



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3J8J
EMDB ID: : EMD-6180
Title : Tilted state of actin, T1
Authors : Galkin, V.E.; Orlova, A.; Vos, M.R.; Schroder, G.F.; Egelman, E.H.
Deposited on : 2014-11-07
Resolution : 12.00 Å(reported)

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

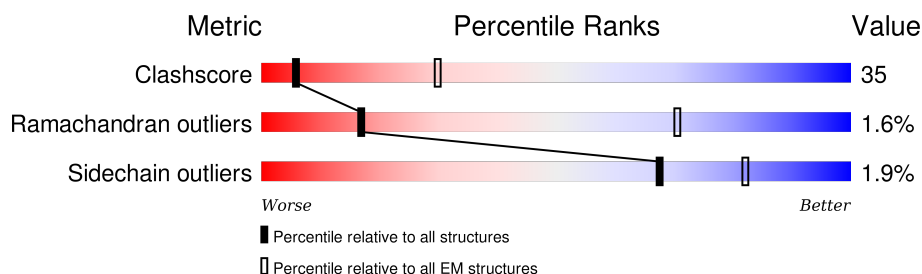
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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	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	377	52%	44% ..
1	B	377	51%	45% ..
1	C	377	51%	45% ..
1	D	377	50%	47% ..
1	E	377	51%	45% ..
1	F	377	51%	46% ..
1	G	377	51%	45% ..
1	H	377	51%	46% ..
1	I	377	50%	46% ..

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Mol	Chain	Length	Quality of chain
1	J	377	<div><div></div><div>51%</div><div>46%</div><div></div></div> <div>• •</div>
1	K	377	<div><div></div><div>52%</div><div>45%</div><div></div></div> <div>• •</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31834 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.

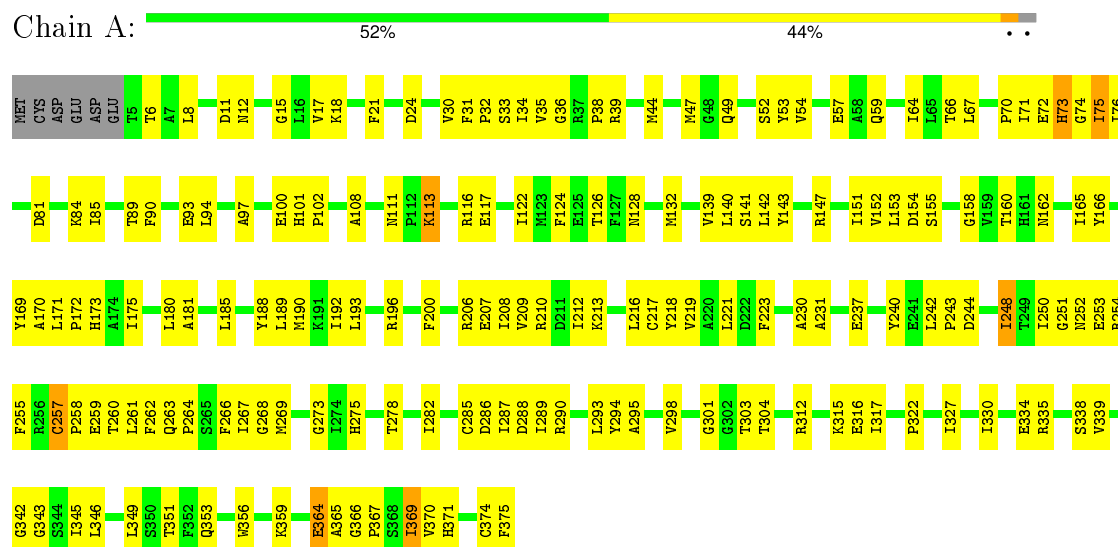
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	B	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	C	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	D	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	E	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	F	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	G	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	H	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	I	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	J	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		
1	K	371	Total	C	N	O	S	0	0
			2894	1833	487	553	21		

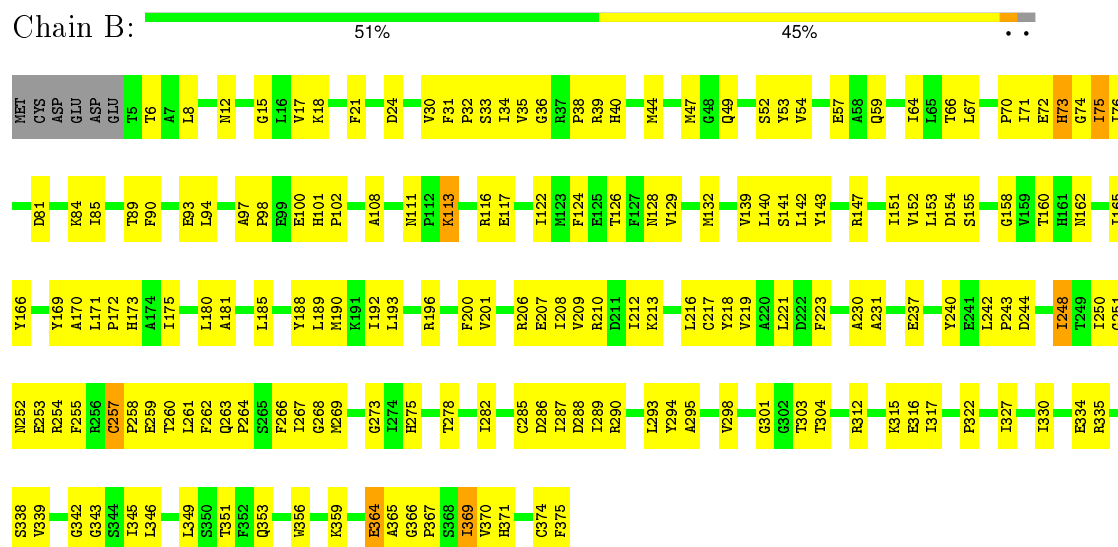
3 Residue-property plots

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. 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.

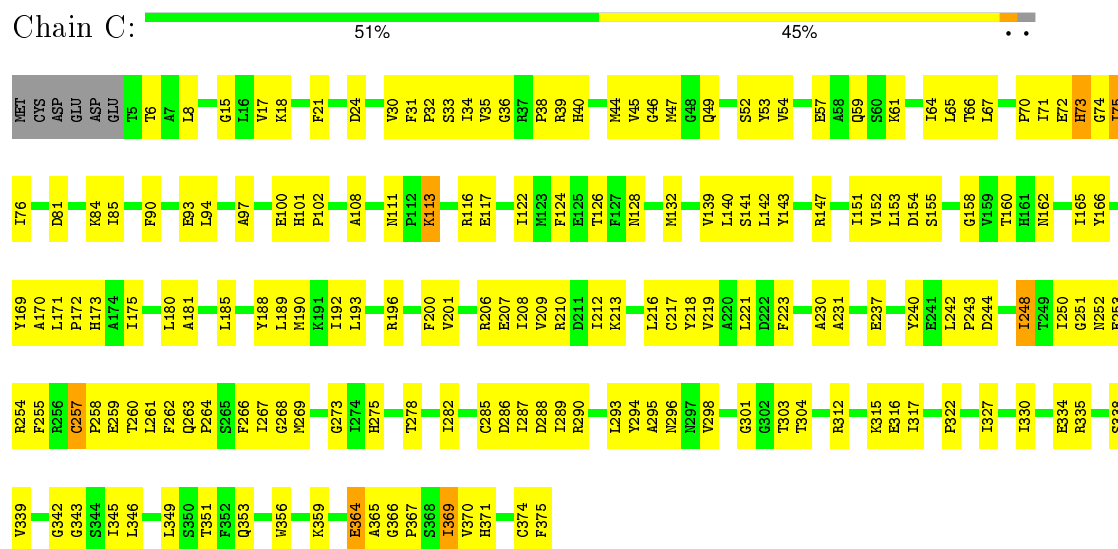
- Molecule 1: Actin, alpha skeletal muscle



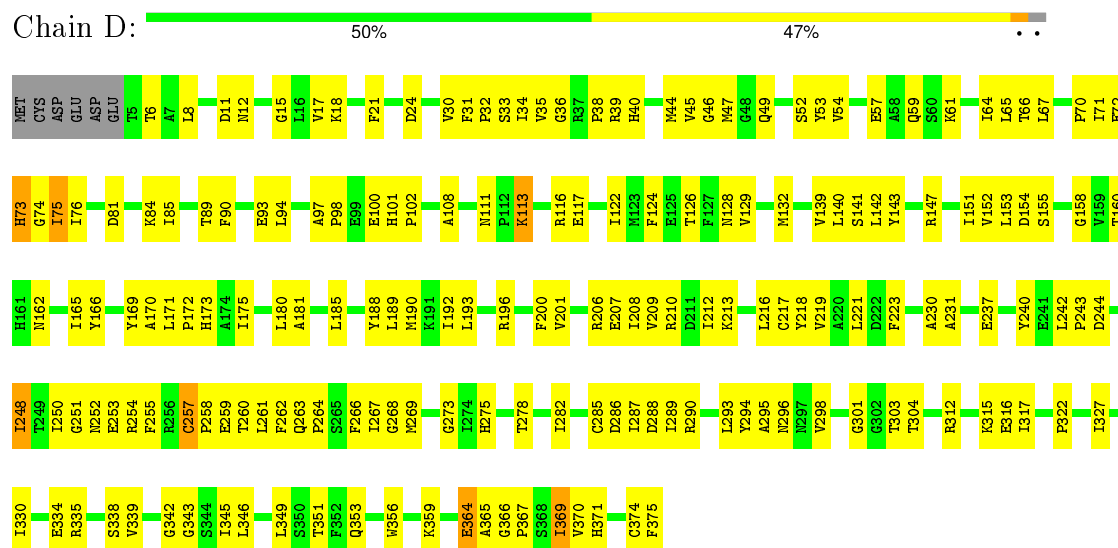
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



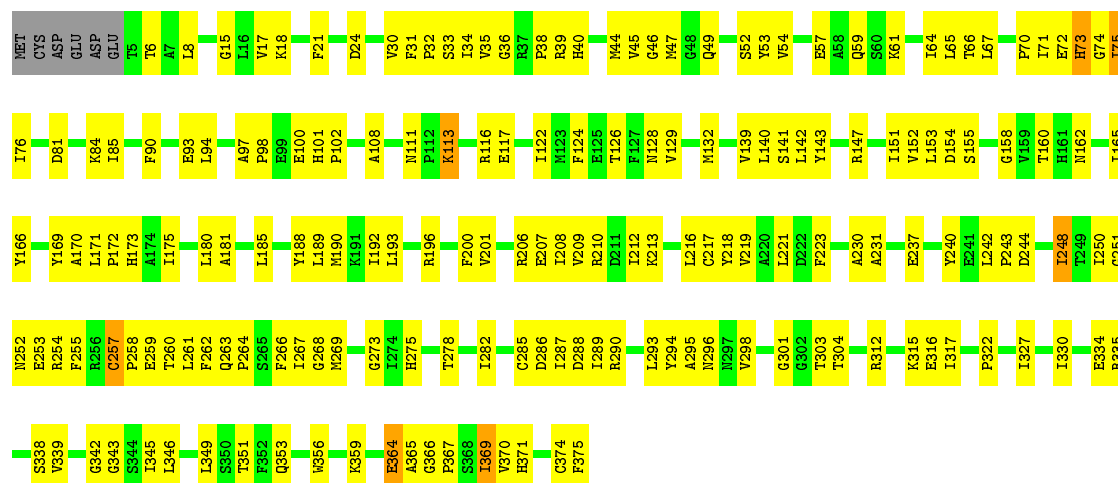
- Molecule 1: Actin, alpha skeletal muscle





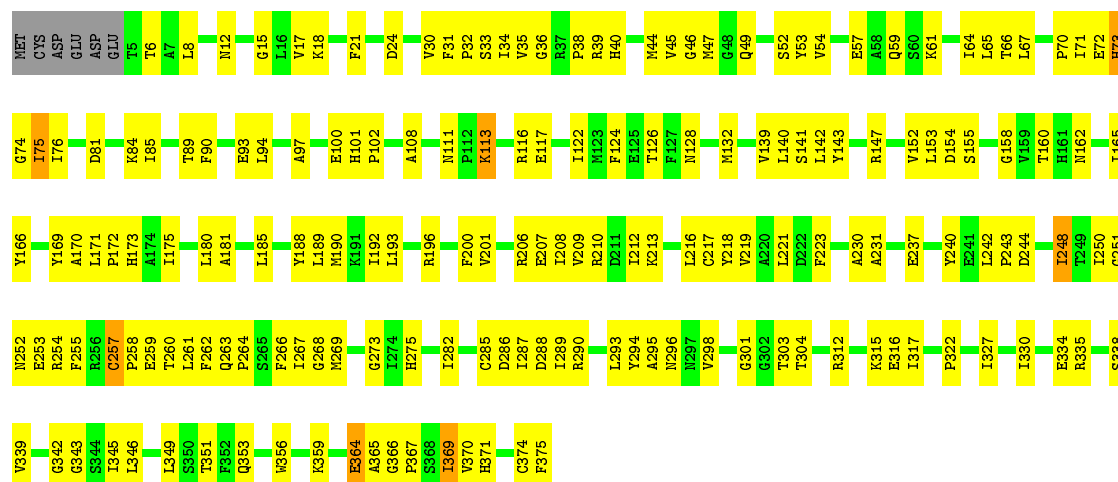
• Molecule 1: Actin, alpha skeletal muscle

Chain F: 51% 46%



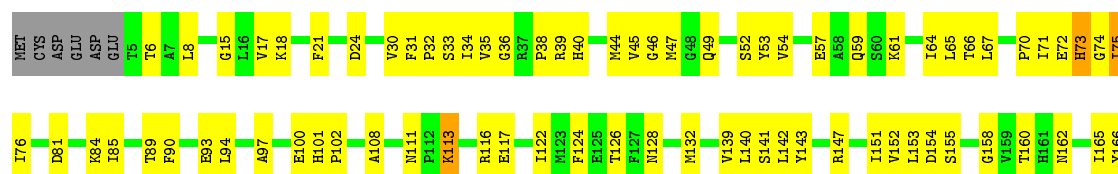
• Molecule 1: Actin, alpha skeletal muscle

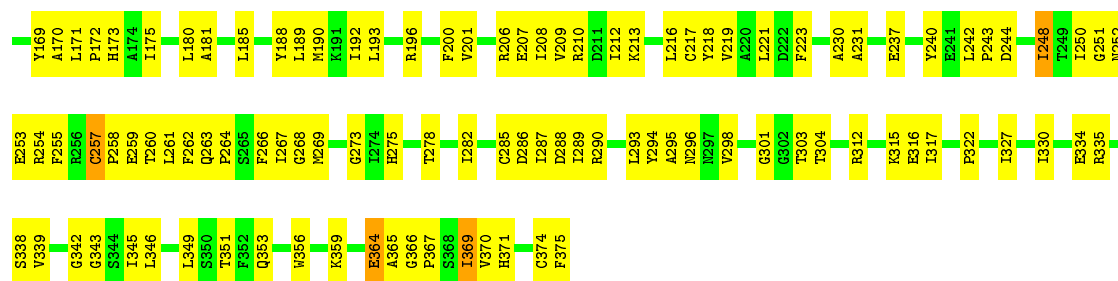
Chain G: 51% 45%



• Molecule 1: Actin, alpha skeletal muscle

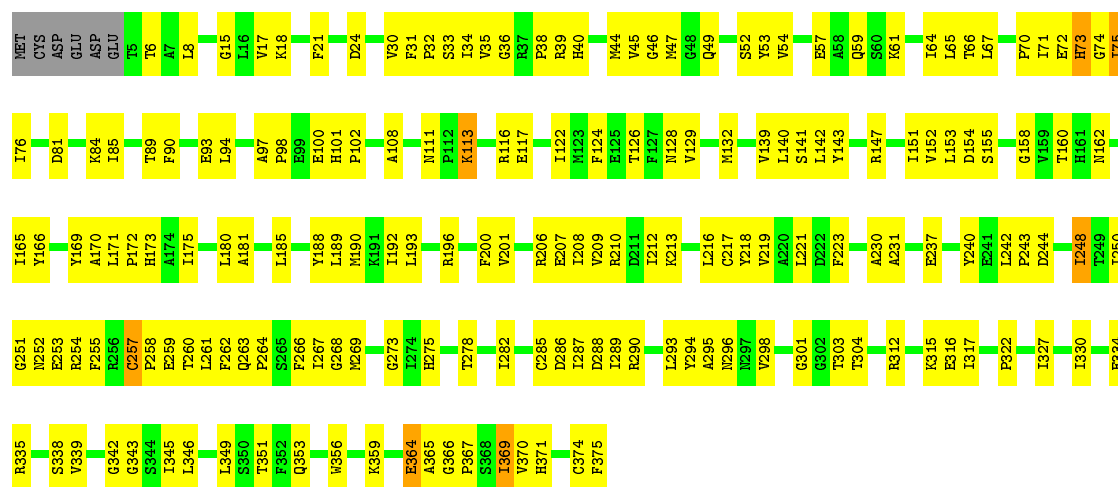
Chain H: 51% 46%





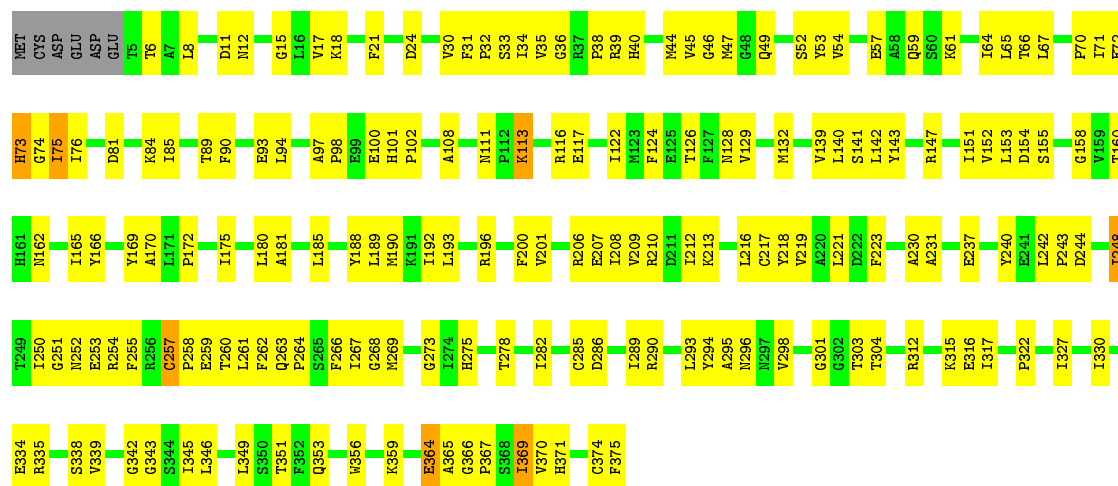
- Molecule 1: Actin, alpha skeletal muscle

Chain I: 50% 46%



- Molecule 1: Actin, alpha skeletal muscle

Chain J: 51% 46%



- Molecule 1: Actin, alpha skeletal muscle

Chain K: 52% 45%



MET	G74	N162	I250	R335
CYS	I75	I165	G251	S338
ASP	I76	Y166	N252	V339
GLU	D81	Y169	E253	
ASP	K84	A170	R254	G342
GLU	I85	L171	R255	G343
TS	A7	P172	C257	S344
T6	T89	I175	P258	I345
L8	F90		E259	L346
			T260	
M12	E93	L180	L261	L349
G15	L94	A181	F262	S350
L16	A97	L185	Q263	T351
V17	P98		P264	F352
K18	E99	Y188	S265	Q353
F21	E100	L189	F266	
	H101	M190	I267	W356
D24	P102	K191	G268	K359
	A108	L193	N269	
V30	N111	R196	G273	E364
F31	F112	F200	I274	A365
P32	K113	V201	H275	G366
S33	R116	R206	T278	P367
I34	E117	E207		S368
V35	I122	I208	I282	I369
G36	M123	V209		V370
R37	F124	D210	C285	G374
P38	E125	R211	D286	F375
R39	T126	I212	I289	
H40	F127	K213	R290	
M44	N128	L216	L293	
V45	V129	C217	Y294	
G46	M132	Y218	A295	
M47		V219	N296	
G48	V139	A220	N297	
Q49	L140	L221	V298	
	S141	D222	G301	
S52	L142	F223	G302	
V53	Y143	A230	T303	
V54	R147	A231	T304	
E57	I151	E237	R312	
A58	V152	Y240	K315	
D59	L153	E241	E316	
S60	D154	L242	I317	
K61	S155	P243	P322	
T64	G158	D244	I327	
L65	V159	I248	I330	
T66	T160	T249	E334	
L67	H161			
P70				
I71				
E72				
H73				

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC and comparison with atomic model	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/2956	0.54	0/4004
1	B	0.37	0/2956	0.54	0/4004
1	C	0.37	0/2956	0.54	0/4004
1	D	0.37	0/2956	0.55	0/4004
1	E	0.37	0/2956	0.54	0/4004
1	F	0.37	0/2956	0.54	0/4004
1	G	0.37	0/2956	0.54	0/4004
1	H	0.37	0/2956	0.55	0/4004
1	I	0.37	0/2956	0.54	0/4004
1	J	0.37	0/2956	0.54	0/4004
1	K	0.37	0/2956	0.55	0/4004
All	All	0.37	0/32516	0.54	0/44044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2894	0	2866	207	0
1	B	2894	0	2866	211	0
1	C	2894	0	2866	265	0
1	D	2894	0	2866	266	0
1	E	2894	0	2866	263	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2894	0	2866	264	0
1	G	2894	0	2866	267	0
1	H	2894	0	2866	266	0
1	I	2894	0	2866	266	0
1	J	2894	0	2866	215	0
1	K	2894	0	2866	210	0
All	All	31834	0	31526	2188	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 35.

The worst 5 of 2188 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:171:LEU:CD2	1:K:45:VAL:HG12	1.60	1.31
1:D:171:LEU:CD2	1:F:45:VAL:HG12	1.60	1.31
1:G:171:LEU:CD2	1:I:45:VAL:HG12	1.61	1.30
1:C:171:LEU:CD2	1:E:45:VAL:HG12	1.60	1.30
1:E:171:LEU:CD2	1:G:45:VAL:HG12	1.61	1.29

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	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	B	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	C	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	D	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	E	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	G	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	H	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	I	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	J	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
1	K	369/377 (98%)	349 (95%)	14 (4%)	6 (2%)	12	56
All	All	4059/4147 (98%)	3839 (95%)	154 (4%)	66 (2%)	17	56

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	B	73	HIS
1	C	73	HIS
1	D	73	HIS
1	E	73	HIS

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	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	B	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	C	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	D	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	E	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	F	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	G	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	H	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	I	313/320 (98%)	307 (98%)	6 (2%)	65	86
1	J	313/320 (98%)	307 (98%)	6 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	313/320 (98%)	307 (98%)	6 (2%)	65 86
All	All	3443/3520 (98%)	3377 (98%)	66 (2%)	67 86

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	364	GLU
1	G	113	LYS
1	K	113	LYS
1	F	113	LYS
1	F	334	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	173	HIS
1	F	354	GLN
1	J	354	GLN
1	E	354	GLN
1	F	92	ASN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.