



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:03 pm GMT

PDB ID : 3ZUF  
Title : PADRON OFF (NON-FLUORESCENT) BTRANS  
Authors : Regis Faro, A.; Carpentier, P.; Bourgeois, D.  
Deposited on : 2011-07-18  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

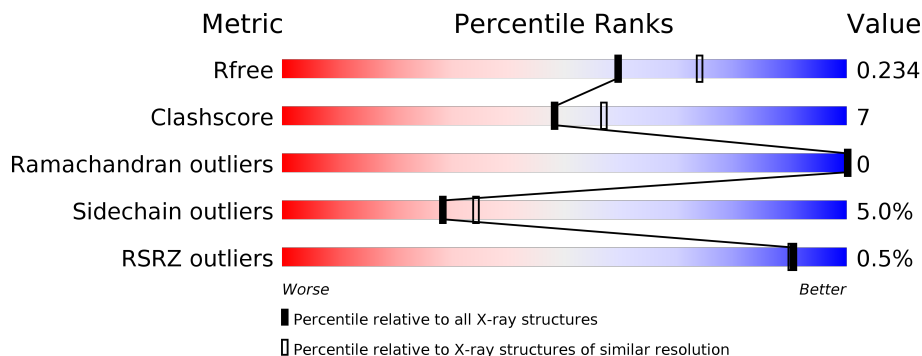
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div style="width: 86%;"></div> <div style="width: 13%;"></div> <div style="width: 1%;"></div> </div> <div>86% 13% .</div>
1	B	215	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>90% 8% .</div>
1	C	215	<div> <div style="width: 80%;"></div> <div style="width: 18%;"></div> <div style="width: 2%;"></div> </div> <div>80% 18% .</div>
1	D	215	<div> <div style="width: 88%;"></div> <div style="width: 11%;"></div> <div style="width: 1%;"></div> </div> <div>88% 11% .</div>
1	E	215	<div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>82% 15% .</div>
1	F	215	<div> <div style="width: 80%;"></div> <div style="width: 17%;"></div> <div style="width: 3%;"></div> </div> <div>80% 17% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GYC	F	63	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11078 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	8	0
			1789	1138	303	338	10			
1	B	214	Total	C	N	O	S	0	4	0
			1761	1121	301	329	10			
1	C	214	Total	C	N	O	S	0	2	0
			1739	1110	293	326	10			
1	D	215	Total	C	N	O	S	0	4	0
			1762	1123	298	331	10			
1	E	214	Total	C	N	O	S	0	5	0
			1764	1124	298	332	10			
1	F	214	Total	C	N	O	S	0	4	0
			1754	1118	296	330	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	THR	CONFLICT	UNP Q5TLG6
A	60	ALA	VAL	CONFLICT	UNP Q5TLG6
A	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
A	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
A	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
A	94	ILE	ASN	CONFLICT	UNP Q5TLG6
A	141	LEU	PRO	CONFLICT	UNP Q5TLG6
A	155	SER	GLY	CONFLICT	UNP Q5TLG6
A	157	GLY	VAL	CONFLICT	UNP Q5TLG6
A	159	TYR	MET	CONFLICT	UNP Q5TLG6
A	190	SER	PHE	CONFLICT	UNP Q5TLG6
B	59	MET	THR	CONFLICT	UNP Q5TLG6
B	60	ALA	VAL	CONFLICT	UNP Q5TLG6
B	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
B	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
B	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
B	94	ILE	ASN	CONFLICT	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	LEU	PRO	CONFLICT	UNP Q5TLG6
B	155	SER	GLY	CONFLICT	UNP Q5TLG6
B	157	GLY	VAL	CONFLICT	UNP Q5TLG6
B	159	TYR	MET	CONFLICT	UNP Q5TLG6
B	190	SER	PHE	CONFLICT	UNP Q5TLG6
C	59	MET	THR	CONFLICT	UNP Q5TLG6
C	60	ALA	VAL	CONFLICT	UNP Q5TLG6
C	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
C	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
C	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
C	94	ILE	ASN	CONFLICT	UNP Q5TLG6
C	141	LEU	PRO	CONFLICT	UNP Q5TLG6
C	155	SER	GLY	CONFLICT	UNP Q5TLG6
C	157	GLY	VAL	CONFLICT	UNP Q5TLG6
C	159	TYR	MET	CONFLICT	UNP Q5TLG6
C	190	SER	PHE	CONFLICT	UNP Q5TLG6
D	59	MET	THR	CONFLICT	UNP Q5TLG6
D	60	ALA	VAL	CONFLICT	UNP Q5TLG6
D	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
D	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
D	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
D	94	ILE	ASN	CONFLICT	UNP Q5TLG6
D	141	LEU	PRO	CONFLICT	UNP Q5TLG6
D	155	SER	GLY	CONFLICT	UNP Q5TLG6
D	157	GLY	VAL	CONFLICT	UNP Q5TLG6
D	159	TYR	MET	CONFLICT	UNP Q5TLG6
D	190	SER	PHE	CONFLICT	UNP Q5TLG6
E	59	MET	THR	CONFLICT	UNP Q5TLG6
E	60	ALA	VAL	CONFLICT	UNP Q5TLG6
E	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
E	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
E	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
E	94	ILE	ASN	CONFLICT	UNP Q5TLG6
E	141	LEU	PRO	CONFLICT	UNP Q5TLG6
E	155	SER	GLY	CONFLICT	UNP Q5TLG6
E	157	GLY	VAL	CONFLICT	UNP Q5TLG6
E	159	TYR	MET	CONFLICT	UNP Q5TLG6
E	190	SER	PHE	CONFLICT	UNP Q5TLG6
F	59	MET	THR	CONFLICT	UNP Q5TLG6
F	60	ALA	VAL	CONFLICT	UNP Q5TLG6
F	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
F	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
F	94	ILE	ASN	CONFLICT	UNP Q5TLG6
F	141	LEU	PRO	CONFLICT	UNP Q5TLG6
F	155	SER	GLY	CONFLICT	UNP Q5TLG6
F	157	GLY	VAL	CONFLICT	UNP Q5TLG6
F	159	TYR	MET	CONFLICT	UNP Q5TLG6
F	190	SER	PHE	CONFLICT	UNP Q5TLG6


- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total 113	O 113	0	0
2	B	72	Total 72	O 72	0	0
2	C	106	Total 106	O 106	0	0
2	D	96	Total 96	O 96	0	0
2	E	63	Total 63	O 63	0	0
2	F	59	Total 59	O 59	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.

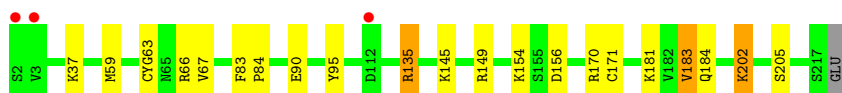
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

Chain A: 




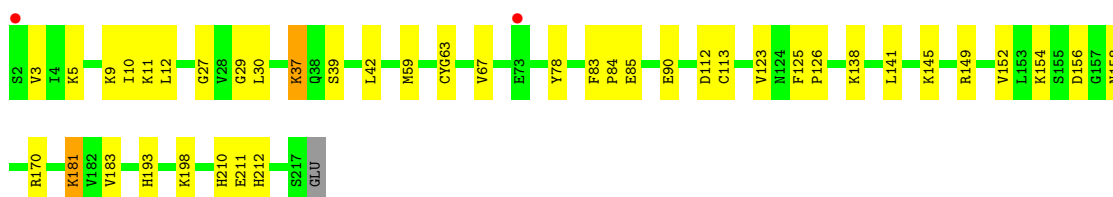
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

Chain B: 




#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

Chain C: 




#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

Chain D: 



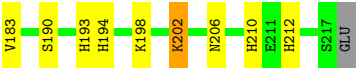
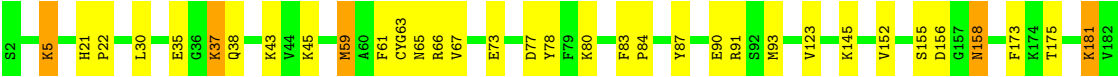
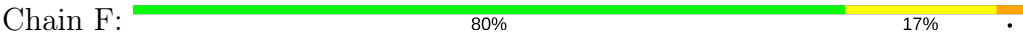
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

Chain E: 





● Molecule 1: FLUORESCENT PROTEIN DRONPA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.32Å 182.00Å 72.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.20 46.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.86-2.20) 99.7 (46.86-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.56 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.187 , 0.240 0.182 , 0.234	Depositor DCC
$R_{free}$ test set	1509 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.20% 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	0.46	0/1813	0.57	0/2445
1	B	0.40	0/1785	0.56	0/2407
1	C	0.42	0/1762	0.55	0/2377
1	D	0.43	0/1786	0.57	0/2410
1	E	0.39	0/1788	0.54	0/2413
1	F	0.38	0/1777	0.53	0/2396
All	All	0.41	0/10711	0.55	0/14448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1789	0	1699	18	0
1	B	1761	0	1679	14	1
1	C	1739	0	1664	34	0
1	D	1762	0	1675	17	0
1	E	1764	0	1679	25	0
1	F	1754	0	1667	47	0
2	A	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	72	0	0	1	0
2	C	106	0	0	3	0
2	D	96	0	0	0	0
2	E	63	0	0	1	0
2	F	59	0	0	2	0
All	All	11078	0	10063	143	1

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 7.

All (143) 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:B:135:ARG:HG3	1:B:135:ARG:HH11	1.10	1.12
1:F:63:GYC:C	1:F:65:ASN:N	2.14	1.09
1:E:37:LYS:HE3	1:E:212[A]:HIS:HB3	1.44	0.99
1:C:12:LEU:O	2:C:2004:HOH:O	1.77	0.99
1:F:61:PHE:O	1:F:63:GYC:N	1.97	0.97
1:F:63:GYC:O	1:F:65:ASN:N	2.02	0.91
1:F:65:ASN:C	1:F:66:ARG:N	2.27	0.88
1:B:135:ARG:HG3	1:B:135:ARG:NH1	1.84	0.87
1:F:61:PHE:C	1:F:63:GYC:N	2.29	0.86
1:F:61:PHE:C	1:F:63:GYC:HN2	1.82	0.81
1:F:61:PHE:O	1:F:63:GYC:CA1	2.30	0.80
1:A:5:LYS:HD2	1:A:5:LYS:N	1.94	0.79
1:F:158:ASN:O	1:F:158:ASN:ND2	2.18	0.77
1:F:59:MET:HG3	2:F:2016:HOH:O	1.88	0.74
1:F:202:LYS:HE2	1:F:202:LYS:HA	1.70	0.73
1:C:149:ARG:HB3	1:C:154:LYS:HD2	1.70	0.72
1:C:198:LYS:HG3	1:C:210:HIS:CD2	2.23	0.72
1:F:91:ARG:HE	1:F:175[B]:THR:HG22	1.55	0.70
1:F:66:ARG:N	1:F:87:TYR:HH	1.88	0.70
1:F:91:ARG:HE	1:F:175[B]:THR:CG2	2.05	0.70
1:F:61:PHE:O	1:F:63:GYC:HA1	1.90	0.69
1:C:3:VAL:HG11	1:C:84:PRO:HG3	1.75	0.69
1:C:67[B]:VAL:HG21	1:C:83:PHE:CE2	2.30	0.67
1:F:63:GYC:HD1	1:F:63:GYC:O2	1.94	0.67
1:B:63:GYC:O2	1:B:63:GYC:HD1	1.95	0.67
2:E:2050:HOH:O	1:F:145:LYS:HE3	1.94	0.67
1:F:61:PHE:CA	1:F:63:GYC:HN2	2.08	0.66
1:F:65:ASN:C	1:F:66:ARG:CA	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:SER:HB3	1:C:210:HIS:CE1	2.32	0.65
1:C:5:LYS:NZ	1:C:112:ASP:HB3	2.12	0.64
1:F:5:LYS:N	1:F:5:LYS:HD2	2.12	0.64
1:A:214[A]:GLU:HG3	1:A:216[A]:HIS:CE1	2.33	0.63
1:A:63:GYC:HD1	1:A:63:GYC:O2	1.99	0.62
1:F:43:LYS:HB2	1:F:45[B]:LYS:HE3	1.80	0.62
1:D:141:LEU:HD22	1:D:193:HIS:O	1.99	0.62
1:B:149:ARG:HB3	1:B:154:LYS:HD2	1.82	0.62
1:D:63:GYC:HD1	1:D:63:GYC:O2	1.99	0.61
1:F:61:PHE:N	1:F:63:GYC:HN2	1.99	0.61
1:E:170:ARG:NE	1:F:156[B]:ASP:OD2	2.35	0.60
1:F:61:PHE:CA	1:F:63:GYC:N	2.65	0.59
1:D:81:GLN:O	1:D:181:LYS:NZ	2.35	0.59
1:C:63:GYC:HD1	1:C:63:GYC:O2	2.02	0.59
1:C:67[B]:VAL:HG21	1:C:83:PHE:HE2	1.67	0.58
1:A:198:LYS:HE2	1:A:210:HIS:CD2	2.39	0.58
1:C:67[B]:VAL:CG2	1:C:83:PHE:HE2	2.17	0.58
1:F:155:SER:HG	1:F:175[B]:THR:HG1	1.53	0.57
1:C:156:ASP:OD2	1:D:170:ARG:NE	2.36	0.57
1:E:149:ARG:HB3	1:E:154:LYS:HD2	1.86	0.57
1:A:149:ARG:O	1:A:152:VAL:HG12	2.05	0.56
1:F:65:ASN:CA	1:F:66:ARG:N	2.69	0.55
1:E:158:ASN:O	1:E:158:ASN:ND2	2.32	0.54
1:E:77:ASP:OD2	1:E:80:LYS:HE2	2.08	0.54
1:E:83:PHE:HB3	1:E:84:PRO:HA	1.89	0.53
1:E:85:GLU:CG	1:E:181:LYS:HD2	2.38	0.53
1:A:195:ILE:HD11	1:A:209:LEU:HD11	1.90	0.53
1:C:37:LYS:HE3	1:C:212:HIS:HB3	1.91	0.53
1:E:27:GLY:HA3	1:E:42:LEU:HD23	1.92	0.52
1:F:198:LYS:HG3	1:F:210:HIS:CD2	2.45	0.52
1:F:83:PHE:HB3	1:F:84:PRO:HA	1.91	0.52
1:B:135:ARG:CG	1:B:135:ARG:NH1	2.62	0.52
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.92	0.52
1:E:63:GYC:O2	1:E:63:GYC:HD1	2.11	0.51
1:F:194:HIS:HB3	1:F:212[B]:HIS:CE1	2.45	0.51
1:D:78:TYR:CE1	1:D:183:VAL:HG22	2.45	0.51
1:F:65:ASN:HA	1:F:66:ARG:N	2.26	0.51
1:F:181:LYS:NZ	1:F:183:VAL:HG12	2.25	0.51
1:F:37:LYS:HG2	1:F:38:GLN:N	2.26	0.51
1:C:170:ARG:NE	1:D:156[B]:ASP:OD2	2.44	0.51
1:F:175[B]:THR:HG23	2:F:2022:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:HB3	1:F:123:VAL:HB	1.93	0.50
1:F:78:TYR:CE1	1:F:183:VAL:CG2	2.95	0.50
1:C:9:LYS:HE3	1:C:113:CYS:HB2	1.93	0.49
1:E:141:LEU:HD22	1:E:193:HIS:O	2.11	0.49
1:A:141:LEU:HD22	1:A:193:HIS:O	2.12	0.49
1:D:37:LYS:HD2	1:D:212[A]:HIS:HB3	1.93	0.49
1:A:78:TYR:CE1	1:A:183:VAL:HG22	2.48	0.49
1:B:149:ARG:HB3	1:B:154:LYS:CD	2.43	0.49
1:C:156:ASP:HB2	1:D:158:ASN:ND2	2.27	0.49
1:F:43:LYS:HG2	1:F:206:ASN:OD1	2.13	0.49
1:A:12:LEU:C	1:A:12:LEU:HD12	2.34	0.48
1:A:11:LYS:HD3	1:A:11:LYS:C	2.34	0.48
1:B:95:TYR:CD2	1:B:171:CYS:HB2	2.49	0.48
1:C:156:ASP:HB2	1:D:158:ASN:HD22	1.79	0.48
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.95	0.47
1:B:205:SER:HB3	2:B:2071:HOH:O	2.14	0.47
1:F:63:GYC:HD2	1:F:193:HIS:CG	2.50	0.47
1:C:211:GLU:HG2	1:C:212:HIS:N	2.28	0.47
1:C:85:GLU:N	1:C:85:GLU:OE1	2.40	0.47
1:C:30:LEU:HD12	1:C:30:LEU:O	2.15	0.47
1:C:39:SER:HB3	1:C:210:HIS:ND1	2.29	0.47
1:E:37:LYS:HE3	1:E:212[A]:HIS:CB	2.31	0.47
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.96	0.47
1:C:149:ARG:HB3	1:C:154:LYS:CD	2.42	0.46
1:C:27:GLY:HA3	1:C:42:LEU:HD23	1.97	0.46
1:D:30:LEU:C	1:D:30:LEU:HD12	2.36	0.46
1:C:125:PHE:HA	1:C:126:PRO:HD3	1.82	0.46
1:F:65:ASN:C	1:F:66:ARG:HA	2.37	0.46
1:E:85:GLU:CD	1:E:85:GLU:H	2.18	0.45
1:B:66:ARG:HH11	1:B:66:ARG:HA	1.82	0.45
1:D:121:ASP:O	1:E:102[B]:ASN:ND2	2.49	0.45
1:F:91:ARG:HG3	1:F:175[B]:THR:HG22	1.99	0.45
1:D:93:MET:HG2	1:D:173:PHE:CE1	2.52	0.45
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.99	0.45
1:A:11:LYS:HD3	1:A:12:LEU:N	2.32	0.45
1:D:90:GLU:HB3	1:E:123:VAL:HB	1.99	0.45
1:C:181:LYS:HD3	2:C:2050:HOH:O	2.16	0.44
1:E:157:GLY:HA2	1:F:158:ASN:OD1	2.17	0.44
1:E:170:ARG:HB3	1:E:170:ARG:CZ	2.48	0.44
1:D:123:VAL:HB	1:E:90:GLU:HB3	1.99	0.44
1:C:141:LEU:HD12	1:C:193:HIS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:HIS:HA	1:F:22:PRO:HD3	1.72	0.43
1:F:61:PHE:N	1:F:63:GYC:N	2.66	0.43
1:D:181:LYS:HE2	1:D:181:LYS:HB3	1.95	0.43
1:E:85:GLU:HG3	1:E:181:LYS:HD2	2.00	0.43
1:C:11:LYS:HE2	1:C:11:LYS:HB3	1.75	0.43
1:C:123:VAL:HB	1:F:90:GLU:HB3	1.99	0.43
1:A:83:PHE:HB3	1:A:84:PRO:HA	2.01	0.42
1:E:5:LYS:N	1:E:5:LYS:HD2	2.33	0.42
1:A:67:VAL:HG21	1:A:83:PHE:CE2	2.55	0.42
1:E:91:ARG:HG3	1:E:175[B]:THR:HG22	2.00	0.42
1:B:37:LYS:HB3	1:B:37:LYS:HE2	1.79	0.42
1:F:93:MET:HG2	1:F:173:PHE:CE1	2.54	0.42
1:C:5:LYS:HZ1	1:C:112:ASP:HB3	1.82	0.42
1:B:183:VAL:HG23	1:B:184:GLN:N	2.35	0.42
1:C:12:LEU:HG	2:C:2004:HOH:O	2.18	0.42
1:E:170:ARG:NH1	1:E:170:ARG:HB3	2.35	0.41
1:A:198:LYS:HE2	1:A:210:HIS:CG	2.55	0.41
1:F:194:HIS:CB	1:F:212[B]:HIS:CE1	3.03	0.41
1:E:37:LYS:HE3	1:E:212[B]:HIS:HB2	2.02	0.41
1:A:141:LEU:C	1:A:141:LEU:HD13	2.40	0.41
1:E:13:ARG:HG3	1:E:26:GLU:HG2	2.01	0.41
1:E:59:MET:HB3	1:E:59:MET:HE2	1.99	0.41
1:B:202:LYS:HB3	1:B:202:LYS:NZ	2.36	0.41
1:A:30:LEU:O	1:A:30:LEU:HD12	2.21	0.41
1:F:66:ARG:N	1:F:87:TYR:OH	2.50	0.41
1:A:39:SER:HB3	1:A:210:HIS:CE1	2.55	0.41
1:E:185:LEU:HA	1:E:186:PRO:HD3	1.84	0.41
1:F:181:LYS:HZ1	1:F:183:VAL:HG12	1.84	0.41
1:C:78:TYR:CE1	1:C:183:VAL:HG22	2.56	0.40
1:F:77:ASP:OD2	1:F:80:LYS:HD2	2.21	0.40
1:C:10:ILE:N	1:C:29:GLY:O	2.43	0.40
1:D:30:LEU:HD12	1:D:30:LEU:O	2.22	0.40
1:C:84:PRO:HD2	1:C:85:GLU:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASP:OD2	1:B:170[A]:ARG:NE[2_555]	2.07	0.13

## 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	219/215 (102%)	216 (99%)	3 (1%)	0	100	100
1	B	215/215 (100%)	213 (99%)	2 (1%)	0	100	100
1	C	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
1	D	216/215 (100%)	214 (99%)	2 (1%)	0	100	100
1	E	216/215 (100%)	213 (99%)	3 (1%)	0	100	100
1	F	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	1291/1290 (100%)	1275 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/184 (103%)	181 (95%)	9 (5%)	30	37
1	B	186/184 (101%)	179 (96%)	7 (4%)	38	47
1	C	184/184 (100%)	177 (96%)	7 (4%)	38	47
1	D	186/184 (101%)	178 (96%)	8 (4%)	33	41
1	E	187/184 (102%)	175 (94%)	12 (6%)	20	23
1	F	185/184 (100%)	173 (94%)	12 (6%)	20	22
All	All	1118/1104 (101%)	1063 (95%)	55 (5%)	28	35

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	LYS
1	A	43	LYS
1	A	59	MET
1	A	180	LYS
1	A	181	LYS
1	A	183	VAL
1	A	190	SER
1	A	202	LYS
1	B	59	MET
1	B	67	VAL
1	B	135	ARG
1	B	145	LYS
1	B	181	LYS
1	B	183	VAL
1	B	202	LYS
1	C	37	LYS
1	C	59	MET
1	C	138	LYS
1	C	145	LYS
1	C	152	VAL
1	C	158	ASN
1	C	181	LYS
1	D	45	LYS
1	D	59	MET
1	D	138	LYS
1	D	145	LYS
1	D	163	LEU
1	D	181	LYS
1	D	183	VAL
1	D	202	LYS
1	E	3	VAL
1	E	8	MET
1	E	45	LYS
1	E	59	MET
1	E	66	ARG
1	E	67	VAL
1	E	134	LYS
1	E	141	LEU
1	E	145	LYS
1	E	158	ASN
1	E	181	LYS

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Mol	Chain	Res	Type
1	E	190	SER
1	F	5	LYS
1	F	30	LEU
1	F	35	GLU
1	F	37	LYS
1	F	59	MET
1	F	67	VAL
1	F	73	GLU
1	F	152	VAL
1	F	158	ASN
1	F	181	LYS
1	F	190	SER
1	F	202	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	C	210	HIS
1	E	194	HIS
1	F	210	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	4.26	7 (31%)	27,30,32	4.27	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GYC	B	63	1	22,22,23	4.26	8 (36%)	27,30,32	4.25	6 (22%)
1	GYC	C	63	1	22,22,23	4.35	6 (27%)	27,30,32	4.29	7 (25%)
1	GYC	D	63	1	22,22,23	4.43	7 (31%)	27,30,32	4.41	6 (22%)
1	GYC	E	63	1	22,22,23	4.45	7 (31%)	27,30,32	4.20	7 (25%)
1	GYC	F	63	-	22,22,23	4.46	7 (31%)	27,30,32	4.59	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	A	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
1	GYC	E	63	1	-	0/9/29/30	0/2/2/2
1	GYC	F	63	-	-	0/9/29/30	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GYC	CA2-C2	-10.72	1.37	1.48
1	D	63	GYC	CA2-C2	-10.72	1.37	1.48
1	F	63	GYC	CA2-C2	-10.23	1.38	1.48
1	B	63	GYC	CA2-C2	-9.99	1.38	1.48
1	E	63	GYC	CA2-C2	-9.88	1.38	1.48
1	A	63	GYC	CA2-C2	-9.78	1.38	1.48
1	B	63	GYC	OH-CZ	-4.84	1.25	1.37
1	A	63	GYC	OH-CZ	-4.78	1.25	1.37
1	E	63	GYC	OH-CZ	-4.77	1.25	1.37
1	F	63	GYC	OH-CZ	-4.60	1.26	1.37
1	C	63	GYC	OH-CZ	-4.53	1.26	1.37
1	D	63	GYC	OH-CZ	-4.35	1.26	1.37
1	F	63	GYC	CA1-C1	-3.44	1.46	1.51
1	E	63	GYC	C2-N3	-2.93	1.32	1.39
1	A	63	GYC	C2-N3	-2.70	1.33	1.39
1	C	63	GYC	C2-N3	-2.65	1.33	1.39
1	B	63	GYC	C2-N3	-2.63	1.33	1.39
1	E	63	GYC	CA1-C1	-2.57	1.47	1.51
1	F	63	GYC	C2-N3	-2.52	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	GYC	CA1-C1	-2.45	1.47	1.51
1	B	63	GYC	CA1-C1	-2.32	1.47	1.51
1	D	63	GYC	C2-N3	-2.25	1.34	1.39
1	A	63	GYC	CA2-N2	-2.04	1.34	1.38
1	B	63	GYC	CA2-N2	-2.01	1.34	1.38
1	C	63	GYC	O2-C2	2.43	1.28	1.23
1	B	63	GYC	C1-N2	2.46	1.36	1.32
1	B	63	GYC	O2-C2	2.61	1.28	1.23
1	E	63	GYC	O2-C2	2.63	1.28	1.23
1	F	63	GYC	O2-C2	2.63	1.28	1.23
1	D	63	GYC	O2-C2	2.65	1.28	1.23
1	A	63	GYC	O2-C2	2.68	1.29	1.23
1	E	63	GYC	C1-N2	2.68	1.36	1.32
1	D	63	GYC	C1-N2	2.71	1.36	1.32
1	F	63	GYC	C1-N2	2.78	1.36	1.32
1	A	63	GYC	C1-N2	2.83	1.36	1.32
1	C	63	GYC	C1-N2	3.15	1.37	1.32
1	B	63	GYC	CB2-CA2	15.62	1.49	1.35
1	C	63	GYC	CB2-CA2	15.68	1.49	1.35
1	A	63	GYC	CB2-CA2	15.74	1.49	1.35
1	D	63	GYC	CB2-CA2	16.26	1.49	1.35
1	F	63	GYC	CB2-CA2	16.41	1.49	1.35
1	E	63	GYC	CB2-CA2	16.63	1.49	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GYC	CB2-CA2-N2	-8.88	115.33	128.79
1	D	63	GYC	O2-C2-CA2	-8.58	126.35	130.97
1	A	63	GYC	CB2-CA2-N2	-8.49	115.93	128.79
1	F	63	GYC	O2-C2-CA2	-7.94	126.69	130.97
1	E	63	GYC	CB2-CA2-N2	-7.76	117.04	128.79
1	C	63	GYC	O2-C2-CA2	-7.59	126.88	130.97
1	C	63	GYC	CB2-CA2-N2	-7.57	117.32	128.79
1	F	63	GYC	CB2-CA2-N2	-7.53	117.39	128.79
1	D	63	GYC	CB2-CA2-N2	-7.33	117.68	128.79
1	E	63	GYC	O2-C2-CA2	-5.80	127.84	130.97
1	B	63	GYC	O2-C2-CA2	-5.57	127.97	130.97
1	A	63	GYC	O2-C2-CA2	-5.39	128.06	130.97
1	F	63	GYC	CG2-CB2-CA2	-3.88	125.68	130.19
1	B	63	GYC	O-C-CA3	-3.31	115.43	126.38
1	F	63	GYC	O-C-CA3	-3.22	115.72	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GYC	O-C-CA3	-2.93	116.68	126.38
1	F	63	GYC	C2-CA2-N2	-2.90	106.81	108.93
1	B	63	GYC	CG2-CB2-CA2	-2.88	126.84	130.19
1	D	63	GYC	C2-CA2-N2	-2.86	106.83	108.93
1	A	63	GYC	O-C-CA3	-2.84	116.99	126.38
1	E	63	GYC	C2-CA2-N2	-2.72	106.94	108.93
1	A	63	GYC	CG2-CB2-CA2	-2.68	127.08	130.19
1	E	63	GYC	O-C-CA3	-2.65	117.60	126.38
1	D	63	GYC	O-C-CA3	-2.52	118.04	126.38
1	C	63	GYC	C2-CA2-N2	-2.49	107.10	108.93
1	E	63	GYC	CG2-CB2-CA2	-2.24	127.58	130.19
1	C	63	GYC	N3-C1-N2	-2.16	109.96	111.45
1	F	63	GYC	CA3-N3-C1	2.44	130.06	127.20
1	A	63	GYC	CA1-C1-N3	2.48	127.72	124.75
1	D	63	GYC	CB2-CA2-C2	10.45	135.46	122.32
1	C	63	GYC	CB2-CA2-C2	10.54	135.58	122.32
1	F	63	GYC	CB2-CA2-C2	10.72	135.80	122.32
1	E	63	GYC	CB2-CA2-C2	10.89	136.01	122.32
1	A	63	GYC	CB2-CA2-C2	11.17	136.37	122.32
1	B	63	GYC	CB2-CA2-C2	11.77	137.12	122.32
1	B	63	GYC	CA2-C2-N3	13.97	109.53	103.30
1	A	63	GYC	CA2-C2-N3	15.03	110.01	103.30
1	E	63	GYC	CA2-C2-N3	15.26	110.11	103.30
1	C	63	GYC	CA2-C2-N3	15.48	110.20	103.30
1	D	63	GYC	CA2-C2-N3	15.89	110.39	103.30
1	F	63	GYC	CA2-C2-N3	16.84	110.81	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	GYC	1	0
1	B	63	GYC	1	0
1	C	63	GYC	1	0
1	D	63	GYC	1	0
1	E	63	GYC	1	0
1	F	63	GYC	13	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](#)

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, 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	213/215 (99%)	-0.67	0 100 100	14, 25, 43, 56	0
1	B	213/215 (99%)	-0.50	3 (1%) 75 73	16, 31, 52, 70	0
1	C	213/215 (99%)	-0.37	2 (0%) 84 83	18, 31, 54, 75	0
1	D	214/215 (99%)	-0.58	0 100 100	17, 28, 49, 64	0
1	E	213/215 (99%)	-0.39	1 (0%) 90 90	21, 35, 56, 78	0
1	F	213/215 (99%)	-0.39	0 100 100	19, 33, 52, 73	0
All	All	1279/1290 (99%)	-0.48	6 (0%) 90 90	14, 31, 52, 78	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	3.7
1	B	2	SER	3.1
1	E	3	VAL	2.6
1	B	3	VAL	2.3
1	C	73	GLU	2.0
1	B	112	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GYC	F	63	21/22	0.95	0.12	-	23,34,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	GYC	A	63	21/22	0.97	0.10	-	16,24,33,34	0
1	GYC	C	63	21/22	0.94	0.12	-	23,28,37,42	0
1	GYC	E	63	21/22	0.95	0.11	-	31,38,46,52	0
1	GYC	D	63	21/22	0.95	0.10	-	19,32,38,48	0
1	GYC	B	63	21/22	0.97	0.09	-	24,30,36,42	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.