



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:14 am GMT

PDB ID : 4QHS  
Title : Crystal structure of AAA+sigma 54 activator domain of the flagellar regulatory protein FlrC of *Vibrio cholerae* in nucleotide free state  
Authors : Dey, S.; Biswas, M.; Sen, U.; Dasgupta, J.  
Deposited on : 2014-05-29  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

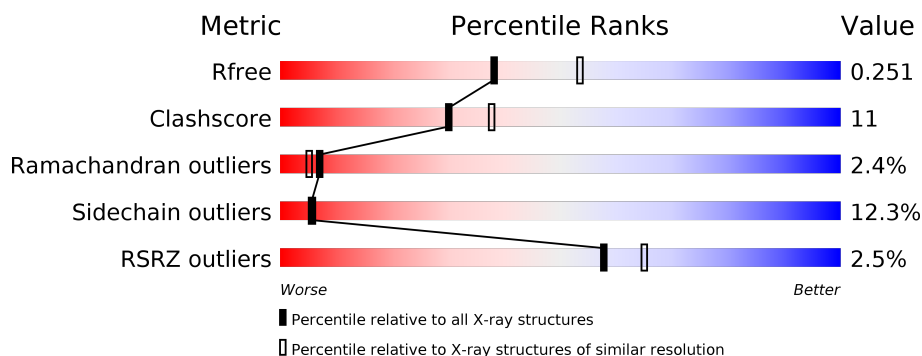
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	267	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	267	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>5%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	267	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	267	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>6%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	267	<div> <div>•</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	267	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	267	<div><div></div><div>2%</div><div>70%</div><div>16%</div><div>• • 9%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14054 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 Flagellar regulatory protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			
1	C	243	Total	C	N	O	S	0	1	0
			1901	1204	340	349	8			
1	B	243	Total	C	N	O	S	0	0	0
			1893	1199	337	349	8			
1	F	242	Total	C	N	O	S	0	0	0
			1888	1196	336	348	8			
1	G	243	Total	C	N	O	S	0	0	0
			1893	1199	337	349	8			
1	E	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			
1	D	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	121	SER	-	EXPRESSION TAG	UNP A5F6D4
A	122	SER	-	EXPRESSION TAG	UNP A5F6D4
A	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
A	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
A	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
A	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
A	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
A	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
A	129	SER	-	EXPRESSION TAG	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	131	MET	-	EXPRESSION TAG	UNP A5F6D4
C	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	121	SER	-	EXPRESSION TAG	UNP A5F6D4
C	122	SER	-	EXPRESSION TAG	UNP A5F6D4
C	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
C	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
C	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
C	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
C	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
C	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
C	129	SER	-	EXPRESSION TAG	UNP A5F6D4
C	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	131	MET	-	EXPRESSION TAG	UNP A5F6D4
B	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	121	SER	-	EXPRESSION TAG	UNP A5F6D4
B	122	SER	-	EXPRESSION TAG	UNP A5F6D4
B	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
B	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
B	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
B	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
B	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
B	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
B	129	SER	-	EXPRESSION TAG	UNP A5F6D4
B	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	131	MET	-	EXPRESSION TAG	UNP A5F6D4
F	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	120	HIS	-	EXPRESSION TAG	UNP A5F6D4

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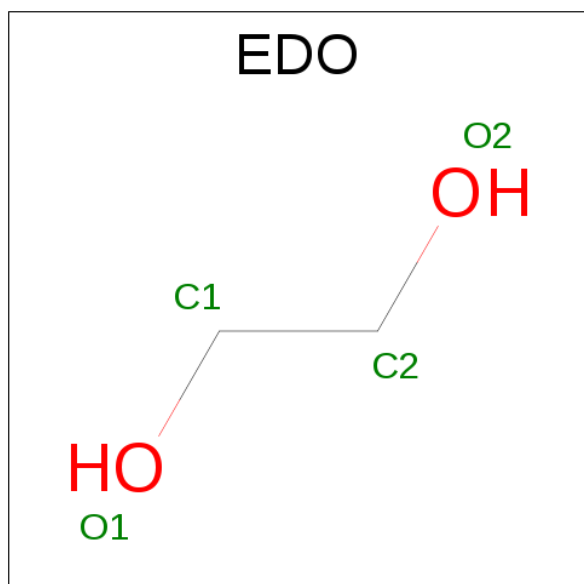
Chain	Residue	Modelled	Actual	Comment	Reference
F	121	SER	-	EXPRESSION TAG	UNP A5F6D4
F	122	SER	-	EXPRESSION TAG	UNP A5F6D4
F	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
F	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
F	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
F	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
F	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
F	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
F	129	SER	-	EXPRESSION TAG	UNP A5F6D4
F	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	131	MET	-	EXPRESSION TAG	UNP A5F6D4
G	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	121	SER	-	EXPRESSION TAG	UNP A5F6D4
G	122	SER	-	EXPRESSION TAG	UNP A5F6D4
G	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
G	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
G	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
G	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
G	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
G	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
G	129	SER	-	EXPRESSION TAG	UNP A5F6D4
G	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	131	MET	-	EXPRESSION TAG	UNP A5F6D4
E	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	121	SER	-	EXPRESSION TAG	UNP A5F6D4
E	122	SER	-	EXPRESSION TAG	UNP A5F6D4
E	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
E	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
E	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
E	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
E	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
E	128	GLY	-	EXPRESSION TAG	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	SER	-	EXPRESSION TAG	UNP A5F6D4
E	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	131	MET	-	EXPRESSION TAG	UNP A5F6D4
D	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	121	SER	-	EXPRESSION TAG	UNP A5F6D4
D	122	SER	-	EXPRESSION TAG	UNP A5F6D4
D	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
D	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
D	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
D	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
D	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
D	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
D	129	SER	-	EXPRESSION TAG	UNP A5F6D4
D	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	131	MET	-	EXPRESSION TAG	UNP A5F6D4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

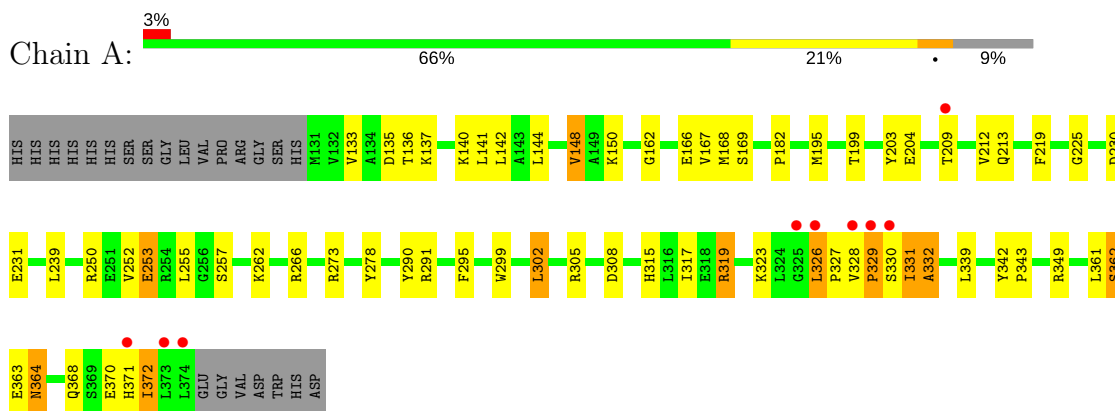
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	C	109	Total O 109 109	0	0
3	B	108	Total O 108 108	0	0
3	F	107	Total O 107 107	0	0
3	G	134	Total O 134 134	0	0
3	E	105	Total O 105 105	0	0
3	D	99	Total O 99 99	0	0



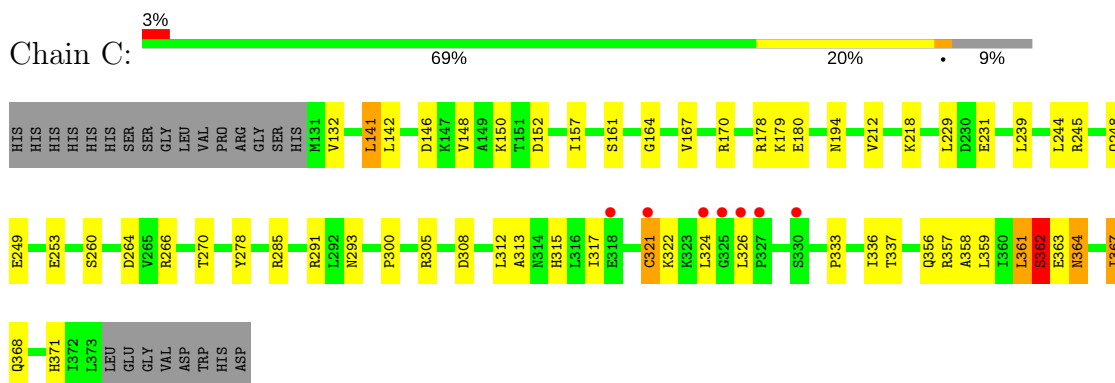
### 3 Residue-property plots [i](#)

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

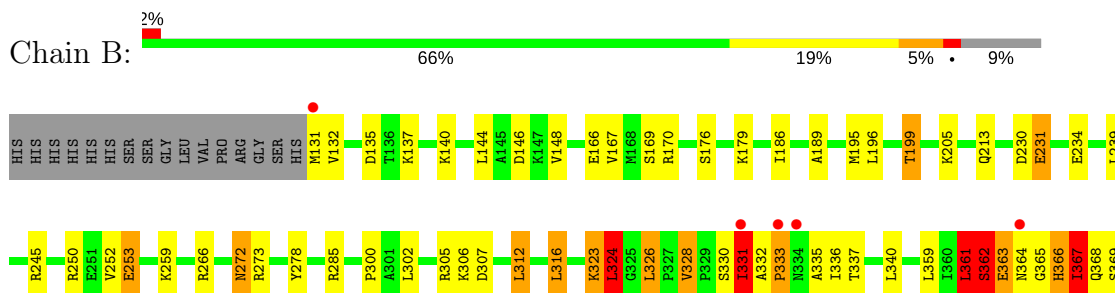
#### • Molecule 1: Flagellar regulatory protein C



#### • Molecule 1: Flagellar regulatory protein C



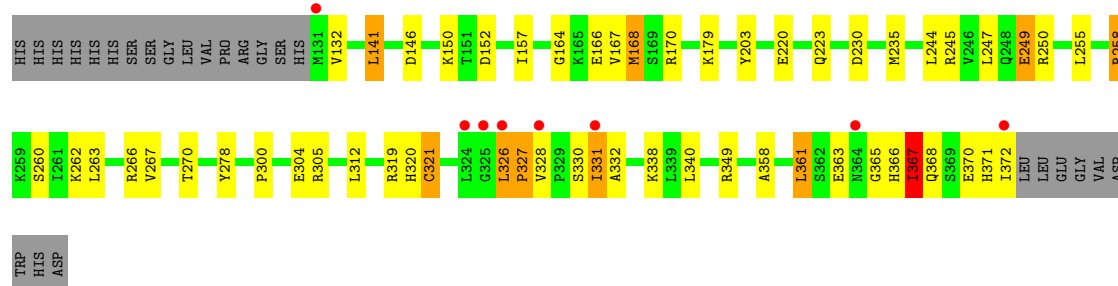
#### • Molecule 1: Flagellar regulatory protein C



E370  
H371  
L372  
L373  
LEU  
GLU  
GLY  
VAL  
ASP  
TRP  
HIS  
ASP

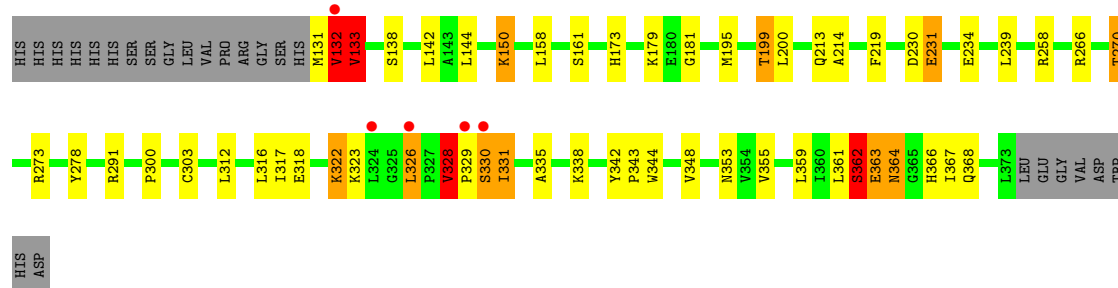
• Molecule 1: Flagellar regulatory protein C

Chain F: 3% 69% 18% 9%



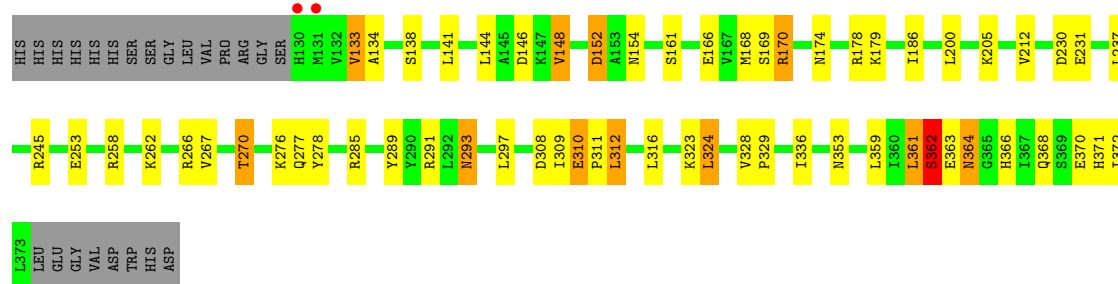
• Molecule 1: Flagellar regulatory protein C

Chain G: 2% 70% 16% 9%



• Molecule 1: Flagellar regulatory protein C

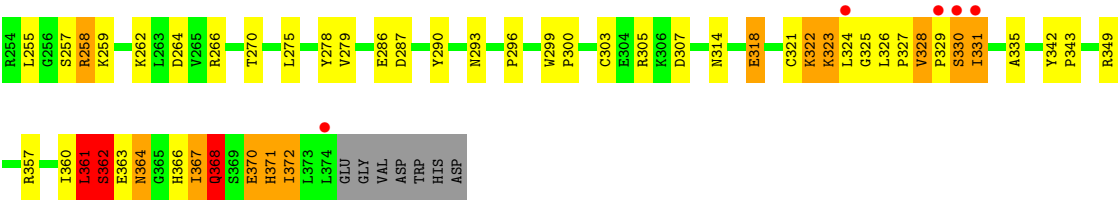
Chain E: % 69% 18% 9%



• Molecule 1: Flagellar regulatory protein C

Chain D: 2% 64% 19% 6% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.29Å 153.28Å 193.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.30 49.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.0 (49.39-2.30) 85.4 (49.39-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.192 , 0.255 0.195 , 0.251	Depositor DCC
$R_{free}$ test set	2003 reflections (2.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.94	1/1932 (0.1%)	0.64	0/2616
1	B	0.66	0/1927	0.62	1/2609 (0.0%)
1	C	0.45	0/1938	0.57	0/2623
1	D	0.61	1/1932 (0.1%)	0.62	0/2616
1	E	0.64	0/1932	0.61	0/2616
1	F	0.78	0/1922	0.59	0/2602
1	G	0.68	1/1927 (0.1%)	0.61	0/2609
All	All	0.69	3/13510 (0.0%)	0.61	1/18291 (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	B	0	2
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	TRP	CB-CG	-5.35	1.40	1.50
1	G	328	VAL	CB-CG1	-5.34	1.41	1.52
1	D	370	GLU	CG-CD	-5.01	1.44	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LEU	Peptide
1	B	362	SER	Peptide
1	C	361	LEU	Peptide
1	F	370	GLU	Peptide
1	G	361	LEU	Peptide

## 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	1898	0	1933	41	0
1	B	1893	0	1931	40	0
1	C	1901	0	1944	39	0
1	D	1898	0	1933	61	0
1	E	1898	0	1933	35	0
1	F	1888	0	1929	30	0
1	G	1893	0	1931	42	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	C	4	0	6	1	0
2	D	4	0	6	0	0
2	E	4	0	6	1	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
3	A	95	0	0	8	0
3	B	108	0	0	9	0
3	C	109	0	0	11	0
3	D	99	0	0	15	0
3	E	105	0	0	7	0
3	F	107	0	0	2	0
3	G	134	0	0	5	0
All	All	14054	0	13576	286	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 11.

The worst 5 of 286 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:273:ARG:NH1	3:A:567:HOH:O	1.77	1.17
1:D:364:ASN:ND2	3:D:501:HOH:O	1.81	1.11
1:D:286:GLU:O	3:D:567:HOH:O	1.76	1.03
1:D:371:HIS:O	1:D:372:ILE:HG23	1.60	0.99
1:F:167:VAL:HG22	1:F:168:MET:N	1.83	0.94

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	242/267 (91%)	222 (92%)	14 (6%)	6 (2%)	6	5
1	B	241/267 (90%)	220 (91%)	13 (5%)	8 (3%)	4	2
1	C	242/267 (91%)	226 (93%)	14 (6%)	2 (1%)	22	26
1	D	242/267 (91%)	223 (92%)	11 (4%)	8 (3%)	4	2
1	E	242/267 (91%)	228 (94%)	11 (4%)	3 (1%)	15	16
1	F	240/267 (90%)	219 (91%)	14 (6%)	7 (3%)	5	3
1	G	241/267 (90%)	219 (91%)	15 (6%)	7 (3%)	5	3
All	All	1690/1869 (90%)	1557 (92%)	92 (5%)	41 (2%)	7	5

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
1	A	330	SER

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Mol	Chain	Res	Type
1	A	362	SER
1	A	364	ASN
1	C	362	SER

### 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	204/227 (90%)	179 (88%)	25 (12%)	5	6
1	B	204/227 (90%)	171 (84%)	33 (16%)	3	2
1	C	205/227 (90%)	189 (92%)	16 (8%)	15	18
1	D	204/227 (90%)	180 (88%)	24 (12%)	6	6
1	E	204/227 (90%)	174 (85%)	30 (15%)	3	3
1	F	204/227 (90%)	179 (88%)	25 (12%)	5	6
1	G	204/227 (90%)	181 (89%)	23 (11%)	7	7
All	All	1429/1589 (90%)	1253 (88%)	176 (12%)	5	6

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	170	ARG
1	F	372	ILE
1	D	250	ARG
1	F	244	LEU
1	F	319	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	315	HIS
1	C	368	GLN
1	B	272	ASN
1	D	364	ASN

*Continued on next page...*



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Mol	Chain	Res	Type
1	D	368	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	A	401	-	3,3,3	0.61	0	2,2,2	0.12	0
2	EDO	B	401	-	3,3,3	0.53	0	2,2,2	0.05	0
2	EDO	C	401	-	3,3,3	0.60	0	2,2,2	0.18	0
2	EDO	D	401	-	3,3,3	0.55	0	2,2,2	0.03	0
2	EDO	E	401	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	F	401	-	3,3,3	0.61	0	2,2,2	0.18	0
2	EDO	G	401	-	3,3,3	0.52	0	2,2,2	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	401	-	-	0/1/1/1	0/0/0/0
2	EDO	B	401	-	-	0/1/1/1	0/0/0/0
2	EDO	C	401	-	-	0/1/1/1	0/0/0/0
2	EDO	D	401	-	-	0/1/1/1	0/0/0/0
2	EDO	E	401	-	-	0/1/1/1	0/0/0/0
2	EDO	F	401	-	-	0/1/1/1	0/0/0/0
2	EDO	G	401	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EDO	1	0
2	C	401	EDO	1	0
2	E	401	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/267 (91%)	-0.14	9 (3%) 42 49	30, 52, 100, 136	0
1	B	243/267 (91%)	-0.16	5 (2%) 64 70	35, 52, 80, 114	0
1	C	243/267 (91%)	-0.06	7 (2%) 52 59	32, 52, 102, 136	0
1	D	244/267 (91%)	-0.15	6 (2%) 58 65	33, 51, 82, 123	0
1	E	244/267 (91%)	-0.27	2 (0%) 86 89	30, 48, 72, 110	0
1	F	242/267 (90%)	-0.13	8 (3%) 47 54	31, 52, 101, 136	0
1	G	243/267 (91%)	-0.13	5 (2%) 64 70	33, 49, 73, 111	0
All	All	1703/1869 (91%)	-0.15	42 (2%) 58 65	30, 51, 88, 136	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	8.0
1	D	330	SER	6.6
1	F	328	VAL	5.5
1	E	130	HIS	4.7
1	F	131	MET	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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
2	EDO	E	401	4/4	0.89	0.15	1.53	51,55,55,56	0
2	EDO	B	401	4/4	0.91	0.15	0.27	43,48,55,57	0
2	EDO	A	401	4/4	0.81	0.17	-	45,51,58,62	0
2	EDO	C	401	4/4	0.82	0.19	-	51,54,59,61	0
2	EDO	G	401	4/4	0.88	0.14	-	44,60,61,68	0
2	EDO	D	401	4/4	0.91	0.21	-	46,51,56,62	0
2	EDO	F	401	4/4	0.89	0.13	-	43,47,49,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.