1:H:173:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:122:GLY:HA2	2.19	0.41
1:B:153:LEU:HB3	1:B:177:TYR:HB2	2.02	0.41
1:C:32:LYS:HB3	1:C:35:GLU:HG3	2.02	0.41
1:F:53:ALA:O	1:F:56:ILE:HG12	2.20	0.41
1:F:89:TRP:HZ3	1:F:91:ARG:HB3	1.86	0.41
1:G:60:VAL:HG13	1:G:89:TRP:CH2	2.55	0.41
1:B:33:PRO:HA	1:B:68:PHE:HA	2.01	0.41
1:C:94:ASN:OD1	1:C:100:ILE:HD12	2.20	0.41
1:E:36:GLY:O	1:E:212:HIS:HA	2.21	0.41
1:A:144:GLU:HB2	1:A:157:VAL:HG22	2.03	0.41
1:C:3:VAL:CG1	1:C:4:ILE:HD12	2.50	0.41
1:H:146:LEU:N	1:H:146:LEU:HD12	2.36	0.41
1:B:139:TRP:CZ3	1:B:159:THR:HG23	2.56	0.41
1:A:12:LEU:HB2	1:A:116:TYR:HB2	2.03	0.41
1:A:183:VAL:HG12	1:A:184:GLN:N	2.36	0.41
1:E:146:LEU:HA	1:E:154:LYS:O	2.21	0.41
1:A:110:ASP:OD2	1:F:45:LYS:NZ	2.53	0.41
1:D:203:ASP:OD2	1:D:205:SER:OG	2.39	0.41
1:F:33:PRO:HA	1:F:68:PHE:HA	2.02	0.41
1:H:128:ASN:HA	1:H:133:GLN:HE21	1.86	0.41
1:C:32:LYS:C	1:C:34:PHE:H	2.29	0.40
1:F:219:LEU:HA	1:F:220:PRO:HD3	1.92	0.40
1:A:42:LEU:O	1:A:43:LYS:HD3	2.20	0.40
1:B:157:VAL:HB	1:B:173:PHE:CB	2.48	0.40
1:C:34:PHE:CE1	1:C:80:LYS:HE2	2.57	0.40
1:E:195:ILE:C	1:E:196:GLU:HG3	2.46	0.40
1:F:81:GLN:O	1:F:181:LYS:NZ	2.49	0.40
1:B:78:TYR:HB2	1:B:186:PRO:HD3	2.04	0.40
1:C:145:LYS:HD2	1:G:158:ASN:O	2.21	0.40
1:D:143:THR:CB	1:H:143:THR:HG21	2.52	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	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	B	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	C	214/255 (84%)	209 (98%)	4 (2%)	1 (0%)	24	36
1	D	213/255 (84%)	209 (98%)	4 (2%)	0	100	100
1	E	213/255 (84%)	209 (98%)	4 (2%)	0	100	100
1	F	212/255 (83%)	207 (98%)	5 (2%)	0	100	100
1	G	211/255 (83%)	204 (97%)	7 (3%)	0	100	100
1	H	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
All	All	1696/2040 (83%)	1660 (98%)	35 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	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	181/216 (84%)	173 (96%)	8 (4%)	25	41
1	B	182/216 (84%)	178 (98%)	4 (2%)	45	66
1	C	179/216 (83%)	174 (97%)	5 (3%)	38	58
1	D	180/216 (83%)	171 (95%)	9 (5%)	22	36
1	E	181/216 (84%)	173 (96%)	8 (4%)	25	41
1	F	185/216 (86%)	173 (94%)	12 (6%)	15	26
1	G	180/216 (83%)	174 (97%)	6 (3%)	33	53
1	H	177/216 (82%)	172 (97%)	5 (3%)	38	58
All	All	1445/1728 (84%)	1388 (96%)	57 (4%)	28	47

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	11	LYS
1	A	30	LEU
1	A	38	GLN
1	A	154	LYS
1	A	180	LYS
1	A	181	LYS
1	A	202	LYS
1	B	132	MET
1	B	180	LYS
1	B	181	LYS
1	B	211	GLU
1	C	30	LEU
1	C	42	LEU
1	C	43	LYS
1	C	94	ASN
1	C	161	LEU
1	D	6	PRO
1	D	32	LYS
1	D	144	GLU
1	D	157	VAL
1	D	158	ASN
1	D	181	LYS
1	D	184	GLN
1	D	195	ILE
1	D	211	GLU
1	E	43	LYS
1	E	66	ARG
1	E	74	ASN
1	E	94[A]	ASN
1	E	94[B]	ASN
1	E	134	LYS
1	E	145	LYS
1	E	181	LYS
1	F	21	HIS
1	F	32	LYS
1	F	38	GLN
1	F	39	SER
1	F	91	ARG
1	F	93	MET
1	F	94	ASN
1	F	117	GLU

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Mol	Chain	Res	Type
1	F	162	SER
1	F	164	GLU
1	F	198	LYS
1	F	202	LYS
1	G	30	LEU
1	G	38	GLN
1	G	39	SER
1	G	43	LYS
1	G	152	VAL
1	G	159	THR
1	H	28	VAL
1	H	30	LEU
1	H	38	GLN
1	H	132	MET
1	H	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	ASN
1	C	212	HIS
1	D	21	HIS
1	D	210	HIS
1	F	21	HIS
1	F	193	HIS
1	F	208	ASN
1	F	210	HIS
1	G	200	HIS
1	H	19	ASN
1	H	102	ASN

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	GYC	A	63	1	21,22,23	1.88	7 (33%)	26,30,32	1.94	5 (19%)
1	GYC	E	63	1	21,22,23	1.94	7 (33%)	26,30,32	2.05	5 (19%)
1	GYC	G	63	1	21,22,23	1.09	1 (4%)	26,30,32	2.32	7 (26%)
1	GYC	B	63	1	21,22,23	1.06	1 (4%)	26,30,32	2.38	6 (23%)
1	GYC	C	63	1	21,22,23	1.14	2 (9%)	26,30,32	2.16	5 (19%)
1	GYC	F	63	1	21,22,23	1.06	1 (4%)	26,30,32	2.42	7 (26%)
1	GYC	H	63	1	21,22,23	1.03	1 (4%)	26,30,32	2.32	7 (26%)
1	GYC	D	63	1	21,22,23	1.06	1 (4%)	26,30,32	2.36	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	A	63	1	-	3/10/29/30	0/2/2/2
1	GYC	E	63	1	-	4/10/29/30	0/2/2/2
1	GYC	G	63	1	-	3/10/29/30	0/2/2/2
1	GYC	B	63	1	-	4/10/29/30	0/2/2/2
1	GYC	C	63	1	-	3/10/29/30	0/2/2/2
1	GYC	F	63	1	-	4/10/29/30	0/2/2/2
1	GYC	H	63	1	-	4/10/29/30	0/2/2/2
1	GYC	D	63	1	-	3/10/29/30	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GYC	CB2-CA2	4.23	1.39	1.35
1	G	63	GYC	CB2-CA2	3.98	1.39	1.35
1	B	63	GYC	CB2-CA2	3.88	1.38	1.35
1	F	63	GYC	CB2-CA2	3.83	1.38	1.35
1	H	63	GYC	CB2-CA2	3.73	1.38	1.35
1	D	63	GYC	CB2-CA2	3.65	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	GYC	C2-N3	-3.60	1.31	1.40
1	E	63	GYC	CB2-CA2	3.59	1.38	1.35
1	A	63	GYC	CA2-C2	-3.45	1.44	1.48
1	A	63	GYC	C2-N3	-3.38	1.32	1.40
1	E	63	GYC	C1-N2	-2.91	1.27	1.32
1	E	63	GYC	CB1-CA1	-2.76	1.50	1.53
1	E	63	GYC	C1-N3	-2.64	1.32	1.37
1	E	63	GYC	CE2-CD2	-2.56	1.34	1.38
1	E	63	GYC	CA2-C2	-2.54	1.45	1.48
1	A	63	GYC	CE1-CD1	-2.47	1.34	1.38
1	A	63	GYC	C1-N2	-2.46	1.28	1.32
1	A	63	GYC	CE2-CD2	-2.44	1.34	1.38
1	A	63	GYC	CA2-N2	-2.24	1.33	1.38
1	A	63	GYC	CE1-CZ	-2.15	1.35	1.39
1	C	63	GYC	C2-N3	-2.08	1.35	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GYC	O2-C2-CA2	-7.23	126.41	131.02
1	F	63	GYC	O2-C2-CA2	-6.83	126.66	131.02
1	D	63	GYC	O2-C2-CA2	-6.70	126.74	131.02
1	H	63	GYC	O2-C2-CA2	-6.61	126.80	131.02
1	E	63	GYC	C2-CA2-N2	-6.29	104.45	108.95
1	G	63	GYC	O2-C2-CA2	-6.12	127.11	131.02
1	C	63	GYC	O2-C2-CA2	-5.97	127.21	131.02
1	G	63	GYC	C2-CA2-N2	-5.30	105.16	108.95
1	C	63	GYC	C2-CA2-N2	-5.20	105.23	108.95
1	F	63	GYC	C2-CA2-N2	-5.19	105.23	108.95
1	B	63	GYC	C2-CA2-N2	-5.10	105.30	108.95
1	F	63	GYC	CG2-CB2-CA2	-5.01	123.91	129.87
1	D	63	GYC	CG2-CB2-CA2	-5.00	123.92	129.87
1	G	63	GYC	CA2-N2-C1	4.91	109.64	105.80
1	H	63	GYC	C2-CA2-N2	-4.86	105.47	108.95
1	A	63	GYC	CA2-N2-C1	4.86	109.60	105.80
1	D	63	GYC	C2-CA2-N2	-4.83	105.49	108.95
1	E	63	GYC	CA2-N2-C1	4.74	109.50	105.80
1	A	63	GYC	O2-C2-CA2	-4.64	128.06	131.02
1	B	63	GYC	CA2-N2-C1	4.62	109.41	105.80
1	F	63	GYC	CA2-N2-C1	4.58	109.38	105.80
1	D	63	GYC	CA2-N2-C1	4.55	109.36	105.80
1	C	63	GYC	CA2-N2-C1	4.43	109.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	GYC	CG2-CB2-CA2	-4.42	124.61	129.87
1	H	63	GYC	CG2-CB2-CA2	-4.35	124.69	129.87
1	A	63	GYC	C2-CA2-N2	-4.13	105.99	108.95
1	H	63	GYC	CA2-N2-C1	4.11	109.02	105.80
1	B	63	GYC	CG2-CB2-CA2	-3.92	125.21	129.87
1	E	63	GYC	O2-C2-CA2	-3.63	128.71	131.02
1	A	63	GYC	O3-C3-CA3	-3.62	109.17	125.47
1	H	63	GYC	CA1-CB1-SG1	-3.39	107.14	114.40
1	C	63	GYC	CG2-CB2-CA2	-3.21	126.05	129.87
1	D	63	GYC	CB2-CA2-C2	3.10	126.11	122.36
1	E	63	GYC	CA2-C2-N3	2.94	105.97	103.50
1	E	63	GYC	CA1-CB1-SG1	-2.87	108.27	114.40
1	G	63	GYC	CB2-CA2-C2	2.85	125.81	122.36
1	H	63	GYC	CA2-C2-N3	2.83	105.88	103.50
1	F	63	GYC	CA2-C2-N3	2.73	105.80	103.50
1	F	63	GYC	CB2-CA2-C2	2.68	125.60	122.36
1	B	63	GYC	CA2-C2-N3	2.67	105.75	103.50
1	G	63	GYC	CA2-C2-N3	2.66	105.73	103.50
1	A	63	GYC	CA2-C2-N3	2.58	105.67	103.50
1	D	63	GYC	CA2-C2-N3	2.57	105.66	103.50
1	F	63	GYC	CA1-CB1-SG1	-2.55	108.95	114.40
1	B	63	GYC	CA1-CB1-SG1	-2.50	109.05	114.40
1	C	63	GYC	CA2-C2-N3	2.50	105.60	103.50
1	D	63	GYC	CA1-CB1-SG1	-2.29	109.50	114.40
1	H	63	GYC	CB2-CA2-C2	2.27	125.11	122.36
1	G	63	GYC	CA1-CB1-SG1	-2.13	109.84	114.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	F	63	GYC	N2-CA2-CB2-CG2
1	F	63	GYC	C2-CA2-CB2-CG2
1	G	63	GYC	C3-CA3-N3-C2
1	G	63	GYC	N2-CA2-CB2-CG2
1	G	63	GYC	C2-CA2-CB2-CG2
1	H	63	GYC	C3-CA3-N3-C2
1	H	63	GYC	N2-CA2-CB2-CG2
1	H	63	GYC	C2-CA2-CB2-CG2
1	A	63	GYC	N2-CA2-CB2-CG2
1	D	63	GYC	N2-CA2-CB2-CG2
1	E	63	GYC	N2-CA2-CB2-CG2
1	A	63	GYC	C3-CA3-N3-C2
1	E	63	GYC	C1-CA1-CB1-SG1
1	E	63	GYC	C3-CA3-N3-C2
1	B	63	GYC	C3-CA3-N3-C1
1	F	63	GYC	C3-CA3-N3-C1
1	H	63	GYC	C3-CA3-N3-C1

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	GYC	2	0
1	E	63	GYC	4	0
1	G	63	GYC	1	0
1	F	63	GYC	1	0
1	H	63	GYC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	215/255 (84%)	0.57	9 (4%)	40	34	18, 34, 60, 70	0
1	B	215/255 (84%)	0.53	6 (2%)	55	50	20, 33, 61, 79	0
1	C	220/255 (86%)	0.83	14 (6%)	25	21	22, 42, 67, 91	0
1	D	219/255 (85%)	0.63	11 (5%)	34	28	19, 36, 60, 73	0
1	E	218/255 (85%)	0.69	9 (4%)	41	35	18, 40, 59, 74	1 (0%)
1	F	218/255 (85%)	0.56	8 (3%)	45	39	18, 34, 60, 77	0
1	G	215/255 (84%)	0.62	8 (3%)	45	39	21, 37, 63, 91	0
1	H	215/255 (84%)	0.63	4 (1%)	66	62	21, 36, 61, 77	0
All	All	1735/2040 (85%)	0.63	69 (3%)	42	35	18, 37, 62, 91	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	220	PRO	4.8
1	A	158	ASN	4.3
1	B	150	ASP	4.1
1	H	213	ALA	3.9
1	H	158	ASN	3.7
1	B	158	ASN	3.5
1	F	158	ASN	3.5
1	C	12	LEU	3.1
1	D	211	GLU	3.0
1	C	7	ASP	3.0
1	D	201	ASP	3.0
1	H	111	GLY	3.0
1	G	158	ASN	2.9
1	C	227	LEU	2.9
1	F	220	PRO	2.9
1	A	90	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	150	ASP	2.9
1	F	150	ASP	2.9
1	F	201	ASP	2.9
1	A	112	ASP	2.8
1	D	71	TYR	2.8
1	E	201	ASP	2.8
1	F	73	GLU	2.8
1	C	195	ILE	2.7
1	C	156	ASP	2.7
1	E	159	THR	2.6
1	C	114	TYR	2.6
1	D	110	ASP	2.5
1	C	150	ASP	2.5
1	D	75	ILE	2.5
1	A	193	HIS	2.5
1	C	117	GLU	2.5
1	A	110	ASP	2.5
1	B	220	PRO	2.4
1	G	94	ASN	2.4
1	G	5	LYS	2.4
1	E	110	ASP	2.4
1	A	143	THR	2.3
1	A	73	GLU	2.3
1	E	214	GLU	2.3
1	E	73	GLU	2.3
1	C	225	ASP	2.3
1	D	225	ASP	2.3
1	C	218	GLY	2.3
1	A	146	LEU	2.3
1	D	74	ASN	2.3
1	G	201	ASP	2.3
1	G	139	TRP	2.3
1	G	67	VAL	2.3
1	A	11	LYS	2.2
1	D	3	VAL	2.2
1	C	33	PRO	2.2
1	B	190	PHE	2.2
1	C	226	GLU	2.2
1	F	74	ASN	2.2
1	G	220	PRO	2.2
1	D	159	THR	2.1
1	B	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	21	HIS	2.1
1	C	228	TYR	2.1
1	C	196	GLU	2.1
1	E	164	GLU	2.1
1	E	165	GLY	2.1
1	D	172	ASP	2.1
1	E	217	SER	2.0
1	B	3	VAL	2.0
1	G	101	CYS	2.0
1	F	69	ALA	2.0
1	D	228	TYR	2.0

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, 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(Å ²)	Q<0.9
1	GYC	E	63	21/22	0.76	0.20	27,41,56,63	0
1	GYC	G	63	21/22	0.88	0.14	24,38,57,58	0
1	GYC	A	63	21/22	0.89	0.12	23,42,48,70	0
1	GYC	C	63	21/22	0.90	0.11	29,32,39,52	0
1	GYC	H	63	21/22	0.90	0.12	7,25,42,50	0
1	GYC	B	63	21/22	0.92	0.14	15,26,37,40	0
1	GYC	D	63	21/22	0.93	0.10	22,29,42,63	0
1	GYC	F	63	21/22	0.93	0.10	19,27,34,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.