

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 05:50 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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

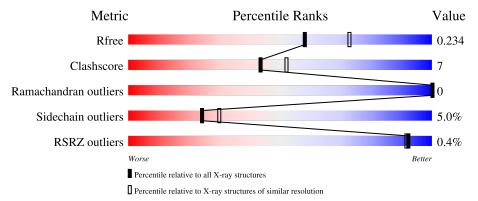
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 of 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 <=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	86%	12%	•
1	В	215	90%	8%	•
1	С	215	80%	18%	
1	D	215	88%	11%	•
1	Е	215	82%	15%	-



M	Iol	Chain	Length	Quality of chain		
	1	F	215	80%	17%	-

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 (i)

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		At	oms			ZeroOcc	AltConf	Trace
1	A	214	Total	С	Ν	О	S	0	8	0
1	Λ	214	1789	1138	303	338	10	0	8	0
1	В	214	Total	С	N	О	S	0	4	0
1	Ъ	214	1761	1121	301	329	10	0	4	0
1	С	214	Total	С	N	О	S	0	2	0
1		214	1739	1110	293	326	10	0		0
1	D	215	Total	С	N	О	S	0	4	0
1	D	210	1762	1123	298	331	10	0	4	0
1	Е	214	Total	С	N	О	S	0	5	0
1	12	214	1764	1124	298	332	10	0	9	0
1	F	214	Total	С	N	О	S	0	4	0
1	I'	214	1754	1118	296	330	10	U	4	U

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
В	59	MET	THR	conflict	UNP Q5TLG6
В	60	ALA	VAL	conflict	UNP Q5TLG6
В	63	GYC	CYS	chromophore	UNP Q5TLG6
В	63	GYC	TYR	chromophore	UNP Q5TLG6
В	63	GYC	GLY	chromophore	UNP Q5TLG6
В	94	ILE	ASN	conflict	UNP Q5TLG6



 $Continued\ from\ previous\ page...$

Chain	Residue	Modelled Modelled	Actual	Comment	Reference
В	141	LEU	PRO	conflict	UNP Q5TLG6
В	155	SER	GLY	conflict	UNP Q5TLG6
В	157	GLY	VAL	conflict	UNP Q5TLG6
В	159	TYR	MET	conflict	UNP Q5TLG6
В	190	SER	PHE	conflict	UNP Q5TLG6
С	59	MET	THR	conflict	UNP Q5TLG6
С	60	ALA	VAL	conflict	UNP Q5TLG6
С	63	GYC	CYS	chromophore	UNP Q5TLG6
С	63	GYC	TYR	chromophore	UNP Q5TLG6
С	63	GYC	GLY	chromophore	UNP Q5TLG6
С	94	ILE	ASN	conflict	UNP Q5TLG6
С	141	LEU	PRO	conflict	UNP Q5TLG6
С	155	SER	GLY	conflict	UNP Q5TLG6
С	157	GLY	VAL	conflict	UNP Q5TLG6
С	159	TYR	MET	conflict	UNP Q5TLG6
С	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
Е	59	MET	THR	conflict	UNP Q5TLG6
Е	60	ALA	VAL	conflict	UNP Q5TLG6
Е	63	GYC	CYS	chromophore	UNP Q5TLG6
Е	63	GYC	TYR	chromophore	UNP Q5TLG6
Е	63	GYC	GLY	chromophore	UNP Q5TLG6
Е	94	ILE	ASN	conflict	UNP Q5TLG6
Е	141	LEU	PRO	conflict	UNP Q5TLG6
Е	155	SER	GLY	conflict	UNP Q5TLG6
Е	157	GLY	VAL	conflict	UNP Q5TLG6
Е	159	TYR	MET	conflict	UNP Q5TLG6
Е	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



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.

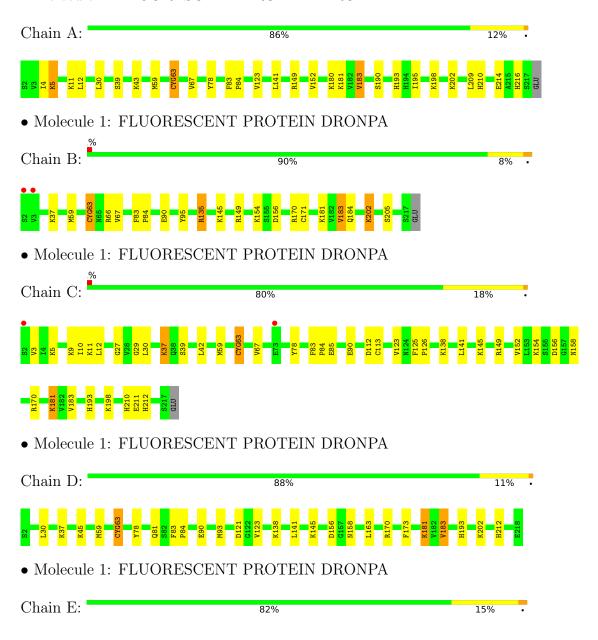
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	В	72	Total O 72 72	0	0
2	С	106	Total O 106 106	0	0
2	D	96	Total O 96 96	0	0
2	Е	63	Total O 63 63	0	0
2	F	59	Total O 59 59	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

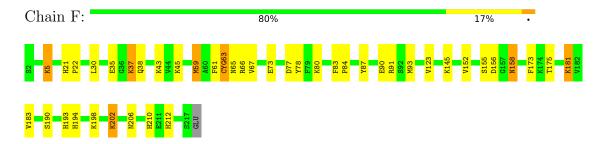
• Molecule 1: FLUORESCENT PROTEIN DRONPA







• Molecule 1: FLUORESCENT PROTEIN DRONPA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	109.32Å 182.00Å 72.88Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 - 2.20	Depositor
resolution (A)	46.86 - 2.20	EDS
% Data completeness	99.7 (46.86-2.20)	Depositor
(in resolution range)	99.7 (46.86-2.20)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.56 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
P.P.	0.187 , 0.240	Depositor
R, R_{free}	0.183 , 0.234	DCC
R_{free} test set	1510 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 34.7	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2> = 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 $(Å^2)$	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.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.46	0/1813	0.57	0/2445	
1	В	0.40	0/1785	0.56	0/2407	
1	С	0.42	0/1762	0.55	0/2377	
1	D	0.43	0/1786	0.57	0/2410	
1	Е	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	1695	18	0
1	В	1761	0	1675	14	1
1	С	1739	0	1660	34	0
1	D	1762	0	1671	17	0
1	Е	1764	0	1675	25	0
1	F	1754	0	1662	43	0
2	A	113	0	0	0	0



I 'omtamalod	trom	mmonia	maaa
Continued	11 0116	DICUIUUS	Daue
	.,	10	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	72	0	0	1	0
2	С	106	0	0	3	0
2	D	96	0	0	0	0
2	Е	63	0	0	1	0
2	F	59	0	0	2	0
All	All	11078	0	10038	139	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.

The worst 5 of 139 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:C3	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:N1	1.97	0.97

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:156:ASP:OD2	1:B:170[A]:ARG:NE[2_555]	2.07	0.13

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	Perce	ntiles
1	A	$217/215 \ (101\%)$	214 (99%)	3 (1%)	0	100	100
1	В	213/215 (99%)	211 (99%)	2 (1%)	0	100	100



Continued	trom	mromonie	maaa
-	110111	DICULUUS	pauc

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	C	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
1	D	214/215 (100%)	212 (99%)	2 (1%)	0	100	100
1	\mathbf{E}	$214/215 \ (100\%)$	212 (99%)	2 (1%)	0	100	100
1	F	212/215~(99%)	209 (99%)	3 (1%)	0	100	100
All	All	1281/1290 (99%)	1266 (99%)	15 (1%)	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	Perce	$_{ m ntiles}$
1	A	190/184~(103%)	181 (95%)	9 (5%)	26	33
1	В	186/184 (101%)	179 (96%)	7 (4%)	33	42
1	С	184/184 (100%)	177 (96%)	7 (4%)	33	42
1	D	186/184 (101%)	178 (96%)	8 (4%)	29	36
1	E	187/184 (102%)	175 (94%)	12 (6%)	17	20
1	F	185/184 (100%)	173 (94%)	12 (6%)	17	19
All	All	1118/1104 (101%)	1063 (95%)	55 (5%)	24	31

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	181	LYS
1	Е	66	ARG
1	F	202	LYS
1	F	73	GLU
1	D	183	VAL

Sometimes 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	С	210	HIS
1	Е	194	HIS
1	F	210	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Tune	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	GYC	В	63	1	22,22,23	4.45	7 (31%)	26,30,32	4.42	8 (30%)
1	GYC	С	63	1	22,22,23	4.55	6 (27%)	26,30,32	4.39	8 (30%)
1	GYC	A	63	1	22,22,23	4.46	7 (31%)	26,30,32	4.45	8 (30%)
1	GYC	Е	63	1	22,22,23	4.65	6 (27%)	26,30,32	4.34	7 (26%)
1	GYC	D	63	1	22,22,23	4.62	6 (27%)	26,30,32	4.55	8 (30%)
1	GYC	F	63	-	22,22,23	4.64	8 (36%)	26,30,32	4.79	9 (34%)

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	В	63	1	-	2/9/29/30	0/2/2/2
1	GYC	С	63	1	-	3/9/29/30	0/2/2/2
1	GYC	A	63	1	-	2/9/29/30	0/2/2/2
1	GYC	E	63	1	-	3/9/29/30	0/2/2/2



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

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	Е	63	GYC	CB2-CA2	17.66	1.49	1.35
1	F	63	GYC	CB2-CA2	17.42	1.49	1.35
1	D	63	GYC	CB2-CA2	17.26	1.49	1.35
1	A	63	GYC	CB2-CA2	16.71	1.49	1.35
1	С	63	GYC	CB2-CA2	16.65	1.49	1.35

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	F	63	GYC	CA2-C2-N3	15.74	110.81	103.37
1	D	63	GYC	CA2-C2-N3	14.85	110.39	103.37
1	С	63	GYC	CA2-C2-N3	14.45	110.20	103.37
1	Е	63	GYC	CA2-C2-N3	14.25	110.11	103.37
1	A	63	GYC	CA2-C2-N3	14.03	110.01	103.37

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	GYC	N2-CA2-CB2-CG2
1	A	63	GYC	C2-CA2-CB2-CG2
1	В	63	GYC	N2-CA2-CB2-CG2
1	В	63	GYC	C2-CA2-CB2-CG2
1	С	63	GYC	N2-CA2-CB2-CG2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	63	GYC	1	0
1	С	63	GYC	1	0
1	A	63	GYC	1	0
1	Е	63	GYC	1	0
1	D	63	GYC	1	0
1	F	63	GYC	9	0



5.5 Carbohydrates (i)

There are no monosaccharides 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	F	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	
1	F	61:PHE	С	63:GYC	N1	2.29
1	F	65:ASN	С	66:ARG	N	2.27
1	F	63:GYC	C3	65:ASN	N	2.14



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^{th} 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>	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
1	A	213/215 (99%)	-0.66	0 100 100	14, 25, 43, 56	0
1	В	213/215 (99%)	-0.50	2 (0%) 84 83	16, 31, 52, 70	0
1	С	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%) 91 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	5 (0%) 92 91	14, 31, 52, 78	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	2	SER	3.8
1	В	2	SER	3.1
1	Ε	3	VAL	2.6
1	В	3	VAL	2.3
1	С	73	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	GYC	С	63	21/22	0.94	0.12	23,28,37,42	0
1	GYC	D	63	21/22	0.95	0.10	19,32,38,48	0
1	GYC	Ε	63	21/22	0.95	0.11	31,38,46,52	0
1	GYC	F	63	21/22	0.95	0.12	23,34,41,45	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
1	GYC	A	63	21/22	0.97	0.10	16,24,33,34	0
1	GYC	В	63	21/22	0.97	0.09	24,30,36,42	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

