Full wwPDB EM Validation Report ⓘ

Sep 27, 2021 – 11:00 am BST

PDB ID	:	7ONI
EMDB ID	:	EMD-12995
Title	:	Structure of Neddylated CUL5 C-terminal region-RBX2-ARIH2*
Authors	:	Kostrhon, S.P.; prabu, J.R.; Schulman, B.A.
Deposited on	:	2021-05-25
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

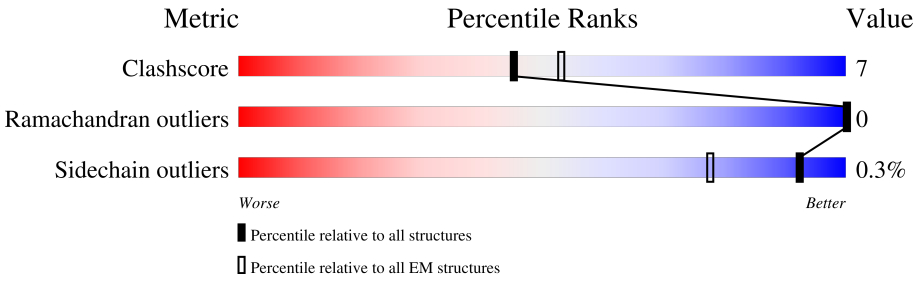
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	C	780	66% 11% 23%
2	H	495	65% 12% 23%
3	R	111	64% 14% 23%
4	N	83	54% 37% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8840 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 Cullin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	599	Total	C	N	O	S	0	0
			4604	2945	792	842	25		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase ARIH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	380	Total	C	N	O	S	0	0
			2965	1875	528	538	24		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP O95376
H	0	SER	-	expression tag	UNP O95376
H	381	ALA	LEU	engineered mutation	UNP O95376
H	382	ALA	GLU	engineered mutation	UNP O95376
H	455	ALA	GLU	engineered mutation	UNP O95376

- Molecule 3 is a protein called RING-box protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	86	Total	C	N	O	S	0	0
			665	414	123	113	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	3	GLY	-	expression tag	UNP Q9UBF6
R	4	SER	-	expression tag	UNP Q9UBF6

- Molecule 4 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	76	Total	C	N	O	S	0	0
			599	378	104	115	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-1	GLY	-	expression tag	UNP Q15843
N	0	SER	-	expression tag	UNP Q15843

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

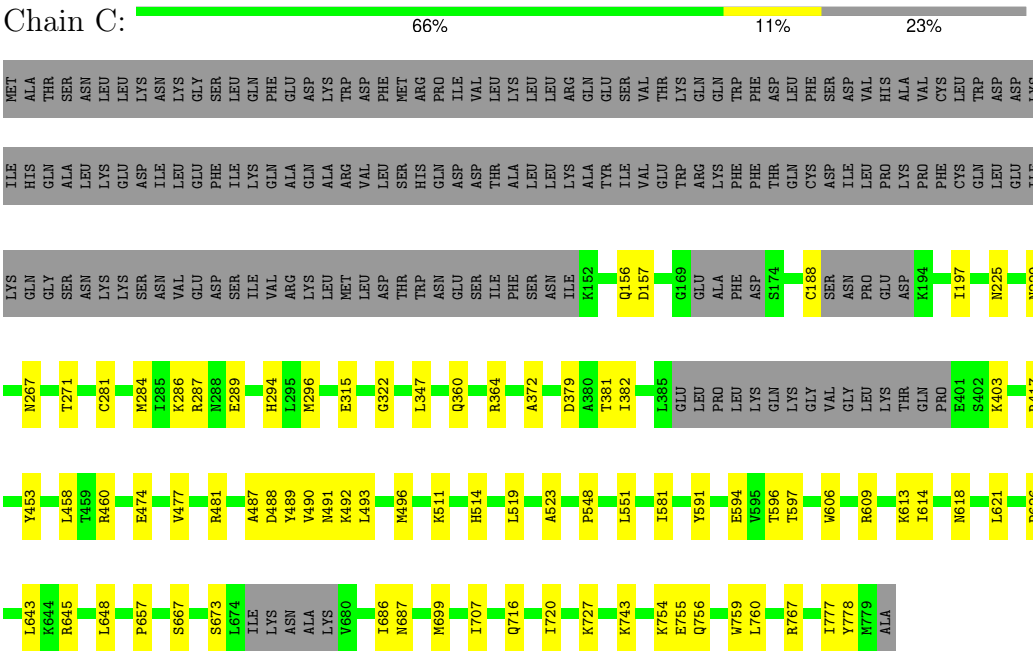
Mol	Chain	Residues	Atoms		AltConf
5	H	4	Total	Zn	0
			4	4	
5	R	3	Total	Zn	0
			3	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

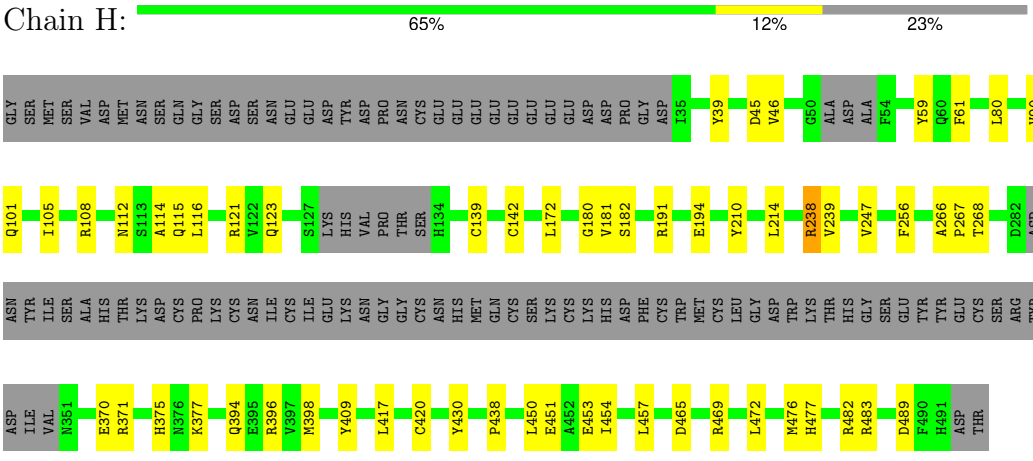
- Molecule 1: Cullin-5

Chain C:



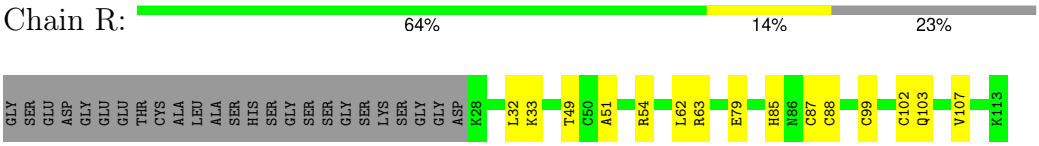
- Molecule 2: E3 ubiquitin-protein ligase ARIH2

Chain H:



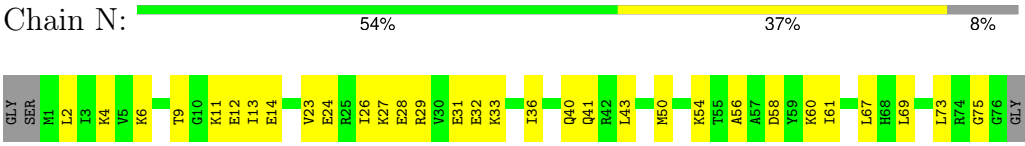
- Molecule 3: RING-box protein 2

Chain R:



• Molecule 4: NEDD8

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191792	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	14.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C	0.25	0/4680	0.46	0/6339
2	H	0.25	0/3032	0.45	0/4118
3	R	0.24	0/681	0.49	0/926
4	N	0.30	0/604	0.55	0/808
All	All	0.26	0/8997	0.46	0/12191

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

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	C	4604	0	4451	50	0
2	H	2965	0	2741	42	0
3	R	665	0	599	9	0
4	N	599	0	638	23	0
5	H	4	0	0	0	0
5	R	3	0	0	0	0
All	All	8840	0	8429	116	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.

All (116) 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)
4:N:24:GLU:HA	4:N:27:LYS:HE2	1.72	0.71
2:H:420:CYS:HB3	2:H:454:ILE:HD11	1.72	0.71
1:C:720:ILE:HD12	4:N:73:LEU:HD22	1.73	0.70
2:H:180:GLY:HA2	2:H:191:ARG:HH21	1.61	0.66
4:N:43:LEU:HD11	4:N:67:LEU:HD13	1.77	0.65
1:C:755:GLU:OE1	1:C:756:GLN:NE2	2.30	0.64
1:C:613:LYS:HD3	1:C:667:SER:HB3	1.80	0.64
2:H:108:ARG:HG3	2:H:115:GLN:HE22	1.61	0.64
2:H:94:ILE:HG22	2:H:105:ILE:HD13	1.80	0.63
2:H:139:CYS:HB3	2:H:142:CYS:SG	2.37	0.63
2:H:194:GLU:OE2	2:H:214:LEU:HD13	1.98	0.63
4:N:4:LYS:HG2	4:N:12:GLU:OE2	1.99	0.62
1:C:621:LEU:HD12	1:C:707:ILE:HG23	1.81	0.62
2:H:121:ARG:HD2	2:H:191:ARG:HH11	1.65	0.62
1:C:594:GLU:OE1	1:C:687:ASN:ND2	2.33	0.60
1:C:460:ARG:NH2	2:H:45:ASP:OD2	2.33	0.60
2:H:268:THR:HG22	2:H:430:TYR:HB2	1.83	0.60
2:H:370:GLU:HG3	2:H:371:ARG:HD2	1.84	0.59
1:C:638:VAL:HG12	1:C:648:LEU:HB2	1.83	0.59
2:H:489:ASP:OD1	3:R:54:ARG:NH1	2.35	0.58
2:H:238:ARG:NH1	2:H:239:VAL:O	2.36	0.58
1:C:267:ASN:O	1:C:271:THR:OG1	2.22	0.58
4:N:61:ILE:HD12	4:N:67:LEU:HD21	1.86	0.57
1:C:492:LYS:O	1:C:496:MET:HG3	2.05	0.57
4:N:28:GLU:HA	4:N:31:GLU:OE1	2.04	0.57
2:H:417:LEU:HD11	2:H:457:LEU:HG	1.88	0.56
1:C:382:ILE:HD13	1:C:403:LYS:HB3	1.88	0.56
1:C:458:LEU:HD23	1:C:493:LEU:HD22	1.87	0.56
2:H:172:LEU:HD12	2:H:181:VAL:HG13	1.87	0.56
1:C:417:ARG:NH1	2:H:39:TYR:OH	2.38	0.56
2:H:101:GLN:O	2:H:105:ILE:HG13	2.05	0.55
1:C:245:ALA:HB2	1:C:261:LEU:HD23	1.88	0.55
1:C:188:CYS:HB3	1:C:197:ILE:HD13	1.90	0.54
2:H:59:TYR:HE2	2:H:61:PHE:HB3	1.73	0.54
1:C:487:ALA:O	1:C:491:ASN:ND2	2.41	0.54
2:H:90:VAL:O	2:H:94:ILE:HG12	2.08	0.53
2:H:396:ARG:NH2	2:H:465:ASP:O	2.42	0.52
4:N:13:ILE:HG23	4:N:33:LYS:HG2	1.92	0.52
4:N:31:GLU:OE2	4:N:41:GLN:NE2	2.43	0.52
4:N:29:ARG:HA	4:N:32:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:472:LEU:O	2:H:476:MET:HG3	2.09	0.51
1:C:315:GLU:HG3	1:C:372:ALA:HB2	1.93	0.51
1:C:645:ARG:NH1	1:C:673:SER:HB2	2.25	0.51
2:H:108:ARG:HB3	2:H:116:LEU:HD13	1.93	0.51
2:H:59:TYR:CE2	2:H:61:PHE:HB3	2.45	0.51
1:C:609:ARG:NH1	1:C:618:ASN:OD1	2.36	0.51
1:C:281:CYS:HA	1:C:296:MET:HE1	1.94	0.50
2:H:453:GLU:OE2	2:H:482:ARG:NH1	2.45	0.50
1:C:322:GLY:HA2	1:C:347:LEU:HD11	1.93	0.49
2:H:482:ARG:HE	3:R:62:LEU:HD12	1.77	0.49
2:H:438:PRO:HG3	3:R:103:GLN:HG2	1.95	0.49
1:C:596:THR:HG22	1:C:597:THR:H	1.77	0.49
1:C:481:ARG:HB2	1:C:490:VAL:HG11	1.94	0.48
1:C:635:TRP:CG	1:C:657:PRO:HG3	2.48	0.48
2:H:394:GLN:O	2:H:398:MET:HG2	2.12	0.48
4:N:23:VAL:HA	4:N:26:ILE:HD12	1.94	0.48
4:N:9:THR:HG23	4:N:11:LYS:H	1.77	0.48
2:H:375:HIS:NE2	2:H:451:GLU:OE2	2.47	0.48
1:C:767:ARG:N	1:C:777:ILE:O	2.43	0.47
1:C:156:GLN:NE2	1:C:157:ASP:OD1	2.48	0.47
3:R:79:GLU:HG3	3:R:107:VAL:HB	1.97	0.47
2:H:59:TYR:CE2	2:H:247:VAL:HG12	2.50	0.47
1:C:488:ASP:OD1	2:H:477:HIS:NE2	2.48	0.47
2:H:112:ASN:O	2:H:115:GLN:NE2	2.44	0.47
1:C:284:MET:HB2	1:C:289:GLU:HG3	1.97	0.46
1:C:759:TRP:HE3	1:C:760:LEU:HD22	1.80	0.46
4:N:2:LEU:HG	4:N:14:GLU:OE2	2.16	0.46
1:C:489:TYR:O	1:C:493:LEU:HG	2.16	0.45
2:H:112:ASN:HB3	2:H:115:GLN:HG3	1.98	0.45
3:R:99:CYS:HB3	3:R:102:CYS:O	2.16	0.45
4:N:43:LEU:HD22	4:N:50:MET:SD	2.56	0.45
3:R:49:THR:HG22	3:R:51:ALA:H	1.81	0.45
1:C:548:PRO:HD2	1:C:551:LEU:HD12	1.98	0.45
4:N:36:ILE:HG13	4:N:41:GLN:HE21	1.82	0.44
4:N:6:LYS:N	4:N:67:LEU:O	2.40	0.44
1:C:626:PRO:HG3	1:C:699:MET:HG2	2.00	0.44
1:C:716:GLN:HG2	1:C:760:LEU:HD21	1.99	0.44
1:C:294:HIS:NE2	1:C:360:GLN:OE1	2.51	0.44
1:C:286:LYS:O	1:C:287:ARG:HG2	2.18	0.44
4:N:31:GLU:HG3	4:N:36:ILE:O	2.17	0.44
1:C:727:LYS:HG3	1:C:778:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:GLU:O	1:C:477:VAL:HG12	2.18	0.43
3:R:32:LEU:HD23	3:R:33:LYS:N	2.33	0.43
4:N:24:GLU:O	4:N:28:GLU:OE1	2.36	0.43
3:R:85:HIS:HB2	3:R:88:CYS:SG	2.59	0.43
1:C:381:THR:HG22	1:C:381:THR:O	2.19	0.43
2:H:472:LEU:HD12	2:H:472:LEU:HA	1.82	0.43
4:N:58:ASP:O	4:N:60:LYS:NZ	2.52	0.43
1:C:606:TRP:CE2	1:C:614:ILE:HD13	2.54	0.42
1:C:225:ASN:HB3	1:C:229:ASN:HB2	2.00	0.42
2:H:266:ALA:HB3	2:H:267:PRO:HD3	2.00	0.42
2:H:80:LEU:HD23	2:H:95:LEU:HG	2.02	0.42
1:C:379:ASP:N	1:C:379:ASP:OD1	2.53	0.42
1:C:441:LEU:HD21	1:C:450:PHE:CE2	2.55	0.42
2:H:114:ALA:O	2:H:123:GLN:NE2	2.53	0.41
1:C:581:ILE:HG12	1:C:594:GLU:HG2	2.02	0.41
1:C:591:TYR:CE2	1:C:673:SER:HA	2.55	0.41
1:C:645:ARG:HH11	1:C:673:SER:HB2	1.85	0.41
2:H:377:LYS:HE3	2:H:377:LYS:HB2	1.84	0.41
4:N:56:ALA:O	4:N:61:ILE:HG22	2.20	0.41
4:N:40:GLN:NE2	4:N:75:GLY:O	2.46	0.41
1:C:643:LEU:HD21	1:C:686:ILE:HD12	2.03	0.41
4:N:54:LYS:HD3	4:N:54:LYS:HA	1.86	0.41
1:C:754:LYS:HB3	1:C:754:LYS:HE2	1.72	0.41
2:H:450:LEU:HD11	2:H:483:ARG:HA	2.02	0.41
1:C:453:TYR:CE1	2:H:46:VAL:HG21	2.55	0.41
1:C:511:LYS:NZ	1:C:523:ALA:O	2.42	0.41
2:H:210:TYR:CZ	2:H:214:LEU:HD11	2.55	0.41
3:R:63:ARG:HH12	3:R:87:CYS:HB3	1.85	0.41
4:N:60:LYS:HA	4:N:60:LYS:HD3	1.88	0.41
2:H:247:VAL:HG22	2:H:256:PHE:O	2.21	0.41
2:H:182:SER:HA	2:H:191:ARG:HA	2.03	0.40
1:C:481:ARG:NH2	1:C:491:ASN:OD1	2.55	0.40
1:C:514:HIS:CE1	1:C:519:LEU:HG	2.56	0.40
4:N:36:ILE:HD11	4:N:69:LEU:HD11	2.03	0.40
2:H:409:TYR:CZ	2:H:469:ARG:HG2	2.57	0.40

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	C	589/780 (76%)	570 (97%)	19 (3%)	0	100	100
2	H	372/495 (75%)	356 (96%)	16 (4%)	0	100	100
3	R	84/111 (76%)	76 (90%)	8 (10%)	0	100	100
4	N	74/83 (89%)	70 (95%)	4 (5%)	0	100	100
All	All	1119/1469 (76%)	1072 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	C	463/710 (65%)	461 (100%)	2 (0%)	91	95
2	H	296/445 (66%)	295 (100%)	1 (0%)	92	97
3	R	70/96 (73%)	70 (100%)	0	100	100
4	N	66/70 (94%)	66 (100%)	0	100	100
All	All	895/1321 (68%)	892 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	364	ARG
1	C	743	LYS
2	H	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	115	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.