Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 01:28 PM EST

PDB ID	:	1XX0
Title	:	Structure of the C-terminal PH domain of human pleckstrin
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Deposited on	:	2004-11-03

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

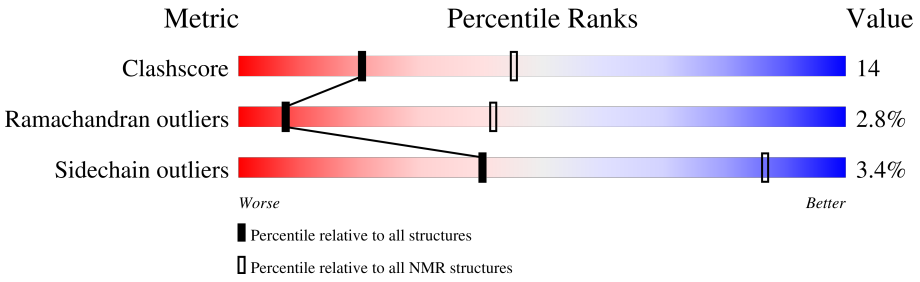
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	127	57% 15% • 19% 8%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:239-A:254, A:261-A:300, A:311-A:347 (93)	0.31	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 7, 8, 10
2	2, 5, 6, 9
Single-model clusters	3

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1905 atoms, of which 956 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pleckstrin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1905	600	956	172	174	3	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	MET	-	expression tag	UNP P08567
A	225	LYS	-	expression tag	UNP P08567
A	226	HIS	-	expression tag	UNP P08567
A	227	HIS	-	expression tag	UNP P08567
A	228	HIS	-	expression tag	UNP P08567
A	229	HIS	-	expression tag	UNP P08567
A	230	HIS	-	expression tag	UNP P08567
A	231	HIS	-	expression tag	UNP P08567
A	232	PRO	-	expression tag	UNP P08567
A	233	MET	-	expression tag	UNP P08567

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Pleckstrin

Chain A: 57% 15% • 19% 8%

MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 Q248 G255 H256 R257 R258 K259 N260 W261 R264 K265 F266 I267 E270 D271 P272 A273 Y274 L275 H276 G282 I290 H291 L292 R293 V300 E301 S302 N303 S304 N305 G306 R307 K308 S309 E310 E311 L314

R335 T336 T348 G349 K350

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Pleckstrin

Chain A: 50% 21% •• 19% 8%

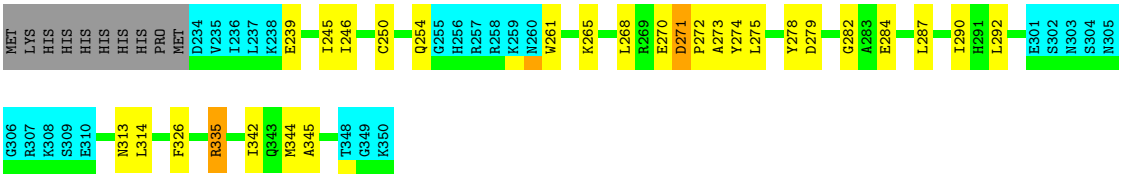
MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 G243 K247 Q248 L251 L252 G255 H256 R257 R258 K259 N260 W261 K262 F266 I267 E270 D271 P272 A273 Y274 L275 D279 G282 A283 I290 H291 L292 R293 E301 S302 N303 S304 N305 G306 R307

K308 S309 E310 E311 L314 K333 T336 E337 W338 T339 K340 M344 A345 T348 G349 K350

4.2.2 Score per residue for model 2

• Molecule 1: Pleckstrin

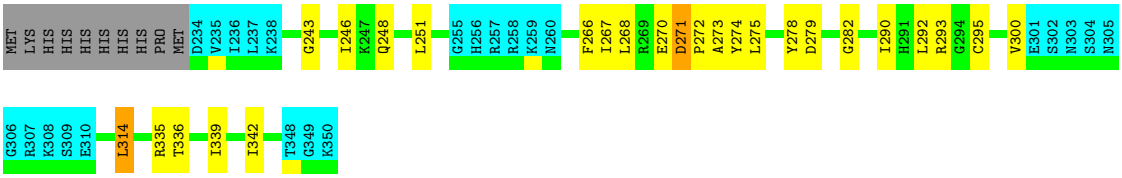
Chain A: 51% 20% • 19% 8%



4.2.3 Score per residue for model 3

- Molecule 1: Pleckstrin

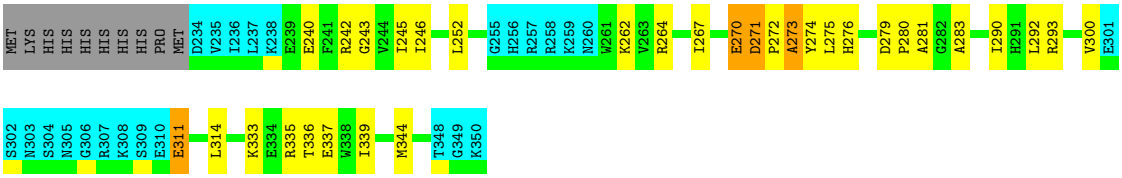
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Pleckstrin

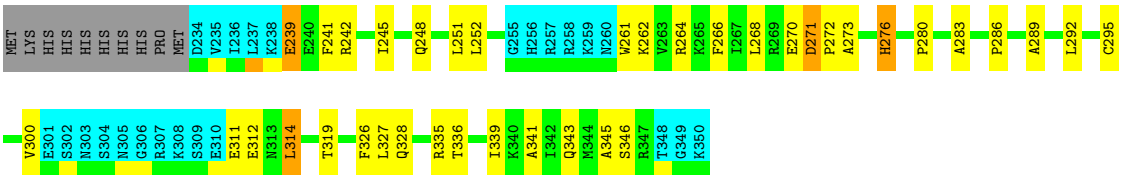
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Pleckstrin

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Pleckstrin

Chain A: 44% 27% • 19% 8%

MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 E239 E240 F241 R242 K247 L252 K253 Q254 G255 H256 R257 R258 K259 N260 W261 K262 V263 R264 K265 F266 I267 L268 R269 E270 D271 P272 A273 Y274 L275 H276 D279 P280 A281 G282 L287 I290 H291 L292 R293

V300 E301 S302 N303 S304 N305 G306 R307 K308 S309 E310 E311 L314 P332 R335 T336 E337 W338 I339 K340 S346 R347 T348 G349 K350

4.2.7 Score per residue for model 7

- Molecule 1: Pleckstrin

Chain A: 51% 20% • 19% 8%

MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 K247 Q248 G249 C250 Q254 G255 H256 R257 R258 K259 N260 W261 R264 K265 D271 P272 A273 Y274 L275 P280 A281 G282 I290 H291 L292 R293 V300 E301 S302 N303 S304 N305 G306 R307 K308 S309 E310 E311

L314 F326 L327 Q328 A329 K333 E334 R335 T336 E337 T348 G349 K350

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Pleckstrin

Chain A: 44% 28% • 19% 8%

MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 E239 E240 F241 R242 G243 Q248 L252 K253 Q254 G255 H256 R257 R258 K259 N260 W261 R264 I267 L268 R269 E270 D271 P272 A273 Y274 L275 H276 Y277 Y278 D279 P280 D285 P286 L287 I290 H291 L292 R293 G294

C295 V300 E301 S302 N303 S304 N305 G306 R307 K308 S309 E310 E311 L314 I318 L327 Q328 R335 T336 K340 A341 I342 T348 G349 K350

4.2.9 Score per residue for model 9

- Molecule 1: Pleckstrin

Chain A: 47% 24% • 19% 8%

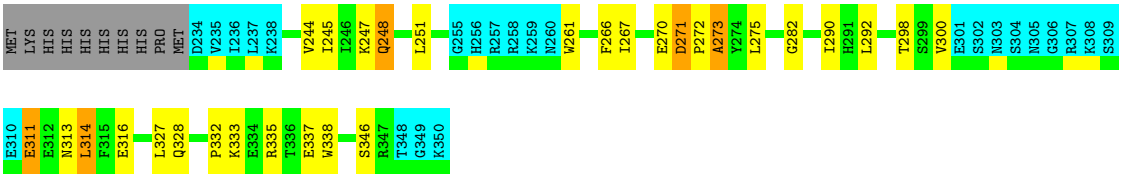
MET LYS HIS HIS HIS HIS HIS HIS PRO MET D234 V235 I236 L237 K238 F241 I245 I246 G255 H256 R257 R258 K259 N260 W261 R264 K265 F266 I267 L268 R269 E270 D271 P272 A273 Y274 L275 H276 Y277 Y278 G282 I290 R293 V300 E301 S302 N303 S304 N305 G306 R307 K308

S309 E310 E311 E312 N313 L314 D321 F326 L327 Q328 P332 R335 T336 I339 K340 S346 R347 T348 G349 K350

4.2.10 Score per residue for model 10

- Molecule 1: Pleckstrin

Chain A:



5 Refinement protocol and experimental data overview (i)

Of the 80 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	759	761	758	21±4
All	All	7590	7610	7580	206

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 14.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:TYR:HA	1:A:287:LEU:HD13	0.88	1.45	2	2
1:A:271:ASP:HB3	1:A:272:PRO:HD3	0.84	1.47	9	8
1:A:300:VAL:HB	1:A:314:LEU:HB3	0.73	1.59	6	7
1:A:278:TYR:HA	1:A:287:LEU:CD1	0.71	2.16	8	2
1:A:311:GLU:HB3	1:A:314:LEU:HD12	0.69	1.63	1	5
1:A:313:ASN:HB2	1:A:335:ARG:HG2	0.69	1.64	2	2
1:A:239:GLU:HG3	1:A:272:PRO:HB3	0.66	1.67	2	1
1:A:273:ALA:HB1	1:A:292:LEU:HB2	0.63	1.69	2	9
1:A:243:GLY:HA3	1:A:270:GLU:O	0.63	1.93	4	4
1:A:266:PHE:O	1:A:267:ILE:HD13	0.62	1.94	6	1
1:A:248:GLN:HB3	1:A:267:ILE:HG12	0.60	1.74	10	2
1:A:252:LEU:HA	1:A:262:LYS:O	0.59	1.97	5	4
1:A:311:GLU:HG2	1:A:314:LEU:HD12	0.58	1.74	8	1
1:A:295:CYS:HA	1:A:318:ILE:O	0.57	2.00	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:313:ASN:HB3	1:A:332:PRO:HA	0.56	1.77	9	1
1:A:271:ASP:CB	1:A:272:PRO:HD3	0.56	2.29	4	8
1:A:268:LEU:HD11	1:A:292:LEU:HD11	0.54	1.79	3	3
1:A:339:ILE:O	1:A:343:GLN:HG3	0.54	2.03	5	1
1:A:264:ARG:HA	1:A:280:PRO:HD3	0.53	1.80	5	4
1:A:336:THR:HG22	1:A:340:LYS:NZ	0.53	2.18	1	1
1:A:311:GLU:HA	1:A:328:GLN:OE1	0.53	2.02	7	3
1:A:264:ARG:HB2	1:A:278:TYR:O	0.53	2.03	9	1
1:A:292:LEU:HD22	1:A:342:ILE:HG23	0.53	1.80	2	3
1:A:329:ALA:HB1	1:A:334:GLU:HB3	0.53	1.80	7	1
1:A:332:PRO:O	1:A:335:ARG:HG3	0.53	2.04	10	2
1:A:270:GLU:O	1:A:271:ASP:HB2	0.52	2.03	1	2
1:A:246:ILE:HD11	1:A:270:GLU:HG2	0.52	1.81	9	3
1:A:335:ARG:HG3	1:A:336:THR:N	0.52	2.20	3	5
1:A:272:PRO:HB2	1:A:274:TYR:CE2	0.51	2.39	7	7
1:A:264:ARG:NH1	1:A:287:LEU:HD13	0.51	2.20	6	1
1:A:313:ASN:CB	1:A:332:PRO:HA	0.51	2.35	9	1
1:A:247:LYS:HE2	1:A:338:TRP:CE2	0.51	2.41	10	1
1:A:279:ASP:HB3	1:A:283:ALA:HB3	0.51	1.82	4	1
1:A:314:LEU:HA	1:A:327:LEU:O	0.50	2.06	8	2
1:A:273:ALA:CB	1:A:346:SER:HA	0.50	2.36	10	3
1:A:276:HIS:CE1	1:A:286:PRO:HB2	0.49	2.42	5	1
1:A:240:GLU:HB3	1:A:276:HIS:CE1	0.49	2.42	6	3
1:A:276:HIS:CE1	1:A:289:ALA:HB2	0.49	2.43	5	1
1:A:311:GLU:H	1:A:311:GLU:CD	0.49	2.11	8	2
1:A:239:GLU:OE1	1:A:242:ARG:HD3	0.49	2.08	5	1
1:A:300:VAL:O	1:A:314:LEU:HB3	0.49	2.08	8	1
1:A:275:LEU:HD23	1:A:290:ILE:HD12	0.49	1.84	1	8
1:A:244:VAL:HG12	1:A:245:ILE:N	0.49	2.23	10	1
1:A:251:LEU:HB2	1:A:266:PHE:CD1	0.48	2.43	10	4
1:A:245:ILE:HA	1:A:268:LEU:O	0.48	2.08	5	3
1:A:245:ILE:HG23	1:A:267:ILE:HG23	0.48	1.85	4	2
1:A:333:LYS:O	1:A:337:GLU:HG2	0.48	2.07	4	4
1:A:279:ASP:HB3	1:A:282:GLY:O	0.48	2.07	2	1
1:A:273:ALA:HB2	1:A:346:SER:HA	0.48	1.86	10	3
1:A:336:THR:HA	1:A:339:ILE:HD12	0.47	1.85	3	3
1:A:246:ILE:HD11	1:A:270:GLU:HB3	0.47	1.86	2	1
1:A:344:MET:HG3	1:A:345:ALA:N	0.47	2.25	2	2
1:A:293:ARG:O	1:A:346:SER:HB2	0.47	2.10	6	1
1:A:239:GLU:HG2	1:A:272:PRO:HG3	0.47	1.87	8	1
1:A:313:ASN:HB3	1:A:335:ARG:HG2	0.47	1.86	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:267:ILE:HG12	1:A:278:TYR:CE1	0.47	2.45	3	1
1:A:268:LEU:HD22	1:A:341:ALA:HB1	0.47	1.87	5	1
1:A:254:GLN:HB2	1:A:261:TRP:CE2	0.47	2.45	6	1
1:A:271:ASP:HB3	1:A:272:PRO:CD	0.47	2.30	6	5
1:A:314:LEU:HD23	1:A:327:LEU:O	0.47	2.10	10	1
1:A:239:GLU:O	1:A:272:PRO:HG3	0.46	2.10	2	1
1:A:295:CYS:CB	1:A:319:THR:HA	0.46	2.40	5	1
1:A:261:TRP:CZ2	1:A:311:GLU:HG3	0.46	2.45	1	2
1:A:279:ASP:OD2	1:A:281:ALA:HB3	0.46	2.11	6	2
1:A:248:GLN:CB	1:A:267:ILE:HG12	0.46	2.40	10	3
1:A:291:HIS:NE2	1:A:293:ARG:HB2	0.46	2.25	8	1
1:A:261:TRP:CH2	1:A:326:PHE:HB3	0.45	2.45	5	4
1:A:335:ARG:O	1:A:339:ILE:HG13	0.45	2.11	5	2
1:A:261:TRP:CZ3	1:A:328:GLN:HG3	0.45	2.46	8	2
1:A:336:THR:O	1:A:340:LYS:HG3	0.45	2.11	8	1
1:A:271:ASP:HB2	1:A:272:PRO:HD3	0.44	1.87	2	1
1:A:266:PHE:HA	1:A:276:HIS:O	0.44	2.12	9	1
1:A:247:LYS:HE2	1:A:338:TRP:NE1	0.44	2.27	6	2
1:A:252:LEU:HB2	1:A:328:GLN:HB2	0.44	1.90	8	2
1:A:253:LYS:O	1:A:261:TRP:HA	0.43	2.13	6	1
1:A:285:ASP:O	1:A:287:LEU:HD12	0.43	2.13	8	1
1:A:336:THR:HG22	1:A:340:LYS:HE2	0.43	1.91	9	2
1:A:298:THR:HG22	1:A:316:GLU:HB3	0.43	1.91	10	1
1:A:254:GLN:HB3	1:A:326:PHE:HB2	0.43	1.88	7	1
1:A:275:LEU:HB3	1:A:290:ILE:HB	0.43	1.91	3	5
1:A:240:GLU:O	1:A:269:ARG:HD2	0.43	2.14	6	1
1:A:337:GLU:HA	1:A:340:LYS:HE2	0.42	1.91	6	1
1:A:279:ASP:CB	1:A:283:ALA:HB3	0.42	2.43	1	1
1:A:270:GLU:HG3	1:A:345:ALA:HA	0.42	1.92	5	1
1:A:240:GLU:HA	1:A:274:TYR:CD2	0.42	2.49	6	1
1:A:250:CYS:HA	1:A:265:LYS:HA	0.42	1.90	7	2
1:A:247:LYS:HE2	1:A:337:GLU:HB3	0.41	1.92	7	1
1:A:247:LYS:HE3	1:A:338:TRP:NE1	0.41	2.30	1	1
1:A:272:PRO:HB2	1:A:274:TYR:CD2	0.40	2.51	2	1
1:A:311:GLU:CD	1:A:311:GLU:H	0.40	2.20	10	1
1:A:292:LEU:HA	1:A:295:CYS:SG	0.40	2.57	3	1
1:A:311:GLU:CG	1:A:314:LEU:HD12	0.40	2.45	8	1
1:A:336:THR:O	1:A:339:ILE:HB	0.40	2.17	6	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	93/127 (73%)	84±2 (90±2%)	6±2 (7±3%)	3±1 (3±1%)	8 42
All	All	930/1270 (73%)	839 (90%)	65 (7%)	26 (3%)	8 42

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	271	ASP	10
1	A	282	GLY	6
1	A	293	ARG	6
1	A	273	ALA	2
1	A	311	GLU	1
1	A	283	ALA	1

6.3.2 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 NMR 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	79/110 (72%)	76±1 (97±1%)	3±1 (3±1%)	40 87
All	All	790/1100 (72%)	763 (97%)	27 (3%)	40 87

All 14 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	314	LEU	6
1	A	248	GLN	4
1	A	270	GLU	4
1	A	335	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	271	ASP	1
1	A	284	GLU	1
1	A	279	ASP	1
1	A	344	MET	1
1	A	239	GLU	1
1	A	276	HIS	1
1	A	241	PHE	1
1	A	277	TYR	1
1	A	321	ASP	1
1	A	311	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided