



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:16 PM GMT

PDB ID : 4QRM  
Title : crystal structure of a binary complex of FliM-FliG middle domains from T.maritima  
Authors : Crane, B.R.; Sircar, R.  
Deposited on : 2014-07-01  
Resolution : 4.32 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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-20026982

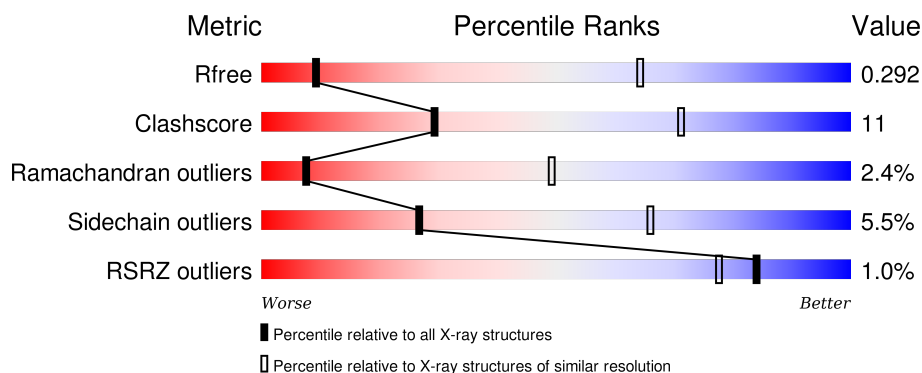
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.32 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.









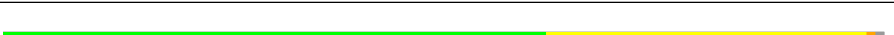
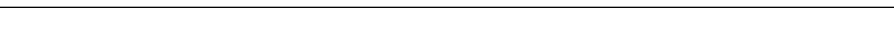
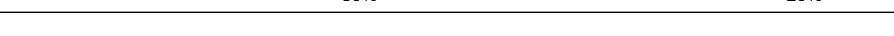
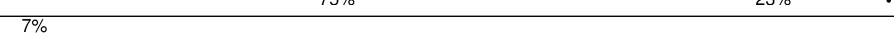
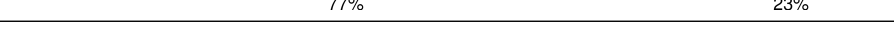






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1062 (5.04-3.60)
Clashscore	102246	1169 (5.04-3.60)
Ramachandran outliers	100387	1108 (5.04-3.60)
Sidechain outliers	100360	1091 (5.04-3.60)
RSRZ outliers	91569	1065 (5.04-3.60)

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	183	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>32%</div> <div>• •</div> </div> </div>
1	C	183	<div> <div></div> <div>67%</div> <div>31%</div> <div>• •</div> </div>
1	E	183	<div> <div></div> <div>64%</div> <div>32%</div> <div>•</div> </div>
1	G	183	<div> <div>2%</div> <div></div> <div>65%</div> <div>32%</div> <div>•</div> </div>
1	I	183	<div> <div>%</div> <div></div> <div>68%</div> <div>31%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	183	 74% 23% .
1	M	183	 69% 29% .
1	O	183	 71% 26% .
1	Q	183	 67% 32% ..
1	S	183	 67% 30% . .
1	U	183	 7% 64% 32% .
2	B	75	 61% 36% ..
2	D	75	 80% 20%
2	F	75	 75% 23% .
2	H	75	 7% 77% 23%
2	J	75	 81% 17% .
2	L	75	 69% 28% .
2	N	75	 81% 17% .
2	P	75	 71% 25% . .
2	R	75	 67% 32% .
2	T	75	 69% 27% .
2	V	75	 53% 41% 5%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22777 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 motor switch protein FliM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	C	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	E	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	G	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	I	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	K	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	M	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	O	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	Q	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	S	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	U	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			584	375	98	110	1			
2	D	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	F	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	J	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	L	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	N	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	P	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	R	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	T	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	V	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
B	114	SER	-	EXPRESSION TAG	UNP Q9WY63
B	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
B	116	MET	-	EXPRESSION TAG	UNP Q9WY63
D	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
D	114	SER	-	EXPRESSION TAG	UNP Q9WY63
D	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
D	116	MET	-	EXPRESSION TAG	UNP Q9WY63
F	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
F	114	SER	-	EXPRESSION TAG	UNP Q9WY63
F	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
F	116	MET	-	EXPRESSION TAG	UNP Q9WY63
H	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
H	114	SER	-	EXPRESSION TAG	UNP Q9WY63
H	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
H	116	MET	-	EXPRESSION TAG	UNP Q9WY63
J	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
J	114	SER	-	EXPRESSION TAG	UNP Q9WY63
J	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
J	116	MET	-	EXPRESSION TAG	UNP Q9WY63
L	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
L	114	SER	-	EXPRESSION TAG	UNP Q9WY63
L	115	HIS	-	EXPRESSION TAG	UNP Q9WY63

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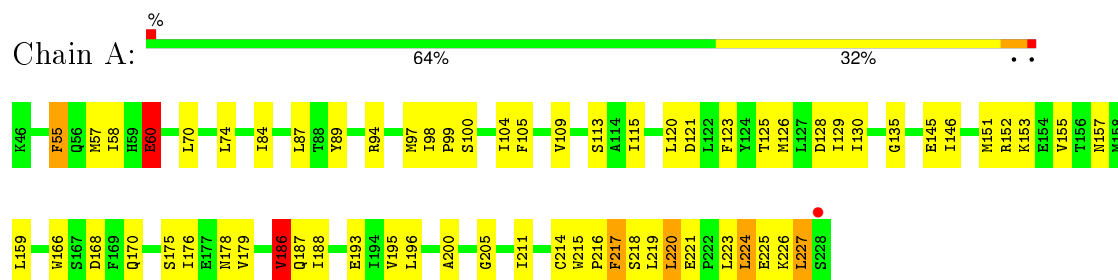
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Chain	Residue	Modelled	Actual	Comment	Reference
L	116	MET	-	EXPRESSION TAG	UNP Q9WY63
N	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
N	114	SER	-	EXPRESSION TAG	UNP Q9WY63
N	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
N	116	MET	-	EXPRESSION TAG	UNP Q9WY63
P	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
P	114	SER	-	EXPRESSION TAG	UNP Q9WY63
P	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
P	116	MET	-	EXPRESSION TAG	UNP Q9WY63
R	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
R	114	SER	-	EXPRESSION TAG	UNP Q9WY63
R	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
R	116	MET	-	EXPRESSION TAG	UNP Q9WY63
T	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
T	114	SER	-	EXPRESSION TAG	UNP Q9WY63
T	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
T	116	MET	-	EXPRESSION TAG	UNP Q9WY63
V	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
V	114	SER	-	EXPRESSION TAG	UNP Q9WY63
V	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
V	116	MET	-	EXPRESSION TAG	UNP Q9WY63

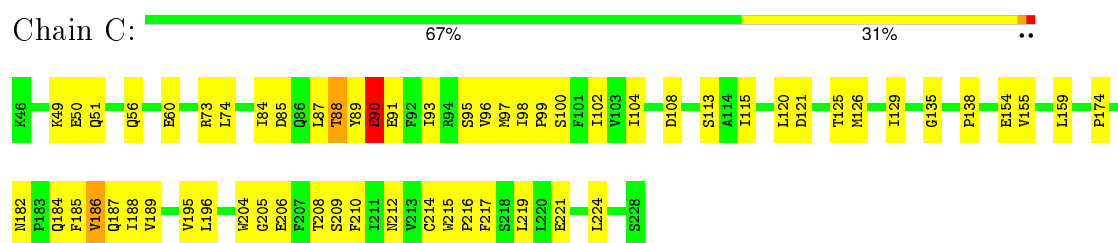
### 3 Residue-property plots

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

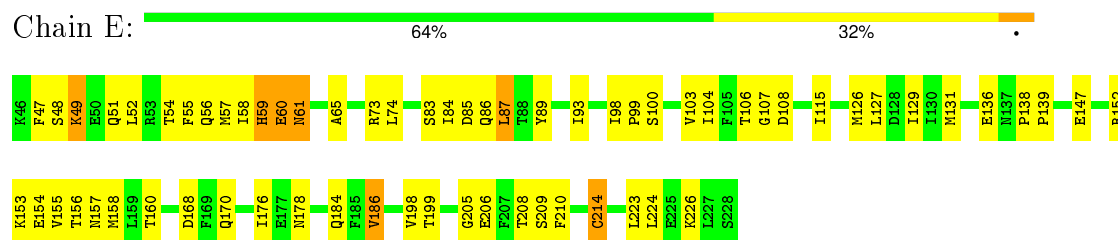
- Molecule 1: Flagellar motor switch protein FliM



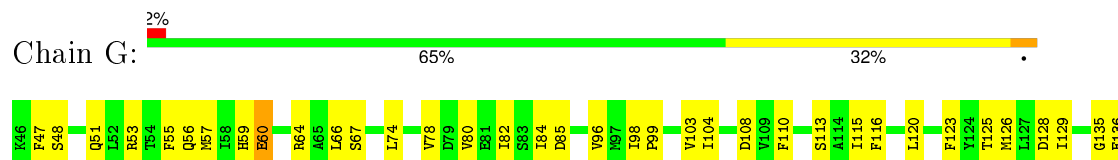
- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM

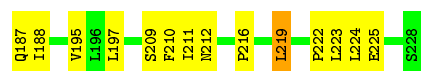




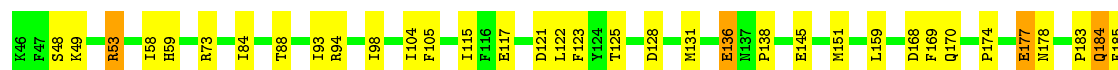
- Molecule 1: Flagellar motor switch protein FliM



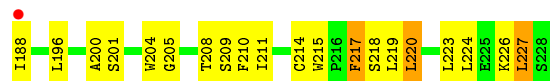
- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM

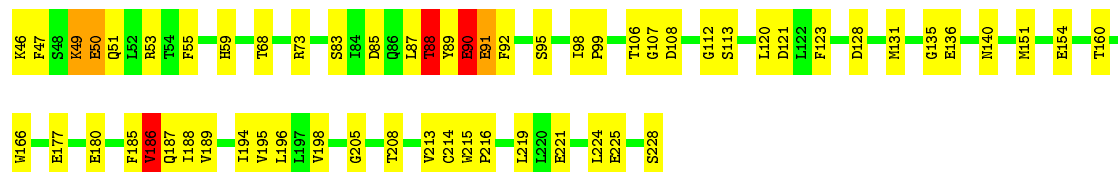






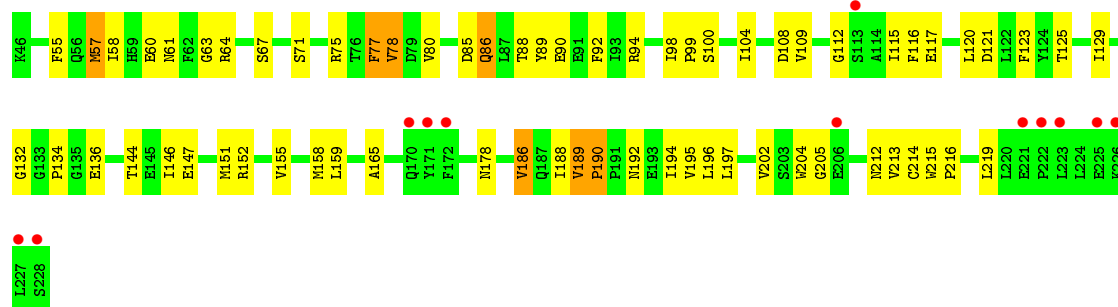
• Molecule 1: Flagellar motor switch protein FliM

Chain S: 67% 30%



• Molecule 1: Flagellar motor switch protein FliM

Chain U: 7% 64% 32%



• Molecule 2: Flagellar motor switch protein FliG

Chain B: 61% 36%



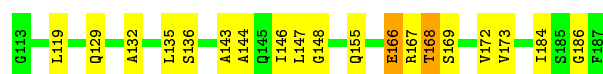
• Molecule 2: Flagellar motor switch protein FliG

Chain D: 80% 20%



• Molecule 2: Flagellar motor switch protein FliG

Chain F: 75% 23%

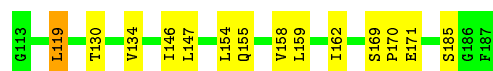
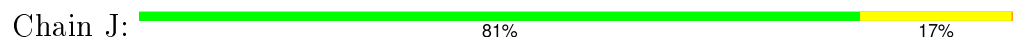


• Molecule 2: Flagellar motor switch protein FliG

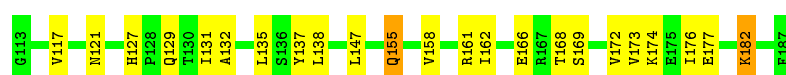
Chain H: 7% 77% 23%



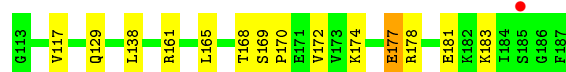
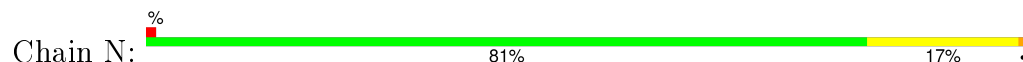
- Molecule 2: Flagellar motor switch protein FliG



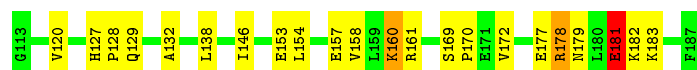
- Molecule 2: Flagellar motor switch protein FliG



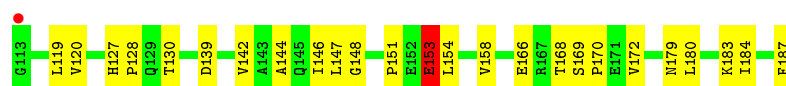
- Molecule 2: Flagellar motor switch protein FliG



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- Molecule 2: Flagellar motor switch protein FliG

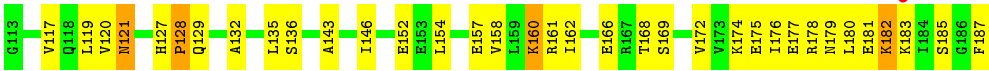


- Molecule 2: Flagellar motor switch protein FliG



- Molecule 2: Flagellar motor switch protein FliG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.40Å 216.25Å 262.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.18 – 4.32 49.98 – 4.31	Depositor EDS
% Data completeness (in resolution range)	89.7 (44.18-4.32) 88.5 (49.98-4.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.209 , 0.291 0.211 , 0.292	Depositor DCC
$R_{free}$ test set	1808 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.5	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 110.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 40680 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	22777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.04% 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 ⓘ

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	0.29	0/1521	0.50	0/2069
1	C	0.29	0/1521	0.46	0/2069
1	E	0.27	0/1521	0.46	0/2069
1	G	0.27	0/1521	0.46	0/2069
1	I	0.29	0/1521	0.44	0/2069
1	K	0.27	0/1521	0.47	0/2069
1	M	0.29	0/1521	0.47	0/2069
1	O	0.27	0/1521	0.44	0/2069
1	Q	0.27	0/1521	0.44	0/2069
1	S	0.30	0/1521	0.48	0/2069
1	U	0.27	0/1521	0.49	0/2069
2	B	0.43	0/593	0.53	0/805
2	D	0.26	0/597	0.46	0/810
2	F	0.26	0/597	0.45	0/810
2	H	0.25	0/597	0.49	0/810
2	J	0.26	0/597	0.48	0/810
2	L	0.27	0/597	0.48	0/810
2	N	0.26	0/597	0.44	0/810
2	P	0.26	0/597	0.54	0/810
2	R	0.28	0/597	0.44	0/810
2	T	0.29	0/597	0.52	0/810
2	V	0.25	0/597	0.51	0/810
All	All	0.28	0/23294	0.47	0/31664

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	E	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	GLU	Peptide
1	E	59	HIS	Peptide
1	G	176	ILE	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	1483	0	1471	47	0
1	C	1483	0	1471	40	0
1	E	1483	0	1471	38	0
1	G	1483	0	1471	32	0
1	I	1483	0	1471	28	0
1	K	1483	0	1471	28	0
1	M	1483	0	1471	32	0
1	O	1483	0	1471	32	0
1	Q	1483	0	1471	34	0
1	S	1483	0	1471	34	0
1	U	1483	0	1471	39	0
2	B	584	0	610	22	0
2	D	588	0	613	8	0
2	F	588	0	613	12	0
2	H	588	0	613	9	0
2	J	588	0	613	7	0
2	L	588	0	613	18	0
2	N	588	0	613	12	0
2	P	588	0	613	19	0
2	R	588	0	613	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	588	0	613	20	0
2	V	588	0	613	23	0
All	All	22777	0	22921	514	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 514 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:I:48:SER:HB3	1:I:51:GLN:HG2	1.49	0.95
1:E:170:GLN:HG3	1:E:223:LEU:HD11	1.61	0.83
1:A:221:GLU:HA	1:A:224:LEU:HB2	1.63	0.81
1:C:195:VAL:HG22	1:C:216:PRO:HA	1.66	0.78
1:Q:68:THR:HG21	1:S:68:THR:HG21	1.66	0.77

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	181/183 (99%)	164 (91%)	14 (8%)	3 (2%)	11	56
1	C	181/183 (99%)	165 (91%)	11 (6%)	5 (3%)	6	46
1	E	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	5	43
1	G	181/183 (99%)	159 (88%)	19 (10%)	3 (2%)	11	56
1	I	181/183 (99%)	170 (94%)	9 (5%)	2 (1%)	17	64
1	K	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	11	56
1	M	181/183 (99%)	163 (90%)	13 (7%)	5 (3%)	6	46
1	O	181/183 (99%)	157 (87%)	19 (10%)	5 (3%)	6	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	181/183 (99%)	166 (92%)	10 (6%)	5 (3%)	6	46
1	S	181/183 (99%)	161 (89%)	13 (7%)	7 (4%)	4	37
1	U	181/183 (99%)	158 (87%)	17 (9%)	6 (3%)	5	43
2	B	72/75 (96%)	67 (93%)	3 (4%)	2 (3%)	6	46
2	D	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	14	59
2	F	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	14	59
2	H	73/75 (97%)	62 (85%)	9 (12%)	2 (3%)	6	47
2	J	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	14	59
2	L	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
2	N	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	14	59
2	P	73/75 (97%)	62 (85%)	7 (10%)	4 (6%)	2	30
2	R	73/75 (97%)	65 (89%)	6 (8%)	2 (3%)	6	47
2	T	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	14	59
2	V	73/75 (97%)	63 (86%)	7 (10%)	3 (4%)	3	36
All	All	2793/2838 (98%)	2508 (90%)	217 (8%)	68 (2%)	7	49

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	C	90	GLU
2	D	181	GLU
1	E	60	GLU
1	G	177	GLU

### 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	170/170 (100%)	160 (94%)	10 (6%)	24	63
1	C	170/170 (100%)	162 (95%)	8 (5%)	32	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	170/170 (100%)	159 (94%)	11 (6%)	21	60
1	G	170/170 (100%)	159 (94%)	11 (6%)	21	60
1	I	170/170 (100%)	158 (93%)	12 (7%)	18	58
1	K	170/170 (100%)	161 (95%)	9 (5%)	28	67
1	M	170/170 (100%)	160 (94%)	10 (6%)	24	63
1	O	170/170 (100%)	162 (95%)	8 (5%)	32	69
1	Q	170/170 (100%)	161 (95%)	9 (5%)	28	67
1	S	170/170 (100%)	154 (91%)	16 (9%)	11	45
1	U	170/170 (100%)	159 (94%)	11 (6%)	21	60
2	B	67/67 (100%)	64 (96%)	3 (4%)	34	70
2	D	67/67 (100%)	67 (100%)	0	100	100
2	F	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	H	67/67 (100%)	64 (96%)	3 (4%)	34	70
2	J	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	L	67/67 (100%)	64 (96%)	3 (4%)	34	70
2	N	67/67 (100%)	66 (98%)	1 (2%)	72	89
2	P	67/67 (100%)	64 (96%)	3 (4%)	34	70
2	R	67/67 (100%)	63 (94%)	4 (6%)	24	63
2	T	67/67 (100%)	64 (96%)	3 (4%)	34	70
2	V	67/67 (100%)	63 (94%)	4 (6%)	24	63
All	All	2607/2607 (100%)	2464 (94%)	143 (6%)	27	66

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	94	ARG
1	M	184	GLN
1	U	146	ILE
1	K	115	ILE
2	L	173	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	86	GLN
1	I	157	ASN
2	L	155	GLN
1	E	51	GLN
2	P	115	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

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, 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	183/183 (100%)	-0.28	1 (0%) 91 88	110, 143, 184, 219	0
1	C	183/183 (100%)	-0.22	0 100 100	117, 155, 191, 233	0
1	E	183/183 (100%)	-0.06	0 100 100	118, 156, 184, 215	0
1	G	183/183 (100%)	-0.01	3 (1%) 74 65	132, 185, 220, 229	0
1	I	183/183 (100%)	-0.18	1 (0%) 91 88	106, 139, 180, 213	0
1	K	183/183 (100%)	-0.03	0 100 100	124, 173, 223, 250	0
1	M	183/183 (100%)	-0.24	1 (0%) 91 88	112, 143, 184, 207	0
1	O	183/183 (100%)	-0.17	1 (0%) 91 88	136, 180, 216, 228	0
1	Q	183/183 (100%)	-0.21	1 (0%) 91 88	115, 154, 194, 223	0
1	S	183/183 (100%)	-0.19	0 100 100	117, 151, 189, 209	0
1	U	183/183 (100%)	0.10	12 (6%) 22 15	147, 201, 239, 273	0
2	B	74/75 (98%)	-0.43	0 100 100	111, 142, 211, 268	0
2	D	75/75 (100%)	-0.37	0 100 100	124, 156, 218, 247	0
2	F	75/75 (100%)	-0.32	0 100 100	134, 166, 230, 246	0
2	H	75/75 (100%)	-0.06	5 (6%) 21 15	133, 171, 256, 290	0
2	J	75/75 (100%)	-0.33	0 100 100	120, 151, 225, 253	0
2	L	75/75 (100%)	0.00	0 100 100	120, 164, 259, 288	0
2	N	75/75 (100%)	-0.30	1 (1%) 79 71	122, 153, 220, 243	0
2	P	75/75 (100%)	-0.30	0 100 100	155, 189, 265, 304	0
2	R	75/75 (100%)	0.12	1 (1%) 79 71	154, 196, 251, 302	0
2	T	75/75 (100%)	-0.44	0 100 100	101, 148, 211, 261	0
2	V	75/75 (100%)	-0.16	1 (1%) 79 71	129, 168, 284, 349	0
All	All	2837/2838 (99%)	-0.16	28 (0%) 84 77	101, 163, 229, 349	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	113	GLY	3.8
1	G	225	GLU	3.5
1	I	228	SER	3.4
2	H	186	GLY	3.2
1	U	228	SER	3.2

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.