



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 13, 2020 – 10:53 AM EST

PDB ID : 6S1K
EMDB ID: : EMD-10050
Title : E. coli Core Signaling Unit, carrying QQQQ receptor mutation
Authors : Cassidy, C.K.
Deposited on : 2019-06-18
Resolution : 8.38 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

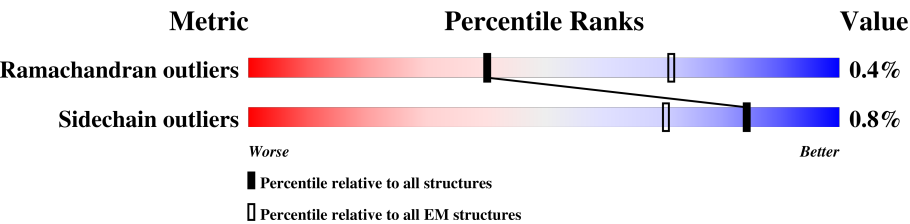
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

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 8.38 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)
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	654	<div><div>57%</div><div>41%</div></div>
1	B	654	<div><div>57%</div><div>41%</div></div>
2	C	167	<div><div>82%</div><div>5%</div><div>13%</div></div>
2	D	167	<div><div>83%</div><div>13%</div></div>
3	E	551	<div><div>19%</div><div>81%</div></div>
3	F	551	<div><div>18%</div><div>81%</div></div>
3	G	551	<div><div>18%</div><div>81%</div></div>
3	H	551	<div><div>18%</div><div>81%</div></div>
3	I	551	<div><div>18%</div><div>81%</div></div>
3	J	551	<div><div>18%</div><div>81%</div></div>
3	K	551	<div><div>19%</div><div>81%</div></div>

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Mol	Chain	Length	Quality of chain
3	L	551	<div><div></div><div>19%</div><div>81%</div></div>
3	M	551	<div><div></div><div>18%</div><div>81%</div></div>
3	N	551	<div><div></div><div>18%</div><div>81%</div></div>
3	O	551	<div><div></div><div>18%</div><div>81%</div></div>
3	P	551	<div><div></div><div>18%</div><div>81%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16884 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		
1	B	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		

- Molecule 2 is a protein called CheW.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		
2	D	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		

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

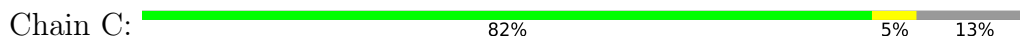
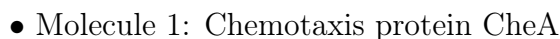
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	F	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	G	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	H	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	I	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	J	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	K	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	L	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	M	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	O	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	P	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

- Molecule 1: Chemotaxis protein CheA





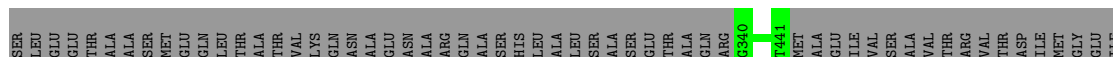
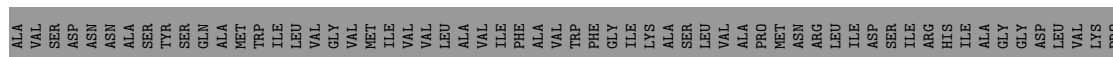
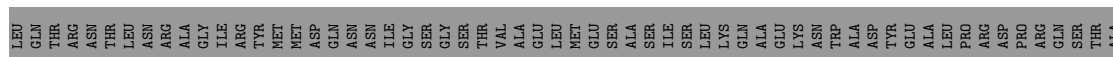
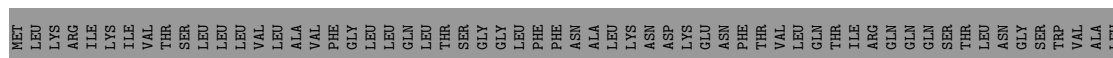
- Molecule 2: CheW

Chain D: 83% 13%



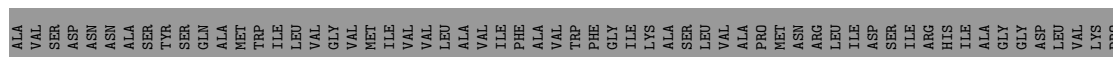
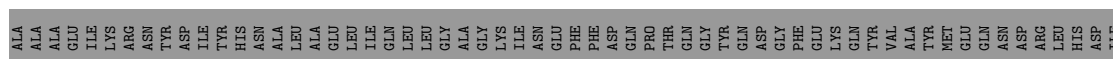
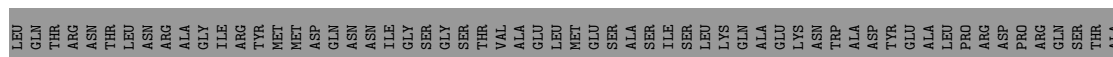
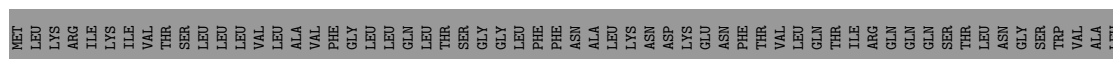
- Molecule 3: Methyl-accepting chemotaxis protein I

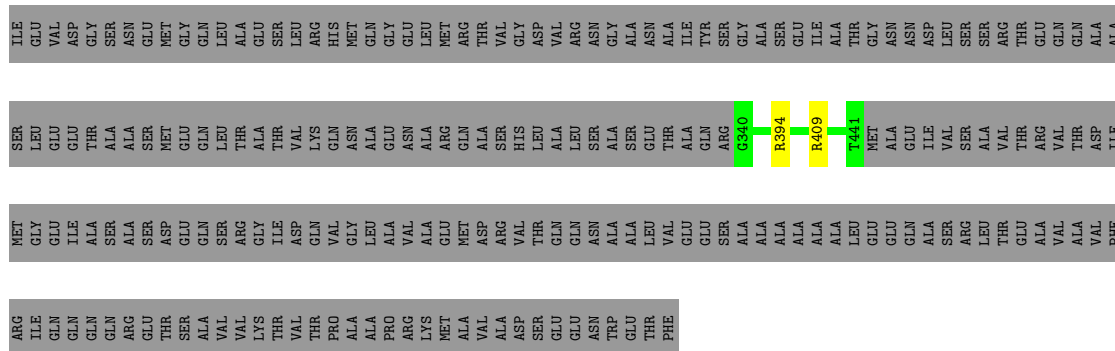
Chain E: 19% 81%



- Molecule 3: Methyl-accepting chemotaxis protein I

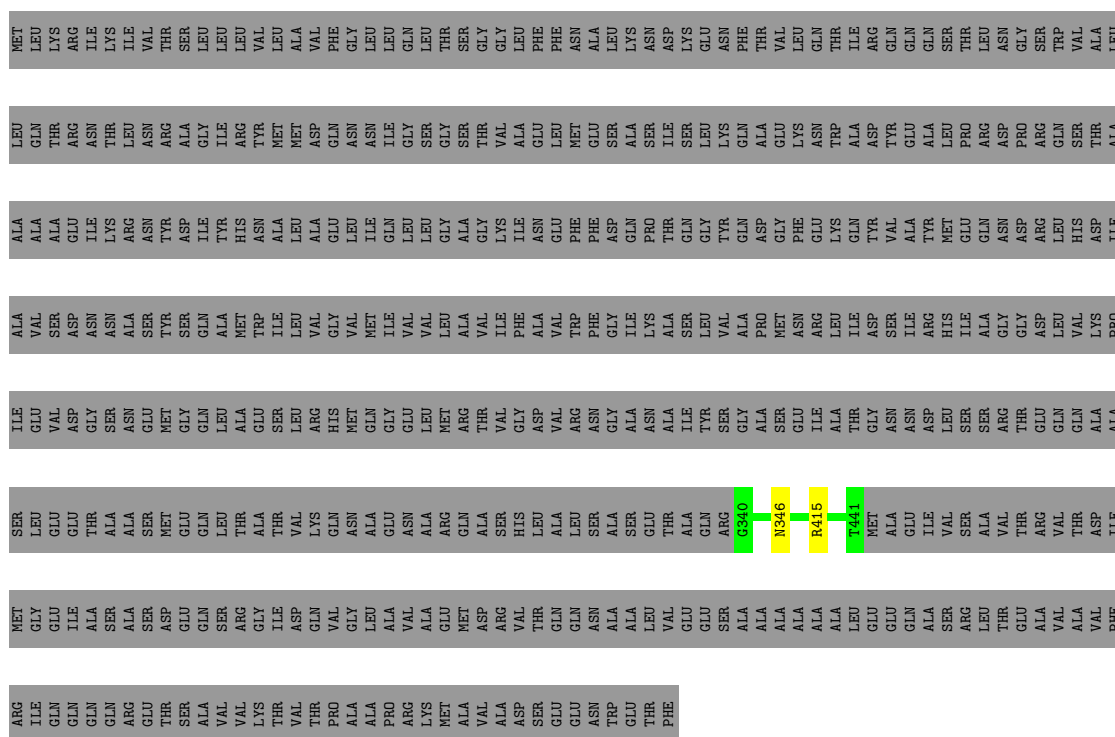
Chain F: 18% 81%





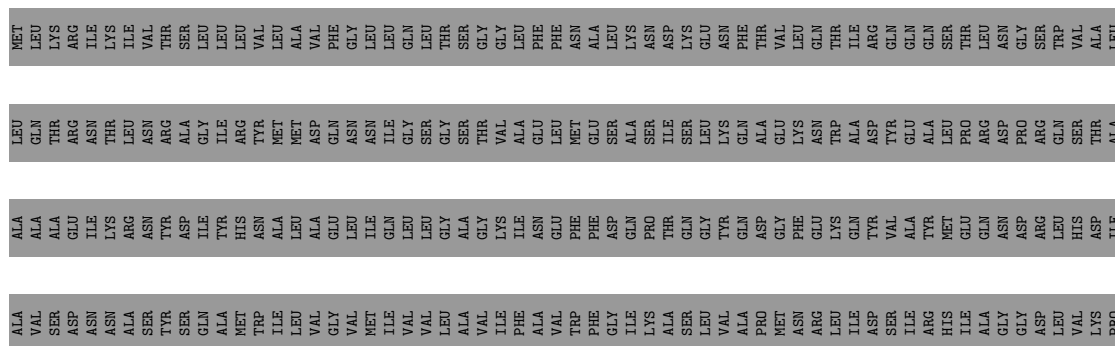
- Molecule 3: Methyl-accepting chemotaxis protein I

Chain G: 18% 81%



- Molecule 3: Methyl-accepting chemotaxis protein I

Chain H:  18% 81%



GLN	GLN	GLN	GLN	GLU	THR	SER	THR	GLN	VAL	LYS	THR	ILE	GLY	LEU	ALA	PRO	ALA	ALA	PRO	ASP	VAL	ASP	MET	GLY	GLN	GLU	GLN	ASN	TRP	GLU	THR	PHE
GLU	ILE	ALA	SER	ALA	ASP	GLU	SER	SER	ARG	GLY	ILE	ASP	GLY	LEU	ALA	VAL	ALA	ASN	ALA	VAL	VAL	GLU	GLU	ALA	ALA	ALA	ALA	GLU	GLU	GLU	GLU	PHE
SER	LEU	GLU	GLU	THR	ALA	ALA	SER	GLU	GLN	LYS	THR	THR	THR	LEU	ALA	ALA	ASN	GLN	ARG	VAL	VAL	MET	GLU	GLN	GLN	GLN	GLU	LEU	ALA	THR	GLU	
ILE	VAL	ASP	GLY	SER	ASN	GLU	MET	GLY	GLN	ARG	ALA	ALA	GLU	LEU	GLU	GLU	ASN	HIS	MET	THR	GLY	LEU	MET	ARG	THR	VAL	GLY	ASP	VAL	GLY	ILE	

- Molecule 3: Methyl-accepting chemotaxis protein I

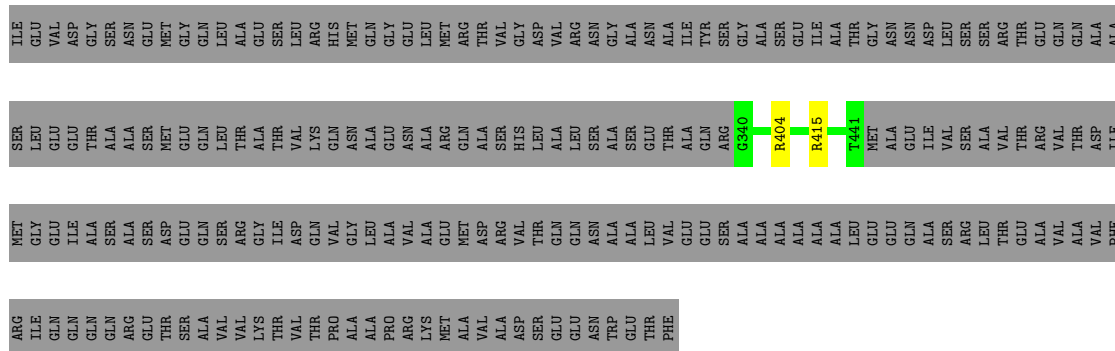
Chain I: 18% 81%

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- Molecule 3: Methyl-accepting chemotaxis protein I

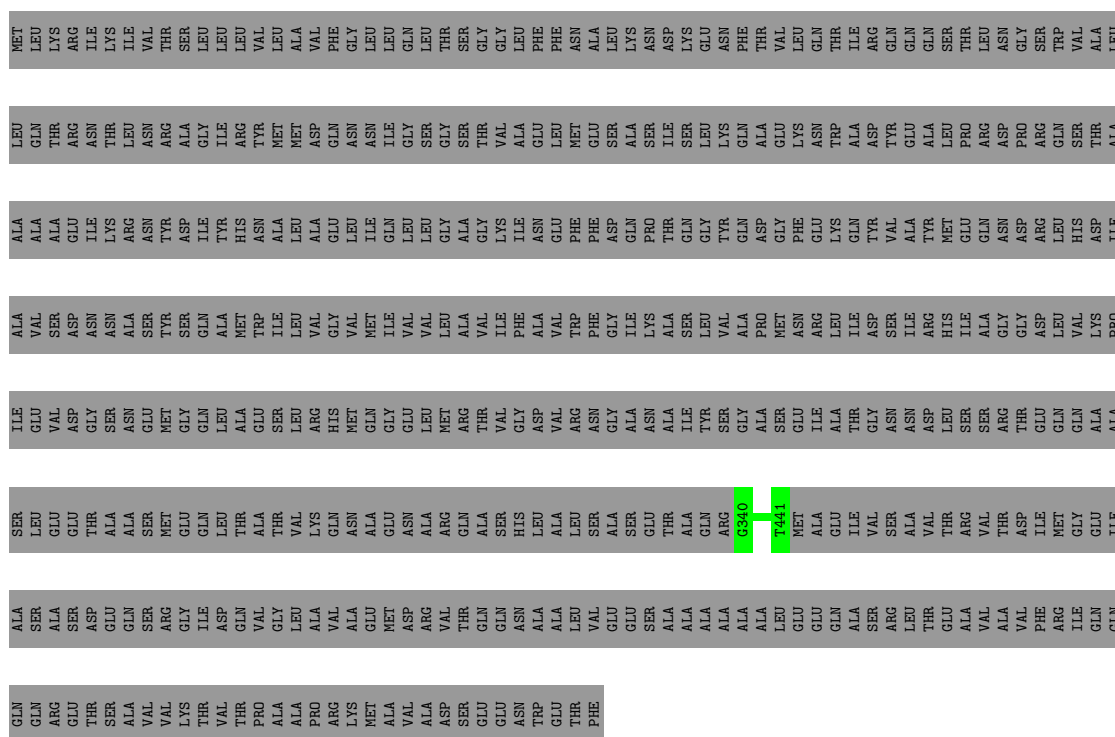
Chain J:  18% 81%

ALA	VAL	VAL	ALA	ALA	LEU	GLN	MET
VAL	SER	ALA	GLU	THR	THR	GLN	LEU
ASP	ASN	ALA	ASN	ARG	ASN	ARG	LYS
ASN	ASN	ILE	LYS	THR	THR	ILE	ILE
ALA	ARG	ARG	LYS	LEU	VAL	VAL	THR
SER	TYR	TYR	ASN	ASN	THR	THR	THR
GLN	GLN	ILE	ILE	GLY	ALA	SER	SER
ALA	ALA	TYR	HIS	ILE	LEU	LEU	LEU
MET	ASN	ASN	ASN	ARG	TYR	LEU	LEU
TRP	TRP	ASN	ASN	THR	MET	VAL	VAL
ILE	ALA	LEU	LEU	MET	MET	ALA	ALA
VAL	VAL	ALA	ASP	ASP	VAL	VAL	PHE
GLY	GLY	LEU	GLU	ASN	GLN	PHE	GLY
VAL	VAL	ILE	LEU	ILE	ASN	GLY	GLY
MET	MET	ILE	GLN	ILE	ASN	THR	SER
ILE	VAL	LEU	LEU	GLY	GLY	THR	THR
VAL	VAL	VAL	LEU	GLY	GLY	GLY	GLY
ALA	ALA	ALA	GLY	ALA	SER	SER	SER
VAL	VAL	GLY	GLY	GLY	THR	GLY	GLY
ILE	ILE	ILE	LYS	VAL	VAL	GLY	GLY
PHE	PHE	ILE	ILE	ALA	ALA	LEU	PHE
ALA	ALA	ASN	ASN	GLU	GLY	PHE	PHE
VAL	VAL	GLU	GLU	LEU	LEU	ASN	ASN
TRP	TRP	PHE	PHE	MET	MET	ASN	ASN
GLY	GLY	ASP	ASP	GLU	GLU	LEU	LEU
ILE	ILE	GLN	GLN	ALA	ALA	LYS	LYS
LYS	LYS	PRO	PRO	SER	SER	ASN	ASN
ALA	ALA	THR	THR	ILE	ILE	ASP	ASP
SER	SER	GLN	GLN	SER	SER	LYS	LYS
LEU	LEU	GLY	GLY	LEU	LEU	GLU	GLU
VAL	VAL	TYR	TYR	LYS	LYS	ASN	ASN
VAL	VAL	GLN	GLN	GLN	GLN	PHE	PHE
PRO	PRO	ASP	ASP	ALA	ALA	THR	THR
MET	MET	GLY	GLY	GLU	GLU	VAL	VAL
ASN	ASN	PHE	PHE	LYS	LYS	LEU	LEU
ARG	ARG	GLU	GLU	ASN	ASN	GLN	GLN
LEU	LEU	LYS	LYS	TRP	TRP	THR	THR
ILE	ILE	GLN	GLN	ALA	ALA	ILE	ILE
ASP	ASP	TYR	TYR	ASP	ASP	ARG	ARG
SER	SER	VAL	VAL	TRR	TRR	GLN	GLN
ILE	ILE	ALA	ALA	GLU	GLU	GLN	GLN
ARG	ARG	TYR	TYR	LEU	LEU	SER	SER
HIS	HIS	MET	MET	LEU	LEU	THR	THR
ILE	ILE	GLU	GLU	GLN	GLN	LEU	LEU
ALA	ALA	GLN	GLN	ASN	ASN	ASP	ASP
GLY	GLY	ASP	ASP	ASP	ASP	GLY	GLY
GLY	GLY	ARG	ARG	ARG	ARG	SER	SER
LEU	LEU	LEU	LEU	GLN	GLN	TRP	TRP
VAL	VAL	HIS	HIS	SER	SER	VAL	VAL
LYS	LYS	ASP	ASP	HIS	HIS	THR	THR
PRO	PRO	ILE	ILE	ALA	ALA	LEU	LEU



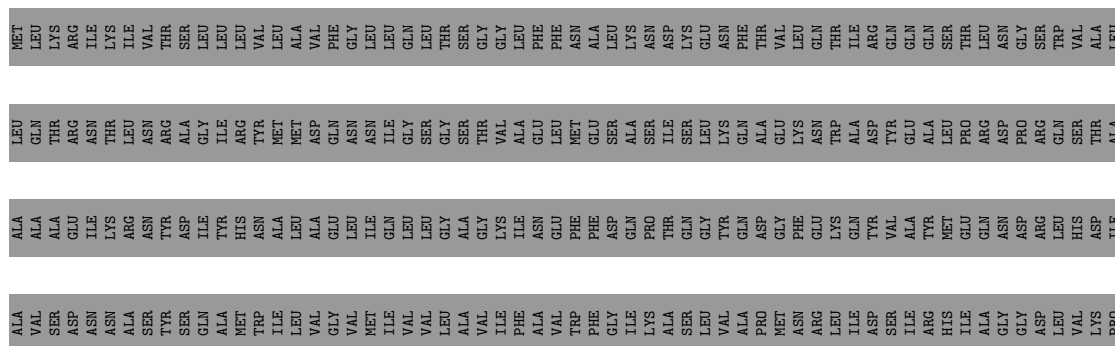
- Molecule 3: Methyl-accepting chemotaxis protein I

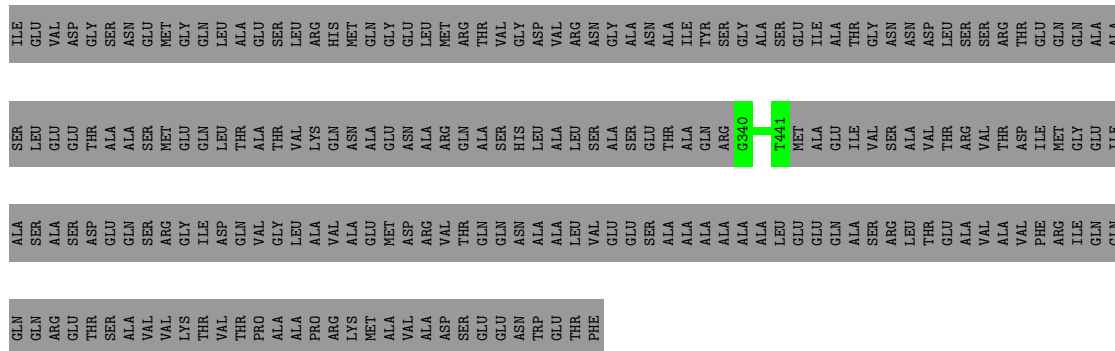
Chain K:  19% 81%



- Molecule 3: Methyl-accepting chemotaxis protein I

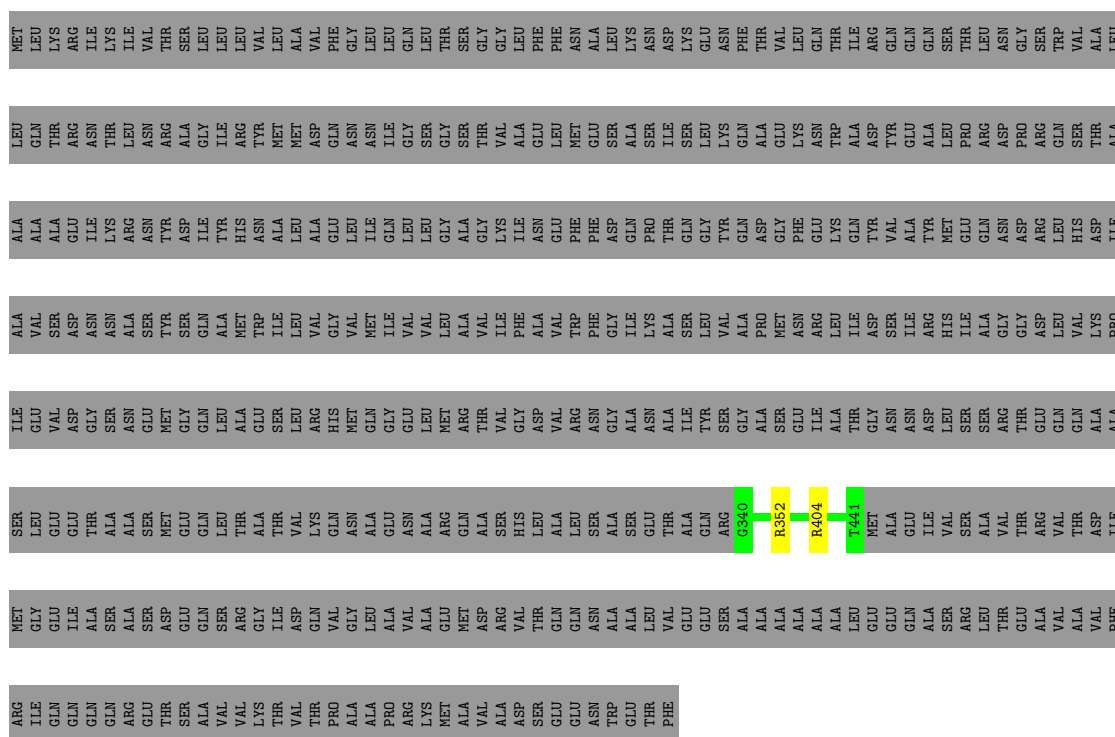
Chain L: 19% 81%





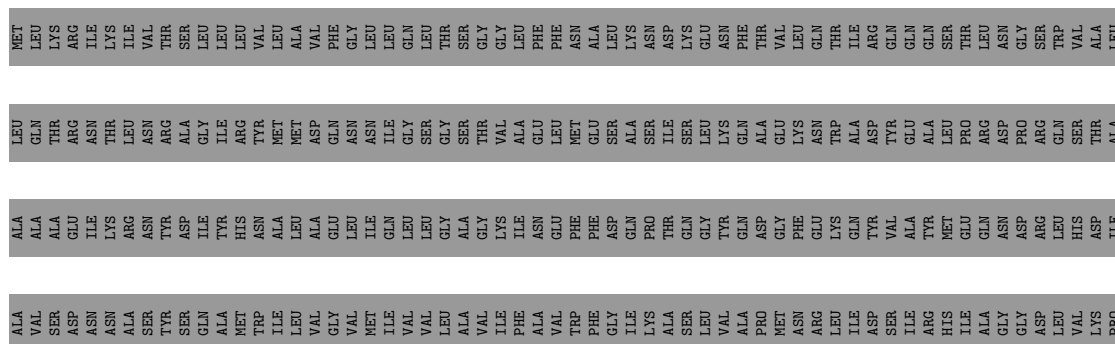
- Molecule 3: Methyl-accepting chemotaxis protein I

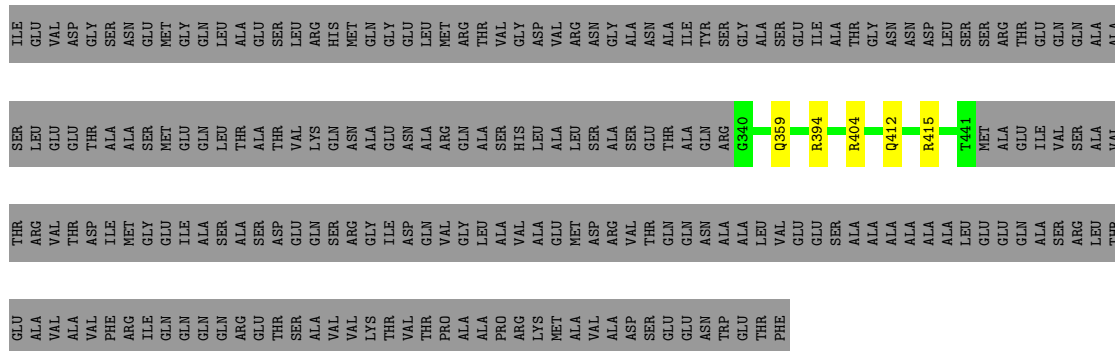
Chain M: 18% 81%



- Molecule 3: Methyl-accepting chemotaxis protein I

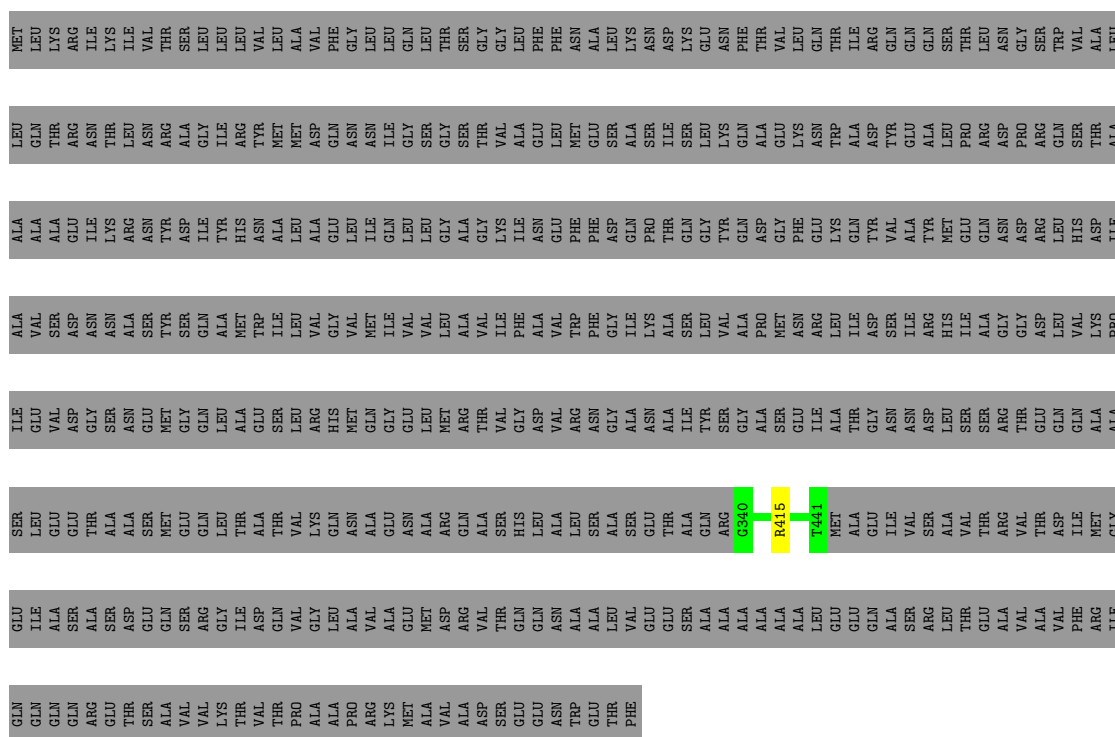
Chain N: 18% . 81%





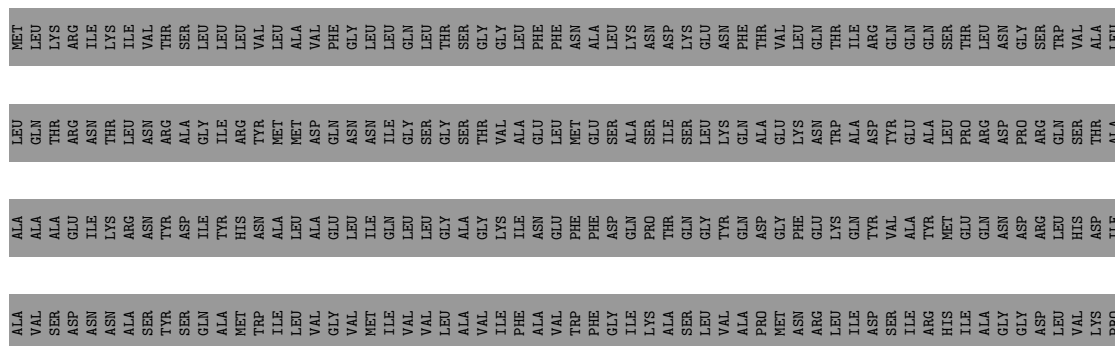
- Molecule 3: Methyl-accepting chemotaxis protein I

Chain O:  18% 81%



- Molecule 3: Methyl-accepting chemotaxis protein I

Chain P: 18% 81%



[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	91636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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	0.70	0/2939	0.91	2/3975 (0.1%)
1	B	0.70	0/2939	0.90	2/3975 (0.1%)
2	C	0.73	0/1130	0.94	1/1537 (0.1%)
2	D	0.72	0/1130	0.94	1/1537 (0.1%)
3	E	0.72	0/737	0.92	0/994
3	F	0.72	0/737	0.91	0/994
3	G	0.71	0/737	0.91	0/994
3	H	0.72	0/737	0.90	0/994
3	I	0.72	0/737	0.90	0/994
3	J	0.73	0/737	0.90	0/994
3	K	0.71	0/737	0.91	0/994
3	L	0.72	0/737	0.92	0/994
3	M	0.73	0/737	0.91	0/994
3	N	0.72	0/737	0.94	0/994
3	O	0.72	0/737	0.92	0/994
3	P	0.73	0/737	0.92	0/994
All	All	0.72	0/16982	0.91	6/22952 (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	A	0	6
1	B	0	5
3	F	0	2
3	G	0	1
3	H	0	1
3	I	0	1
3	J	0	2
3	M	0	2
3	N	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1
3	P	0	1
All	All	0	25

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	PHE	CB-CG-CD1	5.58	124.70	120.80
1	A	333	PHE	CB-CG-CD1	5.45	124.62	120.80
1	B	333	PHE	CB-CG-CD2	-5.32	117.07	120.80
2	D	42	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	C	42	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	333	PHE	CB-CG-CD2	-5.16	117.19	120.80

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	518	ARG	Sidechain
1	A	538	ARG	Sidechain
1	A	614	TYR	Sidechain
1	B	338	ARG	Sidechain
1	B	379	ARG	Sidechain
1	B	480	ARG	Sidechain
1	B	538	ARG	Sidechain
1	B	614	TYR	Sidechain
3	F	394	ARG	Sidechain
3	F	409	ARG	Sidechain
3	G	415	ARG	Sidechain
3	H	404	ARG	Sidechain
3	I	415	ARG	Sidechain
3	J	404	ARG	Sidechain
3	J	415	ARG	Sidechain
3	M	352	ARG	Sidechain
3	M	404	ARG	Sidechain
3	N	394	ARG	Sidechain
3	N	404	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	N	415	ARG	Sidechain
3	O	415	ARG	Sidechain
3	P	409	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2909	0	3009	0	0
1	B	2909	0	3009	0	0
2	C	1117	0	1152	0	0
2	D	1117	0	1152	0	0
3	E	736	0	750	0	0
3	F	736	0	750	0	0
3	G	736	0	750	0	0
3	H	736	0	750	0	0
3	I	736	0	750	0	0
3	J	736	0	750	0	0
3	K	736	0	750	0	0
3	L	736	0	750	0	0
3	M	736	0	750	0	0
3	N	736	0	750	0	0
3	O	736	0	750	0	0
3	P	736	0	750	0	0
All	All	16884	0	17322	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	381/654 (58%)	368 (97%)	10 (3%)	3 (1%)	21	65
1	B	381/654 (58%)	372 (98%)	7 (2%)	2 (0%)	31	74
2	C	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	12	52
2	D	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	12	52
3	E	100/551 (18%)	100 (100%)	0	0	100	100
3	F	100/551 (18%)	100 (100%)	0	0	100	100
3	G	100/551 (18%)	100 (100%)	0	0	100	100
3	H	100/551 (18%)	100 (100%)	0	0	100	100
3	I	100/551 (18%)	100 (100%)	0	0	100	100
3	J	100/551 (18%)	100 (100%)	0	0	100	100
3	K	100/551 (18%)	100 (100%)	0	0	100	100
3	L	100/551 (18%)	100 (100%)	0	0	100	100
3	M	100/551 (18%)	100 (100%)	0	0	100	100
3	N	100/551 (18%)	100 (100%)	0	0	100	100
3	O	100/551 (18%)	100 (100%)	0	0	100	100
3	P	100/551 (18%)	100 (100%)	0	0	100	100
All	All	2248/8254 (27%)	2210 (98%)	29 (1%)	9 (0%)	40	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	ASP
2	D	81	ASP
1	A	618	PRO
1	B	579	GLN
1	B	618	PRO
2	D	121	GLU

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Mol	Chain	Res	Type
1	A	574	LYS
1	A	422	GLY
2	C	124	VAL

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	321/552 (58%)	320 (100%)	1 (0%)	93	96
1	B	321/552 (58%)	320 (100%)	1 (0%)	93	96
2	C	126/143 (88%)	121 (96%)	5 (4%)	34	62
2	D	126/143 (88%)	122 (97%)	4 (3%)	42	68
3	E	77/438 (18%)	77 (100%)	0	100	100
3	F	77/438 (18%)	77 (100%)	0	100	100
3	G	77/438 (18%)	76 (99%)	1 (1%)	71	86
3	H	77/438 (18%)	77 (100%)	0	100	100
3	I	77/438 (18%)	77 (100%)	0	100	100
3	J	77/438 (18%)	77 (100%)	0	100	100
3	K	77/438 (18%)	77 (100%)	0	100	100
3	L	77/438 (18%)	77 (100%)	0	100	100
3	M	77/438 (18%)	77 (100%)	0	100	100
3	N	77/438 (18%)	75 (97%)	2 (3%)	49	73
3	O	77/438 (18%)	77 (100%)	0	100	100
3	P	77/438 (18%)	77 (100%)	0	100	100
All	All	1818/6646 (27%)	1804 (99%)	14 (1%)	84	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	ARG

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Mol	Chain	Res	Type
1	B	483	GLN
2	C	72	ARG
2	C	96	ARG
2	C	115	GLN
2	C	126	LEU
2	C	142	LEU
2	D	72	ARG
2	D	96	ARG
2	D	126	LEU
2	D	142	LEU
3	G	346	ASN
3	N	359	GLN
3	N	412	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no chain breaks in this entry.