



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:48 pm GMT

PDB ID : 3ZUJ  
Title : PADRON ON (FLUORESCENT) ABCIS  
Authors : Regis Faro, A.; Carpentier, P.; Bourgeois, D.  
Deposited on : 2011-07-19  
Resolution : 2.35 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

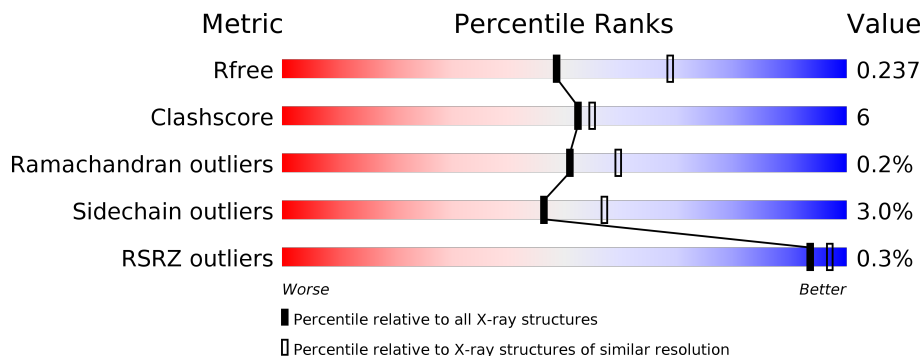
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	214	 86% 13% •
1	B	214	 83% 16% •
1	C	214	 86% 14%
1	D	214	 85% 14% •
1	E	214	 81% 18% •
1	F	214	 84% 15%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11242 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
			1787	1136	301	340	10			
1	B	214	Total	C	N	O	S	0	9	0
			1803	1143	307	343	10			
1	C	213	Total	C	N	O	S	0	10	0
			1794	1141	303	339	11			
1	D	212	Total	C	N	O	S	0	9	0
			1781	1131	300	340	10			
1	E	214	Total	C	N	O	S	0	6	0
			1768	1124	300	333	11			
1	F	214	Total	C	N	O	S	0	6	0
			1775	1129	300	335	11			

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 P42212
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

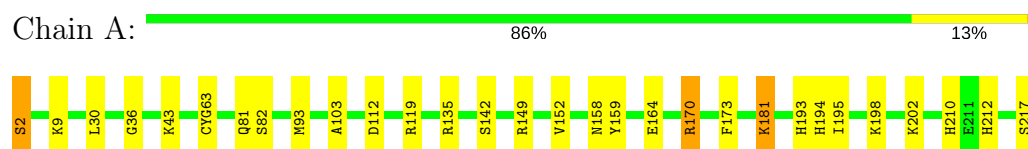
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total 123	O 123	0	0
2	B	80	Total 80	O 80	0	0
2	C	106	Total 106	O 106	0	0
2	D	87	Total 87	O 87	0	0
2	E	67	Total 67	O 67	0	0
2	F	71	Total 71	O 71	0	0

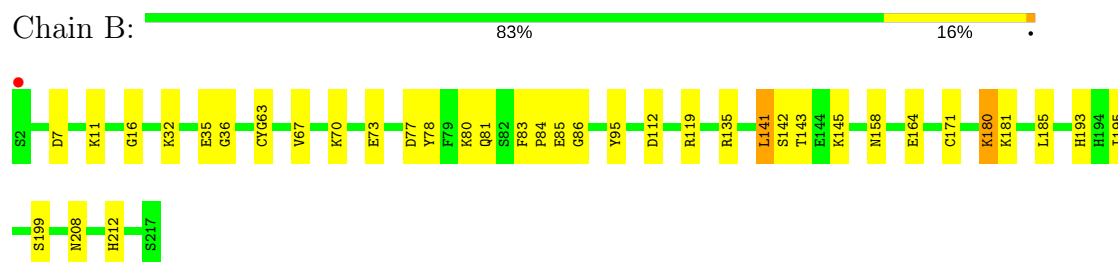
### 3 Residue-property plots [i](#)

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.

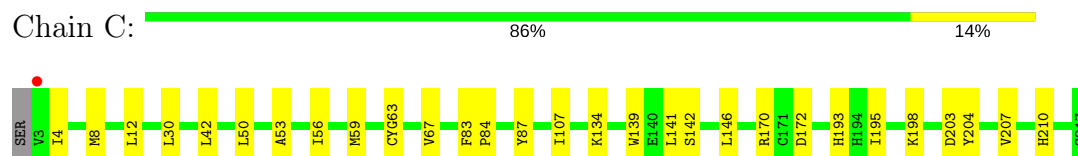
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA



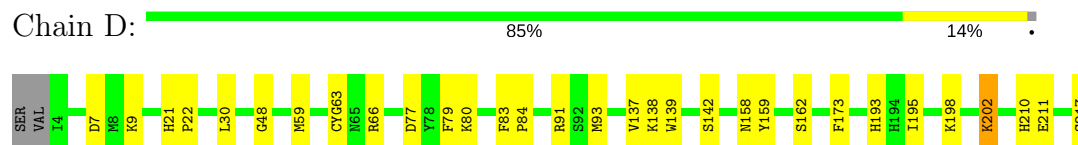
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA



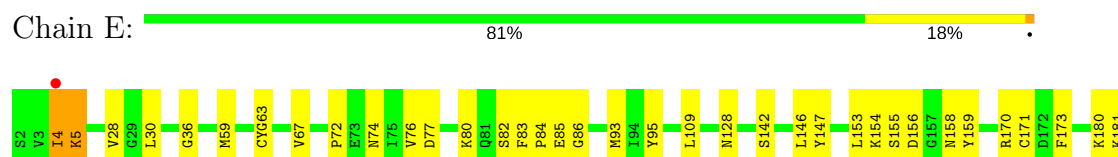
#### • Molecule 1: FLUORESCENT PROTEIN DRONPA



#### • Molecule 1: FLUORESCENT PROTEIN DRONPA

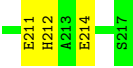
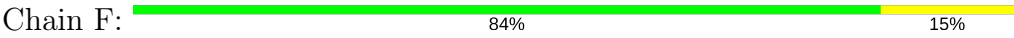


#### • Molecule 1: FLUORESCENT PROTEIN DRONPA





● 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, $\alpha$ , $\beta$ , $\gamma$	109.58Å 181.56Å 72.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.35 46.54 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.54-2.35) 98.9 (46.54-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.189 , 0.250 0.178 , 0.237	Depositor DCC
$R_{free}$ test set	1995 reflections (3.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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	0.45	0/1811	0.58	0/2443
1	B	0.40	0/1827	0.56	0/2463
1	C	0.43	0/1817	0.56	0/2449
1	D	0.41	0/1804	0.56	0/2430
1	E	0.38	0/1792	0.53	0/2415
1	F	0.39	0/1798	0.55	0/2423
All	All	0.41	0/10849	0.56	0/14623

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	1787	0	1697	21	0
1	B	1803	0	1706	25	1
1	C	1794	0	1715	20	0
1	D	1781	0	1692	21	1
1	E	1768	0	1673	25	0
1	F	1775	0	1690	20	0
2	A	123	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	80	0	0	2	0
2	C	106	0	0	2	0
2	D	87	0	0	0	0
2	E	67	0	0	1	0
2	F	71	0	0	0	0
All	All	11242	0	10173	131	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 6.

All (131) 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)
2:C:2088:HOH:O	1:D:158[B]:ASN:OD1	1.81	0.98
1:A:2:SER:N	2:A:2002:HOH:O	1.98	0.94
1:E:4:ILE:HA	1:E:5:LYS:CB	1.99	0.92
1:B:85:GLU:HG2	1:B:181:LYS:HE3	1.62	0.81
1:C:63:GYC:HE1	1:C:195:ILE:HB	1.62	0.81
1:F:63:GYC:HE1	1:F:195:ILE:HB	1.65	0.77
1:D:198:LYS:HG3	1:D:210:HIS:CD2	2.19	0.76
1:B:63:GYC:HE1	1:B:195:ILE:HB	1.68	0.74
1:A:158[B]:ASN:OD1	2:A:2097:HOH:O	2.04	0.74
1:E:4:ILE:HA	1:E:5:LYS:HB2	1.69	0.72
1:D:142[B]:SER:OG	1:D:193:HIS:HB2	1.94	0.68
1:E:4:ILE:HA	1:E:5:LYS:HB3	1.73	0.67
1:A:63:GYC:HE2	1:A:195:ILE:HB	1.76	0.67
1:B:63:GYC:N2	1:B:63:GYC:HD1	2.10	0.67
1:D:63:GYC:HE1	1:D:195:ILE:HB	1.76	0.67
1:E:63:GYC:HE1	1:E:195:ILE:HB	1.79	0.65
1:E:4:ILE:CA	1:E:5:LYS:HB2	2.28	0.64
1:E:4:ILE:CA	1:E:5:LYS:CB	2.76	0.63
1:E:63:GYC:N2	1:E:63:GYC:HD1	2.14	0.61
1:D:63:GYC:HD1	1:D:63:GYC:N2	2.16	0.60
1:A:9:LYS:HE2	1:A:112[A]:ASP:OD2	2.02	0.59
1:B:73[B]:GLU:CD	1:B:73[B]:GLU:H	2.04	0.59
1:C:63:GYC:N2	1:C:63:GYC:HD1	2.19	0.58
1:F:8:MET:O	1:F:30:LEU:HD23	2.05	0.56
1:A:217:SER:O	2:A:2123:HOH:O	2.18	0.56
1:E:128:ASN:ND2	2:E:2039:HOH:O	2.38	0.55
1:A:135:ARG:HB3	1:A:164[A]:GLU:HG2	1.88	0.55
1:F:211:GLU:HG2	1:F:212:HIS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181[B]:LYS:O	1:E:183:VAL:HG23	2.05	0.55
1:D:142[B]:SER:HB2	1:D:159:TYR:CE1	2.42	0.55
1:D:142[A]:SER:HB3	1:D:159:TYR:CE1	2.43	0.54
1:F:63:GYC:HD1	1:F:63:GYC:N2	2.23	0.54
1:C:42:LEU:HB2	1:C:207:VAL:HG22	1.90	0.53
1:C:172:ASP:OD2	2:C:2092:HOH:O	2.18	0.53
1:A:43:LYS:NZ	2:A:2031:HOH:O	2.41	0.53
1:E:142:SER:HB3	1:E:159:TYR:CE1	2.44	0.52
1:B:142:SER:HB2	1:B:193:HIS:HB2	1.91	0.52
1:F:12:LEU:C	1:F:12:LEU:HD12	2.30	0.52
1:E:77:ASP:OD2	1:E:80:LYS:HE2	2.09	0.52
1:B:7:ASP:OD2	1:B:32:LYS:NZ	2.42	0.51
1:C:59:MET:HG2	1:C:63:GYC:CD1	2.40	0.51
1:C:67:VAL:HG21	1:C:83:PHE:CE1	2.46	0.51
1:F:137:VAL:HB	1:F:162[B]:SER:OG	2.11	0.51
1:F:27:GLY:HA3	1:F:42:LEU:HD23	1.93	0.51
1:A:63:GYC:N2	1:A:63:GYC:HD2	2.26	0.51
1:B:77:ASP:O	1:B:81:GLN:HG2	2.11	0.50
1:E:85:GLU:OE1	1:E:181[B]:LYS:NZ	2.39	0.50
1:D:9[B]:LYS:HD2	1:D:30:LEU:HB3	1.92	0.50
1:A:149:ARG:O	1:A:152:VAL:HG12	2.12	0.50
1:F:72:PRO:HG2	1:F:75:ILE:HD12	1.95	0.49
1:E:156:ASP:OD2	1:F:170[A]:ARG:NE	2.45	0.49
1:A:170:ARG:HB3	1:A:170:ARG:CZ	2.42	0.49
1:E:76:VAL:HB	1:E:186:PRO:HA	1.95	0.49
1:C:142:SER:HB2	1:C:193:HIS:HB2	1.95	0.48
1:E:147:TYR:O	1:E:153:LEU:HD12	2.14	0.48
1:F:36:GLY:O	1:F:212:HIS:HA	2.14	0.48
1:A:194:HIS:HB3	1:A:212:HIS:CD2	2.49	0.48
1:C:146:LEU:HD12	1:C:146:LEU:N	2.29	0.47
1:E:59:MET:HG2	1:E:63:GYC:CD1	2.44	0.47
1:B:143:THR:HG22	1:B:145:LYS:HE2	1.97	0.47
1:B:36:GLY:O	1:B:212:HIS:HA	2.14	0.47
1:D:59:MET:HE1	1:D:139:TRP:CD2	2.49	0.47
1:B:145:LYS:NZ	2:B:2065:HOH:O	2.20	0.47
1:D:137:VAL:HB	1:D:162[B]:SER:OG	2.15	0.46
1:D:202:LYS:HD3	1:D:202:LYS:O	2.15	0.46
1:E:170:ARG:CZ	1:E:170:ARG:HB3	2.46	0.46
1:C:50:LEU:O	1:C:134:LYS:NZ	2.48	0.46
1:F:93:MET:HG2	1:F:173:PHE:CE1	2.51	0.46
1:B:143:THR:CG2	1:B:145:LYS:HE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.98	0.45
1:D:93:MET:HG2	1:D:173:PHE:CZ	2.52	0.45
1:A:82:SER:HA	1:A:181:LYS:HE2	1.99	0.45
1:F:93:MET:HG2	1:F:173:PHE:CZ	2.52	0.45
1:B:63:GYC:CZ	1:B:193:HIS:HB3	2.48	0.44
1:B:199:SER:OG	1:B:208:ASN:HB3	2.17	0.44
1:C:87:TYR:CZ	1:C:107:ILE:HD12	2.52	0.44
1:F:125:PHE:CE1	1:F:131:VAL:HG21	2.53	0.44
1:B:158[B]:ASN:N	1:B:158[B]:ASN:OD1	2.49	0.44
1:D:63:GYC:HB12	1:D:211:GLU:OE1	2.17	0.44
1:D:93:MET:HG2	1:D:173:PHE:CE1	2.52	0.44
1:B:83:PHE:CE1	1:B:86:GLY:HA2	2.52	0.44
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.99	0.44
1:C:141:LEU:HD13	1:C:142:SER:N	2.32	0.44
1:F:59[B]:MET:HE1	1:F:139:TRP:CD2	2.53	0.44
1:F:63:GYC:CZ	1:F:193:HIS:HB3	2.48	0.44
1:A:142:SER:HB2	1:A:193:HIS:HB2	1.99	0.44
1:F:63:GYC:CZ	1:F:193:HIS:CB	2.96	0.44
1:A:36:GLY:O	1:A:212:HIS:HA	2.18	0.43
1:C:59:MET:HE1	1:C:139:TRP:CD2	2.53	0.43
1:D:59:MET:HG2	1:D:63:GYC:CD1	2.48	0.43
1:C:198[B]:LYS:HA	1:C:198[B]:LYS:HD3	1.83	0.43
1:B:35[B]:GLU:HA	1:B:70:LYS:NZ	2.34	0.43
1:E:95:TYR:CD1	1:E:171:CYS:HB2	2.54	0.43
1:C:198[A]:LYS:HG3	1:C:210:HIS:CD2	2.53	0.43
1:C:12:LEU:C	1:C:12:LEU:HD12	2.39	0.43
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.01	0.42
1:E:63:GYC:HE1	1:E:195:ILE:CB	2.48	0.42
1:A:142:SER:HB3	1:A:159:TYR:CE1	2.54	0.42
1:A:198:LYS:HG3	1:A:210:HIS:ND1	2.34	0.42
1:E:83:PHE:HB3	1:E:84:PRO:HA	1.99	0.42
1:C:53:ALA:O	1:C:56:ILE:HG12	2.18	0.42
1:E:82[B]:SER:OG	1:E:86:GLY:O	2.36	0.42
1:B:11:LYS:HB2	1:B:11:LYS:HE3	1.57	0.42
1:A:212:HIS:HB2	2:A:2022:HOH:O	2.18	0.42
1:A:158[B]:ASN:N	1:A:158[B]:ASN:OD1	2.50	0.42
1:B:180:LYS:NZ	2:B:2047:HOH:O	2.50	0.42
1:D:63:GYC:HE2	1:D:142[B]:SER:OG	2.20	0.42
1:D:91:ARG:HD3	1:D:173:PHE:CD2	2.55	0.42
1:D:21:HIS:HA	1:D:22:PRO:HD3	1.83	0.42
1:A:103:ALA:HA	1:A:119:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:TYR:HA	1:F:72:PRO:HD2	1.88	0.41
1:E:93:MET:HG2	1:E:173:PHE:CZ	2.55	0.41
1:C:4:ILE:HG13	1:C:8[A]:MET:SD	2.60	0.41
1:D:77:ASP:OD2	1:D:80:LYS:HD2	2.20	0.41
1:B:78:TYR:CE1	1:B:185:LEU:HD23	2.56	0.41
1:C:203:ASP:O	1:C:204:TYR:HB2	2.20	0.41
1:B:141:LEU:HD13	1:B:193:HIS:O	2.20	0.41
1:D:66:ARG:HB3	1:D:79:PHE:CG	2.56	0.41
1:E:36:GLY:O	1:E:212:HIS:HA	2.20	0.41
1:F:63:GYC:HB12	1:F:211:GLU:OE1	2.21	0.41
1:B:85:GLU:HG2	1:B:181:LYS:CE	2.40	0.41
1:F:4:ILE:O	1:F:4:ILE:HG23	2.20	0.41
1:B:77:ASP:OD2	1:B:80:LYS:HD2	2.21	0.40
1:B:16:GLY:HA2	1:B:119:ARG:CZ	2.51	0.40
1:E:146:LEU:HG	1:E:155:SER:HB3	2.04	0.40
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.22	0.40
1:F:139:TRP:CE2	1:F:161:LEU:HD21	2.56	0.40
1:A:63:GYC:CZ	1:A:193:HIS:HB3	2.52	0.40
1:B:95:TYR:CD2	1:B:171:CYS:HB2	2.56	0.40
1:A:93:MET:HG2	1:A:173:PHE:CE1	2.57	0.40
1:C:170:ARG:CZ	1:C:170:ARG:HB3	2.51	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:135[A]:ARG:NE	1:D:48:GLY:O[3_456]	2.08	0.12

## 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	219/214 (102%)	218 (100%)	1 (0%)	0	100	100
1	B	220/214 (103%)	215 (98%)	5 (2%)	0	100	100
1	C	220/214 (103%)	218 (99%)	2 (1%)	0	100	100
1	D	218/214 (102%)	214 (98%)	4 (2%)	0	100	100
1	E	217/214 (101%)	211 (97%)	4 (2%)	2 (1%)	20	20
1	F	217/214 (101%)	214 (99%)	3 (1%)	0	100	100
All	All	1311/1284 (102%)	1290 (98%)	19 (1%)	2 (0%)	51	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	4	ILE
1	E	5	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	191/183 (104%)	184 (96%)	7 (4%)	39	49
1	B	192/183 (105%)	186 (97%)	6 (3%)	45	56
1	C	192/183 (105%)	191 (100%)	1 (0%)	91	95
1	D	190/183 (104%)	186 (98%)	4 (2%)	59	71
1	E	186/183 (102%)	179 (96%)	7 (4%)	38	48
1	F	188/183 (103%)	176 (94%)	12 (6%)	20	23
All	All	1139/1098 (104%)	1102 (97%)	37 (3%)	46	54

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	30	LEU
1	A	81[A]	GLN

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Mol	Chain	Res	Type
1	A	81[B]	GLN
1	A	170	ARG
1	A	181	LYS
1	A	202	LYS
1	B	67	VAL
1	B	112	ASP
1	B	141	LEU
1	B	164[A]	GLU
1	B	164[B]	GLU
1	B	180	LYS
1	C	30	LEU
1	D	7	ASP
1	D	138	LYS
1	D	202	LYS
1	D	217	SER
1	E	28	VAL
1	E	30	LEU
1	E	67	VAL
1	E	109	LEU
1	E	154	LYS
1	E	158	ASN
1	E	180	LYS
1	F	9	LYS
1	F	43	LYS
1	F	73	GLU
1	F	134	LYS
1	F	156	ASP
1	F	158	ASN
1	F	162[A]	SER
1	F	162[B]	SER
1	F	187	ASP
1	F	202	LYS
1	F	214[A]	GLU
1	F	214[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	210	HIS
1	D	210	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	6 (27%)	27,30,32	4.12	6 (22%)
1	GYC	B	63	1	22,22,23	4.52	6 (27%)	27,30,32	4.60	9 (33%)
1	GYC	C	63	1	22,22,23	4.42	6 (27%)	27,30,32	4.06	7 (25%)
1	GYC	D	63	1	22,22,23	4.37	6 (27%)	27,30,32	4.35	8 (29%)
1	GYC	E	63	1	22,22,23	4.54	7 (31%)	27,30,32	4.38	7 (25%)
1	GYC	F	63	1	22,22,23	4.40	6 (27%)	27,30,32	4.08	6 (22%)

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	1	-	0/9/29/30	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	GYC	CA2-C2	-11.76	1.36	1.48
1	E	63	GYC	CA2-C2	-11.54	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GYC	CA2-C2	-11.41	1.37	1.48
1	D	63	GYC	CA2-C2	-11.16	1.37	1.48
1	A	63	GYC	CA2-C2	-11.09	1.37	1.48
1	F	63	GYC	CA2-C2	-10.31	1.38	1.48
1	B	63	GYC	OH-CZ	-4.74	1.26	1.37
1	E	63	GYC	OH-CZ	-4.74	1.26	1.37
1	D	63	GYC	OH-CZ	-4.71	1.26	1.37
1	A	63	GYC	OH-CZ	-4.56	1.26	1.37
1	C	63	GYC	OH-CZ	-4.55	1.26	1.37
1	F	63	GYC	OH-CZ	-4.54	1.26	1.37
1	A	63	GYC	C2-N3	-3.16	1.32	1.39
1	C	63	GYC	C2-N3	-2.97	1.32	1.39
1	F	63	GYC	C2-N3	-2.92	1.32	1.39
1	D	63	GYC	C2-N3	-2.86	1.32	1.39
1	E	63	GYC	C2-N3	-2.80	1.33	1.39
1	B	63	GYC	C2-N3	-2.76	1.33	1.39
1	E	63	GYC	CA1-C1	-2.10	1.48	1.51
1	B	63	GYC	O2-C2	2.42	1.28	1.23
1	C	63	GYC	O2-C2	2.53	1.28	1.23
1	A	63	GYC	O2-C2	2.62	1.28	1.23
1	E	63	GYC	O2-C2	2.65	1.28	1.23
1	D	63	GYC	O2-C2	2.69	1.29	1.23
1	F	63	GYC	O2-C2	2.74	1.29	1.23
1	E	63	GYC	C1-N2	3.39	1.37	1.32
1	C	63	GYC	C1-N2	3.91	1.38	1.32
1	A	63	GYC	C1-N2	3.94	1.38	1.32
1	D	63	GYC	C1-N2	4.07	1.38	1.32
1	F	63	GYC	C1-N2	4.49	1.39	1.32
1	B	63	GYC	C1-N2	4.49	1.39	1.32
1	A	63	GYC	CB2-CA2	14.69	1.48	1.35
1	D	63	GYC	CB2-CA2	15.26	1.48	1.35
1	C	63	GYC	CB2-CA2	15.44	1.48	1.35
1	B	63	GYC	CB2-CA2	15.78	1.49	1.35
1	F	63	GYC	CB2-CA2	15.90	1.49	1.35
1	E	63	GYC	CB2-CA2	16.18	1.49	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GYC	O2-C2-CA2	-12.98	123.97	130.97
1	E	63	GYC	O2-C2-CA2	-12.57	124.19	130.97
1	D	63	GYC	O2-C2-CA2	-11.11	124.98	130.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	O2-C2-CA2	-10.70	125.20	130.97
1	C	63	GYC	O2-C2-CA2	-9.84	125.66	130.97
1	F	63	GYC	O2-C2-CA2	-9.41	125.90	130.97
1	B	63	GYC	CG2-CB2-CA2	-6.37	122.79	130.19
1	E	63	GYC	CG2-CB2-CA2	-5.28	124.05	130.19
1	D	63	GYC	CG2-CB2-CA2	-4.60	124.85	130.19
1	C	63	GYC	CG2-CB2-CA2	-4.36	125.12	130.19
1	A	63	GYC	CG2-CB2-CA2	-3.99	125.56	130.19
1	F	63	GYC	CG2-CB2-CA2	-3.98	125.57	130.19
1	B	63	GYC	O-C-CA3	-3.23	115.69	126.38
1	F	63	GYC	CB2-CA2-N2	-3.20	123.94	128.79
1	A	63	GYC	O-C-CA3	-3.18	115.87	126.38
1	C	63	GYC	O-C-CA3	-2.80	117.11	126.38
1	F	63	GYC	O-C-CA3	-2.72	117.40	126.38
1	E	63	GYC	O-C-CA3	-2.66	117.59	126.38
1	A	63	GYC	CB2-CA2-N2	-2.61	124.83	128.79
1	E	63	GYC	CB2-CA2-N2	-2.61	124.84	128.79
1	C	63	GYC	C2-CA2-N2	-2.59	107.03	108.93
1	D	63	GYC	CB2-CA2-N2	-2.50	125.01	128.79
1	D	63	GYC	O-C-CA3	-2.49	118.14	126.38
1	C	63	GYC	CB2-CA2-N2	-2.44	125.08	128.79
1	B	63	GYC	N3-C1-N2	-2.41	109.79	111.45
1	D	63	GYC	C2-CA2-N2	-2.35	107.21	108.93
1	B	63	GYC	C2-CA2-N2	-2.30	107.24	108.93
1	E	63	GYC	C2-CA2-N2	-2.26	107.27	108.93
1	B	63	GYC	CB2-CA2-N2	-2.16	125.52	128.79
1	B	63	GYC	CA1-C1-N2	2.04	127.67	123.56
1	D	63	GYC	CA3-N3-C1	2.31	129.90	127.20
1	A	63	GYC	CB2-CA2-C2	3.49	126.72	122.32
1	B	63	GYC	CB2-CA2-C2	3.59	126.84	122.32
1	C	63	GYC	CB2-CA2-C2	3.86	127.18	122.32
1	D	63	GYC	CB2-CA2-C2	3.88	127.20	122.32
1	E	63	GYC	CB2-CA2-C2	4.17	127.56	122.32
1	F	63	GYC	CB2-CA2-C2	4.32	127.76	122.32
1	C	63	GYC	CA2-C2-N3	16.67	110.74	103.30
1	A	63	GYC	CA2-C2-N3	16.86	110.82	103.30
1	E	63	GYC	CA2-C2-N3	16.91	110.84	103.30
1	F	63	GYC	CA2-C2-N3	17.07	110.91	103.30
1	B	63	GYC	CA2-C2-N3	17.64	111.17	103.30
1	D	63	GYC	CA2-C2-N3	17.92	111.30	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	GYC	3	0
1	B	63	GYC	3	0
1	C	63	GYC	3	0
1	D	63	GYC	5	0
1	E	63	GYC	4	0
1	F	63	GYC	5	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	213/214 (99%)	-0.35	0 100 100	11, 19, 35, 52	0
1	B	213/214 (99%)	-0.20	1 (0%) 90 95	12, 25, 44, 74	0
1	C	212/214 (99%)	-0.16	1 (0%) 90 95	12, 23, 43, 57	0
1	D	211/214 (98%)	-0.31	0 100 100	13, 23, 40, 59	0
1	E	213/214 (99%)	0.00	1 (0%) 90 95	16, 29, 48, 70	0
1	F	213/214 (99%)	-0.15	1 (0%) 90 95	14, 26, 42, 63	0
All	All	1275/1284 (99%)	-0.19	4 (0%) 93 97	11, 24, 44, 74	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	3.5
1	E	4	ILE	2.1
1	F	166	GLY	2.1
1	C	3	VAL	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. 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	B	63	21/22	0.94	0.12	-	18,27,36,37	0
1	GYC	E	63	21/22	0.93	0.13	-	29,35,50,52	0
1	GYC	D	63	21/22	0.95	0.12	-	23,29,34,40	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	0.13	-	13,21,26,27	0
1	GYC	C	63	21/22	0.95	0.14	-	14,25,34,38	0
1	GYC	F	63	21/22	0.95	0.13	-	20,29,40,41	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.