Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 08:11 AM EST

PDB ID	:	7RRK
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:

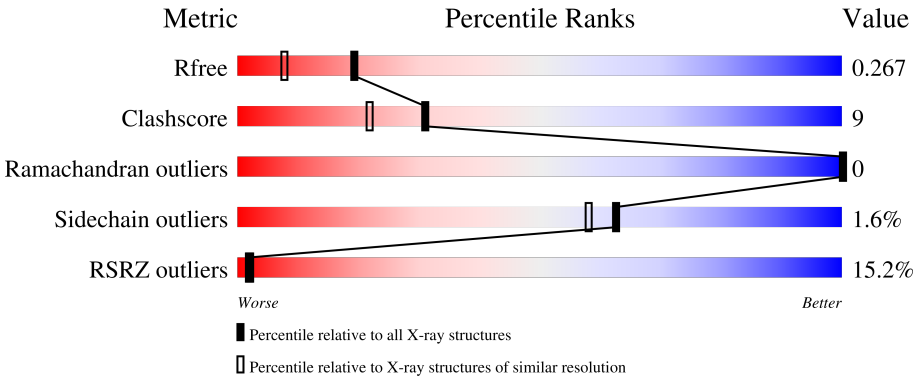
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 <=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	28% 67% 16% • 16%
1	B	255	2% 79% 7% • 13%
1	C	255	21% 67% 15% • 16%
1	D	255	% 77% 7% 16%
1	E	255	23% 67% 15% • 16%

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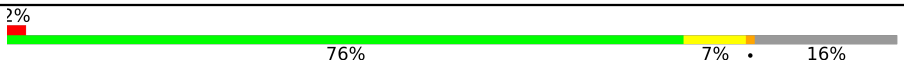
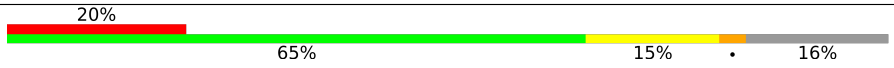
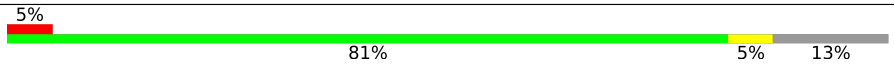
Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	

2 Entry composition (i)

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.

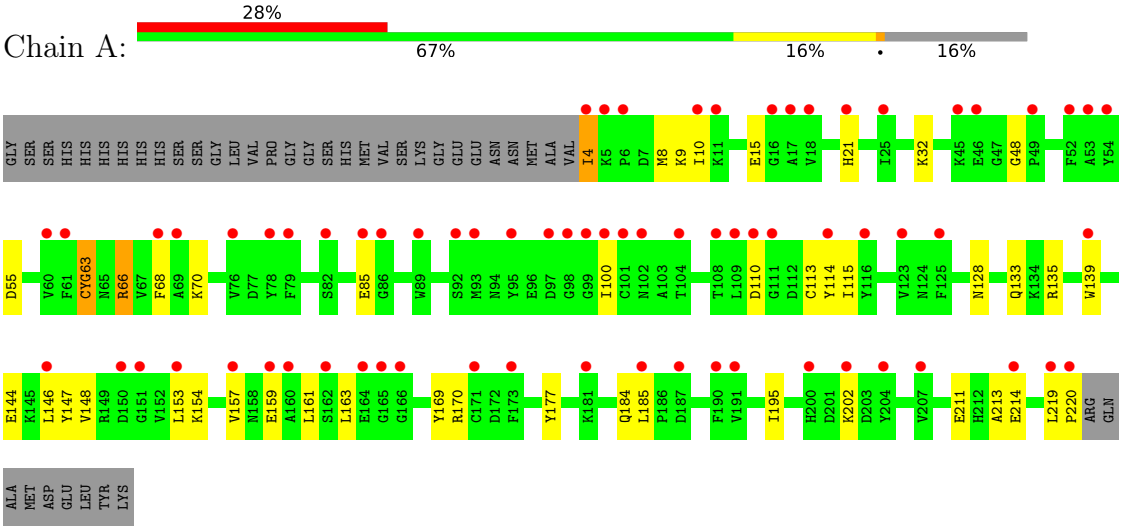
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	223	Total O 223 223	0	0
2	C	108	Total O 108 108	0	0
2	D	215	Total O 215 215	0	0
2	E	101	Total O 101 101	0	0
2	F	197	Total O 197 197	0	0
2	G	102	Total O 102 102	0	0
2	H	203	Total O 203 203	0	0

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.

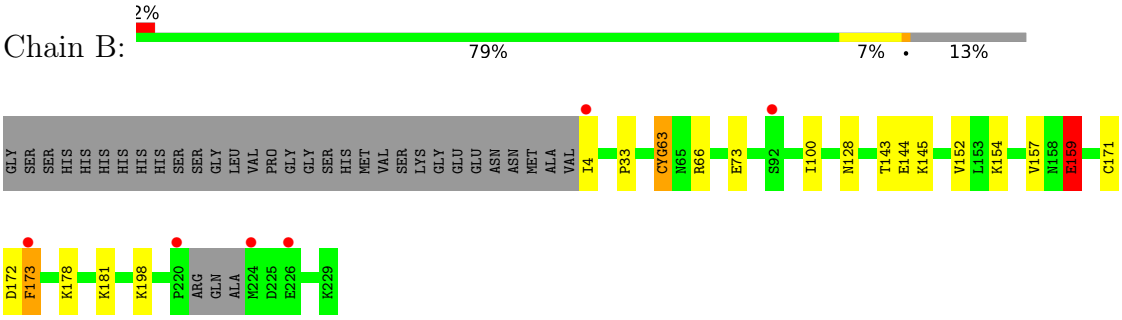
• Molecule 1: Fluorescent protein Dronpa

Chain A:



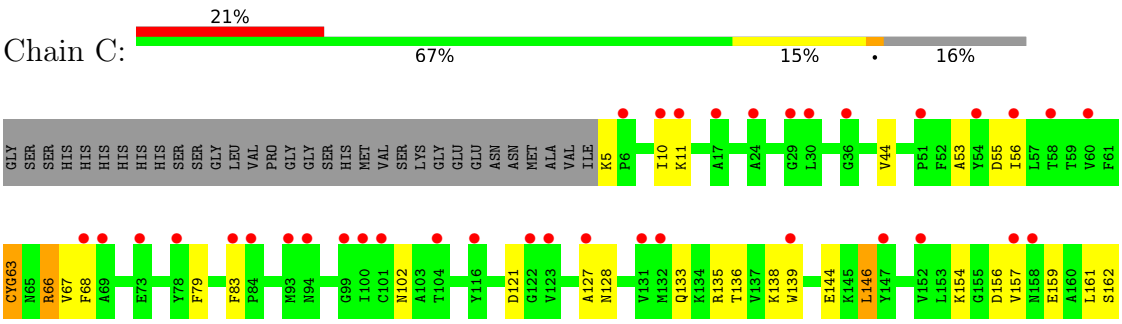
• Molecule 1: Fluorescent protein Dronpa

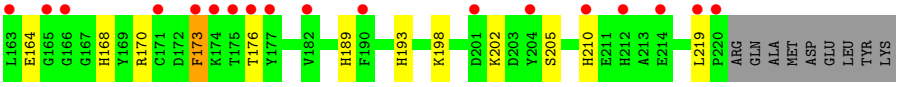
Chain B:



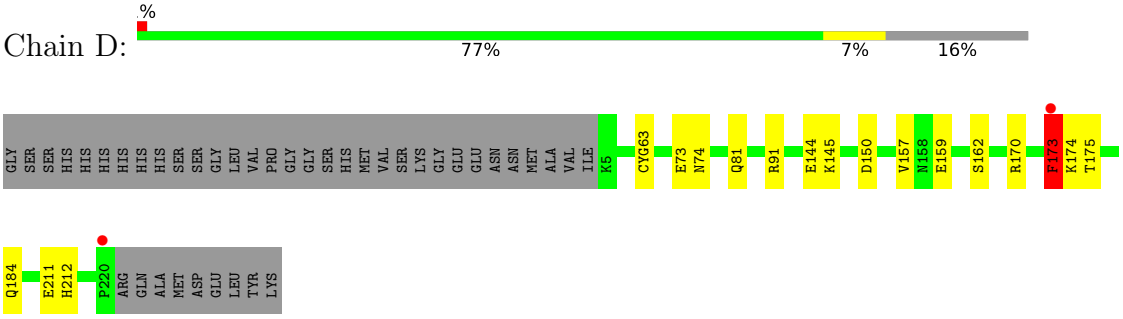
• Molecule 1: Fluorescent protein Dronpa

Chain C:

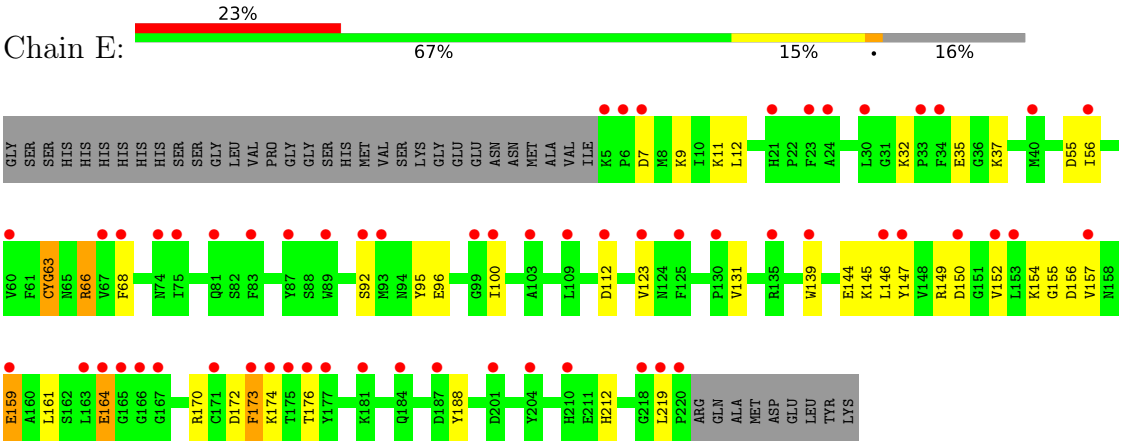




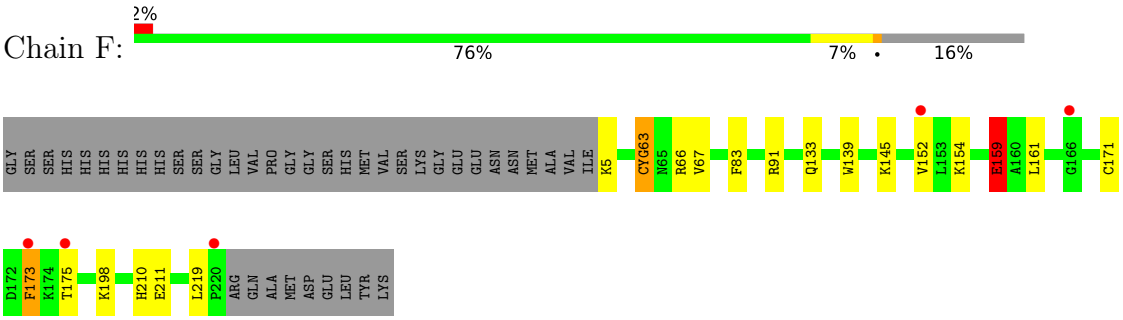
• Molecule 1: Fluorescent protein Dronpa



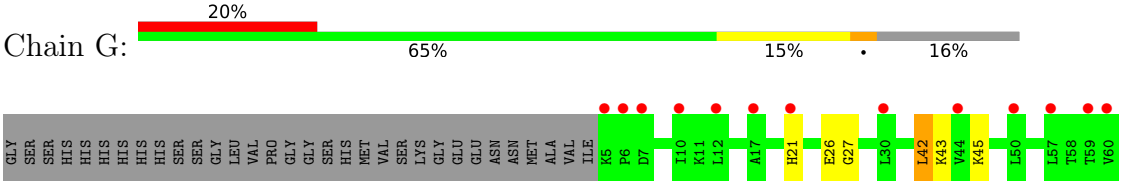
• Molecule 1: Fluorescent protein Dronpa

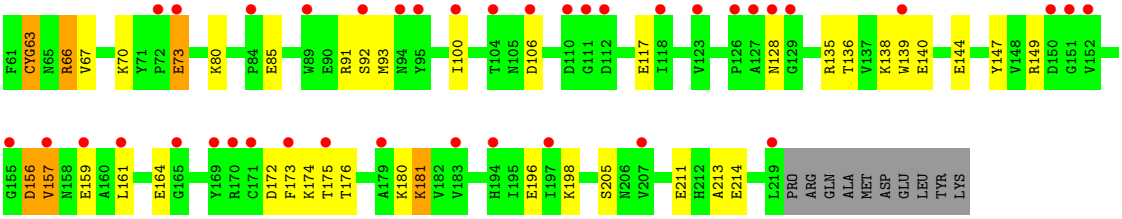


• Molecule 1: Fluorescent protein Dronpa

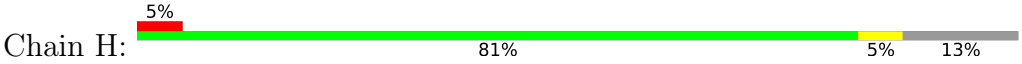


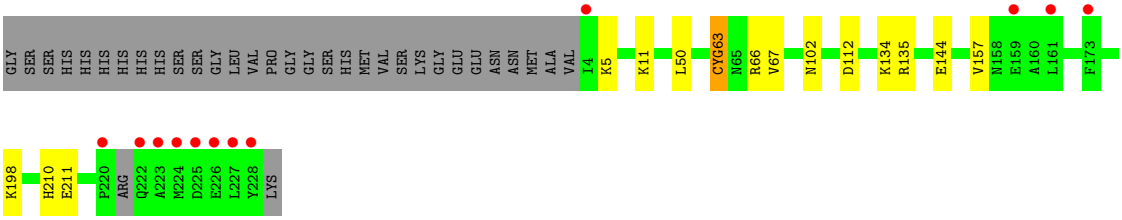
• Molecule 1: Fluorescent protein Dronpa





• Molecule 1: Fluorescent protein Dronpa





4 Data and refinement statistics (i)

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 39.28 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (37.73-1.93) 85.8 (39.28-1.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	1/1775 (0.1%)	0.56	0/2398
1	B	0.52	4/1850 (0.2%)	0.63	2/2496 (0.1%)
1	C	0.58	0/1771	0.68	2/2391 (0.1%)
1	D	0.57	2/1822 (0.1%)	0.64	0/2458
1	E	0.59	1/1778 (0.1%)	0.70	2/2403 (0.1%)
1	F	0.56	2/1785 (0.1%)	0.64	2/2410 (0.1%)
1	G	0.63	0/1788	0.72	0/2414
1	H	0.49	0/1842	0.60	0/2486
All	All	0.55	10/14411 (0.1%)	0.65	8/19456 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	173[A]	PHE	CA-C	6.28	1.69	1.52
1	D	173[B]	PHE	CA-C	6.28	1.69	1.52
1	B	173[A]	PHE	CA-C	5.44	1.67	1.52
1	B	173[B]	PHE	CA-C	5.44	1.67	1.52
1	A	4	ILE	C-N	-5.37	1.21	1.34
1	B	159[A]	GLU	C-O	5.10	1.33	1.23
1	B	159[B]	GLU	C-O	5.10	1.33	1.23
1	E	164	GLU	CD-OE2	5.10	1.31	1.25
1	F	159[A]	GLU	C-O	5.03	1.32	1.23
1	F	159[B]	GLU	C-O	5.03	1.32	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	173[A]	PHE	CB-CA-C	-6.41	97.59	110.40
1	C	173[B]	PHE	CB-CA-C	-6.41	97.59	110.40
1	B	173[A]	PHE	N-CA-CB	-5.92	99.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173[B]	PHE	N-CA-CB	-5.92	99.94	110.60
1	F	173[A]	PHE	CB-CA-C	-5.35	99.69	110.40
1	F	173[B]	PHE	CB-CA-C	-5.35	99.69	110.40
1	E	173[A]	PHE	CA-C-O	5.19	131.00	120.10
1	E	173[B]	PHE	CA-C-O	5.19	131.00	120.10

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	1744	0	1657	41	0
1	B	1807	0	1722	15	0
1	C	1739	0	1657	37	0
1	D	1775	0	1708	19	0
1	E	1743	0	1645	47	0
1	F	1750	0	1670	24	0
1	G	1747	0	1665	68	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	6	0
2	D	215	0	0	4	0
2	E	101	0	0	10	0
2	F	197	0	0	5	0
2	G	102	0	0	5	0
2	H	203	0	0	5	0
All	All	15363	0	13439	250	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 (250) 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: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
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:A:202:LYS:NZ	2:A:303:HOH:O	2.23	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: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:F:154:LYS:NZ	2:F:305:HOH:O	2.27	0.67
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:B:100:ILE:HD13	2:H:354:HOH:O	1.93	0.66
1:G:73:GLU:H	1:G:73:GLU:CD	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:VAL:HG23	1:G:173[A]:PHE:CB	2.21	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:B:198:LYS:NZ	2:B:309:HOH:O	2.31	0.63
1:E:146:LEU:CD2	1:E:155:GLY:HA2	2.30	0.61
1:E:145:LYS:C	1:E:146:LEU:HD23	2.20	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: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:HG3	1:F:175[B]:THR:HG22	1.83	0.60
1:F:91:ARG:HE	1:F:175[B]:THR:CG2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:ILE:HG13	1:A:8:MET:CE	2.38	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
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:73:GLU:CD	1:D:73:GLU:H	2.13	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:C:202:LYS:NZ	2:C:311:HOH:O	2.41	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:136:THR:HB	1:C:161:LEU:HD22	1.94	0.50
1:E:9:LYS:HZ1	1:E:112:ASP:CG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:144:GLU:CD	1:E:146:LEU:HD21	2.33	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:G:93:MET:HG2	1:G:173[A]:PHE:CD1	2.49	0.48
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: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: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:5:LYS:NZ	2:F:307:HOH:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:91:ARG:CG	1:F:175[B]:THR:HG22	2.47	0.45
1:G:196:GLU:HB2	1:G:198:LYS:HZ2	1.81	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
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: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:A:4:ILE:HG13	1:A:8:MET:HE2	2.00	0.42
1:C:157:VAL:O	1:C:173[B]:PHE:HB3	2.19	0.42
1:B:143:THR:H	1:F:145:LYS:HZ3	1.65	0.42
1:A:153:LEU:HB3	1:A:177:TYR:HB2	2.01	0.42
1:D:73:GLU:CD	1:D:73:GLU:N	2.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:LYS:N	1:E:37:LYS:HD2	2.36	0.41
1:G:159[B]:GLU:CD	1:G:173[B]:PHE:HD2	2.24	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
1:G:106:ASP:OD1	1:G:180:LYS:NZ	2.31	0.41
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:A:128:ASN:HA	1:A:133:GLN:CD	2.41	0.40
1:A:170:ARG:HH11	1:E:147:TYR:HH	1.68	0.40
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:G:175:THR:HG22	1:G:176:THR:N	2.35	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 (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	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
All	All	1721/2040 (84%)	1700 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	186/217 (86%)	185 (100%)	1 (0%)	88	89
1	B	192/217 (88%)	186 (97%)	6 (3%)	40	30
1	C	185/217 (85%)	182 (98%)	3 (2%)	62	58
1	D	191/217 (88%)	186 (97%)	5 (3%)	46	37
1	E	185/217 (85%)	182 (98%)	3 (2%)	62	58
1	F	187/217 (86%)	184 (98%)	3 (2%)	62	58
1	G	186/217 (86%)	180 (97%)	6 (3%)	39	29
1	H	190/217 (88%)	188 (99%)	2 (1%)	73	72
All	All	1502/1736 (86%)	1473 (98%)	29 (2%)	62	51

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	B	145	LYS

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Mol	Chain	Res	Type
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	66	ARG
1	C	146	LEU
1	D	145	LYS
1	D	159[A]	GLU
1	D	159[B]	GLU
1	D	173[A]	PHE
1	D	173[B]	PHE
1	E	66	ARG
1	E	159[A]	GLU
1	E	159[B]	GLU
1	F	159[A]	GLU
1	F	159[B]	GLU
1	F	211	GLU
1	G	42	LEU
1	G	66	ARG
1	G	73	GLU
1	G	156	ASP
1	G	157	VAL
1	G	181	LYS
1	H	67	VAL
1	H	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	158	ASN
1	E	158	ASN
1	E	208	ASN
1	E	210	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	E	63	1	22,22,23	1.15	1 (4%)	26,30,32	2.48	7 (26%)
1	GYC	A	63	1	22,22,23	1.18	1 (4%)	26,30,32	2.46	8 (30%)
1	GYC	C	63	1	22,22,23	1.08	1 (4%)	26,30,32	2.41	7 (26%)
1	GYC	B	63	1	22,22,23	1.12	1 (4%)	26,30,32	2.44	5 (19%)
1	GYC	F	63	1	22,22,23	1.07	1 (4%)	26,30,32	2.26	6 (23%)
1	GYC	G	63	1	22,22,23	1.15	1 (4%)	26,30,32	2.48	8 (30%)
1	GYC	H	63	1	22,22,23	1.09	1 (4%)	26,30,32	2.45	6 (23%)
1	GYC	D	63	1	22,22,23	1.06	1 (4%)	26,30,32	2.20	7 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	E	63	1	-	3/9/29/30	0/2/2/2
1	GYC	A	63	1	-	5/9/29/30	0/2/2/2
1	GYC	C	63	1	-	3/9/29/30	0/2/2/2
1	GYC	B	63	1	-	3/9/29/30	0/2/2/2
1	GYC	F	63	1	-	3/9/29/30	0/2/2/2
1	GYC	G	63	1	-	3/9/29/30	0/2/2/2
1	GYC	H	63	1	-	3/9/29/30	0/2/2/2
1	GYC	D	63	1	-	3/9/29/30	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB2-CA2	4.74	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	GYC	CB2-CA2	4.48	1.38	1.35
1	G	63	GYC	CB2-CA2	4.45	1.38	1.35
1	C	63	GYC	CB2-CA2	4.17	1.38	1.35
1	B	63	GYC	CB2-CA2	4.15	1.38	1.35
1	H	63	GYC	CB2-CA2	4.08	1.38	1.35
1	F	63	GYC	CB2-CA2	3.93	1.38	1.35
1	D	63	GYC	CB2-CA2	3.85	1.38	1.35

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	63	GYC	O2-C2-CA2	-7.98	126.48	130.96
1	B	63	GYC	O2-C2-CA2	-7.47	126.76	130.96
1	G	63	GYC	O2-C2-CA2	-7.11	126.97	130.96
1	E	63	GYC	O2-C2-CA2	-7.10	126.97	130.96
1	C	63	GYC	O2-C2-CA2	-7.03	127.01	130.96
1	F	63	GYC	O2-C2-CA2	-6.89	127.09	130.96
1	A	63	GYC	O2-C2-CA2	-6.81	127.14	130.96
1	D	63	GYC	O2-C2-CA2	-6.75	127.17	130.96
1	E	63	GYC	C2-CA2-N2	-5.22	105.27	108.93
1	A	63	GYC	C2-CA2-N2	-5.20	105.29	108.93
1	G	63	GYC	C2-CA2-N2	-5.16	105.32	108.93
1	B	63	GYC	CA2-C2-N3	5.13	105.80	103.37
1	G	63	GYC	CA2-C2-N3	5.13	105.80	103.37
1	A	63	GYC	CA2-N2-C1	5.05	109.50	105.77
1	E	63	GYC	CA2-C2-N3	5.05	105.76	103.37
1	G	63	GYC	CA2-N2-C1	5.04	109.48	105.77
1	B	63	GYC	C2-CA2-N2	-4.99	105.44	108.93
1	E	63	GYC	CA2-N2-C1	4.98	109.44	105.77
1	C	63	GYC	C2-CA2-N2	-4.93	105.48	108.93
1	H	63	GYC	CA2-C2-N3	4.89	105.69	103.37
1	A	63	GYC	CA2-C2-N3	4.84	105.66	103.37
1	C	63	GYC	CA2-C2-N3	4.76	105.62	103.37
1	C	63	GYC	CA2-N2-C1	4.74	109.27	105.77
1	B	63	GYC	CA2-N2-C1	4.73	109.25	105.77
1	H	63	GYC	C2-CA2-N2	-4.52	105.77	108.93
1	H	63	GYC	CA2-N2-C1	4.31	108.95	105.77
1	F	63	GYC	C2-CA2-N2	-4.29	105.93	108.93
1	F	63	GYC	CA2-C2-N3	4.28	105.39	103.37
1	D	63	GYC	CA2-C2-N3	4.26	105.38	103.37
1	F	63	GYC	CA2-N2-C1	4.23	108.89	105.77
1	D	63	GYC	C2-CA2-N2	-4.19	106.00	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	GYC	CA2-N2-C1	4.02	108.74	105.77
1	A	63	GYC	CG2-CB2-CA2	-3.00	126.27	129.94
1	G	63	GYC	CG2-CB2-CA2	-2.66	126.68	129.94
1	C	63	GYC	CA1-CB1-SG1	-2.48	109.09	114.44
1	E	63	GYC	CA1-CB1-SG1	-2.46	109.13	114.44
1	F	63	GYC	O3-C3-CA3	-2.46	118.97	126.39
1	A	63	GYC	CA1-CB1-SG1	-2.40	109.28	114.44
1	D	63	GYC	CA1-CB1-SG1	-2.32	109.44	114.44
1	C	63	GYC	O3-C3-CA3	-2.31	119.42	126.39
1	H	63	GYC	O3-C3-CA3	-2.27	119.52	126.39
1	G	63	GYC	CA1-CB1-SG1	-2.26	109.56	114.44
1	F	63	GYC	CA1-CB1-SG1	-2.25	109.59	114.44
1	A	63	GYC	CB2-CA2-C2	2.22	124.93	122.28
1	E	63	GYC	CG2-CB2-CA2	-2.16	127.29	129.94
1	E	63	GYC	O3-C3-CA3	-2.16	119.87	126.39
1	H	63	GYC	CA1-CB1-SG1	-2.16	109.79	114.44
1	G	63	GYC	O3-C3-CA3	-2.11	120.01	126.39
1	A	63	GYC	O3-C3-CA3	-2.08	120.10	126.39
1	D	63	GYC	CG2-CB2-CA2	-2.07	127.41	129.94
1	B	63	GYC	O3-C3-CA3	-2.07	120.15	126.39
1	G	63	GYC	CB2-CA2-C2	2.05	124.73	122.28
1	D	63	GYC	O3-C3-CA3	-2.05	120.19	126.39
1	C	63	GYC	CG2-CB2-CA2	-2.02	127.47	129.94

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

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Mol	Chain	Res	Type	Atoms
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
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	E	63	GYC	1	0
1	A	63	GYC	2	0
1	C	63	GYC	2	0
1	B	63	GYC	1	0
1	F	63	GYC	1	0
1	G	63	GYC	1	0
1	H	63	GYC	1	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.60	71 (33%) 0 0	52, 60, 75, 89	0
1	B	220/255 (86%)	0.29	6 (2%) 54 57	19, 28, 45, 71	0
1	C	213/255 (83%)	1.61	54 (25%) 0 0	45, 57, 69, 84	0
1	D	213/255 (83%)	0.22	2 (0%) 84 85	16, 26, 42, 55	0
1	E	213/255 (83%)	1.63	59 (27%) 0 0	48, 59, 73, 90	0
1	F	213/255 (83%)	0.28	5 (2%) 60 63	18, 27, 44, 61	0
1	G	212/255 (83%)	1.58	52 (24%) 0 0	48, 59, 72, 77	0
1	H	221/255 (86%)	0.38	12 (5%) 25 29	18, 27, 46, 75	0
All	All	1719/2040 (84%)	0.94	261 (15%) 2 2	16, 49, 70, 90	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173[A]	PHE	6.0
1	E	173[A]	PHE	5.9
1	E	166	GLY	5.6
1	G	127	ALA	5.3
1	G	157	VAL	5.2
1	C	30	LEU	5.2
1	E	152	VAL	5.2
1	E	220	PRO	5.1
1	G	150	ASP	5.1
1	E	164	GLU	4.9
1	E	150[A]	ASP	4.7
1	G	173[A]	PHE	4.7
1	G	95	TYR	4.6
1	F	220	PRO	4.6
1	C	204	TYR	4.5
1	C	165	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	220	PRO	4.2
1	H	224	MET	4.2
1	A	220	PRO	4.2
1	B	224	MET	4.2
1	G	219	LEU	4.1
1	E	74	ASN	4.1
1	A	6	PRO	4.1
1	H	227	LEU	4.0
1	A	10	ILE	3.9
1	E	165	GLY	3.9
1	A	207	VAL	3.9
1	G	30	LEU	3.8
1	A	166	GLY	3.8
1	C	139	TRP	3.8
1	G	89	TRP	3.7
1	G	139	TRP	3.7
1	E	75	ILE	3.7
1	G	21[A]	HIS	3.7
1	G	112	ASP	3.7
1	H	228	TYR	3.6
1	G	60	VAL	3.6
1	G	151	GLY	3.6
1	E	176	THR	3.6
1	C	36	GLY	3.5
1	A	18	VAL	3.5
1	A	165	GLY	3.5
1	B	226	GLU	3.5
1	C	214	GLU	3.5
1	C	201	ASP	3.4
1	E	83	PHE	3.4
1	C	6	PRO	3.4
1	E	103	ALA	3.4
1	E	5	LYS	3.4
1	E	125	PHE	3.4
1	E	184	GLN	3.4
1	G	10	ILE	3.4
1	E	210	HIS	3.3
1	G	207	VAL	3.3
1	C	152	VAL	3.3
1	A	150[A]	ASP	3.2
1	E	219	LEU	3.2
1	G	179	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	100	ILE	3.2
1	G	155	GLY	3.2
1	H	173[A]	PHE	3.2
1	A	191	VAL	3.2
1	C	177	TYR	3.2
1	E	204	TYR	3.2
1	B	220	PRO	3.2
1	C	11	LYS	3.1
1	F	166	GLY	3.1
1	E	177	TYR	3.1
1	A	46	GLU	3.1
1	C	123	VAL	3.1
1	A	181	LYS	3.1
1	G	152	VAL	3.1
1	C	10	ILE	3.1
1	C	58	THR	3.1
1	G	170	ARG	3.0
1	C	73	GLU	3.0
1	C	219	LEU	3.0
1	E	174	LYS	3.0
1	C	175	THR	3.0
1	E	123	VAL	3.0
1	A	114	TYR	3.0
1	C	131	VAL	3.0
1	G	84	PRO	3.0
1	A	25	ILE	2.9
1	A	79	PHE	2.9
1	C	182	VAL	2.9
1	E	187	ASP	2.9
1	A	153	LEU	2.9
1	A	4	ILE	2.9
1	A	214	GLU	2.9
1	G	100	ILE	2.9
1	A	86	GLY	2.9
1	E	6	PRO	2.9
1	E	92[A]	SER	2.8
1	E	30	LEU	2.8
1	G	128	ASN	2.8
1	A	17	ALA	2.8
1	E	153	LEU	2.8
1	G	12	LEU	2.8
1	G	161	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	212	HIS	2.8
1	C	78	TYR	2.8
1	G	44	VAL	2.8
1	A	11	LYS	2.8
1	E	112	ASP	2.8
1	E	24	ALA	2.8
1	A	173	PHE	2.8
1	G	111	GLY	2.8
1	A	99	GLY	2.7
1	G	165	GLY	2.7
1	E	163	LEU	2.7
1	G	72	PRO	2.7
1	E	68	PHE	2.7
1	G	171	CYS	2.7
1	G	5	LYS	2.7
1	G	159[A]	GLU	2.7
1	A	92[A]	SER	2.7
1	A	185	LEU	2.7
1	G	50	LEU	2.7
1	C	84	PRO	2.7
1	E	175	THR	2.7
1	E	34	PHE	2.7
1	C	54	TYR	2.7
1	E	7	ASP	2.6
1	H	4	ILE	2.6
1	A	146	LEU	2.6
1	A	110	ASP	2.6
1	A	151	GLY	2.6
1	A	95	TYR	2.6
1	E	147	TYR	2.6
1	G	7	ASP	2.6
1	G	126	PRO	2.6
1	E	89	TRP	2.6
1	E	100	ILE	2.6
1	G	106	ASP	2.6
1	E	93	MET	2.6
1	D	220	PRO	2.6
1	B	173[A]	PHE	2.6
1	E	139	TRP	2.6
1	E	21	HIS	2.6
1	E	159[A]	GLU	2.6
1	A	204	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	29	GLY	2.6
1	H	220	PRO	2.6
1	A	60	VAL	2.6
1	A	52	PHE	2.5
1	G	92	SER	2.5
1	C	94	ASN	2.5
1	A	171	CYS	2.5
1	G	123	VAL	2.5
1	A	85	GLU	2.5
1	E	201	ASP	2.5
1	C	60	VAL	2.5
1	A	125	PHE	2.5
1	C	83	PHE	2.5
1	A	45	LYS	2.5
1	E	40	MET	2.5
1	A	101	CYS	2.5
1	G	94	ASN	2.5
1	C	157	VAL	2.5
1	D	173[A]	PHE	2.5
1	A	164	GLU	2.5
1	C	24	ALA	2.4
1	G	17	ALA	2.4
1	G	57	LEU	2.4
1	E	181	LYS	2.4
1	A	21	HIS	2.4
1	H	225	ASP	2.4
1	H	226	GLU	2.4
1	A	157	VAL	2.4
1	C	147	TYR	2.4
1	G	169	TYR	2.4
1	C	176	THR	2.4
1	A	123	VAL	2.4
1	F	152	VAL	2.4
1	A	108	THR	2.4
1	A	100	ILE	2.4
1	B	4	ILE	2.4
1	C	210	HIS	2.4
1	G	197	ILE	2.4
1	A	68	PHE	2.4
1	A	187	ASP	2.4
1	F	175[A]	THR	2.4
1	E	33	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	56	ILE	2.4
1	A	78	TYR	2.3
1	A	98	GLY	2.3
1	C	101	CYS	2.3
1	E	157	VAL	2.3
1	E	171	CYS	2.3
1	A	53	ALA	2.3
1	A	109	LEU	2.3
1	A	89	TRP	2.3
1	E	56	ILE	2.3
1	E	60	VAL	2.3
1	C	122	GLY	2.3
1	C	127	ALA	2.3
1	C	166	GLY	2.3
1	A	49	PRO	2.3
1	C	68	PHE	2.3
1	A	102	ASN	2.3
1	A	202	LYS	2.3
1	A	139	TRP	2.3
1	A	159	GLU	2.3
1	E	146	LEU	2.3
1	C	171	CYS	2.3
1	C	104	THR	2.2
1	G	175	THR	2.2
1	G	110	ASP	2.2
1	G	73	GLU	2.2
1	G	6	PRO	2.2
1	G	129	GLY	2.2
1	H	222	GLN	2.2
1	C	174	LYS	2.2
1	A	54	TYR	2.2
1	C	93	MET	2.2
1	E	87	TYR	2.2
1	C	190	PHE	2.2
1	A	200	HIS	2.2
1	A	5	LYS	2.2
1	A	219	LEU	2.2
1	A	116	TYR	2.2
1	A	82	SER	2.2
1	C	51	PRO	2.2
1	A	104	THR	2.2
1	A	111	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	173[A]	PHE	2.2
1	G	183	VAL	2.2
1	G	118	ILE	2.1
1	A	93	MET	2.1
1	C	163	LEU	2.1
1	H	223	ALA	2.1
1	G	104	THR	2.1
1	A	97	ASP	2.1
1	A	16	GLY	2.1
1	E	167	GLY	2.1
1	E	23	PHE	2.1
1	H	159[A]	GLU	2.1
1	A	69	ALA	2.1
1	G	194	HIS	2.1
1	H	161	LEU	2.1
1	C	158	ASN	2.1
1	E	130	PRO	2.1
1	C	132	MET	2.1
1	E	135	ARG	2.1
1	G	59	THR	2.1
1	B	92[A]	SER	2.1
1	C	69	ALA	2.1
1	E	81	GLN	2.1
1	E	109	LEU	2.1
1	A	61	PHE	2.0
1	E	67	VAL	2.0
1	A	160	ALA	2.0
1	C	99	GLY	2.0
1	E	99	GLY	2.0
1	E	218	GLY	2.0
1	C	116	TYR	2.0
1	A	76	VAL	2.0
1	A	190	PHE	2.0
1	C	17	ALA	2.0
1	A	162	SER	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, 95^{th} 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	A	63	21/22	0.71	0.21	36,47,51,52	0
1	GYC	E	63	21/22	0.81	0.21	49,51,52,61	0
1	GYC	C	63	21/22	0.82	0.19	49,50,53,56	0
1	GYC	G	63	21/22	0.82	0.17	47,51,53,59	0
1	GYC	D	63	21/22	0.94	0.12	16,20,22,23	0
1	GYC	F	63	21/22	0.95	0.12	17,21,23,24	0
1	GYC	B	63	21/22	0.95	0.12	16,20,24,25	0
1	GYC	H	63	21/22	0.95	0.13	16,19,22,23	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.