



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:08 AM GMT

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 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

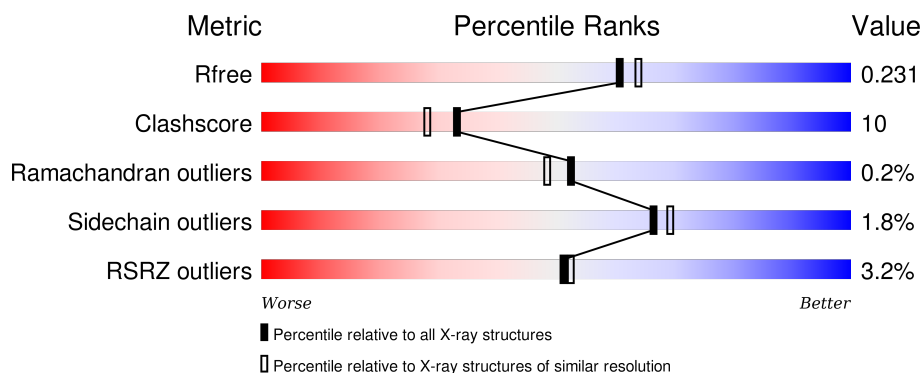
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	223	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	B	223	<div> <div>3%</div> <div>80%</div> <div>14%</div> <div>.</div> </div>
1	C	223	<div> <div>4%</div> <div>72%</div> <div>22%</div> <div>.</div> </div>
1	D	223	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>.</div> </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	CFY	A	66	X	-	-	-
1	CFY	B	66	X	-	-	-
1	CFY	C	66	X	-	-	-
1	CFY	D	66	X	-	-	-

## 2 Entry composition

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
1	A	214	Total	C	N	O	S	0	0	0
			1710	1087	291	321	11			
1	B	214	Total	C	N	O	S	0	0	0
			1710	1087	291	321	11			
1	C	214	Total	C	N	O	S	0	0	0
			1710	1087	291	321	11			
1	D	214	Total	C	N	O	S	0	0	0
			1710	1087	291	321	11			

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

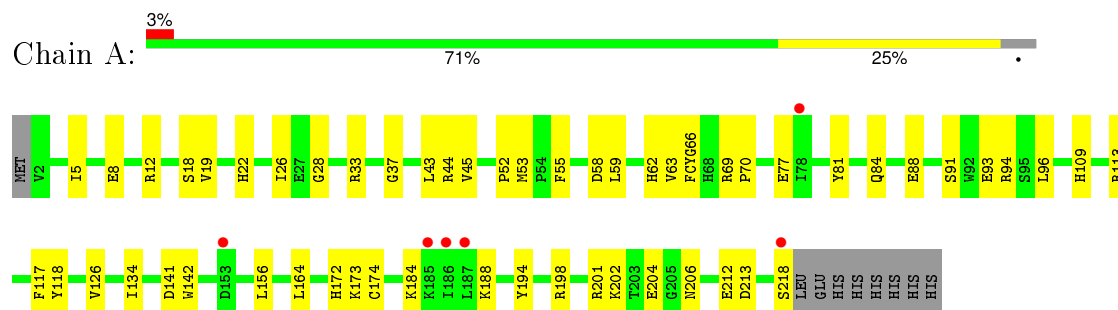
- Molecule 2 is water.

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

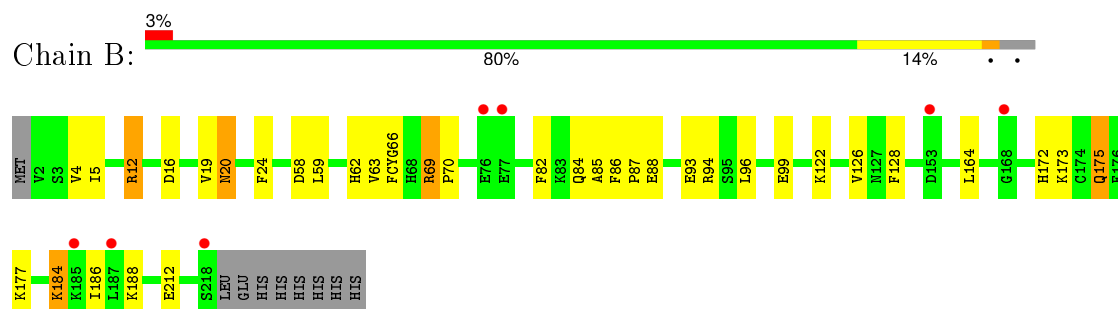
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

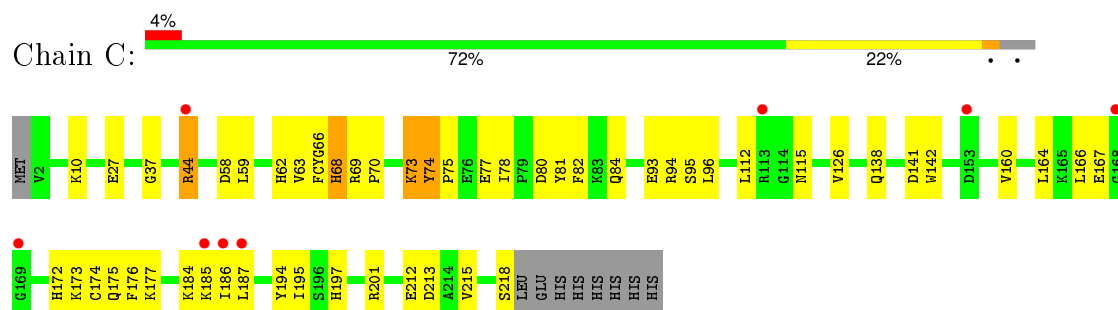
- Molecule 1: Fluorescent protein



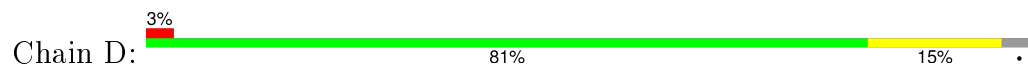
- Molecule 1: Fluorescent protein

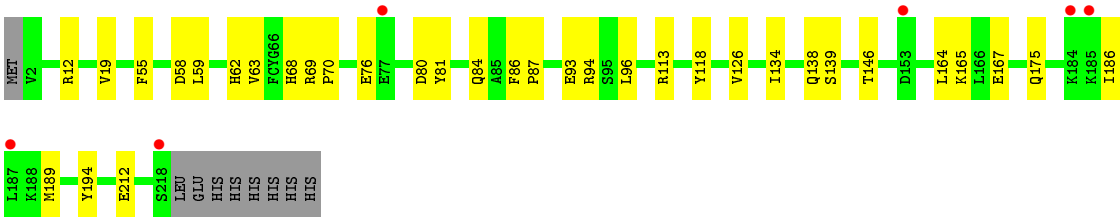


- Molecule 1: Fluorescent protein



- Molecule 1: Fluorescent protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.232 0.197 , 0.231	Depositor DCC
$R_{free}$ test set	3917 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 69.2	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77707 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	1
1	B	1	1
1	C	1	1
1	D	1	1
All	All	4	4

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	C2
1	B	66	CFY	C2
1	C	66	CFY	C2
1	D	66	CFY	C2

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	VAL	Mainchain
1	B	63	VAL	Mainchain
1	C	63	VAL	Mainchain
1	D	63	VAL	Mainchain

## 5.2 Too-close contacts

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	1644	41	0
1	B	1710	0	1644	30	0
1	C	1710	0	1644	42	0
1	D	1710	0	1644	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	6576	138	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.

All (138) 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:HB3	1:B:12:ARG:HH21	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
1:C:69:ARG:HA	1:C:69:ARG:NE	2.02	0.75
1:C:69:ARG:NH1	1:C:195:ILE:HG21	2.00	0.75
1:C:62:HIS:HD2	1:C:94:ARG:HH11	1.33	0.74
1:D:62:HIS:HD2	1:D:94:ARG:HH11	1.36	0.74
1:C:187:LEU:H	1:C:187:LEU:HD12	1.54	0.73
1:B:84:GLN:HE22	1:B:188:LYS:H	1.41	0.68
1:C:27:GLU:O	1:C:44:ARG:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLN:O	1:C:167:GLU:HG3	1.93	0.68
1:B:99:GLU:HB3	1:B:173:LYS:HG2	1.75	0.68
1:A:26:ILE:CD1	1:A:45:VAL:HG22	2.23	0.67
1:A:53:MET:H	1:A:206:ASN:HD21	1.42	0.67
1:C:175:GLN:HG3	2:C:317:HOH:O	1.94	0.67
1:B:62:HIS:HD2	1:B:94:ARG:HH11	1.43	0.67
1:A:19:VAL:HG11	1:A:55:PHE:CD2	2.30	0.66
1:B:88:GLU:HB2	1:B:184:LYS:HD2	1.77	0.65
1:A:141:ASP:OD1	1:A:201:ARG:HG2	1.97	0.64
1:B:20:ASN:HD21	1:B:128:PHE:H	1.43	0.64
1:A:142:TRP:CZ3	1:A:164:LEU:HG	2.34	0.62
1:C:69:ARG:HH12	1:C:195:ILE:HG21	1.63	0.61
1:D:68:HIS:HD2	1:D:70:PRO:HD2	1.67	0.59
1:C:73:LYS:O	1:C:74:TYR:HB2	2.01	0.59
1:A:58:ASP:HB3	1:A:164:LEU:HD21	1.84	0.59
1:C:69:ARG:HA	1:C:69:ARG:HE	1.66	0.59
1:B:59:LEU:O	1:B:62:HIS:HE1	1.86	0.58
1:B:184:LYS:H	1:B:184:LYS:HD3	1.68	0.58
1:C:187:LEU:N	1:C:187:LEU:HD12	2.18	0.58
1:D:138:GLN:O	1:D:167:GLU:HG3	2.04	0.58
1:A:194:TYR:HD2	1:A:218:SER:HB2	1.68	0.57
1:B:62:HIS:CE1	1:B:96:LEU:HD21	2.40	0.57
1:C:44:ARG:CB	1:C:44:ARG:HH11	2.18	0.57
1:A:62:HIS:CE1	1:A:96:LEU:HD21	2.39	0.57
1:A:8:GLU:HG2	1:A:33:ARG:HH11	1.70	0.56
1:D:81:TYR:CD1	1:D:186:ILE:HD13	2.40	0.56
1:D:62:HIS:CE1	1:D:96:LEU:HD21	2.41	0.55
1:A:62:HIS:CD2	1:A:94:ARG:HH11	2.18	0.55
1:A:77:GLU:OE1	1:A:77:GLU:N	2.39	0.55
1:D:139:SER:HB2	1:D:164:LEU:HD22	1.90	0.54
1:C:141:ASP:OD1	1:C:201:ARG:HG2	2.08	0.54
1:C:44:ARG:NH1	1:C:44:ARG:HB2	2.24	0.53
1:C:75:PRO:HG2	1:C:78:ILE:HG12	1.90	0.53
1:B:66:CFY:HB21	1:B:212:GLU:OE1	2.09	0.53
1:C:173:LYS:HG2	1:C:174:CYS:N	2.23	0.53
1:C:142:TRP:CZ3	1:C:164:LEU:HG	2.44	0.53
1:C:68:HIS:HD2	1:C:70:PRO:HD2	1.73	0.52
1:C:62:HIS:CE1	1:C:96:LEU:HD21	2.44	0.52
1:C:59:LEU:O	1:C:62:HIS:HE1	1.93	0.52
1:C:187:LEU:H	1:C:187:LEU:CD1	2.23	0.51
1:C:126:VAL:HB	1:D:93:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ILE:HD11	1:D:189:MET:HA	1.92	0.51
1:C:69:ARG:HB3	1:C:82:PHE:CG	2.46	0.51
1:B:99:GLU:HB3	1:B:173:LYS:CG	2.41	0.51
1:D:80:ASP:O	1:D:84:GLN:HG3	2.11	0.50
1:C:62:HIS:CD2	1:C:94:ARG:HH11	2.23	0.50
1:A:8:GLU:HG2	1:A:33:ARG:NH1	2.26	0.50
1:D:59:LEU:O	1:D:62:HIS:HE1	1.94	0.49
1:D:165:LYS:HD3	2:D:397:HOH:O	2.12	0.49
1:C:194:TYR:HD2	1:C:218:SER:HB2	1.77	0.49
1:A:126:VAL:HB	1:B:93:GLU:HB3	1.94	0.49
1:B:85:ALA:HA	1:B:184:LYS:HE2	1.93	0.49
1:A:69:ARG:NE	1:A:69:ARG:HA	2.28	0.49
1:C:10:LYS:HE2	1:C:115:ASN:HD21	1.78	0.49
1:C:81:TYR:CE1	1:C:186:ILE:HG13	2.49	0.48
1:D:113:ARG:HB2	1:D:118:TYR:HE2	1.77	0.48
1:D:69:ARG:NE	1:D:69:ARG:HA	2.28	0.48
1:D:175:GLN:NE2	2:D:372:HOH:O	2.42	0.48
1:A:202:LYS:HG2	1:A:204:GLU:OE2	2.14	0.48
1:A:113:ARG:HB3	1:A:118:TYR:HE2	1.78	0.47
1:B:177:LYS:HD2	2:B:410:HOH:O	2.13	0.47
1:D:62:HIS:CD2	1:D:94:ARG:HH11	2.25	0.47
1:D:58:ASP:HB3	1:D:164:LEU:HD21	1.96	0.47
1:B:19:VAL:HG23	1:B:24:PHE:HE2	1.80	0.47
1:C:80:ASP:O	1:C:84:GLN:HG3	2.15	0.47
1:A:173:LYS:HG2	1:A:174:CYS:N	2.30	0.47
1:D:12:ARG:HD3	1:D:118:TYR:CE1	2.49	0.46
1:B:84:GLN:HB3	1:B:186:ILE:HD12	1.97	0.46
1:A:44:ARG:HD2	2:A:294:HOH:O	2.16	0.46
1:A:134:ILE:HD13	2:A:227:HOH:O	2.14	0.46
1:B:175:GLN:HE21	1:B:175:GLN:N	2.13	0.46
1:A:8:GLU:CG	1:A:33:ARG:NH1	2.79	0.45
1:A:59:LEU:O	1:A:62:HIS:HE1	2.00	0.45
1:A:37:GLY:O	1:A:213:ASP:HA	2.17	0.45
1:B:173:LYS:HD3	2:B:329:HOH:O	2.17	0.45
1:C:77:GLU:OE2	1:C:77:GLU:N	2.50	0.45
1:D:113:ARG:HB2	1:D:118:TYR:CE2	2.52	0.44
1:C:37:GLY:O	1:C:213:ASP:HA	2.16	0.44
1:A:28:GLY:HA3	1:A:43:LEU:HD23	1.99	0.44
1:C:73:LYS:HB3	1:C:215:VAL:HG13	2.00	0.44
1:A:5:ILE:HD12	1:A:117:PHE:HZ	1.82	0.44
1:A:84:GLN:HE22	1:A:188:LYS:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:O	1:B:62:HIS:CE1	2.71	0.43
1:A:91:SER:OG	1:A:109:HIS:HD2	2.01	0.43
1:A:53:MET:H	1:A:206:ASN:ND2	2.10	0.43
1:B:86:PHE:HB3	1:B:87:PRO:HA	2.01	0.43
1:C:93:GLU:HB3	1:D:126:VAL:HB	2.00	0.43
1:D:58:ASP:CB	1:D:164:LEU:HD21	2.49	0.43
1:C:77:GLU:H	1:C:77:GLU:CD	2.21	0.43
1:A:5:ILE:HD12	1:A:117:PHE:CZ	2.54	0.42
1:D:19:VAL:HG11	1:D:55:PHE:CD2	2.54	0.42
1:A:164:LEU:HB2	1:A:172:HIS:HB3	2.01	0.42
1:C:66:CFY:HB21	1:C:212:GLU:OE2	2.19	0.42
1:B:58:ASP:HB3	1:B:164:LEU:HD21	2.01	0.42
1:A:52:PRO:HA	1:A:206:ASN:HD21	1.85	0.42
1:B:69:ARG:HB3	1:B:82:PHE:CG	2.55	0.42
1:D:69:ARG:N	1:D:70:PRO:CD	2.83	0.42
1:C:58:ASP:HB3	1:C:164:LEU:HD21	2.01	0.42
1:B:164:LEU:HB2	1:B:172:HIS:HB3	2.01	0.42
1:D:134:ILE:N	1:D:134:ILE:HD12	2.34	0.42
1:C:164:LEU:HB2	1:C:172:HIS:HB3	2.02	0.42
1:A:134:ILE:HD12	1:A:134:ILE:N	2.33	0.42
1:B:16:ASP:HB2	1:B:122:LYS:HD3	2.02	0.42
1:B:4:VAL:HG12	1:B:5:ILE:HG13	2.02	0.42
1:C:44:ARG:NH1	1:C:44:ARG:CB	2.82	0.42
1:C:184:LYS:HG2	1:C:185:LYS:N	2.35	0.42
1:A:12:ARG:HD3	1:A:118:TYR:CE1	2.55	0.42
1:A:66:CFY:HB21	1:A:212:GLU:OE2	2.20	0.42
1:A:69:ARG:N	1:A:70:PRO:CD	2.83	0.41
1:A:93:GLU:HB3	1:B:126:VAL:HB	2.02	0.41
1:D:146:THR:HG22	1:D:194:TYR:HD2	1.85	0.41
1:C:160:VAL:HG13	1:C:176:PHE:HB2	2.02	0.41
1:D:86:PHE:HB3	1:D:87:PRO:HA	2.03	0.41
1:D:19:VAL:O	1:D:19:VAL:HG13	2.21	0.41
1:C:95:SER:OG	1:C:177:LYS:HB2	2.21	0.41
1:C:69:ARG:N	1:C:70:PRO:CD	2.84	0.41
1:B:84:GLN:NE2	1:B:188:LYS:H	2.13	0.40
1:D:69:ARG:HD2	2:D:246:HOH:O	2.21	0.40
1:D:134:ILE:HD13	2:D:228:HOH:O	2.20	0.40
1:A:18:SER:HA	1:A:22:HIS:O	2.21	0.40
1:A:58:ASP:CB	1:A:164:LEU:HD21	2.51	0.40
1:B:175:GLN:NE2	1:B:175:GLN:N	2.70	0.40
1:B:69:ARG:N	1:B:70:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:PRO:HB2	1:C:77:GLU:OE1	2.21	0.40
1:A:81:TYR:CB	1:A:156:LEU:HD11	2.51	0.40
1:A:88:GLU:HG2	1:A:184:LYS:HB2	2.04	0.40

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	211/223 (95%)	206 (98%)	5 (2%)	0	100	100
1	B	211/223 (95%)	207 (98%)	4 (2%)	0	100	100
1	C	211/223 (95%)	203 (96%)	6 (3%)	2 (1%)	21	13
1	D	211/223 (95%)	206 (98%)	5 (2%)	0	100	100
All	All	844/892 (95%)	822 (97%)	20 (2%)	2 (0%)	52	48

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%)	90	93
1	B	181/190 (95%)	176 (97%)	5 (3%)	51	50
1	C	181/190 (95%)	176 (97%)	5 (3%)	51	50
1	D	181/190 (95%)	179 (99%)	2 (1%)	80	83
All	All	724/760 (95%)	711 (98%)	13 (2%)	66	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ARG
1	B	12	ARG
1	B	20	ASN
1	B	69	ARG
1	B	175	GLN
1	B	184	LYS
1	C	44	ARG
1	C	68	HIS
1	C	112	LEU
1	C	166	LEU
1	C	197	HIS
1	D	76	GLU
1	D	212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	84	GLN
1	A	109	HIS
1	A	136	GLN
1	A	206	ASN
1	B	20	ASN
1	B	62	HIS
1	B	84	GLN
1	B	109	HIS
1	B	136	GLN
1	B	175	GLN
1	C	62	HIS
1	C	68	HIS
1	C	136	GLN

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Mol	Chain	Res	Type
1	D	62	HIS
1	D	68	HIS
1	D	109	HIS
1	D	136	GLN
1	D	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	66	1	29,35,36	4.57	13 (44%)	28,50,52	2.63	9 (32%)
1	CFY	B	66	1	29,35,36	4.60	13 (44%)	28,50,52	2.61	8 (28%)
1	CFY	C	66	1	29,35,36	4.56	12 (41%)	28,50,52	2.66	9 (32%)
1	CFY	D	66	1	29,35,36	4.54	13 (44%)	28,50,52	2.59	10 (35%)

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	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
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

All (51) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CFY	CB2-SG	-11.79	1.68	1.79
1	B	66	CFY	CB2-SG	-11.54	1.68	1.79
1	C	66	CFY	CB2-SG	-11.52	1.68	1.79
1	D	66	CFY	CB2-SG	-11.17	1.68	1.79
1	D	66	CFY	CA3-C3	-6.99	1.41	1.48
1	A	66	CFY	CA3-C3	-6.86	1.41	1.48
1	B	66	CFY	CA3-C3	-6.61	1.41	1.48
1	C	66	CFY	CA3-C3	-6.59	1.41	1.48
1	A	66	CFY	OH-CZ2	-3.28	1.29	1.37
1	D	66	CFY	OH-CZ2	-3.11	1.29	1.37
1	C	66	CFY	OH-CZ2	-3.07	1.29	1.37
1	B	66	CFY	OH-CZ2	-2.97	1.30	1.37
1	A	66	CFY	CA4-N4	-2.18	1.43	1.47
1	D	66	CFY	CD1-CG1	2.06	1.43	1.38
1	C	66	CFY	CA1-N	2.08	1.50	1.46
1	D	66	CFY	O3-C3	2.27	1.27	1.23
1	B	66	CFY	CA1-N	2.38	1.51	1.46
1	B	66	CFY	O3-C3	2.39	1.28	1.23
1	A	66	CFY	CA1-N	2.41	1.51	1.46
1	B	66	CFY	CE3-CZ2	2.58	1.44	1.38
1	A	66	CFY	CE3-CZ2	2.59	1.44	1.38
1	C	66	CFY	CE3-CZ2	2.61	1.44	1.38
1	D	66	CFY	CE3-CZ2	2.69	1.44	1.38
1	B	66	CFY	CD4-CG2	3.37	1.45	1.39
1	A	66	CFY	CD4-CG2	3.39	1.45	1.39
1	D	66	CFY	CD4-CG2	3.39	1.45	1.39
1	C	66	CFY	CD4-CG2	3.49	1.46	1.39
1	A	66	CFY	CD3-CE3	4.03	1.46	1.38
1	C	66	CFY	CD3-CE3	4.07	1.46	1.38
1	D	66	CFY	CD3-CE3	4.07	1.46	1.38
1	D	66	CFY	CE4-CZ2	4.13	1.47	1.38
1	B	66	CFY	CD3-CE3	4.14	1.46	1.38
1	A	66	CFY	CE4-CZ2	4.16	1.47	1.38
1	B	66	CFY	CE4-CZ2	4.30	1.47	1.38
1	C	66	CFY	CE4-CZ2	4.35	1.47	1.38
1	A	66	CFY	CD4-CE4	5.52	1.48	1.38
1	D	66	CFY	CD3-CG2	5.59	1.50	1.39
1	B	66	CFY	CD3-CG2	5.64	1.50	1.39
1	D	66	CFY	CD4-CE4	5.65	1.48	1.38
1	C	66	CFY	CD3-CG2	5.67	1.50	1.39
1	A	66	CFY	CD3-CG2	5.67	1.50	1.39
1	C	66	CFY	CD4-CE4	5.70	1.49	1.38
1	B	66	CFY	CD4-CE4	5.88	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CFY	CB3-CA3	8.59	1.42	1.35
1	D	66	CFY	CB3-CA3	8.65	1.42	1.35
1	B	66	CFY	CB3-CA3	9.09	1.43	1.35
1	C	66	CFY	CB3-CA3	9.22	1.43	1.35
1	A	66	CFY	CA2-N2	13.42	1.43	1.28
1	C	66	CFY	CA2-N2	13.42	1.43	1.28
1	B	66	CFY	CA2-N2	13.59	1.43	1.28
1	D	66	CFY	CA2-N2	13.65	1.43	1.28

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CFY	O3-C3-CA3	-5.29	128.09	130.95
1	B	66	CFY	O3-C3-CA3	-5.24	128.12	130.95
1	D	66	CFY	O3-C3-CA3	-5.19	128.14	130.95
1	A	66	CFY	O3-C3-CA3	-4.87	128.31	130.95
1	C	66	CFY	CB1-CG1-CD1	-4.21	112.09	120.90
1	C	66	CFY	N4-C2-N3	-4.19	108.52	113.26
1	A	66	CFY	N4-C2-N3	-4.16	108.55	113.26
1	A	66	CFY	CB1-CG1-CD1	-4.13	112.26	120.90
1	D	66	CFY	N4-C2-N3	-4.13	108.58	113.26
1	B	66	CFY	N4-C2-N3	-4.11	108.60	113.26
1	D	66	CFY	CB1-CG1-CD1	-4.07	112.39	120.90
1	B	66	CFY	CB1-CG1-CD1	-4.04	112.45	120.90
1	A	66	CFY	CA4-N4-C3	-3.61	118.12	123.99
1	B	66	CFY	CA4-N4-C3	-3.42	118.42	123.99
1	C	66	CFY	CA4-N4-C3	-3.41	118.45	123.99
1	D	66	CFY	CA4-N4-C3	-3.36	118.51	123.99
1	B	66	CFY	CE1-CD1-CG1	-2.75	116.28	120.65
1	C	66	CFY	CE1-CD1-CG1	-2.71	116.34	120.65
1	A	66	CFY	CE1-CD1-CG1	-2.69	116.37	120.65
1	D	66	CFY	CE1-CD1-CG1	-2.63	116.46	120.65
1	D	66	CFY	CB1-CG1-CD2	2.07	125.24	120.90
1	D	66	CFY	C3-CA3-N3	2.08	110.57	108.91
1	C	66	CFY	CB1-CG1-CD2	2.08	125.26	120.90
1	A	66	CFY	CB1-CG1-CD2	2.11	125.31	120.90
1	C	66	CFY	CZ1-CE1-CD1	2.13	123.30	120.19
1	D	66	CFY	CZ1-CE1-CD1	2.22	123.43	120.19
1	A	66	CFY	CZ1-CE1-CD1	2.24	123.46	120.19
1	B	66	CFY	CZ1-CE1-CD1	2.26	123.49	120.19
1	D	66	CFY	CD2-CG1-CD1	2.65	122.37	118.13
1	A	66	CFY	CD2-CG1-CD1	2.69	122.43	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CFY	CD2-CG1-CD1	2.71	122.47	118.13
1	C	66	CFY	CD2-CG1-CD1	2.82	122.65	118.13
1	D	66	CFY	C-CA4-N4	8.25	131.06	113.00
1	B	66	CFY	C-CA4-N4	8.41	131.41	113.00
1	A	66	CFY	C-CA4-N4	8.62	131.88	113.00
1	C	66	CFY	C-CA4-N4	8.67	131.99	113.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	66	CFY	C2
1	D	66	CFY	C2
1	A	66	CFY	C2
1	C	66	CFY	C2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CFY	1	0
1	B	66	CFY	1	0
1	C	66	CFY	1	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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	213/223 (95%)	-0.05	6 (2%) 56 57	10, 21, 41, 57	0
1	B	213/223 (95%)	-0.18	7 (3%) 50 51	10, 19, 34, 58	0
1	C	213/223 (95%)	0.05	8 (3%) 44 45	10, 21, 43, 60	0
1	D	213/223 (95%)	-0.22	6 (2%) 56 57	10, 19, 35, 56	0
All	All	852/892 (95%)	-0.10	27 (3%) 51 52	10, 20, 40, 60	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	LEU	6.2
1	A	187	LEU	5.8
1	C	187	LEU	5.0
1	C	168	GLY	4.4
1	D	187	LEU	4.2
1	A	218	SER	3.1
1	A	153	ASP	2.9
1	D	185	LYS	2.8
1	A	186	ILE	2.8
1	D	184	LYS	2.7
1	D	153	ASP	2.7
1	A	185	LYS	2.6
1	C	153	ASP	2.6
1	C	169	GLY	2.6
1	D	218	SER	2.6
1	D	77	GLU	2.5
1	C	186	ILE	2.5
1	B	76	GLU	2.4
1	B	168	GLY	2.3
1	C	113	ARG	2.3
1	C	44	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	77	GLU	2.2
1	B	153	ASP	2.2
1	B	185	LYS	2.2
1	C	185	LYS	2.2
1	B	218	SER	2.2
1	A	78	ILE	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	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	A	66	32/33	0.91	0.13	-	13,19,26,26	0
1	CFY	C	66	32/33	0.94	0.12	-	13,20,24,27	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.