



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 1, 2017 – 05:16 PM EDT

PDB ID : 5TBY  
EMDB ID: : EMD-2240  
Title : HUMAN BETA CARDIAC HEAVY MEROMYOSIN INTERACTING-HEADS MOTIF OBTAINED BY HOMOLOGY MODELING (USING SWISS-MODEL) OF HUMAN SEQUENCE FROM APHONOPELMA HOMOLOGY MODEL (PDB-3JBH), RIGIDLY FITTED TO HUMAN BETA-CARDIAC NEGATIVELY STAINED THICK FILAMENT 3D-RECONSTRUCTION (EMD-2240)  
Authors : ALAMO, L.; WARE, J.S.; PINTO, A.; GILLILAN, R.E.; SEIDMAN, J.G.; SEIDMAN, C.E.; PADRON, R.  
Deposited on : unknown  
Resolution : 20.00 Å(reported)  
Based on PDB ID : 3JBH

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](mailto: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.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)

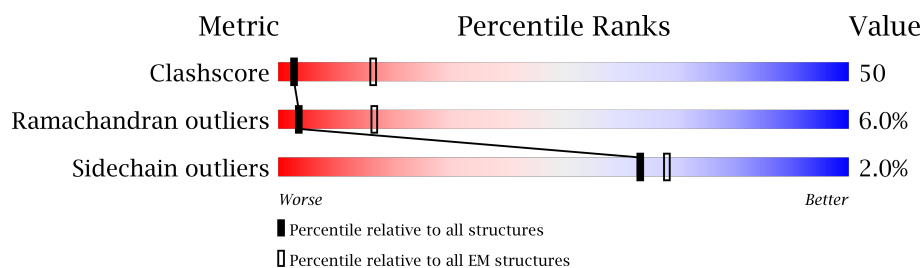
# 1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	1935	
1	B	1935	
2	C	195	
2	D	195	
3	E	166	
3	F	166	

Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20357 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-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	954	Total	C	N	O	S	0	0
			7704	4899	1324	1439	42		
1	B	950	Total	C	N	O	S	0	0
			7673	4877	1320	1435	41		

- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	152	Total	C	N	O	S	0	0
			1212	759	202	240	11		
2	D	152	Total	C	N	O	S	0	0
			1212	759	202	240	11		

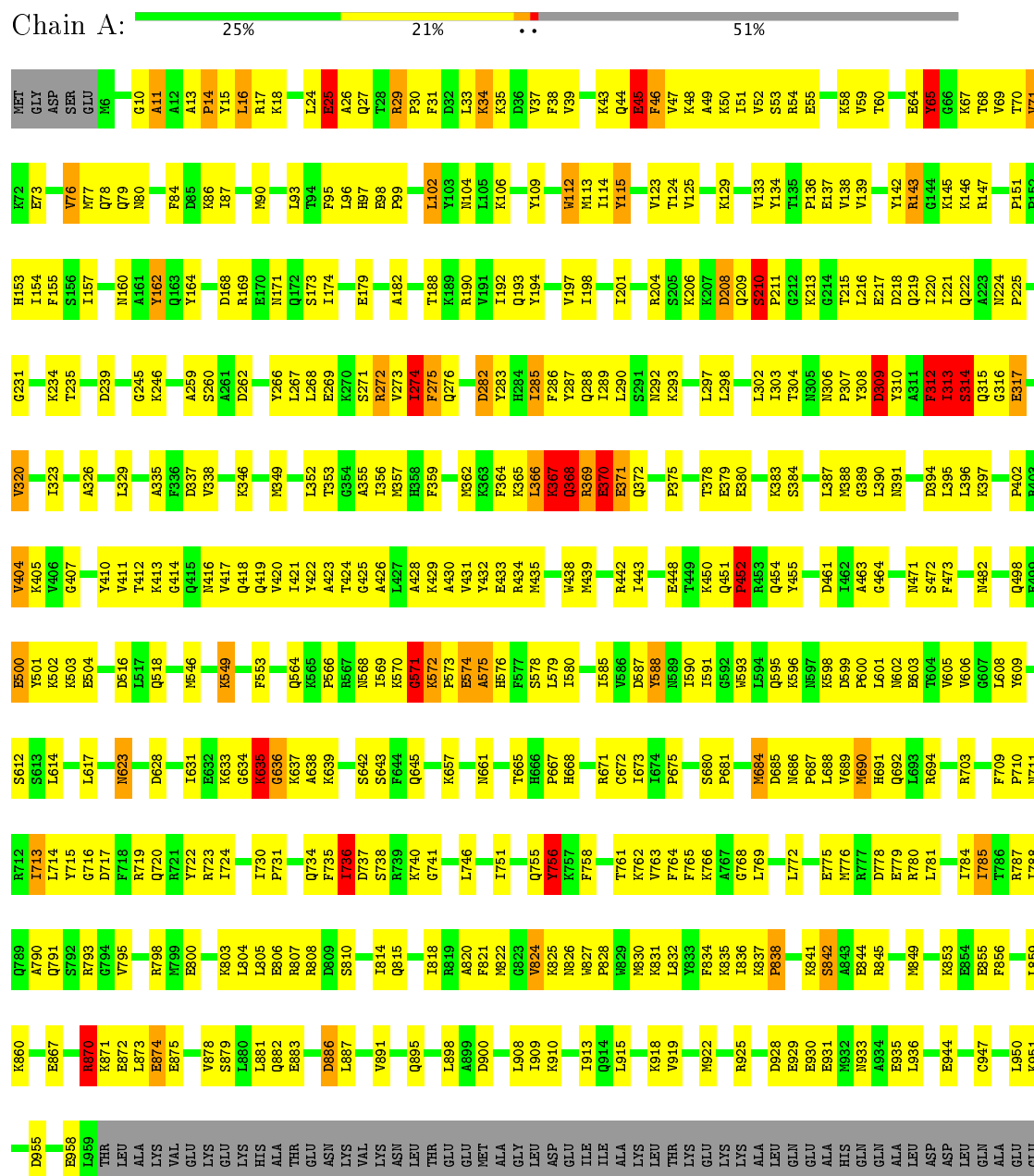
- Molecule 3 is a protein called Myosin regulatory light chain 2, ventricular/cardiac muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	160	Total	C	N	O	S	0	0
			1278	808	212	252	6		
3	F	160	Total	C	N	O	S	0	0
			1278	808	212	252	6		

### 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 the various outlier classes 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.

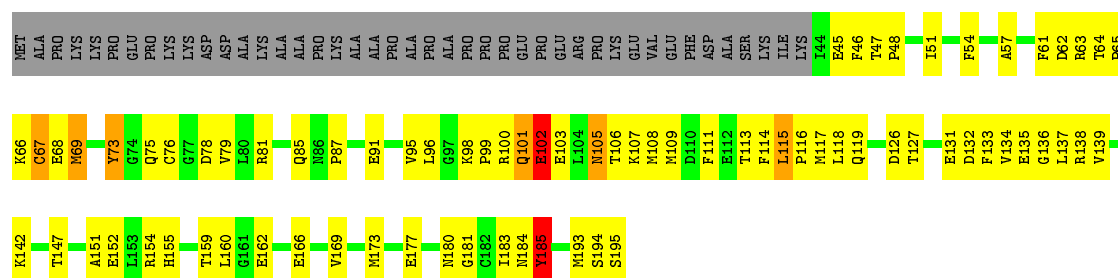
- Molecule 1: Myosin-7



- Molecule 1: Myosin-7

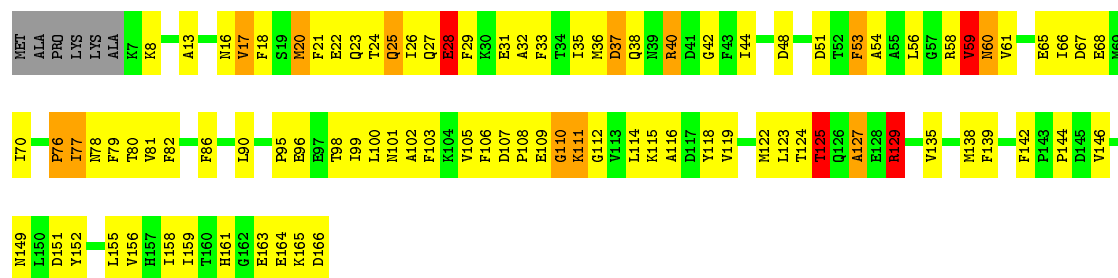
THR	ALA	ASP	ASP	E944	S866	K802	A728	S643	P573	H492	Q418	K351	K278	Q209	A141	E73
ALA	ARG	LEU	ARG	C947	E867	K803	A729	F644	E574	H493	Q419	L352	R281	S210	A142	E76
ALA	ALA	LEU	LEU		A868	L804	F730	Q645	A575	F494	Q420	T353		P211	R143	M77
LYS	ASN	GLN	LYS		R869	L805	F731	T646	H576	V495	I421	G354	D282	G212	K145	Q78
LEU	VAL	ALA	ASP		R870	E806	E732	V647		L496	Y422	A355	Y283	K213	K146	Q79
LYS	LYS	GLU	GLU		K871	R807	G733		L579	E497	A426	K356	H284	G214	R147	N80
LEU	LYS	GLN	GLU		E872	R808	Q734	L850	L580	Q498	A427	K357	P286	E217	F81	
LYS	LEU	D809	F735		L873	E809	F736	H651		Q499	L428	H358		D218	P82	
HIS	ARG	LYS	LYS		E874	S810	I738	R652	T585	E500	A428	F359	Y287	Q219	A150	
ALA	ASP	VAL	ASN		R875	L811	F737			Y501	K430		Q288	Q220	P151	
SER	SER	ASN	THR		N856	V813	S738		Y588	K503	V431		L289	L221	P152	
LEU	LEU	THR	LEU		H666	V814			N569	K504	Y432		L290	L222	H153	
LEU	LEU	THR	LEU		P667	Q815	L744		N590	E504	V433		L287	Q223	I154	
ALA	ARG	LYS	THR		H668	Q816	L745		F591	E505	E433		N292	A224	F155	
GLU	GLU	ALA	ALA		P669	N817	L746		G592	L506	E434		K293	K224	S156	
GLY	GLU	LYS	LYS		F669	N817			W593	E507	M435		K294		I157	
GLU	GLU	ASP	ASP		D750	I818	D750		L594				P295	L227	D158	
GLU	ILE	VAL	VAL		H671	F821	F751		N597	D516	M438		L296	E228	D159	
GLN	LEU	LYS	LYS		C672	M822	H752		K597	L517	M439		L297	A229	N160	
LEU	LEU	LEU	LEU		L674	G823	H753		K598	E370	V440		L298		A161	
ASN	GLU	GLN	GLN		L675	V824	Q755		D599	G372			L302	N232	Y162	
LEU	LEU	ALA	ALA		K825	R824	Y756		L601	A373	I443		L303	A233	G163	
GLN	GLN	LEU	LEU		N826	K825	K757		N602	E374	N444		T303	K234	Y164	
VAL	VAL	ASN	VAL		K827	N826	K758		E603	P375			T304	K235	M165	
GLU	GLU	ASN	ASN		E901	M827	F758		T604		L447			V236	L166	
ARG	ALA	ASP	ASP		E902	W829	G759		V605	E448	E448		D309	R237	T167	
VAL	ALA	ARG	ARG		E903	M829	H760			E525	T449		Y310	N238	D168	
GLN	GLY	GLY	GLY		R904	M830	F761		Y609	K526	K450		F311	D239	R169	
ALA	ALA	GLY	GLY		K831	K831	K762			P527	Q451		F312			
LEU	LEU	ASP	ASP		L832	L832	V763				P452		L313	S242	Q172	
GLU	SER	GLU	SER		Y909	Y833	F764		S612	L530	K453		Q315	R243	S173	
GLU	GLU	LEU	LEU		K910	F834	F765		S613	M531	Q454			R244	S174	
GLU	GLN	GLN	GLN		K835	L835	K766		L614	S532	F455			G245	L175	
ILE	ILE	GLU	GLU		Y913	L836	L769		K615	S533	F456			K246	L176	
LYS	LYS	GLY	GLY		Q914	K837	L770		L616	L534	L457			F247		
GLU	GLU	LYS	LYS		L915	P838	L771		L617		G458					
PHE	ASN	VAL	VAL			L839	G771		S618	C538	V459		S322	L248	E179	
LEU	LYS	ARG	ARG		K918	L840	E774		T619	M539			L323	R249	S180	
LEU	LEU	MET	MET		W919	K841	E774		L620	F540	A463		D325	L250	M113	
LEU	ARG	LEU	LEU		N922	S842	E775		F621		F464		A326	H251	G183	
LEU	LEU	LEU	LEU		E922	E843	M776		A632		F465			T255		
ASP	LYS	GLU	GLU		N923	E844	R777		K623	T544	E466		L329	G256	V186	
ASP	GLU	ARG	ARG		E924	R845	F709		K624					G257		
VAL	PHE	LEU	ALA		R925	E846	L781		A625	T547	F470		R330	K258	R190	
THR	GLN	LEU	LYS		L926	R847	R782		G626	K549	N471		T332	L259	V191	
SER	LYS	ARG	ARG		E927	E848	R783		A627	A550	S472			G260	I192	
ASN	MET	LYS	LYS		D928	M849	L784		D628	X551	F473		A335	L263	Q193	
MET	ARG	ILE	LEU		E929		L785			L552	E474		F336	E264	F195	
GLU	ARG	GLU	GLU		E930	M852	L786		L631	F553	Q475		V338	T265	V197	
GLN	GLY	GLY	GLY		E931		R787		E632		L476		L339	Y286	I198	
ILE	LEU	LEU	LEU		N932	E855	L788		K633	N562	E483			L267	A199	
ILE	GLU	GLU	GLU		N933	F856	Q789		G634	F563	K484			G268		
ALA	ALA	LEU	LEU		E935	L859	A790		K635	O564			T342	L268	A200	
LYS	THR	LEU	LEU		L936	K860	Q791		G636	F565	L485			E269	L201	
ALA	LEU	THR	ALA		T937	E861	S792		K637	F566	Q486			K270	R204	
ASN	GLN	GLU	GLU		A938	E862	R793		A638		F488		K346	I274	S205	
LEU	ALA	GLU	ALA		R939	L863	G794		K639	S569	F489		N347	F275	E137	
HIS	HIS	SER	SER			K864	L795		K640	X570	F489		S348	Q276	F138	
GLU	GLU	ILE	ILE			E864	L726		S641	G571	M400		K349	L277	V139	
THR	THR	THR	THR			K865	P727		S642	S573	R201		T552	L277	L400	





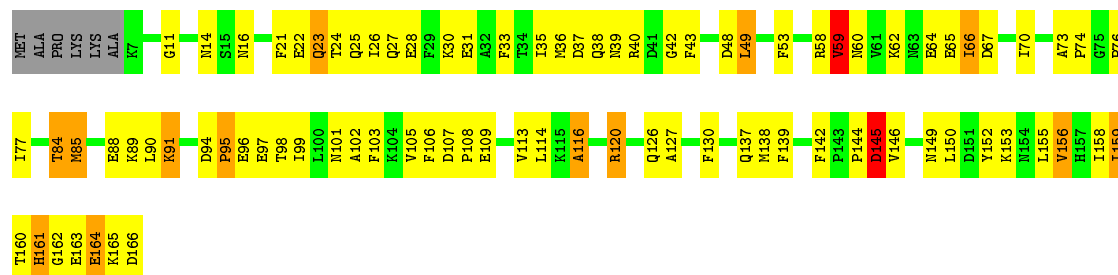
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain E: 40% 46% 7% . .



- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain F: 44% 43% 8% . .





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	10700	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	9	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	0.61	3/7851 (0.0%)	1.11	54/10556 (0.5%)
1	B	0.62	1/7819 (0.0%)	1.11	48/10513 (0.5%)
2	C	0.60	0/1231	1.05	2/1651 (0.1%)
2	D	0.78	4/1231 (0.3%)	1.13	9/1651 (0.5%)
3	E	0.89	3/1301 (0.2%)	1.25	8/1747 (0.5%)
3	F	0.60	0/1301	1.15	6/1747 (0.3%)
All	All	0.65	11/20734 (0.1%)	1.12	127/27865 (0.5%)

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	20
1	B	0	19
2	C	0	2
3	E	0	3
3	F	0	4
All	All	0	48

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	129	ARG	CZ-NH1	-19.60	1.07	1.33
2	D	101	GLN	C-O	-10.93	1.02	1.23
3	E	129	ARG	NE-CZ	9.37	1.45	1.33
3	E	129	ARG	CZ-NH2	9.25	1.45	1.33
1	A	112	TRP	CG-CD1	-8.76	1.24	1.36

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	129	ARG	NE-CZ-NH2	-25.59	107.50	120.30
1	A	756	TYR	CZ-CE2-CD2	15.78	134.00	119.80
1	B	641	GLY	CA-C-O	-13.49	96.31	120.60
3	F	120	ARG	NE-CZ-NH1	12.91	126.76	120.30
1	B	102	LEU	CB-CG-CD2	-12.58	89.62	111.00

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	15	TYR	Sidechain
1	A	162	TYR	Sidechain
1	A	25	GLU	Mainchain
1	A	45	GLU	Mainchain

## 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	7704	0	7735	681	0
1	B	7673	0	7706	1064	0
2	C	1212	0	1182	120	0
2	D	1212	0	1183	234	0
3	E	1278	0	1241	179	0
3	F	1278	0	1239	234	0
All	All	20357	0	20286	2030	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 50.

The worst 5 of 2030 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:804:LEU:CD2	2:D:63:ARG:HD3	1.21	1.56
1:A:714:LEU:HD21	1:B:396:LEU:CD1	1.15	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:LYS:HD3	3:F:163:GLU:CG	1.34	1.55
3:E:8:LYS:CD	3:F:59:VAL:HA	1.33	1.54
1:A:714:LEU:CD2	1:B:396:LEU:HD12	1.33	1.53

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	952/1935 (49%)	759 (80%)	141 (15%)	52 (6%)	2	25
1	B	948/1935 (49%)	781 (82%)	111 (12%)	56 (6%)	2	23
2	C	150/195 (77%)	132 (88%)	12 (8%)	6 (4%)	3	31
2	D	150/195 (77%)	133 (89%)	12 (8%)	5 (3%)	4	35
3	E	158/166 (95%)	111 (70%)	32 (20%)	15 (10%)	1	14
3	F	158/166 (95%)	115 (73%)	27 (17%)	16 (10%)	1	12
All	All	2516/4592 (55%)	2031 (81%)	335 (13%)	150 (6%)	3	23

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	27	GLN
1	A	208	ASP
1	A	272	ARG
1	A	313	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	831/1695 (49%)	811 (98%)	20 (2%)	54	78
1	B	828/1695 (49%)	811 (98%)	17 (2%)	59	80
2	C	133/167 (80%)	132 (99%)	1 (1%)	85	92
2	D	133/167 (80%)	132 (99%)	1 (1%)	85	92
3	E	137/141 (97%)	135 (98%)	2 (2%)	70	85
3	F	137/141 (97%)	133 (97%)	4 (3%)	48	73
All	All	2199/4006 (55%)	2154 (98%)	45 (2%)	63	82

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	ARG
1	B	416	ASN
3	F	25	GLN
1	B	151	PRO
1	B	420	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	589	ASN
1	B	760	HIS
3	F	60	ASN
1	B	597	ASN
1	B	726	ASN

### 5.3.3 RNA ⓘ

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.