



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Dec 20, 2017 – 11:07 AM EST

PDB ID : 6EM9
EMDB ID: : EMD-3894
Title : S.aureus ClpC resting state, asymmetric map
Authors : Carroni, M.; Mogk, A.; Bukau, B.; Franke, K.
Deposited on : 2017-10-01
Resolution : 8.40 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation 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

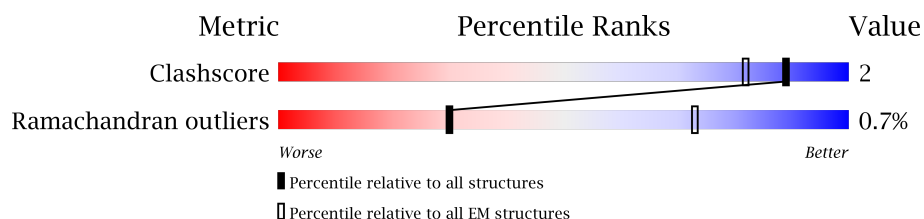
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 8.40 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	818	 89% . 9%
1	B	818	 89% . 9%
1	C	818	 72% . 26%
1	D	818	 51% . 47%
1	E	818	 79% . 19%
1	F	818	 89% . 9%
1	G	818	 89% . 9%
1	H	818	 72% . 26%
1	I	818	 51% . 47%
1	L	818	 80% . 19%

2 Entry composition

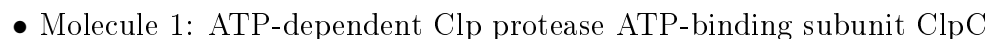
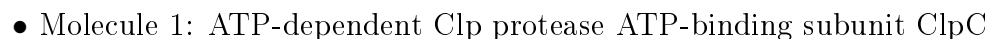
There is only 1 type of molecule in this entry. The entry contains 25512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

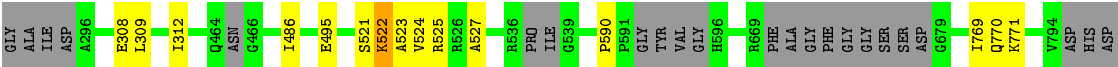
- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	B	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	C	602	Total	C	N	O	0	0
			2408	1204	602	602		
1	D	436	Total	C	N	O	0	0
			1744	872	436	436		
1	E	664	Total	C	N	O	0	0
			2656	1328	664	664		
1	F	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	G	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	I	436	Total	C	N	O	0	0
			1744	872	436	436		
1	H	602	Total	C	N	O	0	0
			2408	1204	602	602		
1	L	662	Total	C	N	O	0	0
			2648	1324	662	662		

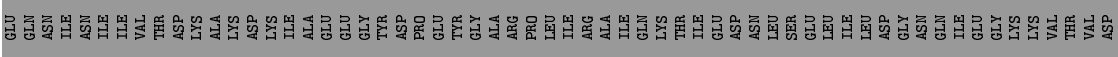
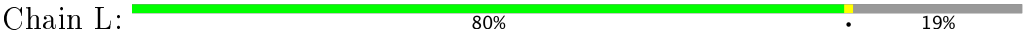
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC



- [illegible]



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



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40000	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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	0.54	0/2960	0.84	0/3672
1	B	0.57	0/2959	0.86	0/3669
1	C	0.56	0/2395	0.88	2/2971 (0.1%)
1	D	0.62	0/1734	0.94	5/2150 (0.2%)
1	E	0.51	0/2641	0.90	1/3275 (0.0%)
1	F	0.57	0/2960	0.95	3/3672 (0.1%)
1	G	0.55	0/2959	0.85	0/3669
1	H	0.54	0/2395	0.88	1/2971 (0.0%)
1	I	0.59	0/1734	0.90	2/2150 (0.1%)
1	L	0.51	0/2634	0.88	0/3268
All	All	0.55	0/25371	0.89	14/31467 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	ARG	N-CA-C	10.16	138.45	111.00
1	I	458	ASN	N-CA-C	6.53	128.63	111.00
1	H	312	ILE	C-N-CA	-6.22	109.24	122.30
1	C	526	ARG	N-CA-C	6.21	127.78	111.00
1	D	458	ASN	N-CA-C	6.07	127.38	111.00
1	D	402	VAL	N-CA-C	5.98	127.13	111.00
1	D	406	SER	N-CA-C	5.86	126.81	111.00
1	F	732	ASN	N-CA-C	5.75	126.53	111.00
1	D	460	TRP	N-CA-C	5.34	125.42	111.00
1	F	495	GLU	N-CA-C	5.34	125.42	111.00
1	D	403	ARG	N-CA-C	5.33	125.38	111.00
1	F	733	ARG	N-CA-C	5.31	125.34	111.00
1	E	130	ASN	N-CA-C	5.10	124.77	111.00
1	I	460	TRP	N-CA-C	5.10	124.76	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2976	0	790	5	0
1	B	2976	0	789	5	0
1	C	2408	0	638	12	0
1	D	1744	0	458	17	0
1	E	2656	0	703	5	0
1	F	2976	0	790	5	0
1	G	2976	0	789	5	0
1	H	2408	0	638	11	0
1	I	1744	0	458	10	0
1	L	2648	0	704	5	0
All	All	25512	0	6757	69	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 2.

All (69) 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:523:ALA:CA	1:D:776:ASN:CA	1.96	1.43
1:C:523:ALA:CA	1:D:776:ASN:C	2.04	1.24
1:C:523:ALA:CA	1:D:776:ASN:O	1.95	1.14
1:C:523:ALA:C	1:D:776:ASN:C	2.13	1.07
1:C:523:ALA:O	1:D:776:ASN:C	2.00	1.00
1:H:523:ALA:CA	1:H:527:ALA:H	1.76	0.98
1:H:523:ALA:O	1:H:527:ALA:N	1.95	0.97
1:C:523:ALA:C	1:D:776:ASN:CA	2.38	0.92
1:H:523:ALA:C	1:H:527:ALA:H	1.77	0.86
1:C:523:ALA:O	1:D:777:LEU:N	2.12	0.81
1:C:523:ALA:O	1:D:777:LEU:CA	2.41	0.69
1:H:521:SER:O	1:H:522:LYS:O	2.14	0.66
1:I:405:LYS:H	1:I:460:TRP:H	1.46	0.64
1:C:224:ALA:O	1:C:226:VAL:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ARG:N	1:D:459:GLU:O	2.36	0.59
1:H:523:ALA:CA	1:H:527:ALA:N	2.57	0.59
1:F:381:TYR:O	1:F:494:THR:N	2.36	0.59
1:I:403:ARG:N	1:I:459:GLU:O	2.39	0.55
1:I:711:PHE:O	1:I:712:HIS:C	2.44	0.55
1:D:405:LYS:N	1:D:459:GLU:H	2.05	0.54
1:D:405:LYS:H	1:D:460:TRP:H	1.56	0.53
1:I:404:LEU:O	1:I:458:ASN:N	2.40	0.53
1:H:521:SER:O	1:H:522:LYS:C	2.48	0.52
1:E:44:GLY:O	1:E:45:ILE:C	2.48	0.52
1:E:532:LYS:N	1:F:729:LYS:O	2.43	0.51
1:C:523:ALA:O	1:D:776:ASN:O	2.29	0.51
1:E:81:THR:O	1:E:83:ARG:N	2.45	0.50
1:E:587:VAL:N	1:F:571:ARG:O	2.45	0.49
1:L:68:ILE:O	1:L:69:GLY:C	2.49	0.49
1:I:404:LEU:O	1:I:457:LYS:N	2.45	0.49
1:L:532:LYS:O	1:L:533:ASP:C	2.51	0.49
1:G:340:ASP:O	1:G:341:GLU:C	2.51	0.48
1:I:405:LYS:N	1:I:459:GLU:H	2.11	0.48
1:B:17:ALA:O	1:B:21:ALA:N	2.48	0.47
1:G:44:GLY:O	1:G:45:ILE:C	2.53	0.47
1:I:404:LEU:C	1:I:459:GLU:H	2.19	0.47
1:A:141:ALA:O	1:A:142:LEU:C	2.52	0.46
1:G:735:SER:O	1:G:736:GLU:C	2.53	0.46
1:D:711:PHE:O	1:D:712:HIS:C	2.54	0.46
1:F:532:LYS:O	1:F:533:ASP:C	2.53	0.46
1:D:404:LEU:H	1:D:459:GLU:C	2.18	0.46
1:I:404:LEU:H	1:I:459:GLU:C	2.19	0.46
1:A:486:ILE:O	1:A:489:THR:N	2.49	0.45
1:L:627:PHE:O	1:L:631:LEU:N	2.50	0.45
1:L:584:SER:O	1:L:601:GLN:N	2.50	0.44
1:H:769:ILE:O	1:H:771:LYS:N	2.50	0.44
1:B:436:PHE:O	1:B:437:GLU:C	2.55	0.44
1:E:574:MET:O	1:E:578:MET:N	2.50	0.44
1:C:532:LYS:O	1:C:533:ASP:C	2.55	0.44
1:D:404:LEU:C	1:D:459:GLU:H	2.20	0.44
1:C:535:LYS:O	1:C:536:ARG:O	2.36	0.43
1:H:523:ALA:C	1:H:525:ARG:N	2.69	0.43
1:F:81:THR:O	1:F:83:ARG:N	2.51	0.43
1:B:735:SER:O	1:B:736:GLU:C	2.57	0.43
1:A:532:LYS:O	1:A:533:ASP:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:VAL:N	1:D:459:GLU:O	2.52	0.43
1:G:463:THR:O	1:G:464:GLN:C	2.57	0.43
1:A:17:ALA:O	1:A:21:ALA:N	2.51	0.42
1:G:436:PHE:O	1:G:439:ALA:N	2.52	0.42
1:H:523:ALA:C	1:H:525:ARG:H	2.23	0.42
1:H:308:GLU:O	1:H:309:LEU:C	2.57	0.42
1:B:80:TYR:O	1:B:81:THR:C	2.58	0.42
1:I:623:HIS:O	1:I:624:PRO:C	2.59	0.41
1:D:581:HIS:O	1:D:585:ARG:N	2.54	0.41
1:B:112:LEU:O	1:B:118:GLY:N	2.53	0.41
1:I:402:VAL:N	1:I:459:GLU:O	2.53	0.41
1:A:43:GLU:O	1:A:44:GLY:C	2.59	0.41
1:L:614:ILE:O	1:L:655:ILE:N	2.50	0.41
1:H:769:ILE:O	1:H:770:GLN:C	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	712/818 (87%)	672 (94%)	36 (5%)	4 (1%)	28	71
1	B	710/818 (87%)	661 (93%)	47 (7%)	2 (0%)	44	81
1	C	576/818 (70%)	548 (95%)	22 (4%)	6 (1%)	18	61
1	D	416/818 (51%)	393 (94%)	19 (5%)	4 (1%)	18	61
1	E	634/818 (78%)	601 (95%)	26 (4%)	7 (1%)	17	60
1	F	712/818 (87%)	660 (93%)	48 (7%)	4 (1%)	28	71
1	G	710/818 (87%)	684 (96%)	24 (3%)	2 (0%)	44	81
1	H	576/818 (70%)	546 (95%)	24 (4%)	6 (1%)	18	61
1	I	416/818 (51%)	391 (94%)	21 (5%)	4 (1%)	18	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	634/818 (78%)	605 (95%)	28 (4%)	1 (0%)	51 84
All	All	6096/8180 (74%)	5761 (94%)	295 (5%)	40 (1%)	30 68

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	ILE
1	C	495	GLU
1	D	590	PRO
1	E	324	ILE
1	E	589	ALA
1	E	590	PRO
1	G	590	PRO
1	I	590	PRO
1	H	522	LYS
1	H	590	PRO
1	L	590	PRO
1	A	590	PRO
1	B	590	PRO
1	C	224	ALA
1	D	625	ASP
1	F	303	ALA
1	I	625	ASP
1	H	495	GLU
1	C	590	PRO
1	E	82	PRO
1	G	546	PRO
1	I	546	PRO
1	A	156	LYS
1	A	486	ILE
1	D	546	PRO
1	F	211	GLY
1	H	232	GLU
1	B	486	ILE
1	C	525	ARG
1	D	486	ILE
1	E	54	ASN
1	F	486	ILE
1	I	406	SER
1	H	486	ILE
1	A	141	ALA
1	E	232	GLU

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Mol	Chain	Res	Type
1	H	524	VAL
1	C	486	ILE
1	E	212	VAL
1	F	82	PRO

5.3.2 Protein sidechains [i](#)

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	7
1	B	7
1	H	6

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Mol	Chain	Number of breaks
1	C	6
1	A	6
1	F	6
1	D	5
1	E	5
1	I	5
1	L	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	487:PRO	C	488:LEU	N	22.78
1	I	487:PRO	C	488:LEU	N	21.40
1	I	410:PRO	C	411:ASN	N	21.31
1	D	410:PRO	C	411:ASN	N	19.73
1	F	712:HIS	C	713:LYS	N	19.70
1	L	487:PRO	C	488:LEU	N	17.16
1	F	487:PRO	C	488:LEU	N	16.20
1	L	410:PRO	C	411:ASN	N	15.13
1	C	410:PRO	C	411:ASN	N	15.01
1	H	410:PRO	C	411:ASN	N	14.95
1	E	410:PRO	C	411:ASN	N	14.12
1	E	342:PRO	C	343:SER	N	13.10
1	E	487:PRO	C	488:LEU	N	12.43
1	I	712:HIS	C	713:LYS	N	12.16
1	D	736:GLU	C	737:GLN	N	10.99
1	F	410:PRO	C	411:ASN	N	10.73
1	B	410:PRO	C	411:ASN	N	10.48
1	D	712:HIS	C	713:LYS	N	10.43
1	G	410:PRO	C	411:ASN	N	10.24
1	F	45:ILE	C	46:ALA	N	9.52
1	L	437:GLU	C	438:ASN	N	8.91
1	A	437:GLU	C	438:ASN	N	7.87
1	B	487:PRO	C	488:LEU	N	7.71
1	H	712:HIS	C	713:LYS	N	7.15
1	F	437:GLU	C	438:ASN	N	6.93
1	A	410:PRO	C	411:ASN	N	6.82
1	D	437:GLU	C	438:ASN	N	6.55
1	A	487:PRO	C	488:LEU	N	6.39
1	C	712:HIS	C	713:LYS	N	6.30
1	C	437:GLU	C	438:ASN	N	6.14
1	B	45:ILE	C	46:ALA	N	6.13
1	H	437:GLU	C	438:ASN	N	5.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	736:GLU	C	737:GLN	N	5.94
1	F	736:GLU	C	737:GLN	N	5.75
1	A	45:ILE	C	46:ALA	N	5.68
1	G	45:ILE	C	46:ALA	N	5.61
1	G	342:PRO	C	343:SER	N	5.56
1	I	437:GLU	C	438:ASN	N	5.51
1	G	712:HIS	C	713:LYS	N	4.94
1	E	45:ILE	C	46:ALA	N	4.85
1	B	437:GLU	C	438:ASN	N	4.80
1	B	342:PRO	C	343:SER	N	4.65
1	C	342:PRO	C	343:SER	N	4.38
1	A	736:GLU	C	737:GLN	N	4.22
1	E	437:GLU	C	438:ASN	N	4.07
1	G	736:GLU	C	737:GLN	N	4.07
1	B	736:GLU	C	737:GLN	N	4.06
1	H	342:PRO	C	343:SER	N	4.05
1	C	736:GLU	C	737:GLN	N	4.04
1	H	736:GLU	C	737:GLN	N	3.98
1	B	712:HIS	C	713:LYS	N	3.90
1	A	712:HIS	C	713:LYS	N	3.83
1	H	487:PRO	C	488:LEU	N	3.66
1	G	437:GLU	C	438:ASN	N	3.55
1	L	45:ILE	C	46:ALA	N	3.45
1	G	487:PRO	C	488:LEU	N	3.21
1	C	487:PRO	C	488:LEU	N	3.20