



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2016 – 07:57 AM EDT

PDB ID : 3VIC  
Title : Green-fluorescent variant of the non-fluorescent chromoprotein Rtms5  
Authors : Battad, J.M.; Traore, D.A.K.; Byres, E.; Wilce, M.; Devenish, R.J.; Rossjohn, J.; Prescott, M.  
Deposited on : 2011-09-28  
Resolution : 2.20 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

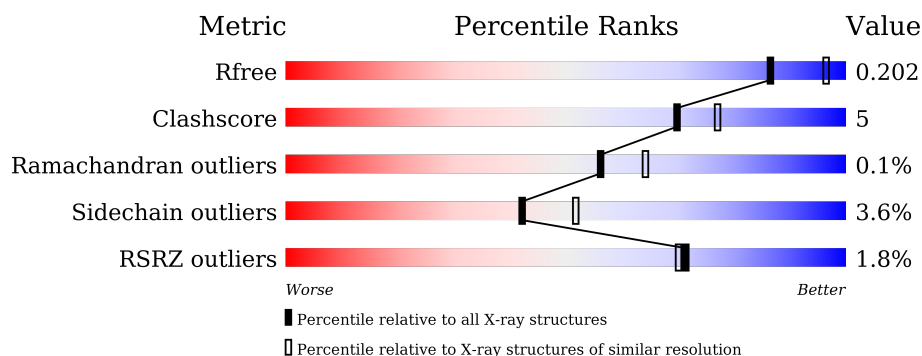
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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	238	<div> <div></div> <div>82%10%8%</div> </div>
1	B	238	<div> <div>3%</div> <div>80%11%8%</div> </div>
1	C	238	<div> <div>2%</div> <div>82%9%8%</div> </div>
1	D	238	<div> <div>2%</div> <div>77%14%8%</div> </div>
1	E	238	<div> <div>2%</div> <div>78%13%8%</div> </div>
1	F	238	<div> <div>%</div> <div>78%13%8%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	238	
1	H	238	

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
3	CL	A	228	-	-	-	X
3	CL	B	228	-	-	-	X
3	CL	C	229	-	-	-	X
3	CL	D	229	-	-	-	X
3	CL	E	228	-	-	-	X
3	CL	F	227	-	-	-	X
3	CL	G	227	-	-	-	X
3	CL	H	228	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15565 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	4	0
			1772	1134	295	330	13			
1	B	219	Total	C	N	O	S	0	3	0
			1766	1130	294	329	13			
1	C	219	Total	C	N	O	S	0	2	0
			1766	1130	294	329	13			
1	D	219	Total	C	N	O	S	0	3	0
			1766	1130	294	329	13			
1	E	218	Total	C	N	O	S	0	3	0
			1761	1127	293	328	13			
1	F	219	Total	C	N	O	S	0	2	0
			1762	1128	293	327	14			
1	G	219	Total	C	N	O	S	0	1	0
			1751	1122	291	325	13			
1	H	218	Total	C	N	O	S	0	2	0
			1754	1123	292	326	13			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP P83690
A	-13	ARG	-	EXPRESSION TAG	UNP P83690
A	-12	GLY	-	EXPRESSION TAG	UNP P83690
A	-11	SER	-	EXPRESSION TAG	UNP P83690
A	-10	HIS	-	EXPRESSION TAG	UNP P83690
A	-9	HIS	-	EXPRESSION TAG	UNP P83690
A	-8	HIS	-	EXPRESSION TAG	UNP P83690
A	-7	HIS	-	EXPRESSION TAG	UNP P83690
A	-6	HIS	-	EXPRESSION TAG	UNP P83690
A	-5	HIS	-	EXPRESSION TAG	UNP P83690
A	-4	THR	-	EXPRESSION TAG	UNP P83690
A	-3	ASP	-	EXPRESSION TAG	UNP P83690
A	-2	PRO	-	EXPRESSION TAG	UNP P83690

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P83690
A	0	SER	-	EXPRESSION TAG	UNP P83690
A	1	ARG	-	EXPRESSION TAG	UNP P83690
A	2	SER	-	EXPRESSION TAG	UNP P83690
A	3	LYS	-	EXPRESSION TAG	UNP P83690
A	4	THR	-	EXPRESSION TAG	UNP P83690
A	66	QFG	GLN	CHROMOPHORE	UNP P83690
A	66	QFG	TYR	CHROMOPHORE	UNP P83690
A	66	QFG	GLY	CHROMOPHORE	UNP P83690
B	-14	MET	-	EXPRESSION TAG	UNP P83690
B	-13	ARG	-	EXPRESSION TAG	UNP P83690
B	-12	GLY	-	EXPRESSION TAG	UNP P83690
B	-11	SER	-	EXPRESSION TAG	UNP P83690
B	-10	HIS	-	EXPRESSION TAG	UNP P83690
B	-9	HIS	-	EXPRESSION TAG	UNP P83690
B	-8	HIS	-	EXPRESSION TAG	UNP P83690
B	-7	HIS	-	EXPRESSION TAG	UNP P83690
B	-6	HIS	-	EXPRESSION TAG	UNP P83690
B	-5	HIS	-	EXPRESSION TAG	UNP P83690
B	-4	THR	-	EXPRESSION TAG	UNP P83690
B	-3	ASP	-	EXPRESSION TAG	UNP P83690
B	-2	PRO	-	EXPRESSION TAG	UNP P83690
B	-1	SER	-	EXPRESSION TAG	UNP P83690
B	0	SER	-	EXPRESSION TAG	UNP P83690
B	1	ARG	-	EXPRESSION TAG	UNP P83690
B	2	SER	-	EXPRESSION TAG	UNP P83690
B	3	LYS	-	EXPRESSION TAG	UNP P83690
B	4	THR	-	EXPRESSION TAG	UNP P83690
B	66	QFG	GLN	CHROMOPHORE	UNP P83690
B	66	QFG	TYR	CHROMOPHORE	UNP P83690
B	66	QFG	GLY	CHROMOPHORE	UNP P83690
C	-14	MET	-	EXPRESSION TAG	UNP P83690
C	-13	ARG	-	EXPRESSION TAG	UNP P83690
C	-12	GLY	-	EXPRESSION TAG	UNP P83690
C	-11	SER	-	EXPRESSION TAG	UNP P83690
C	-10	HIS	-	EXPRESSION TAG	UNP P83690
C	-9	HIS	-	EXPRESSION TAG	UNP P83690
C	-8	HIS	-	EXPRESSION TAG	UNP P83690
C	-7	HIS	-	EXPRESSION TAG	UNP P83690
C	-6	HIS	-	EXPRESSION TAG	UNP P83690
C	-5	HIS	-	EXPRESSION TAG	UNP P83690
C	-4	THR	-	EXPRESSION TAG	UNP P83690

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ASP	-	EXPRESSION TAG	UNP P83690
C	-2	PRO	-	EXPRESSION TAG	UNP P83690
C	-1	SER	-	EXPRESSION TAG	UNP P83690
C	0	SER	-	EXPRESSION TAG	UNP P83690
C	1	ARG	-	EXPRESSION TAG	UNP P83690
C	2	SER	-	EXPRESSION TAG	UNP P83690
C	3	LYS	-	EXPRESSION TAG	UNP P83690
C	4	THR	-	EXPRESSION TAG	UNP P83690
C	66	QFG	GLN	CHROMOPHORE	UNP P83690
C	66	QFG	TYR	CHROMOPHORE	UNP P83690
C	66	QFG	GLY	CHROMOPHORE	UNP P83690
D	-14	MET	-	EXPRESSION TAG	UNP P83690
D	-13	ARG	-	EXPRESSION TAG	UNP P83690
D	-12	GLY	-	EXPRESSION TAG	UNP P83690
D	-11	SER	-	EXPRESSION TAG	UNP P83690
D	-10	HIS	-	EXPRESSION TAG	UNP P83690
D	-9	HIS	-	EXPRESSION TAG	UNP P83690
D	-8	HIS	-	EXPRESSION TAG	UNP P83690
D	-7	HIS	-	EXPRESSION TAG	UNP P83690
D	-6	HIS	-	EXPRESSION TAG	UNP P83690
D	-5	HIS	-	EXPRESSION TAG	UNP P83690
D	-4	THR	-	EXPRESSION TAG	UNP P83690
D	-3	ASP	-	EXPRESSION TAG	UNP P83690
D	-2	PRO	-	EXPRESSION TAG	UNP P83690
D	-1	SER	-	EXPRESSION TAG	UNP P83690
D	0	SER	-	EXPRESSION TAG	UNP P83690
D	1	ARG	-	EXPRESSION TAG	UNP P83690
D	2	SER	-	EXPRESSION TAG	UNP P83690
D	3	LYS	-	EXPRESSION TAG	UNP P83690
D	4	THR	-	EXPRESSION TAG	UNP P83690
D	66	QFG	GLN	CHROMOPHORE	UNP P83690
D	66	QFG	TYR	CHROMOPHORE	UNP P83690
D	66	QFG	GLY	CHROMOPHORE	UNP P83690
E	-14	MET	-	EXPRESSION TAG	UNP P83690
E	-13	ARG	-	EXPRESSION TAG	UNP P83690
E	-12	GLY	-	EXPRESSION TAG	UNP P83690
E	-11	SER	-	EXPRESSION TAG	UNP P83690
E	-10	HIS	-	EXPRESSION TAG	UNP P83690
E	-9	HIS	-	EXPRESSION TAG	UNP P83690
E	-8	HIS	-	EXPRESSION TAG	UNP P83690
E	-7	HIS	-	EXPRESSION TAG	UNP P83690
E	-6	HIS	-	EXPRESSION TAG	UNP P83690

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	EXPRESSION TAG	UNP P83690
E	-4	THR	-	EXPRESSION TAG	UNP P83690
E	-3	ASP	-	EXPRESSION TAG	UNP P83690
E	-2	PRO	-	EXPRESSION TAG	UNP P83690
E	-1	SER	-	EXPRESSION TAG	UNP P83690
E	0	SER	-	EXPRESSION TAG	UNP P83690
E	1	ARG	-	EXPRESSION TAG	UNP P83690
E	2	SER	-	EXPRESSION TAG	UNP P83690
E	3	LYS	-	EXPRESSION TAG	UNP P83690
E	4	THR	-	EXPRESSION TAG	UNP P83690
E	66	QFG	GLN	CHROMOPHORE	UNP P83690
E	66	QFG	TYR	CHROMOPHORE	UNP P83690
E	66	QFG	GLY	CHROMOPHORE	UNP P83690
F	-14	MET	-	EXPRESSION TAG	UNP P83690
F	-13	ARG	-	EXPRESSION TAG	UNP P83690
F	-12	GLY	-	EXPRESSION TAG	UNP P83690
F	-11	SER	-	EXPRESSION TAG	UNP P83690
F	-10	HIS	-	EXPRESSION TAG	UNP P83690
F	-9	HIS	-	EXPRESSION TAG	UNP P83690
F	-8	HIS	-	EXPRESSION TAG	UNP P83690
F	-7	HIS	-	EXPRESSION TAG	UNP P83690
F	-6	HIS	-	EXPRESSION TAG	UNP P83690
F	-5	HIS	-	EXPRESSION TAG	UNP P83690
F	-4	THR	-	EXPRESSION TAG	UNP P83690
F	-3	ASP	-	EXPRESSION TAG	UNP P83690
F	-2	PRO	-	EXPRESSION TAG	UNP P83690
F	-1	SER	-	EXPRESSION TAG	UNP P83690
F	0	SER	-	EXPRESSION TAG	UNP P83690
F	1	ARG	-	EXPRESSION TAG	UNP P83690
F	2	SER	-	EXPRESSION TAG	UNP P83690
F	3	LYS	-	EXPRESSION TAG	UNP P83690
F	4	THR	-	EXPRESSION TAG	UNP P83690
F	66	QFG	GLN	CHROMOPHORE	UNP P83690
F	66	QFG	TYR	CHROMOPHORE	UNP P83690
F	66	QFG	GLY	CHROMOPHORE	UNP P83690
G	-14	MET	-	EXPRESSION TAG	UNP P83690
G	-13	ARG	-	EXPRESSION TAG	UNP P83690
G	-12	GLY	-	EXPRESSION TAG	UNP P83690
G	-11	SER	-	EXPRESSION TAG	UNP P83690
G	-10	HIS	-	EXPRESSION TAG	UNP P83690
G	-9	HIS	-	EXPRESSION TAG	UNP P83690
G	-8	HIS	-	EXPRESSION TAG	UNP P83690

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	HIS	-	EXPRESSION TAG	UNP P83690
G	-6	HIS	-	EXPRESSION TAG	UNP P83690
G	-5	HIS	-	EXPRESSION TAG	UNP P83690
G	-4	THR	-	EXPRESSION TAG	UNP P83690
G	-3	ASP	-	EXPRESSION TAG	UNP P83690
G	-2	PRO	-	EXPRESSION TAG	UNP P83690
G	-1	SER	-	EXPRESSION TAG	UNP P83690
G	0	SER	-	EXPRESSION TAG	UNP P83690
G	1	ARG	-	EXPRESSION TAG	UNP P83690
G	2	SER	-	EXPRESSION TAG	UNP P83690
G	3	LYS	-	EXPRESSION TAG	UNP P83690
G	4	THR	-	EXPRESSION TAG	UNP P83690
G	66	QFG	GLN	CHROMOPHORE	UNP P83690
G	66	QFG	TYR	CHROMOPHORE	UNP P83690
G	66	QFG	GLY	CHROMOPHORE	UNP P83690
H	-14	MET	-	EXPRESSION TAG	UNP P83690
H	-13	ARG	-	EXPRESSION TAG	UNP P83690
H	-12	GLY	-	EXPRESSION TAG	UNP P83690
H	-11	SER	-	EXPRESSION TAG	UNP P83690
H	-10	HIS	-	EXPRESSION TAG	UNP P83690
H	-9	HIS	-	EXPRESSION TAG	UNP P83690
H	-8	HIS	-	EXPRESSION TAG	UNP P83690
H	-7	HIS	-	EXPRESSION TAG	UNP P83690
H	-6	HIS	-	EXPRESSION TAG	UNP P83690
H	-5	HIS	-	EXPRESSION TAG	UNP P83690
H	-4	THR	-	EXPRESSION TAG	UNP P83690
H	-3	ASP	-	EXPRESSION TAG	UNP P83690
H	-2	PRO	-	EXPRESSION TAG	UNP P83690
H	-1	SER	-	EXPRESSION TAG	UNP P83690
H	0	SER	-	EXPRESSION TAG	UNP P83690
H	1	ARG	-	EXPRESSION TAG	UNP P83690
H	2	SER	-	EXPRESSION TAG	UNP P83690
H	3	LYS	-	EXPRESSION TAG	UNP P83690
H	4	THR	-	EXPRESSION TAG	UNP P83690
H	66	QFG	GLN	CHROMOPHORE	UNP P83690
H	66	QFG	TYR	CHROMOPHORE	UNP P83690
H	66	QFG	GLY	CHROMOPHORE	UNP P83690

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total I 2 2	0	0
2	E	1	Total I 1 1	0	0
2	H	1	Total I 1 1	0	0
2	B	1	Total I 1 1	0	0
2	C	2	Total I 2 2	0	0
2	A	1	Total I 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0
3	E	2	Total Cl 2 2	0	0
3	H	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	F	2	Total Cl 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	B	188	Total O 188 188	0	0

*Continued on next page...*

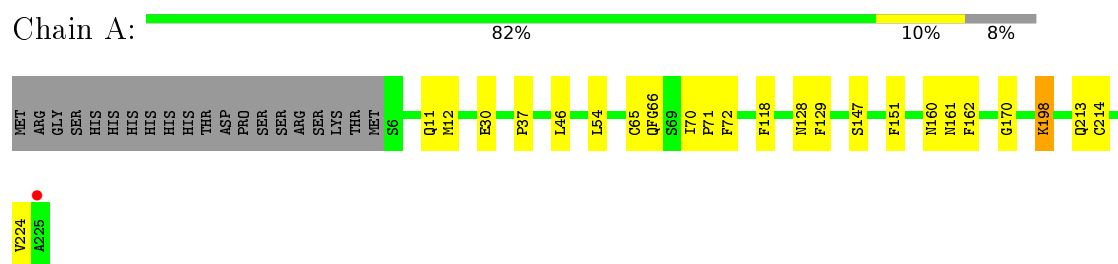
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	169	Total 169	O 169	0	0
4	D	185	Total 185	O 185	0	0
4	E	193	Total 193	O 193	0	0
4	F	189	Total 189	O 189	0	0
4	G	179	Total 179	O 179	0	0
4	H	156	Total 156	O 156	0	0

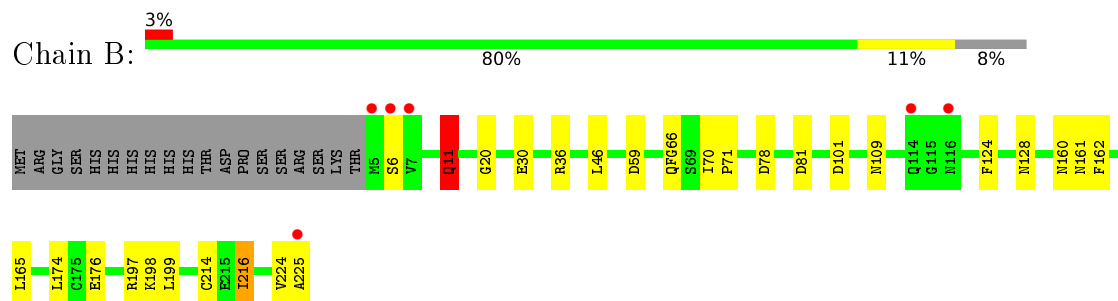
### 3 Residue-property plots [i](#)

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.

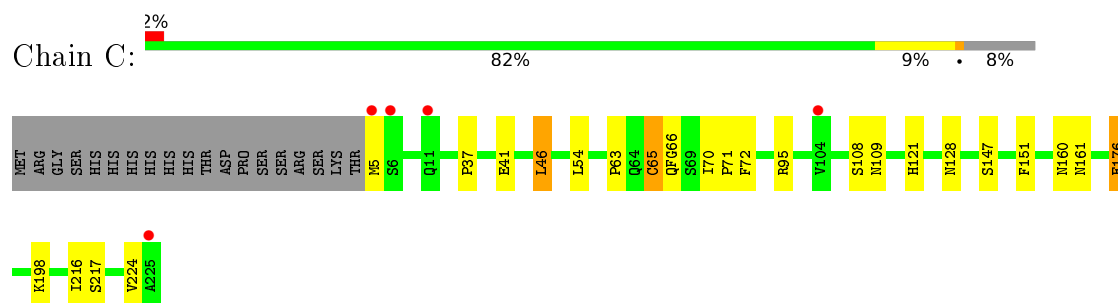
- Molecule 1: GFP-like non-fluorescent chromoprotein



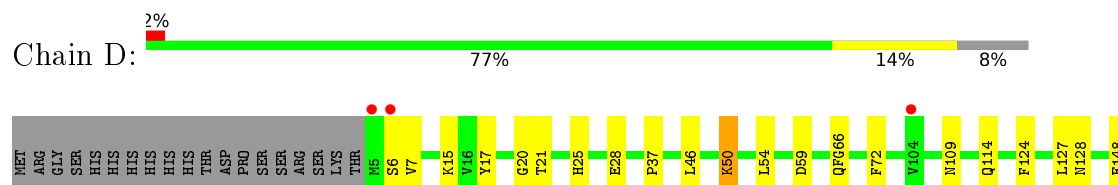
- Molecule 1: GFP-like non-fluorescent chromoprotein



- Molecule 1: GFP-like non-fluorescent chromoprotein

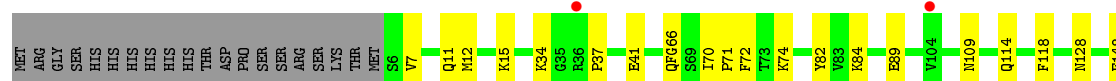
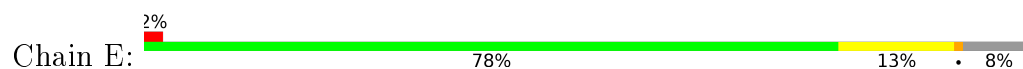


- Molecule 1: GFP-like non-fluorescent chromoprotein

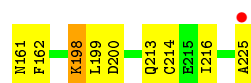
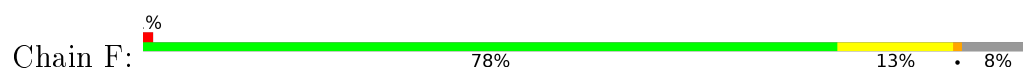




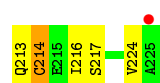
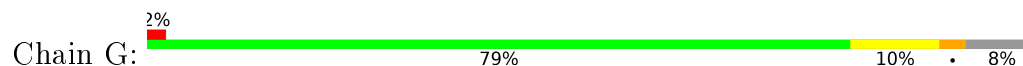
- Molecule 1: GFP-like non-fluorescent chromoprotein



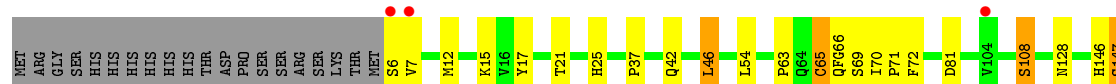
- Molecule 1: GFP-like non-fluorescent chromoprotein



- Molecule 1: GFP-like non-fluorescent chromoprotein



- Molecule 1: GFP-like non-fluorescent chromoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.27Å 186.06Å 185.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.80 – 2.20 55.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.80-2.20) 100.0 (55.74-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.160 , 0.204 0.158 , 0.202	Depositor DCC
$R_{free}$ test set	6587 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: QFG, IOD, CL

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	1.11	1/1798 (0.1%)	0.89	1/2432 (0.0%)
1	B	1.12	2/1795 (0.1%)	0.94	5/2428 (0.2%)
1	C	1.11	2/1792 (0.1%)	0.91	3/2423 (0.1%)
1	D	1.14	0/1795	0.94	2/2428 (0.1%)
1	E	1.19	6/1790 (0.3%)	0.93	3/2421 (0.1%)
1	F	1.15	0/1791	0.92	1/2421 (0.0%)
1	G	1.07	2/1780 (0.1%)	0.88	4/2407 (0.2%)
1	H	1.10	2/1783 (0.1%)	0.94	7/2411 (0.3%)
All	All	1.12	15/14324 (0.1%)	0.92	26/19371 (0.1%)

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	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	176	GLU	CD-OE2	7.61	1.34	1.25
1	E	210	SER	CB-OG	-6.37	1.33	1.42
1	B	176	GLU	CD-OE1	6.19	1.32	1.25
1	B	11	GLN	CG-CD	5.87	1.64	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	89	GLU	CG-CD	5.81	1.60	1.51
1	E	214[A]	CYS	CB-SG	-5.77	1.72	1.81
1	E	214[B]	CYS	CB-SG	-5.77	1.72	1.81
1	C	108	SER	CB-OG	-5.74	1.34	1.42
1	C	176	GLU	CD-OE1	5.63	1.31	1.25
1	H	176	GLU	CD-OE1	5.51	1.31	1.25
1	A	129	PHE	CE2-CZ	5.21	1.47	1.37
1	E	41	GLU	CD-OE1	5.15	1.31	1.25
1	G	62	SER	CB-OG	-5.11	1.35	1.42
1	G	176	GLU	CG-CD	5.05	1.59	1.51
1	E	82	TYR	CD1-CE1	5.05	1.47	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	ILE	CG1-CB-CG2	-8.45	92.81	111.40
1	B	101	ASP	CB-CG-OD1	7.89	125.40	118.30
1	B	161	ASN	CB-CA-C	-6.80	96.79	110.40
1	B	36	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	161	ASN	CB-CA-C	-6.75	96.91	110.40
1	D	161	ASN	CB-CA-C	-6.71	96.97	110.40
1	H	161	ASN	CB-CA-C	-6.34	97.73	110.40
1	C	95	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	H	81	ASP	CB-CG-OD1	6.06	123.75	118.30
1	H	46	LEU	CA-CB-CG	6.05	129.21	115.30
1	F	161	ASN	CB-CA-C	-6.05	98.31	110.40
1	H	65	CYS	CA-CB-SG	-6.04	103.13	114.00
1	C	46	LEU	CA-CB-CG	5.89	128.84	115.30
1	E	161	ASN	CB-CA-C	-5.87	98.66	110.40
1	G	158	ILE	CG1-CB-CG2	-5.87	98.48	111.40
1	G	161	ASN	CB-CA-C	-5.87	98.66	110.40
1	B	78	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	161	ASN	CB-CA-C	-5.75	98.90	110.40
1	E	161	ASN	N-CA-CB	5.72	120.90	110.60
1	B	81	ASP	CB-CG-OD1	5.67	123.40	118.30
1	H	161	ASN	N-CA-CB	5.48	120.46	110.60
1	E	74	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	H	147	SER	N-CA-CB	-5.25	102.63	110.50
1	D	46	LEU	CA-CB-CG	5.18	127.22	115.30
1	G	46	LEU	CA-CB-CG	5.15	127.15	115.30
1	G	65	CYS	CA-CB-SG	-5.06	104.89	114.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	CYS	Mainchain
1	C	65	CYS	Mainchain
1	D	6	SER	Peptide
1	F	65	CYS	Mainchain
1	G	65	CYS	Mainchain
1	H	65	CYS	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	1772	0	1705	17	0
1	B	1766	0	1698	19	0
1	C	1766	0	1700	15	0
1	D	1766	0	1698	20	0
1	E	1761	0	1696	20	0
1	F	1762	0	1699	22	0
1	G	1751	0	1687	16	0
1	H	1754	0	1690	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	184	0	0	6	0
4	B	188	0	0	6	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	169	0	0	5	0
4	D	185	0	0	6	0
4	E	193	0	0	7	0
4	F	189	0	0	6	0
4	G	179	0	0	6	0
4	H	156	0	0	5	0
All	All	15565	0	13573	125	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 5.

All (125) 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:66:QFG:HB2	4:A:1086:HOH:O	1.25	1.35
1:F:66:QFG:HB2	4:F:1218:HOH:O	1.21	1.35
1:D:66:QFG:HB2	4:D:260:HOH:O	1.22	1.34
1:C:66:QFG:HB2	4:C:1217:HOH:O	1.24	1.31
1:G:66:QFG:HB2	4:G:1219:HOH:O	1.25	1.30
1:B:66:QFG:HB2	4:B:1214:HOH:O	1.18	1.30
1:E:66:QFG:HB2	4:E:1146:HOH:O	1.30	1.29
1:D:128[B]:ASN:OD1	4:D:347:HOH:O	1.62	1.15
1:H:66:QFG:HB2	4:H:1220:HOH:O	0.98	1.15
1:F:128[A]:ASN:OD1	4:F:1297:HOH:O	1.69	1.09
1:A:128[B]:ASN:OD1	4:A:466:HOH:O	1.69	1.08
1:A:11:GLN:NE2	4:A:1081:HOH:O	1.97	0.96
1:B:214[B]:CYS:SG	4:B:1252:HOH:O	2.27	0.91
1:G:214[B]:CYS:SG	4:G:1349:HOH:O	2.36	0.83
1:C:176:GLU:OE2	4:C:1439:HOH:O	2.00	0.79
1:F:128[A]:ASN:ND2	4:F:1296:HOH:O	2.06	0.76
1:B:11:GLN:OE1	4:B:1100:HOH:O	2.07	0.72
1:G:214[A]:CYS:SG	4:G:1360:HOH:O	2.48	0.72
1:H:108:SER:OG	4:H:1310:HOH:O	2.08	0.70
1:C:54:LEU:HD12	4:C:1255:HOH:O	1.94	0.68
1:A:170:GLY:O	4:A:1242:HOH:O	2.14	0.66
1:F:5:MET:HB3	1:F:7:VAL:H	1.61	0.64
1:E:37:PRO:HA	1:E:72:PHE:HA	1.85	0.59
1:E:198:LYS:HD3	4:E:393:HOH:O	2.03	0.58
1:A:54:LEU:HD12	4:A:973:HOH:O	2.04	0.57
1:G:54:LEU:HD12	4:G:1403:HOH:O	2.05	0.56
1:E:128[B]:ASN:ND2	4:E:380:HOH:O	2.29	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PHE:CZ	1:D:174:LEU:HD11	2.42	0.55
1:D:214[B]:CYS:SG	4:D:899:HOH:O	2.58	0.55
1:A:30:GLU:OE2	4:A:1432:HOH:O	2.18	0.54
1:F:214[A]:CYS:SG	4:F:1390:HOH:O	2.32	0.54
1:F:54:LEU:HD12	4:F:886:HOH:O	2.07	0.53
1:H:15:LYS:HG2	1:H:17:TYR:CE1	2.44	0.53
1:C:128[B]:ASN:ND2	4:C:664:HOH:O	2.30	0.52
1:E:160:ASN:HB3	1:F:162:PHE:CZ	2.44	0.52
1:G:224:VAL:HG12	1:H:198:LYS:HG2	1.92	0.52
1:E:12:MET:HE2	1:E:118:PHE:CZ	2.45	0.52
1:A:37:PRO:HA	1:A:72:PHE:HA	1.93	0.51
1:D:54:LEU:HD12	4:D:1257:HOH:O	2.10	0.51
1:E:198:LYS:NZ	1:F:225:ALA:C	2.64	0.51
1:F:70:ILE:N	1:F:71:PRO:CD	2.73	0.51
1:G:7:VAL:O	4:G:1340:HOH:O	2.18	0.50
1:G:162:PHE:CZ	1:H:160:ASN:HB3	2.46	0.50
1:E:198:LYS:HZ1	1:F:225:ALA:C	2.15	0.50
1:E:224:VAL:HG12	1:F:198:LYS:HB2	1.94	0.50
1:E:206:LYS:NZ	4:E:1085:HOH:O	2.43	0.49
1:G:198:LYS:HE3	1:G:200:ASP:OD2	2.11	0.49
1:F:116:ASN:HB3	4:F:1417:HOH:O	2.11	0.49
1:G:116:ASN:OD1	4:G:1341:HOH:O	2.20	0.49
1:A:162:PHE:CZ	1:B:160:ASN:HB3	2.48	0.48
1:B:70:ILE:N	1:B:71:PRO:CD	2.76	0.48
1:E:225:ALA:OXT	1:F:198:LYS:HD3	2.12	0.48
1:G:70:ILE:N	1:G:71:PRO:CD	2.76	0.48
1:B:20:GLY:HA3	1:B:124:PHE:O	2.13	0.48
1:E:12:MET:CE	1:E:118:PHE:CE2	2.96	0.48
1:D:162:PHE:HE2	1:D:176:GLU:OE2	1.97	0.48
1:E:11:GLN:NE2	4:E:1103:HOH:O	2.23	0.47
1:A:198:LYS:NZ	1:B:225:ALA:C	2.68	0.47
1:H:42:GLN:HE22	1:H:69:SER:HB3	1.80	0.47
1:E:176:GLU:OE1	4:E:1267:HOH:O	2.20	0.47
1:A:224:VAL:HG12	1:B:198:LYS:HG2	1.95	0.46
1:C:65:CYS:O	1:C:66:QFG:HG1	2.15	0.46
1:E:70:ILE:N	1:E:71:PRO:CD	2.79	0.46
1:G:63:PRO:O	1:G:66:QFG:C2	2.64	0.46
1:H:214[B]:CYS:SG	4:H:1338:HOH:O	2.61	0.46
1:C:224:VAL:HG12	1:D:198:LYS:HG2	1.97	0.46
1:H:54:LEU:HD12	4:H:496:HOH:O	2.15	0.46
1:A:198:LYS:NZ	1:B:225:ALA:OXT	2.39	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:ILE:N	1:H:71:PRO:CD	2.79	0.46
1:A:198:LYS:HZ3	1:B:225:ALA:C	2.19	0.45
1:C:41:GLU:HG2	1:C:216:ILE:HD12	1.98	0.45
1:E:153:ARG:HB3	1:E:158:ILE:CD1	2.46	0.45
1:E:148:GLU:O	1:E:194:TYR:HA	2.16	0.45
1:C:121:HIS:HD2	4:C:1018:HOH:O	2.00	0.45
1:F:5:MET:N	1:F:38:TYR:HH	2.13	0.45
1:H:37:PRO:HA	1:H:72:PHE:HA	1.98	0.45
1:D:176:GLU:HG2	4:D:394:HOH:O	2.17	0.45
1:F:198:LYS:HB3	1:F:198:LYS:HE3	1.62	0.45
1:A:151:PHE:CZ	1:B:174:LEU:HD11	2.52	0.45
1:A:70:ILE:N	1:A:71:PRO:CD	2.80	0.45
1:H:128[B]:ASN:ND2	4:H:342:HOH:O	2.33	0.44
1:G:37:PRO:HA	1:G:72:PHE:HA	1.99	0.44
1:B:160:ASN:ND2	4:B:1264:HOH:O	2.14	0.44
1:D:197:ARG:HA	1:D:216:ILE:O	2.16	0.44
1:E:84:LYS:NZ	4:E:239:HOH:O	2.51	0.44
1:C:70:ILE:N	1:C:71:PRO:CD	2.81	0.44
1:F:198:LYS:HD2	1:F:200:ASP:OD2	2.18	0.44
1:A:160:ASN:HB3	1:B:162:PHE:CZ	2.52	0.43
1:B:30:GLU:OE2	4:B:1247:HOH:O	2.21	0.43
1:B:128[B]:ASN:ND2	4:B:747:HOH:O	2.30	0.43
1:E:12:MET:HE3	1:E:118:PHE:CE2	2.53	0.43
1:H:146:HIS:CG	1:H:163:MET:SD	3.11	0.43
1:C:37:PRO:HA	1:C:72:PHE:HA	2.00	0.43
1:C:198:LYS:HE3	1:C:216:ILE:HG12	2.01	0.43
1:E:12:MET:HE2	1:E:118:PHE:CE2	2.53	0.43
1:H:63:PRO:O	1:H:66:QFG:C2	2.67	0.43
1:D:149:ARG:HD3	1:D:192:TYR:CZ	2.54	0.43
1:D:21:THR:HA	1:D:25:HIS:O	2.19	0.42
1:G:62:SER:HB2	1:G:213:GLN:OE1	2.18	0.42
1:B:59:ASP:HB3	1:B:165:LEU:HD21	2.00	0.42
1:D:20:GLY:HA3	1:D:124:PHE:O	2.19	0.42
1:D:37:PRO:HA	1:D:72:PHE:HA	2.00	0.42
1:D:28:GLU:HB2	1:D:50:LYS:HB2	2.01	0.42
1:A:198:LYS:HB3	1:B:224:VAL:HG12	2.01	0.42
1:C:160:ASN:HB3	1:D:162:PHE:CZ	2.54	0.42
1:F:62:SER:HB2	1:F:213:GLN:OE1	2.19	0.42
1:G:31:GLY:HA3	1:G:46:LEU:HD13	2.01	0.42
1:B:128[B]:ASN:HD22	1:B:128[B]:ASN:HA	1.73	0.42
1:F:66:QFG:CD2	1:F:66:QFG:O2	2.68	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:MET:HE3	1:A:118:PHE:CE2	2.54	0.41
1:D:15:LYS:HG2	1:D:17:TYR:CE1	2.55	0.41
1:F:20:GLY:HA3	1:F:124:PHE:O	2.20	0.41
1:H:12:MET:HG3	1:H:37:PRO:HG3	2.01	0.41
1:D:59:ASP:HB3	1:D:165:LEU:HD21	2.03	0.41
1:G:42:GLN:HE22	1:G:69:SER:HB3	1.85	0.41
1:C:151:PHE:HZ	1:D:174:LEU:HD11	1.83	0.41
1:C:63:PRO:O	1:C:66:QFG:C2	2.68	0.41
1:D:176:GLU:CG	4:D:394:HOH:O	2.68	0.41
1:F:87:PHE:HB3	1:F:88:PRO:HA	2.02	0.40
1:D:148:GLU:O	1:D:194:TYR:HA	2.22	0.40
1:F:15:LYS:HG2	1:F:17:TYR:CE1	2.56	0.40
1:H:21:THR:HA	1:H:25:HIS:O	2.22	0.40
1:B:197:ARG:HA	1:B:216:ILE:O	2.22	0.40
1:F:62:SER:N	1:F:63:PRO:CD	2.85	0.40
1:G:41:GLU:HG2	1:G:216:ILE:HD13	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	219/238 (92%)	214 (98%)	5 (2%)	0	100	100
1	B	219/238 (92%)	215 (98%)	4 (2%)	0	100	100
1	C	218/238 (92%)	214 (98%)	4 (2%)	0	100	100
1	D	219/238 (92%)	216 (99%)	3 (1%)	0	100	100
1	E	218/238 (92%)	212 (97%)	6 (3%)	0	100	100
1	F	218/238 (92%)	213 (98%)	5 (2%)	0	100	100
1	G	217/238 (91%)	211 (97%)	5 (2%)	1 (0%)	34	35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	217/238 (91%)	214 (99%)	3 (1%)	0	100	100
All	All	1745/1904 (92%)	1709 (98%)	35 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	115	GLY

### 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	192/207 (93%)	186 (97%)	6 (3%)	47	59
1	B	191/207 (92%)	185 (97%)	6 (3%)	47	59
1	C	191/207 (92%)	186 (97%)	5 (3%)	54	66
1	D	191/207 (92%)	184 (96%)	7 (4%)	41	50
1	E	191/207 (92%)	183 (96%)	8 (4%)	36	44
1	F	191/207 (92%)	181 (95%)	10 (5%)	29	33
1	G	189/207 (91%)	182 (96%)	7 (4%)	41	50
1	H	190/207 (92%)	183 (96%)	7 (4%)	41	50
All	All	1526/1656 (92%)	1470 (96%)	56 (4%)	42	50

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	147	SER
1	A	198	LYS
1	A	213	GLN
1	A	214[A]	CYS
1	A	214[B]	CYS
1	B	6	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	11	GLN
1	B	46	LEU
1	B	109	ASN
1	B	199	LEU
1	B	216	ILE
1	C	5	MET
1	C	46	LEU
1	C	109	ASN
1	C	147	SER
1	C	217	SER
1	D	7	VAL
1	D	50	LYS
1	D	109	ASN
1	D	114	GLN
1	D	127	LEU
1	D	199	LEU
1	D	217	SER
1	E	7	VAL
1	E	15	LYS
1	E	34	LYS
1	E	109	ASN
1	E	114	GLN
1	E	161	ASN
1	E	198	LYS
1	E	199	LEU
1	F	5	MET
1	F	6	SER
1	F	45	LYS
1	F	109	ASN
1	F	114	GLN
1	F	127	LEU
1	F	158	ILE
1	F	198	LYS
1	F	199	LEU
1	F	216	ILE
1	G	11	GLN
1	G	158	ILE
1	G	198	LYS
1	G	199	LEU
1	G	214[A]	CYS
1	G	214[B]	CYS
1	G	217	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	6	SER
1	H	7	VAL
1	H	46	LEU
1	H	108	SER
1	H	147	SER
1	H	161	ASN
1	H	213	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	ASN
1	F	11	GLN
1	F	109	ASN
1	G	121	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	QFG	A	66	1	23,24,25	2.87	4 (17%)	22,32,34	4.34	6 (27%)
1	QFG	B	66	1	23,24,25	2.65	5 (21%)	22,32,34	4.05	5 (22%)
1	QFG	C	66	1	23,24,25	2.81	4 (17%)	22,32,34	4.76	9 (40%)
1	QFG	D	66	1	23,24,25	2.98	5 (21%)	22,32,34	3.81	8 (36%)
1	QFG	E	66	1	23,24,25	3.47	6 (26%)	22,32,34	4.92	6 (27%)
1	QFG	F	66	1	23,24,25	3.05	6 (26%)	22,32,34	4.49	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	QFG	G	66	1	23,24,25	2.79	10 (43%)	22,32,34	5.17	7 (31%)
1	QFG	H	66	1	23,24,25	3.30	5 (21%)	22,32,34	5.22	7 (31%)

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	QFG	A	66	1	-	0/10/32/33	0/2/2/2
1	QFG	B	66	1	-	0/10/32/33	0/2/2/2
1	QFG	C	66	1	-	0/10/32/33	0/2/2/2
1	QFG	D	66	1	-	0/10/32/33	0/2/2/2
1	QFG	E	66	1	-	0/10/32/33	0/2/2/2
1	QFG	F	66	1	-	0/10/32/33	0/2/2/2
1	QFG	G	66	1	-	0/10/32/33	0/2/2/2
1	QFG	H	66	1	-	0/10/32/33	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	QFG	C2-N3	-2.74	1.32	1.39
1	H	66	QFG	CA2-N2	-2.55	1.32	1.38
1	G	66	QFG	C2-N3	-2.16	1.34	1.39
1	C	66	QFG	C2-N3	-2.07	1.34	1.39
1	B	66	QFG	CA2-C2	-2.01	1.46	1.48
1	E	66	QFG	CE1-CD1	2.01	1.42	1.38
1	G	66	QFG	CD1-CG2	2.02	1.43	1.39
1	B	66	QFG	C1-N2	2.08	1.37	1.33
1	E	66	QFG	CD3-NE1	2.09	1.39	1.32
1	G	66	QFG	CE2-CZ	2.10	1.43	1.38
1	F	66	QFG	C1-N3	2.10	1.42	1.38
1	E	66	QFG	O2-C2	2.11	1.27	1.23
1	B	66	QFG	CE2-CZ	2.13	1.43	1.38
1	A	66	QFG	CE2-CD2	2.14	1.43	1.38
1	C	66	QFG	O2-C2	2.15	1.27	1.23
1	G	66	QFG	CD2-CG2	2.23	1.43	1.39
1	D	66	QFG	CG2-CB2	2.26	1.51	1.46
1	D	66	QFG	C1-N3	2.30	1.43	1.38
1	G	66	QFG	O2-C2	2.33	1.28	1.23
1	E	66	QFG	CG2-CB2	2.36	1.51	1.46
1	F	66	QFG	O2-C2	2.36	1.28	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	QFG	CE2-CD2	2.38	1.43	1.38
1	G	66	QFG	C1-N3	2.41	1.43	1.38
1	F	66	QFG	CG2-CB2	2.65	1.52	1.46
1	F	66	QFG	CE2-CD2	2.67	1.44	1.38
1	H	66	QFG	CE2-CD2	2.85	1.44	1.38
1	G	66	QFG	CG2-CB2	2.92	1.52	1.46
1	H	66	QFG	O2-C2	3.33	1.30	1.23
1	F	66	QFG	C1-N2	3.34	1.39	1.33
1	G	66	QFG	C1-N2	3.91	1.41	1.33
1	D	66	QFG	C1-N2	3.92	1.41	1.33
1	H	66	QFG	C1-N2	4.01	1.41	1.33
1	A	66	QFG	O2-C2	4.08	1.31	1.23
1	D	66	QFG	O2-C2	4.26	1.32	1.23
1	C	66	QFG	C1-N2	4.33	1.41	1.33
1	E	66	QFG	C1-N2	4.49	1.42	1.33
1	A	66	QFG	C1-N2	5.09	1.43	1.33
1	G	66	QFG	CB2-CA2	10.36	1.44	1.35
1	A	66	QFG	CB2-CA2	10.81	1.45	1.35
1	B	66	QFG	CB2-CA2	10.98	1.45	1.35
1	C	66	QFG	CB2-CA2	11.48	1.45	1.35
1	D	66	QFG	CB2-CA2	11.86	1.46	1.35
1	F	66	QFG	CB2-CA2	12.61	1.46	1.35
1	H	66	QFG	CB2-CA2	13.61	1.47	1.35
1	E	66	QFG	CB2-CA2	14.67	1.48	1.35

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	QFG	O2-C2-CA2	-18.63	120.27	130.97
1	G	66	QFG	O2-C2-CA2	-15.08	122.31	130.97
1	A	66	QFG	O2-C2-CA2	-11.28	124.49	130.97
1	F	66	QFG	O2-C2-CA2	-11.26	124.50	130.97
1	B	66	QFG	O2-C2-CA2	-10.23	125.09	130.97
1	E	66	QFG	CG2-CB2-CA2	-10.00	117.62	130.27
1	F	66	QFG	CG2-CB2-CA2	-9.95	117.67	130.27
1	C	66	QFG	O2-C2-CA2	-9.58	125.46	130.97
1	D	66	QFG	CG2-CB2-CA2	-8.56	119.44	130.27
1	E	66	QFG	O2-C2-CA2	-8.43	126.12	130.97
1	G	66	QFG	CG2-CB2-CA2	-7.55	120.72	130.27
1	C	66	QFG	CG2-CB2-CA2	-7.16	121.20	130.27
1	B	66	QFG	CG2-CB2-CA2	-6.45	122.11	130.27
1	H	66	QFG	CG2-CB2-CA2	-6.37	122.21	130.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	QFG	CG2-CB2-CA2	-6.34	122.24	130.27
1	D	66	QFG	O2-C2-CA2	-5.96	127.55	130.97
1	D	66	QFG	CB2-CA2-N2	-5.52	118.93	128.71
1	C	66	QFG	CB2-CA2-N2	-5.00	119.85	128.71
1	G	66	QFG	CB2-CA2-N2	-4.97	119.90	128.71
1	B	66	QFG	CB2-CA2-N2	-4.38	120.95	128.71
1	E	66	QFG	CB2-CA2-N2	-4.01	121.60	128.71
1	A	66	QFG	CB1-CA1-N	-3.89	117.09	124.73
1	A	66	QFG	CB2-CA2-N2	-3.81	121.96	128.71
1	H	66	QFG	CB1-CA1-N	-3.77	117.33	124.73
1	E	66	QFG	C2-CA2-N2	-3.75	106.18	109.03
1	D	66	QFG	CB1-CA1-N	-3.55	117.76	124.73
1	C	66	QFG	CB1-CA1-N	-3.42	118.01	124.73
1	H	66	QFG	CB2-CA2-N2	-3.33	122.81	128.71
1	G	66	QFG	CB1-CA1-N	-3.23	118.38	124.73
1	C	66	QFG	CE2-CD2-CG2	-3.05	116.75	120.66
1	F	66	QFG	CB2-CA2-N2	-3.04	123.32	128.71
1	F	66	QFG	CB1-CA1-N	-2.43	119.95	124.73
1	C	66	QFG	C2-CA2-N2	-2.26	107.31	109.03
1	D	66	QFG	CE1-CD1-CG2	-2.14	117.92	120.66
1	D	66	QFG	CD2-CG2-CD1	2.09	120.76	117.62
1	C	66	QFG	CD2-CG2-CD1	2.09	120.76	117.62
1	H	66	QFG	O2-C2-N3	2.60	130.37	124.70
1	G	66	QFG	C-CA3-N3	3.03	119.23	112.97
1	F	66	QFG	CB2-CA2-C2	4.73	128.90	122.24
1	H	66	QFG	CB2-CA2-C2	4.90	129.14	122.24
1	A	66	QFG	CB2-CA2-C2	5.14	129.48	122.24
1	B	66	QFG	CB2-CA2-C2	6.30	131.10	122.24
1	G	66	QFG	CB2-CA2-C2	6.81	131.82	122.24
1	E	66	QFG	CB2-CA2-C2	7.01	132.11	122.24
1	D	66	QFG	CB2-CA2-C2	7.08	132.20	122.24
1	C	66	QFG	CB2-CA2-C2	7.52	132.81	122.24
1	D	66	QFG	CA2-C2-N3	9.90	108.27	103.37
1	B	66	QFG	CA2-C2-N3	11.86	109.24	103.37
1	H	66	QFG	CA2-C2-N3	12.01	109.32	103.37
1	F	66	QFG	CA2-C2-N3	13.13	109.87	103.37
1	A	66	QFG	CA2-C2-N3	13.14	109.87	103.37
1	G	66	QFG	CA2-C2-N3	14.16	110.38	103.37
1	C	66	QFG	CA2-C2-N3	15.30	110.94	103.37
1	E	66	QFG	CA2-C2-N3	16.35	111.46	103.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	QFG	1	0
1	B	66	QFG	1	0
1	C	66	QFG	3	0
1	D	66	QFG	1	0
1	E	66	QFG	1	0
1	F	66	QFG	2	0
1	G	66	QFG	2	0
1	H	66	QFG	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 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	217/238 (91%)	-0.35	1 (0%) 91 91	22, 32, 44, 57	0
1	B	218/238 (91%)	-0.31	6 (2%) 56 55	21, 31, 45, 56	0
1	C	218/238 (91%)	-0.25	5 (2%) 64 63	22, 33, 46, 62	0
1	D	218/238 (91%)	-0.34	4 (1%) 71 70	20, 30, 42, 54	0
1	E	217/238 (91%)	-0.37	4 (1%) 71 70	21, 30, 42, 50	0
1	F	218/238 (91%)	-0.34	3 (1%) 78 77	22, 31, 42, 53	0
1	G	218/238 (91%)	-0.31	4 (1%) 71 70	20, 31, 44, 53	0
1	H	217/238 (91%)	-0.28	4 (1%) 71 70	21, 33, 47, 63	0
All	All	1741/1904 (91%)	-0.32	31 (1%) 71 70	20, 31, 45, 63	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	SER	5.5
1	C	5	MET	5.4
1	F	6	SER	4.9
1	B	6	SER	4.4
1	H	6	SER	4.1
1	F	5	MET	4.1
1	G	225	ALA	4.0
1	D	5	MET	3.8
1	C	6	SER	3.7
1	G	5	MET	3.3
1	D	225	ALA	3.2
1	A	225	ALA	3.2
1	E	225	ALA	3.1
1	H	225	ALA	3.0
1	B	7	VAL	2.9
1	B	5	MET	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	6	SER	2.7
1	B	225	ALA	2.6
1	H	104	VAL	2.5
1	E	104	VAL	2.4
1	G	7	VAL	2.4
1	B	116	ASN	2.4
1	H	7	VAL	2.4
1	B	114	GLN	2.4
1	C	104	VAL	2.3
1	C	11	GLN	2.3
1	E	36	ARG	2.3
1	E	169	GLY	2.3
1	F	225	ALA	2.2
1	D	104	VAL	2.1
1	C	225	ALA	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	QFG	F	66	23/24	0.92	0.14	-	26,30,34,36	0
1	QFG	D	66	23/24	0.93	0.16	-	28,30,34,37	0
1	QFG	B	66	23/24	0.95	0.18	-	25,31,35,37	0
1	QFG	H	66	23/24	0.91	0.20	-	27,32,38,40	0
1	QFG	C	66	23/24	0.93	0.17	-	30,33,37,39	0
1	QFG	A	66	23/24	0.94	0.19	-	27,31,36,36	0
1	QFG	G	66	23/24	0.91	0.19	-	25,30,35,38	0
1	QFG	E	66	23/24	0.94	0.17	-	24,30,33,38	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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
3	CL	D	229	1/1	0.98	0.42	13.19	36,36,36,36	0
3	CL	E	228	1/1	0.98	0.43	7.22	43,43,43,43	0
3	CL	A	228	1/1	0.98	0.41	6.90	44,44,44,44	0
3	CL	G	227	1/1	0.98	0.26	6.74	33,33,33,33	0
3	CL	B	228	1/1	0.97	0.38	4.64	37,37,37,37	0
3	CL	F	227	1/1	0.99	0.32	4.56	34,34,34,34	0
3	CL	C	229	1/1	0.99	0.34	4.43	33,33,33,33	0
3	CL	H	228	1/1	0.97	0.30	4.34	31,31,31,31	0
2	IOD	C	226	1/1	1.00	0.09	-0.75	34,34,34,34	0
2	IOD	B	226	1/1	1.00	0.09	-0.94	35,35,35,35	0
2	IOD	H	226	1/1	1.00	0.08	-1.03	35,35,35,35	0
2	IOD	D	226	1/1	1.00	0.09	-1.26	32,32,32,32	0
2	IOD	C	227	1/1	1.00	0.09	-1.48	33,33,33,33	0
2	IOD	E	226	1/1	1.00	0.09	-1.54	33,33,33,33	0
2	IOD	A	226	1/1	1.00	0.08	-1.63	33,33,33,33	0
2	IOD	D	227	1/1	1.00	0.08	-2.00	32,32,32,32	0
3	CL	H	227	1/1	0.98	0.21	-	31,31,31,31	0
3	CL	A	227	1/1	0.99	0.21	-	29,29,29,29	0
3	CL	E	227	1/1	0.98	0.24	-	31,31,31,31	0
3	CL	D	228	1/1	0.99	0.19	-	26,26,26,26	0
3	CL	C	228	1/1	0.99	0.25	-	32,32,32,32	0
3	CL	G	226	1/1	0.99	0.25	-	33,33,33,33	0
3	CL	F	226	1/1	0.99	0.20	-	26,26,26,26	0
3	CL	B	227	1/1	0.99	0.22	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.