



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:04 PM UTC

PDB ID : 7RRK / pdb_00007rrk
Title : Crystal structure of fast switching M159E 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 : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

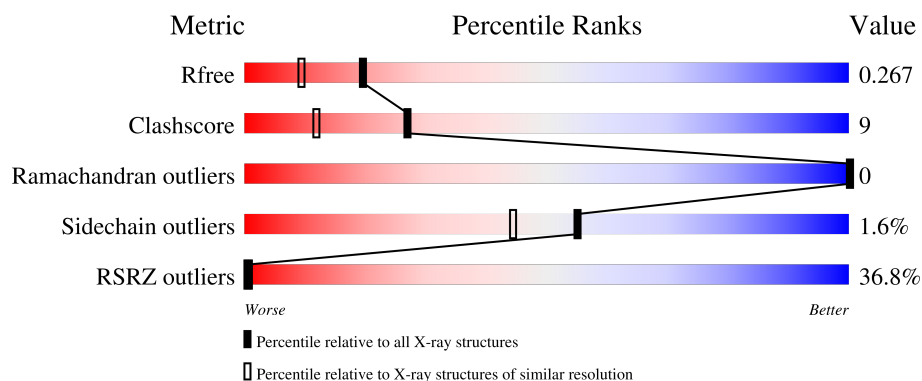
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	60% 66% 17% • 16%
1	B	255	4% 78% 7% • 13%
1	C	255	55% 65% 17% • 16%
1	D	255	2% 76% 5% • 16%
1	E	255	60% 64% 18% • 16%

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Mol	Chain	Length	Quality of chain
1	F	255	3% 76% 7% • 16%
1	G	255	59% 65% 15% • 16%
1	H	255	5% 80% 7% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15363 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	215	Total	C	N	O	S	0	3	0
			1744	1113	292	330	9			
1	B	221	Total	C	N	O	S	0	7	0
			1807	1158	301	339	9			
1	C	214	Total	C	N	O	S	0	2	0
			1739	1113	291	326	9			
1	D	214	Total	C	N	O	S	0	8	0
			1775	1137	297	332	9			
1	E	214	Total	C	N	O	S	0	4	0
			1743	1114	290	330	9			
1	F	214	Total	C	N	O	S	0	4	0
			1750	1120	292	329	9			
1	G	213	Total	C	N	O	S	0	5	0
			1747	1119	292	327	9			
1	H	222	Total	C	N	O	S	0	5	0
			1805	1156	301	339	9			

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	GLU	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	GLU	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	GLU	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	GLU	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	GLU	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	GLU	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	GLU	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

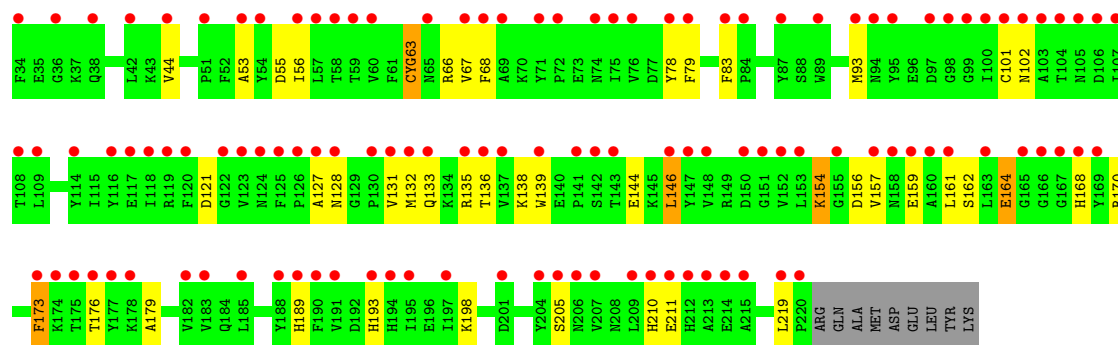
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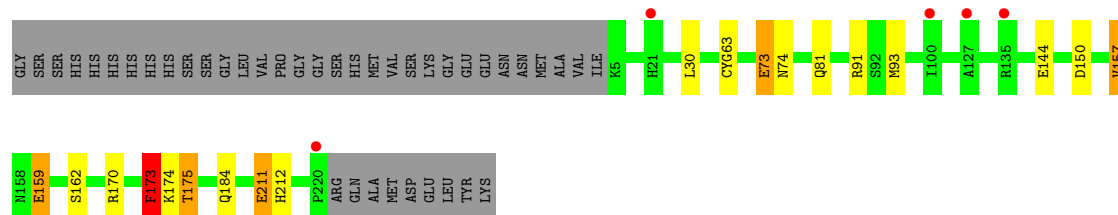
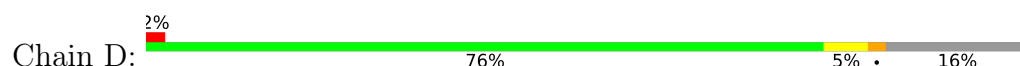
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	GYC	CYS	chromophore	UNP Q5TLG6
H	63	GYC	TYR	chromophore	UNP Q5TLG6
H	63	GYC	GLY	chromophore	UNP Q5TLG6
H	159	GLU	MET	engineered mutation	UNP 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.

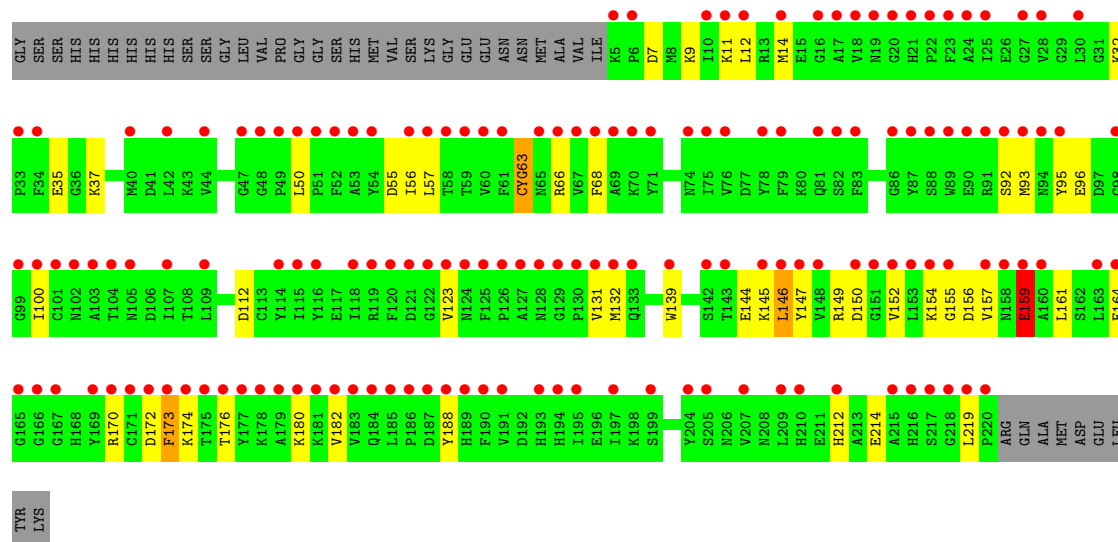
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	223	Total O 223 223	0	0
2	C	108	Total O 108 108	0	0
2	D	215	Total O 215 215	0	0
2	E	101	Total O 101 101	0	0
2	F	197	Total O 197 197	0	0
2	G	102	Total O 102 102	0	0
2	H	203	Total O 203 203	0	0



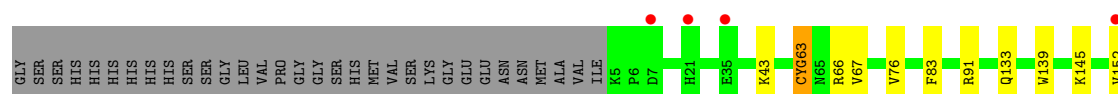
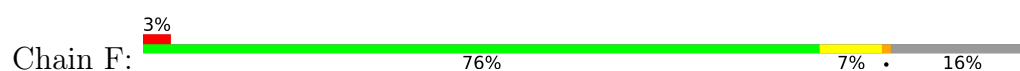
• Molecule 1: Fluorescent protein Dronpa

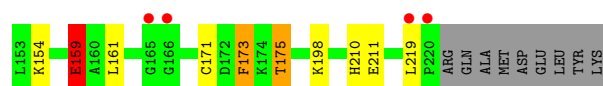


• Molecule 1: Fluorescent protein Dronpa

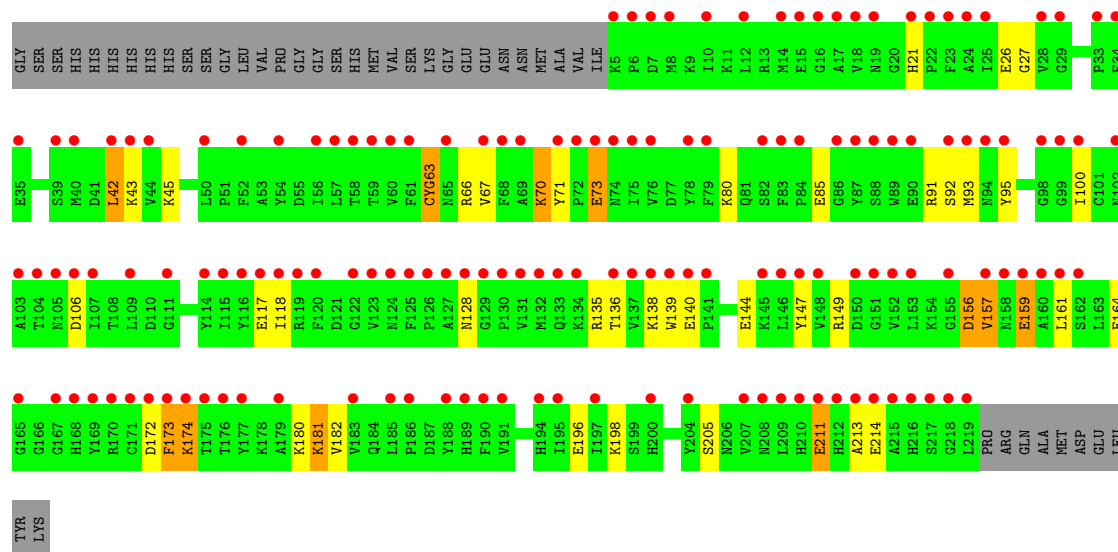


• Molecule 1: Fluorescent protein Dronpa

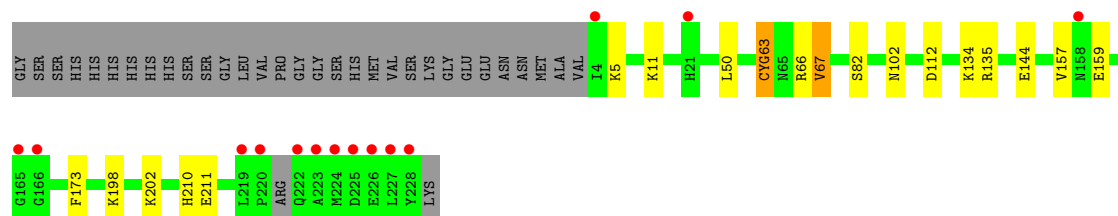
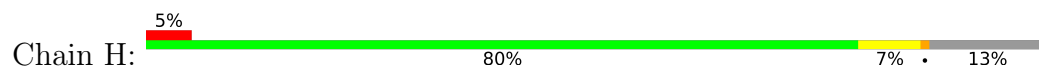




● Molecule 1: Fluorescent protein Dronpa



● 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	79.83Å 85.73Å 143.05Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	37.73 – 1.93 37.73 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (37.73-1.93) 85.7 (37.73-1.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, R_{free}	0.242 , 0.266 0.244 , 0.267	Depositor DCC
R_{free} test set	6941 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15363	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 32.08 % 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 9.9659e-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

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	0.51	1/1775 (0.1%)	0.53	1/2398 (0.0%)
1	B	0.65	9/1850 (0.5%)	0.63	6/2496 (0.2%)
1	C	0.69	3/1771 (0.2%)	0.67	2/2391 (0.1%)
1	D	0.80	12/1822 (0.7%)	0.60	0/2458
1	E	0.70	7/1778 (0.4%)	0.74	6/2403 (0.2%)
1	F	0.79	10/1785 (0.6%)	0.67	8/2410 (0.3%)
1	G	0.80	5/1788 (0.3%)	0.82	10/2414 (0.4%)
1	H	0.60	5/1842 (0.3%)	0.58	2/2486 (0.1%)
All	All	0.70	52/14411 (0.4%)	0.66	35/19456 (0.2%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175[A]	THR	CA-C	10.93	1.65	1.52
1	D	175[B]	THR	CA-C	10.93	1.65	1.52
1	G	174	LYS	CA-C	10.76	1.65	1.52
1	F	173[A]	PHE	CA-C	9.99	1.65	1.52
1	F	173[B]	PHE	CA-C	9.99	1.65	1.52
1	D	173[A]	PHE	CA-C	9.75	1.64	1.52
1	D	173[B]	PHE	CA-C	9.75	1.64	1.52
1	H	173[A]	PHE	CA-C	9.61	1.65	1.52
1	H	173[B]	PHE	CA-C	9.61	1.65	1.52
1	F	175[A]	THR	CA-C	9.41	1.64	1.52
1	F	175[B]	THR	CA-C	9.41	1.64	1.52
1	B	173[A]	PHE	CA-C	9.04	1.63	1.52
1	B	173[B]	PHE	CA-C	9.04	1.63	1.52
1	E	50	LEU	C-N	7.86	1.39	1.33
1	D	159[A]	GLU	CA-C	7.74	1.64	1.53
1	D	159[B]	GLU	CA-C	7.74	1.64	1.53
1	B	159[A]	GLU	C-O	7.73	1.33	1.23
1	B	159[B]	GLU	C-O	7.73	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ILE	C-N	-7.46	1.21	1.33
1	F	159[A]	GLU	C-O	7.39	1.32	1.23
1	F	159[B]	GLU	C-O	7.39	1.32	1.23
1	E	159[A]	GLU	CA-C	7.29	1.63	1.53
1	E	159[B]	GLU	CA-C	7.29	1.63	1.53
1	H	159[A]	GLU	CA-C	7.25	1.63	1.53
1	H	159[B]	GLU	CA-C	7.25	1.63	1.53
1	C	173[A]	PHE	CA-C	7.21	1.61	1.52
1	C	173[B]	PHE	CA-C	7.21	1.61	1.52
1	E	173[A]	PHE	CA-C	7.01	1.61	1.52
1	E	173[B]	PHE	CA-C	7.01	1.61	1.52
1	B	159[A]	GLU	CA-C	6.74	1.61	1.52
1	B	159[B]	GLU	CA-C	6.74	1.61	1.52
1	D	211	GLU	C-O	-6.59	1.16	1.23
1	G	159[A]	GLU	CA-C	6.35	1.62	1.53
1	G	159[B]	GLU	CA-C	6.35	1.62	1.53
1	D	73	GLU	C-O	-6.32	1.16	1.24
1	F	159[A]	GLU	CA-C	6.12	1.60	1.52
1	F	159[B]	GLU	CA-C	6.12	1.60	1.52
1	D	157	VAL	C-O	-5.98	1.18	1.24
1	F	76	VAL	C-O	-5.82	1.18	1.24
1	B	11	LYS	C-O	-5.76	1.17	1.23
1	B	150	ASP	C-O	-5.69	1.16	1.23
1	B	158	ASN	C-O	-5.51	1.16	1.23
1	H	202	LYS	C-O	-5.46	1.17	1.24
1	E	146	LEU	C-O	-5.45	1.17	1.24
1	C	164	GLU	N-CA	-5.29	1.40	1.46
1	F	43	LYS	C-O	-5.25	1.18	1.24
1	G	95	TYR	C-O	-5.24	1.17	1.23
1	E	214	GLU	C-O	-5.22	1.17	1.23
1	D	93	MET	C-O	-5.18	1.18	1.24
1	G	70	LYS	C-O	-5.15	1.17	1.24
1	D	159[A]	GLU	C-O	5.02	1.30	1.23
1	D	159[B]	GLU	C-O	5.02	1.30	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173[A]	PHE	CA-C-O	9.26	131.00	120.54
1	E	173[B]	PHE	CA-C-O	9.26	131.00	120.54
1	G	174	LYS	CA-C-O	9.16	130.10	120.30
1	F	159[A]	GLU	CA-C-O	7.84	129.94	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	159[B]	GLU	CA-C-O	7.84	129.94	120.92
1	B	159[A]	GLU	CA-C-O	7.73	129.38	120.80
1	B	159[B]	GLU	CA-C-O	7.73	129.38	120.80
1	G	173[A]	PHE	CA-C-O	7.47	129.09	120.80
1	G	173[B]	PHE	CA-C-O	7.47	129.09	120.80
1	G	159[A]	GLU	CA-C-O	6.68	129.69	121.81
1	G	159[B]	GLU	CA-C-O	6.68	129.69	121.81
1	F	173[A]	PHE	CB-CA-C	-6.16	99.69	109.80
1	F	173[B]	PHE	CB-CA-C	-6.16	99.69	109.80
1	F	159[A]	GLU	N-CA-C	6.14	120.27	109.96
1	F	159[B]	GLU	N-CA-C	6.14	120.27	109.96
1	C	173[A]	PHE	CA-C-O	6.01	127.54	120.69
1	C	173[B]	PHE	CA-C-O	6.01	127.54	120.69
1	B	173[A]	PHE	CB-CA-C	5.98	119.61	109.75
1	B	173[B]	PHE	CB-CA-C	5.98	119.61	109.75
1	G	118	ILE	N-CA-C	5.95	117.05	108.48
1	E	159[A]	GLU	CA-C-O	5.92	128.80	121.81
1	E	159[B]	GLU	CA-C-O	5.92	128.80	121.81
1	B	159[A]	GLU	N-CA-C	5.76	119.20	109.76
1	B	159[B]	GLU	N-CA-C	5.76	119.20	109.76
1	E	173[A]	PHE	O-C-N	-5.69	116.73	123.22
1	E	173[B]	PHE	O-C-N	-5.69	116.73	123.22
1	H	67	VAL	N-CA-C	-5.44	104.28	111.09
1	G	182	VAL	CB-CA-C	-5.36	104.81	111.08
1	A	158	ASN	N-CA-C	-5.35	99.05	108.20
1	G	71	TYR	CA-C-N	-5.12	115.45	120.52
1	G	71	TYR	C-N-CA	-5.12	115.45	120.52
1	G	174	LYS	O-C-N	-5.10	117.36	123.27
1	F	159[A]	GLU	O-C-N	-5.01	117.35	123.16
1	F	159[B]	GLU	O-C-N	-5.01	117.35	123.16
1	H	82	SER	N-CA-C	5.00	118.48	112.38

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	1744	0	1657	39	0
1	B	1807	0	1722	15	0
1	C	1739	0	1657	39	0
1	D	1775	0	1708	19	0
1	E	1743	0	1645	51	0
1	F	1750	0	1670	24	0
1	G	1747	0	1665	67	0
1	H	1805	0	1715	10	0
2	A	104	0	0	7	0
2	B	223	0	0	4	0
2	C	108	0	0	5	0
2	D	215	0	0	4	0
2	E	101	0	0	12	0
2	F	197	0	0	4	0
2	G	102	0	0	5	0
2	H	203	0	0	5	0
All	All	15363	0	13439	254	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 9.

All (254) 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:G:157:VAL:HG21	1:G:173[B]:PHE:CE2	1.82	1.14
1:G:159[A]:GLU:HG3	1:G:173[A]:PHE:CE2	1.93	1.03
1:G:157:VAL:HG23	1:G:173[A]:PHE:HB2	1.43	0.96
1:G:140:GLU:HB2	2:G:307:HOH:O	1.66	0.95
1:A:4:ILE:HG13	1:A:8:MET:HE2	1.47	0.94
1:F:152:VAL:HA	2:F:337:HOH:O	1.72	0.90
1:F:173[B]:PHE:CE2	1:F:175[B]:THR:HG23	2.08	0.88
1:G:157:VAL:CG2	1:G:173[B]:PHE:CE2	2.57	0.86
1:E:212:HIS:HD2	2:E:394:HOH:O	1.58	0.86
1:G:157:VAL:CG2	1:G:173[B]:PHE:CD2	2.60	0.84
1:G:157:VAL:HG23	1:G:173[B]:PHE:CG	2.13	0.83
1:G:157:VAL:CG2	1:G:173[A]:PHE:HB2	2.09	0.81
1:G:159[A]:GLU:HG3	1:G:173[A]:PHE:CZ	2.14	0.80
1:H:198:LYS:HG3	1:H:210:HIS:CD2	2.18	0.78
1:G:157:VAL:HG21	1:G:173[B]:PHE:CZ	2.17	0.78
1:C:121:ASP:HB2	2:C:301:HOH:O	1.85	0.77
1:C:10:ILE:HD11	1:C:68:PHE:CZ	2.20	0.76
1:G:157:VAL:CG2	1:G:173[B]:PHE:CG	2.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:68:PHE:CE2	2.21	0.75
1:E:37:LYS:HE3	1:E:212:HIS:CE1	2.22	0.74
1:C:135:ARG:HH11	1:C:164:GLU:HG2	1.53	0.74
1:G:157:VAL:HG21	1:G:173[B]:PHE:CD2	2.22	0.74
1:G:157:VAL:CG2	1:G:173[B]:PHE:CZ	2.71	0.74
1:G:181:LYS:HB2	1:G:181:LYS:NZ	2.03	0.72
1:G:144:GLU:HA	1:G:157:VAL:CG1	2.19	0.72
1:G:157:VAL:HG23	1:G:173[B]:PHE:CD2	2.25	0.71
1:E:145:LYS:O	1:E:146:LEU:HD23	1.90	0.70
1:C:93:MET:HE3	1:C:101:CYS:HB2	1.74	0.70
1:G:73:GLU:H	1:G:73:GLU:CD	1.99	0.69
1:F:173[B]:PHE:CE2	1:F:175[B]:THR:CG2	2.76	0.69
1:E:172:ASP:HB3	2:E:360:HOH:O	1.91	0.69
1:C:55[B]:ASP:OD2	1:C:161:LEU:HD21	1.94	0.68
1:C:138:LYS:HG2	1:C:162:SER:HB3	1.73	0.68
1:A:85:GLU:OE1	1:A:85:GLU:N	2.24	0.68
1:D:91:ARG:HE	1:D:175[B]:THR:CG2	2.08	0.67
1:G:159[B]:GLU:OE2	1:G:173[B]:PHE:HD2	1.78	0.67
1:F:159[B]:GLU:OE1	1:F:173[B]:PHE:HB2	1.93	0.67
1:E:100:ILE:HG23	1:E:123:VAL:HG23	1.76	0.66
1:G:211:GLU:OE2	1:G:213:ALA:HB2	1.95	0.66
1:E:145:LYS:C	1:E:146:LEU:HD23	2.20	0.66
1:B:100:ILE:HD13	2:H:354:HOH:O	1.93	0.66
1:G:128:ASN:O	1:G:135:ARG:NH2	2.28	0.66
1:E:55:ASP:HA	2:E:301:HOH:O	1.95	0.65
1:G:157:VAL:HG23	1:G:173[A]:PHE:CB	2.21	0.65
1:A:202:LYS:NZ	2:A:303:HOH:O	2.23	0.65
1:E:144:GLU:HG2	1:E:146:LEU:HD21	1.79	0.65
1:G:157:VAL:HG22	1:G:173[B]:PHE:CE1	2.32	0.64
1:F:154:LYS:NZ	2:F:305:HOH:O	2.27	0.64
1:B:198:LYS:NZ	2:B:309:HOH:O	2.31	0.63
1:E:9:LYS:HZ1	1:E:112:ASP:CG	2.08	0.61
1:E:146:LEU:CD2	1:E:155:GLY:HA2	2.30	0.61
1:E:159[B]:GLU:OE2	1:E:173[B]:PHE:HB2	2.00	0.61
1:F:198:LYS:HG3	1:F:210:HIS:CD2	2.36	0.61
1:A:170:ARG:NH1	1:E:147:TYR:OH	2.32	0.61
1:B:143:THR:H	1:F:145:LYS:HZ3	1.48	0.61
1:C:139:TRP:CE3	1:C:159:GLU:HG3	2.35	0.61
1:E:96:GLU:HB3	1:E:170:ARG:HG2	1.82	0.61
1:F:91:ARG:HE	1:F:175[B]:THR:CG2	2.15	0.60
1:F:91:ARG:HG3	1:F:175[B]:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:ASP:OD1	1:G:180:LYS:NZ	2.31	0.60
1:G:144:GLU:HA	1:G:157:VAL:HG13	1.84	0.60
1:B:143:THR:H	1:F:145:LYS:NZ	1.99	0.59
1:H:50:LEU:O	1:H:134:LYS:NZ	2.35	0.59
1:E:212:HIS:CD2	2:E:394:HOH:O	2.41	0.59
1:A:15:GLU:OE2	2:A:301:HOH:O	2.17	0.59
1:C:198:LYS:HG3	1:C:210:HIS:CD2	2.37	0.59
1:G:181:LYS:HB2	1:G:181:LYS:HZ2	1.66	0.59
1:G:144:GLU:HG3	1:G:157:VAL:HG13	1.83	0.59
1:D:162:SER:HB2	2:D:357:HOH:O	2.03	0.58
1:F:133:GLN:NE2	2:F:310:HOH:O	2.34	0.58
1:F:91:ARG:HE	1:F:175[B]:THR:HG21	1.68	0.58
1:D:91:ARG:HE	1:D:175[B]:THR:HG22	1.68	0.58
1:D:74[A]:ASN:ND2	2:D:305:HOH:O	2.32	0.58
1:A:70:LYS:HB3	1:A:214:GLU:HG3	1.85	0.58
1:C:139:TRP:CZ3	1:C:161:LEU:HG	2.38	0.58
1:H:5:LYS:NZ	1:H:112:ASP:HB3	2.19	0.58
1:D:81:GLN:OE1	1:D:184:GLN:HG2	2.03	0.58
1:A:4:ILE:HD12	1:A:114:TYR:OH	2.05	0.57
1:C:44:VAL:HG12	1:C:205:SER:HA	1.86	0.57
1:B:154:LYS:NZ	2:B:310:HOH:O	2.37	0.57
1:E:144:GLU:CG	1:E:146:LEU:HD21	2.35	0.57
1:E:188:TYR:HB3	2:E:382:HOH:O	2.03	0.57
1:C:102:ASN:HB2	2:C:301:HOH:O	2.04	0.57
1:D:73:GLU:CD	1:D:73:GLU:H	2.13	0.56
1:A:100:ILE:HG12	1:G:100:ILE:HD11	1.87	0.56
1:A:146:LEU:HD23	1:A:153:LEU:HD21	1.88	0.56
1:C:139:TRP:CE3	1:C:161:LEU:HG	2.40	0.56
1:G:43:LYS:HA	1:G:205:SER:O	2.06	0.55
1:G:159[B]:GLU:OE2	1:G:173[B]:PHE:CD2	2.59	0.55
1:A:147:TYR:OH	1:E:170:ARG:NH2	2.36	0.55
1:G:157:VAL:CG2	1:G:173[B]:PHE:CD1	2.89	0.55
1:E:144:GLU:HG2	1:E:146:LEU:CD2	2.36	0.55
1:A:133:GLN:HB2	1:A:135:ARG:HD3	1.88	0.55
1:E:63:GYC:HB2	1:E:66:ARG:NH2	2.21	0.55
1:C:63:GYC:HB2	1:C:66:ARG:NH2	2.21	0.55
1:H:63:GYC:HB2	1:H:66:ARG:NH2	2.22	0.55
1:G:85:GLU:N	1:G:85:GLU:OE2	2.40	0.54
1:A:144:GLU:HA	1:A:157:VAL:HG22	1.89	0.54
1:G:157:VAL:CG2	1:G:173[B]:PHE:CE1	2.90	0.54
1:C:144:GLU:OE2	1:C:193:HIS:NE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:VAL:HG12	1:E:132:MET:HE2	1.89	0.53
1:E:144:GLU:CD	1:E:146:LEU:HD21	2.33	0.53
1:D:91:ARG:HG3	1:D:175[B]:THR:HG22	1.91	0.53
1:E:92[A]:SER:OG	1:E:100:ILE:HD11	2.09	0.53
1:G:144:GLU:HA	1:G:157:VAL:HG12	1.90	0.53
1:E:174:LYS:HG3	2:E:360:HOH:O	2.08	0.52
1:D:91:ARG:CG	1:D:175[B]:THR:HG22	2.39	0.51
1:B:100:ILE:HG22	1:H:102:ASN:HD21	1.74	0.51
1:D:91:ARG:HE	1:D:175[B]:THR:HG21	1.75	0.51
1:B:159[A]:GLU:HG3	1:B:171:CYS:O	2.10	0.50
1:G:91:ARG:HA	1:G:174:LYS:O	2.10	0.50
1:C:78:TYR:HH	1:C:179:ALA:H	1.59	0.50
1:C:136:THR:HB	1:C:161:LEU:HD22	1.94	0.50
1:G:63:GYC:HB2	1:G:66:ARG:NH2	2.27	0.50
1:G:26:GLU:OE1	1:G:45:LYS:NZ	2.36	0.50
1:A:139:TRP:CE3	1:A:161:LEU:HG	2.47	0.50
1:C:154:LYS:HE2	1:C:176:THR:HG23	1.93	0.50
1:E:55:ASP:O	2:E:301:HOH:O	2.19	0.49
1:A:4:ILE:CD1	1:A:114:TYR:OH	2.60	0.49
1:B:4:ILE:HD11	1:B:33:PRO:HB2	1.94	0.49
1:A:139:TRP:CE3	1:A:159:GLU:HG3	2.47	0.49
1:E:55:ASP:CA	2:E:301:HOH:O	2.57	0.49
1:G:67:VAL:HG23	1:G:80:LYS:HG2	1.94	0.49
1:G:157:VAL:HG22	1:G:173[B]:PHE:CD1	2.47	0.49
1:A:32:LYS:HG3	2:A:381:HOH:O	2.13	0.49
1:A:63:GYC:HE2	1:A:195:ILE:HB	1.94	0.49
1:D:91:ARG:NE	1:D:175[B]:THR:CG2	2.75	0.49
1:E:35:GLU:O	1:E:37:LYS:NZ	2.29	0.49
1:E:146:LEU:HD22	1:E:155:GLY:HA2	1.93	0.49
1:B:152:VAL:HG11	1:B:178:LYS:HG2	1.94	0.49
1:C:127:ALA:O	1:C:133:GLN:NE2	2.44	0.49
1:G:196:GLU:HB2	1:G:198:LYS:HZ2	1.77	0.49
1:E:32:LYS:HD3	1:E:35:GLU:OE1	2.13	0.49
1:D:174:LYS:HE3	2:D:452:HOH:O	2.13	0.48
1:C:121:ASP:O	2:C:301:HOH:O	2.20	0.48
1:F:173[B]:PHE:CZ	1:F:175[B]:THR:HG21	2.48	0.48
1:G:181:LYS:NZ	1:G:181:LYS:CB	2.73	0.48
1:F:63:GYC:HB2	1:F:66:ARG:NH2	2.28	0.48
1:C:131:VAL:HG12	1:C:132:MET:HE2	1.94	0.48
1:E:93:MET:HE3	2:E:308:HOH:O	2.13	0.48
1:G:93:MET:HG2	1:G:173[A]:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:HA	1:B:157:VAL:HG22	1.96	0.48
1:G:157:VAL:HG21	1:G:173[A]:PHE:HD2	1.78	0.48
1:H:144:GLU:HA	1:H:157:VAL:HG22	1.96	0.48
1:A:55:ASP:O	1:A:139:TRP:NE1	2.44	0.47
1:E:152:VAL:HG11	1:E:176:THR:HG23	1.96	0.47
1:A:110:ASP:HB2	1:A:115:ILE:HD11	1.96	0.47
1:G:157:VAL:CG2	1:G:173[A]:PHE:CD2	2.97	0.47
1:H:5:LYS:HZ1	1:H:112:ASP:HB3	1.78	0.47
1:C:67:VAL:HG11	1:C:83:PHE:CE2	2.49	0.47
1:A:211:GLU:OE1	1:A:213:ALA:HB2	2.14	0.47
1:B:63:GYC:HB2	1:B:66:ARG:NH2	2.29	0.47
1:G:117:GLU:OE1	2:G:301:HOH:O	2.20	0.47
1:B:73:GLU:OE1	2:B:301:HOH:O	2.20	0.47
1:D:73:GLU:CD	1:D:73:GLU:N	2.73	0.47
1:A:139:TRP:CZ3	1:A:161:LEU:HG	2.50	0.46
1:D:150:ASP:OD2	2:D:301:HOH:O	2.21	0.46
1:F:91:ARG:NE	1:F:175[B]:THR:HG21	2.30	0.46
1:G:172:ASP:O	2:G:302:HOH:O	2.21	0.46
1:G:27:GLY:HA3	1:G:42:LEU:HD23	1.98	0.46
1:A:9:LYS:HB2	1:A:113:CYS:HA	1.97	0.46
1:F:152:VAL:CA	2:F:337:HOH:O	2.48	0.46
1:E:7:ASP:OD1	2:E:303:HOH:O	2.21	0.46
1:E:68:PHE:O	2:E:302:HOH:O	2.21	0.46
1:G:159[B]:GLU:CD	1:G:173[B]:PHE:HD2	2.24	0.46
1:C:67:VAL:HA	2:C:348:HOH:O	2.15	0.46
1:C:154:LYS:HB3	2:C:364:HOH:O	2.14	0.46
1:F:173[B]:PHE:CZ	1:F:175[B]:THR:CG2	2.99	0.46
1:B:100:ILE:CD1	2:H:354:HOH:O	2.58	0.45
1:E:37:LYS:HE3	1:E:212:HIS:ND1	2.29	0.45
1:C:5:LYS:HD3	1:C:5:LYS:N	2.31	0.45
1:E:164:GLU:O	1:E:164:GLU:HG2	2.16	0.45
1:H:198:LYS:CG	1:H:210:HIS:CD2	2.95	0.45
1:A:55:ASP:HB3	1:A:161:LEU:HD21	1.98	0.45
1:B:128[A]:ASN:ND2	2:H:308:HOH:O	2.46	0.45
1:C:67:VAL:HG12	1:C:79:PHE:HB3	1.98	0.45
1:A:163:LEU:HD21	1:A:169:TYR:HB2	1.98	0.45
1:A:128:ASN:HA	1:A:133:GLN:CD	2.41	0.45
1:F:91:ARG:CG	1:F:175[B]:THR:HG22	2.47	0.45
1:D:144:GLU:HA	1:D:157:VAL:HG22	1.99	0.44
1:E:139:TRP:CZ3	1:E:161:LEU:HG	2.52	0.44
1:D:91:ARG:NE	1:D:175[B]:THR:HG22	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:GLU:HB2	1:G:198:LYS:NZ	2.33	0.44
1:C:219:LEU:HD23	1:C:219:LEU:HA	1.69	0.44
1:E:144:GLU:HA	1:E:157:VAL:HG22	1.98	0.44
1:G:157:VAL:HG22	1:G:173[B]:PHE:CZ	2.49	0.44
1:C:128:ASN:HA	1:C:133:GLN:HE21	1.82	0.44
1:A:170:ARG:HE	1:A:170:ARG:HB2	1.62	0.43
1:C:53:ALA:O	1:C:56:ILE:HG12	2.18	0.43
1:G:70:LYS:HD3	1:G:214:GLU:OE2	2.18	0.43
1:C:168:HIS:O	1:G:149:ARG:NH2	2.51	0.43
1:E:92[A]:SER:HG	1:E:100:ILE:HD11	1.82	0.43
1:F:159[B]:GLU:HG3	1:F:171:CYS:O	2.18	0.43
1:G:136:THR:O	2:G:303:HOH:O	2.21	0.43
1:C:170:ARG:HD3	1:G:147:TYR:OH	2.17	0.43
1:A:10:ILE:HD11	1:A:68:PHE:CE2	2.53	0.43
1:C:63:GYC:HB2	1:C:66:ARG:HH22	1.83	0.43
1:G:157:VAL:HG23	1:G:173[A]:PHE:CD2	2.54	0.43
1:A:63:GYC:HB2	1:A:66:ARG:NH2	2.33	0.43
1:D:211:GLU:HG2	1:D:212:HIS:N	2.33	0.43
1:F:67:VAL:HG11	1:F:83:PHE:CE2	2.54	0.43
1:H:135:ARG:NH2	2:H:306:HOH:O	2.37	0.43
1:C:157:VAL:O	1:C:173[B]:PHE:HB3	2.19	0.42
1:A:153:LEU:HB3	1:A:177:TYR:HB2	2.01	0.42
1:A:100:ILE:HG21	1:G:92:SER:HB3	2.01	0.42
1:A:219:LEU:HA	1:A:220:PRO:HD3	1.90	0.42
1:E:56:ILE:HG23	1:E:95:TYR:OH	2.19	0.42
1:E:149:ARG:O	1:E:150[B]:ASP:HB3	2.19	0.42
1:E:172:ASP:C	2:E:360:HOH:O	2.62	0.42
1:G:138:LYS:HG2	1:G:139:TRP:O	2.20	0.42
1:C:67:VAL:HG11	1:C:83:PHE:HE2	1.84	0.42
1:A:154:LYS:NZ	2:A:318:HOH:O	2.52	0.42
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.87	0.41
1:E:146:LEU:HD22	1:E:154:LYS:O	2.20	0.41
1:G:157:VAL:HG23	1:G:173[A]:PHE:CG	2.55	0.41
1:A:184:GLN:NE2	2:A:315:HOH:O	2.46	0.41
1:B:172:ASP:OD2	2:B:302:HOH:O	2.22	0.41
1:A:148:VAL:HG21	1:A:185:LEU:HB3	2.03	0.41
1:G:135:ARG:HA	1:G:164:GLU:OE1	2.19	0.41
1:E:14:MET:HE1	1:E:57:LEU:HD13	2.02	0.41
1:E:37:LYS:N	1:E:37:LYS:HD2	2.36	0.41
1:G:173[B]:PHE:HA	2:G:302:HOH:O	2.20	0.41
1:E:146:LEU:HD22	1:E:155:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:TRP:CE3	1:G:161:LEU:HG	2.55	0.41
1:A:21:HIS:CE1	2:A:306:HOH:O	2.74	0.41
1:C:146:LEU:HD23	1:C:189:HIS:CD2	2.56	0.41
1:E:56:ILE:HD11	1:E:131:VAL:HG22	2.02	0.41
1:F:139:TRP:CZ3	1:F:161:LEU:HG	2.55	0.41
1:C:146:LEU:HD23	1:C:189:HIS:NE2	2.36	0.40
1:E:219:LEU:HD12	1:E:219:LEU:HA	1.88	0.40
1:A:163:LEU:HD21	1:A:169:TYR:CB	2.51	0.40
1:A:48:GLY:N	2:A:313:HOH:O	2.54	0.40
1:F:219:LEU:HD12	1:F:219:LEU:HA	1.84	0.40
1:G:157:VAL:HG21	1:G:173[A]:PHE:CD2	2.54	0.40
1:A:100:ILE:HG21	1:G:92:SER:CB	2.52	0.40
1:C:66:ARG:HB3	1:C:79:PHE:CD1	2.56	0.40
1:E:11:LYS:HD2	1:E:12:LEU:N	2.37	0.40
1:H:11:LYS:HD2	2:H:333:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/255 (84%)	211 (99%)	2 (1%)	0	100	100
1	B	221/255 (87%)	218 (99%)	3 (1%)	0	100	100
1	C	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
1	D	217/255 (85%)	215 (99%)	2 (1%)	0	100	100
1	E	213/255 (84%)	210 (99%)	3 (1%)	0	100	100
1	F	213/255 (84%)	212 (100%)	1 (0%)	0	100	100
1	G	213/255 (84%)	208 (98%)	5 (2%)	0	100	100
1	H	220/255 (86%)	218 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1721/2040 (84%)	1700 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/217 (86%)	185 (100%)	1 (0%)	81	80
1	B	192/217 (88%)	187 (97%)	5 (3%)	40	24
1	C	185/217 (85%)	181 (98%)	4 (2%)	45	32
1	D	191/217 (88%)	186 (97%)	5 (3%)	40	24
1	E	185/217 (85%)	181 (98%)	4 (2%)	45	32
1	F	187/217 (86%)	184 (98%)	3 (2%)	55	44
1	G	186/217 (86%)	180 (97%)	6 (3%)	34	18
1	H	190/217 (88%)	188 (99%)	2 (1%)	65	60
All	All	1502/1736 (86%)	1472 (98%)	30 (2%)	55	35

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	B	159[A]	GLU
1	B	159[B]	GLU
1	B	173[A]	PHE
1	B	173[B]	PHE
1	B	181	LYS
1	C	11	LYS
1	C	146	LEU
1	C	154	LYS
1	C	211	GLU
1	D	30	LEU
1	D	159[A]	GLU

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Mol	Chain	Res	Type
1	D	159[B]	GLU
1	D	173[A]	PHE
1	D	173[B]	PHE
1	E	159[A]	GLU
1	E	159[B]	GLU
1	E	180	LYS
1	E	182	VAL
1	F	159[A]	GLU
1	F	159[B]	GLU
1	F	211	GLU
1	G	42	LEU
1	G	73	GLU
1	G	156	ASP
1	G	157	VAL
1	G	181	LYS
1	G	211	GLU
1	H	67	VAL
1	H	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	B	206	ASN
1	B	212	HIS
1	C	194	HIS
1	D	38	GLN
1	D	158	ASN
1	D	208	ASN
1	E	158	ASN
1	E	210	HIS
1	F	38	GLN
1	G	38	GLN
1	G	184	GLN
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	B	63	1	21,22,23	1.04	2 (9%)	26,30,32	2.12	4 (15%)
1	GYC	F	63	1	21,22,23	1.00	2 (9%)	26,30,32	1.98	5 (19%)
1	GYC	D	63	1	21,22,23	0.99	2 (9%)	26,30,32	1.93	6 (23%)
1	GYC	H	63	1	21,22,23	1.02	1 (4%)	26,30,32	2.12	5 (19%)
1	GYC	E	63	1	21,22,23	1.06	1 (4%)	26,30,32	2.18	6 (23%)
1	GYC	A	63	1	21,22,23	1.09	1 (4%)	26,30,32	2.17	7 (26%)
1	GYC	C	63	1	21,22,23	1.01	1 (4%)	26,30,32	2.11	6 (23%)
1	GYC	G	63	1	21,22,23	1.07	1 (4%)	26,30,32	2.17	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	B	63	1	-	3/10/29/30	0/2/2/2
1	GYC	F	63	1	-	3/10/29/30	0/2/2/2
1	GYC	D	63	1	-	3/10/29/30	0/2/2/2
1	GYC	H	63	1	-	3/10/29/30	0/2/2/2
1	GYC	E	63	1	-	3/10/29/30	0/2/2/2
1	GYC	A	63	1	-	5/10/29/30	0/2/2/2
1	GYC	C	63	1	-	3/10/29/30	0/2/2/2
1	GYC	G	63	1	-	3/10/29/30	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB2-CA2	4.06	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	GYC	CB2-CA2	3.84	1.38	1.35
1	G	63	GYC	CB2-CA2	3.81	1.38	1.35
1	C	63	GYC	CB2-CA2	3.57	1.38	1.35
1	B	63	GYC	CB2-CA2	3.55	1.38	1.35
1	H	63	GYC	CB2-CA2	3.49	1.38	1.35
1	F	63	GYC	CB2-CA2	3.36	1.38	1.35
1	D	63	GYC	CB2-CA2	3.29	1.38	1.35
1	B	63	GYC	C2-N3	-2.05	1.35	1.40
1	D	63	GYC	C2-N3	-2.04	1.35	1.40
1	F	63	GYC	C2-N3	-2.01	1.35	1.40

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	GYC	O2-C2-CA2	-7.12	126.48	131.02
1	B	63	GYC	O2-C2-CA2	-6.67	126.76	131.02
1	G	63	GYC	O2-C2-CA2	-6.35	126.97	131.02
1	E	63	GYC	O2-C2-CA2	-6.35	126.97	131.02
1	C	63	GYC	O2-C2-CA2	-6.28	127.01	131.02
1	F	63	GYC	O2-C2-CA2	-6.16	127.09	131.02
1	A	63	GYC	O2-C2-CA2	-6.09	127.14	131.02
1	D	63	GYC	O2-C2-CA2	-6.03	127.17	131.02
1	E	63	GYC	C2-CA2-N2	-5.13	105.27	108.95
1	A	63	GYC	C2-CA2-N2	-5.11	105.29	108.95
1	G	63	GYC	C2-CA2-N2	-5.07	105.32	108.95
1	B	63	GYC	C2-CA2-N2	-4.91	105.44	108.95
1	C	63	GYC	C2-CA2-N2	-4.85	105.48	108.95
1	A	63	GYC	CA2-N2-C1	4.73	109.50	105.80
1	G	63	GYC	CA2-N2-C1	4.71	109.48	105.80
1	E	63	GYC	CA2-N2-C1	4.66	109.44	105.80
1	H	63	GYC	C2-CA2-N2	-4.44	105.77	108.95
1	C	63	GYC	CA2-N2-C1	4.44	109.27	105.80
1	B	63	GYC	CA2-N2-C1	4.42	109.25	105.80
1	F	63	GYC	C2-CA2-N2	-4.22	105.93	108.95
1	D	63	GYC	C2-CA2-N2	-4.12	106.00	108.95
1	H	63	GYC	CA2-N2-C1	4.03	108.95	105.80
1	F	63	GYC	CA2-N2-C1	3.95	108.89	105.80
1	D	63	GYC	CA2-N2-C1	3.76	108.74	105.80
1	A	63	GYC	CG2-CB2-CA2	-3.02	126.27	129.87
1	B	63	GYC	CA2-C2-N3	2.73	105.80	103.50
1	G	63	GYC	CA2-C2-N3	2.73	105.80	103.50
1	E	63	GYC	CA2-C2-N3	2.69	105.76	103.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	GYC	CG2-CB2-CA2	-2.68	126.68	129.87
1	H	63	GYC	CA2-C2-N3	2.60	105.69	103.50
1	A	63	GYC	CA2-C2-N3	2.57	105.66	103.50
1	C	63	GYC	CA2-C2-N3	2.53	105.62	103.50
1	C	63	GYC	CA1-CB1-SG1	-2.48	109.09	114.40
1	E	63	GYC	CA1-CB1-SG1	-2.46	109.13	114.40
1	A	63	GYC	CA1-CB1-SG1	-2.39	109.28	114.40
1	D	63	GYC	CA1-CB1-SG1	-2.32	109.44	114.40
1	G	63	GYC	CA1-CB1-SG1	-2.26	109.56	114.40
1	F	63	GYC	CA2-C2-N3	2.25	105.39	103.50
1	F	63	GYC	CA1-CB1-SG1	-2.25	109.59	114.40
1	D	63	GYC	CA2-C2-N3	2.24	105.38	103.50
1	E	63	GYC	CG2-CB2-CA2	-2.17	127.29	129.87
1	H	63	GYC	CA1-CB1-SG1	-2.16	109.79	114.40
1	A	63	GYC	CB2-CA2-C2	2.13	124.93	122.36
1	D	63	GYC	CG2-CB2-CA2	-2.07	127.41	129.87
1	C	63	GYC	CG2-CB2-CA2	-2.02	127.47	129.87

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	D	63	GYC	N2-CA2-CB2-CG2
1	E	63	GYC	N2-CA2-CB2-CG2
1	F	63	GYC	N2-CA2-CB2-CG2
1	G	63	GYC	N2-CA2-CB2-CG2
1	H	63	GYC	N2-CA2-CB2-CG2
1	A	63	GYC	N1-CA1-CB1-SG1

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	GYC	1	0
1	F	63	GYC	1	0
1	H	63	GYC	1	0
1	E	63	GYC	1	0
1	A	63	GYC	2	0
1	C	63	GYC	2	0
1	G	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/255 (83%)	2.67	152 (71%) 0 0	27, 60, 75, 89	3 (1%)
1	B	220/255 (86%)	0.64	11 (5%) 34 38	12, 27, 45, 71	7 (3%)
1	C	213/255 (83%)	2.50	139 (65%) 0 0	31, 57, 69, 84	2 (0%)
1	D	213/255 (83%)	0.44	5 (2%) 61 67	8, 26, 42, 55	8 (3%)
1	E	213/255 (83%)	2.59	154 (72%) 0 0	25, 59, 73, 90	4 (1%)
1	F	213/255 (83%)	0.50	8 (3%) 44 49	9, 27, 44, 61	4 (1%)
1	G	212/255 (83%)	2.54	150 (70%) 0 0	32, 59, 72, 77	5 (2%)
1	H	221/255 (86%)	0.58	14 (6%) 26 30	10, 27, 46, 75	5 (2%)
All	All	1719/2040 (84%)	1.55	633 (36%) 1 0	8, 47, 70, 90	38 (2%)

All (633) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103	ALA	7.4
1	G	157	VAL	7.2
1	E	176	THR	6.4
1	E	152	VAL	6.3
1	C	152	VAL	6.0
1	A	89	TRP	6.0
1	G	127	ALA	5.8
1	E	92[A]	SER	5.8
1	C	29	GLY	5.8
1	G	89	TRP	5.8
1	A	220	PRO	5.6
1	H	228	TYR	5.5
1	A	18	VAL	5.4
1	G	219	LEU	5.3
1	E	150[A]	ASP	5.3
1	A	98	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	100	ILE	5.2
1	G	155	GLY	5.1
1	A	197	ILE	5.0
1	C	100	ILE	5.0
1	E	123	VAL	4.9
1	A	10	ILE	4.8
1	C	58	THR	4.8
1	C	123	VAL	4.8
1	G	207	VAL	4.8
1	A	25	ILE	4.8
1	C	36	GLY	4.8
1	C	139	TRP	4.7
1	A	17	ALA	4.7
1	A	104	THR	4.7
1	C	197	ILE	4.7
1	C	219	LEU	4.7
1	H	227	LEU	4.7
1	A	69	ALA	4.7
1	G	150	ASP	4.7
1	G	10	ILE	4.6
1	A	53	ALA	4.6
1	B	220	PRO	4.6
1	E	220	PRO	4.6
1	G	129	GLY	4.5
1	G	95	TYR	4.5
1	E	183	VAL	4.5
1	E	100	ILE	4.5
1	C	177	TYR	4.4
1	E	87	TYR	4.4
1	A	101	CYS	4.4
1	A	99	GLY	4.4
1	E	125	PHE	4.3
1	A	60	VAL	4.3
1	A	92[A]	SER	4.3
1	A	97	ASP	4.3
1	E	75	ILE	4.3
1	A	51	PRO	4.2
1	A	126	PRO	4.2
1	H	220	PRO	4.2
1	A	57	LEU	4.2
1	G	139	TRP	4.2
1	C	173[A]	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	54	TYR	4.2
1	B	224	MET	4.2
1	A	163	LEU	4.2
1	C	101	CYS	4.1
1	C	25	ILE	4.1
1	E	76	VAL	4.1
1	B	229	LYS	4.1
1	E	24	ALA	4.1
1	E	12	LEU	4.1
1	A	125	PHE	4.1
1	E	173[A]	PHE	4.1
1	C	215	ALA	4.1
1	A	44	VAL	4.0
1	C	69	ALA	4.0
1	C	116	TYR	4.0
1	H	224	MET	4.0
1	A	42	LEU	4.0
1	A	191	VAL	4.0
1	E	17	ALA	4.0
1	G	60	VAL	4.0
1	G	44	VAL	4.0
1	E	186	PRO	4.0
1	E	166	GLY	4.0
1	A	34	PHE	4.0
1	A	173	PHE	4.0
1	G	34	PHE	4.0
1	E	5	LYS	3.9
1	E	181	LYS	3.9
1	A	182	VAL	3.9
1	A	48	GLY	3.9
1	E	151	GLY	3.9
1	C	127	ALA	3.9
1	E	167	GLY	3.9
1	E	58	THR	3.8
1	C	67	VAL	3.8
1	C	68	PHE	3.8
1	E	23	PHE	3.8
1	H	222	GLN	3.8
1	E	147	TYR	3.8
1	C	30	LEU	3.8
1	F	220	PRO	3.8
1	A	103	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	79	PHE	3.8
1	G	118	ILE	3.8
1	A	123	VAL	3.8
1	G	123	VAL	3.8
1	C	131	VAL	3.7
1	A	68	PHE	3.7
1	G	72	PRO	3.7
1	A	4	ILE	3.7
1	C	34	PHE	3.7
1	E	153	LEU	3.7
1	A	56	ILE	3.7
1	G	137	VAL	3.7
1	A	166	GLY	3.7
1	D	220	PRO	3.7
1	E	89	TRP	3.7
1	G	12	LEU	3.6
1	C	212	HIS	3.6
1	A	71	TYR	3.6
1	A	67	VAL	3.6
1	A	61	PHE	3.6
1	E	219	LEU	3.6
1	A	204	TYR	3.6
1	C	195	ILE	3.6
1	E	182	VAL	3.6
1	C	79	PHE	3.6
1	G	173[A]	PHE	3.6
1	A	122	GLY	3.6
1	C	10	ILE	3.6
1	C	75	ILE	3.6
1	G	104	THR	3.6
1	G	57	LEU	3.6
1	E	218	GLY	3.5
1	E	197	ILE	3.5
1	G	107	ILE	3.5
1	A	79	PHE	3.5
1	A	219	LEU	3.5
1	E	30	LEU	3.5
1	A	6	PRO	3.5
1	E	67	VAL	3.5
1	G	159[A]	GLU	3.5
1	E	210	HIS	3.5
1	G	21[A]	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	95	TYR	3.5
1	A	169	TYR	3.5
1	C	169	TYR	3.5
1	C	60	VAL	3.5
1	C	146	LEU	3.5
1	E	209	LEU	3.5
1	G	17	ALA	3.5
1	G	153	LEU	3.5
1	C	176	THR	3.4
1	A	65	ASN	3.4
1	E	78	TYR	3.4
1	A	139	TRP	3.4
1	E	83	PHE	3.4
1	G	215	ALA	3.4
1	G	73	GLU	3.4
1	E	169	TYR	3.4
1	G	169	TYR	3.4
1	C	107	ILE	3.4
1	A	207	VAL	3.4
1	C	18	VAL	3.4
1	E	68	PHE	3.4
1	C	102	ASN	3.4
1	E	102	ASN	3.4
1	G	158	ASN	3.4
1	C	104	THR	3.4
1	E	187	ASP	3.4
1	G	25	ILE	3.4
1	H	223	ALA	3.4
1	A	102	ASN	3.4
1	A	146	LEU	3.4
1	C	11	LYS	3.3
1	G	5	LYS	3.3
1	G	138	LYS	3.3
1	C	142	SER	3.3
1	C	209	LEU	3.3
1	E	146	LEU	3.3
1	C	72	PRO	3.3
1	E	54	TYR	3.3
1	A	76	VAL	3.3
1	E	60	VAL	3.3
1	C	214	GLU	3.3
1	A	153	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	57	LEU	3.3
1	A	86	GLY	3.3
1	C	166	GLY	3.3
1	G	151	GLY	3.3
1	G	88	SER	3.3
1	G	87	TYR	3.3
1	E	195	ILE	3.3
1	G	35	GLU	3.3
1	G	197	ILE	3.3
1	A	131	VAL	3.3
1	C	191	VAL	3.3
1	E	21	HIS	3.3
1	G	152	VAL	3.3
1	E	59	THR	3.3
1	E	175	THR	3.3
1	E	6	PRO	3.3
1	G	126	PRO	3.3
1	C	122	GLY	3.3
1	E	16	GLY	3.3
1	A	11	LYS	3.2
1	A	100	ILE	3.2
1	A	116	TYR	3.2
1	G	179	ALA	3.2
1	C	182	VAL	3.2
1	G	131	VAL	3.2
1	E	22	PRO	3.2
1	C	71	TYR	3.2
1	C	97	ASP	3.2
1	A	58	THR	3.2
1	E	57	LEU	3.2
1	E	90	GLU	3.2
1	A	52	PHE	3.2
1	C	99	GLY	3.2
1	C	120	PHE	3.2
1	E	178	LYS	3.2
1	G	125	PHE	3.2
1	E	56	ILE	3.2
1	C	78	TYR	3.2
1	A	183	VAL	3.2
1	C	183	VAL	3.2
1	C	207	VAL	3.2
1	A	50	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLY	3.2
1	A	190	PHE	3.2
1	E	190	PHE	3.2
1	H	225	ASP	3.2
1	A	124	ASN	3.1
1	C	103	ALA	3.1
1	G	213	ALA	3.1
1	A	30	LEU	3.1
1	A	148	VAL	3.1
1	A	218	GLY	3.1
1	E	99	GLY	3.1
1	E	40	MET	3.1
1	A	118	ILE	3.1
1	B	4	ILE	3.1
1	A	16	GLY	3.1
1	A	161	LEU	3.1
1	A	150[A]	ASP	3.1
1	G	106	ASP	3.1
1	C	94	ASN	3.1
1	G	210	HIS	3.1
1	C	118	ILE	3.1
1	C	114	TYR	3.1
1	G	177	TYR	3.1
1	G	76	VAL	3.1
1	G	183	VAL	3.1
1	A	174	LYS	3.1
1	A	151	GLY	3.1
1	G	218	GLY	3.1
1	A	121	ASP	3.0
1	E	107	ILE	3.0
1	C	12	LEU	3.0
1	E	95	TYR	3.0
1	E	177	TYR	3.0
1	A	49	PRO	3.0
1	C	17	ALA	3.0
1	C	185	LEU	3.0
1	G	209	LEU	3.0
1	G	94	ASN	3.0
1	A	23	PHE	3.0
1	C	83	PHE	3.0
1	E	61	PHE	3.0
1	C	175	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	130	PRO	3.0
1	C	160	ALA	3.0
1	E	14	MET	3.0
1	A	158	ASN	3.0
1	E	10	ILE	3.0
1	G	50	LEU	3.0
1	G	185	LEU	3.0
1	A	137	VAL	3.0
1	C	95	TYR	3.0
1	E	116	TYR	3.0
1	E	131	VAL	3.0
1	G	216	HIS	3.0
1	A	59	THR	3.0
1	G	43	LYS	3.0
1	G	175	THR	3.0
1	C	65	ASN	3.0
1	B	227	LEU	2.9
1	A	28	VAL	2.9
1	C	28	VAL	2.9
1	E	48	GLY	2.9
1	A	120	PHE	2.9
1	A	132	MET	2.9
1	A	160	ALA	2.9
1	E	171	CYS	2.9
1	G	24	ALA	2.9
1	C	56	ILE	2.9
1	D	100	ILE	2.9
1	E	174	LYS	2.9
1	C	150	ASP	2.9
1	A	157	VAL	2.9
1	E	191	VAL	2.9
1	G	141	PRO	2.9
1	G	186	PRO	2.9
1	C	190	PHE	2.9
1	E	139	TRP	2.9
1	C	201	ASP	2.9
1	E	164	GLU	2.9
1	C	59	THR	2.9
1	E	165	GLY	2.9
1	G	22	PRO	2.9
1	A	37	LYS	2.9
1	A	164	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	153	LEU	2.9
1	C	163	LEU	2.9
1	C	44	VAL	2.8
1	C	125	PHE	2.8
1	A	159	GLU	2.8
1	E	88	SER	2.8
1	G	39	SER	2.8
1	C	165	GLY	2.8
1	E	86	GLY	2.8
1	G	176	THR	2.8
1	C	76	VAL	2.8
1	G	33	PRO	2.8
1	G	174	LYS	2.8
1	C	54	TYR	2.8
1	E	179	ALA	2.8
1	G	52	PHE	2.8
1	E	184	GLN	2.8
1	A	107	ILE	2.8
1	H	4	ILE	2.8
1	C	159	GLU	2.8
1	C	220	PRO	2.8
1	E	159[A]	GLU	2.8
1	G	18	VAL	2.8
1	A	19	ASN	2.8
1	E	91	ARG	2.8
1	E	20	GLY	2.8
1	G	109	LEU	2.8
1	G	146	LEU	2.8
1	G	130	PRO	2.8
1	E	207	VAL	2.8
1	G	28	VAL	2.8
1	G	82	SER	2.7
1	G	54	TYR	2.7
1	G	114	TYR	2.7
1	C	105	ASN	2.7
1	C	23	PHE	2.7
1	G	98	GLY	2.7
1	H	226	GLU	2.7
1	G	67	VAL	2.7
1	C	89	TRP	2.7
1	G	74	ASN	2.7
1	A	78	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	117	GLU	2.7
1	E	127	ALA	2.7
1	E	188	TYR	2.7
1	G	160	ALA	2.7
1	E	216	HIS	2.7
1	C	20	GLY	2.7
1	F	165	GLY	2.7
1	E	79	PHE	2.7
1	G	161	LEU	2.7
1	E	199	SER	2.7
1	G	128	ASN	2.7
1	D	127	ALA	2.7
1	B	228	TYR	2.7
1	C	204	TYR	2.7
1	E	204	TYR	2.7
1	H	165	GLY	2.7
1	E	120	PHE	2.7
1	G	83	PHE	2.7
1	E	143	THR	2.7
1	A	22	PRO	2.7
1	A	72	PRO	2.7
1	A	162	SER	2.7
1	A	145	LYS	2.7
1	E	74	ASN	2.7
1	G	75	ILE	2.7
1	G	124	ASN	2.7
1	C	137	VAL	2.7
1	E	18	VAL	2.7
1	C	24	ALA	2.6
1	C	155	GLY	2.6
1	E	155	GLY	2.6
1	A	93	MET	2.6
1	B	225	ASP	2.6
1	E	34	PHE	2.6
1	A	202	LYS	2.6
1	E	51	PRO	2.6
1	E	130	PRO	2.6
1	A	94	ASN	2.6
1	E	185	LEU	2.6
1	A	200	HIS	2.6
1	A	47	GLY	2.6
1	C	167	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	157	VAL	2.6
1	A	215	ALA	2.6
1	C	213	ALA	2.6
1	F	7	ASP	2.6
1	C	211	GLU	2.6
1	G	211	GLU	2.6
1	C	147	TYR	2.6
1	E	180	LYS	2.6
1	G	102	ASN	2.6
1	C	51	PRO	2.6
1	G	84	PRO	2.6
1	C	194	HIS	2.6
1	A	12	LEU	2.6
1	C	42	LEU	2.6
1	A	167	GLY	2.6
1	E	27	GLY	2.6
1	G	165	GLY	2.6
1	A	152	VAL	2.6
1	G	69	ALA	2.6
1	A	128	ASN	2.6
1	G	58	THR	2.6
1	A	147	TYR	2.6
1	E	194	HIS	2.6
1	E	49	PRO	2.6
1	G	190	PHE	2.6
1	E	50	LEU	2.6
1	C	132	MET	2.6
1	C	106	ASP	2.6
1	C	151	GLY	2.6
1	E	122	GLY	2.6
1	C	157	VAL	2.6
1	E	28	VAL	2.6
1	E	215	ALA	2.6
1	A	114	TYR	2.5
1	C	38	GLN	2.5
1	E	93	MET	2.5
1	G	68	PHE	2.5
1	G	93	MET	2.5
1	E	25	ILE	2.5
1	A	127	ALA	2.5
1	E	205	SER	2.5
1	C	108	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	143	THR	2.5
1	G	214	GLU	2.5
1	A	87	TYR	2.5
1	E	71	TYR	2.5
1	A	198	LYS	2.5
1	E	145	LYS	2.5
1	C	109	LEU	2.5
1	A	155	GLY	2.5
1	C	158	ASN	2.5
1	C	210	HIS	2.5
1	B	226	GLU	2.5
1	C	148	VAL	2.5
1	G	7	ASP	2.5
1	E	114	TYR	2.5
1	G	204	TYR	2.5
1	A	109	LEU	2.5
1	A	209	LEU	2.5
1	C	16	GLY	2.5
1	E	129	GLY	2.5
1	G	105	ASN	2.5
1	G	119	ARG	2.5
1	G	194	HIS	2.5
1	G	115	ILE	2.5
1	G	162	SER	2.5
1	C	14	MET	2.5
1	G	103	ALA	2.5
1	G	59	THR	2.5
1	A	130	PRO	2.5
1	G	6	PRO	2.5
1	E	66	ARG	2.4
1	G	111	GLY	2.4
1	G	167	GLY	2.4
1	H	166	GLY	2.4
1	C	74	ASN	2.4
1	E	19	ASN	2.4
1	G	71	TYR	2.4
1	G	147	TYR	2.4
1	A	21	HIS	2.4
1	E	109	LEU	2.4
1	F	219	LEU	2.4
1	A	39	SER	2.4
1	A	119	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	27	GLY	2.4
1	G	42	LEU	2.4
1	A	176	THR	2.4
1	G	136	THR	2.4
1	G	191	VAL	2.4
1	A	27	GLY	2.4
1	G	122	GLY	2.4
1	H	21	HIS	2.4
1	G	14	MET	2.4
1	G	92	SER	2.4
1	G	134	LYS	2.4
1	A	177	TYR	2.4
1	B	150	ASP	2.4
1	E	52	PHE	2.4
1	E	53	ALA	2.4
1	C	6	PRO	2.4
1	C	189	HIS	2.4
1	G	8	MET	2.4
1	A	45	LYS	2.4
1	C	9	LYS	2.4
1	C	174	LYS	2.4
1	E	119	ARG	2.3
1	G	116	TYR	2.3
1	G	188	TYR	2.3
1	E	160	ALA	2.3
1	A	33	PRO	2.3
1	A	84	PRO	2.3
1	A	216	HIS	2.3
1	C	168	HIS	2.3
1	G	208	ASN	2.3
1	F	166	GLY	2.3
1	A	199[A]	SER	2.3
1	C	205	SER	2.3
1	E	42	LEU	2.3
1	E	133	GLN	2.3
1	D	21	HIS	2.3
1	E	124	ASN	2.3
1	G	212	HIS	2.3
1	C	84	PRO	2.3
1	G	132	MET	2.3
1	A	66	ARG	2.3
1	G	117	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	108	THR	2.3
1	C	93	MET	2.3
1	E	70	LYS	2.3
1	G	23	PHE	2.3
1	C	98	GLY	2.3
1	G	170	ARG	2.3
1	G	195	ILE	2.3
1	C	133	GLN	2.3
1	F	152	VAL	2.3
1	E	158	ASN	2.3
1	E	189	HIS	2.3
1	E	193	HIS	2.3
1	A	136	THR	2.3
1	E	163	LEU	2.3
1	C	33	PRO	2.2
1	E	98	GLY	2.2
1	E	217	SER	2.2
1	E	148	VAL	2.2
1	C	124	ASN	2.2
1	A	14	MET	2.2
1	G	145	LYS	2.2
1	A	135	ARG	2.2
1	G	171	CYS	2.2
1	A	214	GLU	2.2
1	A	142	SER	2.2
1	A	24	ALA	2.2
1	E	115	ILE	2.2
1	A	189	HIS	2.2
1	A	194	HIS	2.2
1	C	119	ARG	2.2
1	G	90	GLU	2.2
1	E	101	CYS	2.2
1	E	142	SER	2.2
1	G	61	PHE	2.2
1	G	56	ILE	2.2
1	E	11	LYS	2.2
1	E	128	ASN	2.2
1	G	168	HIS	2.2
1	A	91	ARG	2.2
1	A	96	GLU	2.2
1	F	35	GLU	2.2
1	G	140	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	161	LEU	2.2
1	G	29	GLY	2.2
1	H	219	LEU	2.2
1	C	141	PRO	2.2
1	C	53	ALA	2.2
1	A	32	LYS	2.2
1	E	154	LYS	2.2
1	B	173[A]	PHE	2.1
1	E	94	ASN	2.1
1	G	65	ASN	2.1
1	G	120	PHE	2.1
1	C	188	TYR	2.1
1	G	78	TYR	2.1
1	A	195	ILE	2.1
1	A	201	ASP	2.1
1	E	172	ASP	2.1
1	A	171	CYS	2.1
1	E	126	PRO	2.1
1	A	73	GLU	2.1
1	E	132	MET	2.1
1	F	21	HIS	2.1
1	G	15	GLU	2.1
1	C	128	ASN	2.1
1	A	83	PHE	2.1
1	A	156	ASP	2.1
1	B	166	GLY	2.1
1	E	44	VAL	2.1
1	C	193	HIS	2.1
1	C	206	ASN	2.1
1	E	69	ALA	2.1
1	E	81	GLN	2.1
1	E	121	ASP	2.1
1	G	172	ASP	2.1
1	C	135	ARG	2.1
1	D	135	ARG	2.1
1	C	136	THR	2.1
1	A	20	GLY	2.1
1	G	16	GLY	2.1
1	C	8	MET	2.1
1	G	189	HIS	2.1
1	G	19	ASN	2.1
1	C	126	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	2.1
1	A	149	ARG	2.1
1	A	170	ARG	2.1
1	E	170	ARG	2.1
1	A	46	GLU	2.0
1	E	82	SER	2.0
1	E	118	ILE	2.0
1	G	217	SER	2.0
1	A	40	MET	2.0
1	E	104	THR	2.0
1	C	21	HIS	2.0
1	E	212	HIS	2.0
1	G	86	GLY	2.0
1	G	200	HIS	2.0
1	H	158	ASN	2.0
1	E	33	PRO	2.0
1	G	148	VAL	2.0
1	A	185	LEU	2.0
1	C	5	LYS	2.0
1	C	178	LYS	2.0
1	G	40	MET	2.0
1	A	31	GLY	2.0
1	A	175	THR	2.0
1	E	47	GLY	2.0
1	G	99	GLY	2.0
1	G	133	GLN	2.0
1	C	87	TYR	2.0
1	E	65	ASN	2.0
1	E	105	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GYC	A	63	21/22	0.77	0.19	36,47,51,52	0
1	GYC	E	63	21/22	0.84	0.17	49,51,52,61	0
1	GYC	C	63	21/22	0.86	0.17	49,50,53,56	0
1	GYC	G	63	21/22	0.86	0.14	47,51,53,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GYC	B	63	21/22	0.94	0.07	16,20,24,25	0
1	GYC	D	63	21/22	0.94	0.10	16,20,22,23	0
1	GYC	F	63	21/22	0.95	0.08	17,21,23,24	0
1	GYC	H	63	21/22	0.96	0.07	16,19,22,23	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.