Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 01:27 AM EST

PDB ID	:	2Z6Z
Title	:	Crystal structure of a photoswitchable GFP-like protein Dronpa in the bright-state
Authors	:	Kikuchi, A.; Jeyakanthan, J.; Taka, J.; Shiro, Y.; Mizuno, H.; Miyawaki, A.
Deposited on	:	2007-08-09
Resolution	:	1.80 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:

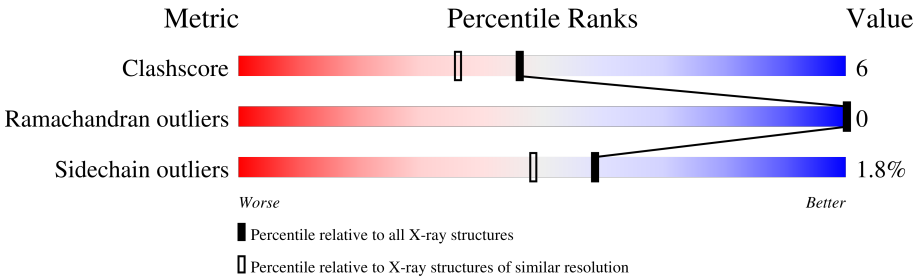
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	255	77% 8% 15%
1	B	255	72% 12% 15%
1	C	255	74% 11% 15%
1	D	255	64% 19% • 16%
1	E	255	73% 12% • 15%
1	F	255	76% 8% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11723 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1749	1117	294	328	10			
1	B	216	Total	C	N	O	S	0	0	0
			1743	1114	293	326	10			
1	C	218	Total	C	N	O	S	0	0	0
			1757	1122	295	329	11			
1	D	214	Total	C	N	O	S	0	0	0
			1727	1103	291	323	10			
1	E	217	Total	C	N	O	S	0	0	0
			1749	1117	294	328	10			
1	F	216	Total	C	N	O	S	0	0	0
			1744	1114	293	327	10			

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	expression tag	UNP Q5TLG6
A	-31	ARG	-	expression tag	UNP Q5TLG6
A	-30	GLY	-	expression tag	UNP Q5TLG6
A	-29	SER	-	expression tag	UNP Q5TLG6
A	-28	HIS	-	expression tag	UNP Q5TLG6
A	-27	HIS	-	expression tag	UNP Q5TLG6
A	-26	HIS	-	expression tag	UNP Q5TLG6
A	-25	HIS	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	GLY	-	expression tag	UNP Q5TLG6
A	-21	MET	-	expression tag	UNP Q5TLG6
A	-20	ALA	-	expression tag	UNP Q5TLG6
A	-19	SER	-	expression tag	UNP Q5TLG6
A	-18	MET	-	expression tag	UNP Q5TLG6
A	-17	THR	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP Q5TLG6
A	-14	GLN	-	expression tag	UNP Q5TLG6
A	-13	GLN	-	expression tag	UNP Q5TLG6
A	-12	MET	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	ARG	-	expression tag	UNP Q5TLG6
A	-9	ASP	-	expression tag	UNP Q5TLG6
A	-8	LEU	-	expression tag	UNP Q5TLG6
A	-7	TYR	-	expression tag	UNP Q5TLG6
A	-6	ASP	-	expression tag	UNP Q5TLG6
A	-5	ASP	-	expression tag	UNP Q5TLG6
A	-4	ASP	-	expression tag	UNP Q5TLG6
A	-3	ASP	-	expression tag	UNP Q5TLG6
A	-2	LYS	-	expression tag	UNP Q5TLG6
A	-1	ASP	-	expression tag	UNP Q5TLG6
A	0	PRO	-	expression tag	UNP Q5TLG6
B	-32	MET	-	expression tag	UNP Q5TLG6
B	-31	ARG	-	expression tag	UNP Q5TLG6
B	-30	GLY	-	expression tag	UNP Q5TLG6
B	-29	SER	-	expression tag	UNP Q5TLG6
B	-28	HIS	-	expression tag	UNP Q5TLG6
B	-27	HIS	-	expression tag	UNP Q5TLG6
B	-26	HIS	-	expression tag	UNP Q5TLG6
B	-25	HIS	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	GLY	-	expression tag	UNP Q5TLG6
B	-21	MET	-	expression tag	UNP Q5TLG6
B	-20	ALA	-	expression tag	UNP Q5TLG6
B	-19	SER	-	expression tag	UNP Q5TLG6
B	-18	MET	-	expression tag	UNP Q5TLG6
B	-17	THR	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	GLY	-	expression tag	UNP Q5TLG6
B	-14	GLN	-	expression tag	UNP Q5TLG6
B	-13	GLN	-	expression tag	UNP Q5TLG6
B	-12	MET	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	ARG	-	expression tag	UNP Q5TLG6
B	-9	ASP	-	expression tag	UNP Q5TLG6
B	-8	LEU	-	expression tag	UNP Q5TLG6
B	-7	TYR	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ASP	-	expression tag	UNP Q5TLG6
B	-5	ASP	-	expression tag	UNP Q5TLG6
B	-4	ASP	-	expression tag	UNP Q5TLG6
B	-3	ASP	-	expression tag	UNP Q5TLG6
B	-2	LYS	-	expression tag	UNP Q5TLG6
B	-1	ASP	-	expression tag	UNP Q5TLG6
B	0	PRO	-	expression tag	UNP Q5TLG6
C	-32	MET	-	expression tag	UNP Q5TLG6
C	-31	ARG	-	expression tag	UNP Q5TLG6
C	-30	GLY	-	expression tag	UNP Q5TLG6
C	-29	SER	-	expression tag	UNP Q5TLG6
C	-28	HIS	-	expression tag	UNP Q5TLG6
C	-27	HIS	-	expression tag	UNP Q5TLG6
C	-26	HIS	-	expression tag	UNP Q5TLG6
C	-25	HIS	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	GLY	-	expression tag	UNP Q5TLG6
C	-21	MET	-	expression tag	UNP Q5TLG6
C	-20	ALA	-	expression tag	UNP Q5TLG6
C	-19	SER	-	expression tag	UNP Q5TLG6
C	-18	MET	-	expression tag	UNP Q5TLG6
C	-17	THR	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	GLY	-	expression tag	UNP Q5TLG6
C	-14	GLN	-	expression tag	UNP Q5TLG6
C	-13	GLN	-	expression tag	UNP Q5TLG6
C	-12	MET	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	ARG	-	expression tag	UNP Q5TLG6
C	-9	ASP	-	expression tag	UNP Q5TLG6
C	-8	LEU	-	expression tag	UNP Q5TLG6
C	-7	TYR	-	expression tag	UNP Q5TLG6
C	-6	ASP	-	expression tag	UNP Q5TLG6
C	-5	ASP	-	expression tag	UNP Q5TLG6
C	-4	ASP	-	expression tag	UNP Q5TLG6
C	-3	ASP	-	expression tag	UNP Q5TLG6
C	-2	LYS	-	expression tag	UNP Q5TLG6
C	-1	ASP	-	expression tag	UNP Q5TLG6
C	0	PRO	-	expression tag	UNP Q5TLG6
D	-32	MET	-	expression tag	UNP Q5TLG6
D	-31	ARG	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	GLY	-	expression tag	UNP Q5TLG6
D	-29	SER	-	expression tag	UNP Q5TLG6
D	-28	HIS	-	expression tag	UNP Q5TLG6
D	-27	HIS	-	expression tag	UNP Q5TLG6
D	-26	HIS	-	expression tag	UNP Q5TLG6
D	-25	HIS	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	GLY	-	expression tag	UNP Q5TLG6
D	-21	MET	-	expression tag	UNP Q5TLG6
D	-20	ALA	-	expression tag	UNP Q5TLG6
D	-19	SER	-	expression tag	UNP Q5TLG6
D	-18	MET	-	expression tag	UNP Q5TLG6
D	-17	THR	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	GLY	-	expression tag	UNP Q5TLG6
D	-14	GLN	-	expression tag	UNP Q5TLG6
D	-13	GLN	-	expression tag	UNP Q5TLG6
D	-12	MET	-	expression tag	UNP Q5TLG6
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	ARG	-	expression tag	UNP Q5TLG6
D	-9	ASP	-	expression tag	UNP Q5TLG6
D	-8	LEU	-	expression tag	UNP Q5TLG6
D	-7	TYR	-	expression tag	UNP Q5TLG6
D	-6	ASP	-	expression tag	UNP Q5TLG6
D	-5	ASP	-	expression tag	UNP Q5TLG6
D	-4	ASP	-	expression tag	UNP Q5TLG6
D	-3	ASP	-	expression tag	UNP Q5TLG6
D	-2	LYS	-	expression tag	UNP Q5TLG6
D	-1	ASP	-	expression tag	UNP Q5TLG6
D	0	PRO	-	expression tag	UNP Q5TLG6
E	-32	MET	-	expression tag	UNP Q5TLG6
E	-31	ARG	-	expression tag	UNP Q5TLG6
E	-30	GLY	-	expression tag	UNP Q5TLG6
E	-29	SER	-	expression tag	UNP Q5TLG6
E	-28	HIS	-	expression tag	UNP Q5TLG6
E	-27	HIS	-	expression tag	UNP Q5TLG6
E	-26	HIS	-	expression tag	UNP Q5TLG6
E	-25	HIS	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	MET	-	expression tag	UNP Q5TLG6
E	-20	ALA	-	expression tag	UNP Q5TLG6
E	-19	SER	-	expression tag	UNP Q5TLG6
E	-18	MET	-	expression tag	UNP Q5TLG6
E	-17	THR	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	GLY	-	expression tag	UNP Q5TLG6
E	-14	GLN	-	expression tag	UNP Q5TLG6
E	-13	GLN	-	expression tag	UNP Q5TLG6
E	-12	MET	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6
E	-10	ARG	-	expression tag	UNP Q5TLG6
E	-9	ASP	-	expression tag	UNP Q5TLG6
E	-8	LEU	-	expression tag	UNP Q5TLG6
E	-7	TYR	-	expression tag	UNP Q5TLG6
E	-6	ASP	-	expression tag	UNP Q5TLG6
E	-5	ASP	-	expression tag	UNP Q5TLG6
E	-4	ASP	-	expression tag	UNP Q5TLG6
E	-3	ASP	-	expression tag	UNP Q5TLG6
E	-2	LYS	-	expression tag	UNP Q5TLG6
E	-1	ASP	-	expression tag	UNP Q5TLG6
E	0	PRO	-	expression tag	UNP Q5TLG6
F	-32	MET	-	expression tag	UNP Q5TLG6
F	-31	ARG	-	expression tag	UNP Q5TLG6
F	-30	GLY	-	expression tag	UNP Q5TLG6
F	-29	SER	-	expression tag	UNP Q5TLG6
F	-28	HIS	-	expression tag	UNP Q5TLG6
F	-27	HIS	-	expression tag	UNP Q5TLG6
F	-26	HIS	-	expression tag	UNP Q5TLG6
F	-25	HIS	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	GLY	-	expression tag	UNP Q5TLG6
F	-21	MET	-	expression tag	UNP Q5TLG6
F	-20	ALA	-	expression tag	UNP Q5TLG6
F	-19	SER	-	expression tag	UNP Q5TLG6
F	-18	MET	-	expression tag	UNP Q5TLG6
F	-17	THR	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	GLY	-	expression tag	UNP Q5TLG6
F	-14	GLN	-	expression tag	UNP Q5TLG6
F	-13	GLN	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	MET	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	ARG	-	expression tag	UNP Q5TLG6
F	-9	ASP	-	expression tag	UNP Q5TLG6
F	-8	LEU	-	expression tag	UNP Q5TLG6
F	-7	TYR	-	expression tag	UNP Q5TLG6
F	-6	ASP	-	expression tag	UNP Q5TLG6
F	-5	ASP	-	expression tag	UNP Q5TLG6
F	-4	ASP	-	expression tag	UNP Q5TLG6
F	-3	ASP	-	expression tag	UNP Q5TLG6
F	-2	LYS	-	expression tag	UNP Q5TLG6
F	-1	ASP	-	expression tag	UNP Q5TLG6
F	0	PRO	-	expression tag	UNP Q5TLG6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	201	Total O 201 201	0	0
2	B	200	Total O 200 200	0	0
2	C	239	Total O 239 239	0	0
2	D	133	Total O 133 133	0	0
2	E	254	Total O 254 254	0	0
2	F	227	Total O 227 227	0	0

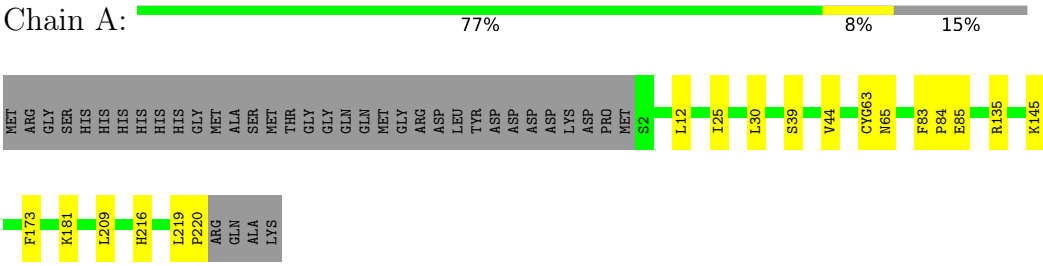
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

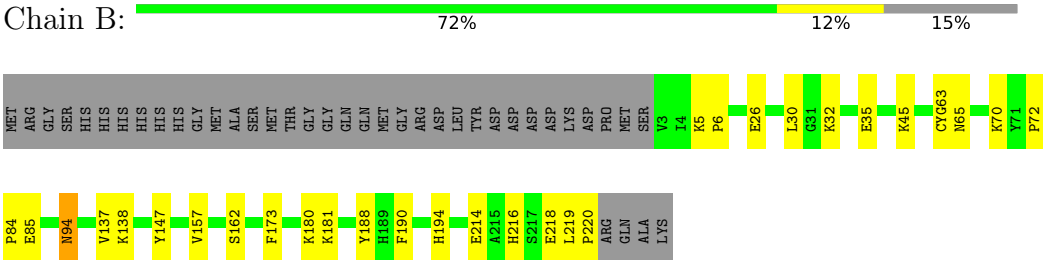
• Molecule 1: Fluorescent protein Dronpa

Chain A:



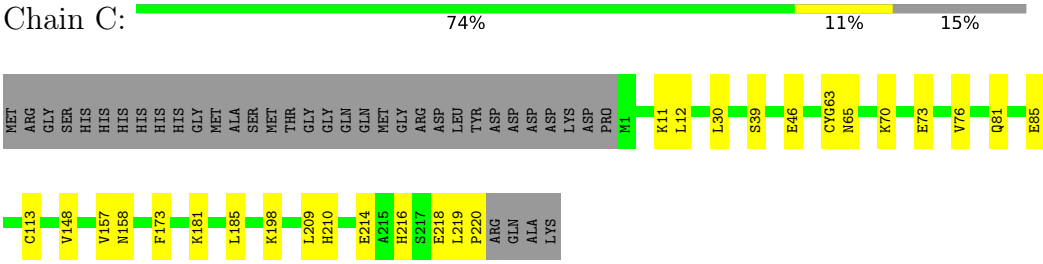
• Molecule 1: Fluorescent protein Dronpa

Chain B:



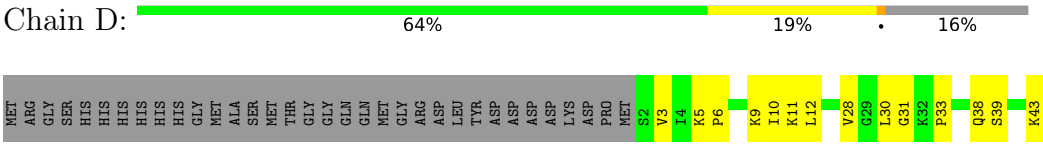
• Molecule 1: Fluorescent protein Dronpa

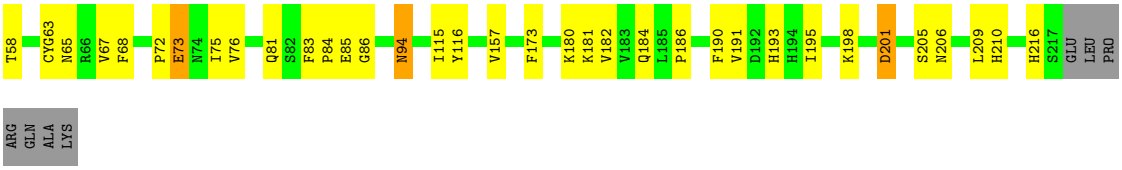
Chain C:



• Molecule 1: Fluorescent protein Dronpa

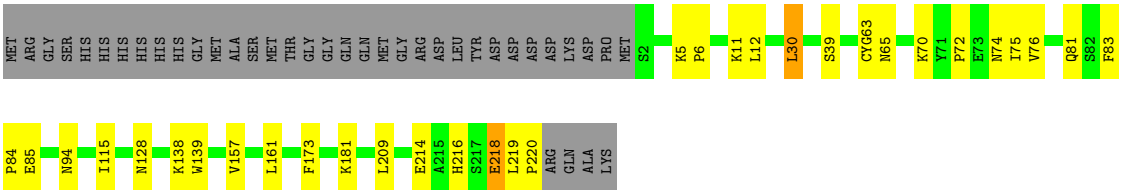
Chain D:





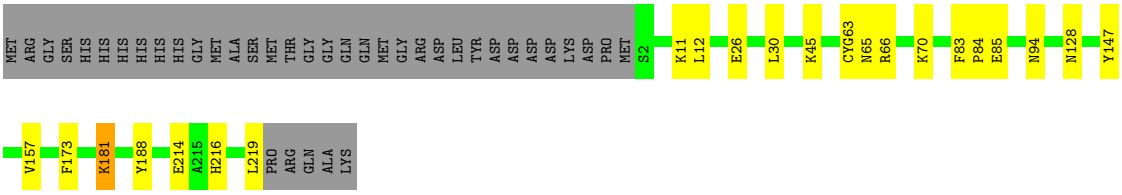
• Molecule 1: Fluorescent protein Dronpa

Chain E:



• Molecule 1: Fluorescent protein Dronpa

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.44Å 182.66Å 72.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.80	Depositor
% Data completeness (in resolution range)	99.8 (19.94-1.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11723	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

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	0.37	0/1773	0.67	0/2393
1	B	0.35	0/1767	0.67	0/2385
1	C	0.35	0/1781	0.67	0/2403
1	D	0.34	0/1751	0.60	0/2363
1	E	0.37	0/1773	0.69	0/2393
1	F	0.37	0/1768	0.68	0/2386
All	All	0.36	0/10613	0.66	0/14323

There are no bond length outliers.

There are no bond angle outliers.

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	1749	0	1669	12	0
1	B	1743	0	1664	23	0
1	C	1757	0	1681	18	0
1	D	1727	0	1651	40	0
1	E	1749	0	1669	21	0
1	F	1744	0	1668	15	0
2	A	201	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	200	0	0	0	0
2	C	239	0	0	1	0
2	D	133	0	0	2	0
2	E	254	0	0	1	0
2	F	227	0	0	4	1
All	All	11723	0	10002	129	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (129) 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:B:219:LEU:HA	1:B:220:PRO:C	1.66	1.11
1:C:219:LEU:O	1:C:220:PRO:CB	2.31	0.79
1:E:219:LEU:O	1:E:220:PRO:CB	2.29	0.79
1:C:181:LYS:HG2	2:C:397:HOH:O	1.86	0.75
1:C:216:HIS:CE1	1:C:219:LEU:HD21	2.27	0.70
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.74	0.69
1:B:219:LEU:CA	1:B:220:PRO:C	2.52	0.68
1:E:72:PRO:HB2	1:E:74:ASN:OD1	1.94	0.67
1:F:26:GLU:HG3	1:F:45:LYS:HG3	1.77	0.66
1:A:219:LEU:O	1:A:220:PRO:CB	2.43	0.66
1:D:86:GLY:O	1:D:180:LYS:HG2	1.96	0.65
1:D:5:LYS:HB3	1:D:6:PRO:HD2	1.80	0.63
1:E:85:GLU:CD	1:E:181:LYS:HD3	2.23	0.59
1:A:216:HIS:CE1	1:A:219:LEU:HD21	2.39	0.58
1:D:12:LEU:CB	1:D:116:TYR:HB2	2.34	0.57
1:B:70:LYS:HB3	1:B:214:GLU:HG2	1.87	0.57
1:E:72:PRO:HG2	1:E:75:ILE:HD12	1.86	0.57
1:D:85:GLU:H	1:D:85:GLU:CD	2.08	0.56
1:B:85:GLU:OE1	1:B:181:LYS:HD3	2.07	0.55
1:F:70:LYS:HB3	1:F:214:GLU:HG2	1.89	0.55
1:D:201:ASP:OD1	1:D:206:ASN:HB2	2.07	0.55
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.89	0.54
1:B:30:LEU:HD12	1:B:30:LEU:C	2.27	0.54
1:D:190:PHE:HB2	1:D:216:HIS:CE1	2.43	0.54
1:B:219:LEU:HA	1:B:220:PRO:O	2.08	0.53
1:B:216:HIS:CE1	1:B:219:LEU:HD21	2.43	0.53
1:A:83:PHE:HB3	1:A:84:PRO:HA	1.90	0.53
1:B:30:LEU:HD12	1:B:30:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:ND2	1:B:94:ASN:C	2.62	0.53
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.91	0.52
1:E:11:LYS:HB2	1:E:115:ILE:HD13	1.91	0.52
1:B:218:GLU:O	1:B:219:LEU:HD23	2.10	0.51
1:A:39:SER:HA	1:A:209:LEU:O	2.10	0.51
1:D:12:LEU:C	1:D:12:LEU:HD12	2.30	0.51
1:D:201:ASP:OD2	1:D:201:ASP:N	2.36	0.51
1:D:72:PRO:HD2	1:D:75:ILE:HD12	1.92	0.51
1:C:218:GLU:O	1:C:219:LEU:HD23	2.10	0.51
1:F:128:ASN:HB3	2:F:416:HOH:O	2.10	0.51
1:D:30:LEU:N	1:D:30:LEU:HD23	2.26	0.50
1:D:73:GLU:H	1:D:73:GLU:CD	2.15	0.50
1:D:86:GLY:C	1:D:180:LYS:HG2	2.32	0.50
1:A:216:HIS:HE1	1:A:219:LEU:HD21	1.76	0.49
1:D:3:VAL:HG11	1:D:84:PRO:HB3	1.93	0.49
1:D:198:LYS:HG3	1:D:210:HIS:CE1	2.47	0.49
1:D:12:LEU:HB2	1:D:116:TYR:HB2	1.94	0.49
1:D:5:LYS:HE3	1:D:6:PRO:HD2	1.94	0.49
1:C:157:VAL:CG1	1:C:173:PHE:HB2	2.43	0.49
1:D:10:ILE:HD11	1:D:68:PHE:CZ	2.47	0.49
1:E:12:LEU:HD12	1:E:12:LEU:C	2.33	0.48
1:E:30:LEU:O	1:E:30:LEU:HD12	2.13	0.48
1:D:76:VAL:HB	1:D:186:PRO:HB3	1.95	0.48
1:D:9:LYS:NZ	1:D:30:LEU:HD13	2.29	0.48
1:D:12:LEU:HB3	1:D:116:TYR:HB2	1.95	0.48
1:C:216:HIS:HE1	1:C:219:LEU:HD21	1.76	0.48
1:B:32:LYS:HB2	1:B:35:GLU:HB2	1.95	0.47
1:C:12:LEU:C	1:C:12:LEU:HD12	2.34	0.47
1:A:85:GLU:CD	1:A:181:LYS:HD3	2.34	0.47
1:A:12:LEU:HD12	1:A:12:LEU:C	2.34	0.47
1:D:76:VAL:HG13	1:D:81:GLN:HE22	1.78	0.47
1:C:46:GLU:HG2	2:F:359:HOH:O	2.15	0.47
1:F:12:LEU:C	1:F:12:LEU:HD12	2.35	0.47
1:A:157:VAL:HG13	1:A:173:PHE:HB2	1.97	0.47
1:B:94:ASN:C	1:B:94:ASN:HD22	2.17	0.47
1:F:157:VAL:CG1	1:F:173:PHE:HB2	2.45	0.47
1:D:181:LYS:HG3	1:D:182:VAL:N	2.30	0.46
1:D:31:GLY:O	1:D:33:PRO:HD3	2.15	0.46
1:A:135:ARG:O	1:A:164:GLU:HG3	2.16	0.46
1:D:10:ILE:O	1:D:28:VAL:HA	2.16	0.46
1:E:157:VAL:CG1	1:E:173:PHE:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLU:CD	1:C:181:LYS:HD3	2.36	0.45
1:E:216:HIS:HE1	1:E:219:LEU:HD13	1.81	0.45
1:C:11:LYS:HG3	1:C:113:CYS:SG	2.57	0.45
1:C:94:ASN:HD22	1:C:100:ILE:CD1	2.29	0.45
1:D:157:VAL:CG1	1:D:173:PHE:HB2	2.46	0.45
1:F:216:HIS:CE1	1:F:219:LEU:HD13	2.51	0.45
1:D:50:LEU:HA	1:D:51:PRO:HD3	1.77	0.45
1:C:76:VAL:HG13	1:C:81:GLN:HE22	1.81	0.45
1:B:157:VAL:CG1	1:B:173:PHE:HB2	2.47	0.44
1:B:85:GLU:HB3	1:B:180:LYS:HB2	1.99	0.44
1:D:43:LYS:HA	1:D:205:SER:O	2.18	0.44
1:D:11:LYS:O	1:D:115:ILE:HA	2.18	0.44
1:E:218:GLU:OE2	1:E:218:GLU:HA	2.17	0.44
1:C:148:VAL:HG21	1:C:185:LEU:HB3	2.00	0.44
1:F:85:GLU:CD	1:F:181:LYS:HD2	2.39	0.44
1:B:137:VAL:HB	1:B:162:SER:OG	2.17	0.44
1:E:138:LYS:HE3	2:E:424:HOH:O	2.18	0.43
1:B:26:GLU:HG3	1:B:45:LYS:HG3	2.00	0.43
1:C:198:LYS:HG3	1:C:210:HIS:CD2	2.53	0.43
1:E:83:PHE:HB3	1:E:84:PRO:HA	1.99	0.43
1:D:191:VAL:HG12	1:D:193:HIS:CE1	2.54	0.43
1:B:72:PRO:HB2	1:B:74:ASN:OD1	2.18	0.43
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.01	0.43
1:E:5:LYS:HE3	1:E:6:PRO:HD2	2.00	0.43
1:C:39:SER:HA	1:C:209:LEU:O	2.19	0.43
1:F:219:LEU:HD12	1:F:219:LEU:HA	1.89	0.43
1:B:190:PHE:HB2	1:B:216:HIS:CE1	2.54	0.42
1:F:30:LEU:HD23	1:F:30:LEU:N	2.34	0.42
1:E:94:ASN:C	1:E:94:ASN:ND2	2.70	0.42
1:F:11:LYS:HE2	2:F:444:HOH:O	2.18	0.42
1:D:65:ASN:CG	1:D:67:VAL:HG12	2.40	0.42
1:D:58:THR:HG21	2:D:253:HOH:O	2.19	0.42
1:F:30:LEU:HB2	2:F:405:HOH:O	2.20	0.42
1:C:157:VAL:HG12	1:C:173:PHE:HB2	2.02	0.42
1:D:9:LYS:HZ3	1:D:30:LEU:HD13	1.83	0.42
1:A:157:VAL:CG1	1:A:173:PHE:HB2	2.50	0.41
1:D:195:ILE:HD11	1:D:209:LEU:HD21	2.03	0.41
1:E:39:SER:HA	1:E:209:LEU:O	2.20	0.41
1:B:157:VAL:HG13	1:B:173:PHE:HB2	2.02	0.41
1:E:216:HIS:CE1	1:E:219:LEU:HD13	2.55	0.41
1:F:30:LEU:HD23	1:F:30:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:VAL:HG13	1:F:173:PHE:HB2	2.01	0.41
1:A:85:GLU:OE1	1:A:85:GLU:N	2.45	0.41
1:B:147:TYR:HB3	1:B:188:TYR:CD1	2.55	0.41
1:D:157:VAL:HG12	1:D:173:PHE:HB2	2.03	0.41
1:F:83:PHE:HB3	1:F:84:PRO:HA	2.03	0.41
1:B:137:VAL:O	1:B:138:LYS:HB3	2.20	0.41
1:D:38:GLN:HG2	2:D:332:HOH:O	2.21	0.41
1:D:39:SER:HA	1:D:209:LEU:O	2.21	0.41
1:D:94:ASN:C	1:D:94:ASN:HD22	2.24	0.41
1:E:139:TRP:CZ3	1:E:161:LEU:HG	2.56	0.41
1:D:76:VAL:CG2	1:D:184:GLN:HE21	2.34	0.41
1:B:5:LYS:HE3	1:B:6:PRO:HD2	2.02	0.40
1:C:158:ASN:HD22	1:C:158:ASN:HA	1.66	0.40
1:D:209:LEU:C	1:D:210:HIS:HD2	2.25	0.40
1:E:11:LYS:HB2	1:E:115:ILE:CD1	2.51	0.40
1:E:76:VAL:HG13	1:E:81:GLN:HE22	1.86	0.40
1:F:147:TYR:HB3	1:F:188:TYR:CD1	2.57	0.40
1:E:157:VAL:HG13	1:E:173:PHE:HB2	2.03	0.40
1:A:25:ILE:HG12	1:A:44:VAL:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:450:HOH:O	2:F:451:HOH:O[2_555]	0.07	2.13

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	212/255 (83%)	210 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	C	213/255 (84%)	211 (99%)	2 (1%)	0	100	100
1	D	209/255 (82%)	203 (97%)	6 (3%)	0	100	100
1	E	212/255 (83%)	210 (99%)	2 (1%)	0	100	100
1	F	211/255 (83%)	209 (99%)	2 (1%)	0	100	100
All	All	1268/1530 (83%)	1250 (99%)	18 (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	186/218 (85%)	183 (98%)	3 (2%)	62	54
1	B	185/218 (85%)	182 (98%)	3 (2%)	62	54
1	C	187/218 (86%)	184 (98%)	3 (2%)	62	54
1	D	184/218 (84%)	181 (98%)	3 (2%)	62	54
1	E	186/218 (85%)	182 (98%)	4 (2%)	52	39
1	F	186/218 (85%)	182 (98%)	4 (2%)	52	39
All	All	1114/1308 (85%)	1094 (98%)	20 (2%)	59	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	65	ASN
1	A	145	LYS
1	B	65	ASN
1	B	94	ASN
1	B	194	HIS
1	C	30	LEU
1	C	65	ASN

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Mol	Chain	Res	Type
1	C	73	GLU
1	D	73	GLU
1	D	94	ASN
1	D	201	ASP
1	E	30	LEU
1	E	65	ASN
1	E	128	ASN
1	E	218	GLU
1	F	65	ASN
1	F	66	ARG
1	F	94	ASN
1	F	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	65	ASN
1	A	102	ASN
1	A	184	GLN
1	A	216	HIS
1	B	21	HIS
1	B	65	ASN
1	B	94	ASN
1	B	102	ASN
1	B	158	ASN
1	B	194	HIS
1	C	38	GLN
1	C	65	ASN
1	C	94	ASN
1	C	102	ASN
1	C	158	ASN
1	D	81	GLN
1	D	94	ASN
1	D	102	ASN
1	D	124	ASN
1	D	184	GLN
1	D	193	HIS
1	E	65	ASN
1	E	94	ASN
1	E	102	ASN
1	E	128	ASN

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Mol	Chain	Res	Type
1	E	184	GLN
1	E	216	HIS
1	F	21	HIS
1	F	65	ASN
1	F	94	ASN
1	F	102	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	GYC	F	63	1	22,22,23	3.72	11 (50%)	26,30,32	2.01	5 (19%)
1	GYC	D	63	1	22,22,23	3.67	13 (59%)	26,30,32	1.94	5 (19%)
1	GYC	C	63	1	22,22,23	3.62	12 (54%)	26,30,32	2.00	5 (19%)
1	GYC	B	63	1	22,22,23	3.83	12 (54%)	26,30,32	2.03	5 (19%)
1	GYC	A	63	1	22,22,23	4.15	12 (54%)	26,30,32	2.03	6 (23%)
1	GYC	E	63	1	22,22,23	3.92	12 (54%)	26,30,32	2.02	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	F	63	1	-	1/9/29/30	0/2/2/2
1	GYC	D	63	1	-	1/9/29/30	0/2/2/2
1	GYC	C	63	1	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	B	63	1	-	2/9/29/30	0/2/2/2
1	GYC	A	63	1	-	1/9/29/30	0/2/2/2
1	GYC	E	63	1	-	2/9/29/30	0/2/2/2

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB1-CA1	-12.61	1.39	1.53
1	E	63	GYC	CB1-CA1	-10.80	1.41	1.53
1	F	63	GYC	CA1-C1	9.62	1.69	1.51
1	B	63	GYC	CA1-C1	8.35	1.67	1.51
1	C	63	GYC	CB1-SG1	-7.58	1.65	1.81
1	B	63	GYC	CA2-C2	-7.58	1.41	1.48
1	E	63	GYC	CA2-C2	-7.51	1.41	1.48
1	F	63	GYC	CA2-C2	-7.44	1.41	1.48
1	A	63	GYC	CA2-C2	-7.34	1.41	1.48
1	D	63	GYC	CA2-C2	-7.29	1.41	1.48
1	D	63	GYC	CB2-CA2	7.27	1.41	1.35
1	D	63	GYC	CA1-C1	7.18	1.65	1.51
1	C	63	GYC	CB2-CA2	7.16	1.41	1.35
1	B	63	GYC	CB1-SG1	-7.07	1.66	1.81
1	C	63	GYC	CA2-C2	-7.01	1.41	1.48
1	A	63	GYC	CA1-C1	6.88	1.64	1.51
1	E	63	GYC	CB2-CA2	6.80	1.40	1.35
1	A	63	GYC	CB2-CA2	6.53	1.40	1.35
1	C	63	GYC	CA1-C1	6.52	1.63	1.51
1	F	63	GYC	CB2-CA2	6.51	1.40	1.35
1	E	63	GYC	CA1-C1	6.12	1.63	1.51
1	B	63	GYC	CB2-CA2	6.12	1.40	1.35
1	D	63	GYC	CB1-SG1	-5.77	1.69	1.81
1	F	63	GYC	CB1-SG1	-5.76	1.69	1.81
1	B	63	GYC	CB1-CA1	-5.71	1.46	1.53
1	D	63	GYC	CB1-CA1	5.61	1.59	1.53
1	A	63	GYC	OH-CZ	-4.39	1.26	1.37
1	B	63	GYC	OH-CZ	-4.37	1.26	1.37
1	D	63	GYC	OH-CZ	-4.31	1.26	1.37
1	C	63	GYC	OH-CZ	-4.29	1.27	1.37
1	E	63	GYC	OH-CZ	-4.24	1.27	1.37
1	F	63	GYC	OH-CZ	-4.10	1.27	1.37
1	F	63	GYC	CA3-N3	-3.98	1.39	1.47
1	E	63	GYC	CA3-N3	-3.95	1.39	1.47
1	B	63	GYC	CA3-N3	-3.90	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	GYC	CA3-N3	-3.77	1.39	1.47
1	C	63	GYC	CA3-N3	-3.71	1.39	1.47
1	A	63	GYC	CA3-N3	-3.68	1.39	1.47
1	C	63	GYC	CB1-CA1	3.46	1.56	1.53
1	F	63	GYC	CG2-CB2	-3.10	1.40	1.46
1	B	63	GYC	CG2-CB2	-3.06	1.41	1.46
1	E	63	GYC	CG2-CB2	-2.95	1.41	1.46
1	A	63	GYC	CG2-CB2	-2.88	1.41	1.46
1	E	63	GYC	CE1-CD1	2.85	1.43	1.38
1	D	63	GYC	CG2-CB2	-2.85	1.41	1.46
1	C	63	GYC	CE1-CD1	2.84	1.43	1.38
1	A	63	GYC	CE1-CD1	2.66	1.43	1.38
1	F	63	GYC	CE1-CD1	2.63	1.43	1.38
1	D	63	GYC	CE2-CD2	2.63	1.43	1.38
1	B	63	GYC	CE1-CD1	2.62	1.43	1.38
1	E	63	GYC	CE2-CD2	2.62	1.43	1.38
1	C	63	GYC	CG2-CB2	-2.60	1.41	1.46
1	F	63	GYC	CE2-CD2	2.55	1.43	1.38
1	C	63	GYC	CE2-CD2	2.55	1.43	1.38
1	D	63	GYC	CE1-CD1	2.50	1.43	1.38
1	C	63	GYC	CD1-CG2	2.43	1.44	1.39
1	A	63	GYC	CE2-CD2	2.43	1.43	1.38
1	B	63	GYC	CE2-CD2	2.41	1.43	1.38
1	C	63	GYC	CE1-CZ	2.39	1.43	1.38
1	E	63	GYC	CD1-CG2	2.36	1.44	1.39
1	F	63	GYC	CE1-CZ	2.34	1.43	1.38
1	B	63	GYC	CD1-CG2	2.32	1.43	1.39
1	D	63	GYC	CD1-CG2	2.17	1.43	1.39
1	E	63	GYC	CE1-CZ	2.15	1.43	1.38
1	A	63	GYC	CE1-CZ	2.10	1.42	1.38
1	A	63	GYC	CD1-CG2	2.09	1.43	1.39
1	F	63	GYC	CD1-CG2	2.08	1.43	1.39
1	B	63	GYC	CE1-CZ	2.05	1.42	1.38
1	D	63	GYC	CD2-CG2	2.05	1.43	1.39
1	A	63	GYC	CD2-CG2	2.04	1.43	1.39
1	E	63	GYC	CD2-CG2	2.02	1.43	1.39
1	D	63	GYC	CE1-CZ	2.01	1.42	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	GYC	CA3-N3-C1	6.22	134.63	127.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	GYC	CA3-N3-C1	6.18	134.58	127.16
1	F	63	GYC	CA3-N3-C1	6.17	134.57	127.16
1	E	63	GYC	CA3-N3-C1	6.11	134.49	127.16
1	C	63	GYC	CA3-N3-C1	6.08	134.46	127.16
1	D	63	GYC	CA3-N3-C1	5.87	134.21	127.16
1	A	63	GYC	C2-CA2-N2	4.47	112.06	108.93
1	B	63	GYC	C2-CA2-N2	4.43	112.04	108.93
1	D	63	GYC	C2-CA2-N2	4.19	111.87	108.93
1	C	63	GYC	C2-CA2-N2	4.19	111.87	108.93
1	F	63	GYC	C2-CA2-N2	4.19	111.87	108.93
1	E	63	GYC	C2-CA2-N2	4.17	111.86	108.93
1	A	63	GYC	CA2-C2-N3	-3.59	101.67	103.37
1	F	63	GYC	CA3-N3-C2	-3.47	115.83	123.80
1	E	63	GYC	CA3-N3-C2	-3.45	115.89	123.80
1	B	63	GYC	CA3-N3-C2	-3.44	115.90	123.80
1	C	63	GYC	CA3-N3-C2	-3.39	116.03	123.80
1	A	63	GYC	CA3-N3-C2	-3.36	116.09	123.80
1	E	63	GYC	C2-N3-C1	3.26	109.62	107.97
1	E	63	GYC	CA2-C2-N3	-3.25	101.83	103.37
1	B	63	GYC	CA2-C2-N3	-3.22	101.85	103.37
1	D	63	GYC	CA3-N3-C2	-3.22	116.41	123.80
1	F	63	GYC	C2-N3-C1	3.22	109.59	107.97
1	C	63	GYC	CA2-C2-N3	-3.12	101.90	103.37
1	C	63	GYC	C2-N3-C1	3.07	109.52	107.97
1	D	63	GYC	CA2-C2-N3	-3.00	101.95	103.37
1	B	63	GYC	C2-N3-C1	2.96	109.47	107.97
1	F	63	GYC	CA2-C2-N3	-2.89	102.00	103.37
1	D	63	GYC	C2-N3-C1	2.80	109.38	107.97
1	A	63	GYC	C2-N3-C1	2.69	109.33	107.97
1	E	63	GYC	CB2-CA2-N2	-2.08	125.95	128.83
1	A	63	GYC	CB2-CA2-N2	-2.05	125.99	128.83
1	E	63	GYC	O3-C3-CA3	-2.02	120.30	126.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	63	GYC	C3-CA3-N3-C2
1	A	63	GYC	C3-CA3-N3-C2
1	F	63	GYC	C3-CA3-N3-C2
1	B	63	GYC	C3-CA3-N3-C2
1	C	63	GYC	C3-CA3-N3-C2

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

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.