



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 21, 2017 – 01:38 PM EST

PDB ID : 6EMW
EMDB ID: : EMD-3897
Title : Structure of S.aureus ClpC in complex with MecA
Authors : Carroni, M.; Mogk, A.; Bukau, B.; Franke, K.
Deposited on : 2017-10-03
Resolution : 11.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

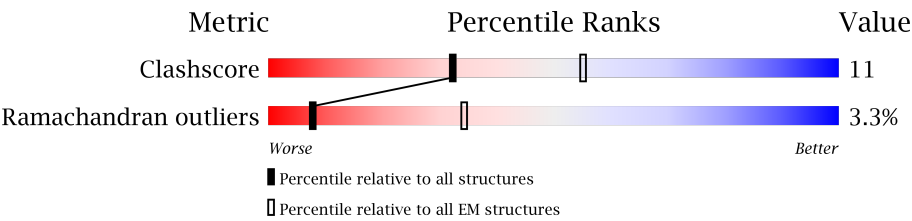
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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.




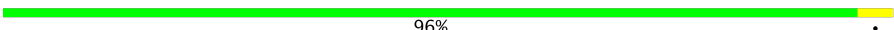
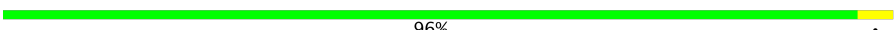
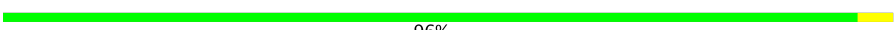
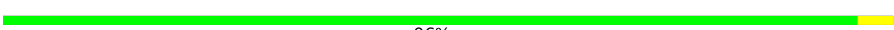





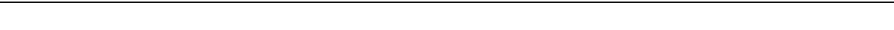

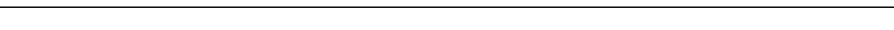
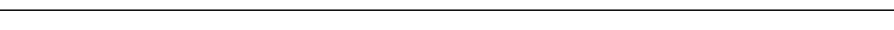











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	82	<div><div>93%7%</div></div>
1	G	82	<div><div>93%7%</div></div>
1	M	82	<div><div>94%6%</div></div>
1	S	82	<div><div>90%10%</div></div>
1	Y	82	<div><div>93%7%</div></div>
1	k	82	<div><div>96%. </div></div>
2	B	225	<div><div>85%7% • 7%</div></div>
2	H	225	<div><div>85%7% • 7%</div></div>
2	N	225	<div><div>84%8% • 7%</div></div>
2	T	225	<div><div>85%7% • 7%</div></div>
2	Z	225	<div><div>85%7% • 7%</div></div>

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Mol	Chain	Length	Quality of chain
2	l	225	 89% . . 7%
3	C	55	 96% .
3	I	55	 96% .
3	O	55	 96% .
3	U	55	 96% .
3	a	55	 96% .
3	m	55	 96% .
4	D	145	 59% . 38%
4	J	145	 59% . 38%
4	P	145	 59% . 38%
4	V	145	 59% . 38%
4	b	145	 61% . 38%
4	n	145	 59% . 38%
5	E	181	 86% 6% 8%
5	K	181	 86% 6% 8%
5	Q	181	 83% 8% 8%
5	W	181	 84% 8% 8%
5	c	181	 89% . 8%
5	o	181	 89% . 8%
6	F	157	 87% 8% . .
6	L	157	 87% 9% . .
6	R	157	 87% 8% . .
6	X	157	 88% 8% . .
6	d	157	 92% 5% .
6	p	157	 92% 5% .

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Mol	Chain	Length	Quality of chain
7	e	90	 100%
7	f	90	 100%
7	g	90	 100%
7	h	90	 100%
7	i	90	 100%
7	j	90	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15210 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms			AltConf	Trace
1	A	82	Total	C	N	0	0
			246	164	82		
1	G	82	Total	C	N	0	0
			246	164	82		
1	M	82	Total	C	N	0	0
			246	164	82		
1	S	82	Total	C	N	0	0
			246	164	82		
1	Y	82	Total	C	N	0	0
			246	164	82		
1	k	82	Total	C	N	0	0
			246	164	82		

- Molecule 2 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms			AltConf	Trace
2	B	210	Total	C	N	0	0
			630	420	210		
2	H	210	Total	C	N	0	0
			630	420	210		
2	N	210	Total	C	N	0	0
			630	420	210		
2	T	210	Total	C	N	0	0
			630	420	210		
2	Z	210	Total	C	N	0	0
			630	420	210		
2	l	210	Total	C	N	0	0
			630	420	210		

- Molecule 3 is a protein called Class III stress response-related ATPase, AAA+ superfamily.

Mol	Chain	Residues	Atoms			AltConf	Trace
3	C	55	Total	C	N	0	0
			165	110	55		

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	I	55	Total	C	N	0	0
			165	110	55		
3	O	55	Total	C	N	0	0
			165	110	55		
3	U	55	Total	C	N	0	0
			165	110	55		
3	a	55	Total	C	N	0	0
			165	110	55		
3	m	55	Total	C	N	0	0
			165	110	55		

- Molecule 4 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms			AltConf	Trace
4	D	90	Total	C	N	0	0
			270	180	90		
4	J	90	Total	C	N	0	0
			270	180	90		
4	P	90	Total	C	N	0	0
			270	180	90		
4	V	90	Total	C	N	0	0
			270	180	90		
4	b	90	Total	C	N	0	0
			270	180	90		
4	n	90	Total	C	N	0	0
			270	180	90		

- Molecule 5 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	E	166	Total	C	N	0	0
			498	332	166		
5	K	166	Total	C	N	0	0
			498	332	166		
5	Q	166	Total	C	N	0	0
			498	332	166		
5	W	166	Total	C	N	0	0
			498	332	166		
5	c	166	Total	C	N	0	0
			498	332	166		
5	o	166	Total	C	N	0	0
			498	332	166		

- Molecule 6 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	F	152	Total 456	C 304	N 152	0	0
6	L	152	Total 456	C 304	N 152	0	0
6	R	152	Total 456	C 304	N 152	0	0
6	X	152	Total 456	C 304	N 152	0	0
6	d	152	Total 456	C 304	N 152	0	0
6	p	152	Total 456	C 304	N 152	0	0

- Molecule 7 is a protein called Adapter protein MecA.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	e	90	Total 270	C 180	N 90	0	0
7	f	90	Total 270	C 180	N 90	0	0
7	g	90	Total 270	C 180	N 90	0	0
7	h	90	Total 270	C 180	N 90	0	0
7	i	90	Total 270	C 180	N 90	0	0
7	j	90	Total 270	C 180	N 90	0	0

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. 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. 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: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain A: 



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain G: 




- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain M: 



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain S: 



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain Y: 



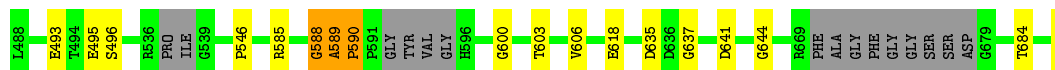
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain k: 



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain B: 85% 7% • 7%



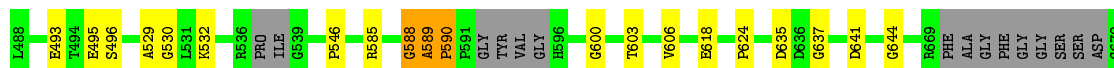
- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain H: 85% 7% • 7%



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain N: 84% 8% • 7%



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain T: 85% 7% • 7%



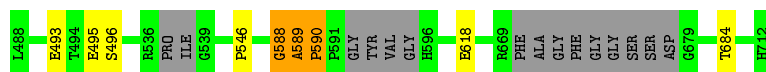
- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain Z: 85% 7% • 7%



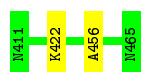
- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain I: 89% • • 7%



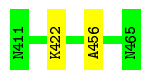
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain C: 96% •



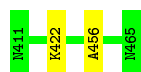
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain I: 96%



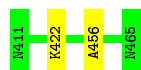
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain O: 96%



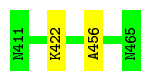
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain U: 96%



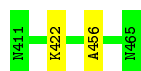
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain a: 96%



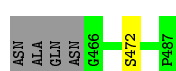
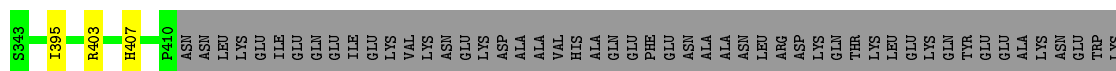
- Molecule 3: Class III stress response-related ATPase, AAA+ superfamily

Chain m: 96%



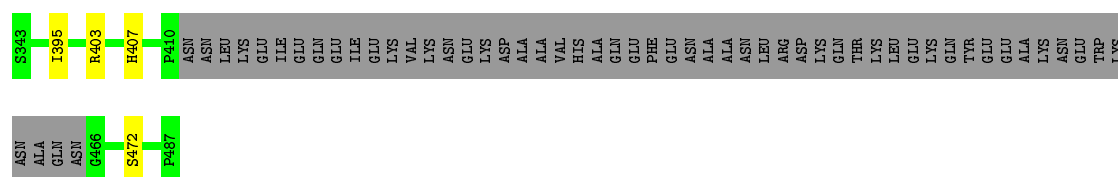
- Molecule 4: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain D: 59%



- Molecule 4: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain J: 59%



- Molecule 4: ATP-dependent Clp protease ATP-binding subunit ClpC



- Molecule 4: ATP-dependent Clp protease ATP-binding subunit ClpC

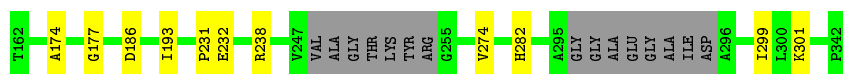


- Molecule 4: ATP-dependent Clp protease ATP-binding subunit ClpC



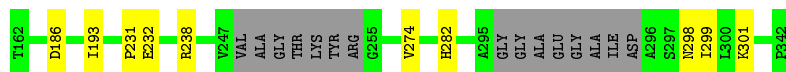
- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC





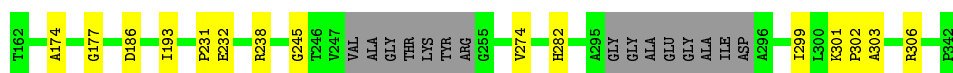
- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain K: 86% 6% 8%



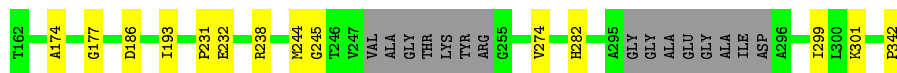
- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain Q: 83% 8% 8%



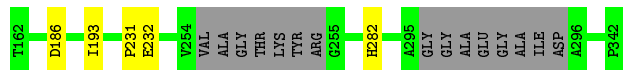
- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain W: 84% 8% 8%



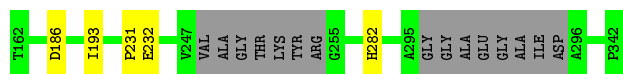
- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain c: 89% 8% 8%



- Molecule 5: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain o: 89% 8% 8%



- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain F: 87% 8% 8%




- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain L: 87% 9% 8%



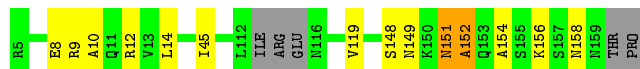
- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain R:  87% 8% ..



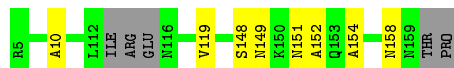
- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain X:  88% 8% ..



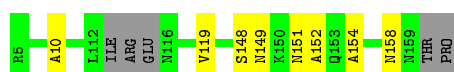
- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain d:  92% 5% .



- Molecule 6: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain p:  92% 5% .



- Molecule 7: Adapter protein MecA

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Adapter protein MecA

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Adapter protein MecA

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Adapter protein MecA

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Adapter protein MecA

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Adapter protein MecA

Chain j:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	A	0.45	0/244	0.67	0/242
1	G	0.45	0/244	0.67	0/242
1	M	0.45	0/244	0.67	0/242
1	S	0.45	0/244	0.67	0/242
1	Y	0.45	0/244	0.67	0/242
1	k	0.45	0/244	0.67	0/242
2	B	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
2	H	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
2	N	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
2	T	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
2	Z	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
2	l	0.63	1/626 (0.2%)	0.81	3/622 (0.5%)
3	C	0.22	0/162	0.49	0/159
3	I	0.22	0/162	0.49	0/159
3	O	0.22	0/162	0.49	0/159
3	U	0.22	0/162	0.49	0/159
3	a	0.22	0/162	0.49	0/159
3	m	0.22	0/162	0.49	0/159
4	D	0.46	0/268	0.73	0/266
4	J	0.46	0/268	0.73	0/266
4	P	0.46	0/268	0.73	0/266
4	V	0.46	0/268	0.73	0/266
4	b	0.46	0/268	0.73	0/266
4	n	0.46	0/268	0.73	0/266
5	E	0.46	0/494	0.74	0/490
5	K	0.46	0/494	0.74	0/490
5	Q	0.46	0/494	0.74	0/490
5	W	0.46	0/494	0.74	0/490
5	c	0.46	0/494	0.74	0/490
5	o	0.46	0/494	0.74	0/490
6	F	0.29	0/452	0.73	0/448
6	L	0.28	0/452	0.73	0/448
6	R	0.28	0/452	0.73	0/448
6	X	0.29	0/452	0.73	0/448

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
6	d	0.28	0/452	0.73	0/448
6	p	0.28	0/452	0.73	0/448
7	e	0.38	0/269	0.87	0/268
7	f	0.38	0/269	0.88	0/268
7	g	0.38	0/269	0.87	0/268
7	h	0.39	0/269	0.87	0/268
7	i	0.39	0/269	0.87	0/268
7	j	0.39	0/269	0.87	0/268
All	All	0.47	6/15090 (0.0%)	0.75	18/14970 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	1	0
2	B	0	1
2	H	0	1
2	N	1	1
2	T	1	1
2	Z	0	1
2	l	0	1
4	n	0	1
5	E	0	2
5	K	0	2
5	Q	0	2
5	W	0	2
5	c	0	2
5	o	0	2
6	F	2	0
6	R	3	0
6	X	1	0
6	p	2	0
7	e	2	0
7	h	1	0
7	j	1	0
All	All	15	19

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	590	PRO	CA-C	-10.01	1.32	1.52
2	I	590	PRO	CA-C	-10.00	1.32	1.52
2	T	590	PRO	CA-C	-9.98	1.32	1.52
2	Z	590	PRO	CA-C	-9.97	1.32	1.52
2	H	590	PRO	CA-C	-9.97	1.32	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	589	ALA	N-CA-C	-8.39	88.34	111.00
2	H	589	ALA	N-CA-C	-8.39	88.36	111.00
2	Z	589	ALA	N-CA-C	-8.38	88.38	111.00
2	N	589	ALA	N-CA-C	-8.38	88.39	111.00
2	T	589	ALA	N-CA-C	-8.37	88.39	111.00

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	122	ARG	CA
6	F	123	VAL	CA
2	N	531	LEU	CA
6	R	81	THR	CA,CA
6	R	83	ARG	CA

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	618	GLU	Peptide
5	E	231	PRO	Peptide
5	E	282	HIS	Peptide
2	H	618	GLU	Peptide
5	K	231	PRO	Peptide

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	246	0	86	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	246	0	86	4	0
1	M	246	0	86	1	0
1	S	246	0	85	6	0
1	Y	246	0	86	6	0
1	k	246	0	86	0	0
2	B	630	0	227	8	0
2	H	630	0	227	7	0
2	N	630	0	227	10	0
2	T	630	0	227	5	0
2	Z	630	0	227	9	0
2	l	630	0	227	0	0
3	C	165	0	52	0	0
3	I	165	0	52	0	0
3	O	165	0	52	0	0
3	U	165	0	52	0	0
3	a	165	0	52	0	0
3	m	165	0	52	0	0
4	D	270	0	93	2	0
4	J	270	0	93	2	0
4	P	270	0	93	2	0
4	V	270	0	93	5	0
4	b	270	0	93	0	0
4	n	270	0	93	0	0
5	E	498	0	179	4	0
5	K	498	0	179	5	0
5	Q	498	0	179	19	0
5	W	498	0	179	20	0
5	c	498	0	179	0	0
5	o	498	0	179	0	0
6	F	456	0	164	12	0
6	L	456	0	164	12	0
6	R	456	0	165	6	0
6	X	456	0	164	6	0
6	d	456	0	165	0	0
6	p	456	0	161	0	0
7	e	270	0	95	0	0
7	f	270	0	99	0	0
7	g	270	0	97	0	0
7	h	270	0	99	0	0
7	i	270	0	99	0	0
7	j	270	0	97	0	0
All	All	15210	0	5390	114	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 114 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)
5:Q:302:PRO:C	5:W:245:GLY:HA2	1.12	1.49
5:Q:302:PRO:C	5:W:245:GLY:CA	1.87	1.42
4:V:343:SER:N	5:W:342:PRO:C	1.71	1.40
5:Q:303:ALA:N	5:W:245:GLY:CA	1.87	1.38
2:N:624:PRO:CA	2:T:575:SER:CA	2.04	1.33

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 PDB entries followed by that with respect to all EM entries.

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	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
1	G	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
1	M	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
1	S	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
1	Y	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
1	k	78/82 (95%)	55 (70%)	20 (26%)	3 (4%)	4	32
2	B	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31
2	H	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31
2	N	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31
2	T	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31
2	Z	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31
2	l	202/225 (90%)	162 (80%)	32 (16%)	8 (4%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
3	I	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
3	O	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
3	U	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
3	a	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
3	m	50/55 (91%)	45 (90%)	3 (6%)	2 (4%)	3	31
4	D	86/145 (59%)	68 (79%)	16 (19%)	2 (2%)	7	43
4	J	86/145 (59%)	68 (79%)	16 (19%)	2 (2%)	7	43
4	P	86/145 (59%)	68 (79%)	15 (17%)	3 (4%)	4	34
4	V	86/145 (59%)	68 (79%)	16 (19%)	2 (2%)	7	43
4	b	86/145 (59%)	68 (79%)	16 (19%)	2 (2%)	7	43
4	n	86/145 (59%)	68 (79%)	15 (17%)	3 (4%)	4	34
5	E	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
5	K	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
5	Q	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
5	W	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
5	c	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
5	o	158/181 (87%)	131 (83%)	24 (15%)	3 (2%)	9	47
6	F	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
6	L	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
6	R	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
6	X	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
6	d	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
6	p	144/157 (92%)	116 (81%)	20 (14%)	8 (6%)	2	25
7	e	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
7	f	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
7	g	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
7	h	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
7	i	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
7	j	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
All	All	4836/5610 (86%)	3942 (82%)	736 (15%)	158 (3%)	8	35

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	493	GLU
2	B	495	GLU
2	B	589	ALA
2	B	590	PRO
6	F	10	ALA

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	X	2
6	p	2

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Mol	Chain	Number of breaks
6	R	2
3	I	2
3	a	2
3	U	2
6	L	2
3	m	2
6	d	2
3	C	2
3	O	2
6	F	2
5	K	1
5	c	1
5	W	1
5	o	1
1	S	1
1	k	1
5	E	1
1	A	1
1	M	1
1	G	1
5	Q	1
1	Y	1

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	464:GLN	C	465:ASN	N	12.34
1	I	464:GLN	C	465:ASN	N	12.34
1	O	464:GLN	C	465:ASN	N	12.34
1	U	464:GLN	C	465:ASN	N	12.34
1	a	464:GLN	C	465:ASN	N	12.34