wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 12:08 AM EST

PDB ID	:	2ZMW
Title	:	Crystal Structure of Monomeric Kusabira-Orange (MKO), Orange-Emitting GFP-like Protein, at pH 6.0
Authors	:	Kikuchi, A.; Fukumura, E.; Karasawa, S.; Mizuno, H.; Miyawaki, A.; Shiro, Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2008-04-21
Resolution	:	2.00 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:

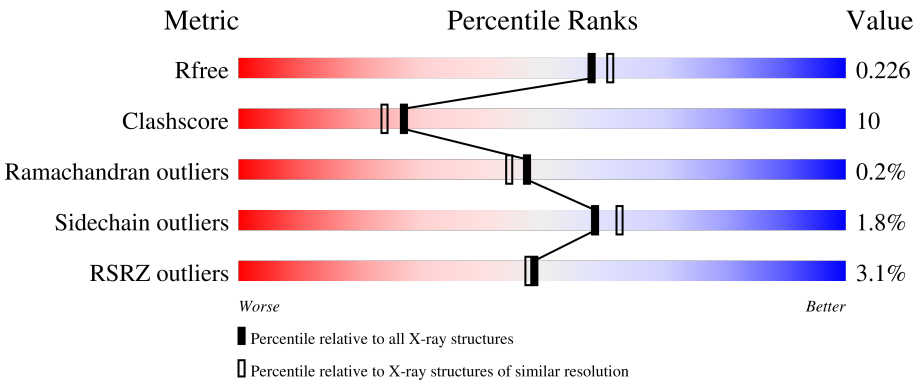
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	223	2%, 72%, 24%, •
1	B	223	3%, 81%, 13%, • •
1	C	223	4%, 73%, 21%, • •
1	D	223	3%, 81%, 15%, •

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	CFY	A	66	X	-	-	-
1	CFY	B	66	X	-	-	-
1	CFY	C	66	X	-	-	-
1	CFY	D	66	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7562 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1710	1087	291	321	11	0	0	0
1	B	214	1710	1087	291	321	11	0	0	0
1	C	214	1710	1087	291	321	11	0	0	0
1	D	214	1710	1087	291	321	11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CFY	PHE	chromophore	UNP Q6I7B2
A	66	CFY	CYS	chromophore	UNP Q6I7B2
A	66	CFY	TYR	chromophore	UNP Q6I7B2
A	66	CFY	GLY	chromophore	UNP Q6I7B2
A	219	LEU	-	expression tag	UNP Q6I7B2
A	220	GLU	-	expression tag	UNP Q6I7B2
A	221	HIS	-	expression tag	UNP Q6I7B2
A	222	HIS	-	expression tag	UNP Q6I7B2
A	223	HIS	-	expression tag	UNP Q6I7B2
A	224	HIS	-	expression tag	UNP Q6I7B2
A	225	HIS	-	expression tag	UNP Q6I7B2
A	226	HIS	-	expression tag	UNP Q6I7B2
B	66	CFY	PHE	chromophore	UNP Q6I7B2
B	66	CFY	CYS	chromophore	UNP Q6I7B2
B	66	CFY	TYR	chromophore	UNP Q6I7B2
B	66	CFY	GLY	chromophore	UNP Q6I7B2
B	219	LEU	-	expression tag	UNP Q6I7B2
B	220	GLU	-	expression tag	UNP Q6I7B2
B	221	HIS	-	expression tag	UNP Q6I7B2
B	222	HIS	-	expression tag	UNP Q6I7B2
B	223	HIS	-	expression tag	UNP Q6I7B2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	UNP Q6I7B2
B	225	HIS	-	expression tag	UNP Q6I7B2
B	226	HIS	-	expression tag	UNP Q6I7B2
C	66	CFY	PHE	chromophore	UNP Q6I7B2
C	66	CFY	CYS	chromophore	UNP Q6I7B2
C	66	CFY	TYR	chromophore	UNP Q6I7B2
C	66	CFY	GLY	chromophore	UNP Q6I7B2
C	219	LEU	-	expression tag	UNP Q6I7B2
C	220	GLU	-	expression tag	UNP Q6I7B2
C	221	HIS	-	expression tag	UNP Q6I7B2
C	222	HIS	-	expression tag	UNP Q6I7B2
C	223	HIS	-	expression tag	UNP Q6I7B2
C	224	HIS	-	expression tag	UNP Q6I7B2
C	225	HIS	-	expression tag	UNP Q6I7B2
C	226	HIS	-	expression tag	UNP Q6I7B2
D	66	CFY	PHE	chromophore	UNP Q6I7B2
D	66	CFY	CYS	chromophore	UNP Q6I7B2
D	66	CFY	TYR	chromophore	UNP Q6I7B2
D	66	CFY	GLY	chromophore	UNP Q6I7B2
D	219	LEU	-	expression tag	UNP Q6I7B2
D	220	GLU	-	expression tag	UNP Q6I7B2
D	221	HIS	-	expression tag	UNP Q6I7B2
D	222	HIS	-	expression tag	UNP Q6I7B2
D	223	HIS	-	expression tag	UNP Q6I7B2
D	224	HIS	-	expression tag	UNP Q6I7B2
D	225	HIS	-	expression tag	UNP Q6I7B2
D	226	HIS	-	expression tag	UNP Q6I7B2

- Molecule 2 is water.

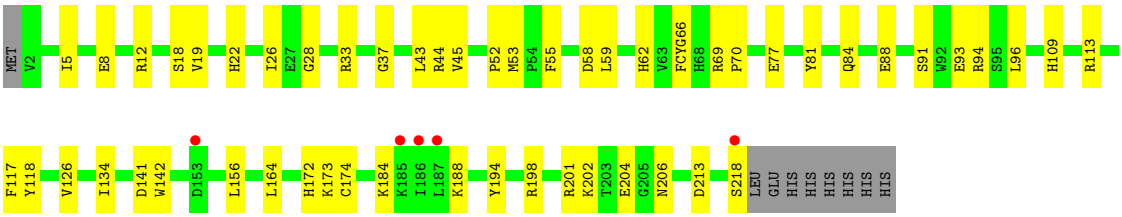
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	162	162	162	0	0
			Total	O		
2	B	214	214	214	0	0
			Total	O		
2	C	176	176	176	0	0
			Total	O		
2	D	170	170	170	0	0

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.

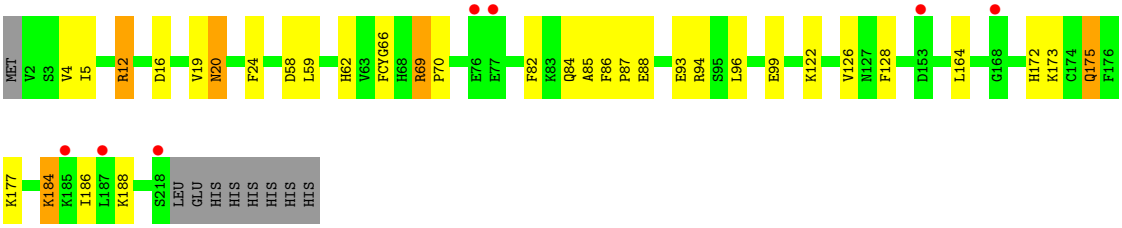
• Molecule 1: Fluorescent protein

Chain A:



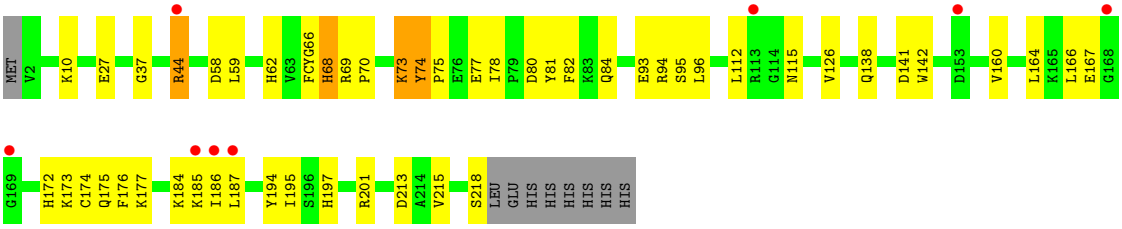
• Molecule 1: Fluorescent protein

Chain B:



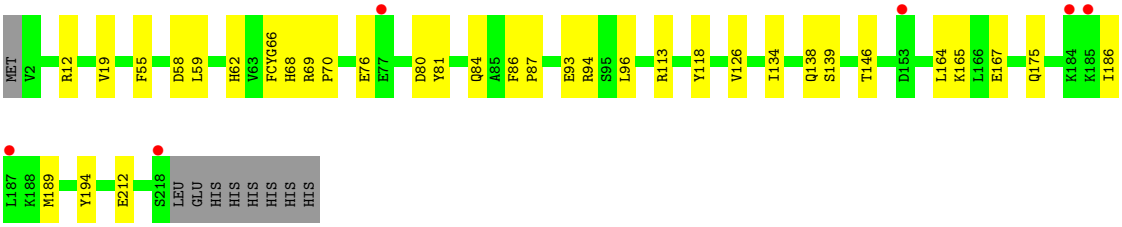
• Molecule 1: Fluorescent protein

Chain C:



• Molecule 1: Fluorescent protein

Chain D:


MET
V2
R12
V19
F55
D58
L59
H62
V63
FCYG66
H68
R69
P70
E76
E77
D80
Y81
Q84
A85
F86
P87
E93
R94
S95
L96
R113
Y118
V126
I134
Q138
S139
T146
D153
L164
K165
L166
E167
Q175
K184
K185
I186
L187
K188
M189
Y194
E212
S218
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.57Å 72.11Å 90.27Å 90.00° 102.72° 90.00°	Depositor
Resolution (Å)	19.99 – 2.00 31.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.99-2.00) 98.2 (31.99-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.232 0.192 , 0.226	Depositor DCC
R_{free} test set	3917 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 69.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7562	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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: CFY

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	0.33	0/1722	0.64	0/2320
1	B	0.33	0/1722	0.64	0/2320
1	C	0.32	0/1722	0.64	0/2320
1	D	0.33	0/1722	0.64	0/2320
All	All	0.33	0/6888	0.64	0/9280

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	66	CFY	C1
1	B	66	CFY	C1
1	C	66	CFY	C1
1	D	66	CFY	C1

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	1710	0	1635	40	0
1	B	1710	0	1635	29	0
1	C	1710	0	1635	41	0
1	D	1710	0	1635	29	0
2	A	162	0	0	2	0
2	B	214	0	0	2	0
2	C	176	0	0	1	0
2	D	170	0	0	5	0
All	All	7562	0	6540	135	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 10.

The worst 5 of 135 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:A:26:ILE:HD12	1:A:45:VAL:HG22	1.42	1.00
1:B:12:ARG:HH21	1:B:12:ARG:HB3	1.34	0.92
1:B:12:ARG:HB3	1:B:12:ARG:NH2	1.92	0.82
1:A:62:HIS:HD2	1:A:94:ARG:HH11	1.28	0.80
1:D:175:GLN:HG2	2:D:315:HOH:O	1.81	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/223 (94%)	205 (98%)	4 (2%)	0	100	100
1	B	209/223 (94%)	206 (99%)	3 (1%)	0	100	100
1	C	209/223 (94%)	202 (97%)	5 (2%)	2 (1%)	15	9
1	D	209/223 (94%)	205 (98%)	4 (2%)	0	100	100
All	All	836/892 (94%)	818 (98%)	16 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	73	LYS
1	C	74	TYR

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	181/190 (95%)	180 (99%)	1 (1%)	86	90
1	B	181/190 (95%)	176 (97%)	5 (3%)	43	44
1	C	181/190 (95%)	176 (97%)	5 (3%)	43	44
1	D	181/190 (95%)	179 (99%)	2 (1%)	73	78
All	All	724/760 (95%)	711 (98%)	13 (2%)	59	63

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68	HIS
1	C	112	LEU
1	D	212	GLU
1	C	197	HIS
1	D	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	62	HIS
1	D	136	GLN
1	D	175	GLN
1	D	109	HIS
1	B	109	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)

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	CFY	C	66	1	29,35,36	5.29	13 (44%)	31,50,52	2.10	14 (45%)
1	CFY	D	66	1	29,35,36	5.29	15 (51%)	31,50,52	2.07	15 (48%)
1	CFY	A	66	1	29,35,36	5.24	14 (48%)	31,50,52	2.06	13 (41%)
1	CFY	B	66	1	29,35,36	5.31	14 (48%)	31,50,52	2.07	15 (48%)

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	CFY	C	66	1	1/1/7/9	0/10/48/49	0/4/4/4
1	CFY	D	66	1	1/1/7/9	0/10/48/49	0/4/4/4
1	CFY	A	66	1	1/1/7/9	0/10/48/49	0/4/4/4
1	CFY	B	66	1	1/1/7/9	0/10/48/49	0/4/4/4

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CFY	CB1-CA1	15.67	1.63	1.50
1	D	66	CFY	CA1-N1	15.58	1.43	1.28
1	B	66	CFY	CB1-CA1	15.55	1.63	1.50
1	B	66	CFY	CA1-N1	15.52	1.43	1.28
1	D	66	CFY	CB1-CA1	15.50	1.63	1.50

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	CFY	O2-C2-CA2	-5.11	128.09	130.96
1	B	66	CFY	O2-C2-CA2	-5.06	128.12	130.96
1	D	66	CFY	O2-C2-CA2	-5.02	128.14	130.96
1	A	66	CFY	O2-C2-CA2	-4.71	128.31	130.96
1	C	66	CFY	CB0-CG1-CD1	-4.44	112.09	120.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	66	CFY	C1
1	B	66	CFY	C1
1	C	66	CFY	C1
1	D	66	CFY	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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	213/223 (95%)	-0.10	5 (2%)	60	59	10, 21, 41, 57	0
1	B	213/223 (95%)	-0.23	7 (3%)	46	45	10, 19, 34, 58	0
1	C	213/223 (95%)	-0.00	8 (3%)	40	39	10, 21, 43, 60	0
1	D	213/223 (95%)	-0.26	6 (2%)	53	51	10, 19, 35, 56	0
All	All	852/892 (95%)	-0.15	26 (3%)	49	48	10, 20, 40, 60	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	LEU	6.0
1	A	187	LEU	5.6
1	C	187	LEU	4.8
1	C	168	GLY	4.2
1	D	187	LEU	3.9

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	CFY	A	66	32/33	0.91	0.13	13,19,26,26	0
1	CFY	B	66	32/33	0.93	0.12	10,18,22,26	0
1	CFY	D	66	32/33	0.93	0.12	12,19,22,24	0
1	CFY	C	66	32/33	0.94	0.12	13,20,24,27	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.