



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:12 am BST

PDB ID : 4TZG
Title : Crystal structure of eCGP123, an extremely thermostable green fluorescent protein
Authors : Close, D.W.; Don Paul, C.; Traore, D.A.K.; Wilce, M.C.J.; Prescott, M.; Bradbury, A.R.M.
Deposited on : 2014-07-10
Resolution : 2.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

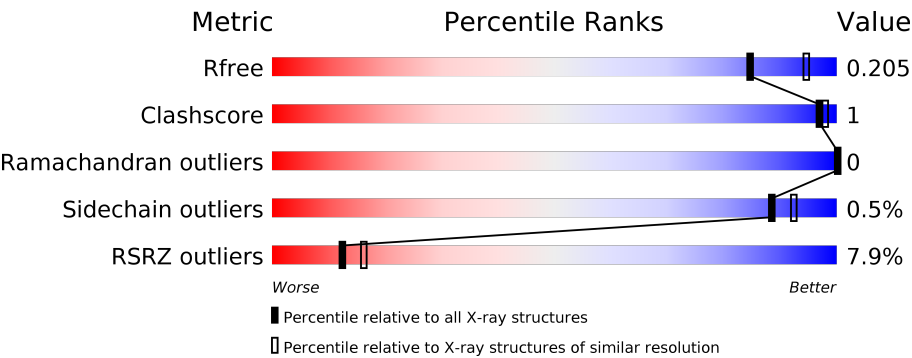
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	245	<div><div>5%</div><div><div></div><div>85%</div><div></div><div>11%</div></div><div></div></div>
1	B	245	<div><div>2%</div><div><div></div><div>88%</div><div></div><div>10%</div></div><div></div></div>
1	C	245	<div><div>4%</div><div><div></div><div>88%</div><div></div><div>10%</div></div><div></div></div>
1	D	245	<div><div>4%</div><div><div></div><div>89%</div><div></div><div>10%</div></div><div></div></div>
1	E	245	<div><div>9%</div><div><div></div><div>87%</div><div></div><div>11%</div></div><div></div></div>
1	F	245	<div><div>8%</div><div><div></div><div>86%</div><div></div><div>10%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	245	<div><div></div><div>10%</div><div>87%</div><div>•</div><div>10%</div></div>
1	H	245	<div><div></div><div>13%</div><div>88%</div><div>•</div><div>10%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29280 atoms, of which 13908 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	219	Total	C	H	N	O	S	0	0	0
			3523	1147	1734	298	333	11			
1	B	220	Total	C	H	N	O	S	0	0	0
			3542	1150	1747	299	335	11			
1	C	220	Total	C	H	N	O	S	0	0	0
			3542	1150	1747	299	335	11			
1	D	220	Total	C	H	N	O	S	0	0	0
			3541	1150	1746	299	335	11			
1	E	218	Total	C	H	N	O	S	0	0	0
			3509	1142	1727	297	332	11			
1	F	220	Total	C	H	N	O	S	0	0	0
			3541	1150	1746	299	335	11			
1	G	220	Total	C	H	N	O	S	0	0	0
			3514	1150	1719	299	335	11			
1	H	220	Total	C	H	N	O	S	0	0	0
			3537	1150	1742	299	335	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	160	Total	O	0	0
			160	160		
2	C	166	Total	O	0	0
			166	166		
2	D	120	Total	O	0	0
			120	120		
2	E	124	Total	O	0	0
			124	124		
2	F	126	Total	O	0	0
			126	126		

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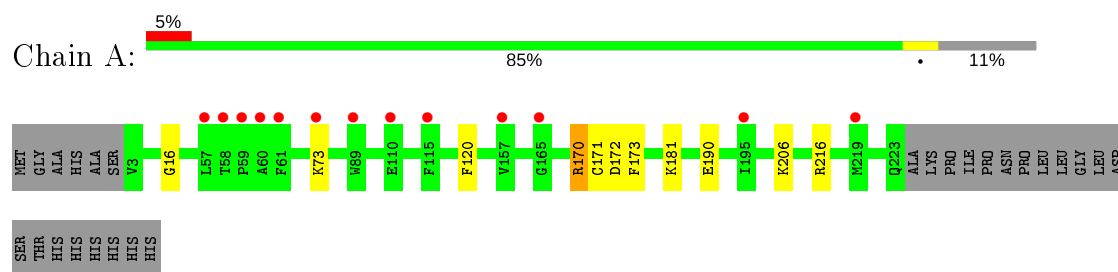
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	94	Total	O	0	0
			94	94		
2	H	99	Total	O	0	0
			99	99		

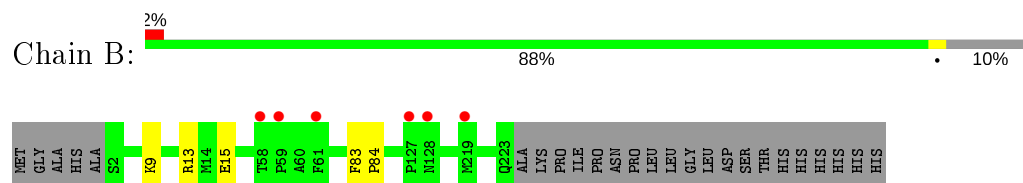
3 Residue-property plots

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.

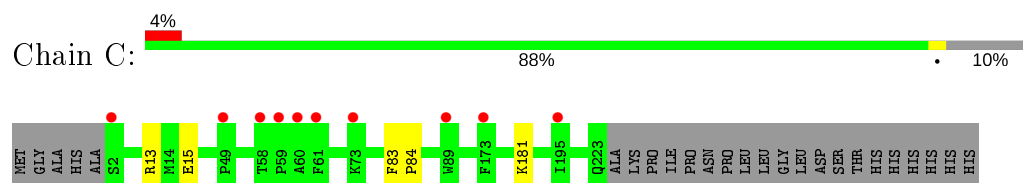
• Molecule 1: Fluorescent Protein



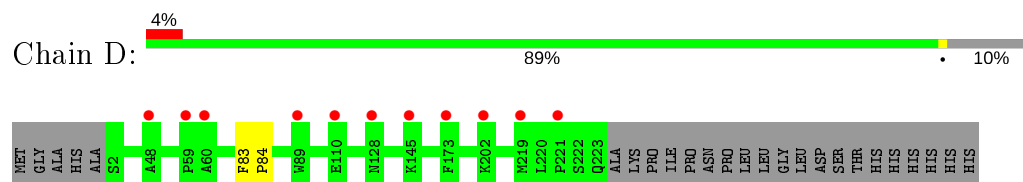
• Molecule 1: Fluorescent Protein



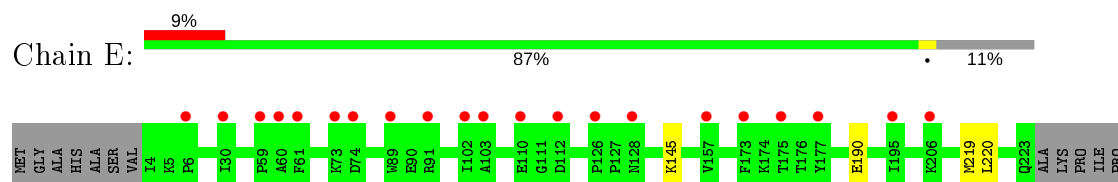
• Molecule 1: Fluorescent Protein



• Molecule 1: Fluorescent Protein




• Molecule 1: Fluorescent Protein



ASN
PRO
LEU
LEU
GLY
LEU
ASP
SER
HIS
HIS
HIS
HIS
HIS


• Molecule 1: Fluorescent Protein

Chain F:  8% 86% 10%

MET GLY ALA HIS THR HIS HIS HIS HIS
S2 V3 D41 T58 P59 A60 F61 R66 P72 K73 D74 F83 P84 R89 E90 R91 A103 G111 H128 V157 C171 D172 F173 K174 T175 R184 L185 K202 R208 L209 Q223
ALA LYS PRO ILE PRO ASN PRO LEU

GLY
LEU
ASP
SER
THR
HIS
HIS
HIS
HIS


• Molecule 1: Fluorescent Protein

Chain G:  10% 87% 10%

MET GLY ALA HIS THR HIS HIS HIS HIS
S2 V3 I4 K5 P6 E26 T30 G31 K32 K45 P59 A60 F61 QY62 R65 K73 R89 E110 P127 H128 E144 K145 V157 E164 F173 Y177 R184 E190 K202 Y217 S218 P219 L220 P221 S222 Q223
ALA LYS

PRO
ILE
PRO
ASN
PRO
LEU
LEU
GLY
LEU
ASP
SER
THR
HIS
HIS
HIS
HIS

• Molecule 1: Fluorescent Protein

Chain H:  13% 88% 10%

MET GLY ALA HIS THR HIS HIS HIS HIS
S2 V3 I4 K5 P6 K22 T30 Y34 V44 P49 L57 T58 P59 A60 F61 K73 D74 F83 P84 R89 E90 R91 I100 C101 I102 A103 E110 G111 Y116 P126 H139 V152 V157 F173 K174 T175 Y177

D182 V183 R184 L185 K202 S222 Q223
ALA LYS PRO ILE PRO ASN PRO LEU LEU GLY ASP SER THR HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.63 Å 75.38 Å 84.51 Å 90.96° 89.82° 104.03°	Depositor
Resolution (Å)	29.85 – 2.10 29.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.85-2.10) 94.4 (29.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.9_1685	Depositor
R, R_{free}	0.167 , 0.203 0.171 , 0.205	Depositor DCC
R_{free} test set	4888 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.001 for -k,-h,-l 0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29280	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/1811	0.46	0/2441
1	B	0.27	0/1817	0.47	0/2449
1	C	0.28	0/1817	0.46	0/2449
1	D	0.27	0/1817	0.46	0/2449
1	E	0.26	0/1804	0.45	0/2431
1	F	0.27	0/1817	0.45	0/2449
1	G	0.25	0/1817	0.46	1/2449 (0.0%)
1	H	0.25	0/1817	0.43	0/2449
All	All	0.27	0/14517	0.45	1/19566 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	218	SER	C-N-CA	7.10	139.44	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1789	1734	1743	6	0
1	B	1795	1747	1748	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1795	1747	1748	3	0
1	D	1795	1746	1748	1	0
1	E	1782	1727	1734	1	0
1	F	1795	1746	1748	7	0
1	G	1795	1719	1748	3	0
1	H	1795	1742	1747	2	0
2	A	142	0	0	2	0
2	B	160	0	0	1	0
2	C	166	0	0	1	0
2	D	120	0	0	0	0
2	E	124	0	0	0	0
2	F	126	0	0	2	0
2	G	94	0	0	1	0
2	H	99	0	0	0	0
All	All	15372	13908	13964	26	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 1.

All (26) 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:G:145:LYS:NZ	1:G:190:GLU:OE2	2.29	0.66
1:C:181:LYS:NZ	2:C:301:HOH:O	2.32	0.61
1:F:41:ASP:OD1	1:F:208:ARG:NH1	2.34	0.60
1:C:13:ARG:NH1	1:C:15:GLU:OE2	2.35	0.59
1:A:73:LYS:NZ	2:A:301:HOH:O	2.36	0.58
1:F:73:LYS:NZ	2:F:414:HOH:O	2.38	0.56
1:A:171:CYS:HG	1:A:173:PHE:HE1	1.57	0.52
1:E:145:LYS:NZ	1:E:190:GLU:OE2	2.41	0.52
1:F:208:ARG:NH1	2:F:418:HOH:O	2.43	0.52
1:G:32:LYS:NZ	2:G:366:HOH:O	2.44	0.51
1:A:170:ARG:NH2	1:A:172:ASP:OD1	2.42	0.50
1:G:26:GLU:OE1	1:G:45:LYS:NZ	2.43	0.49
1:H:100:ILE:HG13	1:H:101:CYS:N	2.28	0.48
1:F:171:CYS:HG	1:F:173:PHE:HE1	1.62	0.47
1:B:9:LYS:NZ	2:B:442:HOH:O	2.48	0.46
1:F:2:SER:N	1:F:3:VAL:HA	2.31	0.45
1:B:13:ARG:NH1	1:B:15:GLU:OE1	2.48	0.45
1:A:190:GLU:OE1	1:A:216:ARG:NH1	2.51	0.43
1:F:83:PHE:HB3	1:F:84:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.01	0.43
1:A:206:LYS:NZ	2:A:410:HOH:O	2.45	0.42
1:C:83:PHE:HB3	1:C:84:PRO:HA	2.02	0.42
1:F:66:ARG:NE	1:F:66:ARG:HA	2.35	0.41
1:A:16:GLY:HA3	1:A:120:PHE:O	2.19	0.41
1:H:83:PHE:HB3	1:H:84:PRO:HA	2.02	0.41
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	216/245 (88%)	216 (100%)	0	0	100	100
1	B	217/245 (89%)	217 (100%)	0	0	100	100
1	C	217/245 (89%)	217 (100%)	0	0	100	100
1	D	217/245 (89%)	216 (100%)	1 (0%)	0	100	100
1	E	215/245 (88%)	214 (100%)	1 (0%)	0	100	100
1	F	217/245 (89%)	216 (100%)	1 (0%)	0	100	100
1	G	217/245 (89%)	215 (99%)	2 (1%)	0	100	100
1	H	217/245 (89%)	215 (99%)	2 (1%)	0	100	100
All	All	1733/1960 (88%)	1726 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	190/211 (90%)	188 (99%)	2 (1%)	73	79
1	B	191/211 (90%)	191 (100%)	0	100	100
1	C	191/211 (90%)	191 (100%)	0	100	100
1	D	191/211 (90%)	191 (100%)	0	100	100
1	E	189/211 (90%)	187 (99%)	2 (1%)	73	79
1	F	191/211 (90%)	191 (100%)	0	100	100
1	G	191/211 (90%)	190 (100%)	1 (0%)	88	92
1	H	191/211 (90%)	189 (99%)	2 (1%)	76	82
All	All	1525/1688 (90%)	1518 (100%)	7 (0%)	88	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ARG
1	A	181	LYS
1	E	219	MET
1	E	220	LEU
1	G	30	ILE
1	H	100	ILE
1	H	116	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	CRQ	D	62	1	24,25,26	3.15	9 (37%)	27,34,36	2.23	9 (33%)
1	CRQ	H	62	1	24,25,26	3.30	10 (41%)	27,34,36	2.44	7 (25%)
1	CRQ	A	62	1	24,25,26	3.15	10 (41%)	27,34,36	2.25	8 (29%)
1	CRQ	B	62	1	24,25,26	3.08	9 (37%)	27,34,36	2.13	9 (33%)
1	CRQ	C	62	1	24,25,26	3.13	10 (41%)	27,34,36	2.07	7 (25%)
1	CRQ	E	62	1	24,25,26	3.19	10 (41%)	27,34,36	2.20	7 (25%)
1	CRQ	F	62	1	24,25,26	3.51	9 (37%)	27,34,36	2.37	7 (25%)
1	CRQ	G	62	1	24,25,26	3.27	10 (41%)	27,34,36	2.38	7 (25%)

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	CRQ	D	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	H	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	B	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	E	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	F	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	G	62	1	-	4/10/32/33	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	CRQ	CA2-C2	11.39	1.59	1.48
1	E	62	CRQ	CA2-C2	11.05	1.59	1.48
1	G	62	CRQ	CA2-C2	11.03	1.59	1.48
1	H	62	CRQ	CA2-C2	11.01	1.59	1.48
1	D	62	CRQ	CA2-C2	10.68	1.59	1.48
1	A	62	CRQ	CA2-C2	10.63	1.59	1.48
1	C	62	CRQ	CA2-C2	10.61	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	CRQ	CA2-C2	10.39	1.58	1.48
1	F	62	CRQ	CB2-CA2	7.41	1.41	1.35
1	H	62	CRQ	CB2-CA2	6.13	1.40	1.35
1	G	62	CRQ	CB2-CA2	5.72	1.39	1.35
1	A	62	CRQ	CB2-CA2	5.16	1.39	1.35
1	C	62	CRQ	CD3-NE1	5.01	1.49	1.32
1	D	62	CRQ	CD3-NE1	5.01	1.49	1.32
1	H	62	CRQ	CD3-NE1	5.00	1.49	1.32
1	G	62	CRQ	CD3-NE1	4.99	1.49	1.32
1	D	62	CRQ	CB2-CA2	4.96	1.39	1.35
1	A	62	CRQ	CD3-NE1	4.91	1.48	1.32
1	E	62	CRQ	CB2-CA2	4.89	1.39	1.35
1	E	62	CRQ	CD3-NE1	4.89	1.48	1.32
1	C	62	CRQ	CB2-CA2	4.88	1.39	1.35
1	B	62	CRQ	CB2-CA2	4.81	1.39	1.35
1	B	62	CRQ	CD3-NE1	4.75	1.48	1.32
1	F	62	CRQ	CD3-NE1	4.69	1.48	1.32
1	F	62	CRQ	CA1-N	4.17	1.37	1.27
1	B	62	CRQ	CA3-N3	-4.06	1.39	1.47
1	F	62	CRQ	C2-N3	3.94	1.49	1.39
1	G	62	CRQ	C2-N3	3.93	1.49	1.39
1	H	62	CRQ	C2-N3	3.92	1.49	1.39
1	A	62	CRQ	C2-N3	3.83	1.48	1.39
1	C	62	CRQ	C2-N3	3.81	1.48	1.39
1	D	62	CRQ	CA3-N3	-3.73	1.39	1.47
1	E	62	CRQ	C2-N3	3.73	1.48	1.39
1	H	62	CRQ	CA3-N3	-3.73	1.39	1.47
1	H	62	CRQ	CG2-CB2	3.71	1.54	1.46
1	C	62	CRQ	CA3-N3	-3.71	1.39	1.47
1	G	62	CRQ	CA3-N3	-3.70	1.39	1.47
1	D	62	CRQ	C2-N3	3.70	1.48	1.39
1	E	62	CRQ	CA3-N3	-3.66	1.40	1.47
1	B	62	CRQ	CA1-N	3.60	1.36	1.27
1	B	62	CRQ	C2-N3	3.58	1.48	1.39
1	D	62	CRQ	CA1-N	3.55	1.36	1.27
1	G	62	CRQ	CA1-N	3.55	1.36	1.27
1	F	62	CRQ	CG2-CB2	3.53	1.53	1.46
1	A	62	CRQ	CA3-N3	-3.52	1.40	1.47
1	G	62	CRQ	CG2-CB2	3.52	1.53	1.46
1	C	62	CRQ	CA1-N	3.45	1.35	1.27
1	F	62	CRQ	CA3-N3	-3.45	1.40	1.47
1	A	62	CRQ	CA1-N	3.44	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CRQ	CG2-CB2	3.44	1.53	1.46
1	E	62	CRQ	CA1-N	3.44	1.35	1.27
1	A	62	CRQ	CG2-CB2	3.41	1.53	1.46
1	H	62	CRQ	CA1-N	3.41	1.35	1.27
1	E	62	CRQ	CG2-CB2	3.33	1.53	1.46
1	F	62	CRQ	C1-N3	3.26	1.43	1.38
1	B	62	CRQ	CG2-CB2	3.24	1.53	1.46
1	D	62	CRQ	CG2-CB2	3.21	1.53	1.46
1	F	62	CRQ	CA3-C	2.69	1.58	1.49
1	H	62	CRQ	CA3-C	2.37	1.57	1.49
1	D	62	CRQ	C1-N3	2.34	1.42	1.38
1	E	62	CRQ	CA3-C	2.31	1.57	1.49
1	G	62	CRQ	CA3-C	2.29	1.57	1.49
1	A	62	CRQ	CA3-C	2.29	1.57	1.49
1	E	62	CRQ	CA2-N2	-2.28	1.33	1.38
1	B	62	CRQ	CA2-N2	-2.25	1.33	1.38
1	A	62	CRQ	CA2-N2	-2.24	1.33	1.38
1	G	62	CRQ	CA2-N2	-2.20	1.33	1.38
1	B	62	CRQ	CA3-C	2.19	1.56	1.49
1	C	62	CRQ	CA3-C	2.16	1.56	1.49
1	D	62	CRQ	CA3-C	2.16	1.56	1.49
1	H	62	CRQ	CA2-N2	-2.09	1.34	1.38
1	G	62	CRQ	C1-N3	2.08	1.41	1.38
1	E	62	CRQ	C1-N3	2.08	1.41	1.38
1	H	62	CRQ	C1-N3	2.05	1.41	1.38
1	A	62	CRQ	C1-N3	2.04	1.41	1.38
1	C	62	CRQ	C1-N3	2.03	1.41	1.38
1	C	62	CRQ	CA2-N2	-2.02	1.34	1.38

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	62	CRQ	O2-C2-CA2	-6.54	127.29	130.96
1	A	62	CRQ	O2-C2-CA2	-6.42	127.36	130.96
1	G	62	CRQ	O2-C2-CA2	-6.40	127.36	130.96
1	F	62	CRQ	O2-C2-CA2	-6.24	127.46	130.96
1	D	62	CRQ	O2-C2-CA2	-6.17	127.50	130.96
1	H	62	CRQ	C2-CA2-N2	-6.14	104.64	108.93
1	F	62	CRQ	C2-CA2-N2	-6.07	104.68	108.93
1	G	62	CRQ	C2-CA2-N2	-5.83	104.85	108.93
1	E	62	CRQ	O2-C2-CA2	-5.75	127.73	130.96
1	B	62	CRQ	O2-C2-CA2	-5.59	127.82	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	CRQ	O2-C2-CA2	-5.14	128.07	130.96
1	E	62	CRQ	C2-CA2-N2	-5.03	105.41	108.93
1	F	62	CRQ	CA2-N2-C1	4.80	113.10	104.33
1	A	62	CRQ	C2-CA2-N2	-4.75	105.61	108.93
1	H	62	CRQ	CA2-N2-C1	4.61	112.77	104.33
1	G	62	CRQ	CA2-N2-C1	4.61	112.76	104.33
1	C	62	CRQ	C2-CA2-N2	-4.52	105.77	108.93
1	H	62	CRQ	CG2-CB2-CA2	-4.46	124.47	129.94
1	G	62	CRQ	CG2-CB2-CA2	-4.22	124.77	129.94
1	E	62	CRQ	CA2-N2-C1	4.12	111.86	104.33
1	A	62	CRQ	CA2-N2-C1	4.07	111.77	104.33
1	B	62	CRQ	C2-CA2-N2	-4.06	106.09	108.93
1	C	62	CRQ	CA2-N2-C1	4.01	111.67	104.33
1	D	62	CRQ	C2-CA2-N2	-3.96	106.16	108.93
1	B	62	CRQ	CA2-N2-C1	3.94	111.54	104.33
1	D	62	CRQ	CA2-N2-C1	3.81	111.30	104.33
1	D	62	CRQ	O-C-CA3	-3.79	114.94	126.39
1	C	62	CRQ	O-C-CA3	-3.78	114.98	126.39
1	D	62	CRQ	CG2-CB2-CA2	-3.65	125.47	129.94
1	B	62	CRQ	O-C-CA3	-3.63	115.43	126.39
1	A	62	CRQ	O-C-CA3	-3.59	115.56	126.39
1	E	62	CRQ	CG2-CB2-CA2	-3.30	125.91	129.94
1	F	62	CRQ	O-C-CA3	-3.27	116.52	126.39
1	B	62	CRQ	CG2-CB2-CA2	-3.24	125.97	129.94
1	G	62	CRQ	O-C-CA3	-3.15	116.88	126.39
1	E	62	CRQ	O-C-CA3	-3.12	116.97	126.39
1	F	62	CRQ	CG2-CB2-CA2	-3.11	126.14	129.94
1	H	62	CRQ	O-C-CA3	-2.89	117.65	126.39
1	A	62	CRQ	CG2-CB2-CA2	-2.89	126.40	129.94
1	A	62	CRQ	CA3-N3-C2	2.77	130.15	123.80
1	C	62	CRQ	CG2-CB2-CA2	-2.76	126.56	129.94
1	F	62	CRQ	CA2-C2-N3	2.69	104.64	103.37
1	D	62	CRQ	CB2-CA2-N2	2.51	132.31	128.83
1	B	62	CRQ	CA3-N3-C2	2.47	129.47	123.80
1	D	62	CRQ	CA3-N3-C2	2.47	129.46	123.80
1	E	62	CRQ	CA3-N3-C2	2.45	129.43	123.80
1	G	62	CRQ	CA3-N3-C2	2.36	129.21	123.80
1	B	62	CRQ	O2-C2-N3	2.34	129.00	124.35
1	D	62	CRQ	O2-C2-N3	2.33	128.97	124.35
1	H	62	CRQ	CA2-C2-N3	2.30	104.46	103.37
1	C	62	CRQ	CA3-N3-C2	2.27	129.00	123.80
1	B	62	CRQ	CD2-CG2-CD1	2.26	120.98	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	CRQ	CB2-CA2-N2	2.25	131.95	128.83
1	D	62	CRQ	CD2-CG2-CD1	2.22	120.93	117.64
1	A	62	CRQ	O2-C2-N3	2.20	128.72	124.35
1	H	62	CRQ	CA3-N3-C2	2.19	128.82	123.80
1	B	62	CRQ	CB2-CA2-N2	2.17	131.84	128.83
1	G	62	CRQ	O2-C2-N3	2.07	128.46	124.35
1	C	62	CRQ	CB2-CA2-N2	2.05	131.67	128.83
1	A	62	CRQ	CD2-CG2-CD1	2.05	120.67	117.64
1	E	62	CRQ	CG1-CB1-CA1	-2.00	107.31	113.53

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	62	CRQ	C-CA3-N3-C2
1	H	62	CRQ	C-CA3-N3-C2
1	A	62	CRQ	C-CA3-N3-C2
1	B	62	CRQ	C-CA3-N3-C2
1	C	62	CRQ	C-CA3-N3-C2
1	E	62	CRQ	C1-CA1-CB1-CG1
1	E	62	CRQ	C-CA3-N3-C2
1	F	62	CRQ	C-CA3-N3-C2
1	G	62	CRQ	C-CA3-N3-C2
1	H	62	CRQ	C-CA3-N3-C1
1	B	62	CRQ	C-CA3-N3-C1
1	E	62	CRQ	C-CA3-N3-C1
1	G	62	CRQ	C-CA3-N3-C1
1	D	62	CRQ	C-CA3-N3-C1
1	A	62	CRQ	C-CA3-N3-C1
1	C	62	CRQ	C-CA3-N3-C1
1	F	62	CRQ	C-CA3-N3-C1
1	D	62	CRQ	C1-CA1-CB1-CG1
1	G	62	CRQ	C1-CA1-CB1-CG1
1	H	62	CRQ	CA1-CB1-CG1-CD3
1	G	62	CRQ	CA1-CB1-CG1-CD3

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	218/245 (88%)	0.30	13 (5%) 21 27	27, 36, 50, 65	0
1	B	219/245 (89%)	0.17	6 (2%) 54 60	24, 33, 46, 57	0
1	C	219/245 (89%)	0.28	10 (4%) 32 38	25, 34, 47, 70	0
1	D	219/245 (89%)	0.30	11 (5%) 28 34	26, 38, 51, 64	0
1	E	217/245 (88%)	0.57	21 (9%) 7 10	29, 42, 58, 71	0
1	F	219/245 (89%)	0.59	20 (9%) 9 12	27, 42, 62, 89	0
1	G	219/245 (89%)	0.68	24 (10%) 5 7	33, 46, 64, 82	0
1	H	219/245 (89%)	0.93	33 (15%) 2 3	30, 49, 67, 83	0
All	All	1749/1960 (89%)	0.48	138 (7%) 12 16	24, 40, 59, 89	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	SER	5.7
1	H	89	TRP	5.4
1	H	60	ALA	5.3
1	H	3	VAL	5.1
1	G	184	ARG	4.4
1	H	2	SER	4.4
1	C	2	SER	4.4
1	E	60	ALA	4.3
1	F	89	TRP	4.3
1	E	89	TRP	4.3
1	H	111	GLY	4.2
1	F	60	ALA	4.0
1	G	2	SER	3.9
1	D	219	MET	3.8
1	H	59	PRO	3.8
1	F	59	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	59	PRO	3.7
1	F	184	ARG	3.7
1	H	61	PHE	3.6
1	H	91	ARG	3.6
1	F	74	ASP	3.5
1	G	89	TRP	3.5
1	F	111	GLY	3.5
1	H	73	LYS	3.5
1	G	59	PRO	3.5
1	H	202	LYS	3.4
1	A	60	ALA	3.4
1	G	30	ILE	3.4
1	G	221	PRO	3.4
1	F	185	LEU	3.3
1	D	110	GLU	3.3
1	A	110	GLU	3.3
1	E	73	LYS	3.2
1	G	6	PRO	3.1
1	E	173	PHE	3.1
1	H	157	VAL	3.1
1	G	110	GLU	3.1
1	F	61	PHE	3.1
1	H	34	TYR	3.1
1	E	110	GLU	3.1
1	B	128	ASN	3.0
1	D	59	PRO	3.0
1	F	173	PHE	3.0
1	H	184	ARG	3.0
1	D	48	ALA	3.0
1	G	177	TYR	2.9
1	A	165	GLY	2.9
1	F	128	ASN	2.8
1	A	59	PRO	2.8
1	H	44	VAL	2.8
1	G	60	ALA	2.8
1	H	173	PHE	2.8
1	F	58	THR	2.8
1	H	74	ASP	2.8
1	B	59	PRO	2.7
1	E	128	ASN	2.7
1	C	60	ALA	2.7
1	A	58	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	202	LYS	2.7
1	G	173	PHE	2.6
1	H	6	PRO	2.6
1	C	58	THR	2.6
1	E	195	ILE	2.6
1	A	61	PHE	2.6
1	G	157	VAL	2.6
1	E	126	PRO	2.6
1	F	157	VAL	2.5
1	F	103	ALA	2.5
1	C	195	ILE	2.5
1	C	61	PHE	2.5
1	G	61	PHE	2.5
1	E	103	ALA	2.5
1	H	152	VAL	2.5
1	B	219	MET	2.5
1	H	4	ILE	2.5
1	E	61	PHE	2.5
1	E	74	ASP	2.5
1	G	3	VAL	2.5
1	B	61	PHE	2.5
1	B	127	PRO	2.4
1	E	157	VAL	2.4
1	E	91	ARG	2.4
1	H	139	TRP	2.4
1	G	217	TYR	2.4
1	H	175	THR	2.4
1	G	73	LYS	2.4
1	E	6	PRO	2.4
1	H	110	GLU	2.4
1	A	73	LYS	2.4
1	C	59	PRO	2.3
1	F	72	PRO	2.3
1	H	177	TYR	2.3
1	D	60	ALA	2.3
1	G	65	ASN	2.3
1	H	58	THR	2.3
1	E	175	THR	2.3
1	F	91	ARG	2.3
1	H	126	PRO	2.3
1	F	209	LEU	2.3
1	H	182	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	MET	2.2
1	H	103	ALA	2.2
1	D	173	PHE	2.2
1	C	89	TRP	2.2
1	H	49	PRO	2.2
1	A	115	PHE	2.2
1	D	145	LYS	2.2
1	A	89	TRP	2.2
1	H	30	ILE	2.2
1	B	58	THR	2.2
1	H	22	LYS	2.2
1	H	185	LEU	2.2
1	G	127	PRO	2.2
1	H	222	SER	2.2
1	G	128	ASN	2.2
1	G	144	GLU	2.2
1	C	49	PRO	2.2
1	E	30	ILE	2.1
1	C	173	PHE	2.1
1	D	128	ASN	2.1
1	E	102	ILE	2.1
1	E	206	LYS	2.1
1	F	202	LYS	2.1
1	H	57	LEU	2.1
1	D	221	PRO	2.1
1	D	202	LYS	2.1
1	E	177	TYR	2.1
1	A	195	ILE	2.0
1	G	219	MET	2.0
1	F	175	THR	2.0
1	D	89	TRP	2.0
1	A	57	LEU	2.0
1	E	112	ASP	2.0
1	F	73	LYS	2.0
1	G	164	GLU	2.0
1	A	157	VAL	2.0
1	C	73	LYS	2.0
1	G	5	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
1	CRQ	G	62	24/25	0.91	0.38	37,40,51,56	0
1	CRQ	H	62	24/25	0.93	0.42	39,44,58,58	0
1	CRQ	A	62	24/25	0.93	0.28	26,29,35,35	0
1	CRQ	B	62	24/25	0.93	0.25	22,27,33,34	0
1	CRQ	E	62	24/25	0.93	0.35	30,36,48,48	0
1	CRQ	D	62	24/25	0.93	0.29	26,29,36,36	0
1	CRQ	F	62	24/25	0.95	0.39	30,35,44,47	0
1	CRQ	C	62	24/25	0.95	0.29	25,26,33,34	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.