WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2022 – 01:50 AM EST

PDB ID : 1TRL

Title : NMR SOLUTION STRUCTURE OF THE C-TERMINAL FRAGMENT 255-316 OF THERMOLYSIN: A DIMER FORMED BY SUBUNITS HAVING THE NATIVE STRUCTURE

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Deposited on : 1994-09-02

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

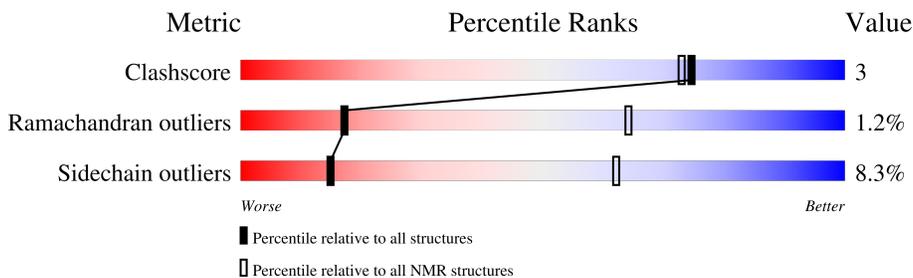|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		1.2%
Sidechain outliers		8.3%

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	62	65% 19% 16%
1	B	62	71% 13% 16%

2 Ensemble composition and analysis ⓘ

This entry contains 8 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:262-A:313, B:262-B:313 (104)	0.40	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1168 atoms, of which 232 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called THERMOLYSIN FRAGMENT 255 - 316.

| Mol	Chain	Residues	Atoms					Trace
1	A	62	Total	C	H	N	O	0
			584	296	116	81	91	
1	B	62	Total	C	H	N	O	0
			584	296	116	81	91	

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: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316
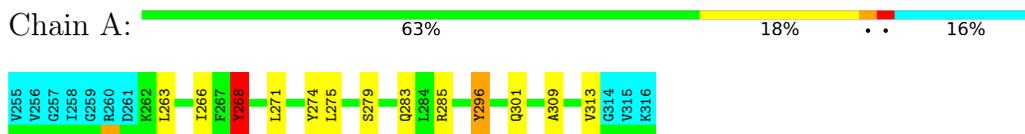
Chain B:
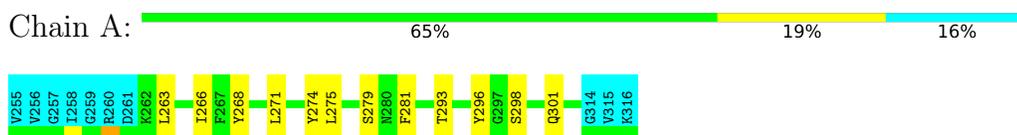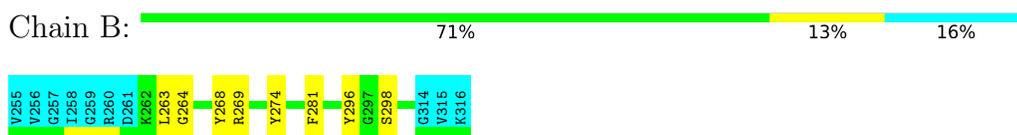
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:
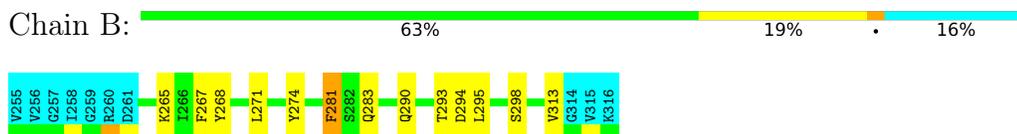
4.2.2 Score per residue for model 2

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:
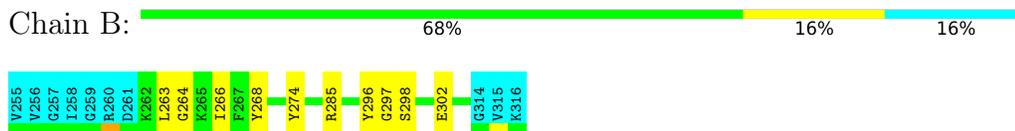
4.2.3 Score per residue for model 3

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:
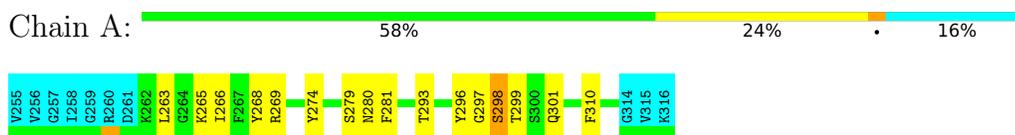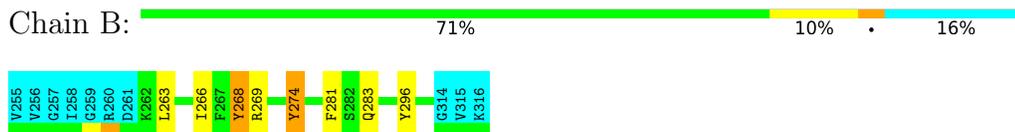
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:

4.2.5 Score per residue for model 5
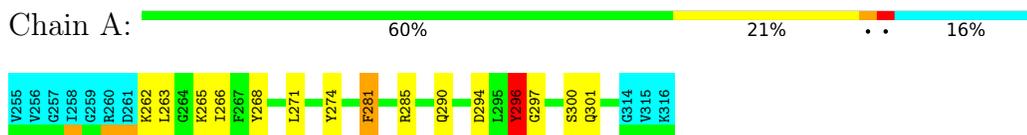
• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

60%   19%   5%   16%

V255 V256 G257 I258 G259 R260 D261 K262 L263 G264 K265 I266 F267 Y268 R269 Y274 L275 T276 F281 A286 T293 Y296 G297 S298 E302 V306 G314 V315 K316

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:

63%   19%   •   16%
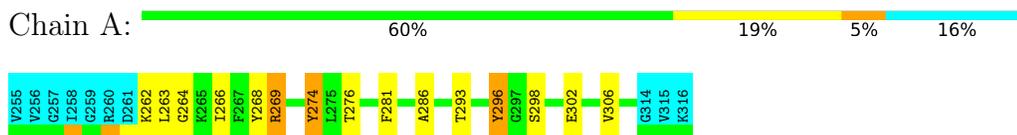
V255 V256 G257 I258 G259 R260 D261 K262 L263 G264 K265 I266 R269 S279 N280 F281 S282 Q283 T293 Y296 G297 S298 F310 V313 G314 V315 K316
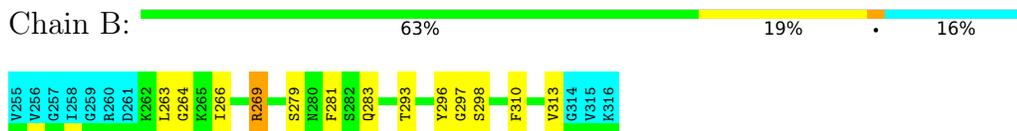
4.2.6 Score per residue for model 6

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

60%   23%   •   16%

V255 V256 G257 I258 G259 R260 D261 K262 L263 G264 K265 I266 F267 Y268 Q273 Y274 L275 S279 N280 F281 Y296 T299 S300 Q301 S305 G314 V315 K316

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:

68%   15%   •   16%
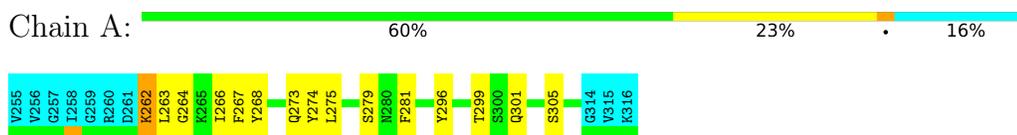
V255 V256 G257 I258 G259 R260 D261 K262 L263 G264 R269 A270 L271 T272 Q273 Y274 Q283 Y296 S305 Q308 G314 V315 K316

4.2.7 Score per residue for model 7

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain A:

65%   19%   16%

V255 V256 G257 I258 G259 R260 D261 K262 L263 Y268 L271 Y274 L275 T276 P277 T278 S279 N280 F281 R285 T293 Y296 G297 S298 G314 V315 K316

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:

61%   19%   •   16%
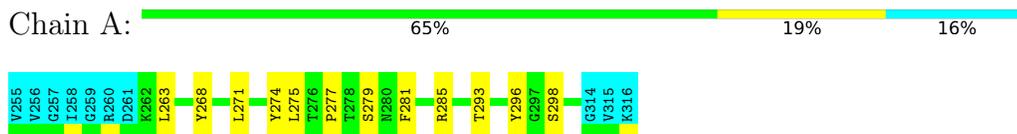
V255 V256 G257 I258 G259 R260 D261 K265 Y268 L271 Y274 L275 R285 Q290 Y296 G297 S298 Q301 E302 V303 A304 S305 V306 K307 G314 V315 K316
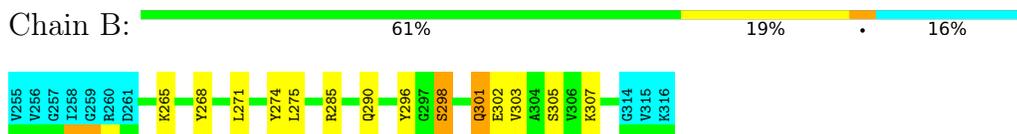
4.2.8 Score per residue for model 8

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316
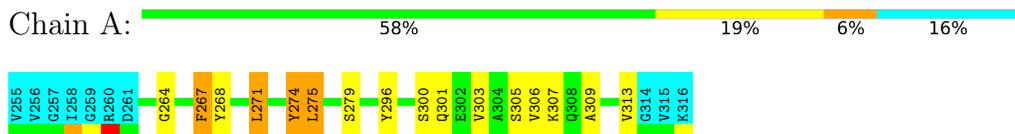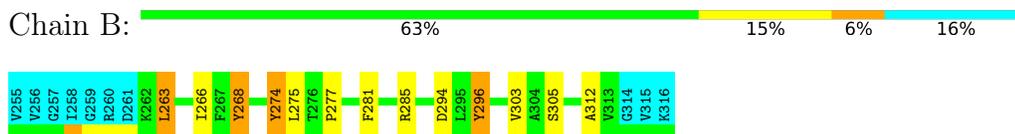
Chain A:

• Molecule 1: THERMOLYSIN FRAGMENT 255 - 316

Chain B:

5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 8 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
GROMOS	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.81±0.01	0±0/405 (0.0± 0.0%)	1.26±0.10	3±2/550 (0.6± 0.4%)
1	B	0.81±0.02	0±0/405 (0.0± 0.0%)	1.24±0.08	2±2/550 (0.5± 0.3%)
All	All	0.81	0/6480 (0.0%)	1.25	46/8800 (0.5%)

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	Planarity
1	A	0.0±0.0	3.1±1.5
1	B	0.0±0.0	2.6±1.6
All	All	0	46

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	301	GLN	CG-CD-OE1	10.35	142.31	121.60	4	1
1	A	301	GLN	CG-CD-NE2	-8.56	96.14	116.70	4	1
1	A	274	TYR	CB-CG-CD2	-8.16	116.11	121.00	4	7
1	B	268	TYR	CB-CG-CD2	-7.54	116.48	121.00	3	1
1	A	285	ARG	NE-CZ-NH2	7.35	123.97	120.30	7	1
1	B	285	ARG	CD-NE-CZ	7.29	133.80	123.60	4	1
1	B	268	TYR	CB-CG-CD1	-7.28	116.63	121.00	4	1
1	B	269	ARG	NE-CZ-NH1	7.24	123.92	120.30	5	3
1	A	285	ARG	NE-CZ-NH1	6.87	123.73	120.30	1	2
1	A	296	TYR	CB-CG-CD2	-6.67	117.00	121.00	2	5
1	B	303	VAL	CG1-CB-CG2	-6.26	100.89	110.90	4	1
1	B	281	PHE	CB-CG-CD2	-6.24	116.43	120.80	5	3
1	B	296	TYR	CB-CG-CD2	-6.13	117.32	121.00	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	B	274	TYR	CB-CG-CD2	-6.08	117.35	121.00	6	4
1	A	267	PHE	CB-CG-CD1	-6.01	116.60	120.80	4	2
1	B	285	ARG	CG-CD-NE	-5.96	99.29	111.80	4	1
1	B	285	ARG	NE-CZ-NH1	5.89	123.25	120.30	8	1
1	A	268	TYR	CB-CG-CD2	-5.89	117.47	121.00	1	3
1	A	281	PHE	CB-CG-CD2	-5.87	116.69	120.80	2	2
1	A	296	TYR	CB-CG-CD1	-5.74	117.56	121.00	2	1
1	A	269	ARG	NE-CZ-NH1	5.42	123.01	120.30	5	1
1	B	267	PHE	CB-CG-CD1	-5.31	117.08	120.80	1	1
1	B	310	PHE	CB-CG-CD1	-5.28	117.10	120.80	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	268	TYR	Sidechain	5
1	A	296	TYR	Sidechain	5
1	B	274	TYR	Sidechain	5
1	B	296	TYR	Sidechain	5
1	B	268	TYR	Sidechain	4
1	B	281	PHE	Sidechain	3
1	A	281	PHE	Sidechain	3
1	A	310	PHE	Sidechain	2
1	A	274	TYR	Sidechain	2
1	A	279	SER	Mainchain	1
1	A	267	PHE	Sidechain	1
1	A	306	VAL	Mainchain	1
1	B	277	PRO	Mainchain	1
1	B	312	ALA	Mainchain	1
1	A	286	ALA	Mainchain	1
1	B	310	PHE	Sidechain	1
1	B	313	VAL	Mainchain	1
1	A	278	THR	Mainchain	1
1	A	308	GLN	Sidechain	1
1	A	309	ALA	Mainchain	1
1	A	313	VAL	Mainchain	1

6.2 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 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	398	96	399	4±2
1	B	398	96	399	3±1
All	All	6368	1536	6384	41

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:264:GLY:HA2	1:B:263:LEU:HB3	0.69	1.64	4	2
1:A:264:GLY:HA2	1:B:263:LEU:HB2	0.66	1.64	8	1
1:A:263:LEU:HA	1:A:266:ILE:HD12	0.62	1.70	6	6
1:B:269:ARG:CZ	1:B:273:GLN:HE22	0.59	2.09	6	1
1:A:263:LEU:HB2	1:B:264:GLY:HA2	0.58	1.76	8	1
1:A:293:THR:HG23	1:A:298:SER:HB3	0.57	1.76	5	3
1:B:293:THR:HG23	1:B:298:SER:HB3	0.54	1.80	5	2
1:A:263:LEU:HD22	1:B:264:GLY:HA2	0.52	1.80	6	3
1:B:265:LYS:HB3	1:B:295:LEU:HD13	0.50	1.82	1	1
1:A:300:SER:HB3	1:A:303:VAL:HG23	0.49	1.84	4	1
1:A:281:PHE:HB2	1:B:279:SER:HB2	0.49	1.84	5	1
1:B:263:LEU:HA	1:B:266:ILE:HD12	0.47	1.85	3	4
1:A:309:ALA:O	1:A:313:VAL:HG23	0.47	2.10	1	2
1:B:266:ILE:HD11	1:B:302:GLU:HG2	0.46	1.85	2	1
1:A:305:SER:HA	1:A:308:GLN:OE1	0.44	2.12	8	1
1:A:266:ILE:HG21	1:A:306:VAL:HG21	0.44	1.90	5	1
1:A:275:LEU:HB3	1:B:313:VAL:HG13	0.43	1.89	1	1
1:A:303:VAL:HG12	1:A:307:LYS:HE3	0.43	1.90	4	1
1:A:297:GLY:O	1:A:300:SER:HB2	0.43	2.13	2	1
1:B:271:LEU:HA	1:B:275:LEU:HB2	0.42	1.90	7	1
1:A:264:GLY:HA2	1:B:263:LEU:HD12	0.41	1.90	5	1
1:B:269:ARG:NH2	1:B:273:GLN:HE22	0.41	2.12	6	1
1:A:275:LEU:HG	1:A:279:SER:OG	0.41	2.15	6	1
1:B:298:SER:HA	1:B:303:VAL:HG21	0.41	1.91	7	1
1:A:293:THR:HG22	1:A:298:SER:HA	0.41	1.91	8	1
1:A:271:LEU:HA	1:A:275:LEU:HB2	0.41	1.93	4	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	52/62 (84%)	48±2 (92±3%)	3±2 (6±3%)	1±1 (2±2%)	13	56
1	B	52/62 (84%)	48±1 (91±2%)	4±1 (8±2%)	0±0 (1±1%)	26	73
All	All	832/992 (84%)	764 (92%)	58 (7%)	10 (1%)	17	64

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	299	THR	3
1	B	297	GLY	2
1	A	296	TYR	1
1	A	297	GLY	1
1	A	298	SER	1
1	A	279	SER	1
1	B	264	GLY	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	42/49 (86%)	38±1 (91±2%)	4±1 (9±2%)	14	61
1	B	42/49 (86%)	39±2 (92±4%)	3±2 (8±4%)	16	63
All	All	672/784 (86%)	616 (92%)	56 (8%)	15	62

All 36 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	271	LEU	5
1	B	283	GLN	4
1	A	301	GLN	3
1	A	265	LYS	3
1	A	279	SER	2
1	B	271	LEU	2
1	B	290	GLN	2
1	B	294	ASP	2
1	A	262	LYS	2
1	B	285	ARG	2
1	B	298	SER	2
1	A	275	LEU	2
1	B	263	LEU	2
1	A	268	TYR	1
1	A	283	GLN	1
1	A	290	GLN	1
1	A	294	ASP	1
1	A	280	ASN	1
1	B	268	TYR	1
1	B	275	LEU	1
1	A	269	ARG	1
1	A	276	THR	1
1	A	302	GLU	1
1	B	269	ARG	1
1	A	273	GLN	1
1	B	305	SER	1
1	B	308	GLN	1
1	A	263	LEU	1
1	A	277	PRO	1
1	B	265	LYS	1
1	B	301	GLN	1
1	B	302	GLU	1
1	B	307	LYS	1
1	A	293	THR	1
1	B	273	GLN	1
1	B	299	THR	1

6.3.3 RNA (i)

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 (i)

No chemical shift data were provided