WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 03:11 PM EDT

PDB ID	:	2LGC
BMRB ID	:	6468
Title	:	Joint NMR and X-ray refinement reveals the structure of a novel dibenzo[a,d] cycloheptenone inhibitor/p38 MAP kinase complex in solution
Authors	:	Habeck, M.
Deposited on	:	2011-07-25

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

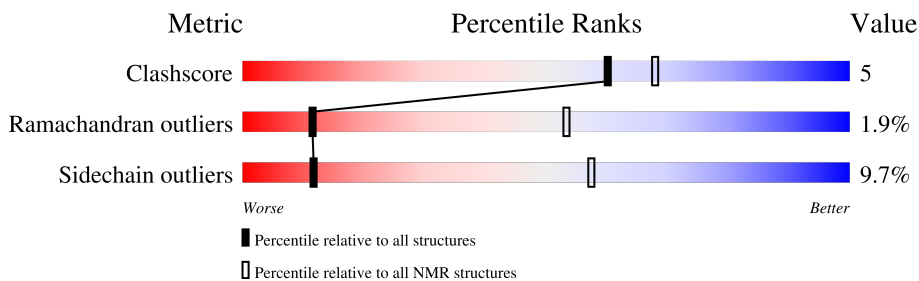|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 22%.

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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		1.9%
Sidechain outliers		9.7%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	359	82% 14% •

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *best r-free*.

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:-4-A:354 (359)	0.10	4

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 1 clusters and 7 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3242 atoms, of which 344 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	359	3242	1851	344	494	538	15	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP Q16539
A	-3	HIS	-	expression tag	UNP Q16539
A	-2	MET	-	expression tag	UNP Q16539
A	-1	LEU	-	expression tag	UNP Q16539
A	0	GLU	-	expression tag	UNP Q16539
A	1	MET	-	expression tag	UNP Q16539

4 Residue-property plots ⓘ

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: Mitogen-activated protein kinase 14
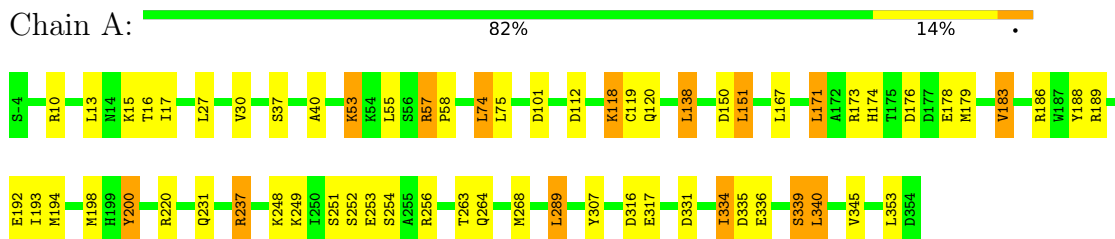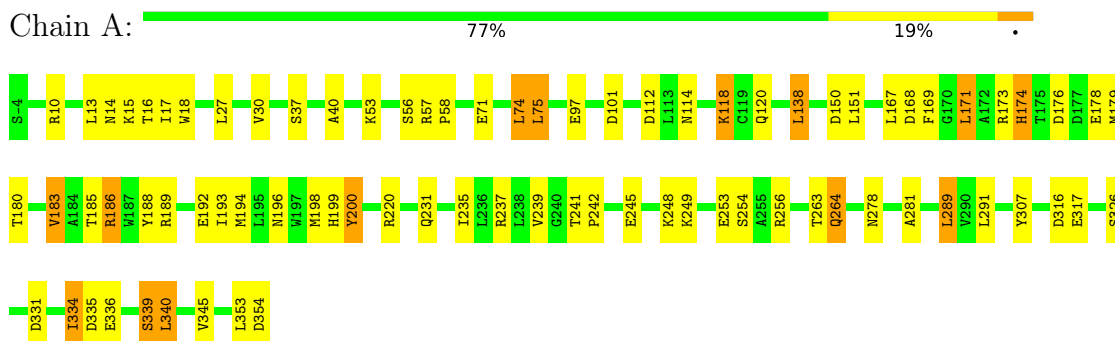

4.2 Scores per residue for each member of the ensemble
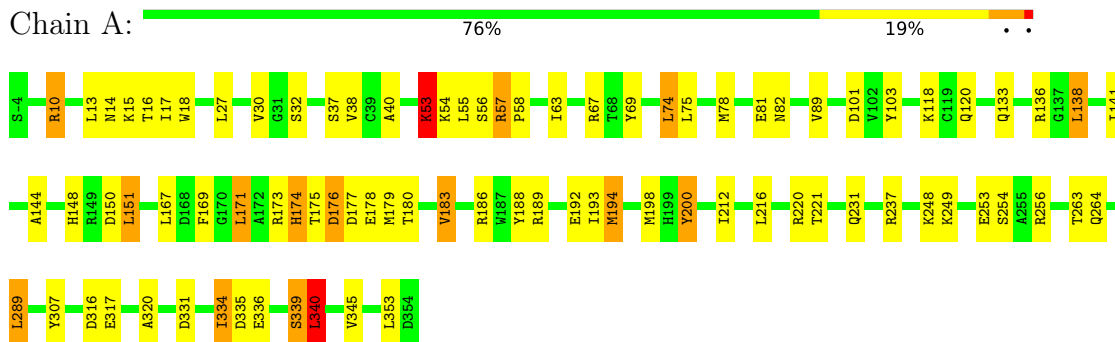
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1
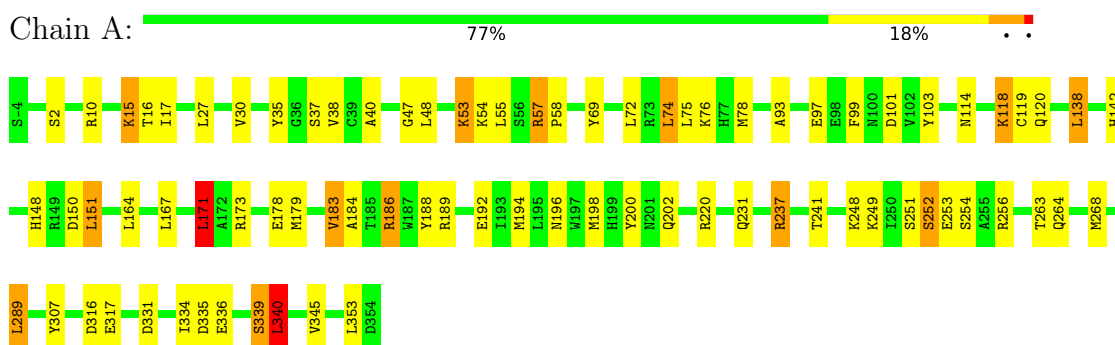
• Molecule 1: Mitogen-activated protein kinase 14

4.2.2 Score per residue for model 2

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 76% 19%

S-4 R10 L13 N14 K15 T16 I17 W18 L27 V30 G31 S32 S37 V38 C39 A40 K53 K54 L55 S56 R57 P58 I63 R67 T68 Y69 L74 L75 M78 E81 N82 V89 D101 V102 Y103 K118 C119 Q120 Q133 R136 G137 L138 I141

A144 H148 R149 D150 L151 L167 D168 F169 G170 L171 A172 R173 H174 T175 D176 D177 E178 M179 T180 V183 R186 W187 Y188 R189 E192 I193 M194 M198 H199 Y200 I212 L216 R220 T221 Q231 R237 K248 K249 E253 S254 R256 T263 Q264

L289 Y307 D316 E317 A320 D331 I334 D335 E336 S339 L340 V345 L353 D364

4.2.3 Score per residue for model 3

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 77% 18%

S-4 S2 R10 K15 T16 I17 L27 V30 Y35 G36 S37 V38 C39 A40 G47 L48 K53 K54 L55 S56 R57 P58 Y69 L72 R73 L74 L75 K76 H77 M78 A93 E97 E98 F99 N100 D101 V102 Y103 N114 K118 C119 Q120 L138 H142

H148 R149 D150 L151 L164 L167 L171 A172 R173 E178 M179 V183 A184 T185 R186 W187 Y188 R189 E192 I193 M194 L195 N196 W197 M198 H199 Y200 N201 Q202 R220 Q231 R237 T241 K248 K249 I250 S251 S252 E253 S254 A255 R256 T263 Q264 M268

L289 Y307 D316 E317 D331 I334 D335 E336 S339 L340 V345 L353 D364

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 80% 16%

S-4 R10 K15 T16 I17 L27 V30 S37 V38 C39 A40 K53 K54 L55 S56 R57 P58 L72 R73 L74 L75 K76 D101 V102 Y103 D112 L113 N114 N115 K118 C119 Q120 L138 D150 L151 L164 L167 L171 A172 R173 E178 M179 V183

R186 W187 Y188 E192 I193 M194 M198 H199 Y200 R220 Q231 R237 K248 K249 I250 S251 S252 E253 S254 A255 R256 T263 Q264 M268 N269 F270 E286 L289 A306 Y307 D316 E317 D331 I334 D335 E336 S339 L340 V345 L353 D364
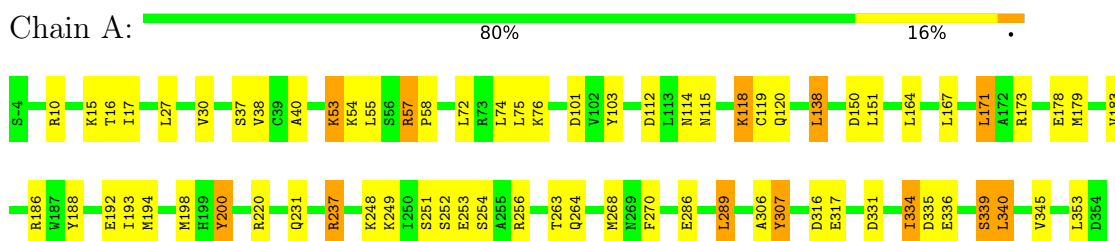
4.2.5 Score per residue for model 5

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 77% 19%

S-4 R10 L13 N14 K15 T16 I17 L27 V30 S37 V38 C39 A40 K53 K54 L55 S56 R57 P58 K66 L74 L75 I84 D101 V102 Y103 D112 L113 N114 N115 K118 C119 Q120 L138 A144 H148 R149 D150 L151 L164 L167 L171

A172 R173 E178 M179 V183 R186 W187 Y188 R189 E192 I193 M194 M198 H199 Y200 N201 V204 R220 Q231 R237 K248 K249 I250 S251 S252 E253 S254 A255 R256 T263 Q264 M268 N269 F270 E286 L289 D292 K295 A306 Y307 D316 E317

A320 E328 D331 L332 L333 I334 D335 E336 S339 L340 V345 L353 D354

4.2.6　Score per residue for model 6

● Molecule 1: Mitogen-activated protein kinase 14

Chain A:　　　79%　　　18%　　•

S-4 R10 L13 N14 K15 T16 I17 W18 L27 V30 G31 S32 S37 A40 A41 K53 K54 L55 S56 R57 P58 L74 L75 M78 I84 E97 D101 K118 C119 Q120 L138 A144 D150 L151 K152 L167 D168 L171 A172 R173 H174 T175

D176 D177 E178 M179 Y182 V183 A184 T185 R186 W187 Y188 E192 M198 H199 Y200 R220 F223 Q231 R237 L246 L247 K248 K249 S252 E253 R256 T263 Q264 M268 L289 Y307 D316 E317 P318 V319 A320 S326 D331 L332 L333 I334 D335 E336

S339 L340 V345 L353 D354

4.2.7　Score per residue for model 7

● Molecule 1: Mitogen-activated protein kinase 14

Chain A:　　　77%　　　19%　　••

S-4 R10 K15 T16 I17 P21 L27 V30 G31 S32 G36 S37 V38 C39 A40 A41 K53 K54 L55 S56 R57 P58 Y69 L74 L75 M78 E81 F90 E97 D101 K118 C119 Q120 D124 Q128 R136 G137 L138 K139 I146 I147

H148 R149 D150 L151 K152 L167 L171 A172 R173 H174 T175 D176 D177 E178 M179 Y182 V183 R186 W187 Y188 E192 I193 M194 L195 N196 W197 M198 H199 Y200 R220 T226 Q231 R237 T241 K248 K249 I250 S251 S252 E253 R256 Q260 T263 Q264 L289

Y307 D316 E317 P318 V319 D331 L332 L333 I334 D335 E336 S339 L340 V345 L353 D354

4.2.8　Score per residue for model 8

● Molecule 1: Mitogen-activated protein kinase 14

Chain A:　　　78%　　　19%　　•

S-4 R5 P6 R10 L13 N14 K15 T16 I17 L27 V30 G31 S32 S37 A40 K53 R57 P58 L72 R73 L74 L75 K76 D101 D112 N115 K118 C119 Q120 K121 L138 A144 H148 R149 D150 L151 K152 L167 D168 F169 G170 L171

A172 R173 H174 T175 D176 D177 E178 M179 V183 Y188 E192 I193 M194 M198 H199 Y200 D205 V209 R220 Q231 R237 T241 P242 K248 K249 I250 S251 S252 E253 R256 T263 Q264 L289 V290 L291 Y307 D316 E317 A320 D331 I334

D335 E336 S339 L340 V345 L353 D354

4.2.9 Score per residue for model 9

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 78% 19% •

S-4 R10 L13 N14 K15 T16 I17 L27 V30 S37 A40 K53 K54 L55 S56 R57 P58 F59 K66 Y69 L74 L75 A93 F99 N100 D101 D112 L113 N114 N115 K118 C119 Q120 L138 D150 L151 L164 L167 L171 A172 R173

E178 M179 V183 R186 W187 Y188 R189 E192 I193 M194 L195 N196 W197 M198 H199 Y200 N201 V204 R220 Q231 R237 K248 K249 I250 S251 S252 E253 S254 A255 R256 T263 Q264 M268 L289 A306 Y307 D316 E317 E328 D331 L332 L333 I334 D335

E336 W337 K338 S339 L340 V345 L353 D354

4.2.10 Score per residue for model 10

• Molecule 1: Mitogen-activated protein kinase 14

Chain A: 77% 20% •

S-4 R10 Q11 E12 L13 N14 K15 T16 I17 W18 L27 V30 G31 S32 S37 A40 A41 K53 S56 R57 P58 Y69 L74 L75 E81 I84 E97 D101 D112 N115 K118 C119 Q120 R136 G137 L138 D150 L151 K152 L167

L171 A172 R173 H174 T175 D176 D177 E178 M179 V183 R186 W187 Y188 R189 E192 I193 M194 L195 N196 W197 M198 H199 Y200 R220 Q231 R237 L238 T241 K248 K249 S252 E253 S254 A255 R256 T263 Q264 M268 N278 A281 L289 D292 K295

Y307 D316 E317 D331 L332 L333 I334 D335 E336 S339 L340 V345 L353 D354

5 Refinement protocol and experimental data overview ⓘ

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

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *lowest R-free.*

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

Software name	Classification	Version
ISD	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1112
Number of shifts mapped to atoms	1112
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

6 Model quality ⓘ

6.1 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 (average) 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	A	1.08±0.00	7±0/2965 (0.2± 0.0%)	1.09±0.00	20±0/4023 (0.5± 0.0%)
All	All	1.08	70/29650 (0.2%)	1.09	202/40230 (0.5%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	A	15	LYS	CA-CB	-10.84	1.30	1.53	4	10
1	A	339	SER	CA-CB	7.89	1.64	1.52	6	10
1	A	53	LYS	CB-CG	-6.06	1.36	1.52	10	10
1	A	192	GLU	CB-CG	-5.35	1.42	1.52	7	10
1	A	307	TYR	CD2-CE2	-5.33	1.31	1.39	8	10
1	A	345	VAL	CB-CG1	5.22	1.63	1.52	6	10
1	A	188	TYR	CD1-CE1	5.08	1.47	1.39	7	1
1	A	188	TYR	CD2-CE2	5.07	1.47	1.39	8	9

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Total
1	A	10	ARG	NE-CZ-NH2	-15.02	112.79	120.30	7	10
1	A	10	ARG	NE-CZ-NH1	12.22	126.41	120.30	7	10
1	A	339	SER	N-CA-CB	8.19	122.78	110.50	7	10
1	A	15	LYS	N-CA-CB	7.91	124.84	110.60	7	10
1	A	74	LEU	CB-CG-CD2	-7.28	98.63	111.00	6	10
1	A	289	LEU	CB-CG-CD1	6.97	122.86	111.00	9	10
1	A	15	LYS	CA-CB-CG	-6.85	98.33	113.40	10	10
1	A	167	LEU	CB-CG-CD2	-6.75	99.52	111.00	9	10
1	A	10	ARG	CG-CD-NE	-6.34	98.50	111.80	2	10
1	A	150	ASP	CB-CG-OD1	6.25	123.93	118.30	6	10
1	A	150	ASP	CB-CA-C	6.25	122.89	110.40	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	138	LEU	CB-CG-CD1	6.25	121.62	111.00	3	10
1	A	192	GLU	CB-CA-C	-5.91	98.59	110.40	5	10
1	A	101	ASP	CB-CG-OD1	5.80	123.52	118.30	4	10
1	A	15	LYS	CB-CA-C	-5.67	99.06	110.40	1	10
1	A	220	ARG	NE-CZ-NH2	-5.51	117.55	120.30	7	10
1	A	171	LEU	CA-CB-CG	5.38	127.67	115.30	7	10
1	A	167	LEU	CA-CB-CG	5.33	127.56	115.30	10	10
1	A	340	LEU	CB-CG-CD2	5.13	119.72	111.00	5	10
1	A	167	LEU	CB-CA-C	-5.05	100.60	110.20	6	10
1	A	340	LEU	CB-CG-CD1	5.01	119.52	111.00	9	2

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	2898	344	2884	27±3
All	All	28980	3440	28840	271

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:248:LYS:HA	1:A:256:ARG:HH21	0.92	1.23	7	10
1:A:16:THR:HG22	1:A:17:ILE:N	0.71	2.00	5	9
1:A:248:LYS:HA	1:A:256:ARG:NH2	0.69	2.03	7	3
1:A:114:ASN:O	1:A:118:LYS:HD2	0.66	1.90	3	5
1:A:334:ILE:O	1:A:336:GLU:N	0.64	2.31	1	10
1:A:16:THR:HG22	1:A:17:ILE:H	0.62	1.52	9	10
1:A:63:ILE:O	1:A:67:ARG:HG3	0.61	1.96	2	1
1:A:316:ASP:O	1:A:317:GLU:HG3	0.60	1.95	1	10
1:A:57:ARG:N	1:A:58:PRO:CD	0.60	2.65	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:HIS:CE1	1:A:151:LEU:H	0.58	2.17	2	5
1:A:186:ARG:HG2	1:A:194:MET:HE1	0.58	1.73	1	3
1:A:27:LEU:HA	1:A:40:ALA:O	0.57	2.00	1	10
1:A:81:GLU:HB2	1:A:136:ARG:HH12	0.56	1.60	7	3
1:A:72:LEU:O	1:A:76:LYS:HG3	0.56	2.01	3	3
1:A:112:ASP:H	1:A:115:ASN:ND2	0.56	1.98	8	5
1:A:189:ARG:HB3	1:A:194:MET:HE3	0.56	1.76	5	4
1:A:241:THR:OG1	1:A:264:GLN:HG3	0.56	2.01	1	4
1:A:170:GLY:HA2	1:A:173:ARG:HG2	0.54	1.78	8	1
1:A:152:LYS:NZ	1:A:173:ARG:HH21	0.54	2.00	7	4
1:A:248:LYS:CA	1:A:256:ARG:HH21	0.54	2.12	6	2
1:A:71:GLU:HG2	1:A:75:LEU:HD22	0.54	1.78	1	1
1:A:193:ILE:HG22	1:A:200:TYR:CD2	0.53	2.38	1	2
1:A:38:VAL:HG22	1:A:53:LYS:HB3	0.53	1.80	7	5
1:A:84:ILE:HG13	1:A:167:LEU:HD23	0.53	1.81	6	3
1:A:27:LEU:HG	1:A:41:ALA:HB2	0.52	1.82	7	3
1:A:237:ARG:O	1:A:268:MET:HG3	0.52	2.05	4	5
1:A:74:LEU:HD22	1:A:169:PHE:CE2	0.51	2.41	8	2
1:A:47:GLY:O	1:A:48:LEU:HD23	0.51	2.06	3	1
1:A:13:LEU:HD12	1:A:18:TRP:CG	0.50	2.41	10	2
1:A:53:LYS:NZ	1:A:174:HIS:HE1	0.50	2.04	2	1
1:A:54:LYS:HE3	1:A:103:TYR:OH	0.50	2.06	3	4
1:A:212:ILE:O	1:A:216:LEU:HG	0.50	2.06	2	1
1:A:168:ASP:OD2	1:A:174:HIS:NE2	0.50	2.44	6	2
1:A:16:THR:CG2	1:A:17:ILE:N	0.49	2.72	5	6
1:A:183:VAL:HG12	1:A:184:ALA:H	0.49	1.67	6	2
1:A:74:LEU:O	1:A:78:MET:HG2	0.49	2.08	3	3
1:A:186:ARG:HG2	1:A:194:MET:CE	0.49	2.36	4	3
1:A:334:ILE:C	1:A:336:GLU:H	0.48	2.11	1	9
1:A:334:ILE:C	1:A:336:GLU:N	0.48	2.67	10	10
1:A:97:GLU:H	1:A:97:GLU:CD	0.48	2.11	7	5
1:A:195:LEU:HB2	1:A:197:TRP:NE1	0.48	2.24	10	3
1:A:139:LYS:HE2	1:A:319:VAL:CG1	0.47	2.40	7	1
1:A:141:ILE:HD13	1:A:169:PHE:HE1	0.47	1.68	2	1
1:A:13:LEU:HB2	1:A:18:TRP:CD1	0.47	2.45	1	3
1:A:193:ILE:HG22	1:A:200:TYR:CD1	0.47	2.45	8	5
1:A:66:LYS:HE2	1:A:328:GLU:OE1	0.47	2.10	5	2
1:A:256:ARG:O	1:A:260:GLN:HG3	0.46	2.10	7	1
1:A:333:LEU:O	1:A:336:GLU:HB2	0.45	2.11	6	5
1:A:189:ARG:HB3	1:A:194:MET:CE	0.45	2.42	10	2
1:A:164:LEU:C	1:A:164:LEU:HD23	0.45	2.32	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:21:PRO:HD3	1:A:90:PHE:CE1	0.45	2.46	7	1
1:A:27:LEU:N	1:A:27:LEU:HD12	0.45	2.27	1	3
1:A:59:PHE:CD2	1:A:338:LYS:HD2	0.45	2.46	9	1
1:A:93:ALA:HB2	1:A:99:PHE:HA	0.45	1.89	3	2
1:A:112:ASP:H	1:A:115:ASN:HD22	0.45	1.52	5	4
1:A:13:LEU:O	1:A:14:ASN:HB2	0.45	2.11	5	3
1:A:201:ASN:O	1:A:204:VAL:HG22	0.44	2.12	9	2
1:A:74:LEU:HD21	1:A:146:ILE:HD13	0.44	1.89	7	1
1:A:5:ARG:HG3	1:A:6:PRO:HD2	0.44	1.88	8	1
1:A:242:PRO:HB3	1:A:291:LEU:HD23	0.44	1.89	8	2
1:A:223:PHE:HB2	1:A:231:GLN:NE2	0.44	2.27	6	1
1:A:144:ALA:HB2	1:A:320:ALA:CB	0.44	2.42	5	4
1:A:292:ASP:HB3	1:A:295:LYS:HB2	0.44	1.90	10	2
1:A:270:PHE:CD2	1:A:286:GLU:HG3	0.43	2.48	5	2
1:A:69:TYR:CE1	1:A:340:LEU:HB3	0.43	2.48	7	5
1:A:112:ASP:OD1	1:A:112:ASP:C	0.43	2.57	9	3
1:A:317:GLU:N	1:A:318:PRO:CD	0.43	2.82	7	2
1:A:142:HIS:HB3	1:A:202:GLN:NE2	0.42	2.29	3	1
1:A:74:LEU:HD13	1:A:169:PHE:HD2	0.42	1.74	1	1
1:A:278:ASN:O	1:A:281:ALA:HB3	0.42	2.15	10	2
1:A:252:SER:O	1:A:256:ARG:HB2	0.42	2.15	3	1
1:A:124:ASP:OD2	1:A:128:GLN:NE2	0.42	2.52	7	1
1:A:112:ASP:OD1	1:A:114:ASN:HB2	0.42	2.15	1	1
1:A:78:MET:HA	1:A:78:MET:HE2	0.42	1.92	7	1
1:A:205:ASP:O	1:A:209:VAL:HG23	0.42	2.14	8	1
1:A:151:LEU:HD12	1:A:151:LEU:HA	0.41	1.80	7	1
1:A:238:LEU:HA	1:A:268:MET:HG3	0.41	1.92	10	1
1:A:185:THR:O	1:A:189:ARG:NH2	0.41	2.54	1	1
1:A:36:GLY:N	1:A:174:HIS:CE1	0.41	2.88	7	1
1:A:152:LYS:NZ	1:A:173:ARG:NH2	0.41	2.68	7	1
1:A:306:ALA:O	1:A:307:TYR:C	0.41	2.59	5	3
1:A:182:TYR:OH	1:A:226:THR:HG22	0.41	2.16	7	1
1:A:235:ILE:O	1:A:239:VAL:HG22	0.40	2.15	1	1
1:A:171:LEU:CD2	1:A:171:LEU:N	0.40	2.84	3	1
1:A:82:ASN:ND2	1:A:133:GLN:HB3	0.40	2.32	2	1
1:A:12:GLU:HA	1:A:16:THR:O	0.40	2.16	10	1
1:A:57:ARG:N	1:A:58:PRO:HD3	0.40	2.31	2	1
1:A:164:LEU:HD23	1:A:164:LEU:C	0.40	2.36	3	1

6.3 Torsion angles ⓘ

6.3.1 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 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	357/359 (99%)	331±2 (93±1%)	20±2 (6±1%)	7±1 (2±0%)	11	53
All	All	3570/3590 (99%)	3306 (93%)	197 (6%)	67 (2%)	11	53

All 12 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	151	LEU	10
1	A	183	VAL	10
1	A	200	TYR	10
1	A	335	ASP	9
1	A	57	ARG	9
1	A	334	ILE	8
1	A	174	HIS	3
1	A	177	ASP	3
1	A	196	ASN	2
1	A	176	ASP	1
1	A	2	SER	1
1	A	35	TYR	1

6.3.2 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 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	319/319 (100%)	288±3 (90±1%)	31±3 (10±1%)	12	57
All	All	3190/3190 (100%)	2882 (90%)	308 (10%)	12	57

All 49 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	30	VAL	10
1	A	37	SER	10
1	A	75	LEU	10
1	A	118	LYS	10
1	A	120	GLN	10
1	A	138	LEU	10
1	A	171	LEU	10
1	A	173	ARG	10
1	A	178	GLU	10
1	A	179	MET	10
1	A	198	MET	10
1	A	231	GLN	10
1	A	237	ARG	10
1	A	249	LYS	10
1	A	253	GLU	10
1	A	263	THR	10
1	A	264	GLN	10
1	A	289	LEU	10
1	A	331	ASP	10
1	A	339	SER	10
1	A	340	LEU	10
1	A	353	LEU	10
1	A	119	CYS	8
1	A	186	ARG	7
1	A	254	SER	7
1	A	55	LEU	7
1	A	252	SER	7
1	A	176	ASP	6
1	A	251	SER	6
1	A	56	SER	5
1	A	32	SER	5
1	A	183	VAL	3
1	A	199	HIS	3
1	A	53	LYS	3
1	A	194	MET	3
1	A	14	ASN	2
1	A	180	THR	2
1	A	326	SER	2
1	A	175	THR	2
1	A	245	GLU	1
1	A	354	ASP	1
1	A	10	ARG	1
1	A	89	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	221	THR	1
1	A	15	LYS	1
1	A	241	THR	1
1	A	182	TYR	1
1	A	246	LEU	1
1	A	121	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 22% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1112
Number of shifts mapped to atoms	1112
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	232	0.47 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_\beta$	219	1.03 ± 0.12	Should be checked
$^{13}C'$	227	0.18 ± 0.11	None needed (< 0.5 ppm)
^{15}N	217	1.11 ± 0.30	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 1112 atoms were assigned a chemical shift out of a possible 5021. 0 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	893/1776 (50%)	217/716 (30%)	459/718 (64%)	217/342 (63%)
Sidechain	219/2847 (8%)	0/1857 (0%)	219/886 (25%)	0/104 (0%)

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PROTEIN DATA BANK

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	0/398 (0%)	0/207 (0%)	0/191 (0%)	0/0 (—%)
Overall	1112/5021 (22%)	217/2780 (8%)	678/1795 (38%)	217/446 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 22%, i.e. 1112 atoms were assigned a chemical shift out of a possible 5021. 0 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|	**Total**	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	893/1776 (50%)	217/716 (30%)	459/718 (64%)	217/342 (63%)
Sidechain	219/2847 (8%)	0/1857 (0%)	219/886 (25%)	0/104 (0%)
Aromatic	0/398 (0%)	0/207 (0%)	0/191 (0%)	0/0 (—%)
Overall	1112/5021 (22%)	217/2780 (8%)	678/1795 (38%)	217/446 (49%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	**Chain**	**Res**	**Type**	**Atom**	**Shift, *ppm***	**Expected range, *ppm***	**Z-score**
1	A	91	THR	C	184.43	166.08 – 183.07	5.8

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:
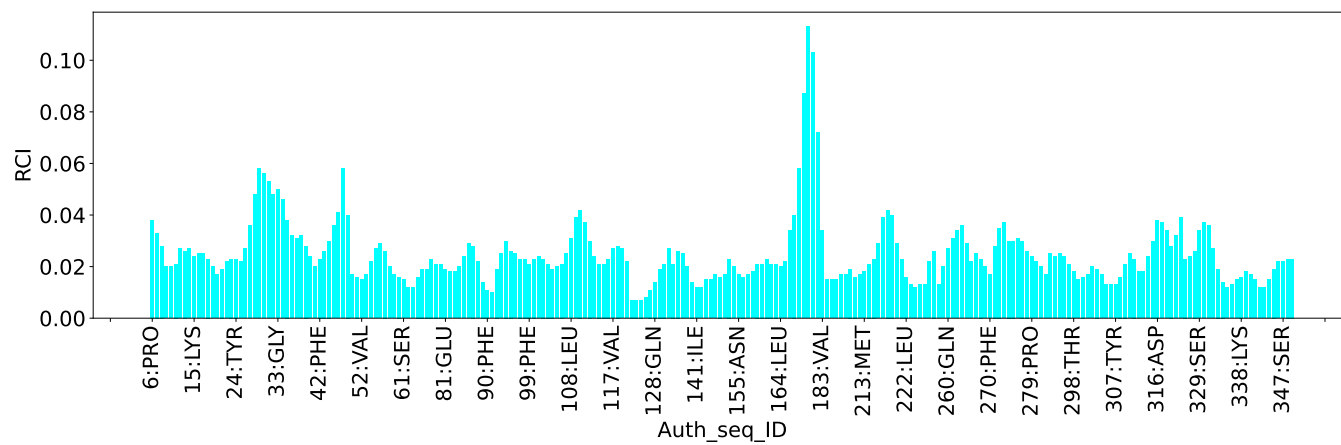
8 NMR restraints analysis ⓘ

No restraints data found

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found