



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:53 PM UTC

PDB ID : 4UTS / pdb\_00004uts  
Title : Room temperature crystal structure of the fast switching M159T mutant of fluorescent protein Dronpa  
Authors : Kaucikas, M.; Fitzpatrick, A.; Bryan, E.; Struve, A.; Henning, R.; Kosheleva, I.; Srajer, V.; van Thor, J.J.  
Deposited on : 2014-07-22  
Resolution : 2.03 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.

The types of validation reports are described at

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

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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

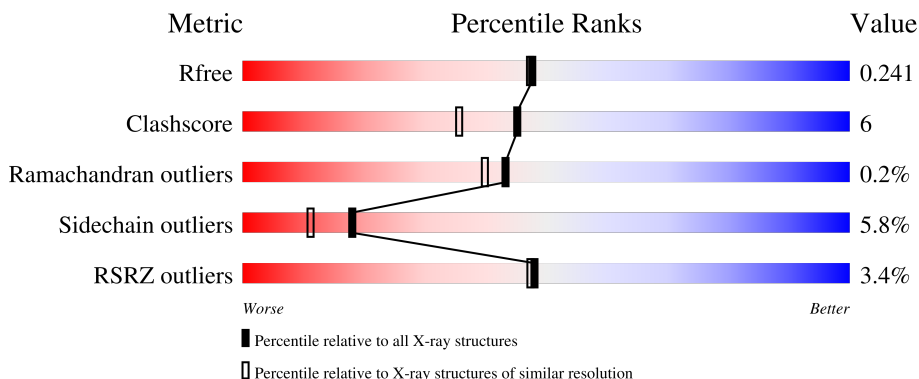
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


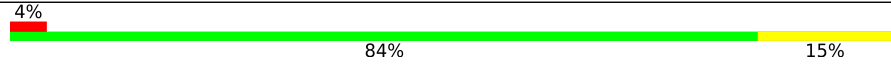
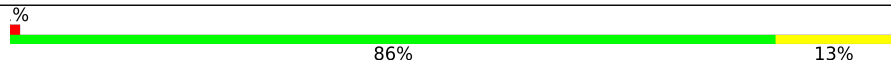

The reported resolution of this entry is 2.03 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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  $\geq 3$ , 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	214	
1	B	214	
1	C	214	
1	D	214	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7146 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
			Total	C	N	O	S			
1	A	214	1726	1102	291	324	9	0	0	0
1	B	214	1726	1102	291	324	9	0	0	0
1	C	214	1726	1102	291	324	9	0	0	0
1	D	214	1726	1102	291	324	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GYC	CYS	chromophore	UNP Q5TLG6
A	63	GYC	TYR	chromophore	UNP Q5TLG6
A	63	GYC	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	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	THR	MET	engineered mutation	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	THR	MET	engineered mutation	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	THR	MET	engineered mutation	UNP Q5TLG6

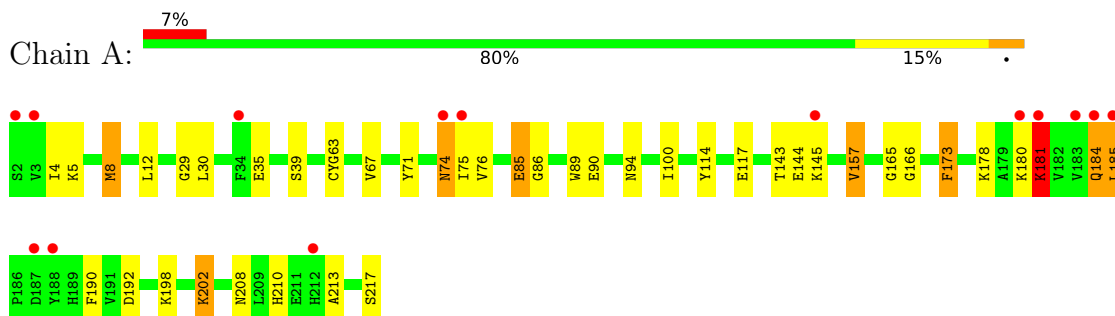
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	55	Total O 55 55	0	0
2	C	62	Total O 62 62	0	0
2	D	56	Total O 56 56	0	0

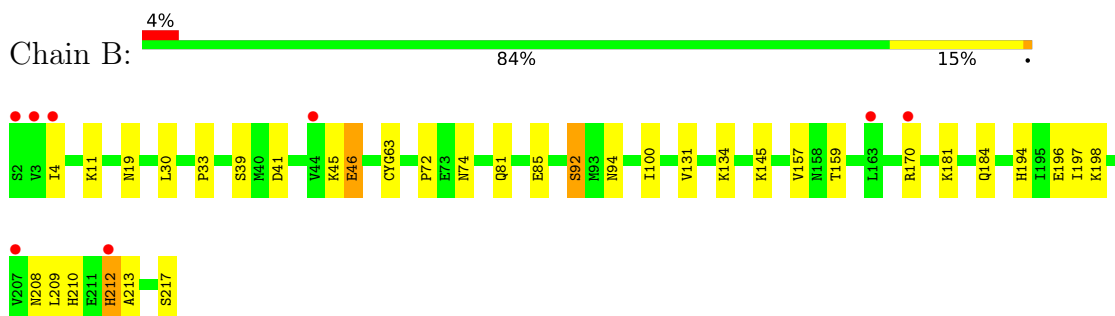
### 3 Residue-property plots [i](#)

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.

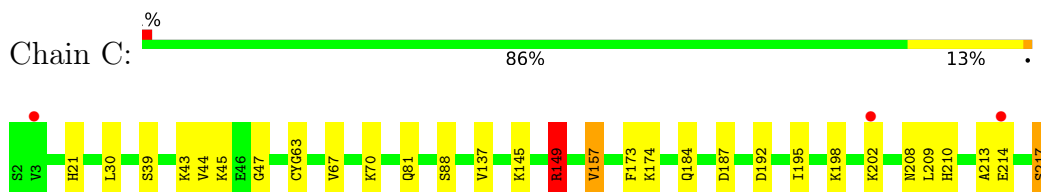
- Molecule 1: FLUORESCENT PROTEIN DRONPA



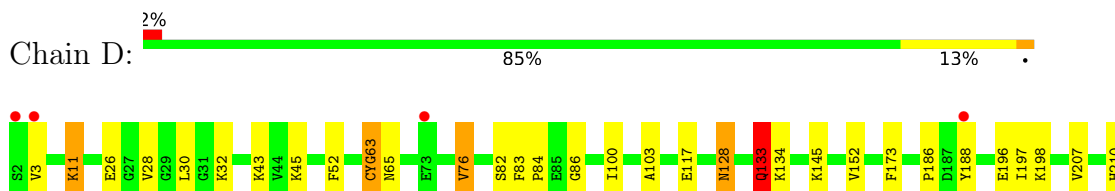
- Molecule 1: FLUORESCENT PROTEIN DRONPA



- 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, $\alpha$ , $\beta$ , $\gamma$	75.66Å 111.14Å 117.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.63 – 2.03 55.63 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.8 (55.63-2.03) 98.9 (55.63-2.03)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.172 , 0.213 (Not available) , 0.241	Depositor DCC
$R_{free}$ test set	3286 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 i

### 5.1 Standard geometry i

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	1.26	2/1750 (0.1%)	1.25	10/2363 (0.4%)
1	B	1.19	4/1750 (0.2%)	1.12	1/2363 (0.0%)
1	C	1.35	4/1750 (0.2%)	1.16	5/2363 (0.2%)
1	D	1.35	6/1750 (0.3%)	1.17	4/2363 (0.2%)
All	All	1.29	16/7000 (0.2%)	1.18	20/9452 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLY	N-CA	6.79	1.54	1.45
1	D	52	PHE	C-O	-6.22	1.16	1.23
1	B	197	ILE	CA-C	6.01	1.59	1.52
1	D	133	GLN	C-O	6.01	1.31	1.24
1	C	45	LYS	C-O	-6.00	1.16	1.24
1	C	44	VAL	C-O	-5.93	1.18	1.24
1	C	195	ILE	C-O	-5.80	1.18	1.24
1	D	117	GLU	CA-C	5.60	1.59	1.52
1	A	89	TRP	C-O	5.59	1.30	1.23
1	B	213	ALA	CA-C	-5.52	1.45	1.52
1	B	92	SER	N-CA	-5.45	1.39	1.46
1	D	103	ALA	CA-C	5.40	1.59	1.52
1	D	207	VAL	N-CA	-5.37	1.39	1.46
1	D	197	ILE	N-CA	-5.37	1.40	1.46
1	B	45	LYS	CA-C	-5.34	1.49	1.52
1	C	137	VAL	C-O	-5.24	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ARG	NE-CZ-NH2	-9.16	110.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ARG	NE-CZ-NH1	7.96	129.46	121.50
1	A	166	GLY	N-CA-C	-7.61	104.72	111.95
1	D	212	HIS	CB-CA-C	7.56	122.24	110.14
1	B	92	SER	CA-CB-OG	-7.46	96.17	111.10
1	D	173	PHE	CB-CA-C	-7.05	95.91	109.37
1	A	71	TYR	CA-C-N	-6.41	114.18	120.52
1	A	71	TYR	C-N-CA	-6.41	114.18	120.52
1	D	100	ILE	CB-CA-C	-6.33	100.29	110.28
1	A	185	LEU	CA-C-N	-6.18	114.40	120.52
1	A	185	LEU	C-N-CA	-6.18	114.40	120.52
1	A	185	LEU	CA-CB-CG	5.91	136.98	116.30
1	A	173	PHE	CB-CA-C	-5.44	99.59	109.38
1	C	173	PHE	CB-CA-C	-5.28	99.88	109.38
1	A	157	VAL	CB-CA-C	5.25	118.57	110.28
1	C	137	VAL	CB-CA-C	-5.23	106.47	111.44
1	A	100	ILE	CB-CA-C	-5.15	102.81	110.33
1	A	12	LEU	N-CA-C	5.11	116.84	109.07
1	D	133	GLN	N-CA-C	5.05	119.44	113.28
1	C	157	VAL	CA-CB-CG1	5.03	118.94	110.40

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	1726	0	1649	22	0
1	B	1726	0	1650	27	0
1	C	1726	0	1650	15	0
1	D	1726	0	1649	15	0
2	A	69	0	0	10	0
2	B	55	0	0	9	0
2	C	62	0	0	6	0
2	D	56	0	0	5	0
All	All	7146	0	6598	78	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 6.

All (78) 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:C:88:SER:HB3	2:C:2030:HOH:O	1.13	1.24
1:C:187:ASP:HB3	2:C:2058:HOH:O	1.38	1.21
1:D:82:SER:HB2	2:D:2028:HOH:O	1.41	1.20
1:A:192:ASP:OD1	2:A:2054:HOH:O	1.61	1.17
1:C:88:SER:CB	2:C:2030:HOH:O	1.67	1.16
1:B:217:SER:O	2:B:2055:HOH:O	1.70	1.09
1:B:19:ASN:CG	2:B:2006:HOH:O	1.94	1.08
1:A:86:GLY:O	2:A:2029:HOH:O	1.70	1.08
1:B:19:ASN:ND2	2:B:2006:HOH:O	1.84	1.05
1:B:46:GLU:OE2	2:B:2003:HOH:O	1.91	0.89
1:A:85:GLU:CD	1:A:181:LYS:HD2	1.99	0.87
1:A:143:THR:HG23	2:A:2054:HOH:O	1.75	0.86
1:D:63:GYC:CA3	1:D:65:ASN:N	2.41	0.84
1:B:94:ASN:HD22	1:B:100:ILE:CD1	1.99	0.76
1:D:128:ASN:HB3	2:D:2040:HOH:O	1.89	0.71
2:A:2058:HOH:O	1:C:145:LYS:NZ	2.24	0.70
1:B:46:GLU:N	1:B:46:GLU:CD	2.51	0.69
1:C:81:GLN:HE22	1:C:184:GLN:H	1.41	0.69
1:A:29:GLY:HA2	2:A:2006:HOH:O	1.93	0.67
1:C:217:SER:O	2:C:2062:HOH:O	2.13	0.67
2:A:2060:HOH:O	1:C:149:ARG:HD3	1.94	0.67
1:B:94:ASN:HD22	1:B:100:ILE:HD11	1.59	0.66
1:B:46:GLU:CD	1:B:46:GLU:H	2.04	0.66
1:D:63:GYC:C3	1:D:65:ASN:CA	2.75	0.64
1:C:217:SER:C	2:C:2062:HOH:O	2.39	0.64
1:B:41:ASP:OD2	2:B:2007:HOH:O	2.15	0.63
1:B:196:GLU:CD	2:B:2052:HOH:O	2.44	0.61
1:A:85:GLU:CD	1:A:181:LYS:CD	2.74	0.60
1:D:26:GLU:OE1	1:D:45:LYS:NZ	2.34	0.60
1:B:198:LYS:HG3	1:B:210:HIS:CD2	2.37	0.59
1:A:4:ILE:HG23	1:A:8:MET:HE2	1.84	0.59
1:B:81:GLN:HE22	1:B:184:GLN:H	1.50	0.59
1:B:46:GLU:N	1:B:46:GLU:OE1	2.35	0.59
1:D:196:GLU:CD	2:D:2051:HOH:O	2.48	0.57
1:D:76:VAL:HB	1:D:186:PRO:HB3	1.87	0.56
1:B:94:ASN:HD22	1:B:100:ILE:HD13	1.69	0.56
1:D:188:TYR:HB2	2:D:2048:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:NZ	2:A:2066:HOH:O	2.39	0.55
1:B:145:LYS:HD3	2:B:2041:HOH:O	2.07	0.54
1:A:217:SER:HA	2:A:2068:HOH:O	2.07	0.54
1:B:94:ASN:ND2	1:B:100:ILE:HD11	2.23	0.53
1:A:85:GLU:CG	1:A:181:LYS:HD2	2.38	0.53
1:A:4:ILE:HG23	1:A:8:MET:CE	2.39	0.52
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.91	0.52
1:B:194:HIS:HB3	1:B:212:HIS:HD2	1.73	0.52
1:A:180:LYS:N	2:A:2029:HOH:O	2.05	0.52
1:B:134:LYS:C	2:B:2035:HOH:O	2.52	0.52
1:D:11:LYS:HD2	1:D:28:VAL:HG12	1.92	0.52
1:D:86:GLY:O	2:D:2028:HOH:O	2.20	0.49
1:D:30:LEU:HD12	1:D:30:LEU:O	2.13	0.49
1:A:90:GLU:OE1	1:B:19:ASN:ND2	2.43	0.49
1:D:198:LYS:HG3	1:D:210:HIS:CD2	2.48	0.48
1:C:21:HIS:HE1	1:C:47:GLY:O	1.97	0.48
1:D:30:LEU:HD12	1:D:30:LEU:C	2.39	0.48
1:B:4:ILE:HD11	1:B:33:PRO:CB	2.44	0.47
1:B:72:PRO:HB2	1:B:74:ASN:OD1	2.14	0.47
1:B:159:THR:O	1:B:170:ARG:NH1	2.47	0.47
1:D:133:GLN:O	1:D:134:LYS:HB2	2.14	0.47
1:B:4:ILE:HD11	1:B:33:PRO:HB3	1.97	0.47
1:A:198:LYS:HB2	1:A:208:ASN:HD22	1.80	0.46
1:A:39:SER:HB2	1:A:210:HIS:CD2	2.51	0.46
1:B:198:LYS:HB2	1:B:208:ASN:HD22	1.81	0.45
1:B:85:GLU:OE1	1:B:181:LYS:NZ	2.42	0.45
1:C:39:SER:HA	1:C:209:LEU:O	2.16	0.45
1:B:46:GLU:CD	2:B:2003:HOH:O	2.52	0.44
1:A:76:VAL:HG11	1:A:184:GLN:HB2	2.00	0.43
1:A:192:ASP:O	1:A:213:ALA:HA	2.18	0.43
1:C:192:ASP:O	1:C:213:ALA:HA	2.18	0.43
1:A:8:MET:HE3	1:A:114:TYR:OH	2.19	0.43
1:C:88:SER:OG	2:C:2030:HOH:O	2.02	0.43
1:C:198:LYS:HG3	1:C:210:HIS:CD2	2.54	0.43
1:A:198:LYS:HG3	1:A:210:HIS:CD2	2.55	0.42
1:C:43:LYS:HB2	1:C:43:LYS:HE2	1.93	0.42
1:B:39:SER:HA	1:B:209:LEU:O	2.18	0.41
1:A:180:LYS:CB	2:A:2029:HOH:O	2.68	0.41
1:A:94:ASN:C	1:A:94:ASN:HD22	2.28	0.40
1:C:198:LYS:HB2	1:C:208:ASN:HD22	1.86	0.40
1:A:144:GLU:O	1:A:190:PHE:HA	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	209/214 (98%)	200 (96%)	7 (3%)	2 (1%)	12	5
1	B	209/214 (98%)	207 (99%)	2 (1%)	0	100	100
1	C	209/214 (98%)	208 (100%)	1 (0%)	0	100	100
1	D	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
All	All	836/856 (98%)	820 (98%)	14 (2%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	181	LYS

### 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	184/184 (100%)	167 (91%)	17 (9%)	8	3
1	B	184/184 (100%)	177 (96%)	7 (4%)	29	23
1	C	184/184 (100%)	175 (95%)	9 (5%)	22	15
1	D	184/184 (100%)	174 (95%)	10 (5%)	20	13
All	All	736/736 (100%)	693 (94%)	43 (6%)	18	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	MET
1	A	30	LEU
1	A	35	GLU
1	A	67	VAL
1	A	74	ASN
1	A	75	ILE
1	A	85	GLU
1	A	117	GLU
1	A	145	LYS
1	A	157	VAL
1	A	173	PHE
1	A	178	LYS
1	A	181	LYS
1	A	184	GLN
1	A	185	LEU
1	A	202	LYS
1	B	11	LYS
1	B	30	LEU
1	B	46	GLU
1	B	92	SER
1	B	131	VAL
1	B	157	VAL
1	B	212	HIS
1	C	30	LEU
1	C	67	VAL
1	C	70	LYS
1	C	149	ARG
1	C	157	VAL
1	C	174	LYS
1	C	202	LYS
1	C	214	GLU
1	C	217	SER
1	D	3	VAL
1	D	11	LYS
1	D	32	LYS
1	D	43	LYS
1	D	76	VAL
1	D	128	ASN
1	D	133	GLN
1	D	145	LYS
1	D	152	VAL

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Mol	Chain	Res	Type
1	D	212	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	94	ASN
1	A	102	ASN
1	A	206	ASN
1	A	208	ASN
1	A	212	HIS
1	A	216	HIS
1	B	19	ASN
1	B	81	GLN
1	B	94	ASN
1	B	102	ASN
1	B	194	HIS
1	B	206	ASN
1	B	208	ASN
1	B	210	HIS
1	B	212	HIS
1	C	21	HIS
1	C	81	GLN
1	C	102	ASN
1	C	158	ASN
1	C	194	HIS
1	C	208	ASN
1	D	38	GLN
1	D	102	ASN
1	D	128	ASN
1	D	208	ASN
1	D	210	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	63	1	21,22,23	2.67	5 (23%)	26,30,32	2.52	11 (42%)
1	GYC	B	63	1	21,22,23	2.68	8 (38%)	26,30,32	2.70	10 (38%)
1	GYC	D	63	1	21,22,23	3.63	9 (42%)	26,30,32	3.30	11 (42%)
1	GYC	A	63	1	21,22,23	4.08	8 (38%)	26,30,32	3.13	8 (30%)

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	63	1	-	3/10/29/30	0/2/2/2
1	GYC	B	63	1	-	2/10/29/30	0/2/2/2
1	GYC	D	63	1	-	2/10/29/30	0/2/2/2
1	GYC	A	63	1	-	2/10/29/30	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB2-CA2	13.54	1.48	1.35
1	D	63	GYC	CB2-CA2	12.17	1.46	1.35
1	B	63	GYC	CB2-CA2	8.48	1.43	1.35
1	C	63	GYC	CB2-CA2	7.89	1.42	1.35
1	A	63	GYC	CB1-CA1	-7.72	1.44	1.53
1	D	63	GYC	CA2-C2	-5.92	1.42	1.48
1	A	63	GYC	C1-N2	5.71	1.40	1.32
1	D	63	GYC	C1-N2	5.41	1.40	1.32
1	C	63	GYC	C1-N2	4.63	1.39	1.32
1	A	63	GYC	CA2-C2	-4.46	1.43	1.48
1	C	63	GYC	CA2-C2	-4.22	1.44	1.48
1	D	63	GYC	CB1-CA1	-4.17	1.48	1.53
1	C	63	GYC	CB1-CA1	-4.16	1.48	1.53
1	A	63	GYC	O2-C2	3.98	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	GYC	C2-N3	-3.80	1.31	1.40
1	A	63	GYC	CB1-SG1	-3.65	1.73	1.81
1	C	63	GYC	O2-C2	3.60	1.30	1.23
1	B	63	GYC	CA2-C2	-3.50	1.44	1.48
1	B	63	GYC	CB1-CA1	-3.48	1.49	1.53
1	D	63	GYC	O2-C2	3.46	1.30	1.23
1	D	63	GYC	C2-N3	-3.16	1.32	1.40
1	B	63	GYC	C1-N2	3.08	1.36	1.32
1	B	63	GYC	CA2-N2	-2.82	1.32	1.38
1	D	63	GYC	C1-N3	2.71	1.41	1.37
1	A	63	GYC	CA2-N2	-2.50	1.33	1.38
1	B	63	GYC	O2-C2	2.43	1.28	1.23
1	A	63	GYC	C1-N3	2.28	1.41	1.37
1	D	63	GYC	CA2-N2	-2.25	1.33	1.38
1	B	63	GYC	CA3-N3	-2.15	1.43	1.47
1	D	63	GYC	CA1-N1	-2.09	1.38	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	O2-C2-CA2	-10.68	124.21	131.02
1	D	63	GYC	O2-C2-CA2	-10.39	124.39	131.02
1	B	63	GYC	O2-C2-CA2	-7.79	126.05	131.02
1	D	63	GYC	CA2-C2-N3	6.38	108.86	103.50
1	C	63	GYC	CB2-CA2-N2	-6.13	120.43	128.76
1	C	63	GYC	CB2-CA2-C2	5.79	129.38	122.36
1	B	63	GYC	CB2-CA2-C2	5.64	129.19	122.36
1	D	63	GYC	CB2-CA2-C2	5.61	129.16	122.36
1	A	63	GYC	CA2-C2-N3	5.29	107.94	103.50
1	A	63	GYC	N3-C1-N2	-5.14	107.43	111.48
1	D	63	GYC	N3-C1-N2	-5.04	107.51	111.48
1	D	63	GYC	CB2-CA2-N2	-4.74	122.33	128.76
1	C	63	GYC	O2-C2-CA2	-4.64	128.06	131.02
1	B	63	GYC	CB2-CA2-N2	-4.59	122.53	128.76
1	B	63	GYC	CA2-C2-N3	4.21	107.03	103.50
1	A	63	GYC	CB2-CA2-C2	4.06	127.28	122.36
1	C	63	GYC	C3-CA3-N3	3.99	121.50	112.43
1	A	63	GYC	CA2-N2-C1	3.70	108.69	105.80
1	A	63	GYC	CA1-C1-N3	3.49	129.38	124.84
1	A	63	GYC	C3-CA3-N3	3.39	120.15	112.43
1	A	63	GYC	CB2-CA2-N2	-3.10	124.55	128.76
1	D	63	GYC	C3-CA3-N3	3.04	119.35	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GYC	C2-N3-C1	2.96	109.44	108.07
1	B	63	GYC	CA1-C1-N3	2.88	128.59	124.84
1	C	63	GYC	CD1-CG2-CB2	-2.86	111.39	121.22
1	B	63	GYC	CD2-CE2-CZ	2.83	122.88	119.88
1	C	63	GYC	N3-C1-N2	-2.78	109.29	111.48
1	C	63	GYC	CD1-CE1-CZ	2.52	122.55	119.88
1	B	63	GYC	N3-C1-N2	-2.52	109.50	111.48
1	D	63	GYC	CA1-C1-N2	2.50	128.46	123.57
1	B	63	GYC	CD1-CG2-CB2	-2.46	112.77	121.22
1	D	63	GYC	CD1-CG2-CB2	-2.43	112.86	121.22
1	D	63	GYC	CA2-N2-C1	2.40	107.68	105.80
1	D	63	GYC	CE2-CD2-CG2	-2.40	118.13	121.22
1	C	63	GYC	CD2-CG2-CB2	2.35	129.28	121.22
1	B	63	GYC	CE2-CD2-CG2	-2.32	118.23	121.22
1	C	63	GYC	CE1-CD1-CG2	-2.19	118.39	121.22
1	D	63	GYC	CA1-CB1-SG1	2.08	118.84	114.40
1	B	63	GYC	CA3-N3-C2	2.07	128.22	123.67
1	C	63	GYC	CA2-C2-N3	2.06	105.23	103.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	GYC	C3-CA3-N3-C2
1	B	63	GYC	C3-CA3-N3-C1
1	B	63	GYC	C3-CA3-N3-C2
1	C	63	GYC	C3-CA3-N3-C2
1	D	63	GYC	C3-CA3-N3-C1
1	D	63	GYC	C3-CA3-N3-C2
1	A	63	GYC	C3-CA3-N3-C1
1	C	63	GYC	C3-CA3-N3-C1
1	C	63	GYC	N1-CA1-CB1-SG1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	63	GYC	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	63:GYC	C3	65:ASN	N	1.79
1	A	63:GYC	C3	65:ASN	N	1.66
1	B	63:GYC	C3	65:ASN	N	1.61

## 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	213/214 (99%)	0.25	14 (6%) 24 23	19, 34, 71, 126	0
1	B	213/214 (99%)	0.34	8 (3%) 44 43	22, 39, 64, 87	0
1	C	213/214 (99%)	-0.25	3 (1%) 73 73	17, 27, 46, 80	0
1	D	213/214 (99%)	-0.01	4 (1%) 66 66	17, 31, 58, 88	0
All	All	852/856 (99%)	0.08	29 (3%) 48 47	17, 33, 63, 126	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	5.8
1	A	185	LEU	5.6
1	A	187	ASP	3.4
1	A	183	VAL	3.4
1	A	188	TYR	3.1
1	D	3	VAL	3.0
1	B	4	ILE	2.9
1	B	3	VAL	2.7
1	A	2	SER	2.6
1	A	75	ILE	2.6
1	B	2	SER	2.6
1	A	145	LYS	2.5
1	A	184	GLN	2.5
1	A	34	PHE	2.5
1	B	170	ARG	2.4
1	A	74	ASN	2.3
1	D	2	SER	2.3
1	C	214	GLU	2.2
1	D	188	TYR	2.2
1	A	180	LYS	2.2
1	C	202	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	73	GLU	2.1
1	B	44	VAL	2.1
1	B	207	VAL	2.1
1	B	163	LEU	2.1
1	A	181	LYS	2.1
1	C	3	VAL	2.1
1	B	212	HIS	2.0
1	A	212	HIS	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(Å <sup>2</sup> )	Q<0.9
1	GYC	B	63	21/22	0.94	0.09	29,33,37,45	0
1	GYC	A	63	21/22	0.96	0.07	22,24,29,31	0
1	GYC	D	63	21/22	0.96	0.06	20,23,29,30	0
1	GYC	C	63	21/22	0.97	0.06	17,19,24,27	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.