



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3J8K
EMDB ID: : EMD-6181
Title : Tilted state of actin, T2
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

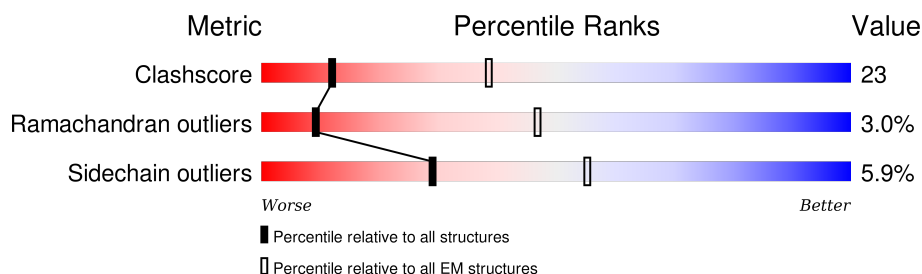
1 Overall quality at a glance

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	58% 37% . .
1	B	377	63% 33% . .
1	C	377	60% 36% . .
1	D	377	51% 43% 5% .
1	E	377	55% 41% . .
1	F	377	54% 40% 5% . .
1	G	377	57% 38% . .
1	H	377	55% 40% . .
1	I	377	51% 46% . .

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Mol	Chain	Length	Quality of chain
1	J	377	<div><div></div><div>50%</div><div>46%</div><div>..</div></div>

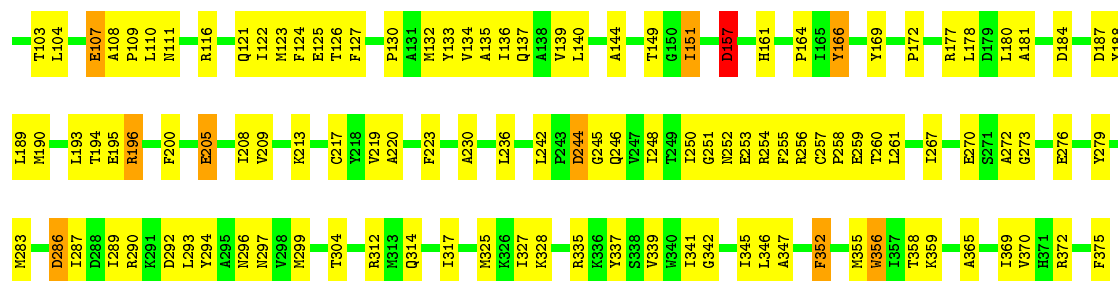
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29330 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.

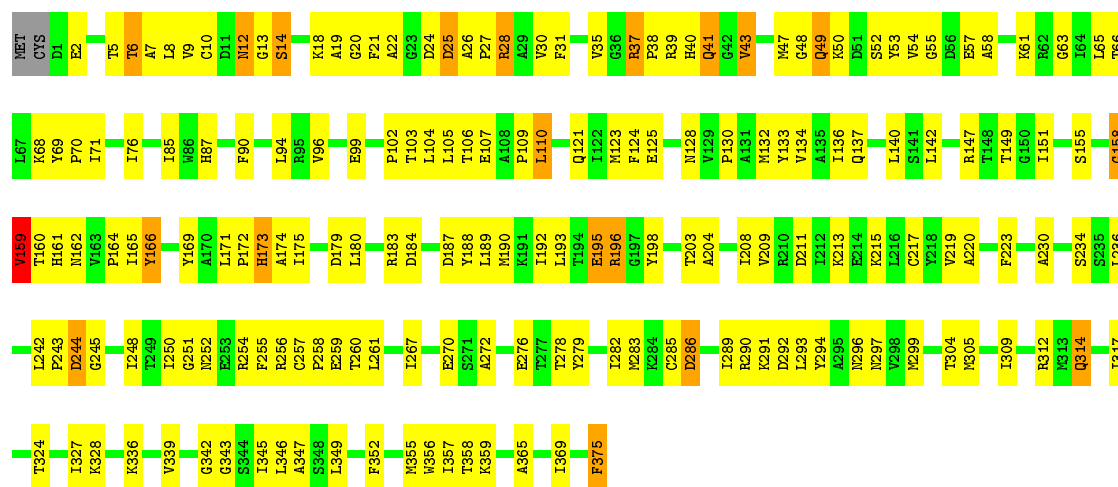
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		



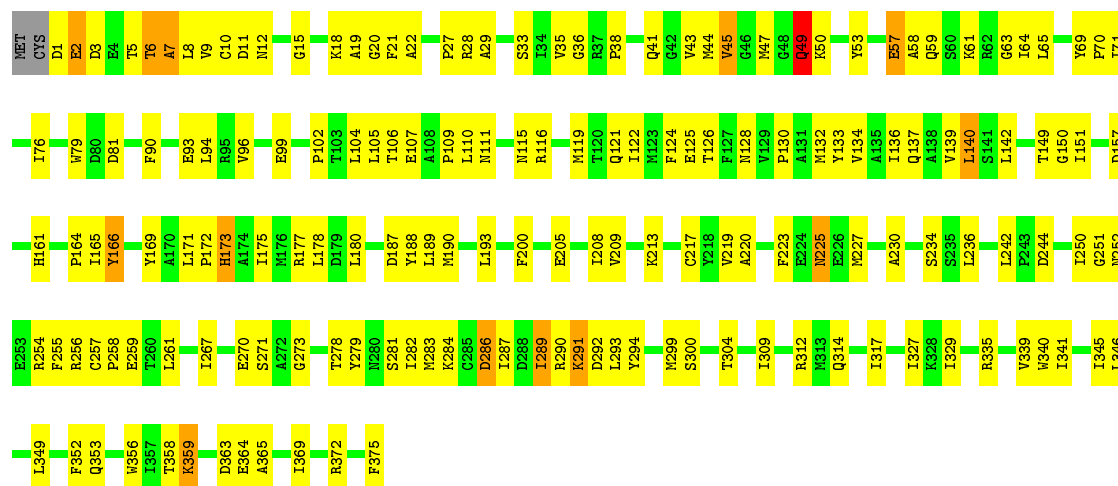
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 51% 43% 5% •



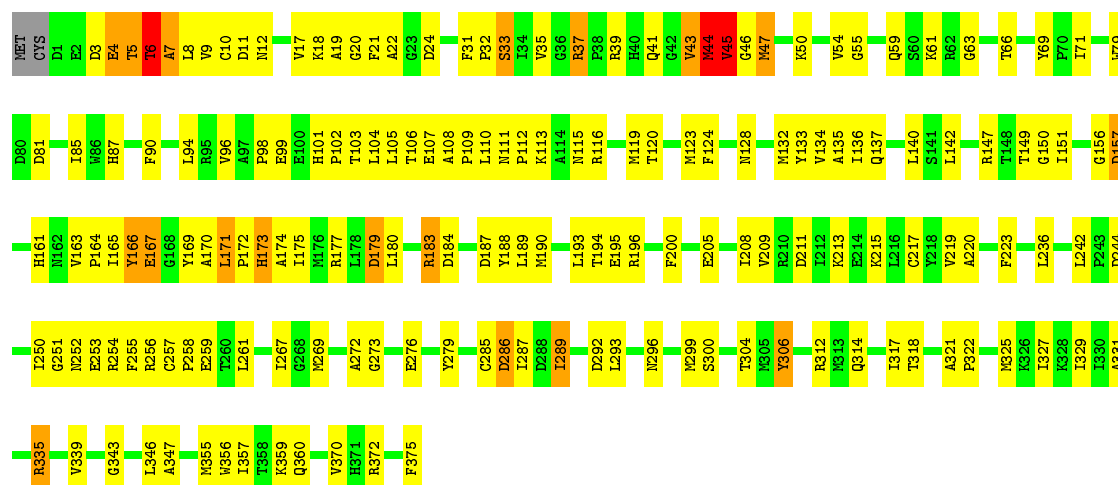
- Molecule 1: Actin, alpha skeletal muscle

Chain E: 55% 41% • •



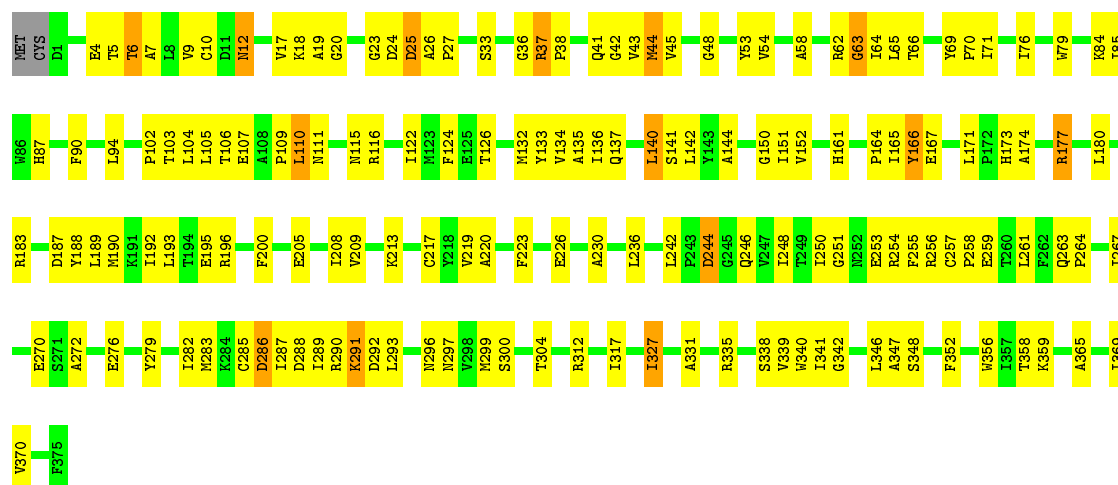
- Molecule 1: Actin, alpha skeletal muscle

Chain F: 54% 40% 5% • •



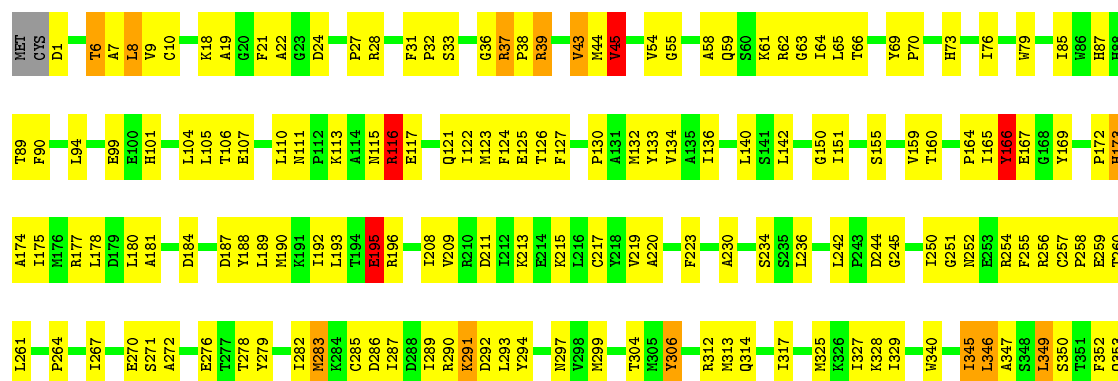
- Molecule 1: Actin, alpha skeletal muscle

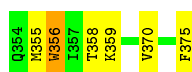
Chain G: 57% 38%



- Molecule 1: Actin, alpha skeletal muscle

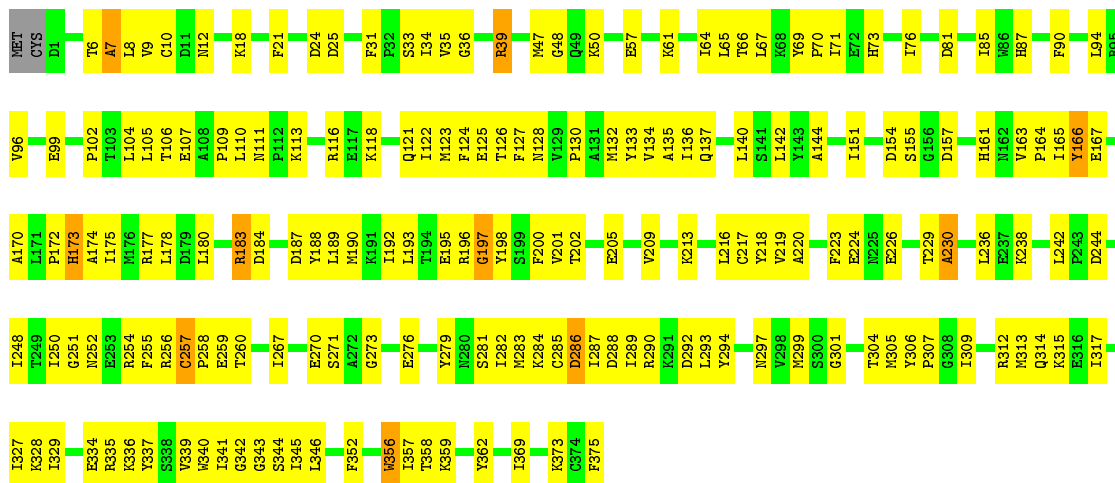
Chain H: 55% 40%





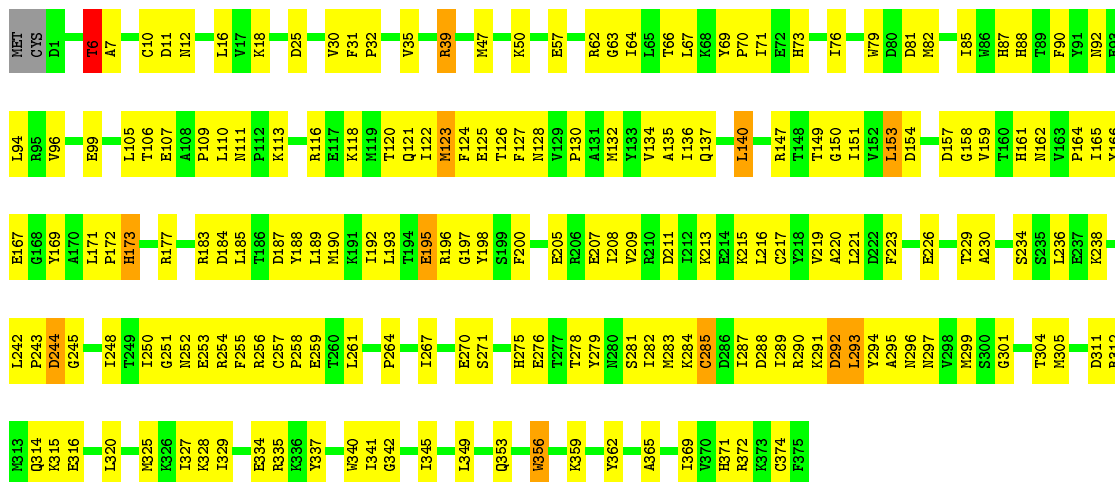
• Molecule 1: Actin, alpha skeletal muscle

Chain I: 51% 46%



• Molecule 1: Actin, alpha skeletal muscle

Chain J: 50% 46%



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	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	0.41	0/2996	0.63	0/4058
1	B	0.42	0/2996	0.66	1/4058 (0.0%)
1	C	0.41	0/2996	0.64	0/4058
1	D	0.42	0/2996	0.66	0/4058
1	E	0.40	0/2996	0.65	0/4058
1	F	0.41	0/2996	0.64	0/4058
1	G	0.43	0/2996	0.66	0/4058
1	H	0.44	0/2996	0.68	1/4058 (0.0%)
1	I	0.40	0/2996	0.60	0/4058
1	J	0.38	0/2996	0.58	0/4058
All	All	0.41	0/29960	0.64	2/40580 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	116	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	362	TYR	CB-CG-CD1	-5.20	117.88	121.00

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	2933	0	2894	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2933	0	2894	113	0
1	C	2933	0	2894	121	0
1	D	2933	0	2894	149	0
1	E	2933	0	2894	126	0
1	F	2933	0	2894	140	0
1	G	2933	0	2894	140	0
1	H	2933	0	2894	150	0
1	I	2933	0	2894	148	0
1	J	2933	0	2894	164	0
All	All	29330	0	28940	1317	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 23.

The worst 5 of 1317 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:A:63:GLY:HA3	1:C:287:ILE:HG21	1.34	1.06
1:B:7:ALA:HB1	1:B:104:LEU:HB2	1.40	1.00
1:G:58:ALA:HB1	1:G:65:LEU:HD21	1.46	0.97
1:C:58:ALA:HB1	1:C:65:LEU:HD21	1.47	0.95
1:H:151:ILE:HB	1:H:293:LEU:HD22	1.48	0.95

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	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	7	47
1	B	373/377 (99%)	349 (94%)	11 (3%)	13 (4%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	7	47
1	D	373/377 (99%)	340 (91%)	17 (5%)	16 (4%)	3	34
1	E	373/377 (99%)	339 (91%)	18 (5%)	16 (4%)	3	34
1	F	373/377 (99%)	343 (92%)	17 (5%)	13 (4%)	4	39
1	G	373/377 (99%)	343 (92%)	19 (5%)	11 (3%)	6	43
1	H	373/377 (99%)	347 (93%)	15 (4%)	11 (3%)	6	43
1	I	373/377 (99%)	348 (93%)	18 (5%)	7 (2%)	10	52
1	J	373/377 (99%)	344 (92%)	21 (6%)	8 (2%)	9	50
All	All	3730/3770 (99%)	3453 (93%)	164 (4%)	113 (3%)	9	42

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	B	6	THR
1	B	7	ALA
1	B	41	GLN
1	B	43	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	318/320 (99%)	302 (95%)	16 (5%)	30	66
1	B	318/320 (99%)	301 (95%)	17 (5%)	28	64
1	C	318/320 (99%)	297 (93%)	21 (7%)	21	57
1	D	318/320 (99%)	296 (93%)	22 (7%)	19	56
1	E	318/320 (99%)	301 (95%)	17 (5%)	28	64
1	F	318/320 (99%)	295 (93%)	23 (7%)	18	55
1	G	318/320 (99%)	300 (94%)	18 (6%)	25	62
1	H	318/320 (99%)	298 (94%)	20 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	318/320 (99%)	299 (94%)	19 (6%)	24	60
1	J	318/320 (99%)	302 (95%)	16 (5%)	30	66
All	All	3180/3200 (99%)	2991 (94%)	189 (6%)	29	61

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	227	MET
1	F	171	LEU
1	J	39	ARG
1	E	291	LYS
1	F	33	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	92	ASN
1	F	40	HIS
1	J	92	ASN
1	E	137	GLN
1	E	297	ASN

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.