



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 08:22 pm GMT

PDB ID : 2GX0  
Title : Crystal structural and functional analysis of GFP-like fluorescent protein  
Authors : Hwang, K.Y.; Nam, K.-H.; Park, S.-Y.; Sugiyama, K.  
Deposited on : 2006-05-08  
Resolution : 1.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

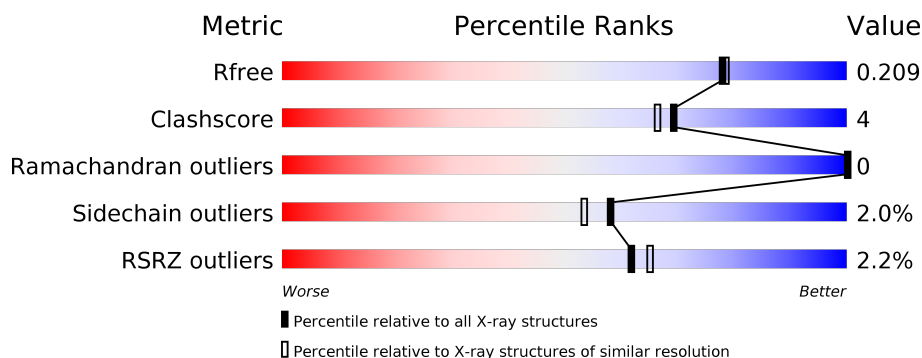
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	241	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	241	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	241	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	D	241	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7621 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	218	Total	C	N	O	S	0	0	0
			1762	1125	298	329	10			
1	B	215	Total	C	N	O	S	0	0	0
			1736	1108	292	326	10			
1	C	218	Total	C	N	O	S	0	0	0
			1762	1125	298	329	10			
1	D	217	Total	C	N	O	S	0	0	0
			1751	1119	294	328	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
A	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
A	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
A	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
A	62	GYC	CYS	CHROMOPHORE	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
A	62	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
B	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
B	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
B	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
B	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
B	62	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
B	62	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
B	62	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
C	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
C	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
C	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
C	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
C	62	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
C	62	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
C	62	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
D	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
D	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
D	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
D	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
D	62	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
D	62	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
D	62	GYC	GLY	CHROMOPHORE	UNP Q5TLG6

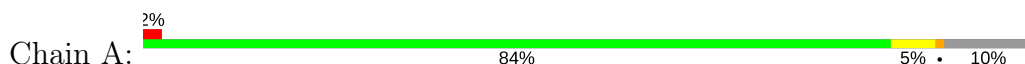
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	155	Total O 155 155	0	0
2	B	162	Total O 162 162	0	0
2	C	148	Total O 148 148	0	0
2	D	145	Total O 145 145	0	0

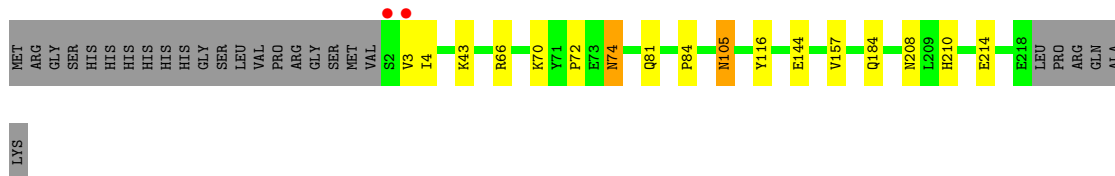
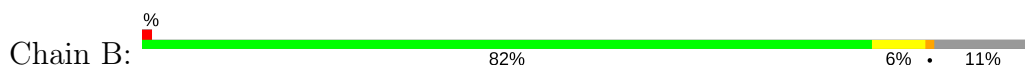
### 3 Residue-property plots [i](#)

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

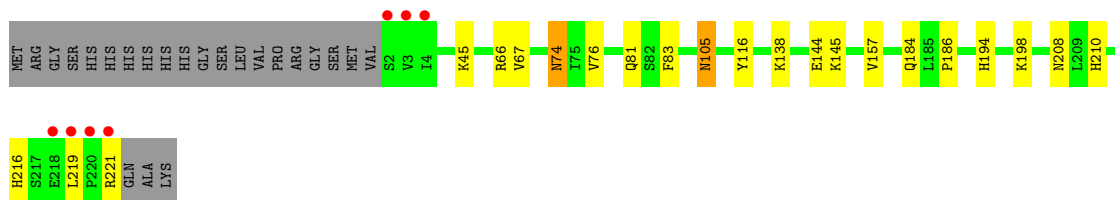
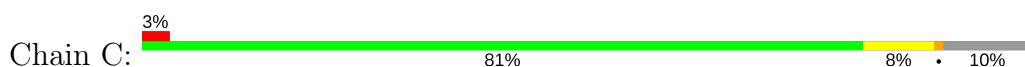
- Molecule 1: fluorescent protein Dronpa



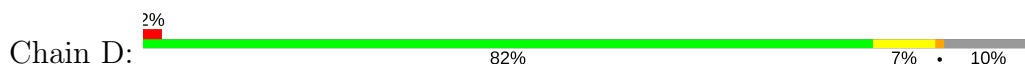
- Molecule 1: fluorescent protein Dronpa



- Molecule 1: fluorescent protein Dronpa



- Molecule 1: fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.59Å 103.59Å 122.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 30.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-1.90) 91.8 (30.58-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.178 , 0.211 0.178 , 0.209	Depositor DCC
$R_{free}$ test set	6907 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.35	0/1787	0.66	0/2412
1	B	0.34	0/1760	0.65	0/2375
1	C	0.33	0/1787	0.65	0/2412
1	D	0.33	0/1776	0.63	0/2398
All	All	0.34	0/7110	0.65	0/9597

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	1762	0	1692	14	0
1	B	1736	0	1661	13	0
1	C	1762	0	1692	15	0
1	D	1751	0	1679	15	0
2	A	155	0	0	0	0
2	B	162	0	0	0	0
2	C	148	0	0	0	0
2	D	145	0	0	0	0
All	All	7621	0	6724	55	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 4.

All (55) 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:A:208:ASN:HD21	1:A:210:HIS:HE1	1.28	0.79
1:B:208:ASN:HD21	1:B:210:HIS:HE1	1.36	0.72
1:C:81:GLN:HE22	1:C:184:GLN:H	1.39	0.69
1:D:67:VAL:HG11	1:D:83:PHE:HE1	1.63	0.64
1:D:67:VAL:HG11	1:D:83:PHE:CE1	2.33	0.64
1:C:216:HIS:CE1	1:C:219:LEU:HD21	2.35	0.61
1:A:208:ASN:HD21	1:A:210:HIS:CE1	2.14	0.61
1:B:74:ASN:H	1:B:74:ASN:HD22	1.48	0.60
1:C:208:ASN:HD21	1:C:210:HIS:HE1	1.49	0.60
1:A:74:ASN:H	1:A:74:ASN:HD22	1.49	0.60
1:B:72:PRO:HB2	1:B:74:ASN:ND2	2.18	0.58
1:D:94:ASN:HD22	1:D:94:ASN:C	2.06	0.58
1:C:221:ARG:HG2	1:D:192:ASP:OD2	2.05	0.57
1:C:81:GLN:NE2	1:C:184:GLN:H	2.05	0.55
1:B:208:ASN:HD21	1:B:210:HIS:CE1	2.23	0.54
1:C:208:ASN:HD21	1:C:210:HIS:CE1	2.27	0.53
1:C:74:ASN:HD22	1:C:74:ASN:H	1.56	0.53
1:B:105:ASN:HD21	1:B:116:TYR:HB3	1.73	0.52
1:A:72:PRO:HD2	1:A:75:ILE:HD12	1.91	0.52
1:A:208:ASN:ND2	1:A:210:HIS:HE1	2.03	0.51
1:D:70:LYS:HB3	1:D:214:GLU:HG2	1.93	0.50
1:A:74:ASN:N	1:A:74:ASN:HD22	2.05	0.50
1:A:198:LYS:HB2	1:A:208:ASN:HD22	1.76	0.49
1:C:74:ASN:N	1:C:74:ASN:HD22	2.10	0.49
1:C:198:LYS:HB2	1:C:208:ASN:HD22	1.78	0.49
1:B:70:LYS:HB3	1:B:214:GLU:HG2	1.95	0.49
1:C:67:VAL:HG21	1:C:83:PHE:CE1	2.48	0.48
1:A:216:HIS:CD2	1:A:219:LEU:HD21	2.49	0.47
1:A:208:ASN:ND2	1:A:210:HIS:CE1	2.82	0.47
1:B:74:ASN:N	1:B:74:ASN:HD22	2.10	0.46
1:D:190:PHE:HB2	1:D:216:HIS:CE1	2.50	0.46
1:D:81:GLN:HE22	1:D:184:GLN:H	1.64	0.46
1:D:72:PRO:HD2	1:D:75:ILE:HD12	1.98	0.46
1:B:3:VAL:HG23	1:B:4:ILE:HG13	1.99	0.45
1:C:105:ASN:HD21	1:C:116:TYR:HB3	1.82	0.45
1:D:75:ILE:HD11	1:D:217:SER:N	2.32	0.44
1:A:105:ASN:HD22	1:A:106:ASP:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:CG1	1:D:83:PHE:HE1	2.29	0.44
1:B:144:GLU:HG3	1:B:157:VAL:HG22	1.99	0.43
1:B:208:ASN:ND2	1:B:210:HIS:HE1	2.11	0.43
1:A:219:LEU:HA	1:A:220:PRO:C	2.39	0.43
1:D:216:HIS:CE1	1:D:219:LEU:HD21	2.54	0.42
1:D:30:LEU:N	1:D:30:LEU:HD23	2.34	0.42
1:A:216:HIS:NE2	1:A:219:LEU:HD21	2.35	0.41
1:C:145:LYS:NZ	1:D:143:THR:H	2.18	0.41
1:C:45:LYS:HE2	1:C:45:LYS:HA	2.03	0.41
1:D:105:ASN:HD22	1:D:106:ASP:N	2.18	0.41
1:B:81:GLN:HE22	1:B:184:GLN:H	1.69	0.40
1:C:144:GLU:HA	1:C:157:VAL:HB	2.02	0.40
1:B:3:VAL:HG11	1:B:84:PRO:HD3	2.02	0.40
1:C:76:VAL:HB	1:C:186:PRO:HB3	2.03	0.40
1:B:208:ASN:ND2	1:B:210:HIS:CE1	2.89	0.40
1:A:157:VAL:CG1	1:A:173:PHE:HB2	2.51	0.40
1:D:81:GLN:NE2	1:D:184:GLN:H	2.19	0.40
1:A:71:TYR:HA	1:A:72:PRO:HD3	1.90	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	215/241 (89%)	212 (99%)	3 (1%)	0	100	100
1	B	212/241 (88%)	211 (100%)	1 (0%)	0	100	100
1	C	215/241 (89%)	213 (99%)	2 (1%)	0	100	100
1	D	214/241 (89%)	211 (99%)	3 (1%)	0	100	100
All	All	856/964 (89%)	847 (99%)	9 (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	188/207 (91%)	185 (98%)	3 (2%)	65	62
1	B	185/207 (89%)	181 (98%)	4 (2%)	55	49
1	C	188/207 (91%)	183 (97%)	5 (3%)	48	40
1	D	187/207 (90%)	184 (98%)	3 (2%)	65	62
All	All	748/828 (90%)	733 (98%)	15 (2%)	58	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	105	ASN
1	A	212	HIS
1	B	43	LYS
1	B	66	ARG
1	B	74	ASN
1	B	105	ASN
1	C	66	ARG
1	C	74	ASN
1	C	105	ASN
1	C	138	LYS
1	C	194	HIS
1	D	66	ARG
1	D	94	ASN
1	D	105	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	105	ASN
1	A	184	GLN
1	A	194	HIS

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Mol	Chain	Res	Type
1	A	208	ASN
1	A	210	HIS
1	A	216	HIS
1	B	38	GLN
1	B	74	ASN
1	B	81	GLN
1	B	105	ASN
1	B	158	ASN
1	B	184	GLN
1	B	194	HIS
1	B	208	ASN
1	B	210	HIS
1	C	74	ASN
1	C	81	GLN
1	C	105	ASN
1	C	194	HIS
1	C	208	ASN
1	D	38	GLN
1	D	81	GLN
1	D	94	ASN
1	D	105	ASN
1	D	124	ASN
1	D	194	HIS
1	D	210	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GYC	A	62	1	22,22,23	3.31	8 (36%)	27,30,32	2.18	6 (22%)
1	GYC	B	62	1	22,22,23	3.38	8 (36%)	27,30,32	2.06	7 (25%)
1	GYC	C	62	1	22,22,23	3.38	7 (31%)	27,30,32	2.15	7 (25%)
1	GYC	D	62	1	22,22,23	3.39	8 (36%)	27,30,32	2.12	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	A	62	1	-	0/9/29/30	0/2/2/2
1	GYC	B	62	1	-	0/9/29/30	0/2/2/2
1	GYC	C	62	1	-	0/9/29/30	0/2/2/2
1	GYC	D	62	1	-	0/9/29/30	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GYC	CB1-SG1	-12.81	1.54	1.81
1	D	62	GYC	CB1-SG1	-12.50	1.55	1.81
1	B	62	GYC	CB1-SG1	-12.39	1.55	1.81
1	A	62	GYC	CB1-SG1	-12.18	1.55	1.81
1	D	62	GYC	CA2-C2	-4.52	1.44	1.48
1	B	62	GYC	CA2-C2	-4.44	1.44	1.48
1	C	62	GYC	CA2-C2	-4.05	1.44	1.48
1	A	62	GYC	CA2-C2	-3.98	1.44	1.48
1	B	62	GYC	CG2-CB2	-3.31	1.40	1.46
1	C	62	GYC	CG2-CB2	-3.28	1.40	1.46
1	D	62	GYC	CG2-CB2	-3.15	1.40	1.46
1	A	62	GYC	CG2-CB2	-2.75	1.41	1.46
1	D	62	GYC	CE1-CZ	2.02	1.42	1.38
1	A	62	GYC	CE2-CD2	2.09	1.42	1.38
1	B	62	GYC	CE1-CZ	2.14	1.43	1.38
1	B	62	GYC	CD1-CG2	2.16	1.43	1.39
1	D	62	GYC	CE2-CD2	2.18	1.42	1.38
1	B	62	GYC	CE2-CD2	2.29	1.42	1.38
1	C	62	GYC	CE1-CZ	2.36	1.43	1.38
1	A	62	GYC	CE1-CZ	2.42	1.43	1.38
1	A	62	GYC	CD1-CG2	2.42	1.44	1.39
1	D	62	GYC	CD1-CG2	2.42	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GYC	CD1-CG2	2.54	1.44	1.39
1	C	62	GYC	CD2-CG2	2.61	1.44	1.39
1	D	62	GYC	CD2-CG2	2.69	1.44	1.39
1	A	62	GYC	CD2-CG2	2.85	1.44	1.39
1	B	62	GYC	CD2-CG2	2.96	1.45	1.39
1	C	62	GYC	CB2-CA2	4.78	1.39	1.35
1	A	62	GYC	CB2-CA2	5.33	1.39	1.35
1	B	62	GYC	CB2-CA2	5.42	1.39	1.35
1	D	62	GYC	CB2-CA2	5.60	1.39	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GYC	N3-C1-N2	-3.42	109.08	111.45
1	B	62	GYC	N3-C1-N2	-3.30	109.17	111.45
1	D	62	GYC	N3-C1-N2	-2.85	109.48	111.45
1	C	62	GYC	CA2-C2-N3	-2.72	102.12	103.30
1	B	62	GYC	CA2-C2-N3	-2.64	102.16	103.30
1	A	62	GYC	CA2-C2-N3	-2.59	102.18	103.30
1	C	62	GYC	N3-C1-N2	-2.57	109.67	111.45
1	D	62	GYC	CA1-C1-N3	-2.57	121.67	124.75
1	C	62	GYC	CA1-C1-N3	-2.45	121.81	124.75
1	D	62	GYC	CA2-C2-N3	-2.33	102.29	103.30
1	B	62	GYC	CA1-C1-N3	-2.20	122.11	124.75
1	D	62	GYC	O-C-CA3	-2.05	119.61	126.38
1	C	62	GYC	CB1-CA1-C1	2.08	114.59	110.44
1	B	62	GYC	CB1-CA1-C1	2.10	114.63	110.44
1	A	62	GYC	CB1-CA1-C1	2.20	114.84	110.44
1	D	62	GYC	CB1-CA1-C1	2.23	114.89	110.44
1	A	62	GYC	CA1-C1-N2	2.25	128.10	123.56
1	C	62	GYC	CA1-C1-N2	2.37	128.33	123.56
1	B	62	GYC	CA1-C1-N2	2.48	128.56	123.56
1	D	62	GYC	CA1-C1-N2	2.55	128.69	123.56
1	D	62	GYC	CA2-N2-C1	3.72	108.56	105.75
1	C	62	GYC	CA2-N2-C1	3.76	108.60	105.75
1	B	62	GYC	CA2-N2-C1	3.95	108.74	105.75
1	A	62	GYC	CA2-N2-C1	4.19	108.92	105.75
1	B	62	GYC	O2-C2-CA2	7.14	134.77	130.97
1	D	62	GYC	O2-C2-CA2	7.75	135.09	130.97
1	A	62	GYC	O2-C2-CA2	8.01	135.22	130.97
1	C	62	GYC	O2-C2-CA2	8.09	135.27	130.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	217/241 (90%)	-0.19	4 (1%) 68 71	11, 19, 39, 70	0
1	B	214/241 (88%)	-0.24	2 (0%) 84 86	13, 19, 40, 76	0
1	C	217/241 (90%)	0.09	7 (3%) 47 51	14, 22, 40, 74	0
1	D	216/241 (89%)	0.10	6 (2%) 53 56	14, 25, 47, 73	0
All	All	864/964 (89%)	-0.06	19 (2%) 62 65	11, 21, 41, 76	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	5.2
1	A	2	SER	4.6
1	D	2	SER	4.0
1	A	220	PRO	3.7
1	B	3	VAL	3.6
1	C	3	VAL	3.4
1	A	3	VAL	3.1
1	C	220	PRO	3.0
1	D	219	LEU	2.9
1	C	218	GLU	2.8
1	B	2	SER	2.6
1	A	219	LEU	2.4
1	C	221	ARG	2.3
1	C	219	LEU	2.3
1	D	73	GLU	2.2
1	C	4	ILE	2.2
1	D	165	GLY	2.1
1	D	3	VAL	2.1
1	D	6	PRO	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<sup>th</sup> 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	D	62	21/22	0.92	0.16	19,21,23,28	0
1	GYC	B	62	21/22	0.95	0.13	16,17,18,19	0
1	GYC	C	62	21/22	0.96	0.14	15,18,20,23	0
1	GYC	A	62	21/22	0.98	0.13	13,14,15,16	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.