



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:45 am BST

PDB ID : 4UTS
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

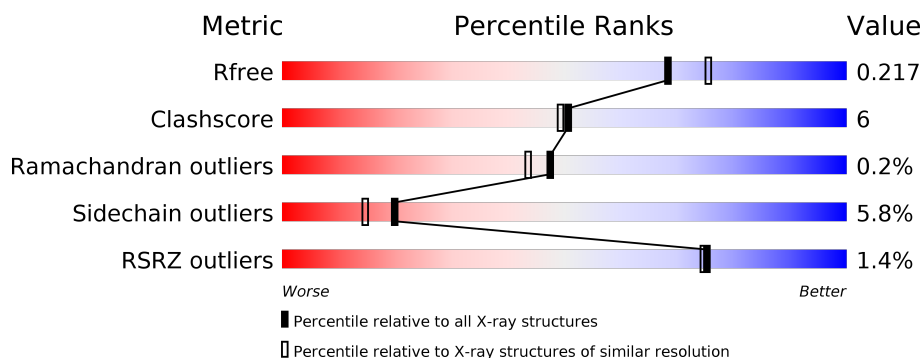
1 Overall quality at a glance

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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (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 on 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	214	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> </div>
1	B	214	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div> </div>
1	C	214	<div> <div></div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	D	214	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div> </div>

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
1	A	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	B	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	C	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			
1	D	214	Total	C	N	O	S	0	0	0
			1726	1102	291	324	9			

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

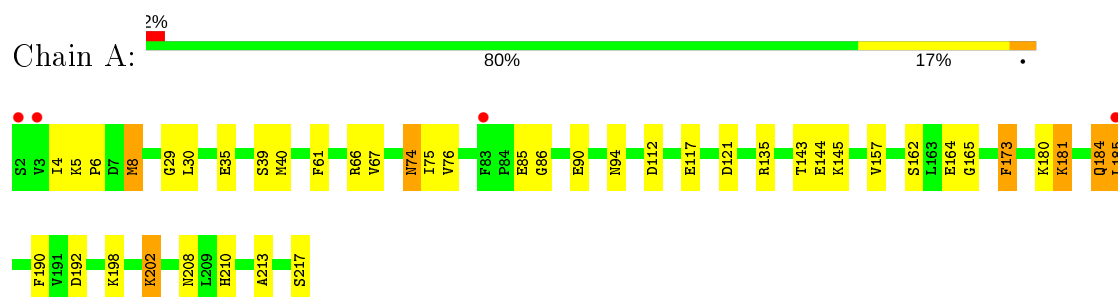
- Molecule 2 is water.

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

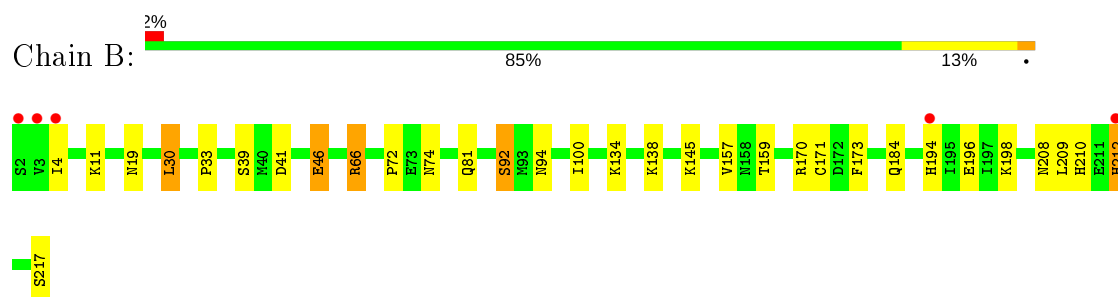
3 Residue-property plots [i](#)

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.

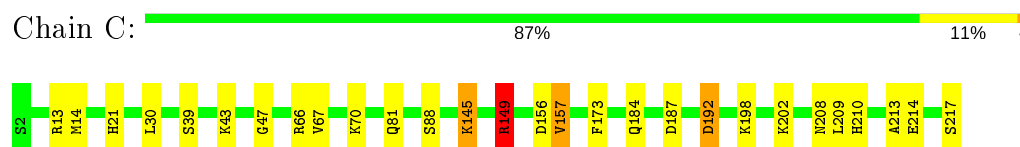
• Molecule 1: FLUORESCENT PROTEIN DRONPA



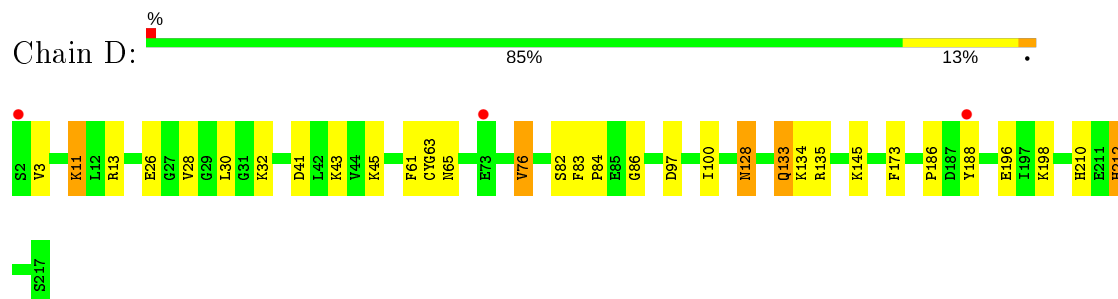
• Molecule 1: FLUORESCENT PROTEIN DRONPA



• 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, α , β , γ	75.66Å 111.14Å 117.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.63 – 2.03 55.57 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.8 (55.63-2.03) 98.8 (55.57-2.03)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.213 0.181 , 0.217	Depositor DCC
R_{free} test set	3241 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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.*

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	0.95	2/1750 (0.1%)	1.08	8/2363 (0.3%)
1	B	0.89	0/1750	0.97	3/2363 (0.1%)
1	C	1.02	0/1750	1.15	14/2363 (0.6%)
1	D	1.01	0/1750	1.03	7/2363 (0.3%)
All	All	0.97	2/7000 (0.0%)	1.06	32/9452 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	SER	CB-OG	-5.84	1.34	1.42
1	A	165	GLY	N-CA	5.37	1.54	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	C	149	ARG	NE-CZ-NH1	18.31	129.46	120.30
1	A	185	LEU	CA-CB-CG	9.43	136.98	115.30
1	D	173	PHE	CB-CA-C	-7.25	95.91	110.40
1	B	30	LEU	CA-CB-CG	7.12	131.68	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	D	135	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	112	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	173	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	C	13	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	192	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	212	HIS	CB-CA-C	5.92	122.24	110.40
1	A	164	GLU	C-N-CA	-5.90	109.91	122.30
1	C	145	LYS	CD-CE-NZ	5.89	125.24	111.70
1	C	173	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	D	100	ILE	CB-CA-C	-5.66	100.29	111.60
1	A	40	MET	CG-SD-CE	5.58	109.12	100.20
1	B	92	SER	CA-CB-OG	-5.57	96.17	111.20
1	D	97	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	173	PHE	CB-CA-C	-5.40	99.59	110.40
1	C	157	VAL	CA-CB-CG1	5.36	118.94	110.90
1	C	156	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	41	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	149	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	121	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	173	PHE	CB-CA-C	-5.26	99.88	110.40
1	C	14	MET	CG-SD-CE	5.16	108.45	100.20
1	C	173	PHE	CB-CG-CD1	5.14	124.40	120.80
1	C	157	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	D	173	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	B	66	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	135	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	PHE	Mainchain
1	D	61	PHE	Mainchain

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	1726	0	1652	20	0
1	B	1726	0	1653	27	0
1	C	1726	0	1654	15	0
1	D	1726	0	1653	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	6612	76	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 (76) 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: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	1.07
1:B:19:ASN:CG	2:B:2006:HOH:O	1.94	1.06
1:B:46:GLU:OE2	2:B:2003:HOH:O	1.91	0.89
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:A:85:GLU:CD	1:A:181:LYS:HD2	1.99	0.83
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: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:N	1:B:46:GLU:CD	2.51	0.65
1:D:63:GYC:C	1:D:65:ASN:CA	2.75	0.64
1:B:41:ASP:OD2	2:B:2007:HOH:O	2.15	0.63
1:D:26:GLU:OE1	1:D:45:LYS:NZ	2.34	0.60
1:B:46:GLU:H	1:B:46:GLU:CD	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LYS:HG3	1:B:210:HIS:CD2	2.37	0.59
1:C:217:SER:C	2:C:2062:HOH:O	2.39	0.59
1:B:81:GLN:HE22	1:B:184:GLN:H	1.50	0.59
1:B:46:GLU:OE1	1:B:46:GLU:N	2.35	0.59
1:A:4:ILE:HG23	1:A:8:MET:HE2	1.86	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:A:85:GLU:CD	1:A:181:LYS:CD	2.74	0.56
1:B:196:GLU:CD	2:B:2052:HOH:O	2.44	0.55
1:D:188:TYR:HB2	2:D:2048:HOH:O	2.07	0.55
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:D:11:LYS:HD2	1:D:28:VAL:HG12	1.92	0.52
1:D:196:GLU:CD	2:D:2051:HOH:O	2.48	0.51
1:D:86:GLY:O	2:D:2028:HOH:O	2.20	0.49
1:D:30:LEU:O	1:D:30:LEU:HD12	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:B:4:ILE:HD11	1:B:33:PRO:CB	2.44	0.47
1:D:133:GLN:O	1:D:134:LYS:HB2	2.14	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:B:134:LYS:C	2:B:2035:HOH:O	2.52	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:171:CYS:HG	1:B:173:PHE:HE1	1.63	0.45
1:C:39:SER:HA	1:C:209:LEU:O	2.16	0.45
1:D:30:LEU:C	1:D:30:LEU:HD12	2.39	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LYS:HG3	1:C:210:HIS:CD2	2.54	0.43
1:C:88:SER:OG	2:C:2030:HOH:O	2.02	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:46:GLU:CD	2:B:2003:HOH:O	2.52	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: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	211/214 (99%)	202 (96%)	7 (3%)	2 (1%)	17	10
1	B	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
1	C	211/214 (99%)	210 (100%)	1 (0%)	0	100	100
1	D	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	844/856 (99%)	828 (98%)	14 (2%)	2 (0%)	47	43

All (2) Ramachandran outliers are listed below:

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

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	184/184 (100%)	167 (91%)	17 (9%)	9	5
1	B	184/184 (100%)	176 (96%)	8 (4%)	29	25
1	C	184/184 (100%)	176 (96%)	8 (4%)	29	25
1	D	184/184 (100%)	174 (95%)	10 (5%)	22	17
All	All	736/736 (100%)	693 (94%)	43 (6%)	20	15

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

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	PRO
1	A	8	MET
1	A	30	LEU
1	A	35	GLU
1	A	66	ARG
1	A	67	VAL
1	A	74	ASN
1	A	75	ILE
1	A	94	ASN
1	A	117	GLU
1	A	145	LYS
1	A	157	VAL
1	A	173	PHE
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	66	ARG
1	B	92	SER
1	B	138	LYS
1	B	157	VAL

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Mol	Chain	Res	Type
1	B	212	HIS
1	C	30	LEU
1	C	66	ARG
1	C	67	VAL
1	C	70	LYS
1	C	149	ARG
1	C	157	VAL
1	C	202	LYS
1	C	214	GLU
1	D	3	VAL
1	D	11	LYS
1	D	13	ARG
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	212	HIS

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	81	GLN
1	A	94	ASN
1	A	102	ASN
1	A	133	GLN
1	A	206	ASN
1	A	208	ASN
1	A	210	HIS
1	A	216	HIS
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

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Mol	Chain	Res	Type
1	C	158	ASN
1	C	208	ASN
1	D	102	ASN
1	D	128	ASN
1	D	158	ASN
1	D	206	ASN
1	D	208	ASN
1	D	210	HIS
1	D	216	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	D	63	1	22,22,23	3.94	10 (45%)	26,30,32	3.96	11 (42%)
1	GYC	A	63	1	22,22,23	4.35	8 (36%)	26,30,32	3.71	8 (30%)
1	GYC	C	63	1	22,22,23	2.80	5 (22%)	26,30,32	2.57	10 (38%)
1	GYC	B	63	1	22,22,23	2.86	9 (40%)	26,30,32	3.14	10 (38%)

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	D	63	1	-	2/9/29/30	0/2/2/2
1	GYC	A	63	1	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	C	63	1	-	3/9/29/30	0/2/2/2
1	GYC	B	63	1	-	2/9/29/30	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CB2-CA2	15.64	1.48	1.35
1	D	63	GYC	CB2-CA2	14.06	1.46	1.35
1	B	63	GYC	CB2-CA2	9.81	1.43	1.35
1	C	63	GYC	CB2-CA2	9.14	1.42	1.35
1	A	63	GYC	CB1-CA1	-7.61	1.44	1.53
1	D	63	GYC	CA2-C2	-6.57	1.42	1.48
1	A	63	GYC	C1-N2	5.69	1.40	1.32
1	D	63	GYC	C1-N2	5.38	1.40	1.32
1	A	63	GYC	CA2-C2	-4.97	1.43	1.48
1	C	63	GYC	CA2-C2	-4.71	1.44	1.48
1	C	63	GYC	C1-N2	4.61	1.39	1.32
1	D	63	GYC	CB1-CA1	-4.11	1.48	1.53
1	C	63	GYC	CB1-CA1	-4.10	1.48	1.53
1	B	63	GYC	CA2-C2	-3.92	1.44	1.48
1	A	63	GYC	O2-C2	3.83	1.31	1.23
1	B	63	GYC	C2-N3	-3.65	1.31	1.39
1	A	63	GYC	CB1-SG1	-3.61	1.73	1.81
1	C	63	GYC	O2-C2	3.46	1.30	1.23
1	B	63	GYC	CB1-CA1	-3.43	1.49	1.53
1	D	63	GYC	O2-C2	3.32	1.30	1.23
1	D	63	GYC	CA1-C1	-3.15	1.44	1.51
1	B	63	GYC	C1-N2	3.06	1.36	1.32
1	D	63	GYC	C2-N3	-3.03	1.32	1.39
1	B	63	GYC	CA2-N2	-2.79	1.32	1.38
1	D	63	GYC	C1-N3	2.76	1.41	1.37
1	A	63	GYC	CA2-N2	-2.47	1.33	1.38
1	A	63	GYC	C1-N3	2.33	1.41	1.37
1	B	63	GYC	O2-C2	2.33	1.28	1.23
1	D	63	GYC	CA2-N2	-2.22	1.33	1.38
1	B	63	GYC	CA1-C1	-2.15	1.46	1.51
1	D	63	GYC	CA1-N	-2.08	1.38	1.48
1	B	63	GYC	CA3-N3	-2.02	1.43	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	O2-C2-CA2	-12.03	124.21	130.96
1	D	63	GYC	O2-C2-CA2	-11.70	124.39	130.96
1	D	63	GYC	CA2-C2-N3	11.61	108.86	103.37
1	A	63	GYC	CA2-C2-N3	9.66	107.94	103.37
1	B	63	GYC	O2-C2-CA2	-8.75	126.05	130.96
1	B	63	GYC	CA2-C2-N3	7.75	107.03	103.37
1	C	63	GYC	CB2-CA2-N2	-6.05	120.43	128.83
1	C	63	GYC	CB2-CA2-C2	5.95	129.38	122.28
1	A	63	GYC	N3-C1-N2	-5.81	107.43	111.45
1	B	63	GYC	CB2-CA2-C2	5.79	129.19	122.28
1	D	63	GYC	CB2-CA2-C2	5.77	129.16	122.28
1	D	63	GYC	N3-C1-N2	-5.69	107.51	111.45
1	C	63	GYC	O2-C2-CA2	-5.16	128.06	130.96
1	D	63	GYC	CB2-CA2-N2	-4.68	122.33	128.83
1	B	63	GYC	CB2-CA2-N2	-4.54	122.53	128.83
1	A	63	GYC	CB2-CA2-C2	4.19	127.28	122.28
1	A	63	GYC	CA2-N2-C1	3.97	108.69	105.77
1	C	63	GYC	CA2-C2-N3	3.94	105.23	103.37
1	A	63	GYC	CA1-C1-N3	3.48	129.38	124.85
1	C	63	GYC	N3-C1-N2	-3.12	109.29	111.45
1	A	63	GYC	CB2-CA2-N2	-3.08	124.55	128.83
1	C	63	GYC	C2-N3-C1	2.91	109.44	107.97
1	B	63	GYC	CA3-N3-C1	-2.90	123.69	127.16
1	C	63	GYC	CD1-CG2-CB2	-2.89	111.39	121.22
1	A	63	GYC	O-C-CA3	-2.88	117.68	126.39
1	B	63	GYC	CA1-C1-N3	2.87	128.59	124.85
1	B	63	GYC	N3-C1-N2	-2.82	109.50	111.45
1	B	63	GYC	CD2-CE2-CZ	2.74	122.88	119.88
1	D	63	GYC	O-C-CA3	-2.60	118.53	126.39
1	D	63	GYC	CA2-N2-C1	2.58	107.68	105.77
1	B	63	GYC	CD1-CG2-CB2	-2.48	112.77	121.22
1	D	63	GYC	CD1-CG2-CB2	-2.45	112.86	121.22
1	C	63	GYC	CD1-CE1-CZ	2.44	122.55	119.88
1	D	63	GYC	CA1-C1-N2	2.43	128.46	123.56
1	D	63	GYC	CE2-CD2-CG2	-2.39	118.13	121.25
1	C	63	GYC	CD2-CG2-CB2	2.37	129.28	121.22
1	B	63	GYC	CE2-CD2-CG2	-2.31	118.23	121.25
1	C	63	GYC	CE1-CD1-CG2	-2.19	118.39	121.25
1	D	63	GYC	CA1-CB1-SG1	2.04	118.84	114.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	63	GYC	C-CA3-N3-C1
1	D	63	GYC	C-CA3-N3-C2
1	A	63	GYC	C-CA3-N3-C2
1	C	63	GYC	C-CA3-N3-C2
1	B	63	GYC	C-CA3-N3-C1
1	B	63	GYC	C-CA3-N3-C2
1	A	63	GYC	C-CA3-N3-C1
1	C	63	GYC	C-CA3-N3-C1
1	C	63	GYC	N-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 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](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

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	213/214 (99%)	-0.00	4 (1%) 66 66	19, 34, 71, 126	0
1	B	213/214 (99%)	-0.12	5 (2%) 60 59	22, 39, 64, 87	0
1	C	213/214 (99%)	-0.43	0 100 100	17, 27, 46, 80	0
1	D	213/214 (99%)	-0.23	3 (1%) 75 74	17, 31, 58, 88	0
All	All	852/856 (99%)	-0.19	12 (1%) 75 74	17, 33, 63, 126	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	LEU	3.6
1	A	2	SER	3.5
1	B	212	HIS	2.9
1	A	3	VAL	2.8
1	B	2	SER	2.8
1	D	188	TYR	2.7
1	D	2	SER	2.5
1	B	3	VAL	2.4
1	D	73	GLU	2.3
1	B	4	ILE	2.2
1	A	83	PHE	2.1
1	B	194	HIS	2.1

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(\AA^2)	Q<0.9
1	GYC	D	63	21/22	0.97	0.10	20,23,29,30	0
1	GYC	A	63	21/22	0.97	0.11	22,24,29,31	0
1	GYC	C	63	21/22	0.97	0.09	17,19,24,27	0
1	GYC	B	63	21/22	0.97	0.14	29,33,37,45	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.