



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 8, 2016 – 12:27 PM EST

PDB ID : 3JBH
EMDB ID: : EMD-1950
Title : TWO HEAVY MEROMYOSIN INTERACTING-HEADS MOTIFS FLEX-
IBLE DOCKED INTO TARANTULA THICK FILAMENT 3D-MAP AL-
LWS IN DEPTH STUDY OF INTRA- AND INTERMOLECULAR INTER-
ACTIONS
Authors : Alamo, L.; Qi, D.; Wriggers, W.; Pinto, A.; Zhu, J.; Bilbao, A.; Gillilan, R.E.;
Hu, S.; Padron, R.
Deposited on : 2015-09-01
Resolution : 20.00 Å(reported)
Based on PDB ID : 3DTP

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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
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)

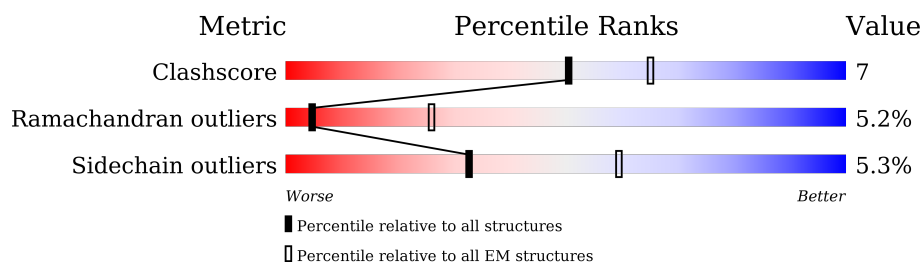
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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	1953	
1	B	1953	
1	G	1953	
1	H	1953	
2	C	156	
2	D	156	
2	I	156	
2	J	156	

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Mol	Chain	Length	Quality of chain
3	E	196	 73% 24% •
3	F	196	 64% 29% 6% •
3	K	196	 78% 19% •
3	L	196	 63% 28% 7% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41968 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 MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	B	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		
1	G	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	H	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		

- Molecule 2 is a protein called MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	D	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	I	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	J	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		

- Molecule 3 is a protein called MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	F	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	K	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	L	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		

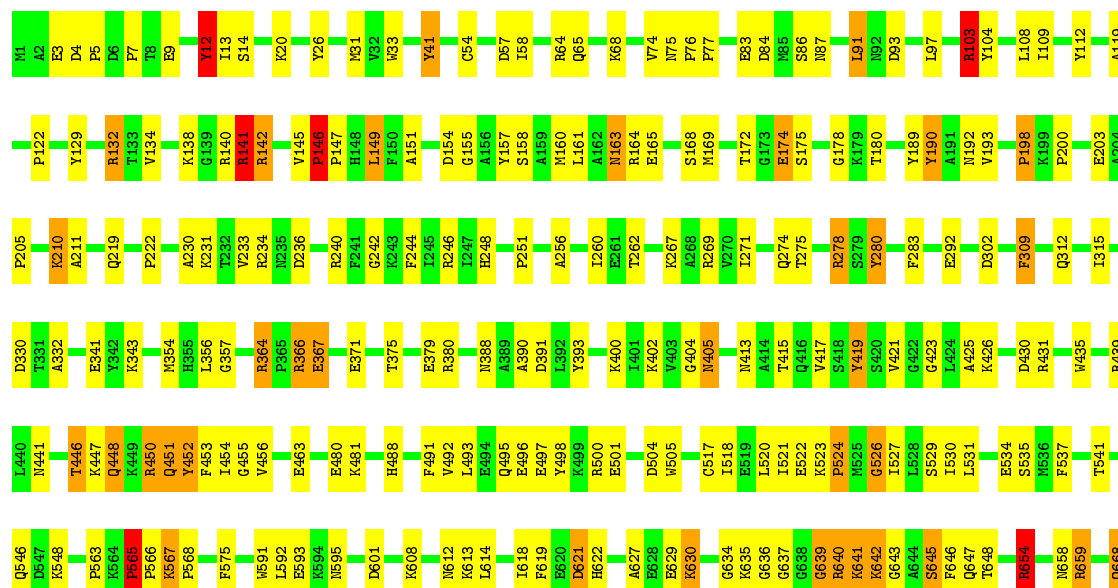
● Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE



[illegible]

- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE

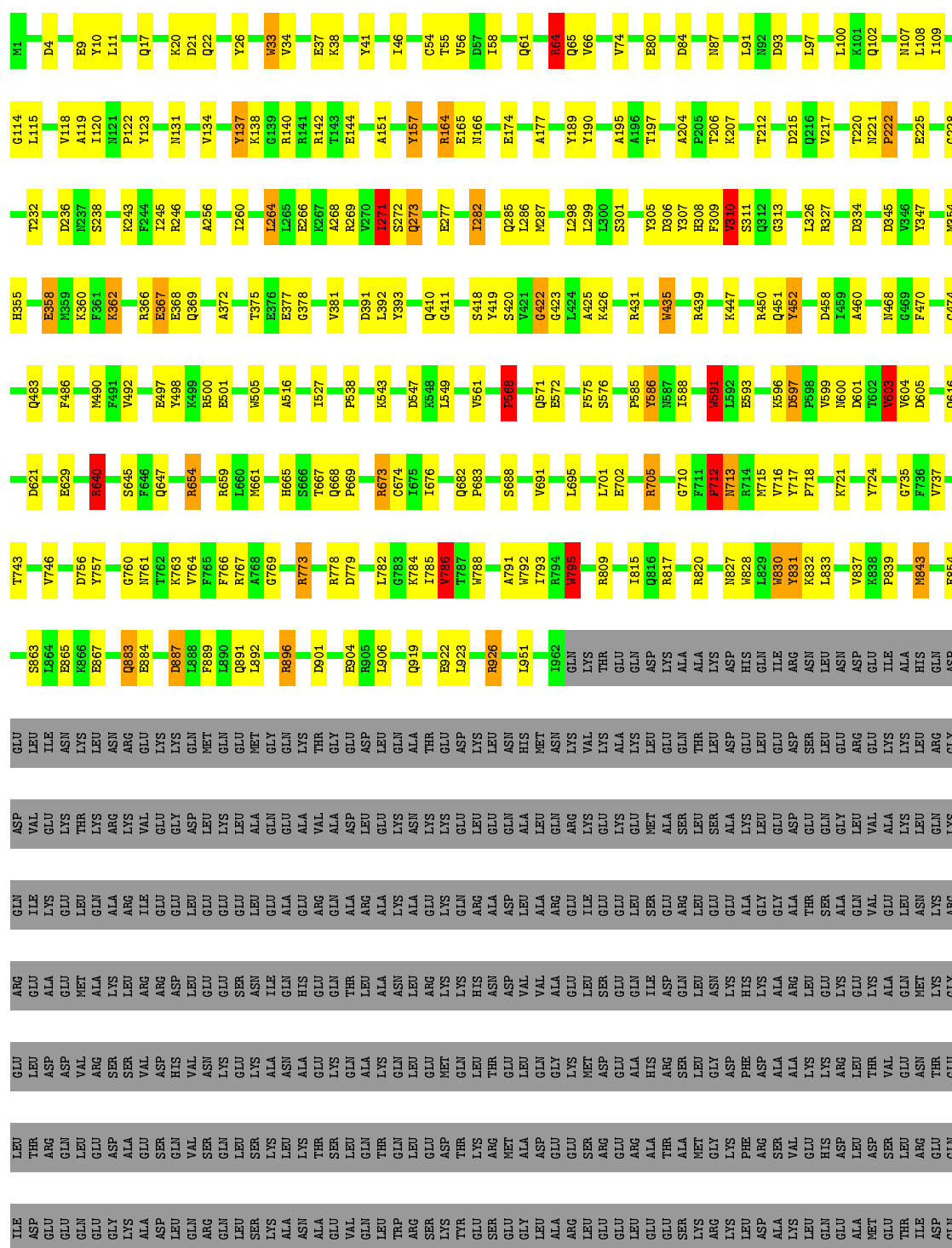
Chain B: 33% 13% . 51%



[illegible]

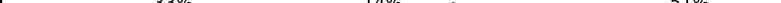
- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE

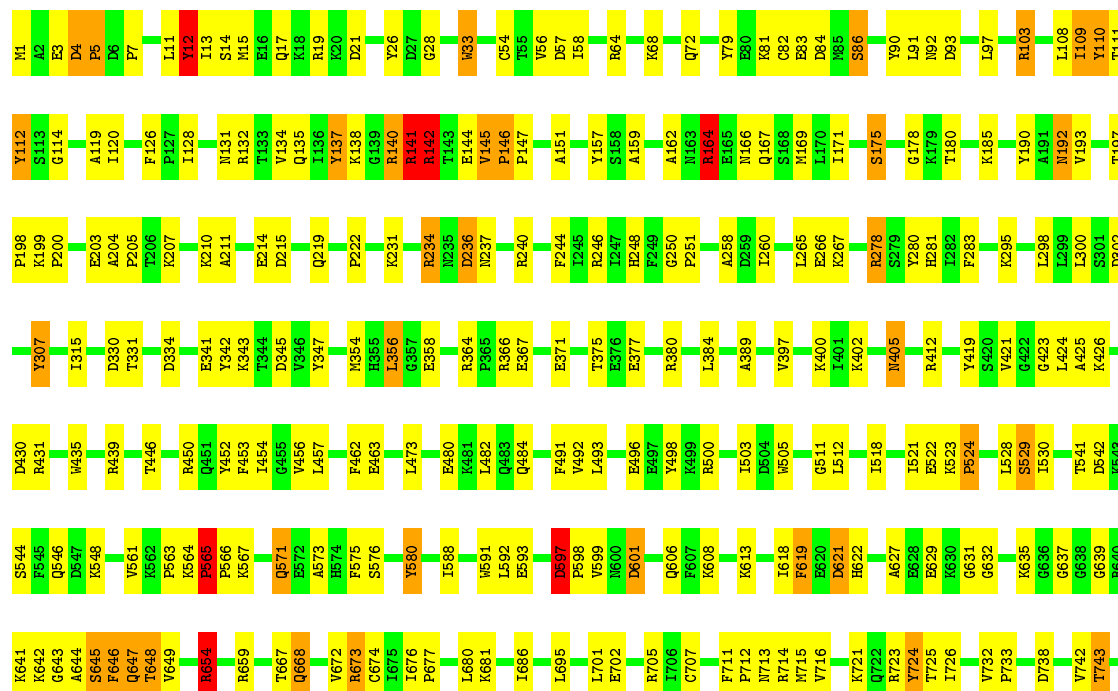
Chain G:



[illegible]

- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE

Chain H:  33% 14% 51%



[illegible]


SER
LYS
ILE
ASP
GLU
GLU

• Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

Chain C:  86% 12%




• Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

Chain D:  83% 15%



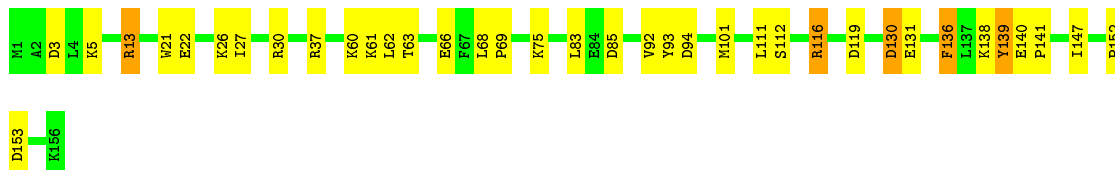
• Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

Chain I:  83% 15%



• Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

Chain J:  76% 21%



• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE

Chain E:  73% 24%



• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE

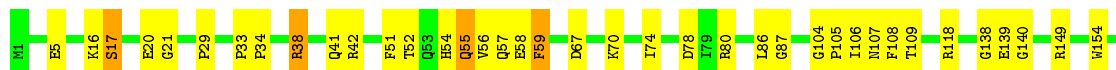
Chain F:  64% 29% 6%





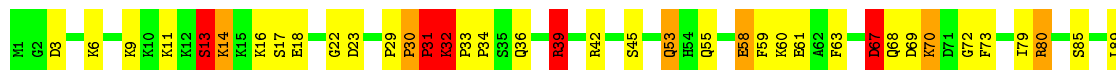
• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE

Chain K: 78% 19%



• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE

Chain L: 63% 28% 7%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1950	Depositor
Maximum defocus (nm)	1950	Depositor
Magnification	35000	Depositor
Image detector	KODAK SO-163 FILM	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	0.65	0/7867	1.36	93/10591 (0.9%)
1	B	0.64	0/7885	1.35	68/10614 (0.6%)
1	G	0.64	0/7867	1.33	75/10591 (0.7%)
1	H	0.64	0/7885	1.34	64/10614 (0.6%)
2	C	0.66	0/1251	1.20	6/1674 (0.4%)
2	D	0.66	0/1251	1.19	8/1674 (0.5%)
2	I	0.64	0/1251	1.21	9/1674 (0.5%)
2	J	0.65	0/1251	1.21	7/1674 (0.4%)
3	E	0.64	0/1554	1.20	10/2081 (0.5%)
3	F	0.64	0/1554	1.30	11/2081 (0.5%)
3	K	0.65	0/1554	1.24	9/2081 (0.4%)
3	L	0.69	0/1554	1.40	17/2081 (0.8%)
All	All	0.65	0/42724	1.32	377/57430 (0.7%)

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	32
1	B	0	20
1	G	0	25
1	H	0	19
2	D	0	1
2	I	0	1
2	J	0	4
3	E	0	1
3	F	0	3
3	K	0	2
3	L	0	8
All	All	0	116

There are no bond length outliers.

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	PRO	CA-N-CD	-13.39	92.75	111.50
1	B	380	ARG	NE-CZ-NH1	-12.71	113.94	120.30
1	G	140	ARG	NE-CZ-NH1	-10.79	114.91	120.30
1	B	654	ARG	NE-CZ-NH1	-10.67	114.97	120.30
1	G	367	GLU	CA-C-N	10.62	140.56	117.20

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	142	ARG	Sidechain
1	A	157	TYR	Sidechain
1	A	41	TYR	Sidechain
1	A	64	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	7721	0	7778	123	0
1	B	7739	0	7799	165	0
1	G	7721	0	7778	108	0
1	H	7739	0	7799	130	0
2	C	1233	0	1227	9	0
2	D	1233	0	1227	9	0
2	I	1233	0	1227	10	0
2	J	1233	0	1227	14	0
3	E	1529	0	1491	27	0
3	F	1529	0	1491	28	0
3	K	1529	0	1491	23	0
3	L	1529	0	1491	47	0
All	All	41968	0	42026	606	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 7.

The worst 5 of 606 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:B:641:LYS:HE3	1:B:642:LYS:NZ	1.21	1.52
1:B:641:LYS:CE	1:B:642:LYS:NZ	2.16	1.08
1:A:364:ARG:HA	3:L:31:PRO:HG2	1.42	1.00
1:B:641:LYS:CE	1:B:642:LYS:HZ1	1.70	0.99
1:A:364:ARG:HA	3:L:31:PRO:CG	1.95	0.94

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	960/1953 (49%)	772 (80%)	149 (16%)	39 (4%)	3	35
1	B	962/1953 (49%)	779 (81%)	128 (13%)	55 (6%)	2	28
1	G	960/1953 (49%)	783 (82%)	136 (14%)	41 (4%)	3	34
1	H	962/1953 (49%)	779 (81%)	125 (13%)	58 (6%)	2	26
2	C	154/156 (99%)	137 (89%)	13 (8%)	4 (3%)	7	45
2	D	154/156 (99%)	139 (90%)	11 (7%)	4 (3%)	7	45
2	I	154/156 (99%)	135 (88%)	16 (10%)	3 (2%)	10	52
2	J	154/156 (99%)	131 (85%)	19 (12%)	4 (3%)	7	45
3	E	194/196 (99%)	139 (72%)	40 (21%)	15 (8%)	1	20
3	F	194/196 (99%)	136 (70%)	41 (21%)	17 (9%)	1	17
3	K	194/196 (99%)	144 (74%)	37 (19%)	13 (7%)	1	24
3	L	194/196 (99%)	129 (66%)	46 (24%)	19 (10%)	1	14
All	All	5236/9220 (57%)	4203 (80%)	761 (14%)	272 (5%)	5	30

5 of 272 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	22	GLN
1	A	138	LYS
1	A	269	ARG
1	A	310	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	833/1689 (49%)	792 (95%)	41 (5%)	31	67
1	B	835/1689 (49%)	780 (93%)	55 (7%)	21	57
1	G	833/1689 (49%)	798 (96%)	35 (4%)	36	70
1	H	835/1689 (49%)	785 (94%)	50 (6%)	24	60
2	C	132/132 (100%)	126 (96%)	6 (4%)	34	69
2	D	132/132 (100%)	126 (96%)	6 (4%)	34	69
2	I	132/132 (100%)	127 (96%)	5 (4%)	40	73
2	J	132/132 (100%)	125 (95%)	7 (5%)	28	64
3	E	164/164 (100%)	157 (96%)	7 (4%)	35	70
3	F	164/164 (100%)	150 (92%)	14 (8%)	13	48
3	K	164/164 (100%)	160 (98%)	4 (2%)	57	82
3	L	164/164 (100%)	154 (94%)	10 (6%)	23	60
All	All	4520/7940 (57%)	4280 (95%)	240 (5%)	33	64

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	18	GLU
1	G	215	ASP
2	J	94	ASP
3	E	58	GLU

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Mol	Chain	Res	Type
3	F	55	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	130	ASN
1	G	665	HIS
2	I	73	GLN
1	G	87	ASN
1	G	670	HIS

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.