Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 04:30 PM EST

PDB ID	:	2CPX
Title	:	solution structure of RNA binding domain in Hypothetical protein FLJ11016
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Deposited on	:	2005-05-19

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:

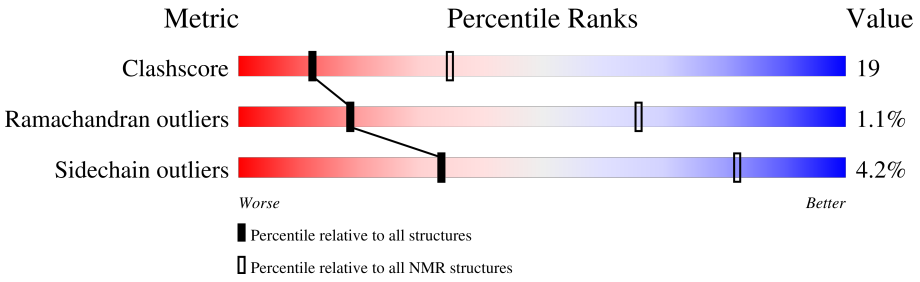
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	115	42% 17% 42%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:307-A:332, A:340-A:345, A:351-A:385 (67)	0.21	5

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 9, 10, 11, 13
2	8, 15, 17
3	16, 18, 20
4	12, 14
Single-model clusters	2; 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1847 atoms, of which 935 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein FLJ11016.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1847	583	935	164	161	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLY	-	cloning artifact	UNP Q96IZ5
A	285	SER	-	cloning artifact	UNP Q96IZ5
A	286	SER	-	cloning artifact	UNP Q96IZ5
A	287	GLY	-	cloning artifact	UNP Q96IZ5
A	288	SER	-	cloning artifact	UNP Q96IZ5
A	289	SER	-	cloning artifact	UNP Q96IZ5
A	290	GLY	-	cloning artifact	UNP Q96IZ5
A	393	SER	-	cloning artifact	UNP Q96IZ5
A	394	GLY	-	cloning artifact	UNP Q96IZ5
A	395	PRO	-	cloning artifact	UNP Q96IZ5
A	396	SER	-	cloning artifact	UNP Q96IZ5
A	397	SER	-	cloning artifact	UNP Q96IZ5
A	398	GLY	-	cloning artifact	UNP Q96IZ5

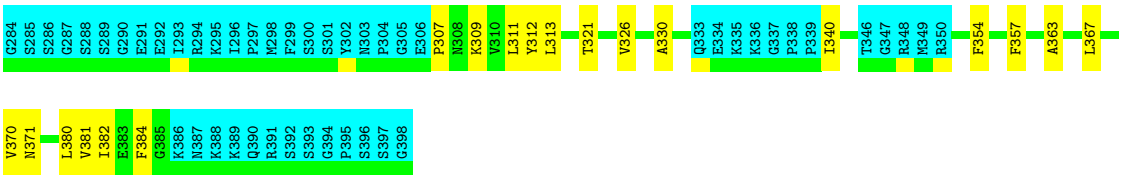
4 Residue-property plots (i)

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: Hypothetical protein FLJ11016

Chain A: 42% 17% 42%



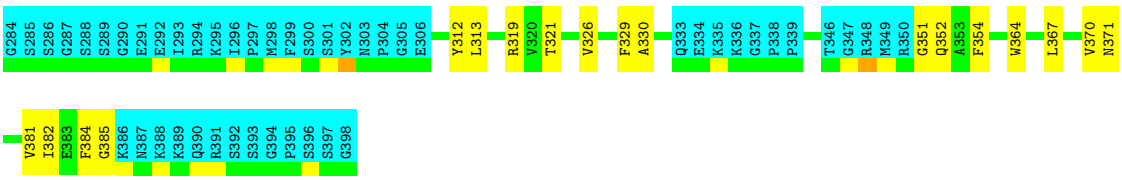
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hypothetical protein FLJ11016

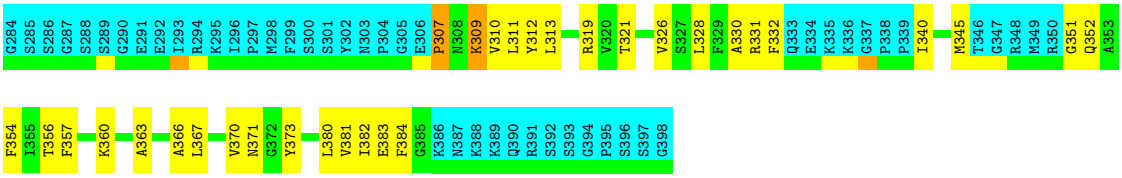
Chain A: 43% 16% 42%



4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical protein FLJ11016

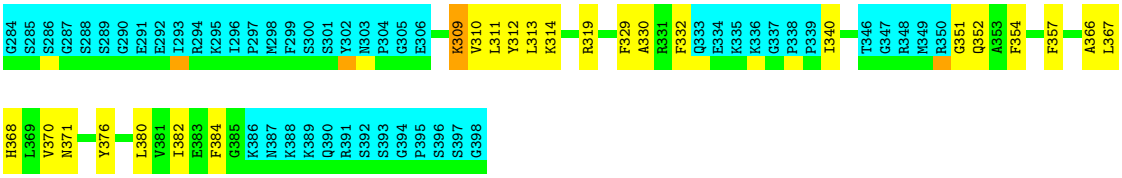
Chain A: 30% 26% • 42%



4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein FLJ11016

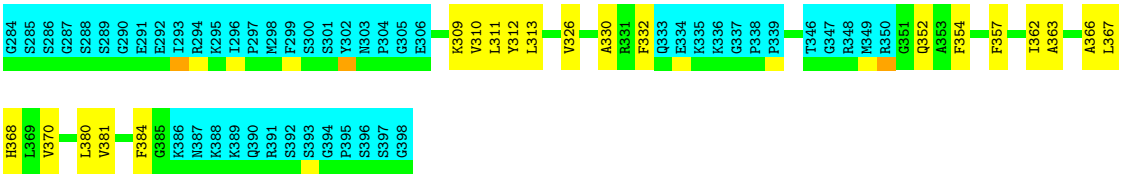
Chain A: 37% 20% • 42%



4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein FLJ11016

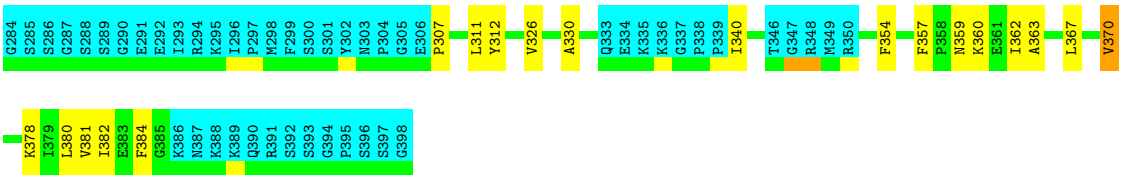
Chain A: 41% 17% 42%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 42% 16% • 42%



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 30% 29% 42%

G284 S285 S286 G287 S288 S289 G290 E291 E292 I293 R294 K295 I296 P297 M298 F299 S300 S301 Y302 N303 P304 G305 E306 L311 Y312 L313 K314 T321 E322 R323 D324 L325 V326 S327 L328 F329 A330 R331 F332 Q333 E334 K335 K336 G337 P338 P339 I340 Q341 F342 M345 T346 G347 R348 M349 R350 F354

F357 P358 N359 I362 A363 W364 Q365 A366 L367 H368 L369 V370 N371 G372 Y373 K374 L375 Y376 L380 V381 I382 E383 F384 G385 K386 N387 K388 K389 Q390 R391 S392 S393 G394 P395 S396 S397 G398

4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 40% 17% • 42%

G284 S285 S286 G287 S288 S289 G290 E291 E292 I293 R294 K295 I296 P297 M298 F299 S300 S301 Y302 N303 P304 G305 E306 K309 V310 L311 Y312 L313 K314 R319 V320 T321 V326 F329 A330 R331 F332 Q333 E334 K335 K336 G337 P338 P339 M345 T346 G347 R348 M349 R350 F354 F357

A366 L367 V370 N371 L380 V381 F384 G385 K386 N387 K388 K389 Q390 R391 S392 S393 G394 P395 S396 S397 G398

4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 40% 17% • 42%

G284 S285 S286 G287 S288 S289 G290 E291 E292 I293 R294 K295 I296 P297 M298 F299 S300 S301 Y302 N303 P304 G305 E306 P307 N308 K309 Y312 L313 L316 V326 S327 L328 F329 A330 Q333 E334 K335 K336 G337 P338 P339 I340 T346 G347 R348 M349 R350 F354 I355 T356 A366 L367 H368

L369 V370 N371 G372 Y373 K374 L375 L380 F384 G385 K386 N387 K388 K389 Q390 R391 S392 S393 G394 P395 S396 S397 G398

4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 41% 17% • 42%

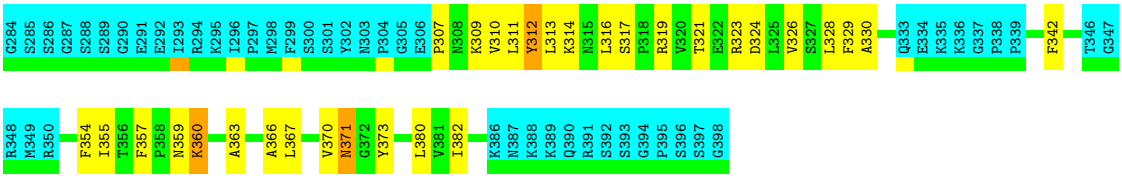
G284 S285 S286 G287 S288 S289 G290 E291 E292 I293 R294 K295 I296 P297 M298 F299 S300 S301 Y302 N303 P304 G305 E306 P307 N308 K309 Y310 L311 Y312 L313 K314 V326 A330 Q333 E334 K335 K336 G337 P338 P339 I340 T346 G347 R348 M349 R350 G351 Q352 A353 F354 F357 A363 L367

H368 K378 I379 L380 V381 I382 E383 F384 G385 K386 N387 K388 K389 Q390 R391 S392 S393 G394 P395 S396 S397 G398

4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 31% 24% • 42%



4.2.11 Score per residue for model 11

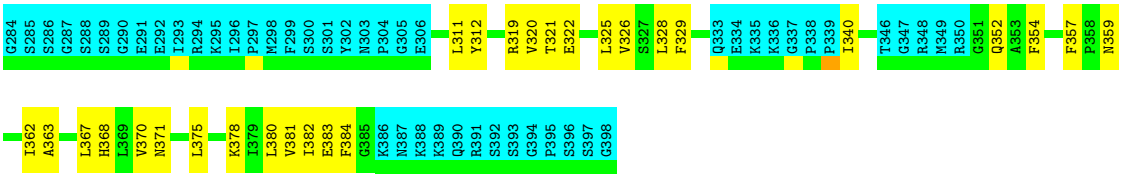
- Molecule 1: Hypothetical protein FLJ11016

Chain A: 39% 18% • 42%

4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein FLJ11016

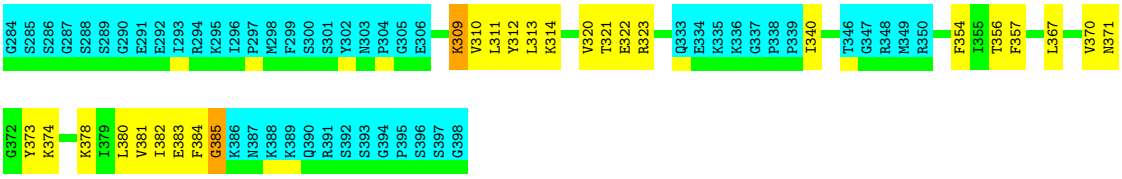
Chain A: 34% 24% 42%



4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein FLJ11016

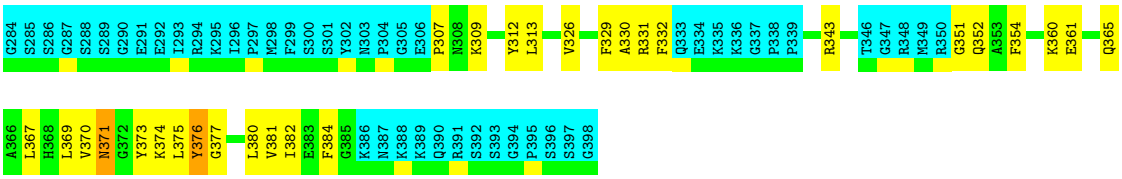
Chain A: 36% 21% • 42%



4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein FLJ11016

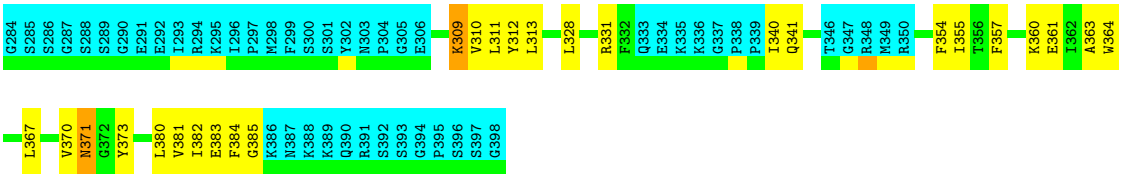
Chain A: 33% 23% • 42%



4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein FLJ11016

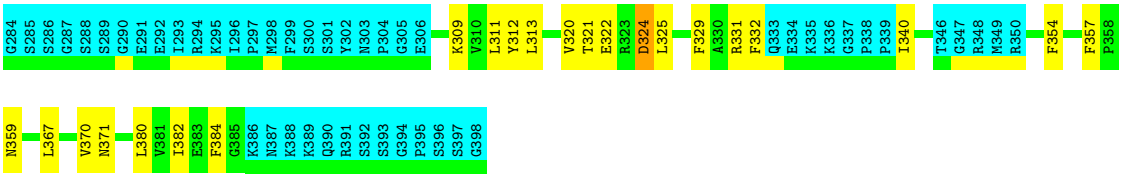
Chain A: 36% 21% • 42%



4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein FLJ11016

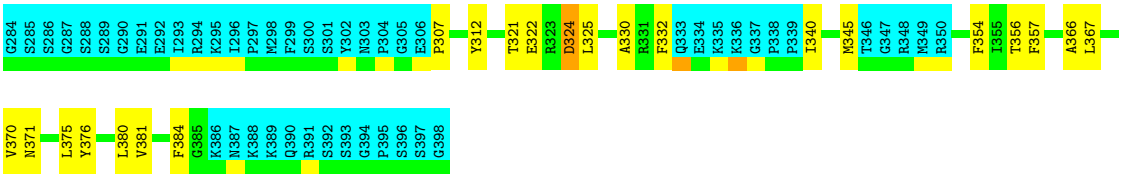
Chain A: 39% 18% • 42%



4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical protein FLJ11016

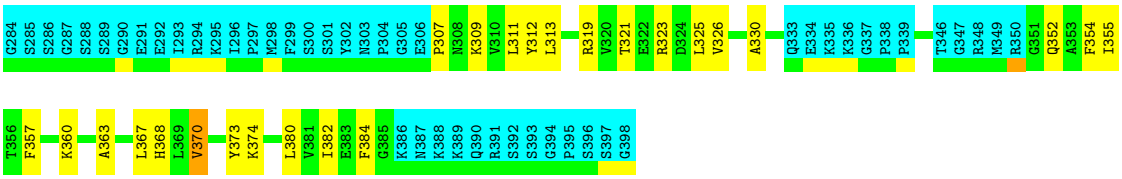
Chain A: 39% 18% • 42%



4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 37% 21% • 42%



4.2.19 Score per residue for model 19

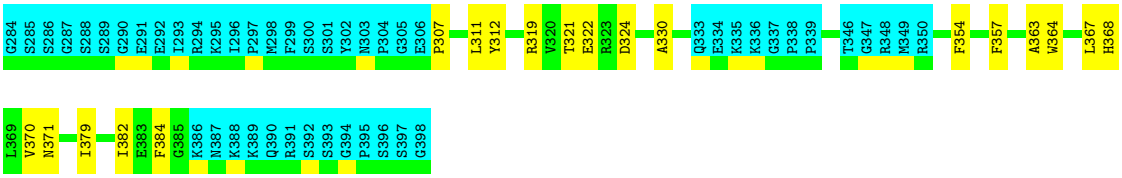
- Molecule 1: Hypothetical protein FLJ11016

Chain A: 40% 17% • 42%

4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein FLJ11016

Chain A: 42% 17% 42%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, restrainted molecular dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations.*

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	555	579	579	22±4
All	All	11100	11580	11580	435

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:367:LEU:HD13	1:A:384:PHE:CZ	0.86	2.05	8	18
1:A:312:TYR:CD1	1:A:354:PHE:CE1	0.80	2.70	8	16
1:A:312:TYR:CE1	1:A:354:PHE:CE2	0.80	2.70	20	11
1:A:312:TYR:CD1	1:A:354:PHE:CZ	0.80	2.70	14	15
1:A:312:TYR:CD1	1:A:354:PHE:CE2	0.79	2.70	1	7
1:A:312:TYR:CE1	1:A:354:PHE:CZ	0.79	2.70	15	16
1:A:311:LEU:HD12	1:A:357:PHE:CE1	0.79	2.13	10	8
1:A:322:GLU:OE1	1:A:325:LEU:HD12	0.76	1.80	16	2
1:A:312:TYR:CE1	1:A:354:PHE:CE1	0.76	2.74	14	4
1:A:340:ILE:HD13	1:A:357:PHE:CE2	0.75	2.16	19	7
1:A:312:TYR:CG	1:A:354:PHE:CE1	0.69	2.80	18	10
1:A:313:LEU:HD23	1:A:380:LEU:HD11	0.69	1.65	11	4
1:A:367:LEU:HD13	1:A:384:PHE:CE2	0.69	2.23	18	5
1:A:332:PHE:O	1:A:340:ILE:HD11	0.68	1.89	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:LEU:HA	1:A:328:LEU:HD12	0.66	1.66	12	1
1:A:370:VAL:HG12	1:A:370:VAL:O	0.66	1.89	3	9
1:A:329:PHE:CD1	1:A:366:ALA:HB1	0.65	2.27	7	2
1:A:340:ILE:HG22	1:A:342:PHE:CE1	0.65	2.26	6	1
1:A:357:PHE:HB2	1:A:363:ALA:HB2	0.65	1.67	2	8
1:A:328:LEU:HD21	1:A:373:TYR:CE2	0.65	2.27	8	5
1:A:367:LEU:C	1:A:367:LEU:HD23	0.64	2.12	17	16
1:A:322:GLU:O	1:A:326:VAL:HG23	0.64	1.93	12	1
1:A:366:ALA:O	1:A:370:VAL:HG23	0.63	1.92	2	3
1:A:311:LEU:CD1	1:A:357:PHE:CE1	0.63	2.82	10	1
1:A:326:VAL:O	1:A:330:ALA:HB2	0.61	1.94	11	9
1:A:325:LEU:HD22	1:A:355:ILE:HD11	0.61	1.72	18	1
1:A:313:LEU:HD21	1:A:329:PHE:CE1	0.61	2.31	8	2
1:A:380:LEU:C	1:A:380:LEU:HD23	0.60	2.16	14	13
1:A:312:TYR:CD1	1:A:354:PHE:CD1	0.60	2.90	8	5
1:A:311:LEU:HD12	1:A:357:PHE:HE2	0.59	1.58	3	1
1:A:367:LEU:HD23	1:A:368:HIS:N	0.58	2.13	18	8
1:A:313:LEU:CD1	1:A:313:LEU:N	0.58	2.65	9	1
1:A:367:LEU:HD23	1:A:367:LEU:C	0.58	2.19	18	2
1:A:313:LEU:N	1:A:313:LEU:HD12	0.58	2.12	9	1
1:A:313:LEU:HD12	1:A:313:LEU:N	0.58	2.14	2	7
1:A:312:TYR:CZ	1:A:314:LYS:CG	0.57	2.87	19	1
1:A:381:VAL:HG12	1:A:383:GLU:OE1	0.57	1.99	13	3
1:A:370:VAL:O	1:A:370:VAL:HG12	0.56	1.99	19	6
1:A:373:TYR:CE1	1:A:374:LYS:O	0.55	2.60	18	3
1:A:311:LEU:HD12	1:A:357:PHE:CE2	0.55	2.37	3	1
1:A:380:LEU:HD23	1:A:381:VAL:N	0.55	2.17	11	5
1:A:380:LEU:HD23	1:A:380:LEU:C	0.54	2.23	5	3
1:A:355:ILE:HG22	1:A:357:PHE:CE1	0.54	2.37	10	1
1:A:367:LEU:HD13	1:A:384:PHE:CE1	0.53	2.38	15	3
1:A:340:ILE:HG23	1:A:356:THR:O	0.53	2.03	8	2
1:A:340:ILE:CG2	1:A:342:PHE:CE1	0.53	2.91	6	1
1:A:329:PHE:CE1	1:A:370:VAL:HG21	0.52	2.38	14	4
1:A:370:VAL:O	1:A:382:ILE:HD11	0.52	2.05	18	7
1:A:307:PRO:HA	1:A:384:PHE:CE1	0.52	2.40	18	1
1:A:313:LEU:N	1:A:313:LEU:CD1	0.51	2.74	2	3
1:A:320:VAL:HG22	1:A:375:LEU:HD21	0.51	1.82	12	1
1:A:311:LEU:HD22	1:A:367:LEU:HD12	0.51	1.82	18	3
1:A:331:ARG:HG3	1:A:332:PHE:CE2	0.50	2.41	2	1
1:A:313:LEU:HD23	1:A:380:LEU:HD21	0.50	1.83	3	1
1:A:329:PHE:HD1	1:A:366:ALA:HB1	0.50	1.66	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:311:LEU:HD21	1:A:363:ALA:HB1	0.50	1.83	15	1
1:A:364:TRP:O	1:A:367:LEU:N	0.50	2.45	19	3
1:A:351:GLY:C	1:A:352:GLN:CD	0.50	2.70	2	2
1:A:345:MET:CE	1:A:354:PHE:CD2	0.50	2.95	2	1
1:A:345:MET:SD	1:A:354:PHE:CE2	0.49	3.06	2	1
1:A:371:ASN:O	1:A:371:ASN:ND2	0.49	2.46	8	2
1:A:324:ASP:CG	1:A:325:LEU:N	0.49	2.66	17	1
1:A:319:ARG:O	1:A:321:THR:HG23	0.49	2.08	2	7
1:A:341:GLN:O	1:A:355:ILE:HG23	0.48	2.09	15	1
1:A:312:TYR:CE2	1:A:354:PHE:CE2	0.48	3.01	10	1
1:A:380:LEU:HD21	1:A:382:ILE:CG1	0.48	2.39	10	2
1:A:309:LYS:CD	1:A:310:VAL:HG23	0.48	2.39	7	3
1:A:309:LYS:HD3	1:A:310:VAL:HG23	0.48	1.86	7	2
1:A:380:LEU:HD21	1:A:382:ILE:HG12	0.47	1.85	10	1
1:A:312:TYR:CD2	1:A:314:LYS:HD2	0.47	2.44	19	1
1:A:342:PHE:N	1:A:342:PHE:CD1	0.47	2.82	6	1
1:A:311:LEU:CD2	1:A:384:PHE:CE1	0.47	2.98	20	2
1:A:378:LYS:CG	1:A:378:LYS:O	0.47	2.62	12	1
1:A:342:PHE:CE2	1:A:355:ILE:HD13	0.46	2.46	10	1
1:A:375:LEU:HG	1:A:376:TYR:CD2	0.46	2.45	17	2
1:A:309:LYS:HD2	1:A:310:VAL:HG23	0.46	1.86	11	3
1:A:370:VAL:O	1:A:382:ILE:CD1	0.46	2.64	18	5
1:A:326:VAL:O	1:A:330:ALA:N	0.46	2.49	9	6
1:A:331:ARG:CG	1:A:332:PHE:CE2	0.46	2.99	2	1
1:A:382:ILE:C	1:A:383:GLU:OE1	0.46	2.54	2	2
1:A:320:VAL:HG22	1:A:376:TYR:CD2	0.46	2.46	11	1
1:A:321:THR:O	1:A:322:GLU:C	0.46	2.54	16	5
1:A:313:LEU:HD21	1:A:329:PHE:CZ	0.45	2.46	11	2
1:A:313:LEU:HD13	1:A:355:ILE:HG13	0.45	1.87	10	1
1:A:380:LEU:CD2	1:A:382:ILE:CG1	0.45	2.95	10	4
1:A:371:ASN:O	1:A:371:ASN:CG	0.45	2.55	14	4
1:A:367:LEU:O	1:A:371:ASN:N	0.45	2.49	2	3
1:A:312:TYR:CD2	1:A:314:LYS:HE2	0.45	2.46	13	3
1:A:311:LEU:HD21	1:A:384:PHE:CE1	0.45	2.46	13	3
1:A:319:ARG:HB3	1:A:376:TYR:CE2	0.45	2.46	3	1
1:A:322:GLU:O	1:A:323:ARG:C	0.45	2.55	19	2
1:A:311:LEU:HD12	1:A:357:PHE:HE1	0.44	1.71	5	1
1:A:312:TYR:CD1	1:A:314:LYS:HE2	0.44	2.47	10	1
1:A:373:TYR:HE2	1:A:375:LEU:HD13	0.44	1.71	8	1
1:A:313:LEU:HD21	1:A:329:PHE:HZ	0.44	1.72	11	1
1:A:309:LYS:HG3	1:A:310:VAL:HG23	0.44	1.90	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:367:LEU:CD1	1:A:384:PHE:CE2	0.44	2.99	18	1
1:A:313:LEU:HD21	1:A:329:PHE:CE2	0.44	2.47	1	1
1:A:362:ILE:O	1:A:363:ALA:C	0.44	2.56	6	4
1:A:331:ARG:HG3	1:A:332:PHE:CD1	0.44	2.48	6	1
1:A:312:TYR:CG	1:A:354:PHE:CE2	0.44	3.06	14	2
1:A:367:LEU:C	1:A:367:LEU:CD2	0.44	2.86	15	6
1:A:320:VAL:HG22	1:A:376:TYR:HD2	0.44	1.72	11	1
1:A:370:VAL:O	1:A:371:ASN:C	0.44	2.56	17	2
1:A:332:PHE:CZ	1:A:366:ALA:HA	0.44	2.48	7	3
1:A:309:LYS:O	1:A:356:THR:HG23	0.44	2.13	2	1
1:A:380:LEU:CD2	1:A:382:ILE:HG13	0.43	2.43	10	5
1:A:320:VAL:O	1:A:321:THR:HG23	0.43	2.12	13	1
1:A:312:TYR:CD1	1:A:354:PHE:CD2	0.43	3.05	1	1
1:A:309:LYS:NZ	1:A:356:THR:HG23	0.43	2.28	13	1
1:A:352:GLN:N	1:A:352:GLN:CD	0.43	2.72	12	1
1:A:311:LEU:HD12	1:A:357:PHE:CZ	0.43	2.47	10	1
1:A:307:PRO:HA	1:A:384:PHE:CZ	0.43	2.49	19	2
1:A:328:LEU:HD21	1:A:373:TYR:CD2	0.43	2.49	10	1
1:A:322:GLU:O	1:A:325:LEU:N	0.43	2.51	19	1
1:A:323:ARG:O	1:A:324:ASP:C	0.43	2.57	10	2
1:A:322:GLU:OE1	1:A:322:GLU:C	0.43	2.57	12	1
1:A:367:LEU:CD2	1:A:368:HIS:N	0.42	2.82	9	3
1:A:313:LEU:HD21	1:A:329:PHE:HE2	0.42	1.74	1	1
1:A:351:GLY:C	1:A:352:GLN:OE1	0.42	2.58	1	2
1:A:375:LEU:O	1:A:376:TYR:C	0.42	2.57	14	1
1:A:380:LEU:C	1:A:380:LEU:CD2	0.42	2.88	14	2
1:A:365:GLN:O	1:A:369:LEU:CG	0.42	2.68	6	2
1:A:375:LEU:O	1:A:377:GLY:N	0.42	2.52	14	1
1:A:307:PRO:HA	1:A:384:PHE:CE2	0.42	2.50	19	1
1:A:360:LYS:O	1:A:361:GLU:C	0.42	2.58	14	2
1:A:312:TYR:CD2	1:A:354:PHE:CE2	0.42	3.08	10	1
1:A:307:PRO:O	1:A:360:LYS:NZ	0.42	2.51	10	1
1:A:344:MET:C	1:A:345:MET:CE	0.42	2.88	11	1
1:A:312:TYR:CE2	1:A:314:LYS:CD	0.41	3.03	19	1
1:A:330:ALA:O	1:A:332:PHE:N	0.41	2.53	14	1
1:A:370:VAL:O	1:A:370:VAL:CG1	0.41	2.69	19	1
1:A:329:PHE:CE1	1:A:370:VAL:CG2	0.41	3.04	14	1
1:A:331:ARG:HG3	1:A:332:PHE:N	0.41	2.31	16	1
1:A:331:ARG:HB2	1:A:331:ARG:CZ	0.41	2.46	15	1
1:A:363:ALA:O	1:A:364:TRP:C	0.41	2.58	20	1
1:A:380:LEU:HD23	1:A:380:LEU:O	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:331:ARG:CG	1:A:332:PHE:CD1	0.41	3.04	6	1
1:A:329:PHE:CD1	1:A:329:PHE:N	0.41	2.89	8	1
1:A:352:GLN:OE1	1:A:352:GLN:N	0.41	2.54	2	1
1:A:316:LEU:O	1:A:317:SER:C	0.40	2.60	10	1
1:A:351:GLY:C	1:A:352:GLN:NE2	0.40	2.75	14	1
1:A:384:PHE:O	1:A:385:GLY:C	0.40	2.59	13	1
1:A:316:LEU:HD21	1:A:380:LEU:HG	0.40	1.94	8	1
1:A:320:VAL:CG1	1:A:324:ASP:OD1	0.40	2.69	16	1
1:A:332:PHE:CE2	1:A:366:ALA:HB2	0.40	2.51	17	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	67/115 (58%)	57±2 (86±3%)	9±2 (13±3%)	1±1 (1±1%)	18	66
All	All	1340/2300 (58%)	1146 (86%)	179 (13%)	15 (1%)	18	66

All 7 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	307	PRO	6
1	A	385	GLY	3
1	A	370	VAL	2
1	A	340	ILE	1
1	A	331	ARG	1
1	A	376	TYR	1
1	A	379	ILE	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	59/99 (60%)	57±1 (96±2%)	2±1 (4±2%)	33 82
All	All	1180/1980 (60%)	1131 (96%)	49 (4%)	33 82

All 13 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	371	ASN	11
1	A	309	LYS	11
1	A	359	ASN	6
1	A	360	LYS	5
1	A	378	LYS	3
1	A	314	LYS	3
1	A	324	ASP	3
1	A	345	MET	2
1	A	312	TYR	1
1	A	368	HIS	1
1	A	343	ARG	1
1	A	361	GLU	1
1	A	323	ARG	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