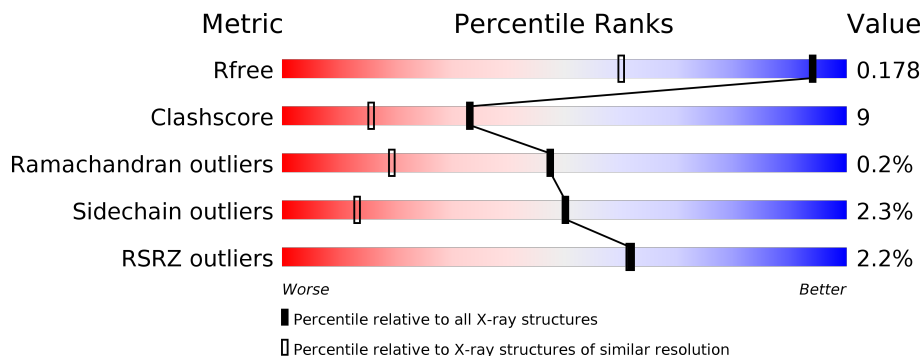# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	Percentile Ranks	Value
Rfree		0.178
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		2.3%
RSRZ outliers		2.2%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 >=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	73	66% 21% · 12%
1	C	73	3% 70% 10% · 19%
2	B	168	5% 80% 18% ·
2	D	168	88% 11% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4390 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 GFP-like non-fluorescent chromoprotein FP595 chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	2	0
			501	320	81	96	4			
1	C	59	Total	C	N	O	S	2	1	0
			463	299	73	87	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q9GZ28
A	-9	ARG	-	EXPRESSION TAG	UNP Q9GZ28
A	-8	GLY	-	EXPRESSION TAG	UNP Q9GZ28
A	-7	SER	-	EXPRESSION TAG	UNP Q9GZ28
A	-6	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	-5	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	-4	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	-3	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	-2	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	-1	HIS	-	EXPRESSION TAG	UNP Q9GZ28
A	0	GLY	-	EXPRESSION TAG	UNP Q9GZ28
A	1	SER	-	EXPRESSION TAG	UNP Q9GZ28
C	-10	MET	-	EXPRESSION TAG	UNP Q9GZ28
C	-9	ARG	-	EXPRESSION TAG	UNP Q9GZ28
C	-8	GLY	-	EXPRESSION TAG	UNP Q9GZ28
C	-7	SER	-	EXPRESSION TAG	UNP Q9GZ28
C	-6	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	-5	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	-4	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	-3	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	-2	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	-1	HIS	-	EXPRESSION TAG	UNP Q9GZ28
C	0	GLY	-	EXPRESSION TAG	UNP Q9GZ28
C	1	SER	-	EXPRESSION TAG	UNP Q9GZ28

- Molecule 2 is a protein called GFP-like non-fluorescent chromoprotein FP595 chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total 1377	C 875	N 236	O 256	S 10	5	4	0
2	D	168	Total 1390	C 884	N 238	O 258	S 10	9	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	NRQ	MET	CHROMOPHORE	UNP Q9GZ28
B	65	NRQ	TYR	CHROMOPHORE	UNP Q9GZ28
B	65	NRQ	GLY	CHROMOPHORE	UNP Q9GZ28
D	65	NRQ	MET	CHROMOPHORE	UNP Q9GZ28
D	65	NRQ	TYR	CHROMOPHORE	UNP Q9GZ28
D	65	NRQ	GLY	CHROMOPHORE	UNP Q9GZ28

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total 109	O 109	0	0
3	B	237	Total 237	O 237	0	0
3	C	85	Total 85	O 85	0	0
3	D	228	Total 228	O 228	0	0

3 Residue-property plots ⓘ

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.
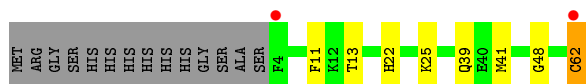
- Molecule 1: GFP-like non-fluorescent chromoprotein FP595 chain 1
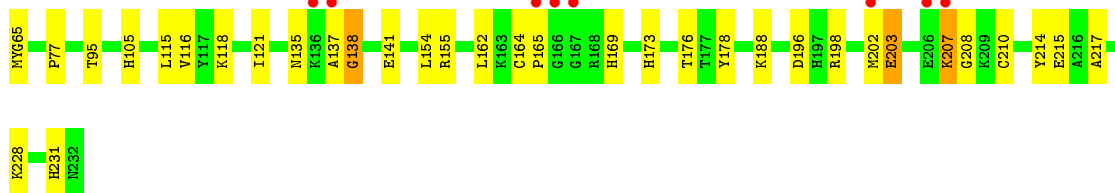
Chain A:

- Molecule 1: GFP-like non-fluorescent chromoprotein FP595 chain 1
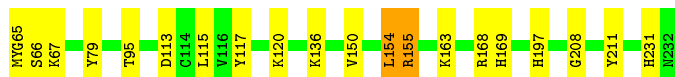
Chain C:

- Molecule 2: GFP-like non-fluorescent chromoprotein FP595 chain 2

Chain B:

- Molecule 2: GFP-like non-fluorescent chromoprotein FP595 chain 2

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	76.17Å 126.50Å 94.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.30 65.26 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.30) 99.5 (65.26-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.179 0.152 , 0.178	Depositor DCC
R_{free} test set	5551 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.0	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4390	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ

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	0.59	0/514	0.65	0/690
1	C	0.66	1/475 (0.2%)	0.65	0/637
2	B	0.64	2/1390 (0.1%)	0.74	0/1873
2	D	0.59	0/1404	0.70	0/1894
All	All	0.62	3/3783 (0.1%)	0.70	0/5094

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CYS	CB-SG	-5.77	1.72	1.81
2	B	203	GLU	CA-CB	5.76	1.66	1.53
2	B	164	CYS	CB-SG	5.09	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	501	0	489	15	0
1	C	463	0	455	6	0
2	B	1377	0	1326	31	1
2	D	1390	0	1332	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	109	0	0	5	0
3	B	237	0	0	9	0
3	C	85	0	0	1	0
3	D	228	0	0	9	1
All	All	4390	0	3602	63	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 9.

The worst 5 of 63 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:B:207:LYS:HB3	2:B:208:GLY:HA3	1.12	1.09
2:B:95[A]:THR:HG21	3:B:338:HOH:O	1.57	1.01
2:B:207:LYS:HB3	2:B:208:GLY:CA	1.93	0.98
2:B:162:LEU:HG	3:B:437:HOH:O	1.76	0.86
2:B:137:ALA:O	2:B:165:PRO:HD3	1.76	0.86

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)
2:B:228[A]:LYS:NZ	3:D:350:HOH:O[5_555]	1.85	0.35

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	64/73 (88%)	64 (100%)	0	0	100	100
1	C	58/73 (80%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	169/168 (101%)	162 (96%)	6 (4%)	1 (1%)	25	4
2	D	170/168 (101%)	163 (96%)	7 (4%)	0	100	100
All	All	461/482 (96%)	447 (97%)	13 (3%)	1 (0%)	47	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	138	GLY

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	55/61 (90%)	54 (98%)	1 (2%)	59	24
1	C	51/61 (84%)	51 (100%)	0	100	100
2	B	144/140 (103%)	140 (97%)	4 (3%)	43	8
2	D	145/140 (104%)	140 (97%)	5 (3%)	37	5
All	All	395/402 (98%)	385 (98%)	10 (2%)	50	10

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	207	LYS
2	D	113	ASP
2	D	155[A]	ARG
2	B	203	GLU
2	D	154	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	232	ASN

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Mol	Chain	Res	Type
1	C	22	HIS
2	D	169	HIS
2	B	197	HIS
2	B	231	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)

2 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	$\#|Z| > 2$
2	NRQ	D	65	2	23,24,25	4.09	5 (21%)	23,32,34	3.96	4 (17%)
2	NRQ	B	65	2	23,24,25	3.94	5 (21%)	23,32,34	4.06	4 (17%)

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
2	NRQ	D	65	2	-	3/9/31/32	0/2/2/2
2	NRQ	B	65	2	-	3/9/31/32	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	NRQ	CB2-CA2	15.79	1.48	1.35
2	D	65	NRQ	CB2-CA2	15.51	1.48	1.35
2	D	65	NRQ	CA2-C2	-10.28	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	NRQ	CA2-C2	-8.39	1.40	1.48
2	D	65	NRQ	OH-CZ	-3.70	1.28	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	65	NRQ	CA2-C2-N3	12.08	109.08	103.37
2	B	65	NRQ	CB2-CA2-C2	11.75	136.31	122.28
2	B	65	NRQ	CA2-C2-N3	11.15	108.64	103.37
2	D	65	NRQ	CB2-CA2-C2	10.76	135.12	122.28
2	B	65	NRQ	CB2-CA2-N2	-9.39	115.80	128.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	65	NRQ	N2-CA2-CB2-CG2
2	D	65	NRQ	C2-CA2-CB2-CG2
2	B	65	NRQ	C2-CA2-CB2-CG2
2	B	65	NRQ	N2-CA2-CB2-CG2
2	B	65	NRQ	C3-CA3-N3-C1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	65	NRQ	2	0
2	B	65	NRQ	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 (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(Å²)	Q<0.9
1	A	64/73 (87%)	-0.43	0	100	100	12, 18, 23, 26	0
1	C	59/73 (80%)	-0.13	2 (3%)	45	42	13, 21, 27, 39	1 (1%)
2	B	167/168 (99%)	-0.17	8 (4%)	30	28	10, 14, 31, 47	1 (0%)
2	D	167/168 (99%)	-0.39	0	100	100	11, 17, 31, 35	3 (1%)
All	All	457/482 (94%)	-0.28	10 (2%)	62	61	10, 17, 30, 47	5 (1%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	137	ALA	7.6
2	B	207	LYS	4.9
1	C	4	PHE	3.9
2	B	202	MET	3.8
2	B	165	PRO	3.7

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(Å²)	Q<0.9
2	NRQ	D	65	23/24	0.97	0.06	12,13,17,21	0
2	NRQ	B	65	23/24	0.98	0.05	10,12,14,18	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.