



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:07 PM UTC

PDB ID : 2GX0 / pdb_00002gx0
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

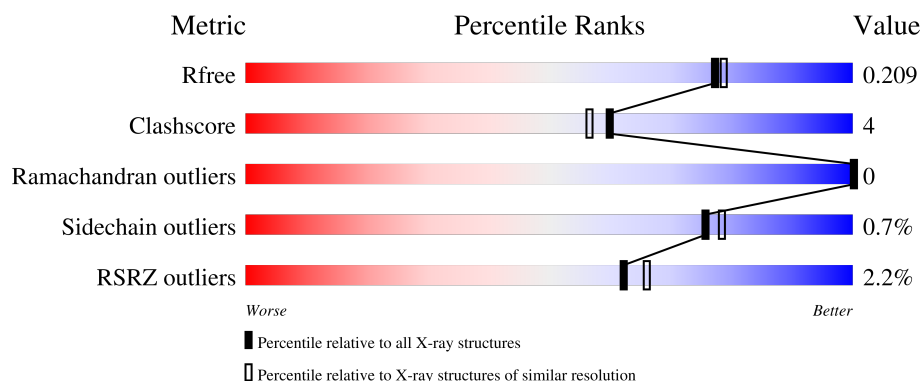
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	2% 82% 8% 10%
1	B	241	2% 79% 9% 11%
1	C	241	2% 80% 10% 10%
1	D	241	2% 80% 10% 10%

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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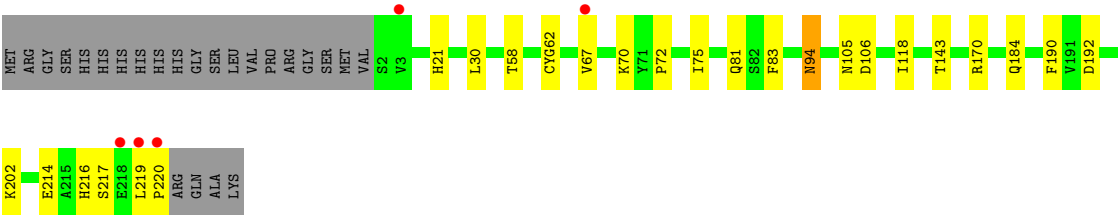
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q5TLG6
C	0	MET	-	expression tag	UNP Q5TLG6
C	1	VAL	-	expression tag	UNP Q5TLG6
C	62	GYC	CYS	chromophore	UNP Q5TLG6
C	62	GYC	TYR	chromophore	UNP Q5TLG6
C	62	GYC	GLY	chromophore	UNP Q5TLG6
D	-18	MET	-	expression tag	UNP Q5TLG6
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

- 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, α , β , γ	73.59Å 103.59Å 122.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-1.90) 91.8 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	17.8	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GYC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/1787	0.90	5/2412 (0.2%)
1	B	0.35	0/1760	0.90	8/2375 (0.3%)
1	C	0.35	0/1787	0.89	6/2412 (0.2%)
1	D	0.34	0/1776	0.88	6/2398 (0.3%)
All	All	0.35	0/7110	0.90	25/9597 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	N-CA-C	8.05	121.07	111.33
1	D	58	THR	N-CA-C	8.05	120.77	111.11
1	C	58	THR	N-CA-C	7.99	120.99	111.33
1	B	58	THR	N-CA-C	7.56	120.48	111.33
1	D	118	ILE	N-CA-C	6.57	118.05	108.53
1	B	202	LYS	N-CA-C	6.32	118.69	111.11
1	A	118	ILE	N-CA-C	6.10	117.37	108.53
1	A	166	GLY	N-CA-C	6.07	117.71	111.95
1	D	21	HIS	CA-C-N	5.86	125.77	119.85
1	D	21	HIS	C-N-CA	5.86	125.77	119.85
1	B	118	ILE	N-CA-C	5.79	116.92	108.53
1	D	202	LYS	N-CA-C	5.47	117.68	111.11
1	C	79	PHE	N-CA-C	5.41	118.00	111.40
1	C	21	HIS	CA-C-N	5.34	125.24	119.85
1	C	21	HIS	C-N-CA	5.34	125.24	119.85
1	A	67	VAL	N-CA-C	-5.32	104.59	112.04
1	B	170	ARG	N-CA-C	5.30	118.33	110.48
1	C	118	ILE	N-CA-C	5.29	116.20	108.53
1	B	67	VAL	N-CA-C	-5.27	104.50	111.09
1	A	170	ARG	N-CA-C	5.21	118.18	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	LYS	N-CA-C	5.19	117.34	111.11
1	B	124	ASN	N-CA-C	5.17	118.85	112.24
1	D	170	ARG	N-CA-C	5.04	117.94	110.48
1	B	32	LYS	CA-C-N	5.03	125.05	119.32
1	B	32	LYS	C-N-CA	5.03	125.05	119.32

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	1688	15	0
1	B	1736	0	1657	14	0
1	C	1762	0	1688	16	0
1	D	1751	0	1675	16	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	6708	59	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 (59) 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:D:94:ASN:C	1:D:94:ASN:HD22	2.06	0.63
1:C:216:HIS:CE1	1:C:219:LEU:HD21	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:A:74:ASN:H	1.49	0.60
1:B:72:PRO:HB2	1:B:74:ASN:ND2	2.18	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:H	1:C:74:ASN:HD22	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:HD22	1:A:74:ASN:N	2.05	0.50
1:A:198:LYS:HB2	1:A:208:ASN:HD22	1.76	0.49
1:C:74:ASN:HD22	1:C:74:ASN:N	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:219:LEU:HA	1:A:220:PRO:C	2.39	0.47
1:A:208:ASN:ND2	1:A:210:HIS:CE1	2.82	0.47
1:B:74:ASN:HD22	1:B:74:ASN:N	2.10	0.46
1:D:81:GLN:HE22	1:D:184:GLN:H	1.64	0.46
1:D:190:PHE:HB2	1:D:216:HIS:CE1	2.50	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
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:D:216:HIS:CE1	1:D:219:LEU:HD21	2.54	0.42
1:A:12:LEU:HD12	1:A:12:LEU:C	2.45	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:B:12:LEU:C	1:B:12:LEU:HD12	2.45	0.41
1:C:45:LYS:HA	1:C:45:LYS:HE2	2.03	0.41
1:C:145:LYS:NZ	1:D:143:THR:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD12	1:C:12:LEU:C	2.46	0.41
1:D:105:ASN:HD22	1:D:106:ASP:N	2.18	0.41
1:D:219:LEU:HA	1:D:220:PRO:C	2.45	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 [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	213/241 (88%)	211 (99%)	2 (1%)	0	100	100
1	B	210/241 (87%)	209 (100%)	1 (0%)	0	100	100
1	C	213/241 (88%)	211 (99%)	2 (1%)	0	100	100
1	D	212/241 (88%)	210 (99%)	2 (1%)	0	100	100
All	All	848/964 (88%)	841 (99%)	7 (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	188/207 (91%)	187 (100%)	1 (0%)	81	84
1	B	185/207 (89%)	183 (99%)	2 (1%)	65	67
1	C	188/207 (91%)	187 (100%)	1 (0%)	81	84
1	D	187/207 (90%)	186 (100%)	1 (0%)	81	84
All	All	748/828 (90%)	743 (99%)	5 (1%)	76	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	B	74	ASN
1	B	157	VAL
1	C	74	ASN
1	D	94	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	94	ASN
1	A	105	ASN
1	A	128	ASN
1	A	158	ASN
1	A	184	GLN
1	A	194	HIS
1	A	208	ASN
1	A	210	HIS
1	A	216	HIS
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	21	HIS
1	C	38	GLN

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Mol	Chain	Res	Type
1	C	74	ASN
1	C	81	GLN
1	C	94	ASN
1	C	105	ASN
1	C	158	ASN
1	C	194	HIS
1	C	208	ASN
1	C	210	HIS
1	D	81	GLN
1	D	94	ASN
1	D	105	ASN
1	D	124	ASN
1	D	158	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	C	62	1	21,22,23	3.48	8 (38%)	26,30,32	2.24	7 (26%)
1	GYC	A	62	1	21,22,23	3.38	8 (38%)	26,30,32	2.30	6 (23%)
1	GYC	D	62	1	21,22,23	3.46	8 (38%)	26,30,32	2.24	7 (26%)
1	GYC	B	62	1	21,22,23	3.46	8 (38%)	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	C	62	1	-	2/10/29/30	0/2/2/2
1	GYC	A	62	1	-	1/10/29/30	0/2/2/2
1	GYC	D	62	1	-	1/10/29/30	0/2/2/2
1	GYC	B	62	1	-	2/10/29/30	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GYC	CB1-SG1	-13.18	1.54	1.81
1	D	62	GYC	CB1-SG1	-12.85	1.55	1.81
1	B	62	GYC	CB1-SG1	-12.74	1.55	1.81
1	A	62	GYC	CB1-SG1	-12.53	1.55	1.81
1	D	62	GYC	CB2-CA2	4.89	1.39	1.35
1	B	62	GYC	CB2-CA2	4.73	1.39	1.35
1	A	62	GYC	CB2-CA2	4.65	1.39	1.35
1	C	62	GYC	CB2-CA2	4.16	1.39	1.35
1	D	62	GYC	CA2-C2	-4.09	1.44	1.48
1	B	62	GYC	CA2-C2	-4.02	1.44	1.48
1	C	62	GYC	CA2-C2	-3.67	1.44	1.48
1	B	62	GYC	CG2-CB2	-3.61	1.40	1.46
1	A	62	GYC	CA2-C2	-3.60	1.44	1.48
1	C	62	GYC	CG2-CB2	-3.58	1.40	1.46
1	D	62	GYC	CG2-CB2	-3.44	1.40	1.46
1	A	62	GYC	CG2-CB2	-3.00	1.41	1.46
1	B	62	GYC	CD2-CG2	2.80	1.45	1.39
1	A	62	GYC	CD2-CG2	2.70	1.44	1.39
1	D	62	GYC	CD2-CG2	2.54	1.44	1.39
1	C	62	GYC	CD2-CG2	2.47	1.44	1.39
1	B	62	GYC	CE2-CD2	2.46	1.42	1.38
1	A	62	GYC	CE1-CZ	2.44	1.43	1.39
1	C	62	GYC	CD1-CG2	2.40	1.44	1.39
1	C	62	GYC	CE1-CZ	2.38	1.43	1.39
1	D	62	GYC	CE2-CD2	2.34	1.42	1.38
1	D	62	GYC	CD1-CG2	2.29	1.44	1.39
1	A	62	GYC	CD1-CG2	2.29	1.44	1.39
1	A	62	GYC	CE2-CD2	2.24	1.42	1.38
1	B	62	GYC	CE1-CZ	2.15	1.43	1.39
1	C	62	GYC	CE2-CD2	2.08	1.42	1.38
1	B	62	GYC	CD1-CG2	2.04	1.43	1.39
1	D	62	GYC	CE1-CZ	2.03	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	GYC	O2-C2-CA2	6.65	135.27	131.02
1	A	62	GYC	O2-C2-CA2	6.59	135.22	131.02
1	D	62	GYC	O2-C2-CA2	6.38	135.09	131.02
1	B	62	GYC	O2-C2-CA2	5.87	134.77	131.02
1	A	62	GYC	C2-N3-C1	5.15	110.45	108.07
1	B	62	GYC	C2-N3-C1	5.01	110.39	108.07
1	D	62	GYC	C2-N3-C1	4.84	110.31	108.07
1	C	62	GYC	C3-CA3-N3	4.71	123.14	112.43
1	D	62	GYC	C3-CA3-N3	4.58	122.86	112.43
1	A	62	GYC	C3-CA3-N3	4.54	122.75	112.43
1	C	62	GYC	C2-N3-C1	4.47	110.14	108.07
1	B	62	GYC	C3-CA3-N3	4.44	122.53	112.43
1	A	62	GYC	CA2-N2-C1	4.00	108.92	105.80
1	B	62	GYC	CA2-N2-C1	3.76	108.74	105.80
1	C	62	GYC	CA2-N2-C1	3.58	108.60	105.80
1	D	62	GYC	CA2-N2-C1	3.54	108.56	105.80
1	A	62	GYC	N3-C1-N2	-3.04	109.08	111.48
1	B	62	GYC	N3-C1-N2	-2.94	109.17	111.48
1	D	62	GYC	CA1-C1-N2	2.63	128.69	123.57
1	B	62	GYC	CA1-C1-N2	2.56	128.56	123.57
1	D	62	GYC	N3-C1-N2	-2.54	109.48	111.48
1	C	62	GYC	CA1-C1-N2	2.44	128.33	123.57
1	D	62	GYC	CA1-C1-N3	-2.43	121.67	124.84
1	C	62	GYC	CA1-C1-N3	-2.33	121.81	124.84
1	A	62	GYC	CA1-C1-N2	2.32	128.10	123.57
1	C	62	GYC	N3-C1-N2	-2.30	109.67	111.48
1	B	62	GYC	CA1-C1-N3	-2.10	122.11	124.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	GYC	C3-CA3-N3-C2
1	B	62	GYC	C3-CA3-N3-C2
1	C	62	GYC	C3-CA3-N3-C2
1	D	62	GYC	C3-CA3-N3-C2
1	C	62	GYC	C3-CA3-N3-C1
1	B	62	GYC	C3-CA3-N3-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/241 (90%)	-0.28	4 (1%) 67 71	11, 19, 39, 70	0
1	B	214/241 (88%)	-0.36	4 (1%) 66 70	13, 19, 40, 76	0
1	C	217/241 (90%)	-0.11	6 (2%) 55 59	14, 22, 40, 74	0
1	D	216/241 (89%)	-0.00	5 (2%) 61 65	14, 25, 47, 73	0
All	All	864/964 (89%)	-0.19	19 (2%) 62 66	11, 21, 41, 76	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	3.4
1	D	219	LEU	3.3
1	A	220	PRO	3.3
1	C	220	PRO	3.0
1	D	220	PRO	2.6
1	D	218	GLU	2.5
1	B	4	ILE	2.4
1	C	4	ILE	2.4
1	D	67	VAL	2.4
1	A	219	LEU	2.3
1	C	2	SER	2.2
1	A	182	VAL	2.2
1	C	221	ARG	2.2
1	C	30	LEU	2.2
1	D	3	VAL	2.1
1	A	3	VAL	2.1
1	B	73	GLU	2.1
1	C	3	VAL	2.1
1	B	2	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GYC	D	62	21/22	0.92	0.07	19,21,23,28	0
1	GYC	C	62	21/22	0.96	0.06	15,18,20,23	0
1	GYC	B	62	21/22	0.96	0.06	16,17,18,19	0
1	GYC	A	62	21/22	0.97	0.05	13,14,15,16	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.