



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 AM GMT

PDB ID : 2WHT  
Title : Fluorescent Protein mKeima at pH 5.6  
Authors : Violot, S.; Carpentier, P.; Blanchoin, L.; Bourgeois, D.  
Deposited on : 2009-05-06  
Resolution : 1.90 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

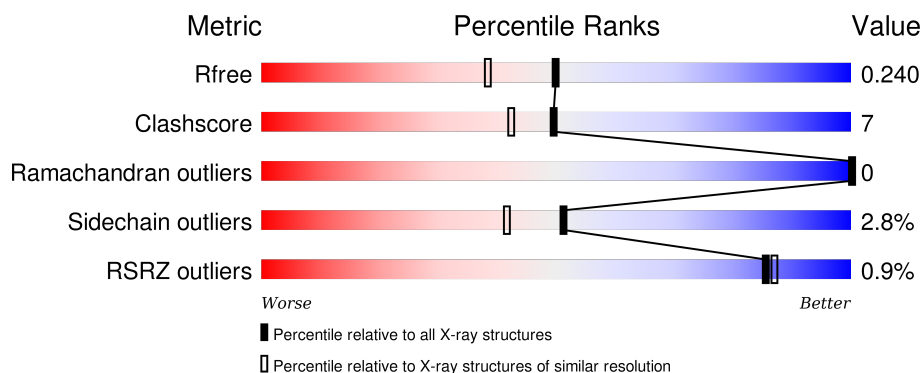
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	240	 78% 11% • 10%
1	B	240	 78% 11% • 10%
1	C	240	 77% 12% • 10%
1	D	240	 80% 10% • 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8339 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 LARGE STOKES SHIFT FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	1	0
			1757	1118	294	334	11			
1	B	217	Total	C	N	O	S	0	1	0
			1765	1124	295	335	11			
1	C	216	Total	C	N	O	S	0	1	0
			1757	1118	294	334	11			
1	D	216	Total	C	N	O	S	0	1	0
			1757	1118	294	334	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	CRQ	GLN	CHROMOPHORE	UNP Q1JV70
A	62	CRQ	TYR	CHROMOPHORE	UNP Q1JV70
A	62	CRQ	GLY	CHROMOPHORE	UNP Q1JV70
B	62	CRQ	GLN	CHROMOPHORE	UNP Q1JV70
B	62	CRQ	TYR	CHROMOPHORE	UNP Q1JV70
B	62	CRQ	GLY	CHROMOPHORE	UNP Q1JV70
C	62	CRQ	GLN	CHROMOPHORE	UNP Q1JV70
C	62	CRQ	TYR	CHROMOPHORE	UNP Q1JV70
C	62	CRQ	GLY	CHROMOPHORE	UNP Q1JV70
D	62	CRQ	GLN	CHROMOPHORE	UNP Q1JV70
D	62	CRQ	TYR	CHROMOPHORE	UNP Q1JV70
D	62	CRQ	GLY	CHROMOPHORE	UNP Q1JV70

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	351	Total	O	0	0
			351	351		
2	B	345	Total	O	0	0
			345	345		

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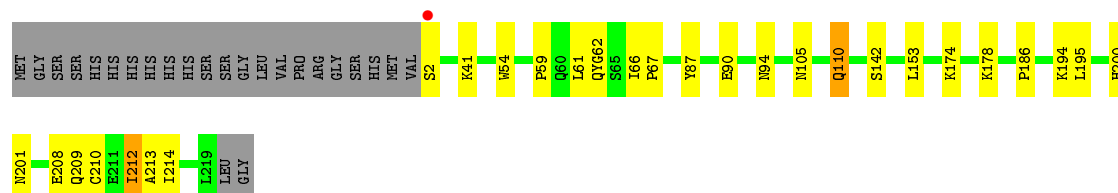
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	283	Total 283	O 283	0	0
2	D	324	Total 324	O 324	0	0

### 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.

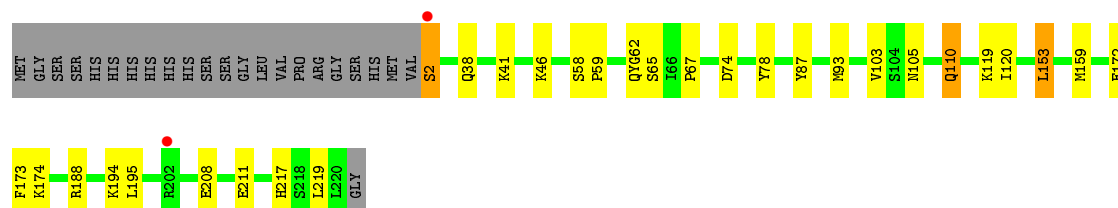
#### • Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

Chain A: 




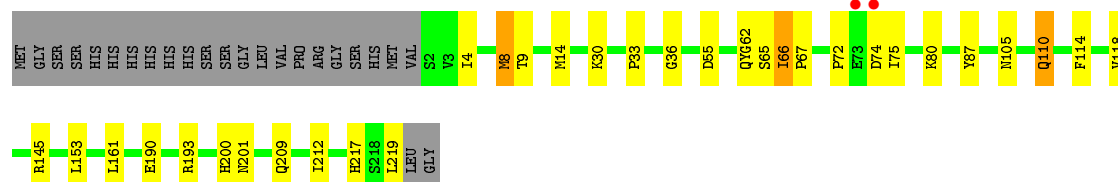
#### • Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

Chain B: 




#### • Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

Chain C: 



#### • Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

Chain D: 



R188	S199	H200	N201	Q209	S218	L219	LEU	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.46 Å   55.56 Å   90.56 Å 90.00°   108.47°   90.00°	Depositor
Resolution (Å)	45.13 – 1.90 45.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.13-1.90) 99.6 (45.12-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.183   ,   0.239 0.183   ,   0.240	Depositor DCC
$R_{free}$ test set	4256 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84623 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: 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	0.79	1/1754 (0.1%)	0.79	0/2369
1	B	0.74	0/1762	0.77	1/2380 (0.0%)
1	C	0.71	0/1754	0.72	0/2369
1	D	0.69	0/1754	0.71	1/2369 (0.0%)
All	All	0.73	1/7024 (0.0%)	0.75	2/9487 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	CYS	CB-SG	-5.02	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	MET	CG-SD-CE	5.11	108.37	100.20
1	D	118	VAL	CB-CA-C	-5.03	101.85	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	61	LEU	Mainchain

## 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	1757	0	1676	25	0
1	B	1765	0	1687	28	0
1	C	1757	0	1676	28	0
1	D	1757	0	1676	16	0
2	A	351	0	0	8	0
2	B	345	0	0	9	0
2	C	283	0	0	6	0
2	D	324	0	0	5	0
All	All	8339	0	6715	97	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 7.

All (97) 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:C:72:PRO:HG2	1:C:75:ILE:HD12	1.14	1.06
1:C:72:PRO:CG	1:C:75:ILE:HD12	1.92	0.99
1:C:4:ILE:HG23	1:C:8:MET:HE1	1.52	0.89
1:D:54:TRP:HE1	1:D:209:GLN:HE21	1.16	0.88
1:A:90:GLU:HG3	2:A:2182:HOH:O	1.77	0.83
1:A:54:TRP:HE1	1:A:209:GLN:NE2	1.78	0.81
1:A:54:TRP:HE1	1:A:209:GLN:HE21	1.22	0.81
1:B:46:LYS:HE2	2:B:2113:HOH:O	1.85	0.76
1:D:54:TRP:HE1	1:D:209:GLN:NE2	1.82	0.75
1:A:194:LYS:HG3	2:A:2317:HOH:O	1.85	0.74
1:D:218:SER:HB3	2:D:2324:HOH:O	1.89	0.72
1:A:110:GLN:NE2	2:A:2202:HOH:O	2.25	0.69
1:A:90:GLU:CG	2:A:2182:HOH:O	2.37	0.68
1:C:219:LEU:C	2:C:2283:HOH:O	2.33	0.67
1:D:67:PRO:HD3	1:D:87:TYR:OH	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:HIS:HD2	1:C:201:ASN:O	1.77	0.67
1:B:93:MET:HE3	1:B:173:PHE:CZ	2.29	0.66
1:B:74:ASP:OD2	1:B:217:HIS:HE1	1.79	0.64
1:B:62[A]:CRQ:HE2	1:B:195:LEU:HB2	1.80	0.63
1:C:8:MET:HE3	1:C:114:PHE:CZ	2.33	0.63
1:A:212:ILE:HD13	1:A:213:ALA:N	2.15	0.62
1:C:67:PRO:HD3	1:C:87:TYR:OH	2.00	0.62
1:D:119:LYS:HE3	2:D:2031:HOH:O	1.99	0.61
1:C:72:PRO:HG2	1:C:75:ILE:CD1	2.09	0.61
1:B:2:SER:HB2	2:B:2003:HOH:O	2.01	0.60
1:C:145:ARG:HG2	1:C:190:GLU:HG2	1.82	0.59
1:B:174:LYS:HE3	2:B:2288:HOH:O	2.02	0.59
1:B:194:LYS:NZ	2:B:2313:HOH:O	2.36	0.58
1:A:62[B]:CRQ:HA31	1:A:62[B]:CRQ:N	2.19	0.57
1:B:41:LYS:HE3	2:B:2339:HOH:O	2.03	0.57
1:A:90:GLU:CD	2:A:2182:HOH:O	2.44	0.55
1:A:67:PRO:HD3	1:A:87:TYR:OH	2.06	0.55
1:B:93:MET:HE2	1:B:173:PHE:CE1	2.43	0.55
1:D:66:ILE:N	1:D:67:PRO:CD	2.70	0.54
1:A:62[B]:CRQ:HE2	1:A:195:LEU:HB2	1.91	0.53
1:A:178:LYS:HE3	2:A:2289:HOH:O	2.08	0.53
1:C:8:MET:CE	1:C:114:PHE:CZ	2.93	0.52
1:C:66:ILE:HG13	2:C:2147:HOH:O	2.09	0.51
1:B:62[A]:CRQ:HE2	1:B:195:LEU:CB	2.39	0.50
1:A:200:HIS:HD2	1:A:201:ASN:O	1.94	0.50
1:D:2:SER:HB3	2:D:2008:HOH:O	2.11	0.50
1:B:93:MET:CE	1:B:173:PHE:CE1	2.95	0.49
1:B:62[A]:CRQ:HG12	1:B:211:GLU:OE2	2.13	0.49
1:A:62[A]:CRQ:O2	1:A:62[A]:CRQ:HD2	2.13	0.49
1:A:174:LYS:HE3	2:A:2283:HOH:O	2.12	0.49
1:C:66:ILE:N	1:C:67:PRO:CD	2.76	0.48
1:B:194:LYS:HG3	2:B:2316:HOH:O	2.12	0.48
1:A:212:ILE:HD13	1:A:213:ALA:H	1.77	0.48
1:C:65:SER:C	1:C:67:PRO:HD2	2.34	0.48
1:C:8:MET:HG3	1:C:33:PRO:HG2	1.94	0.48
1:B:67:PRO:HD3	1:B:87:TYR:OH	2.13	0.48
1:C:55:ASP:HB3	1:C:161:LEU:HD21	1.97	0.47
1:B:110:GLN:NE2	2:B:2212:HOH:O	2.47	0.47
1:A:212:ILE:CD1	1:A:214:ILE:HG13	2.45	0.47
1:B:172:GLU:CD	1:B:174:LYS:HE2	2.36	0.46
1:C:200:HIS:HE1	2:C:2125:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:O	1:A:62[B]:CRQ:C2	2.63	0.46
1:C:4:ILE:HG23	1:C:8:MET:CE	2.36	0.46
1:A:110:GLN:O	1:A:110:GLN:HG3	2.16	0.46
1:C:62[B]:CRQ:HD2	1:C:62[B]:CRQ:O2	2.16	0.46
1:B:172:GLU:OE2	1:B:174:LYS:HE2	2.17	0.46
1:C:14:MET:HB2	1:C:118:VAL:HG13	1.97	0.46
1:D:10:TYR:OH	1:D:40:VAL:HB	2.16	0.45
1:B:217:HIS:HD2	2:B:2308:HOH:O	1.98	0.45
1:A:66:ILE:N	1:A:67:PRO:CD	2.79	0.45
1:D:62[B]:CRQ:HD2	1:D:62[B]:CRQ:O2	2.17	0.45
1:C:4:ILE:HD13	1:C:80:LYS:HG2	1.98	0.44
1:C:145:ARG:NE	1:C:190:GLU:OE1	2.48	0.44
1:B:62[B]:CRQ:O2	1:B:62[B]:CRQ:HD1	2.17	0.44
1:B:59:PRO:O	1:B:62[A]:CRQ:C2	2.65	0.44
1:C:217:HIS:HD2	2:C:2248:HOH:O	2.01	0.44
1:D:55:ASP:HB3	1:D:161:LEU:HD21	2.00	0.43
1:D:126:PRO:HA	1:D:127:PRO:HD3	1.94	0.43
1:C:66:ILE:HD13	1:C:193:ARG:NH1	2.33	0.43
1:D:93:MET:CE	1:D:173:PHE:CE1	3.01	0.43
1:B:41:LYS:HG2	1:B:208:GLU:HG2	2.01	0.43
1:B:103:VAL:HG22	1:B:120:ILE:HG13	2.01	0.42
1:B:59:PRO:O	1:B:62[B]:CRQ:C2	2.67	0.42
1:C:74:ASP:OD1	2:C:2129:HOH:O	2.22	0.42
1:A:62[B]:CRQ:OH	1:A:142:SER:OG	2.33	0.42
1:B:219:LEU:HD23	1:B:219:LEU:HA	1.87	0.42
1:C:9:THR:HA	1:C:30:LYS:HA	2.02	0.42
1:A:153:LEU:HD11	1:A:186:PRO:HG2	2.01	0.41
1:A:41:LYS:HG2	1:A:208:GLU:HG2	2.02	0.41
1:D:93:MET:HE3	1:D:173:PHE:CE1	2.56	0.41
1:B:78:TYR:CG	1:B:153:LEU:HD22	2.55	0.41
1:A:94:ASN:ND2	2:A:2185:HOH:O	2.53	0.41
1:D:62[A]:CRQ:OH	2:D:2146:HOH:O	2.22	0.41
1:C:110:GLN:NE2	2:C:2176:HOH:O	2.54	0.41
1:A:62[B]:CRQ:CA3	1:A:62[B]:CRQ:N	2.81	0.41
1:B:58:SER:OG	1:B:59:PRO:HD3	2.21	0.40
1:C:8:MET:HE2	1:C:114:PHE:CE2	2.57	0.40
1:D:200:HIS:HD2	1:D:201:ASN:O	2.04	0.40
1:B:38:GLN:HE22	1:B:65:SER:HB3	1.87	0.40
1:B:119:LYS:HE3	2:B:2016:HOH:O	2.20	0.40
1:C:36:GLY:O	1:C:212:ILE:HA	2.21	0.40
1:D:188:ARG:NH1	2:D:2286:HOH:O	2.54	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	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
1	B	214/240 (89%)	212 (99%)	2 (1%)	0	100	100
1	C	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
1	D	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
All	All	853/960 (89%)	842 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	187/207 (90%)	183 (98%)	4 (2%)	61	55
1	B	188/207 (91%)	183 (97%)	5 (3%)	52	43
1	C	187/207 (90%)	181 (97%)	6 (3%)	46	35
1	D	187/207 (90%)	181 (97%)	6 (3%)	46	35
All	All	749/828 (90%)	728 (97%)	21 (3%)	51	41

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	105	ASN
1	A	110	GLN
1	A	212	ILE
1	B	2	SER
1	B	105	ASN
1	B	110	GLN
1	B	153	LEU
1	B	188	ARG
1	C	8	MET
1	C	66	ILE
1	C	105	ASN
1	C	110	GLN
1	C	153	LEU
1	C	209	GLN
1	D	105	ASN
1	D	110	GLN
1	D	118	VAL
1	D	153	LEU
1	D	188	ARG
1	D	199	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	110	GLN
1	A	200	HIS
1	A	209	GLN
1	B	110	GLN
1	B	200	HIS
1	B	217	HIS
1	C	105	ASN
1	C	110	GLN
1	C	112	ASN
1	C	200	HIS
1	C	217	HIS
1	D	105	ASN
1	D	110	GLN
1	D	112	ASN
1	D	200	HIS
1	D	209	GLN

### 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	A	62[A]	1	24,25,26	3.43	5 (20%)	25,34,36	3.82	7 (28%)
1	CRQ	A	62[B]	1	24,25,26	3.47	6 (25%)	25,34,36	4.21	5 (20%)
1	CRQ	B	62[A]	1	24,25,26	3.54	6 (25%)	25,34,36	4.44	7 (28%)
1	CRQ	B	62[B]	1	24,25,26	3.73	6 (25%)	25,34,36	3.79	7 (28%)
1	CRQ	C	62[A]	1	24,25,26	3.72	6 (25%)	25,34,36	4.48	6 (24%)
1	CRQ	C	62[B]	1	24,25,26	3.44	6 (25%)	25,34,36	3.90	7 (28%)
1	CRQ	D	62[A]	1	24,25,26	3.53	6 (25%)	25,34,36	3.79	5 (20%)
1	CRQ	D	62[B]	1	24,25,26	3.66	5 (20%)	25,34,36	3.88	7 (28%)

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	A	62[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	A	62[B]	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	62[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	62[B]	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	62[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	62[B]	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	62[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	62[B]	1	-	0/10/32/33	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62[A]	CRQ	OH-CZ	-5.29	1.24	1.37
1	C	62[B]	CRQ	OH-CZ	-5.26	1.24	1.37
1	A	62[B]	CRQ	OH-CZ	-5.04	1.25	1.37
1	B	62[B]	CRQ	OH-CZ	-5.01	1.25	1.37
1	A	62[A]	CRQ	OH-CZ	-4.88	1.25	1.37
1	C	62[A]	CRQ	OH-CZ	-4.65	1.26	1.37
1	D	62[B]	CRQ	OH-CZ	-4.54	1.26	1.37
1	B	62[A]	CRQ	OH-CZ	-4.38	1.26	1.37
1	D	62[A]	CRQ	C2-N3	-3.33	1.32	1.39
1	A	62[B]	CRQ	C2-N3	-3.29	1.32	1.39
1	C	62[B]	CRQ	C2-N3	-3.26	1.32	1.39
1	C	62[A]	CRQ	C2-N3	-3.26	1.32	1.39
1	B	62[A]	CRQ	C2-N3	-3.11	1.33	1.39
1	B	62[A]	CRQ	CA2-C2	-3.08	1.45	1.48
1	A	62[A]	CRQ	C2-N3	-2.92	1.33	1.39
1	D	62[B]	CRQ	C2-N3	-2.91	1.33	1.39
1	A	62[B]	CRQ	CA2-C2	-2.91	1.45	1.48
1	D	62[A]	CRQ	CA2-C2	-2.77	1.45	1.48
1	B	62[B]	CRQ	C2-N3	-2.72	1.34	1.39
1	C	62[B]	CRQ	CA2-N2	-2.34	1.33	1.38
1	C	62[A]	CRQ	CA2-C2	-2.29	1.46	1.48
1	A	62[A]	CRQ	CA2-N2	-2.23	1.33	1.38
1	B	62[B]	CRQ	CA2-N2	-2.06	1.33	1.38
1	A	62[B]	CRQ	O2-C2	2.12	1.27	1.23
1	C	62[B]	CRQ	C1-N2	2.39	1.38	1.33
1	D	62[B]	CRQ	C1-N2	2.44	1.38	1.33
1	A	62[B]	CRQ	C1-N2	2.50	1.38	1.33
1	C	62[B]	CRQ	O2-C2	2.57	1.28	1.23
1	A	62[A]	CRQ	O2-C2	2.59	1.28	1.23
1	B	62[A]	CRQ	C1-N2	2.63	1.38	1.33
1	C	62[A]	CRQ	O2-C2	2.64	1.28	1.23
1	B	62[A]	CRQ	O2-C2	2.76	1.29	1.23
1	D	62[A]	CRQ	C1-N2	2.81	1.39	1.33
1	D	62[A]	CRQ	O2-C2	2.84	1.29	1.23
1	B	62[B]	CRQ	O2-C2	2.88	1.29	1.23
1	D	62[B]	CRQ	O2-C2	2.89	1.29	1.23
1	C	62[A]	CRQ	C1-N2	3.58	1.40	1.33
1	B	62[B]	CRQ	CA3-N3	4.38	1.54	1.47
1	C	62[B]	CRQ	CB2-CA2	14.82	1.48	1.35
1	A	62[B]	CRQ	CB2-CA2	14.97	1.48	1.35
1	A	62[A]	CRQ	CB2-CA2	15.03	1.48	1.35
1	D	62[A]	CRQ	CB2-CA2	15.20	1.48	1.35
1	B	62[A]	CRQ	CB2-CA2	15.56	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62[B]	CRQ	CB2-CA2	15.99	1.49	1.35
1	C	62[A]	CRQ	CB2-CA2	16.22	1.49	1.35
1	D	62[B]	CRQ	CB2-CA2	16.30	1.49	1.35

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62[A]	CRQ	O2-C2-CA2	-16.64	121.96	130.95
1	C	62[A]	CRQ	O2-C2-CA2	-15.43	122.61	130.95
1	A	62[B]	CRQ	O2-C2-CA2	-14.38	123.18	130.95
1	D	62[A]	CRQ	O2-C2-CA2	-12.62	124.13	130.95
1	C	62[B]	CRQ	O2-C2-CA2	-9.52	125.80	130.95
1	B	62[B]	CRQ	O2-C2-CA2	-9.22	125.97	130.95
1	A	62[A]	CRQ	O2-C2-CA2	-8.18	126.53	130.95
1	D	62[B]	CRQ	O2-C2-CA2	-7.45	126.92	130.95
1	B	62[B]	CRQ	CB2-CA2-N2	-6.11	117.75	128.67
1	A	62[A]	CRQ	CB2-CA2-N2	-5.80	118.30	128.67
1	C	62[B]	CRQ	CB2-CA2-N2	-5.15	119.46	128.67
1	D	62[B]	CRQ	CB2-CA2-N2	-5.10	119.55	128.67
1	D	62[B]	CRQ	C2-CA2-N2	-4.78	105.09	108.91
1	C	62[A]	CRQ	CB1-CA1-N	-4.59	116.50	124.94
1	A	62[B]	CRQ	CB1-CA1-N	-4.57	116.55	124.94
1	B	62[A]	CRQ	CB1-CA1-N	-4.50	116.67	124.94
1	C	62[A]	CRQ	C2-CA2-N2	-4.49	105.33	108.91
1	D	62[B]	CRQ	CB1-CA1-N	-4.23	117.17	124.94
1	D	62[A]	CRQ	CB1-CA1-N	-4.08	117.44	124.94
1	C	62[B]	CRQ	C2-CA2-N2	-3.91	105.79	108.91
1	B	62[B]	CRQ	C2-CA2-N2	-3.85	105.84	108.91
1	A	62[A]	CRQ	C2-CA2-N2	-3.81	105.87	108.91
1	A	62[A]	CRQ	CG2-CB2-CA2	-3.63	125.50	130.22
1	B	62[B]	CRQ	CB1-CA1-N	-3.58	118.35	124.94
1	A	62[A]	CRQ	CB1-CA1-N	-3.50	118.51	124.94
1	A	62[B]	CRQ	C2-CA2-N2	-3.46	106.15	108.91
1	B	62[A]	CRQ	C2-CA2-N2	-3.42	106.18	108.91
1	C	62[B]	CRQ	CB1-CA1-N	-3.37	118.75	124.94
1	C	62[B]	CRQ	CG2-CB2-CA2	-3.26	125.99	130.22
1	D	62[A]	CRQ	C2-CA2-N2	-2.86	106.63	108.91
1	C	62[A]	CRQ	N3-C1-N2	-2.31	110.64	113.26
1	B	62[B]	CRQ	CG2-CB2-CA2	-2.25	127.29	130.22
1	B	62[A]	CRQ	CE2-CD2-CG2	-2.22	118.52	121.29
1	D	62[A]	CRQ	CE2-CD2-CG2	-2.10	118.66	121.29
1	B	62[A]	CRQ	N3-C1-N2	-2.04	110.95	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62[A]	CRQ	CB2-CA2-C2	2.03	125.33	122.36
1	D	62[B]	CRQ	C-CA3-N3	2.05	117.49	113.00
1	B	62[A]	CRQ	CB2-CA2-C2	2.13	125.48	122.36
1	A	62[B]	CRQ	CB2-CA2-C2	2.49	126.00	122.36
1	C	62[B]	CRQ	CB2-CA2-C2	8.45	134.74	122.36
1	D	62[B]	CRQ	CB2-CA2-C2	8.88	135.36	122.36
1	A	62[A]	CRQ	CB2-CA2-C2	9.17	135.79	122.36
1	B	62[B]	CRQ	CB2-CA2-C2	9.59	136.41	122.36
1	B	62[B]	CRQ	CA2-C2-N3	10.05	108.44	103.40
1	A	62[A]	CRQ	CA2-C2-N3	11.23	109.03	103.40
1	C	62[B]	CRQ	CA2-C2-N3	11.94	109.38	103.40
1	D	62[A]	CRQ	CA2-C2-N3	12.38	109.61	103.40
1	B	62[A]	CRQ	CA2-C2-N3	12.51	109.67	103.40
1	D	62[B]	CRQ	CA2-C2-N3	12.65	109.74	103.40
1	A	62[B]	CRQ	CA2-C2-N3	13.45	110.14	103.40
1	C	62[A]	CRQ	CA2-C2-N3	14.18	110.51	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	62[A]	CRQ	1	0
1	A	62[B]	CRQ	5	0
1	B	62[A]	CRQ	4	0
1	B	62[B]	CRQ	2	0
1	C	62[B]	CRQ	1	0
1	D	62[A]	CRQ	1	0
1	D	62[B]	CRQ	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

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 [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, 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	215/240 (89%)	-0.44	1 (0%) 91 92	5, 10, 20, 33	0
1	B	216/240 (90%)	-0.36	2 (0%) 85 87	7, 14, 24, 34	0
1	C	215/240 (89%)	-0.17	2 (0%) 85 87	7, 17, 28, 34	0
1	D	215/240 (89%)	-0.26	3 (1%) 78 80	10, 17, 28, 35	0
All	All	861/960 (89%)	-0.31	8 (0%) 85 87	5, 14, 26, 35	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	ASP	5.1
1	A	2	SER	5.0
1	B	2	SER	3.7
1	D	165	GLY	3.0
1	D	166	GLY	2.6
1	B	202	ARG	2.4
1	C	73	GLU	2.3
1	D	164	GLU	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	CRQ	A	62[B]	24/25	0.96	0.12	-	6,8,10,11	24
1	CRQ	D	62[B]	24/25	0.96	0.11	-	7,11,13,14	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CRQ	D	62[A]	24/25	0.96	0.11	-	10,14,15,17	24
1	CRQ	C	62[A]	24/25	0.96	0.11	-	11,13,14,15	24
1	CRQ	B	62[A]	24/25	0.95	0.11	-	2,7,12,14	24
1	CRQ	A	62[A]	24/25	0.96	0.12	-	2,5,6,6	24
1	CRQ	C	62[B]	24/25	0.96	0.11	-	6,11,13,13	24
1	CRQ	B	62[B]	24/25	0.95	0.11	-	6,11,14,14	24

### 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.