



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 02:45 PM UTC

PDB ID : 2KUI / pdb_00002kui
Title : NMR structure of the PASTA domain of Mycobacterium tuberculosis of PknB
Authors : Barthe, P.; Mukamolova, G.; Roumestand, C.; Cohen-Gonsaud, M.
Deposited on : 2010-02-17

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

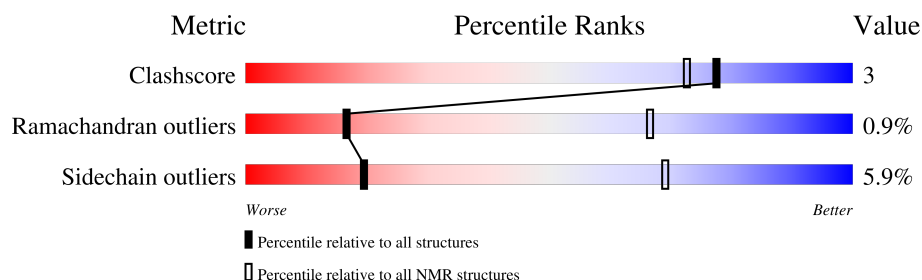
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	275	

2 Ensemble composition and analysis

This entry contains 28 models. Model 16 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:359-A:423 (65)	0.90	16
2	A:426-A:490 (65)	0.62	18
3	A:492-A:626 (135)	2.23	16

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. No single-model clusters were found.

Cluster number	Models
1	1, 10, 12, 13, 14, 15, 17, 18, 21, 23, 25, 28
2	2, 3, 8, 11, 16, 19, 20, 22, 26, 27
3	5, 7, 9, 24
4	4, 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3990 atoms, of which 1988 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase pknB.

Mol	Chain	Residues	Atoms						Trace
1	A	272	Total	C	H	N	O	S	0
			3990	1243	1988	354	402	3	

There are 3 discrepancies between the modelled and reference sequences:

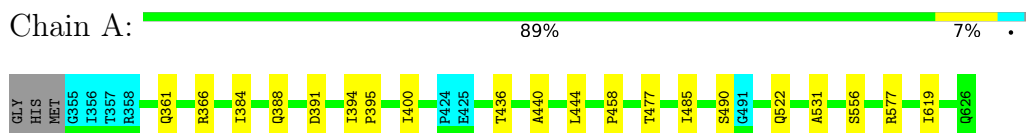
Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	expression tag	UNP P0A5S4
A	353	HIS	-	expression tag	UNP P0A5S4
A	354	MET	-	expression tag	UNP P0A5S4

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: Serine/threonine-protein kinase pknB

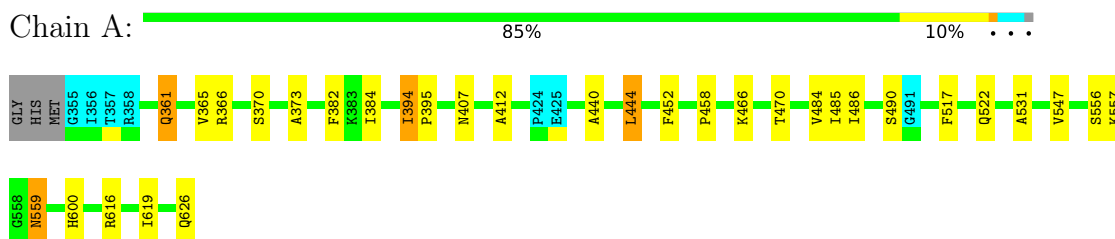


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

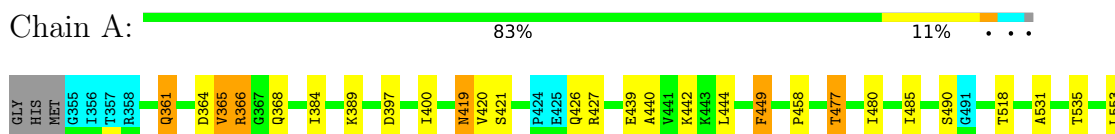
4.2.1 Score per residue for model 1

- Molecule 1: Serine/threonine-protein kinase pknB



4.2.2 Score per residue for model 2

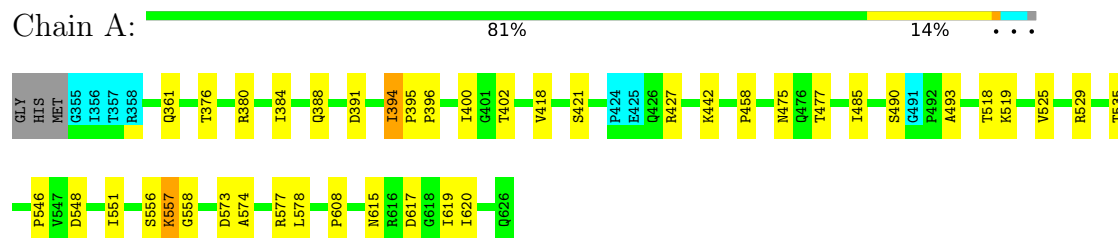
- Molecule 1: Serine/threonine-protein kinase pknB





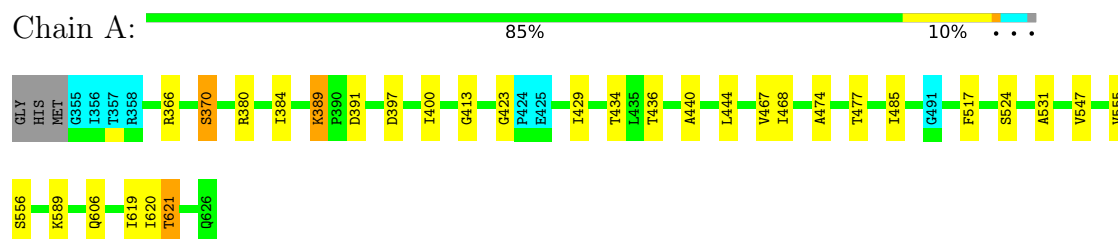
4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase pknB



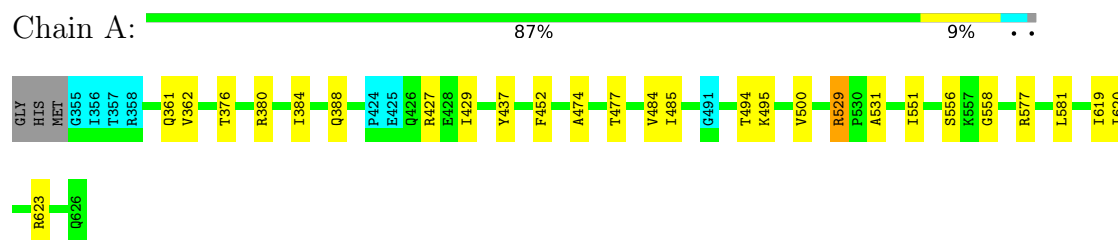
4.2.4 Score per residue for model 4

- Molecule 1: Serine/threonine-protein kinase pknB



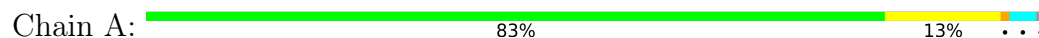
4.2.5 Score per residue for model 5

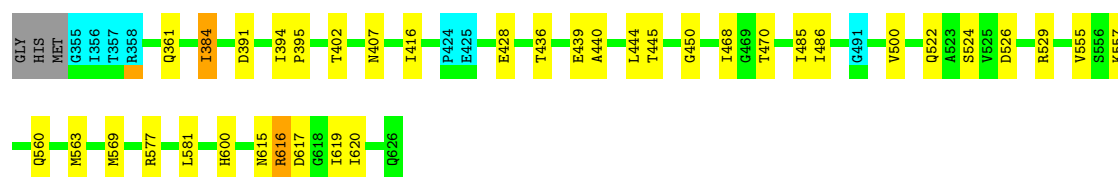
- Molecule 1: Serine/threonine-protein kinase pknB



4.2.6 Score per residue for model 6

- Molecule 1: Serine/threonine-protein kinase pknB

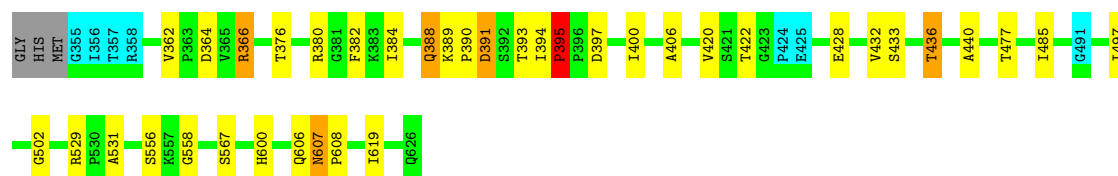




4.2.7 Score per residue for model 7

- Molecule 1: Serine/threonine-protein kinase pknB

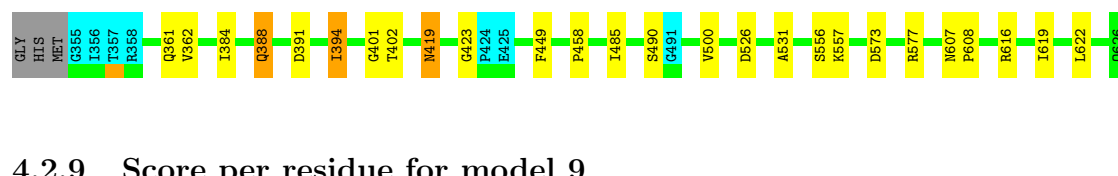
Chain A: 83% 12% . . .



4.2.8 Score per residue for model 8

- Molecule 1: Serine/threonine-protein kinase pknB

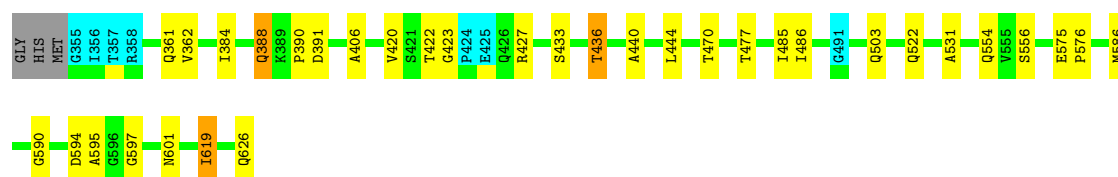
Chain A: 87% 8% . . .



4.2.9 Score per residue for model 9

- Molecule 1: Serine/threonine-protein kinase pknB

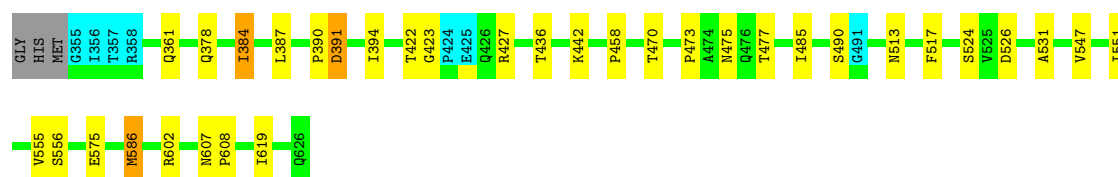
Chain A: 84% 11% . . .



4.2.10 Score per residue for model 10

- Molecule 1: Serine/threonine-protein kinase pknB

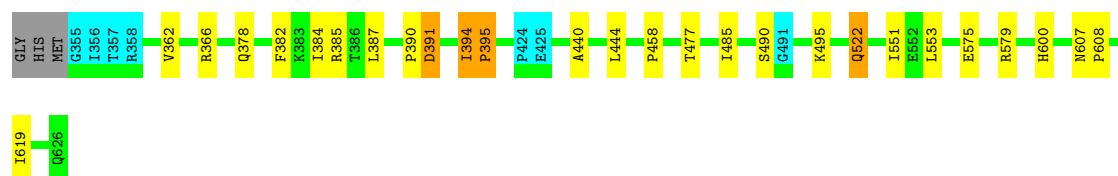
Chain A: 84% 11% . . .



4.2.11 Score per residue for model 11

- Molecule 1: Serine/threonine-protein kinase pknB

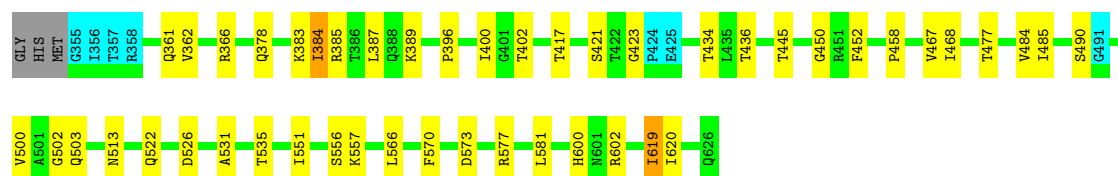
Chain A: 87% 8% ...



4.2.12 Score per residue for model 12

- Molecule 1: Serine/threonine-protein kinase pknB

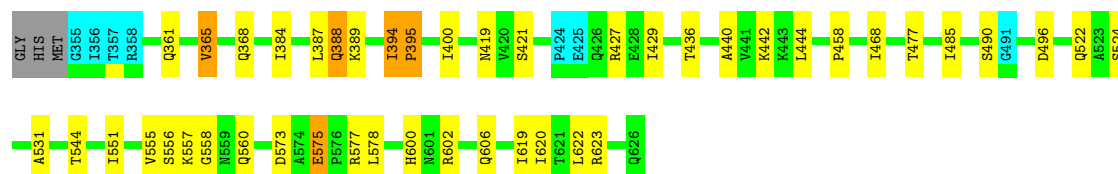
Chain A: 79% 16% ...



4.2.13 Score per residue for model 13

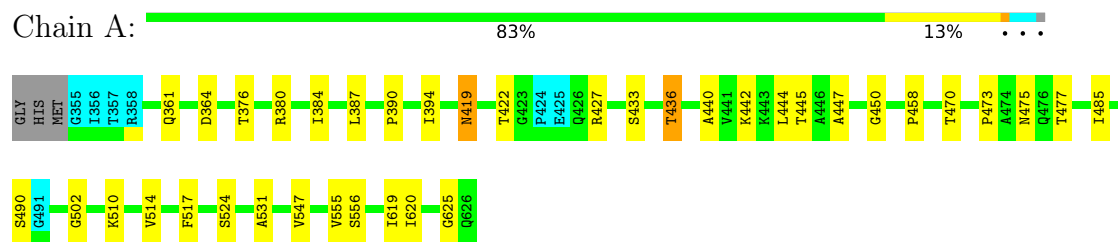
- Molecule 1: Serine/threonine-protein kinase pknB

Chain A: 80% 15% ...



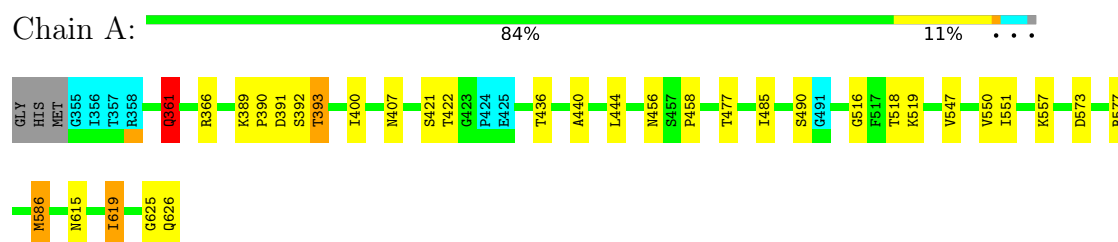
4.2.14 Score per residue for model 14

- Molecule 1: Serine/threonine-protein kinase pknB



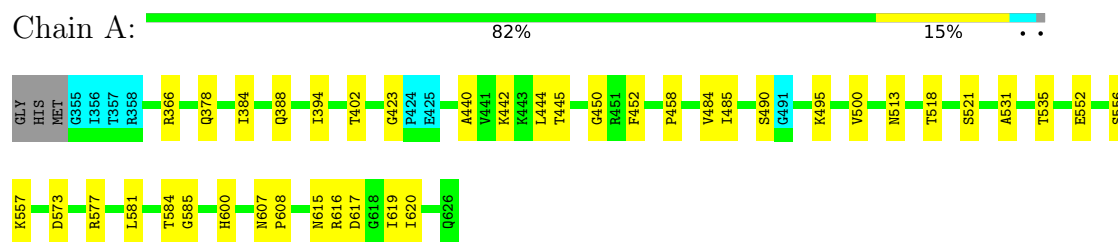
4.2.15 Score per residue for model 15

- Molecule 1: Serine/threonine-protein kinase pknB



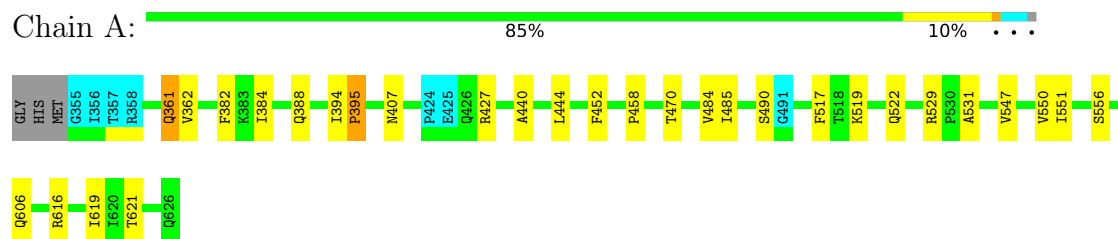
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Serine/threonine-protein kinase pknB



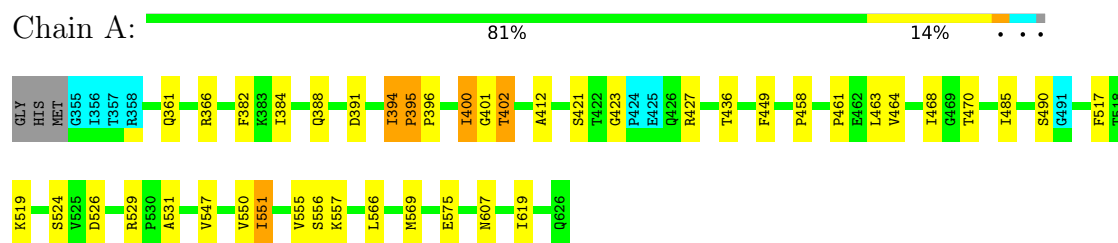
4.2.17 Score per residue for model 17

- Molecule 1: Serine/threonine-protein kinase pknB



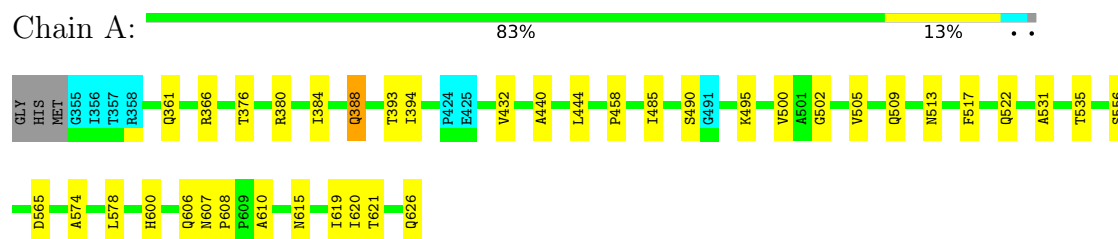
4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein kinase pknB



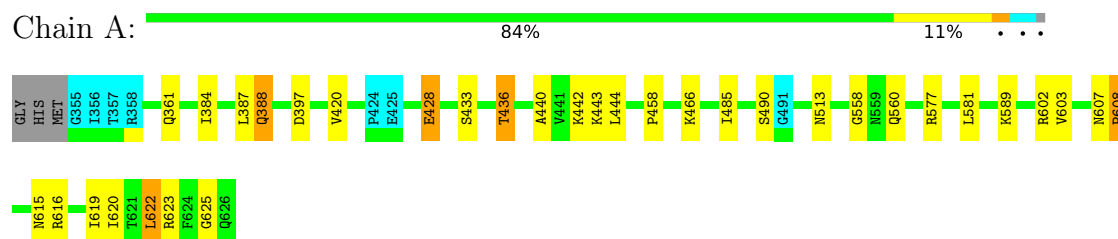
4.2.19 Score per residue for model 19

- Molecule 1: Serine/threonine-protein kinase pknB



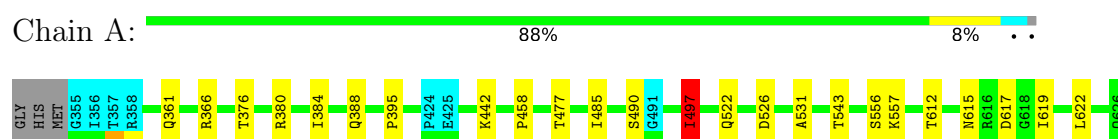
4.2.20 Score per residue for model 20

- Molecule 1: Serine/threonine-protein kinase pknB



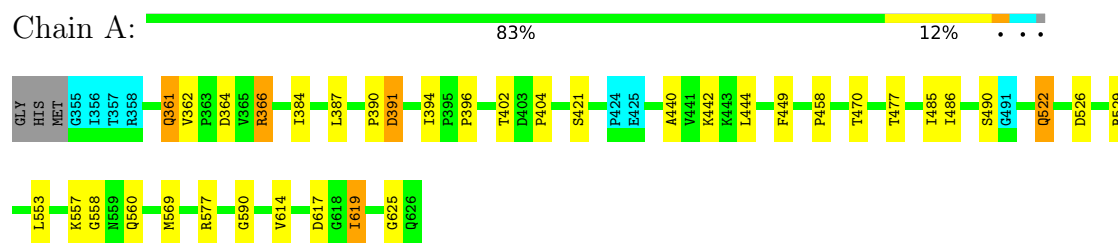
4.2.21 Score per residue for model 21

- Molecule 1: Serine/threonine-protein kinase pknB



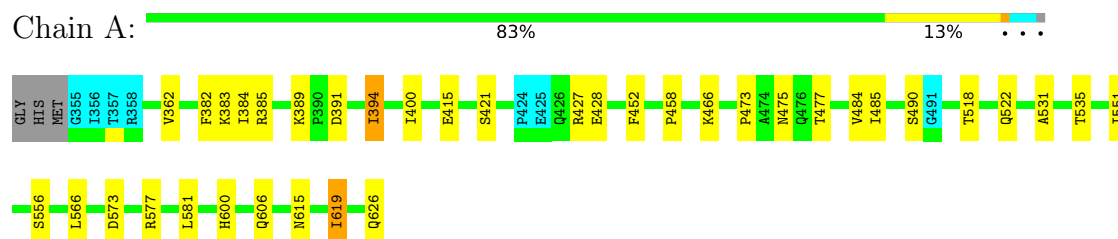
4.2.22 Score per residue for model 22

- Molecule 1: Serine/threonine-protein kinase pknB



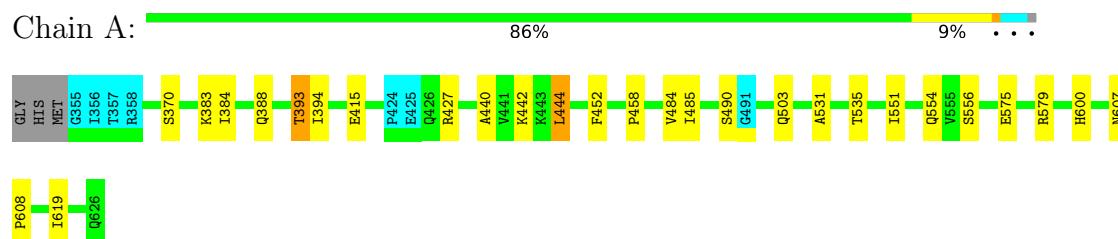
4.2.23 Score per residue for model 23

- Molecule 1: Serine/threonine-protein kinase pknB



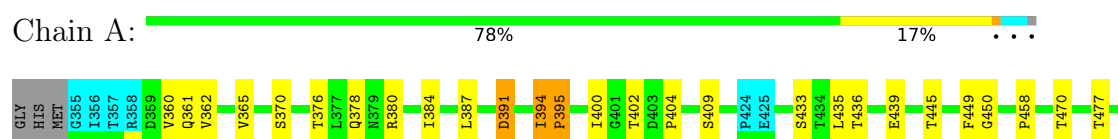
4.2.24 Score per residue for model 24

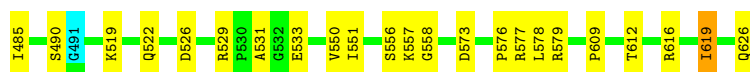
- Molecule 1: Serine/threonine-protein kinase pknB



4.2.25 Score per residue for model 25

- Molecule 1: Serine/threonine-protein kinase pknB

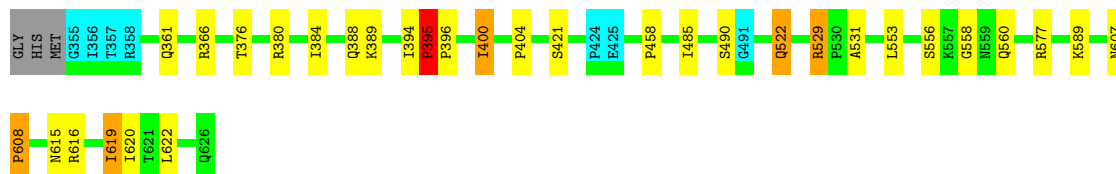




4.2.26 Score per residue for model 26

- Molecule 1: Serine/threonine-protein kinase pknB

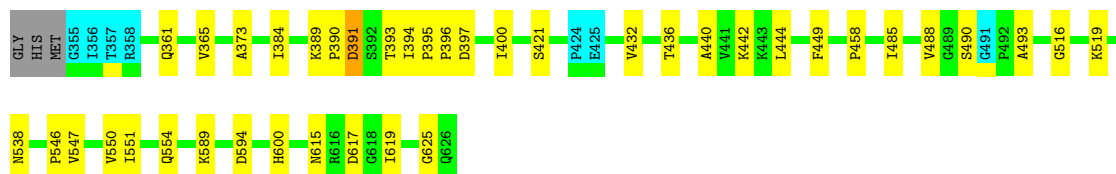
Chain A: 85% 9% . . .



4.2.27 Score per residue for model 27

- Molecule 1: Serine/threonine-protein kinase pknB

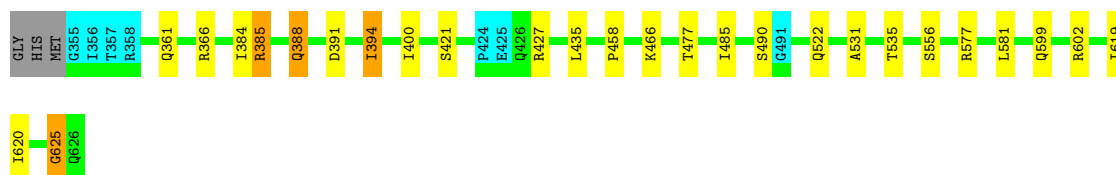
Chain A: 82% 14% . .



4.2.28 Score per residue for model 28

- Molecule 1: Serine/threonine-protein kinase pknB

Chain A: 87% 8% . . .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained molecular dynamics in a hydrated environment*.

Of the 30 calculated structures, 28 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
CNS	refinement	1.2

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	1.17±0.03	2±1/1989 (0.1± 0.1%)	0.99±0.02	1±1/2718 (0.0± 0.0%)
All	All	1.17	45/55692 (0.1%)	0.99	32/76104 (0.0%)

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	0.3±0.5
All	All	0	8

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	361	GLN	C-N	-7.87	1.25	1.33	5	12
1	A	395	PRO	CA-C	7.35	1.58	1.52	17	2
1	A	362	VAL	N-CA	-6.62	1.40	1.46	5	5
1	A	401	GLY	CA-C	-6.57	1.44	1.51	8	1
1	A	575	GLU	CA-C	6.27	1.59	1.52	18	3
1	A	612	THR	C-N	-6.23	1.30	1.33	21	1
1	A	385	ARG	C-N	-6.16	1.25	1.33	28	3
1	A	402	THR	N-CA	-6.14	1.38	1.46	8	1
1	A	401	GLY	C-N	-5.83	1.25	1.33	8	2
1	A	361	GLN	N-CA	-5.80	1.38	1.46	5	2
1	A	429	ILE	N-CA	-5.59	1.42	1.46	13	1
1	A	622	LEU	C-N	-5.46	1.25	1.33	20	1
1	A	477	THR	N-CA	-5.42	1.39	1.45	12	1
1	A	364	ASP	C-N	-5.42	1.28	1.34	14	1
1	A	619	ILE	CA-CB	5.37	1.60	1.53	12	4
1	A	384	ILE	C-N	-5.37	1.26	1.33	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	401	GLY	N-CA	-5.10	1.40	1.45	18	1
1	A	623	ARG	C-N	-5.09	1.26	1.33	20	1
1	A	394	ILE	N-CA	-5.07	1.41	1.46	23	1

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	559	ASN	CA-CB-CG	7.81	120.41	112.60	1	1
1	A	400	ILE	N-CA-C	-7.12	105.84	112.96	26	1
1	A	395	PRO	N-CA-C	6.20	118.26	110.70	13	5
1	A	497	ILE	N-CA-CB	6.14	116.80	110.23	21	1
1	A	468	ILE	N-CA-C	-6.05	106.61	111.81	18	5
1	A	391	ASP	N-CA-CB	6.04	119.01	109.71	15	1
1	A	394	ILE	CA-C-N	6.02	126.58	120.38	13	5
1	A	394	ILE	C-N-CA	6.02	126.58	120.38	13	5
1	A	497	ILE	N-CA-C	6.01	113.80	108.63	21	2
1	A	500	VAL	N-CA-C	-5.90	106.98	112.83	19	3
1	A	419	ASN	CA-CB-CG	5.75	118.35	112.60	2	3

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	616	ARG	Sidechain	2
1	A	366	ARG	Sidechain	2
1	A	623	ARG	Sidechain	1
1	A	602	ARG	Sidechain	1
1	A	427	ARG	Sidechain	1
1	A	577	ARG	Sidechain	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	1952	1938	1938	11±3
All	All	54656	54264	54264	318

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:390:PRO:HA	1:A:422:THR:O	0.64	1.92	15	5
1:A:429:ILE:HB	1:A:474:ALA:O	0.64	1.93	4	2
1:A:458:PRO:HA	1:A:490:SER:O	0.62	1.94	18	23
1:A:388:GLN:HA	1:A:420:VAL:O	0.60	1.97	9	2
1:A:365:VAL:HB	1:A:368:GLN:NE2	0.59	2.12	13	2
1:A:389:LYS:O	1:A:421:SER:HA	0.57	1.98	13	7
1:A:531:ALA:HA	1:A:556:SER:O	0.57	2.00	16	21
1:A:535:THR:HB	1:A:556:SER:OG	0.57	2.00	16	8
1:A:362:VAL:HG22	1:A:382:PHE:CZ	0.57	2.35	7	4
1:A:517:PHE:HA	1:A:547:VAL:O	0.57	2.00	17	4
1:A:427:ARG:NE	1:A:427:ARG:HA	0.56	2.15	9	9
1:A:376:THR:O	1:A:380:ARG:HG2	0.55	2.01	19	8
1:A:383:LYS:O	1:A:415:GLU:HA	0.55	2.01	23	2
1:A:470:THR:HG22	1:A:486:ILE:HG12	0.54	1.80	22	4
1:A:574:ALA:O	1:A:578:LEU:HG	0.53	2.03	3	2
1:A:606:GLN:HA	1:A:621:THR:O	0.53	2.04	17	3
1:A:573:ASP:O	1:A:577:ARG:HG2	0.53	2.03	8	7
1:A:445:THR:HA	1:A:450:GLY:CA	0.52	2.35	14	5
1:A:440:ALA:O	1:A:444:LEU:HG	0.52	2.05	20	10
1:A:440:ALA:O	1:A:444:LEU:HD22	0.51	2.06	1	2
1:A:370:SER:HB3	1:A:397:ASP:O	0.51	2.06	4	1
1:A:382:PHE:CZ	1:A:412:ALA:HA	0.51	2.41	18	2
1:A:452:PHE:HA	1:A:484:VAL:O	0.51	2.06	24	7
1:A:505:VAL:O	1:A:509:GLN:HG3	0.51	2.06	19	1
1:A:428:GLU:CD	1:A:428:GLU:H	0.51	2.13	20	1
1:A:433:SER:HB2	1:A:436:THR:OG1	0.50	2.06	7	5
1:A:615:ASN:ND2	1:A:617:ASP:HB3	0.50	2.22	3	2
1:A:594:ASP:HA	1:A:626:GLN:OE1	0.49	2.07	9	1
1:A:599:GLN:O	1:A:625:GLY:HA3	0.49	2.07	28	1
1:A:364:ASP:OD2	1:A:366:ARG:HD2	0.49	2.08	7	1
1:A:396:PRO:HA	1:A:421:SER:OG	0.49	2.07	3	5
1:A:394:ILE:HG12	1:A:421:SER:OG	0.49	2.08	28	1
1:A:397:ASP:HA	1:A:420:VAL:HG13	0.49	1.83	20	3
1:A:607:ASN:HB3	1:A:608:PRO:HD3	0.49	1.83	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:388:GLN:N	1:A:388:GLN:HE21	0.49	2.06	9	6
1:A:622:LEU:O	1:A:623:ARG:HD2	0.49	2.08	13	1
1:A:517:PHE:CD1	1:A:547:VAL:HA	0.48	2.43	1	3
1:A:390:PRO:O	1:A:391:ASP:HB2	0.48	2.06	10	4
1:A:529:ARG:O	1:A:558:GLY:HA2	0.48	2.08	26	6
1:A:496:ASP:OD1	1:A:544:THR:HB	0.48	2.08	13	1
1:A:392:SER:O	1:A:393:THR:HB	0.48	2.08	15	1
1:A:434:THR:HB	1:A:467:VAL:O	0.48	2.09	4	2
1:A:432:VAL:HG11	1:A:440:ALA:HB2	0.48	1.86	27	3
1:A:524:SER:HA	1:A:555:VAL:O	0.47	2.09	10	6
1:A:565:ASP:HA	1:A:610:ALA:HB1	0.47	1.84	19	1
1:A:573:ASP:O	1:A:577:ARG:HD3	0.47	2.09	3	1
1:A:566:LEU:O	1:A:569:MET:HG3	0.47	2.09	18	1
1:A:563:MET:SD	1:A:620:ILE:HD12	0.47	2.50	6	1
1:A:362:VAL:HG22	1:A:382:PHE:CE1	0.47	2.45	7	1
1:A:575:GLU:O	1:A:579:ARG:HG2	0.47	2.10	11	1
1:A:364:ASP:OD1	1:A:366:ARG:HG2	0.47	2.10	22	1
1:A:597:GLY:O	1:A:601:ASN:HB2	0.46	2.10	9	1
1:A:525:VAL:O	1:A:557:LYS:HB3	0.46	2.10	3	1
1:A:577:ARG:O	1:A:581:LEU:HG	0.46	2.11	23	7
1:A:391:ASP:OD2	1:A:393:THR:HG22	0.46	2.11	27	1
1:A:361:GLN:NE2	1:A:407:ASN:HA	0.46	2.24	15	4
1:A:497:ILE:HD13	1:A:543:THR:O	0.46	2.11	21	1
1:A:617:ASP:OD2	1:A:619:ILE:HB	0.46	2.11	22	1
1:A:461:PRO:O	1:A:464:VAL:HG22	0.45	2.11	18	1
1:A:575:GLU:OE2	1:A:579:ARG:HD3	0.45	2.11	24	1
1:A:391:ASP:HB3	1:A:394:ILE:CD1	0.45	2.41	25	1
1:A:389:LYS:HB2	1:A:389:LYS:NZ	0.45	2.27	4	1
1:A:364:ASP:OD2	1:A:366:ARG:HB3	0.45	2.12	2	1
1:A:519:LYS:O	1:A:550:VAL:HA	0.45	2.11	18	5
1:A:594:ASP:HA	1:A:600:HIS:NE2	0.45	2.27	27	1
1:A:463:LEU:O	1:A:463:LEU:HD13	0.44	2.11	18	1
1:A:394:ILE:H	1:A:394:ILE:HD13	0.44	1.72	3	3
1:A:526:ASP:HA	1:A:557:LYS:HG2	0.44	1.89	8	5
1:A:615:ASN:HD21	1:A:619:ILE:HG22	0.44	1.73	23	2
1:A:493:ALA:O	1:A:546:PRO:HA	0.44	2.13	3	2
1:A:362:VAL:HB	1:A:406:ALA:HA	0.44	1.88	7	2
1:A:391:ASP:OD1	1:A:393:THR:HG22	0.44	2.13	7	1
1:A:569:MET:HE2	1:A:569:MET:HA	0.43	1.90	6	1
1:A:575:GLU:O	1:A:578:LEU:HG	0.43	2.12	13	1
1:A:473:PRO:C	1:A:475:ASN:H	0.43	2.21	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:600:HIS:HB2	1:A:626:GLN:H	0.43	1.74	19	1
1:A:513:ASN:HA	1:A:517:PHE:O	0.43	2.13	19	1
1:A:600:HIS:C	1:A:602:ARG:H	0.43	2.21	13	1
1:A:521:SER:O	1:A:552:GLU:HA	0.43	2.14	16	1
1:A:366:ARG:HD2	1:A:366:ARG:O	0.43	2.14	19	1
1:A:569:MET:SD	1:A:577:ARG:HD3	0.43	2.53	22	1
1:A:427:ARG:HG3	1:A:447:ALA:O	0.43	2.14	14	1
1:A:578:LEU:O	1:A:581:LEU:HG	0.43	2.14	2	1
1:A:575:GLU:HB2	1:A:576:PRO:HD3	0.43	1.91	9	1
1:A:570:PHE:CD2	1:A:602:ARG:HB3	0.43	2.49	12	1
1:A:516:GLY:O	1:A:547:VAL:HB	0.42	2.14	27	2
1:A:440:ALA:O	1:A:444:LEU:HD13	0.42	2.15	14	4
1:A:558:GLY:C	1:A:560:GLN:H	0.42	2.22	13	3
1:A:522:GLN:HA	1:A:553:LEU:O	0.42	2.14	26	3
1:A:519:LYS:O	1:A:551:ILE:HD13	0.42	2.14	18	1
1:A:602:ARG:HD2	1:A:603:VAL:O	0.42	2.12	20	1
1:A:393:THR:HG22	1:A:393:THR:O	0.42	2.14	24	1
1:A:391:ASP:HB3	1:A:394:ILE:HG12	0.42	1.91	6	1
1:A:366:ARG:HB3	1:A:402:THR:OG1	0.42	2.14	18	1
1:A:519:LYS:HD2	1:A:548:ASP:O	0.42	2.15	3	1
1:A:586:MET:HA	1:A:586:MET:HE3	0.42	1.91	10	2
1:A:439:GLU:CD	1:A:442:LYS:HE3	0.42	2.39	2	1
1:A:529:ARG:HB2	1:A:556:SER:HB3	0.42	1.92	3	1
1:A:436:THR:HG22	1:A:439:GLU:HB3	0.42	1.91	6	2
1:A:585:GLY:HA3	1:A:617:ASP:O	0.41	2.15	16	1
1:A:615:ASN:ND2	1:A:617:ASP:HB2	0.41	2.29	27	1
1:A:380:ARG:NE	1:A:380:ARG:HA	0.41	2.30	4	1
1:A:366:ARG:HD3	1:A:402:THR:OG1	0.41	2.16	16	1
1:A:385:ARG:O	1:A:417:THR:HA	0.41	2.15	12	1
1:A:578:LEU:HD12	1:A:579:ARG:N	0.41	2.31	25	1
1:A:526:ASP:HA	1:A:557:LYS:HB3	0.41	1.91	12	1
1:A:600:HIS:HA	1:A:626:GLN:O	0.41	2.16	1	1
1:A:384:ILE:HA	1:A:416:ILE:O	0.41	2.15	6	1
1:A:510:LYS:O	1:A:514:VAL:HG23	0.41	2.15	14	1
1:A:449:PHE:HB3	1:A:480:ILE:HA	0.41	1.92	2	1
1:A:456:ASN:HB2	1:A:490:SER:OG	0.41	2.16	15	1
1:A:609:PRO:HB2	1:A:612:THR:OG1	0.41	2.16	25	1
1:A:529:ARG:HD3	1:A:533:GLU:OE2	0.41	2.15	25	1
1:A:538:ASN:CA	1:A:554:GLN:HE22	0.41	2.28	27	1
1:A:360:VAL:O	1:A:409:SER:HA	0.40	2.16	25	1
1:A:365:VAL:CG2	1:A:373:ALA:HA	0.40	2.45	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:426:GLN:OE1	1:A:477:THR:HB	0.40	2.15	2	1
1:A:396:PRO:HA	1:A:421:SER:O	0.40	2.16	27	1
1:A:560:GLN:HA	1:A:614:VAL:O	0.40	2.17	22	1
1:A:586:MET:HA	1:A:586:MET:HE2	0.40	1.91	9	1
1:A:400:ILE:H	1:A:400:ILE:HD13	0.40	1.76	18	1
1:A:616:ARG:HG3	1:A:617:ASP:N	0.40	2.31	6	1
1:A:573:ASP:O	1:A:576:PRO:HD2	0.40	2.16	25	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	264/275 (96%)	247±2 (94±1%)	15±2 (6±1%)	2±1 (1±0%)	16	66
All	All	7392/7700 (96%)	6913 (94%)	409 (6%)	70 (1%)	16	66

All 18 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	391	ASP	13
1	A	395	PRO	10
1	A	423	GLY	7
1	A	600	HIS	6
1	A	625	GLY	6
1	A	502	GLY	4
1	A	365	VAL	3
1	A	608	PRO	3
1	A	500	VAL	3
1	A	393	THR	3
1	A	404	PRO	3
1	A	607	ASN	2
1	A	590	GLY	2
1	A	601	ASN	1
1	A	413	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	595	ALA	1
1	A	615	ASN	1
1	A	397	ASP	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	215/222 (97%)	202±2 (94±1%)	13±2 (6±1%)	19 69
All	All	6020/6216 (97%)	5662 (94%)	358 (6%)	19 69

All 62 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	485	ILE	28
1	A	619	ILE	28
1	A	384	ILE	27
1	A	394	ILE	17
1	A	477	THR	16
1	A	388	GLN	15
1	A	522	GLN	14
1	A	400	ILE	13
1	A	551	ILE	13
1	A	361	GLN	12
1	A	620	ILE	11
1	A	436	THR	11
1	A	442	LYS	10
1	A	366	ARG	9
1	A	387	LEU	8
1	A	557	LYS	6
1	A	449	PHE	6
1	A	402	THR	6
1	A	616	ARG	6
1	A	518	THR	5
1	A	529	ARG	5
1	A	378	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	470	THR	5
1	A	370	SER	4
1	A	466	LYS	4
1	A	419	ASN	4
1	A	589	LYS	4
1	A	495	LYS	4
1	A	428	GLU	4
1	A	615	ASN	4
1	A	395	PRO	4
1	A	622	LEU	4
1	A	513	ASN	4
1	A	606	GLN	3
1	A	503	GLN	3
1	A	626	GLN	3
1	A	444	LEU	2
1	A	389	LYS	2
1	A	554	GLN	2
1	A	526	ASP	2
1	A	586	MET	2
1	A	566	LEU	2
1	A	435	LEU	2
1	A	559	ASN	1
1	A	553	LEU	1
1	A	577	ARG	1
1	A	418	VAL	1
1	A	475	ASN	1
1	A	621	THR	1
1	A	437	TYR	1
1	A	494	THR	1
1	A	560	GLN	1
1	A	567	SER	1
1	A	427	ARG	1
1	A	383	LYS	1
1	A	584	THR	1
1	A	600	HIS	1
1	A	443	LYS	1
1	A	497	ILE	1
1	A	488	VAL	1
1	A	385	ARG	1
1	A	602	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 oligosaccharides 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

No chemical shift data were provided