



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:46 PM EST

PDB ID : 7RRJ
Title : Crystal structure of fast switching M159Q 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 : 2.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

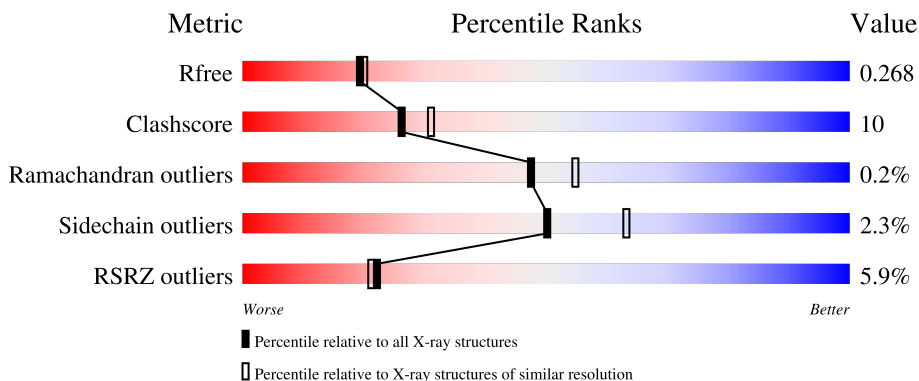
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



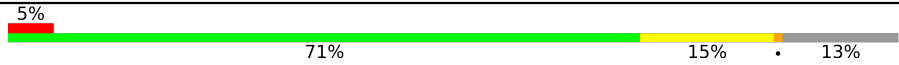

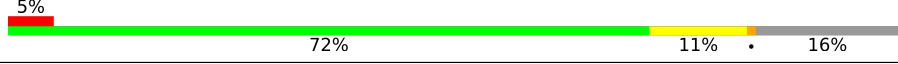
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 75% 9% • 15%
1	B	255	 4% 74% 9% • 16%
1	C	255	 5% 72% 13% • 14%
1	D	255	 7% 75% 11% • 13%
1	E	255	 6% 76% 10% • 12%

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Mol	Chain	Length	Quality of chain
1	F	255	 5% 71% 15% • 13%
1	G	255	 6% 73% 11% • 15%
1	H	255	 5% 72% 11% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15127 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
			Total	C	N	O	S			
1	A	217	Total 1782	C 1140	N 301	O 331	S 10	0	4	0
1	B	215	Total 1740	C 1112	N 294	O 325	S 9	0	1	0
1	C	219	Total 1814	C 1159	N 308	O 337	S 10	0	7	0
1	D	223	Total 1819	C 1164	N 307	O 338	S 10	0	4	0
1	E	224	Total 1834	C 1170	N 310	O 344	S 10	0	5	0
1	F	223	Total 1792	C 1142	N 303	O 337	S 10	0	2	0
1	G	216	Total 1762	C 1127	N 297	O 328	S 10	0	1	0
1	H	215	Total 1740	C 1113	N 294	O 324	S 9	0	1	0

There are 320 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	159	GLN	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
B	-13	PRO	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	159	GLN	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

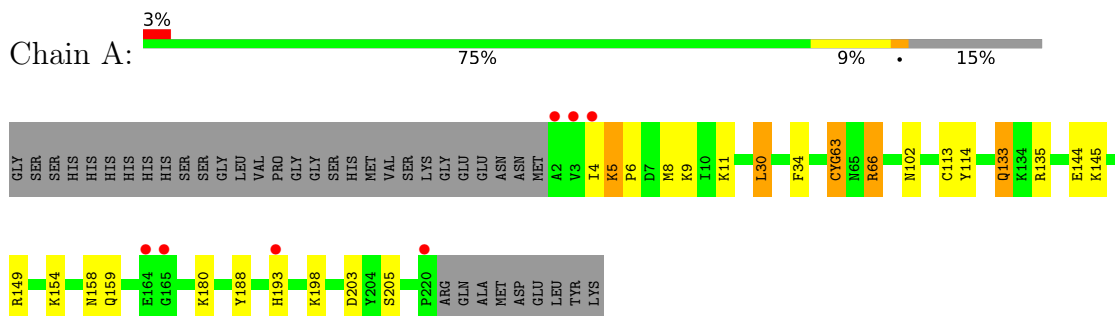
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	105	Total O 105 105	0	0
2	C	98	Total O 98 98	0	0
2	D	111	Total O 111 111	0	0
2	E	95	Total O 95 95	0	0
2	F	102	Total O 102 102	0	0
2	G	102	Total O 102 102	0	0
2	H	112	Total O 112 112	0	0

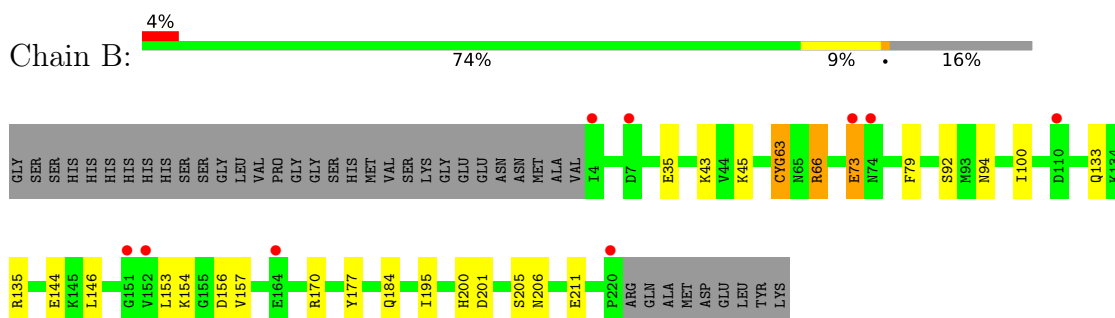
3 Residue-property plots [i](#)

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.

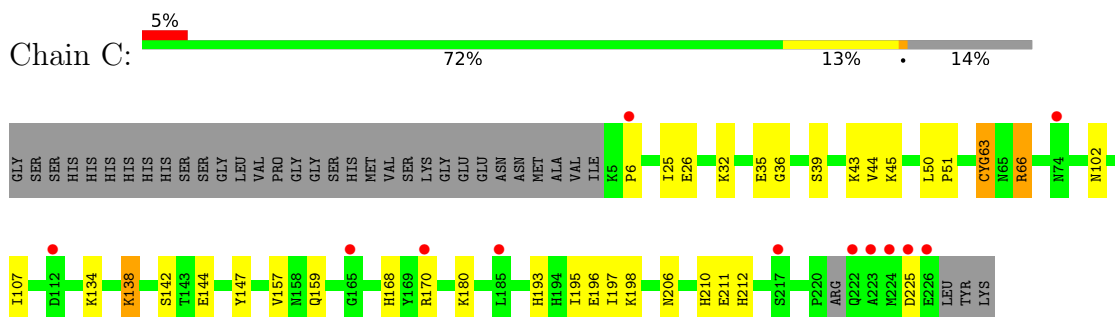
- Molecule 1: Fluorescent protein Dronpa



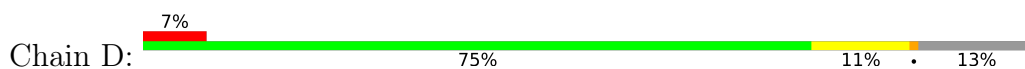
- Molecule 1: Fluorescent protein Dronpa

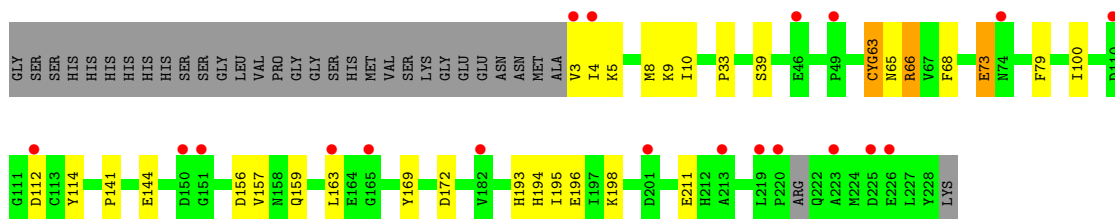


- Molecule 1: Fluorescent protein Dronpa

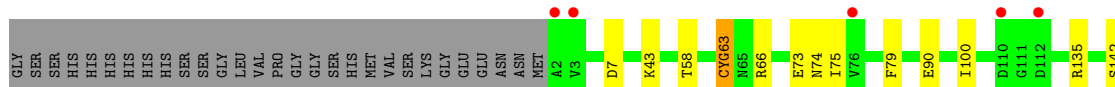
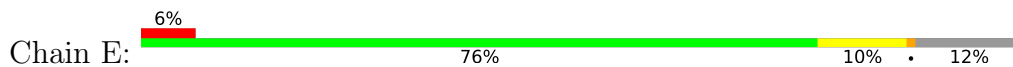


- Molecule 1: Fluorescent protein Dronpa





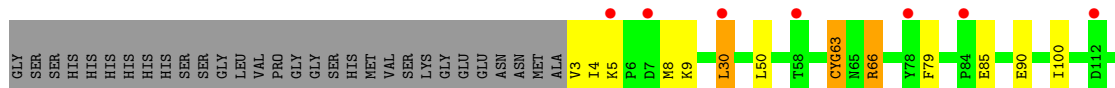
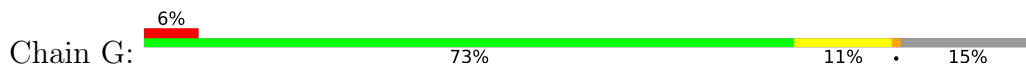
• Molecule 1: Fluorescent protein Dronpa



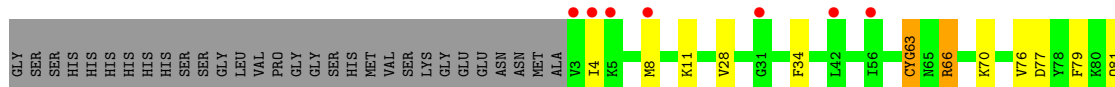
• Molecule 1: Fluorescent protein Dronpa

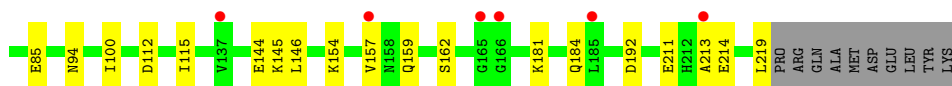


• Molecule 1: Fluorescent protein Dronpa



• 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	79.75Å 85.79Å 144.04Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	36.89 – 2.20 39.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (36.89-2.20) 81.6 (39.44-2.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.13RC2_2986	Depositor
R, R_{free}	0.242 , 0.271 0.241 , 0.268	Depositor DCC
R_{free} test set	4630 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15127	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 44.04 % 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 1.6154e-04. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/1793	0.62	0/2422
1	B	0.56	0/1768	0.59	0/2387
1	C	0.58	0/1833	0.60	0/2471
1	D	0.64	1/1831 (0.1%)	0.63	0/2471
1	E	0.57	0/1841	0.62	0/2486
1	F	0.53	0/1816	0.58	0/2451
1	G	0.49	0/1766	0.57	0/2385
1	H	0.58	0/1767	0.66	0/2384
All	All	0.57	1/14415 (0.0%)	0.61	0/19457

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	65	ASN	C-N	-5.83	1.20	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1691	45	0
1	B	1740	0	1665	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1814	0	1724	39	0
1	D	1819	0	1726	35	0
1	E	1834	0	1722	41	1
1	F	1792	0	1695	39	0
1	G	1762	0	1674	43	0
1	H	1740	0	1672	30	0
2	A	119	0	0	4	0
2	B	105	0	0	1	0
2	C	98	0	0	4	0
2	D	111	0	0	3	0
2	E	95	0	0	4	0
2	F	102	0	0	4	0
2	G	102	0	0	3	0
2	H	112	0	0	2	0
All	All	15127	0	13569	290	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ARG:HH22	1:E:193[A]:HIS:CE1	1.25	1.51
1:D:66[B]:ARG:NH1	1:D:193:HIS:CE1	1.78	1.50
1:E:66:ARG:NH2	1:E:193[A]:HIS:HE1	1.02	1.45
1:D:66[B]:ARG:NH1	1:D:193:HIS:NE2	1.64	1.45
1:D:66[B]:ARG:CZ	1:D:193:HIS:NE2	1.91	1.33
1:D:66[B]:ARG:NH2	1:D:193:HIS:NE2	1.77	1.30
1:D:66[B]:ARG:HH22	1:D:193:HIS:CD2	1.49	1.28
1:E:66:ARG:NH2	1:E:193[A]:HIS:CE1	1.94	1.15
1:G:9:LYS:CG	1:G:30:LEU:HD11	1.78	1.14
1:G:63[B]:GYC:HD1	1:G:66:ARG:HH22	1.03	1.12
1:C:63[B]:GYC:HE1	1:C:193[B]:HIS:CE1	1.86	1.09
1:G:9:LYS:HG3	1:G:30:LEU:HD11	1.19	1.07
1:E:159:GLN:HE22	1:E:193[B]:HIS:CE1	1.72	1.06
1:G:9:LYS:HG3	1:G:30:LEU:CD1	1.86	1.04
1:B:43:LYS:CE	1:B:45:LYS:HE2	1.88	1.02
1:F:63:GYC:HB2	1:F:66:ARG:NH2	1.71	1.02
1:B:43:LYS:HE3	1:B:45:LYS:CE	1.93	0.98
1:C:63[B]:GYC:CE1	1:C:193[B]:HIS:CE1	2.46	0.98
1:F:95:TYR:HB3	1:F:169:TYR:OH	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[B]:GYC:HD2	1:A:66:ARG:NH2	1.80	0.97
1:G:9:LYS:CG	1:G:30:LEU:CD1	2.44	0.96
1:C:138[B]:LYS:HE2	1:C:197:ILE:H	1.28	0.95
1:B:43:LYS:HE3	1:B:45:LYS:HE2	0.97	0.95
1:E:142[B]:SER:HB2	1:E:193[B]:HIS:CE1	2.01	0.94
1:G:63[B]:GYC:CD1	1:G:66:ARG:HH22	1.78	0.94
1:A:9:LYS:HZ2	1:A:30:LEU:HD23	1.33	0.94
1:G:63[B]:GYC:HD1	1:G:66:ARG:NH2	1.81	0.94
1:D:66[B]:ARG:NH2	1:D:193:HIS:CD2	2.30	0.90
1:E:66:ARG:CZ	1:E:193[A]:HIS:HE1	1.85	0.90
1:F:95:TYR:CD2	1:F:169:TYR:CE2	2.61	0.89
1:G:63[B]:GYC:CD1	1:G:66:ARG:NH2	2.35	0.89
1:D:66[B]:ARG:NH1	1:D:193:HIS:HE1	1.62	0.89
1:A:159:GLN:HE22	1:A:193[B]:HIS:HE1	1.21	0.88
1:A:9:LYS:HZ2	1:A:30:LEU:CD2	1.86	0.88
1:D:63[A]:GYC:HB2	1:D:66[A]:ARG:HH12	1.38	0.88
1:E:142[B]:SER:CB	1:E:193[B]:HIS:CE1	2.57	0.88
1:D:63[A]:GYC:HB12	1:D:211:GLU:HG3	1.57	0.86
1:H:63:GYC:HE1	1:H:159:GLN:HE22	1.41	0.84
1:A:4:ILE:HD13	1:A:34:PHE:CZ	2.13	0.83
1:F:66:ARG:NH1	1:F:193:HIS:CE1	2.46	0.83
1:G:8:MET:O	1:G:30:LEU:HD12	1.79	0.83
1:A:9:LYS:NZ	1:A:30:LEU:CD2	2.42	0.82
1:C:138[B]:LYS:CE	1:C:197:ILE:H	1.91	0.82
1:E:66:ARG:HG2	1:E:79:PHE:CE1	2.14	0.82
1:F:63:GYC:HB2	1:F:66:ARG:HH22	1.41	0.80
1:C:138[B]:LYS:HE2	1:C:197:ILE:N	1.97	0.79
1:H:63:GYC:HE1	1:H:159:GLN:NE2	1.98	0.78
1:H:81:GLN:OE1	1:H:184:GLN:HG2	1.85	0.77
1:G:9:LYS:HA	1:G:30:LEU:HD13	1.67	0.77
1:F:95:TYR:HD2	1:F:169:TYR:CE2	2.03	0.76
1:D:4:ILE:HD11	1:D:33:PRO:HG2	1.65	0.76
1:A:9:LYS:NZ	1:A:30:LEU:HD23	1.99	0.76
1:A:63[A]:GYC:HB2	1:A:66:ARG:NH2	2.00	0.75
1:A:9:LYS:NZ	1:A:30:LEU:HB3	2.01	0.75
1:B:73:GLU:H	1:B:73:GLU:CD	1.90	0.75
1:F:95:TYR:CB	1:F:169:TYR:OH	2.35	0.74
1:A:9:LYS:HZ2	1:A:30:LEU:HB3	1.53	0.74
1:D:63[A]:GYC:HB2	1:D:66[A]:ARG:NH1	2.01	0.74
1:D:159:GLN:HG2	2:D:325:HOH:O	1.89	0.73
1:E:66:ARG:CZ	1:E:193[A]:HIS:CE1	2.65	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LYS:HG2	1:G:30:LEU:HD11	1.69	0.73
1:H:76:VAL:HG13	1:H:81:GLN:HE22	1.54	0.73
1:E:159:GLN:HE22	1:E:193[B]:HIS:HE1	1.34	0.72
1:E:73:GLU:OE2	1:E:73:GLU:N	2.19	0.72
1:D:66[B]:ARG:NH1	1:D:144:GLU:OE2	2.15	0.72
1:B:63:GYC:HB2	1:B:66:ARG:NH2	2.03	0.72
1:F:95:TYR:HB3	1:F:169:TYR:CZ	2.25	0.72
1:A:159:GLN:NE2	1:A:193[B]:HIS:HE1	1.88	0.71
1:E:66:ARG:HG2	1:E:79:PHE:CZ	2.25	0.71
1:F:66:ARG:NH1	1:F:193:HIS:NE2	2.39	0.71
1:G:9:LYS:HG2	1:G:30:LEU:CD1	2.21	0.71
1:C:138[B]:LYS:HE2	1:C:196:GLU:HA	1.72	0.70
1:F:67:VAL:HG11	1:F:83:PHE:HE2	1.57	0.70
1:A:63[B]:GYC:HE1	1:A:193[B]:HIS:CE1	2.27	0.70
1:E:159:GLN:NE2	1:E:193[B]:HIS:CE1	2.55	0.70
1:E:142[B]:SER:HB3	1:E:193[B]:HIS:NE2	2.08	0.69
1:H:4:ILE:HG22	1:H:34:PHE:CZ	2.27	0.69
1:C:159:GLN:HG2	2:C:349:HOH:O	1.91	0.69
1:F:26:GLU:HG3	1:F:45:LYS:HG3	1.75	0.69
1:A:63[B]:GYC:HD2	1:A:66:ARG:HH22	1.56	0.68
1:D:8:MET:HE2	1:D:112:ASP:HB3	1.74	0.68
1:A:4:ILE:HD13	1:A:34:PHE:HZ	1.58	0.67
1:G:170:ARG:NH1	2:G:302:HOH:O	2.23	0.67
1:E:74:ASN:OD1	1:E:75:ILE:HG13	1.95	0.67
1:F:95:TYR:CD2	1:F:169:TYR:HE2	2.10	0.67
1:B:201:ASP:OD1	1:B:206:ASN:N	2.25	0.67
1:B:63:GYC:HB2	1:B:66:ARG:HH22	1.57	0.67
1:E:66:ARG:HG2	1:E:79:PHE:CD1	2.29	0.67
1:E:198:LYS:HG3	1:E:210:HIS:ND1	2.09	0.66
1:F:66:ARG:HB3	1:F:79:PHE:CG	2.31	0.66
1:H:66:ARG:HB3	1:H:79:PHE:CG	2.31	0.66
1:E:63[B]:GYC:HE2	1:E:193[B]:HIS:CE1	2.31	0.66
1:E:142[B]:SER:HB3	1:E:193[B]:HIS:CE1	2.30	0.66
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.79	0.65
1:G:154:LYS:NZ	2:G:307:HOH:O	2.29	0.65
1:A:9:LYS:NZ	1:A:30:LEU:CB	2.60	0.65
1:A:135:ARG:NH2	2:A:303:HOH:O	2.28	0.65
1:G:66:ARG:HB3	1:G:79:PHE:CG	2.33	0.64
1:F:198:LYS:HG3	1:F:210:HIS:ND1	2.15	0.62
1:A:159:GLN:OE1	1:A:193[B]:HIS:CE1	2.53	0.62
1:H:66:ARG:HH11	1:H:66:ARG:HA	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:VAL:HG11	1:F:83:PHE:CE2	2.35	0.61
1:H:63:GYC:HB2	1:H:66:ARG:NH2	2.15	0.61
1:B:66:ARG:HB3	1:B:79:PHE:CG	2.34	0.61
1:G:66:ARG:HG2	1:G:79:PHE:CZ	2.35	0.61
1:H:11:LYS:HE2	1:H:28:VAL:HG22	1.83	0.61
1:A:9:LYS:HZ2	1:A:30:LEU:CB	2.13	0.60
1:H:63:GYC:HB2	1:H:66:ARG:HH22	1.67	0.60
1:A:5:LYS:HD2	1:A:8:MET:SD	2.41	0.60
1:C:63[A]:GYC:HB2	1:C:66[A]:ARG:NH2	2.17	0.59
1:A:154[B]:LYS:NZ	2:A:306:HOH:O	2.35	0.59
1:G:3:VAL:HG13	1:G:4:ILE:HD12	1.84	0.59
1:D:63[A]:GYC:OH	1:D:159:GLN:NE2	2.35	0.59
1:G:144:GLU:HA	1:G:157:VAL:HB	1.85	0.59
1:A:4:ILE:CD1	1:A:34:PHE:HZ	2.14	0.59
1:C:51:PRO:HG2	2:C:359:HOH:O	2.03	0.59
1:A:63[A]:GYC:HB2	1:A:66:ARG:CZ	2.33	0.59
1:C:198:LYS:HG3	1:C:210:HIS:ND1	2.18	0.58
1:G:9:LYS:CG	1:G:30:LEU:HD13	2.33	0.58
1:H:85:GLU:OE1	1:H:181:LYS:NZ	2.34	0.58
1:G:63[B]:GYC:HD1	1:G:63[B]:GYC:O2	2.04	0.58
1:E:66:ARG:HB3	1:E:79:PHE:CD2	2.39	0.58
1:B:66:ARG:HB3	1:B:79:PHE:CD2	2.40	0.57
1:C:25:ILE:HG12	1:C:44:VAL:HG22	1.86	0.57
1:G:128:ASN:ND2	2:G:313:HOH:O	2.38	0.57
1:D:163:LEU:HD11	1:D:169:TYR:HB2	1.86	0.57
1:E:66:ARG:NH1	1:E:193[A]:HIS:CE1	2.72	0.57
1:F:128:ASN:HA	1:F:133:GLN:OE1	2.05	0.57
1:C:147:TYR:OH	1:G:170:ARG:NH1	2.37	0.57
1:F:66:ARG:NH1	1:F:144:GLU:OE2	2.38	0.57
1:H:4:ILE:HG22	1:H:34:PHE:CE2	2.41	0.56
1:H:4:ILE:CG2	1:H:34:PHE:CZ	2.88	0.56
1:D:4:ILE:HD13	1:D:114:TYR:OH	2.06	0.56
1:E:63[B]:GYC:HB2	1:E:211:GLU:OE2	2.06	0.55
1:C:63[A]:GYC:HE2	1:C:195:ILE:HB	1.88	0.55
1:E:66:ARG:NH2	2:E:305:HOH:O	2.30	0.55
1:B:144:GLU:HA	1:B:157:VAL:HB	1.88	0.55
1:F:66:ARG:HB3	1:F:79:PHE:CD2	2.41	0.55
1:H:63:GYC:OH	2:H:301:HOH:O	2.18	0.55
1:A:63[B]:GYC:CE1	1:A:193[B]:HIS:CE1	2.90	0.55
1:G:85:GLU:OE2	1:G:181:LYS:CE	2.55	0.55
1:G:5:LYS:HD3	1:G:8:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:NZ	1:A:30:LEU:HD22	2.21	0.55
1:C:26:GLU:HG3	1:C:45:LYS:HG3	1.89	0.55
1:H:66:ARG:HB3	1:H:79:PHE:CD2	2.42	0.55
1:H:77:ASP:C	1:H:81:GLN:HE21	2.10	0.55
1:A:9:LYS:O	1:A:114:TYR:N	2.33	0.54
1:G:66:ARG:CG	1:G:79:PHE:CE1	2.90	0.54
1:B:66:ARG:HA	1:B:66:ARG:HH11	1.73	0.54
1:B:94:ASN:HA	1:B:100:ILE:HD12	1.90	0.54
1:A:145:LYS:HD2	1:A:188:TYR:OH	2.08	0.54
1:D:10:ILE:HD11	1:D:68:PHE:CZ	2.42	0.54
1:D:5:LYS:HB2	1:D:8:MET:HE3	1.90	0.54
1:G:219:LEU:HD12	1:G:220:PRO:HD2	1.89	0.53
1:C:159:GLN:NE2	1:C:193[B]:HIS:HE1	2.06	0.53
1:B:133:GLN:HG3	1:B:135:ARG:NH1	2.22	0.53
1:C:168:HIS:O	1:G:149:ARG:NH2	2.41	0.53
1:F:212:HIS:CE1	1:F:214:GLU:OE2	2.62	0.53
1:C:26:GLU:HG3	1:C:45:LYS:HE2	1.90	0.52
1:E:144:GLU:HA	1:E:157:VAL:HB	1.91	0.52
1:G:66:ARG:HB3	1:G:79:PHE:CD2	2.44	0.52
1:F:66:ARG:HG2	1:F:79:PHE:CZ	2.44	0.52
1:C:170:ARG:NH1	1:G:147:TYR:OH	2.42	0.52
1:G:90:GLU:OE2	1:G:178:LYS:NZ	2.43	0.52
1:C:107:ILE:O	1:C:180:LYS:NZ	2.43	0.52
1:E:66:ARG:HH12	1:E:193[A]:HIS:CE1	2.28	0.52
1:D:10:ILE:HD11	1:D:68:PHE:CE2	2.45	0.52
1:E:63[B]:GYC:CE2	1:E:193[B]:HIS:CE1	2.93	0.52
1:C:142[A]:SER:HB2	1:G:145:LYS:HZ3	1.74	0.52
1:F:50:LEU:HD12	1:F:52:PHE:CE2	2.44	0.52
1:A:4:ILE:O	1:A:4:ILE:HD12	2.10	0.51
1:F:81:GLN:HE22	1:F:184:GLN:H	1.58	0.51
1:H:66:ARG:CG	1:H:79:PHE:CE1	2.93	0.51
1:F:90:GLU:HG3	2:F:357:HOH:O	2.09	0.51
1:C:63[A]:GYC:OH	1:C:159:GLN:NE2	2.44	0.51
1:C:66[B]:ARG:HH12	1:C:193[B]:HIS:CD2	2.29	0.51
1:A:30:LEU:C	1:A:30:LEU:HD12	2.31	0.50
1:A:30:LEU:HD12	1:A:30:LEU:O	2.11	0.50
1:G:85:GLU:OE2	1:G:181:LYS:HE3	2.10	0.50
1:B:66:ARG:HG2	1:B:79:PHE:CZ	2.47	0.50
1:B:153:LEU:HB3	1:B:177:TYR:HB2	1.93	0.50
1:G:8:MET:O	1:G:30:LEU:CD1	2.53	0.50
1:D:144:GLU:HA	1:D:157:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:HG3	1:A:135:ARG:NH2	2.26	0.50
1:A:159:GLN:HE22	1:A:193[B]:HIS:CE1	2.13	0.49
1:B:66:ARG:CG	1:B:79:PHE:CE1	2.95	0.49
1:D:66[A]:ARG:HA	1:D:66[A]:ARG:HH21	1.78	0.49
1:E:227:LEU:N	1:E:227:LEU:HD12	2.28	0.49
1:C:138[B]:LYS:NZ	2:C:305:HOH:O	2.33	0.49
1:G:63[A]:GYC:OH	1:G:159:GLN:NE2	2.46	0.48
1:F:7:ASP:OD1	2:F:301:HOH:O	2.20	0.48
1:C:63[B]:GYC:CE1	1:C:193[B]:HIS:NE2	2.74	0.48
1:G:66:ARG:HG3	1:G:79:PHE:CE1	2.48	0.48
1:G:66:ARG:CG	1:G:79:PHE:CZ	2.97	0.48
1:H:144:GLU:HA	1:H:157:VAL:HB	1.95	0.48
1:E:66:ARG:HG2	1:E:79:PHE:CE2	2.49	0.48
1:C:39:SER:HB2	1:C:210:HIS:CD2	2.49	0.48
1:A:158:ASN:HB3	2:E:381:HOH:O	2.14	0.48
1:F:66:ARG:CG	1:F:79:PHE:CE1	2.96	0.47
1:G:9:LYS:HA	1:G:30:LEU:CD1	2.43	0.47
1:C:144:GLU:HA	1:C:157:VAL:HB	1.97	0.47
1:B:66:ARG:HG2	1:B:79:PHE:CE1	2.48	0.47
1:E:90:GLU:OE1	2:E:301:HOH:O	2.20	0.47
1:A:9:LYS:O	1:A:113:CYS:HA	2.14	0.47
1:D:156:ASP:OD1	2:D:301:HOH:O	2.21	0.47
1:C:43:LYS:HD3	1:C:206:ASN:OD1	2.15	0.47
1:H:8:MET:HE3	1:H:112:ASP:O	2.15	0.46
1:H:94:ASN:HA	1:H:100:ILE:HD12	1.96	0.46
1:A:203:ASP:OD2	1:A:205:SER:HB3	2.14	0.46
1:C:102:ASN:HD21	1:E:100:ILE:HG22	1.79	0.46
1:C:142[B]:SER:OG	1:C:159:GLN:CG	2.64	0.46
1:E:43:LYS:HA	1:E:205:SER:O	2.16	0.46
1:D:172:ASP:OD1	2:D:302:HOH:O	2.21	0.46
1:E:159:GLN:NE2	1:E:193[B]:HIS:HE1	2.02	0.46
1:B:43:LYS:HG2	1:B:45:LYS:CE	2.45	0.46
1:G:50:LEU:O	1:G:134:LYS:NZ	2.40	0.46
1:H:34:PHE:O	2:H:302:HOH:O	2.21	0.45
1:B:66:ARG:HA	1:B:66:ARG:HD3	1.65	0.45
1:F:66:ARG:HG3	1:F:79:PHE:CE1	2.51	0.45
1:H:66:ARG:HG2	1:H:79:PHE:CZ	2.51	0.45
1:E:66:ARG:NE	1:E:66:ARG:HA	2.31	0.45
1:D:196:GLU:OE1	1:D:198:LYS:NZ	2.48	0.45
1:F:144:GLU:HA	1:F:157:VAL:HB	1.98	0.45
1:D:141:PRO:HD3	1:D:194:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:LEU:HA	1:F:154:LYS:O	2.17	0.45
1:G:66:ARG:HA	1:G:66:ARG:HD3	1.52	0.45
1:E:58:THR:HG21	2:E:346:HOH:O	2.16	0.45
1:C:138[B]:LYS:HE2	1:C:196:GLU:CA	2.42	0.44
1:A:63[B]:GYC:CD2	1:A:66:ARG:NH2	2.68	0.44
1:D:100:ILE:HG21	1:F:92[A]:SER:OG	2.18	0.44
1:F:4:ILE:HG23	1:F:4:ILE:O	2.17	0.44
1:H:11:LYS:O	1:H:115:ILE:HA	2.17	0.44
1:C:26:GLU:CG	1:C:45:LYS:HE2	2.48	0.44
1:D:63[A]:GYC:CB1	1:D:211:GLU:HG3	2.39	0.44
1:A:9:LYS:HD3	1:A:30:LEU:HB3	1.99	0.44
1:A:159:GLN:OE1	1:A:193[B]:HIS:NE2	2.50	0.44
1:F:81:GLN:NE2	1:F:184:GLN:H	2.16	0.44
1:A:9:LYS:HZ3	1:A:30:LEU:CB	2.29	0.44
1:H:66:ARG:HA	1:H:66:ARG:HD3	1.51	0.44
1:H:66:ARG:HH11	1:H:66:ARG:CA	2.29	0.44
1:B:170:ARG:HG2	2:B:371:HOH:O	2.18	0.44
1:B:43:LYS:HG2	1:B:45:LYS:HE3	2.00	0.43
1:D:8:MET:CE	1:D:112:ASP:HB3	2.44	0.43
1:D:66[A]:ARG:HB3	1:D:79:PHE:CD2	2.53	0.43
1:A:102:ASN:HD21	1:G:100:ILE:HG23	1.82	0.43
1:F:191:VAL:HG12	1:F:193:HIS:NE2	2.33	0.43
1:C:63[B]:GYC:HB2	1:C:211:GLU:OE2	2.19	0.43
1:D:66[A]:ARG:HA	1:D:66[A]:ARG:HD3	1.84	0.43
1:F:146:LEU:HD23	1:F:153:LEU:HD21	2.01	0.43
1:A:6:PRO:HB3	2:A:409:HOH:O	2.18	0.43
1:D:66[B]:ARG:HB3	1:D:79:PHE:CG	2.54	0.43
1:E:66:ARG:HG2	1:E:79:PHE:CG	2.53	0.43
1:A:63[B]:GYC:OH	1:A:159:GLN:OE1	2.37	0.42
1:B:43:LYS:HA	1:B:205:SER:O	2.19	0.42
1:C:138[B]:LYS:HA	1:C:138[B]:LYS:HD3	1.83	0.42
1:A:11:LYS:HB3	1:A:11:LYS:HE2	1.84	0.42
1:A:144:GLU:HB2	1:A:193[A]:HIS:CD2	2.54	0.42
1:D:63[A]:GYC:HB11	1:D:195:ILE:HD12	2.01	0.42
2:A:354:HOH:O	1:E:145:LYS:HD2	2.18	0.42
1:B:92:SER:OG	1:H:100:ILE:HG21	2.18	0.42
1:B:94:ASN:CA	1:B:100:ILE:HD12	2.50	0.42
1:F:220:PRO:HG2	1:F:223:ALA:HB2	2.01	0.42
1:G:146:LEU:HA	1:G:154:LYS:O	2.20	0.42
1:D:73:GLU:O	1:D:73:GLU:HG3	2.18	0.42
1:F:3:VAL:N	2:F:318:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LEU:O	1:C:134:LYS:NZ	2.53	0.42
1:B:146:LEU:HA	1:B:154:LYS:O	2.19	0.42
1:B:63:GYC:HE2	1:B:195:ILE:HB	2.02	0.41
1:E:227:LEU:N	1:E:227:LEU:CD1	2.82	0.41
1:F:85:GLU:OE2	1:F:85:GLU:N	2.44	0.41
1:F:41:ASP:OD2	2:F:302:HOH:O	2.21	0.41
1:H:146:LEU:HA	1:H:154:LYS:O	2.20	0.41
1:C:26:GLU:HG3	1:C:45:LYS:CG	2.50	0.41
1:A:63[A]:GYC:HB2	1:A:66:ARG:HH22	1.80	0.41
1:A:149:ARG:NH2	1:E:168:HIS:O	2.54	0.41
1:G:85:GLU:OE2	1:G:85:GLU:N	2.47	0.41
1:H:192:ASP:O	1:H:213:ALA:HA	2.20	0.41
1:D:66[B]:ARG:HB3	1:D:79:PHE:CD2	2.56	0.41
1:C:63[A]:GYC:HB2	1:C:66[A]:ARG:HH22	1.84	0.41
1:E:219:LEU:HA	1:E:220:PRO:HD3	1.80	0.41
1:E:58:THR:O	1:E:63[B]:GYC:N1	2.54	0.41
1:F:95:TYR:CD2	1:F:171:CYS:HB2	2.56	0.41
1:B:200:HIS:ND1	1:B:201:ASP:O	2.45	0.40
1:E:63[A]:GYC:HB11	1:E:195:ILE:HD12	2.03	0.40
1:C:6:PRO:O	1:C:32:LYS:HA	2.21	0.40
1:C:35[B]:GLU:OE1	2:C:301:HOH:O	2.22	0.40
1:F:9:LYS:HA	1:F:30:LEU:HA	2.02	0.40
1:H:66:ARG:HG3	1:H:79:PHE:CE1	2.57	0.40
1:C:36:GLY:O	1:C:212:HIS:HA	2.21	0.40
1:G:66:ARG:HB3	1:G:79:PHE:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ARG:NH2	1:E:222:GLN:OE1[2_646]	2.10	0.10

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	215/255 (84%)	214 (100%)	1 (0%)	0	100	100
1	B	211/255 (83%)	210 (100%)	1 (0%)	0	100	100
1	C	218/255 (86%)	215 (99%)	2 (1%)	1 (0%)	29	31
1	D	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
1	E	221/255 (87%)	215 (97%)	5 (2%)	1 (0%)	29	31
1	F	218/255 (86%)	214 (98%)	3 (1%)	1 (0%)	29	31
1	G	211/255 (83%)	209 (99%)	2 (1%)	0	100	100
1	H	211/255 (83%)	210 (100%)	1 (0%)	0	100	100
All	All	1724/2040 (84%)	1704 (99%)	17 (1%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	ASP
1	E	227	LEU
1	F	227	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/217 (86%)	181 (97%)	6 (3%)	39	50
1	B	185/217 (85%)	178 (96%)	7 (4%)	33	42
1	C	190/217 (88%)	186 (98%)	4 (2%)	53	67
1	D	189/217 (87%)	183 (97%)	6 (3%)	39	50
1	E	190/217 (88%)	187 (98%)	3 (2%)	62	76
1	F	188/217 (87%)	185 (98%)	3 (2%)	62	76
1	G	185/217 (85%)	181 (98%)	4 (2%)	52	65
1	H	185/217 (85%)	180 (97%)	5 (3%)	44	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1499/1736 (86%)	1461 (98%)	38 (2%)	50 60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	30	LEU
1	A	66	ARG
1	A	133	GLN
1	A	180	LYS
1	A	198	LYS
1	B	35	GLU
1	B	66	ARG
1	B	73	GLU
1	B	156	ASP
1	B	184[A]	GLN
1	B	184[B]	GLN
1	B	211	GLU
1	C	66[A]	ARG
1	C	66[B]	ARG
1	C	138[A]	LYS
1	C	138[B]	LYS
1	D	3	VAL
1	D	9	LYS
1	D	39	SER
1	D	66[A]	ARG
1	D	66[B]	ARG
1	D	73	GLU
1	E	7	ASP
1	E	145	LYS
1	E	194	HIS
1	F	66	ARG
1	F	145	LYS
1	F	194	HIS
1	G	30	LEU
1	G	66	ARG
1	G	156	ASP
1	G	180	LYS
1	H	66	ARG
1	H	145	LYS
1	H	162	SER
1	H	211	GLU

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Mol	Chain	Res	Type
1	H	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

13 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	F	63	1	22,22,23	1.07	1 (4%)	26,30,32	2.66	9 (34%)
1	GYC	E	63[A]	1	22,22,23	1.10	1 (4%)	26,30,32	2.50	7 (26%)
1	GYC	E	63[B]	1	22,22,23	1.05	1 (4%)	26,30,32	2.81	9 (34%)
1	GYC	H	63	1	22,22,23	1.09	1 (4%)	26,30,32	2.49	7 (26%)
1	GYC	C	63[A]	1	22,22,23	1.05	1 (4%)	26,30,32	2.46	8 (30%)
1	GYC	C	63[B]	1	22,22,23	1.00	1 (4%)	26,30,32	2.57	8 (30%)
1	GYC	A	63[A]	1	22,22,23	1.11	1 (4%)	26,30,32	2.36	8 (30%)
1	GYC	B	63	1	22,22,23	1.09	1 (4%)	26,30,32	2.48	7 (26%)
1	GYC	A	63[B]	1	22,22,23	1.03	1 (4%)	26,30,32	2.60	8 (30%)
1	GYC	G	63[B]	1	22,22,23	1.14	1 (4%)	26,30,32	2.75	8 (30%)
1	GYC	D	63[B]	1	22,22,23	1.00	1 (4%)	26,30,32	2.57	8 (30%)
1	GYC	G	63[A]	1	22,22,23	1.09	1 (4%)	26,30,32	2.41	8 (30%)
1	GYC	D	63[A]	1	22,22,23	1.04	1 (4%)	26,30,32	2.46	8 (30%)

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	F	63	1	-	4/9/29/30	0/2/2/2
1	GYC	E	63[A]	1	-	3/9/29/30	0/2/2/2
1	GYC	E	63[B]	1	-	6/9/29/30	0/2/2/2
1	GYC	H	63	1	-	3/9/29/30	0/2/2/2
1	GYC	C	63[A]	1	-	3/9/29/30	0/2/2/2
1	GYC	C	63[B]	1	-	5/9/29/30	0/2/2/2
1	GYC	A	63[A]	1	-	2/9/29/30	0/2/2/2
1	GYC	B	63	1	-	3/9/29/30	0/2/2/2
1	GYC	A	63[B]	1	-	4/9/29/30	0/2/2/2
1	GYC	G	63[B]	1	-	3/9/29/30	0/2/2/2
1	GYC	D	63[B]	1	-	5/9/29/30	0/2/2/2
1	GYC	G	63[A]	1	-	4/9/29/30	0/2/2/2
1	GYC	D	63[A]	1	-	3/9/29/30	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63[B]	GYC	CB2-CA2	4.27	1.38	1.35
1	A	63[A]	GYC	CB2-CA2	4.23	1.38	1.35
1	E	63[A]	GYC	CB2-CA2	4.22	1.38	1.35
1	G	63[A]	GYC	CB2-CA2	4.13	1.38	1.35
1	F	63	GYC	CB2-CA2	4.10	1.38	1.35
1	B	63	GYC	CB2-CA2	4.06	1.38	1.35
1	H	63	GYC	CB2-CA2	4.04	1.38	1.35
1	C	63[A]	GYC	CB2-CA2	3.86	1.38	1.35
1	D	63[A]	GYC	CB2-CA2	3.79	1.38	1.35
1	E	63[B]	GYC	CB2-CA2	3.68	1.38	1.35
1	A	63[B]	GYC	CB2-CA2	3.65	1.38	1.35
1	C	63[B]	GYC	CB2-CA2	3.24	1.37	1.35
1	D	63[B]	GYC	CB2-CA2	3.24	1.37	1.35

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	GYC	O2-C2-CA2	-7.99	126.47	130.96
1	G	63[B]	GYC	CB2-CA2-C2	7.81	131.60	122.28
1	E	63[A]	GYC	O2-C2-CA2	-7.56	126.72	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	GYC	O2-C2-CA2	-7.18	126.93	130.96
1	B	63	GYC	O2-C2-CA2	-7.18	126.93	130.96
1	C	63[A]	GYC	O2-C2-CA2	-7.11	126.97	130.96
1	D	63[A]	GYC	O2-C2-CA2	-7.09	126.98	130.96
1	E	63[B]	GYC	CB2-CA2-C2	6.96	130.58	122.28
1	G	63[A]	GYC	O2-C2-CA2	-6.55	127.28	130.96
1	A	63[B]	GYC	CB2-CA2-C2	6.47	130.00	122.28
1	D	63[B]	GYC	CB2-CA2-C2	6.34	129.84	122.28
1	C	63[B]	GYC	CB2-CA2-C2	6.32	129.82	122.28
1	A	63[A]	GYC	O2-C2-CA2	-6.21	127.47	130.96
1	E	63[B]	GYC	CA2-N2-C1	5.82	110.06	105.77
1	E	63[B]	GYC	O2-C2-CA2	-5.81	127.70	130.96
1	G	63[B]	GYC	CA2-N2-C1	5.77	110.02	105.77
1	A	63[B]	GYC	O2-C2-CA2	-5.63	127.80	130.96
1	G	63[B]	GYC	C2-CA2-N2	-5.58	105.02	108.93
1	A	63[B]	GYC	CA2-N2-C1	5.52	109.84	105.77
1	C	63[B]	GYC	O2-C2-CA2	-5.41	127.92	130.96
1	D	63[B]	GYC	O2-C2-CA2	-5.40	127.93	130.96
1	D	63[B]	GYC	CA2-N2-C1	5.19	109.60	105.77
1	C	63[B]	GYC	CA2-N2-C1	5.17	109.58	105.77
1	E	63[B]	GYC	C2-CA2-N2	-5.05	105.39	108.93
1	H	63	GYC	CA2-N2-C1	4.95	109.42	105.77
1	B	63	GYC	CA2-N2-C1	4.94	109.41	105.77
1	H	63	GYC	C2-CA2-N2	-4.89	105.51	108.93
1	G	63[A]	GYC	C2-CA2-N2	-4.87	105.52	108.93
1	B	63	GYC	C2-CA2-N2	-4.87	105.52	108.93
1	A	63[A]	GYC	C2-CA2-N2	-4.85	105.54	108.93
1	A	63[A]	GYC	CA2-N2-C1	4.84	109.34	105.77
1	A	63[B]	GYC	C2-CA2-N2	-4.82	105.55	108.93
1	E	63[A]	GYC	CA2-N2-C1	4.81	109.32	105.77
1	E	63[A]	GYC	C2-CA2-N2	-4.80	105.57	108.93
1	G	63[A]	GYC	CA2-N2-C1	4.79	109.30	105.77
1	E	63[A]	GYC	CA2-C2-N3	4.75	105.62	103.37
1	C	63[A]	GYC	CA2-N2-C1	4.74	109.27	105.77
1	D	63[A]	GYC	CA2-N2-C1	4.73	109.25	105.77
1	H	63	GYC	CA2-C2-N3	4.72	105.60	103.37
1	F	63	GYC	C2-CA2-N2	-4.71	105.64	108.93
1	B	63	GYC	CA2-C2-N3	4.70	105.59	103.37
1	C	63[A]	GYC	C2-CA2-N2	-4.69	105.64	108.93
1	G	63[A]	GYC	CA2-C2-N3	4.69	105.59	103.37
1	D	63[A]	GYC	C2-CA2-N2	-4.69	105.65	108.93
1	A	63[A]	GYC	CA2-C2-N3	4.62	105.56	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	GYC	CA2-C2-N3	4.59	105.54	103.37
1	F	63	GYC	CA2-C2-N3	4.56	105.53	103.37
1	F	63	GYC	CA2-N2-C1	4.54	109.12	105.77
1	C	63[A]	GYC	CA2-C2-N3	4.53	105.51	103.37
1	C	63[B]	GYC	C2-CA2-N2	-4.37	105.87	108.93
1	D	63[B]	GYC	C2-CA2-N2	-4.37	105.87	108.93
1	F	63	GYC	CG2-CB2-CA2	-4.33	124.64	129.94
1	G	63[B]	GYC	CA2-C2-N3	4.32	105.41	103.37
1	C	63[A]	GYC	CG2-CB2-CA2	-4.09	124.93	129.94
1	D	63[A]	GYC	CG2-CB2-CA2	-4.08	124.95	129.94
1	E	63[B]	GYC	CA2-C2-N3	4.06	105.29	103.37
1	G	63[B]	GYC	CB2-CA2-N2	-3.94	123.36	128.83
1	A	63[B]	GYC	CA2-C2-N3	3.81	105.17	103.37
1	A	63[A]	GYC	CG2-CB2-CA2	-3.65	125.47	129.94
1	G	63[B]	GYC	O2-C2-CA2	-3.58	128.95	130.96
1	E	63[A]	GYC	CG2-CB2-CA2	-3.53	125.62	129.94
1	C	63[B]	GYC	CA2-C2-N3	3.50	105.03	103.37
1	G	63[A]	GYC	CG2-CB2-CA2	-3.49	125.67	129.94
1	D	63[B]	GYC	CA2-C2-N3	3.48	105.02	103.37
1	B	63	GYC	CG2-CB2-CA2	-3.48	125.68	129.94
1	E	63[B]	GYC	CB2-CA2-N2	-3.48	124.00	128.83
1	H	63	GYC	CG2-CB2-CA2	-3.47	125.69	129.94
1	E	63[B]	GYC	CG2-CB2-CA2	-3.39	125.80	129.94
1	D	63[B]	GYC	CG2-CB2-CA2	-3.34	125.85	129.94
1	C	63[B]	GYC	CG2-CB2-CA2	-3.32	125.88	129.94
1	D	63[B]	GYC	CB2-CA2-N2	-3.29	124.26	128.83
1	C	63[B]	GYC	CB2-CA2-N2	-3.28	124.28	128.83
1	G	63[B]	GYC	CG2-CB2-CA2	-3.21	126.02	129.94
1	A	63[B]	GYC	CB2-CA2-N2	-3.18	124.41	128.83
1	F	63	GYC	CA1-CB1-SG1	-2.72	108.58	114.44
1	G	63[A]	GYC	CB2-CA2-C2	2.71	125.51	122.28
1	A	63[B]	GYC	CG2-CB2-CA2	-2.67	126.68	129.94
1	C	63[A]	GYC	CB2-CA2-C2	2.60	125.37	122.28
1	D	63[A]	GYC	CB2-CA2-C2	2.59	125.37	122.28
1	A	63[A]	GYC	CB2-CA2-C2	2.55	125.32	122.28
1	F	63	GYC	CB2-CA2-C2	2.53	125.30	122.28
1	G	63[A]	GYC	CA1-CB1-SG1	-2.50	109.05	114.44
1	H	63	GYC	CA1-CB1-SG1	-2.40	109.28	114.44
1	B	63	GYC	CA1-CB1-SG1	-2.39	109.30	114.44
1	F	63	GYC	O3-C3-CA3	-2.30	119.45	126.39
1	G	63[A]	GYC	O3-C3-CA3	-2.24	119.63	126.39
1	A	63[A]	GYC	O3-C3-CA3	-2.19	119.78	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	GYC	CA1-CB1-SG1	-2.19	109.72	114.44
1	B	63	GYC	O3-C3-CA3	-2.19	119.78	126.39
1	H	63	GYC	O3-C3-CA3	-2.18	119.79	126.39
1	E	63[A]	GYC	O3-C3-CA3	-2.18	119.80	126.39
1	E	63[B]	GYC	CA1-C1-N3	2.17	127.69	124.85
1	E	63[A]	GYC	CA1-CB1-SG1	-2.17	109.76	114.44
1	C	63[A]	GYC	CA1-CB1-SG1	-2.17	109.76	114.44
1	F	63	GYC	CA3-N3-C1	-2.16	124.57	127.16
1	A	63[B]	GYC	O3-C3-CA3	-2.15	119.89	126.39
1	A	63[A]	GYC	CA1-CB1-SG1	-2.14	109.82	114.44
1	G	63[B]	GYC	O3-C3-CA3	-2.13	119.97	126.39
1	C	63[A]	GYC	O3-C3-CA3	-2.08	120.12	126.39
1	D	63[A]	GYC	O3-C3-CA3	-2.08	120.12	126.39
1	C	63[B]	GYC	O3-C3-CA3	-2.06	120.17	126.39
1	D	63[B]	GYC	O3-C3-CA3	-2.05	120.20	126.39
1	E	63[B]	GYC	O3-C3-CA3	-2.00	120.34	126.39

There are no chirality outliers.

All (48) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	E	63[B]	GYC	C2-CA2-CB2-CG2
1	F	63	GYC	C3-CA3-N3-C2
1	F	63	GYC	N2-CA2-CB2-CG2
1	F	63	GYC	C2-CA2-CB2-CG2
1	G	63[A]	GYC	N2-CA2-CB2-CG2
1	G	63[A]	GYC	C2-CA2-CB2-CG2
1	G	63[B]	GYC	N2-CA2-CB2-CG2
1	G	63[B]	GYC	C2-CA2-CB2-CG2
1	H	63	GYC	N2-CA2-CB2-CG2
1	H	63	GYC	C2-CA2-CB2-CG2
1	B	63	GYC	C3-CA3-N3-C2
1	C	63[B]	GYC	C3-CA3-N3-C2
1	D	63[B]	GYC	C3-CA3-N3-C2
1	G	63[B]	GYC	C3-CA3-N3-C2
1	H	63	GYC	C3-CA3-N3-C2
1	F	63	GYC	C3-CA3-N3-C1
1	G	63[A]	GYC	CA2-CB2-CG2-CD1
1	A	63[B]	GYC	CA2-CB2-CG2-CD1
1	A	63[B]	GYC	CA2-CB2-CG2-CD2
1	G	63[A]	GYC	CA2-CB2-CG2-CD2
1	C	63[B]	GYC	CA2-CB2-CG2-CD1
1	D	63[B]	GYC	CA2-CB2-CG2-CD1
1	E	63[B]	GYC	CA2-CB2-CG2-CD2
1	C	63[B]	GYC	CA2-CB2-CG2-CD2
1	D	63[B]	GYC	CA2-CB2-CG2-CD2
1	E	63[B]	GYC	CA2-CB2-CG2-CD1
1	E	63[B]	GYC	C1-CA1-CB1-SG1

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	63	GYC	2	0
1	E	63[A]	GYC	1	0
1	E	63[B]	GYC	4	0
1	H	63	GYC	5	0
1	C	63[A]	GYC	4	0
1	C	63[B]	GYC	4	0
1	A	63[A]	GYC	3	0
1	B	63	GYC	3	0
1	A	63[B]	GYC	6	0
1	G	63[B]	GYC	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	63[A]	GYC	1	0
1	D	63[A]	GYC	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.66	7 (3%) 47 45	21, 35, 55, 77	1 (0%)
1	B	214/255 (83%)	0.61	9 (4%) 36 34	22, 34, 52, 73	0
1	C	218/255 (85%)	0.87	12 (5%) 25 24	25, 40, 62, 84	0
1	D	222/255 (87%)	0.73	19 (8%) 10 9	22, 35, 56, 82	0
1	E	223/255 (87%)	0.82	15 (6%) 17 16	23, 37, 62, 81	0
1	F	222/255 (87%)	0.73	12 (5%) 25 24	23, 35, 55, 100	0
1	G	215/255 (84%)	0.77	16 (7%) 14 13	25, 37, 57, 77	0
1	H	214/255 (83%)	0.74	13 (6%) 21 20	22, 36, 58, 102	0
All	All	1744/2040 (85%)	0.74	103 (5%) 22 21	21, 36, 58, 102	1 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	ILE	7.9
1	C	224	MET	7.0
1	E	3	VAL	5.6
1	D	220	PRO	5.4
1	F	224	MET	5.3
1	D	3	VAL	5.1
1	H	3	VAL	4.9
1	C	165	GLY	4.8
1	E	220	PRO	4.8
1	A	4	ILE	4.8
1	A	3	VAL	4.7
1	C	223	ALA	4.6
1	E	165	GLY	4.6
1	G	220	PRO	4.6
1	A	220	PRO	4.5
1	F	222	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	220	PRO	4.5
1	F	182	VAL	4.3
1	D	4	ILE	4.3
1	E	224	MET	4.2
1	B	4	ILE	4.0
1	E	225	ASP	3.9
1	D	182	VAL	3.9
1	F	223	ALA	3.9
1	B	7	ASP	3.9
1	B	220	PRO	3.8
1	G	7	ASP	3.7
1	E	150	ASP	3.6
1	E	202	LYS	3.4
1	G	219	LEU	3.4
1	D	151	GLY	3.3
1	H	213	ALA	3.3
1	F	111	GLY	3.2
1	D	112	ASP	3.2
1	G	164	GLU	3.2
1	C	112	ASP	3.2
1	E	227	LEU	3.2
1	D	110	ASP	3.1
1	F	226	GLU	3.1
1	C	222	GLN	3.1
1	G	30	LEU	3.1
1	A	164	GLU	3.0
1	A	2	ALA	3.0
1	D	223	ALA	3.0
1	B	164	GLU	3.0
1	D	150	ASP	3.0
1	D	225	ASP	3.0
1	C	226	GLU	2.9
1	E	222	GLN	2.9
1	B	151	GLY	2.8
1	G	78	TYR	2.8
1	B	73	GLU	2.8
1	D	226	GLU	2.8
1	E	223	ALA	2.8
1	C	225	ASP	2.8
1	F	112	ASP	2.8
1	E	112	ASP	2.7
1	A	165	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	225	ASP	2.6
1	C	74	ASN	2.6
1	B	74	ASN	2.6
1	A	193[A]	HIS	2.6
1	C	6	PRO	2.5
1	D	201	ASP	2.5
1	F	4	ILE	2.5
1	C	185	LEU	2.5
1	F	98	GLY	2.5
1	H	165	GLY	2.5
1	G	182	VAL	2.5
1	E	110	ASP	2.5
1	H	42	LEU	2.4
1	E	2	ALA	2.4
1	D	165	GLY	2.4
1	D	74	ASN	2.4
1	D	46	GLU	2.3
1	H	5	LYS	2.3
1	G	218	GLY	2.3
1	G	202	LYS	2.3
1	H	166	GLY	2.3
1	G	5	LYS	2.3
1	H	8	MET	2.3
1	G	157	VAL	2.2
1	G	112	ASP	2.2
1	G	156	ASP	2.2
1	D	49	PRO	2.2
1	H	31	GLY	2.2
1	E	157	VAL	2.1
1	H	137	VAL	2.1
1	B	110	ASP	2.1
1	E	76	VAL	2.1
1	G	217	SER	2.1
1	C	170	ARG	2.1
1	C	217	SER	2.1
1	G	84	PRO	2.1
1	D	163	LEU	2.1
1	G	58	THR	2.1
1	D	219	LEU	2.1
1	H	56	ILE	2.1
1	D	213	ALA	2.1
1	H	157	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	201	ASP	2.0
1	B	152	VAL	2.0
1	H	185	LEU	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	G	63[A]	21/22	0.82	0.25	30,36,40,41	21
1	GYC	G	63[B]	21/22	0.82	0.25	30,36,40,42	21
1	GYC	H	63	21/22	0.86	0.22	22,33,54,69	0
1	GYC	C	63[B]	21/22	0.87	0.23	32,35,41,52	21
1	GYC	C	63[A]	21/22	0.87	0.23	32,35,41,41	21
1	GYC	E	63[A]	21/22	0.88	0.21	28,33,36,38	21
1	GYC	E	63[B]	21/22	0.88	0.21	26,33,36,41	21
1	GYC	B	63	21/22	0.88	0.19	22,33,54,69	0
1	GYC	A	63[A]	21/22	0.88	0.24	27,36,42,42	21
1	GYC	A	63[B]	21/22	0.88	0.24	27,36,42,56	21
1	GYC	D	63[B]	21/22	0.89	0.23	32,35,41,52	21
1	GYC	D	63[A]	21/22	0.89	0.23	32,35,41,41	21
1	GYC	F	63	21/22	0.91	0.17	20,30,54,59	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.