



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2019 – 03:06 PM EDT

PDB ID : 6NQJ
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2)
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on : 2019-01-21
Resolution : 2.00 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
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) : rb-20031633

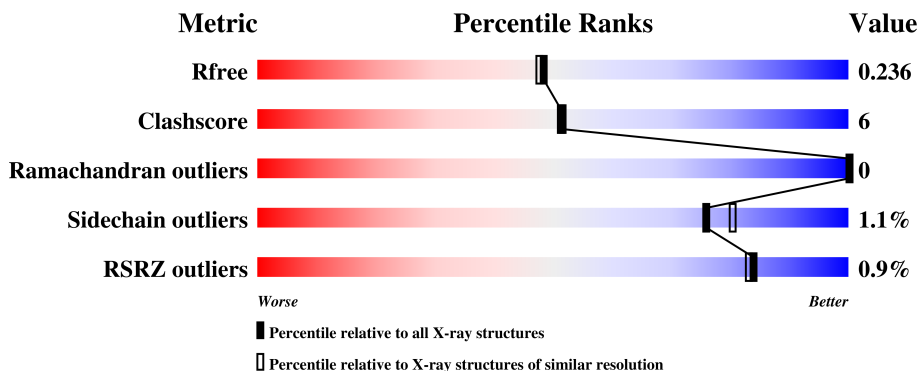
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	255	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	B	255	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>
1	C	255	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>12%</div> </div> </div>
1	D	255	<div> <div></div> <div> <div>77%</div> <div>7%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7746 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	224	Total	C	N	O	S	0	2	0
			1799	1148	304	338	9			
1	B	218	Total	C	N	O	S	0	2	0
			1766	1128	298	331	9			
1	C	224	Total	C	N	O	S	0	1	0
			1791	1144	304	334	9			
1	D	216	Total	C	N	O	S	0	2	0
			1748	1117	295	327	9			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP Q5TLG6
A	-26	SER	-	expression tag	UNP Q5TLG6
A	-25	SER	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	HIS	-	expression tag	UNP Q5TLG6
A	-21	HIS	-	expression tag	UNP Q5TLG6
A	-20	HIS	-	expression tag	UNP Q5TLG6
A	-19	HIS	-	expression tag	UNP Q5TLG6
A	-18	SER	-	expression tag	UNP Q5TLG6
A	-17	SER	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	LEU	-	expression tag	UNP Q5TLG6
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
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
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
A	224	MET	-	expression tag	UNP Q5TLG6
A	225	ASP	-	expression tag	UNP Q5TLG6
A	226	GLU	-	expression tag	UNP Q5TLG6
A	227	LEU	-	expression tag	UNP Q5TLG6
A	228	TYR	-	expression tag	UNP Q5TLG6
A	229	LYS	-	expression tag	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	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
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	224	MET	-	expression tag	UNP Q5TLG6
B	225	ASP	-	expression tag	UNP Q5TLG6
B	226	GLU	-	expression tag	UNP Q5TLG6
B	227	LEU	-	expression tag	UNP Q5TLG6
B	228	TYR	-	expression tag	UNP Q5TLG6
B	229	LYS	-	expression tag	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	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
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	224	MET	-	expression tag	UNP Q5TLG6
C	225	ASP	-	expression tag	UNP Q5TLG6
C	226	GLU	-	expression tag	UNP Q5TLG6
C	227	LEU	-	expression tag	UNP Q5TLG6
C	228	TYR	-	expression tag	UNP Q5TLG6
C	229	LYS	-	expression tag	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	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
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	224	MET	-	expression tag	UNP Q5TLG6
D	225	ASP	-	expression tag	UNP Q5TLG6
D	226	GLU	-	expression tag	UNP Q5TLG6
D	227	LEU	-	expression tag	UNP Q5TLG6
D	228	TYR	-	expression tag	UNP Q5TLG6
D	229	LYS	-	expression tag	UNP Q5TLG6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	175	Total O 175 175	0	0
2	B	177	Total O 177 177	0	0
2	C	152	Total O 152 152	0	0
2	D	138	Total O 138 138	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.03Å 85.80Å 78.58Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	38.28 – 2.00 38.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.28-2.00) 97.8 (38.28-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.174 , 0.237 0.178 , 0.236	Depositor DCC
R_{free} test set	2918 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7746	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.97% 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 [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	0.46	0/1824	0.67	0/2464
1	B	0.52	0/1791	0.65	0/2419
1	C	0.49	0/1816	0.68	2/2454 (0.1%)
1	D	0.49	0/1773	0.66	1/2396 (0.0%)
All	All	0.49	0/7204	0.66	3/9733 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ASN	N-CA-C	-7.19	91.59	111.00
1	C	227	LEU	CA-CB-CG	6.35	129.91	115.30
1	C	226	GLU	C-N-CA	5.45	135.32	121.70

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	1799	0	1715	20	0
1	B	1766	0	1693	25	0
1	C	1791	0	1707	21	0
1	D	1748	0	1669	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	175	0	0	5	0
2	B	177	0	0	3	0
2	C	152	0	0	5	0
2	D	138	0	0	4	0
All	All	7746	0	6784	85	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 (85) 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:D:190:PHE:HB2	1:D:216:HIS:CE1	1.73	1.23
1:B:3:VAL:CG2	1:B:4:ILE:HD12	1.70	1.22
1:A:85:GLU:OE1	1:A:181:LYS:NZ	1.92	1.01
1:B:3:VAL:HG22	1:B:4:ILE:HD12	1.38	1.00
1:D:190:PHE:CB	1:D:216:HIS:CE1	2.47	0.98
1:A:144:GLU:HB2	1:A:157:VAL:HG22	1.47	0.95
1:D:190:PHE:HB2	1:D:216:HIS:NE2	1.80	0.94
1:C:225:ASP:HA	2:C:368:HOH:O	1.67	0.91
1:B:3:VAL:CG2	1:B:4:ILE:CD1	2.55	0.83
1:B:3:VAL:CG2	1:B:4:ILE:N	2.56	0.69
1:D:145:LYS:HD2	1:D:190:PHE:CD1	2.29	0.68
1:D:190:PHE:CG	1:D:216:HIS:CE1	2.81	0.68
1:B:14:MET:HE2	1:B:23:PHE:HE2	1.57	0.68
1:D:29:GLY:O	1:D:30:LEU:HD22	1.94	0.68
1:C:198:LYS:NZ	2:C:304:HOH:O	2.26	0.68
1:A:158:ASN:OD1	1:B:158:ASN:ND2	2.27	0.68
1:D:190:PHE:CB	1:D:216:HIS:NE2	2.55	0.64
1:A:85:GLU:OE2	2:A:301:HOH:O	2.15	0.64
1:A:145:LYS:HD2	1:A:188:TYR:OH	1.98	0.63
1:C:220:PRO:HB2	1:C:223:ALA:HB2	1.81	0.63
1:A:144:GLU:CB	1:A:157:VAL:HG22	2.27	0.62
1:B:14:MET:CE	1:B:23:PHE:HE2	2.12	0.62
1:D:75:ILE:HD11	1:D:216:HIS:O	2.02	0.60
1:B:3:VAL:HG23	1:B:4:ILE:HD12	1.78	0.59
1:C:77:ASP:O	1:C:81:GLN:HG3	2.02	0.59
1:D:75:ILE:CD1	1:D:216:HIS:O	2.51	0.58
1:A:196:GLU:OE1	1:A:198:LYS:NZ	2.35	0.58
1:D:145:LYS:HD2	1:D:190:PHE:HD1	1.67	0.57
1:B:3:VAL:HG22	1:B:4:ILE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:OD1	2:A:302:HOH:O	2.18	0.56
1:B:14:MET:HE1	1:B:57:LEU:HD13	1.87	0.56
1:D:219:LEU:O	2:D:301:HOH:O	2.18	0.55
1:B:3:VAL:HG22	1:B:4:ILE:H	1.71	0.55
1:B:3:VAL:HG23	1:B:4:ILE:CD1	2.37	0.55
1:A:144:GLU:HB2	1:A:157:VAL:CG2	2.31	0.54
1:C:157:VAL:HG13	1:C:173:PHE:HB2	1.90	0.54
1:B:145:LYS:HG2	2:B:378:HOH:O	2.08	0.53
1:B:39:SER:HB3	1:B:210:HIS:CD2	2.43	0.53
1:A:221:ARG:N	2:A:309:HOH:O	2.43	0.52
1:A:4:ILE:HD13	1:A:80:LYS:HG2	1.90	0.52
1:A:195:ILE:HG22	2:A:336:HOH:O	2.10	0.52
1:C:135:ARG:NE	2:C:309:HOH:O	2.33	0.52
1:C:148:VAL:HG11	1:C:185:LEU:HD13	1.92	0.51
1:A:145:LYS:HG3	1:A:145:LYS:O	2.09	0.51
1:C:77:ASP:OD2	1:C:80:LYS:HD2	2.10	0.51
1:B:14:MET:CE	1:B:23:PHE:CE2	2.94	0.51
1:C:131:VAL:HG12	1:C:132:MET:HE2	1.92	0.51
1:D:190:PHE:CD2	1:D:216:HIS:CE1	2.99	0.50
1:B:94:ASN:HA	1:B:100:ILE:HD13	1.93	0.50
1:C:3:VAL:HG11	1:C:84:PRO:HG3	1.93	0.50
1:A:158:ASN:OD1	1:B:158:ASN:CG	2.50	0.49
1:B:3:VAL:HG21	1:B:4:ILE:HD12	1.80	0.49
1:D:157:VAL:HG13	1:D:173:PHE:HB2	1.95	0.48
1:D:70:LYS:HG2	2:D:393:HOH:O	2.12	0.48
1:C:90:GLU:OE2	1:C:178:LYS:NZ	2.40	0.47
1:C:12:LEU:O	1:C:26:GLU:HG3	2.15	0.47
1:C:198:LYS:HG3	1:C:210:HIS:ND1	2.31	0.46
1:A:227:LEU:N	1:A:227:LEU:HD12	2.30	0.46
1:B:154:LYS:NZ	2:B:317:HOH:O	2.48	0.45
1:A:100:ILE:HG21	1:C:100:ILE:HD11	1.97	0.45
1:A:36:GLY:O	1:A:212:HIS:HA	2.18	0.44
1:A:77:ASP:OD1	1:A:80:LYS:HD2	2.17	0.44
1:C:11:LYS:HG3	1:C:113:CYS:SG	2.57	0.44
1:D:220:PRO:C	2:D:301:HOH:O	2.55	0.44
1:C:158:ASN:OD1	1:C:158:ASN:O	2.36	0.44
1:D:145:LYS:HD2	1:D:190:PHE:CE1	2.53	0.43
1:B:128:ASN:OD1	2:B:301:HOH:O	2.21	0.43
1:B:3:VAL:HG23	1:B:4:ILE:N	2.32	0.43
1:C:154:LYS:HE2	1:C:176:THR:HG23	2.00	0.42
1:B:29:GLY:O	1:B:30:LEU:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ASN:OD1	1:D:116:TYR:HB3	2.19	0.42
1:C:5:LYS:H	1:C:8:MET:HE1	1.84	0.42
1:A:145:LYS:HZ3	1:A:156:ASP:HB2	1.84	0.42
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.73	0.42
1:A:51:PRO:HG2	2:A:419:HOH:O	2.20	0.42
1:C:21:HIS:CD2	2:C:307:HOH:O	2.73	0.42
1:C:26:GLU:HG2	2:C:417:HOH:O	2.18	0.42
1:D:145:LYS:N	1:D:145:LYS:HD3	2.34	0.42
1:D:65:ASN:CG	1:D:67:VAL:HG12	2.40	0.42
1:B:81[A]:GLN:O	1:B:181:LYS:NZ	2.43	0.41
1:D:11:LYS:NZ	2:D:317:HOH:O	2.53	0.41
1:C:45:LYS:HD3	1:C:45:LYS:HA	1.85	0.41
1:B:145:LYS:HD3	1:B:188:TYR:OH	2.20	0.41
1:B:136:THR:HG21	1:B:161:LEU:HD13	2.02	0.41
1:D:13:ARG:NH1	1:D:26:GLU:OE2	2.52	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	223/255 (88%)	218 (98%)	5 (2%)	0	100	100
1	B	217/255 (85%)	215 (99%)	2 (1%)	0	100	100
1	C	222/255 (87%)	219 (99%)	3 (1%)	0	100	100
1	D	215/255 (84%)	211 (98%)	4 (2%)	0	100	100
All	All	877/1020 (86%)	863 (98%)	14 (2%)	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	189/217 (87%)	187 (99%)	2 (1%)	76	80
1	B	187/217 (86%)	185 (99%)	2 (1%)	76	80
1	C	187/217 (86%)	185 (99%)	2 (1%)	76	80
1	D	185/217 (85%)	183 (99%)	2 (1%)	76	80
All	All	748/868 (86%)	740 (99%)	8 (1%)	76	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	194	HIS
1	B	3	VAL
1	B	66	ARG
1	C	66	ARG
1	C	157	VAL
1	D	66	ARG
1	D	157	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A	63	1	22,22,23	3.09	6 (27%)	28,30,32	3.55	8 (28%)
1	GYC	B	63	1	22,22,23	2.99	5 (22%)	28,30,32	3.12	8 (28%)
1	GYC	C	63	1	22,22,23	2.95	7 (31%)	28,30,32	3.01	4 (14%)
1	GYC	D	63	1	22,22,23	1.85	9 (40%)	28,30,32	2.70	11 (39%)

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	63	1	-	0/9/29/30	0/2/2/2
1	GYC	B	63	1	-	0/9/29/30	0/2/2/2
1	GYC	C	63	1	-	0/9/29/30	0/2/2/2
1	GYC	D	63	1	-	0/9/29/30	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	CA2-C2	-12.60	1.36	1.48
1	B	63	GYC	CA2-C2	-12.15	1.36	1.48
1	C	63	GYC	CA2-C2	-11.41	1.37	1.48
1	D	63	GYC	C2-N3	-3.57	1.31	1.39
1	C	63	GYC	C2-N3	-3.50	1.31	1.39
1	D	63	GYC	C1-N2	-3.29	1.27	1.32
1	C	63	GYC	CB2-CA2	-3.25	1.32	1.35
1	B	63	GYC	C2-N3	-3.12	1.32	1.39
1	D	63	GYC	O2-C2	-3.05	1.16	1.23
1	A	63	GYC	C2-N3	-3.00	1.32	1.39
1	A	63	GYC	CA2-N2	-2.96	1.32	1.38
1	B	63	GYC	CB2-CA2	-2.78	1.32	1.35
1	A	63	GYC	CB2-CA2	-2.48	1.33	1.35
1	C	63	GYC	CA2-N2	-2.48	1.33	1.38
1	D	63	GYC	CE1-CD1	-2.46	1.34	1.38
1	D	63	GYC	CA3-N3	-2.37	1.42	1.47
1	B	63	GYC	CA2-N2	-2.31	1.33	1.38
1	D	63	GYC	CA2-N2	-2.14	1.34	1.38
1	C	63	GYC	O2-C2	-2.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GYC	O2-C2	-2.05	1.18	1.23
1	D	63	GYC	OH-CZ	-2.04	1.32	1.37
1	D	63	GYC	C1-N3	-2.04	1.33	1.37
1	C	63	GYC	C1-N2	2.41	1.35	1.32
1	D	63	GYC	CB2-CA2	2.65	1.37	1.35
1	A	63	GYC	CG2-CB2	3.29	1.53	1.46
1	B	63	GYC	CG2-CB2	3.35	1.53	1.46
1	C	63	GYC	CG2-CB2	3.36	1.53	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	O2-C2-CA2	-12.60	123.89	130.96
1	B	63	GYC	O2-C2-CA2	-10.97	124.81	130.96
1	C	63	GYC	O2-C2-CA2	-9.51	125.62	130.96
1	D	63	GYC	C2-CA2-N2	-6.41	104.43	108.92
1	D	63	GYC	O-C-CA3	-5.72	109.13	126.39
1	B	63	GYC	N3-C1-N2	-5.43	107.69	111.45
1	D	63	GYC	O2-C2-CA2	-4.06	128.68	130.96
1	A	63	GYC	N3-C1-N2	-3.85	108.79	111.45
1	C	63	GYC	N3-C1-N2	-3.74	108.86	111.45
1	D	63	GYC	CA3-N3-C1	-3.50	123.10	127.20
1	B	63	GYC	O-C-CA3	-3.35	116.27	126.39
1	B	63	GYC	CA3-N3-C1	-2.80	123.91	127.20
1	D	63	GYC	CA1-C1-N3	-2.73	121.29	124.85
1	A	63	GYC	C2-N3-C1	-2.60	106.62	107.97
1	C	63	GYC	O-C-CA3	-2.41	119.12	126.39
1	A	63	GYC	CG2-CB2-CA2	-2.36	127.13	130.01
1	A	63	GYC	CA1-CB1-SG1	-2.35	109.14	114.42
1	B	63	GYC	CG2-CB2-CA2	-2.16	127.38	130.01
1	A	63	GYC	O-C-CA3	-2.14	119.93	126.39
1	D	63	GYC	CG2-CB2-CA2	2.08	132.56	130.01
1	B	63	GYC	CA1-C1-N2	2.11	127.81	123.56
1	D	63	GYC	CA1-C1-N2	2.36	128.32	123.56
1	A	63	GYC	CA2-N2-C1	2.52	107.63	105.77
1	D	63	GYC	CB2-CA2-C2	2.57	125.38	122.28
1	B	63	GYC	CA2-N2-C1	2.75	107.80	105.77
1	D	63	GYC	C2-N3-C1	3.04	109.55	107.97
1	D	63	GYC	CA2-C2-N3	3.47	105.01	103.35
1	D	63	GYC	CA2-N2-C1	6.57	110.62	105.77
1	B	63	GYC	CA2-C2-N3	8.45	107.40	103.35
1	C	63	GYC	CA2-C2-N3	11.26	108.74	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	CA2-C2-N3	11.61	108.91	103.35

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 [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	223/255 (87%)	-0.35	2 (0%) 84 83	14, 24, 50, 74	0
1	B	217/255 (85%)	-0.32	2 (0%) 84 83	15, 25, 48, 71	0
1	C	223/255 (87%)	-0.23	3 (1%) 77 76	16, 28, 53, 66	0
1	D	215/255 (84%)	-0.26	1 (0%) 90 90	16, 28, 51, 63	0
All	All	878/1020 (86%)	-0.29	8 (0%) 84 83	14, 27, 51, 74	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.0
1	C	223	ALA	3.4
1	D	216	HIS	3.4
1	A	3	VAL	3.3
1	A	221	ARG	3.3
1	B	2	ALA	3.2
1	B	3	VAL	2.5
1	C	166	GLY	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(Å ²)	Q<0.9
1	GYC	C	63	21/22	0.95	0.08	11,23,29,33	0
1	GYC	D	63	21/22	0.96	0.07	17,26,29,30	0
1	GYC	B	63	21/22	0.96	0.08	16,19,26,28	0
1	GYC	A	63	21/22	0.97	0.08	9,16,25,27	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.