wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:47 PM BST

PDB ID	:	3J5R
EMDB ID:	:	EMD-5777
Title	:	Reconstruction of TRPV1 ion channel in complex with capsaicin by single particle cryo-microscopy
Authors	:	Liao, M.; Cao, E.; Julius, D.; Cheng, Y.
Deposited on	:	2013-10-28
Resolution	:	4.20 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

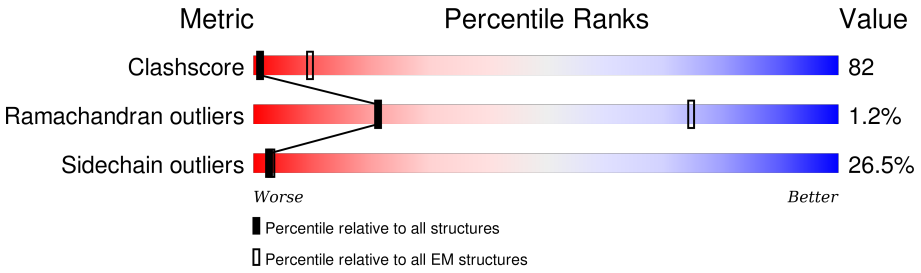
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	598	41% 41% 17% ••
1	B	598	41% 40% 17% •
1	C	598	42% 40% 17% ••
1	D	598	41% 41% 17% ••

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17564 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 Transient receptor potential cation channel subfamily V member 1.

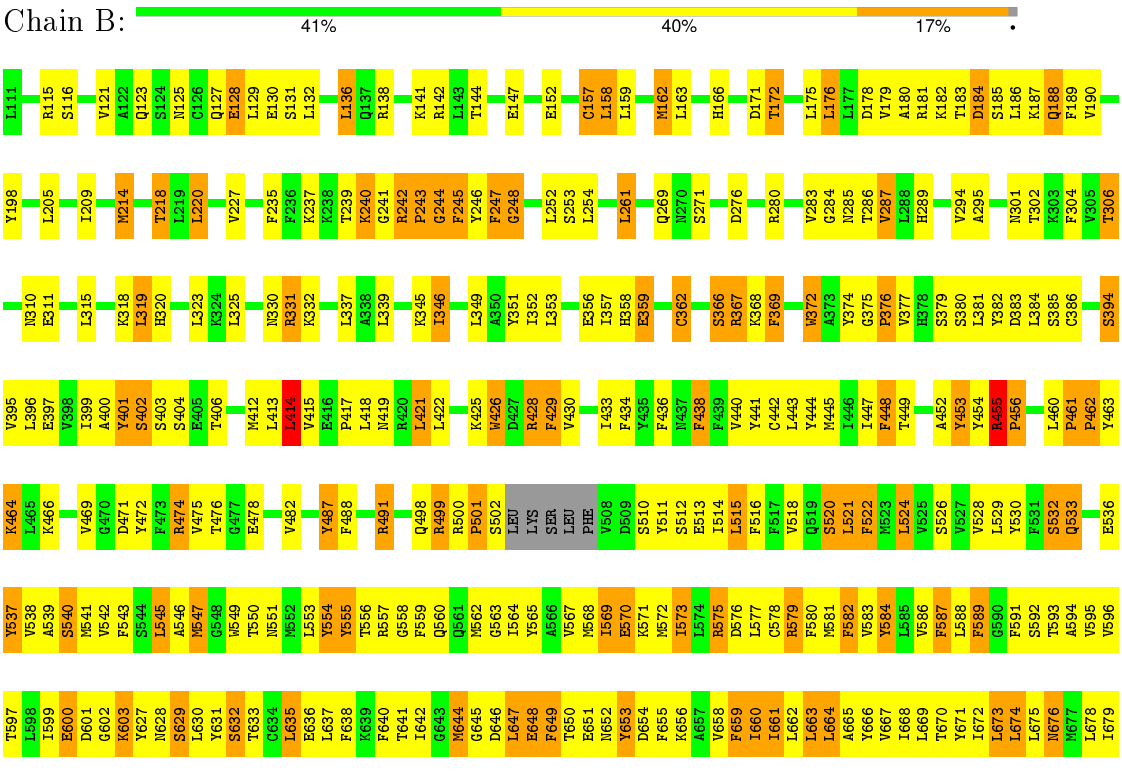
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	592	Total	C	N	O	S	0	0
			4391	2847	726	798	20		
1	A	592	Total	C	N	O	S	0	0
			4391	2847	726	798	20		
1	C	592	Total	C	N	O	S	0	0
			4391	2847	726	798	20		
1	D	592	Total	C	N	O	S	0	0
			4391	2847	726	798	20		

3 Residue-property plots (i)

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.

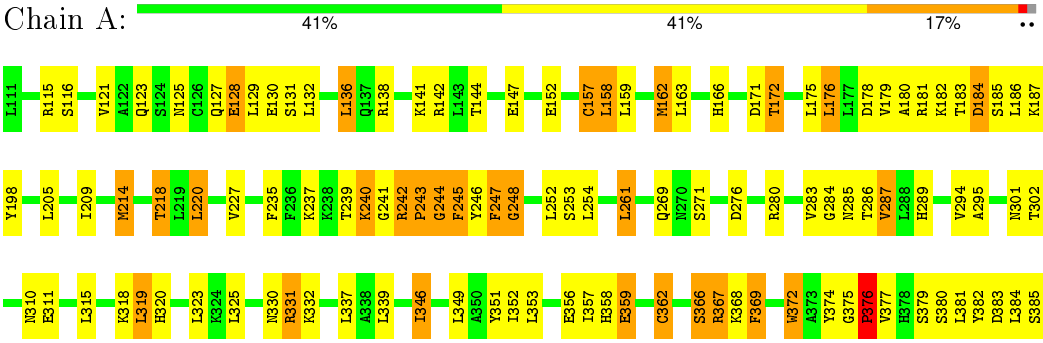
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

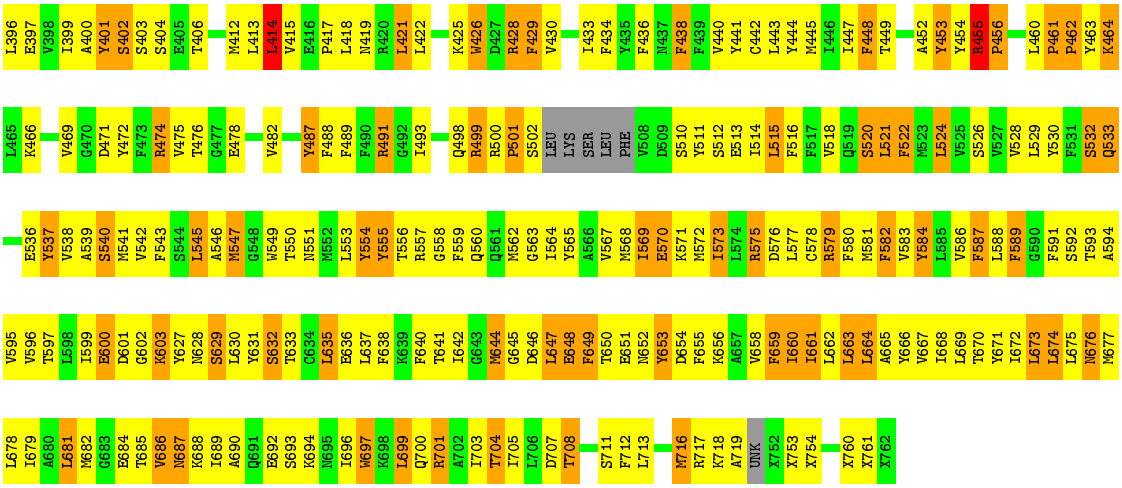
Chain B:



- Molecule 1: Transient receptor potential cation channel subfamily V member 1

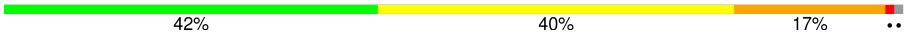
Chain A:

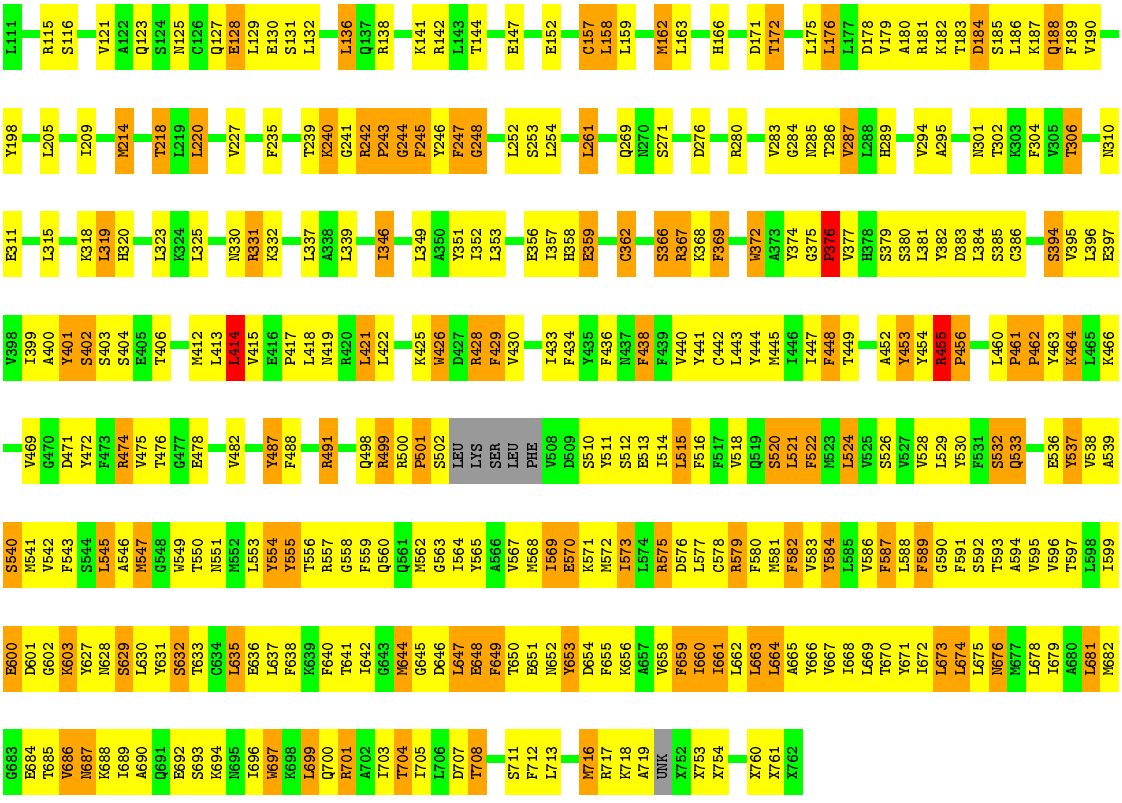




• Molecule 1: Transient receptor potential cation channel subfamily V member 1

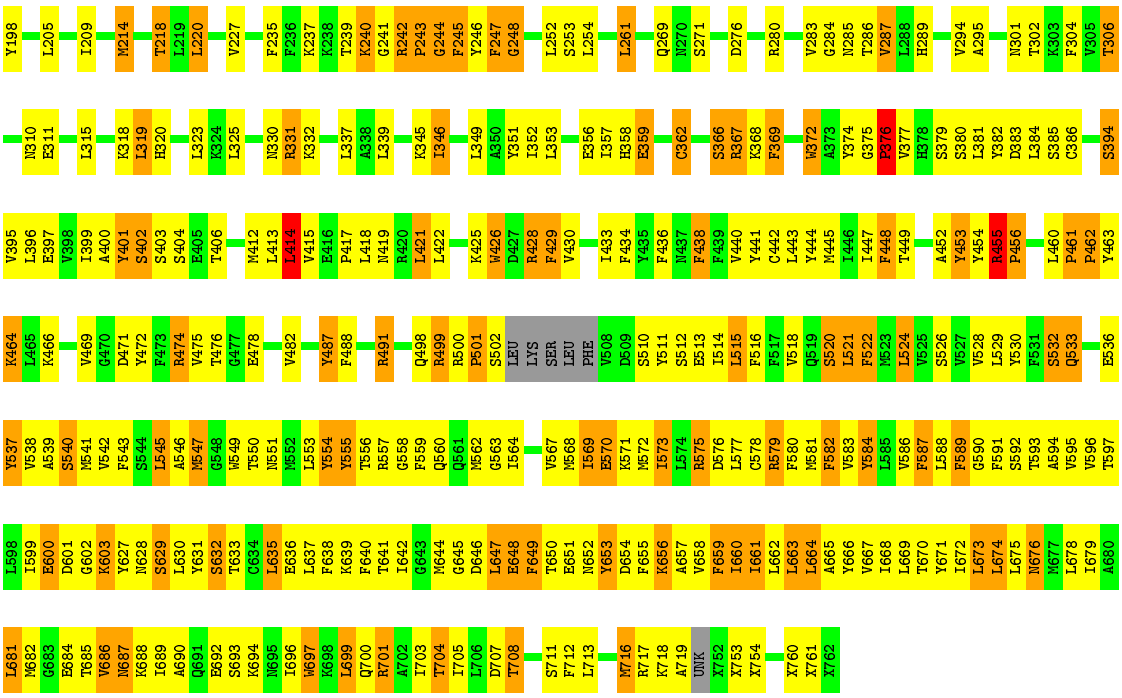
Chain C:





• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D:


Y198 L205 I209 M214 T218 L219 L220 V227 F235 F236 K237 K238 T239 K240 G241 R242 P243 G244 F245 Y246 F247 G248 L252 S253 L254 L261 Q269 N270 S271 D276 R280 V283 G284 N285 T286 V287 L288 H289 V294 A295 N301 T302 K303 F304 V305 T306
N310 E311 L315 K318 L319 H320 L323 K324 L325 N330 R331 K332 L337 A338 L339 K345 I346 L349 A350 Y351 I352 L353 E356 I357 H358 E359 C362 S366 R367 K368 F369 W372 A373 Y374 G375 P376 V377 H378 S379 S380 L381 Y382 D383 L384 S385 C386 S394
V395 L396 E397 V398 I399 A400 Y401 S402 S403 S404 E405 T406 M412 L413 L414 V415 E416 P417 L418 N419 R420 L421 L422 K425 W426 D427 R428 F429 V430 I433 F434 Y435 F436 N437 F438 F439 V440 Y441 C442 L443 Y444 M445 I446 I447 F448 T449 A452 Y453 Y454 R455 P456 L460 P461 P462 Y463
K464 L465 K466 V469 G470 D471 Y472 F473 R474 V475 T476 G477 E478 V482 Y487 F488 R491 Q498 R499 R500 P501 S502 LEU LYS SER LEU PHE V508 D509 S510 Y511 S512 E513 I514 L515 F516 F517 V518 Q519 S520 L521 F522 M523 L524 V525 S526 V527 V528 L529 Y530 P531 S532 Q533 E536
Y537 V538 A539 S540 M541 V542 F543 S544 L545 A546 M547 G548 W549 T550 N551 M552 L553 Y554 Y555 T556 R557 G558 F559 Q560 Q561 M562 G563 I564 V567 M568 I569 E570 K571 M572 I573 L574 R575 D576 L577 C578 R579 F580 M581 F582 V583 Y584 L585 V586 F587 L588 F589 G590 F591 S592 T593 A594 V595 V596 T597
L598 I599 E600 D601 G602 K603 Y627 N628 S629 L630 Y631 S632 T633 C634 L635 E636 L637 F638 K639 F640 T641 I642 G643 M644 G645 D646 L647 E648 F649 T650 E651 N652 Y653 D654 F655 K656 A657 V658 F659 I660 I661 L662 L663 L664 A665 Y666 V667 I668 L669 T670 Y671 I672 L673 L674 L675 N676 M677 L678 I679 A680
L681 M682 G683 E684 T685 V686 N687 K688 I689 A690 Q691 E692 S693 K694 M695 I696 W697 K698 L699 Q700 R701 A702 I703 T704 I705 L706 D707 T708 S711 F712 L713 M716 R717 K718 A719 UNK X752 X753 X754 X760 X761 X762

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	33238	Depositor
Resolution determination method	Gold standard FSC at 0.143 criteria	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	31000	Depositor
Image detector	Gatan K2 Summit	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	0.50	6/4425 (0.1%)	0.66	6/6016 (0.1%)
1	B	0.50	5/4425 (0.1%)	0.66	6/6016 (0.1%)
1	C	0.50	6/4425 (0.1%)	0.66	6/6016 (0.1%)
1	D	0.50	6/4425 (0.1%)	0.66	6/6016 (0.1%)
All	All	0.50	23/17700 (0.1%)	0.66	24/24064 (0.1%)

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	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	MET	CG-SD	7.70	2.01	1.81
1	D	162	MET	CG-SD	7.69	2.01	1.81
1	B	162	MET	CG-SD	7.68	2.01	1.81
1	C	162	MET	CG-SD	7.66	2.01	1.81
1	B	214	MET	CG-SD	6.28	1.97	1.81

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	359	GLU	C-N-CD	5.83	140.65	128.40
1	C	359	GLU	C-N-CD	5.83	140.65	128.40
1	B	359	GLU	C-N-CD	5.83	140.65	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	359	GLU	C-N-CD	5.83	140.63	128.40
1	A	460	LEU	C-N-CD	5.56	140.08	128.40

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	243	PRO	Peptide
1	B	244	GLY	Peptide
1	B	247	PHE	Peptide
1	B	248	GLY	Peptide
1	B	376	PRO	Peptide

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	4391	0	4117	749	0
1	B	4391	0	4117	751	0
1	C	4391	0	4117	739	0
1	D	4391	0	4117	758	0
All	All	17564	0	16468	2807	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 82.

The worst 5 of 2807 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:376:PRO:HG3	1:D:245:PHE:CD2	1.23	1.70
1:A:655:PHE:CE2	1:C:536:GLU:HA	1.29	1.66
1:C:655:PHE:CE1	1:D:539:ALA:HB2	1.15	1.64
1:B:539:ALA:HB2	1:D:655:PHE:CE1	1.18	1.62
1:B:376:PRO:CG	1:D:245:PHE:CD2	1.76	1.62

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	577/598 (96%)	525 (91%)	45 (8%)	7 (1%)	16	62
1	B	577/598 (96%)	525 (91%)	45 (8%)	7 (1%)	16	62
1	C	577/598 (96%)	525 (91%)	45 (8%)	7 (1%)	16	62
1	D	577/598 (96%)	525 (91%)	45 (8%)	7 (1%)	16	62
All	All	2308/2392 (96%)	2100 (91%)	180 (8%)	28 (1%)	21	62

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	LEU
1	B	417	PRO
1	B	466	LYS
1	B	537	TYR
1	B	653	TYR

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	419/519 (81%)	308 (74%)	111 (26%)	0	5
1	B	419/519 (81%)	308 (74%)	111 (26%)	0	5
1	C	419/519 (81%)	308 (74%)	111 (26%)	0	5
1	D	419/519 (81%)	308 (74%)	111 (26%)	0	5
All	All	1676/2076 (81%)	1232 (74%)	444 (26%)	3	5

5 of 444 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	644	MET
1	C	287	VAL
1	D	575	ARG
1	A	659	PHE
1	C	131	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	C	188	GLN
1	D	423	GLN
1	A	687	ASN
1	C	125	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

There are no chain breaks in this entry.