



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:58 PM BST

PDB ID : 3JA6
EMDB ID: : EMD-6319
Title : Cryo-electron Tomography and All-atom Molecular Dynamics Simulations Reveal a Novel Kinase Conformational Switch in Bacterial Chemotaxis Signaling
Authors : Cassidy, C.K.; Himes, B.A.; Alvarez, F.J.; Ma, J.; Zhao, G.; Perilla, J.R.; Schulten, K.; Zhang, P.
Deposited on : 2015-04-21
Resolution : 12.70 Å (reported)
Based on PDB ID : 1QU7

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

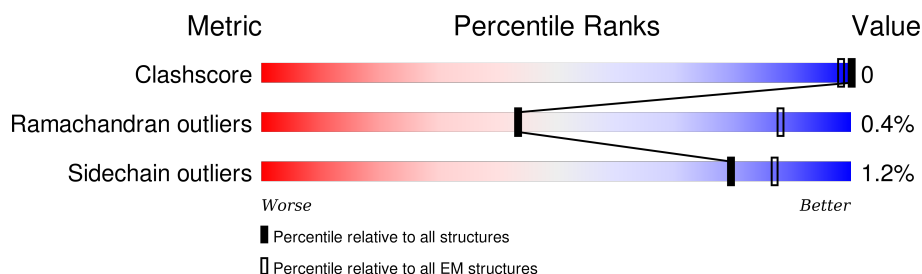
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.70 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.



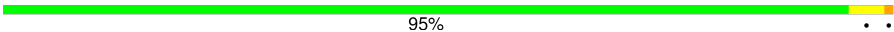
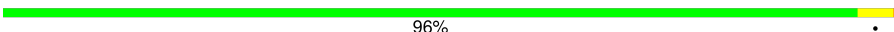
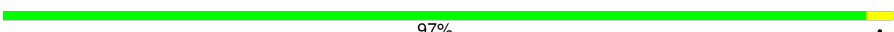
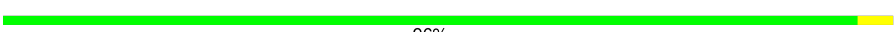




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	139	91% 6% .
1	B	139	94% . .
1	D	139	94% . .
1	F	139	94% . .
2	C	379	95% 5%
2	E	379	93% 6% .
3	G	309	96% . .
3	I	309	95% 5% .
3	K	309	95% 5%

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Mol	Chain	Length	Quality of chain
3	M	309	 95% . .
3	O	309	 96% . .
3	Q	309	 97% .
4	H	307	 95% .
4	J	307	 96% .
4	L	307	 96% .
4	N	307	 96% .
4	P	307	 95% . .
4	R	307	 96% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 77014 atoms, of which 38700 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 Chemotaxis protein CheW.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	B	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	D	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	F	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		

- Molecule 2 is a protein called Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	379	Total	C	H	N	O	S	0	0
			6110	1889	3131	513	567	10		
2	E	379	Total	C	H	N	O	S	0	0
			6110	1889	3131	513	567	10		

- Molecule 3 is a protein called Methyl-accepting chemotaxis protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	I	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	K	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	M	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	O	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	Q	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		

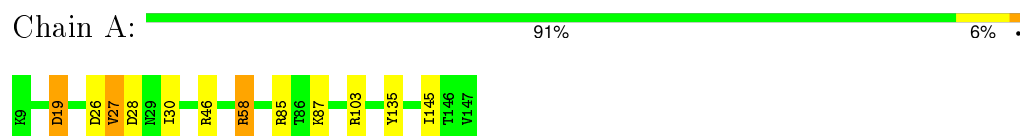
- Molecule 4 is a protein called Methyl-accepting chemotaxis protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	J	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	L	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	N	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	P	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	R	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0

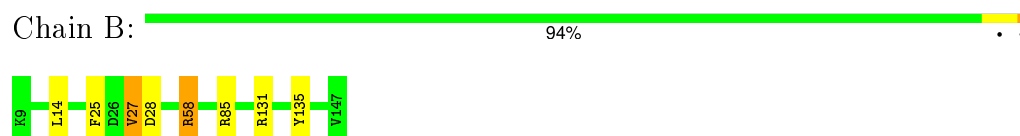
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

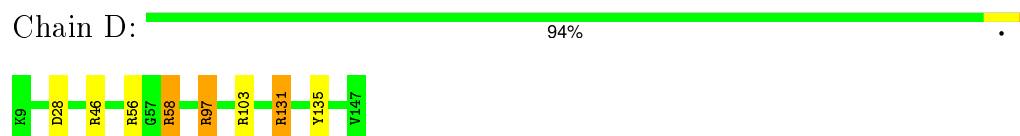
- Molecule 1: Chemotaxis protein CheW



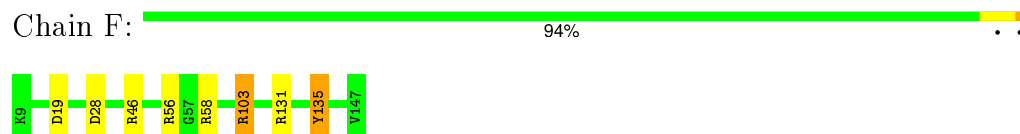
- Molecule 1: Chemotaxis protein CheW



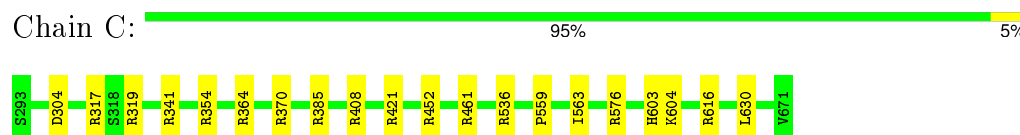
- Molecule 1: Chemotaxis protein CheW



- Molecule 1: Chemotaxis protein CheW



- Molecule 2: Chemotaxis protein CheA



- Molecule 2: Chemotaxis protein CheA





- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain G: 96% ..



- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain I: 95% 5% .



- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain K: 95% 5% .



- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain M: 95% . .



- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain O: 96% . .



- Molecule 3: Methyl-accepting chemotaxis protein 2

Chain Q: 97% .

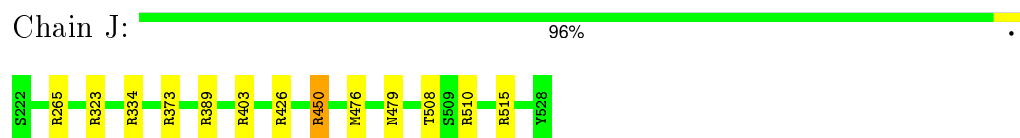


- Molecule 4: Methyl-accepting chemotaxis protein 2

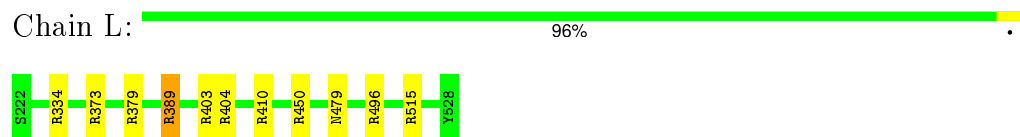
Chain H: 95% .



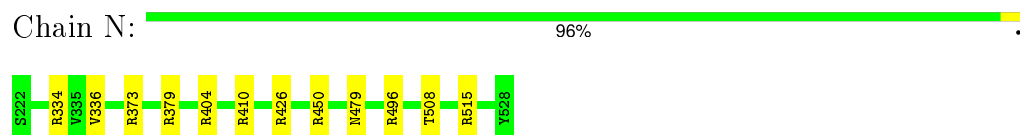
- Molecule 4: Methyl-accepting chemotaxis protein 2



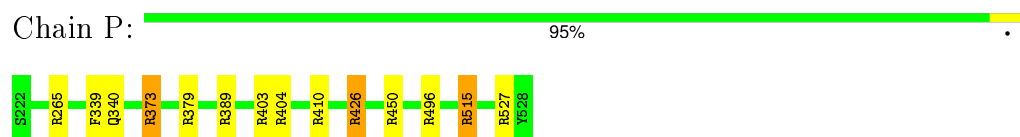
- Molecule 4: Methyl-accepting chemotaxis protein 2



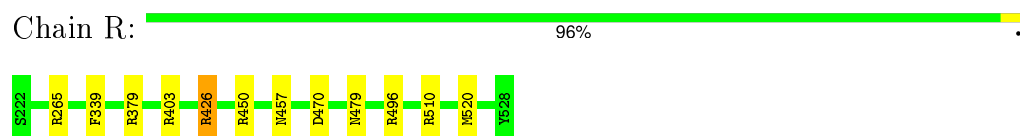
- Molecule 4: Methyl-accepting chemotaxis protein 2



- Molecule 4: Methyl-accepting chemotaxis protein 2



- Molecule 4: Methyl-accepting chemotaxis protein 2



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	4000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	TomoCTF (strip-based periodogram)	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	39000	Depositor
Image detector	GATAN UltraScan 4000 (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	0.67	0/1116	1.09	8/1501 (0.5%)
1	B	0.68	0/1116	1.05	7/1501 (0.5%)
1	D	0.67	0/1116	1.16	12/1501 (0.8%)
1	F	0.68	0/1116	1.08	6/1501 (0.4%)
2	C	0.66	0/3009	1.08	19/4051 (0.5%)
2	E	0.66	0/3009	1.09	24/4051 (0.6%)
3	G	0.67	0/2340	1.07	15/3153 (0.5%)
3	I	0.66	0/2340	1.05	13/3153 (0.4%)
3	K	0.66	0/2340	1.09	18/3153 (0.6%)
3	M	0.67	0/2340	1.06	16/3153 (0.5%)
3	O	0.67	0/2340	1.07	12/3153 (0.4%)
3	Q	0.68	0/2340	1.03	5/3153 (0.2%)
4	H	0.67	0/2328	1.09	15/3138 (0.5%)
4	J	0.66	0/2328	1.04	9/3138 (0.3%)
4	L	0.67	0/2328	1.03	10/3138 (0.3%)
4	N	0.67	0/2328	1.02	8/3138 (0.3%)
4	P	0.67	0/2328	1.04	14/3138 (0.4%)
4	R	0.66	0/2328	1.05	13/3138 (0.4%)
All	All	0.67	0/38490	1.06	224/51852 (0.4%)

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	B	0	1
1	D	0	2
1	F	0	2
2	C	0	1
2	E	0	4
3	G	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2
3	K	0	1
3	M	0	5
3	O	0	3
3	Q	0	2
4	H	0	2
4	J	0	1
4	L	0	3
4	N	0	1
4	P	0	2
All	All	0	35

There are no bond length outliers.

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	421	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	97	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	D	135	TYR	CB-CG-CD2	-8.52	115.89	121.00
4	R	403	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	D	103	ARG	NE-CZ-NH1	8.45	124.53	120.30

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ARG	Sidechain
1	B	58	ARG	Sidechain
2	C	319	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	97	ARG	Sidechain

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1105	1169	1166	0	0
1	B	1105	1169	1166	0	0
1	D	1105	1169	1166	0	0
1	F	1105	1169	1166	0	0
2	C	2979	3131	3128	2	0
2	E	2979	3131	3128	0	0
3	G	2334	2322	2319	0	0
3	I	2334	2322	2319	0	0
3	K	2334	2322	2319	0	0
3	M	2334	2322	2319	0	0
3	O	2334	2322	2319	0	0
3	Q	2334	2322	2319	0	0
4	H	2322	2305	2302	0	0
4	J	2322	2305	2302	0	0
4	L	2322	2305	2302	0	0
4	N	2322	2305	2302	0	0
4	P	2322	2305	2302	0	0
4	R	2322	2305	2302	0	0
All	All	38314	38700	38646	2	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 0.

All (2) 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)
2:C:603:HIS:CG	2:C:604:LYS:H	2.35	0.44
2:C:603:HIS:CG	2:C:604:LYS:N	2.89	0.41

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	137/139 (99%)	120 (88%)	13 (10%)	4 (3%)	6	43
1	B	137/139 (99%)	118 (86%)	17 (12%)	2 (2%)	13	57
1	D	137/139 (99%)	122 (89%)	14 (10%)	1 (1%)	26	71
1	F	137/139 (99%)	123 (90%)	13 (10%)	1 (1%)	26	71
2	C	377/379 (100%)	355 (94%)	19 (5%)	3 (1%)	24	69
2	E	377/379 (100%)	354 (94%)	19 (5%)	4 (1%)	17	63
3	G	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
3	I	307/309 (99%)	301 (98%)	4 (1%)	2 (1%)	26	71
3	K	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
3	M	307/309 (99%)	306 (100%)	1 (0%)	0	100	100
3	O	307/309 (99%)	301 (98%)	4 (1%)	2 (1%)	26	71
3	Q	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
4	H	305/307 (99%)	301 (99%)	4 (1%)	0	100	100
4	J	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	L	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	N	305/307 (99%)	301 (99%)	4 (1%)	0	100	100
4	P	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	R	305/307 (99%)	299 (98%)	6 (2%)	0	100	100
All	All	4974/5010 (99%)	4816 (97%)	139 (3%)	19 (0%)	43	80

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	28	ASP
1	B	27	VAL
1	B	28	ASP
2	C	563	ILE

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

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	127/127 (100%)	124 (98%)	3 (2%)	57	82
1	B	127/127 (100%)	125 (98%)	2 (2%)	70	88
1	D	127/127 (100%)	126 (99%)	1 (1%)	86	94
1	F	127/127 (100%)	125 (98%)	2 (2%)	70	88
2	C	337/337 (100%)	335 (99%)	2 (1%)	90	95
2	E	337/337 (100%)	332 (98%)	5 (2%)	72	88
3	G	253/253 (100%)	251 (99%)	2 (1%)	86	94
3	I	253/253 (100%)	250 (99%)	3 (1%)	78	90
3	K	253/253 (100%)	250 (99%)	3 (1%)	78	90
3	M	253/253 (100%)	251 (99%)	2 (1%)	86	94
3	O	253/253 (100%)	252 (100%)	1 (0%)	93	96
3	Q	253/253 (100%)	250 (99%)	3 (1%)	78	90
4	H	252/252 (100%)	249 (99%)	3 (1%)	78	90
4	J	252/252 (100%)	247 (98%)	5 (2%)	63	85
4	L	252/252 (100%)	251 (100%)	1 (0%)	93	96
4	N	252/252 (100%)	248 (98%)	4 (2%)	70	88
4	P	252/252 (100%)	249 (99%)	3 (1%)	78	90
4	R	252/252 (100%)	248 (98%)	4 (2%)	70	88
All	All	4212/4212 (100%)	4163 (99%)	49 (1%)	79	90

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	409	ILE
4	J	508	THR
4	R	426	ARG
4	J	426	ARG
3	K	224	MET

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

Mol	Chain	Res	Type
2	C	578	GLN

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Mol	Chain	Res	Type
2	E	409	ASN
2	E	413	HIS
3	M	223	HIS
4	P	465	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](#)

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.