Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 01:17 PM EST

PDB ID	:	2BPR
Title	:	NMR STRUCTURE OF THE SUBSTRATE BINDING DOMAIN OF DNAK, 25 STRUCTURES
Authors	:	Wang, H.; Kurochkin, A.V.; Pang, Y.; Hu, W.; Flynn, G.C.; Zuiderweg, E.R.P.
Deposited on	:	1998-08-11

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:

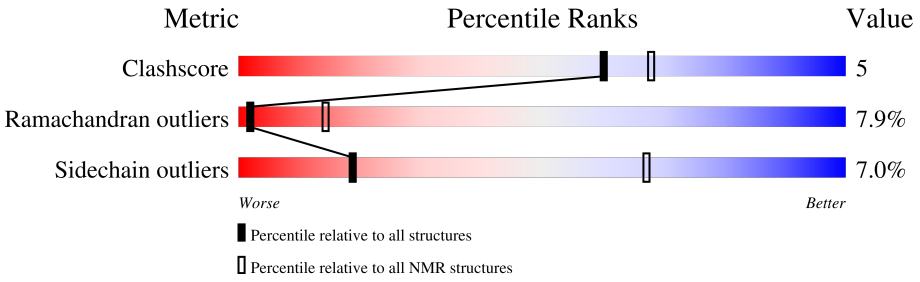
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	191	71% 13% • 6% 9%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 8 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:386-A:546 (161)	1.06	8

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 7, 12, 17, 20, 21, 22, 25
2	2, 6, 8, 9, 10, 11, 13, 14, 15
3	5, 18, 19, 23
Single-model clusters	16; 24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2656 atoms, of which 1331 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNAK.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	173	2656	812	1331	239	270	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	SER	VAL	conflict	UNP P0A6Y8
A	382	ILE	LEU	conflict	UNP P0A6Y8
A	383	GLU	THR	conflict	UNP P0A6Y8
A	385	ARG	ASP	conflict	UNP P0A6Y8

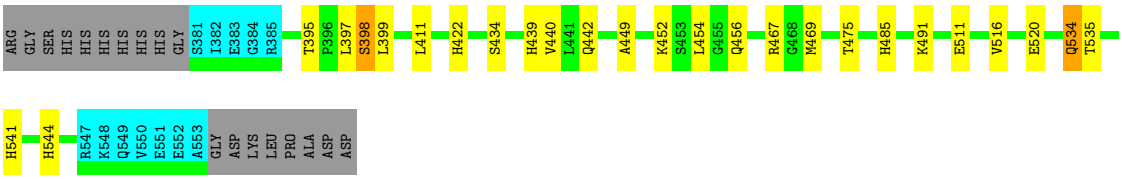
4 Residue-property plots (i)

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: DNAK

Chain A: 71% 13% • 6% 9%



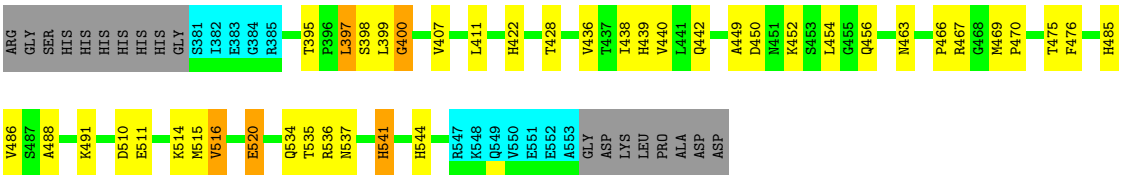
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNAK

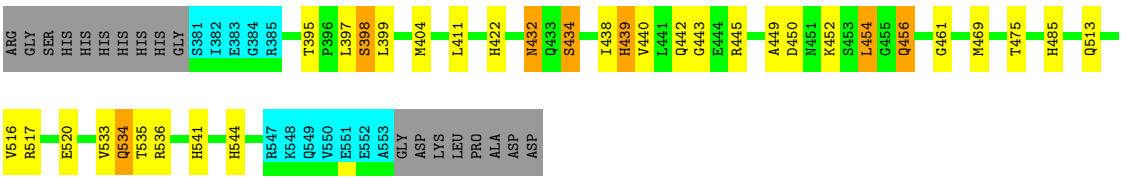
Chain A: 62% 19% • 6% 9%



4.2.2 Score per residue for model 2

• Molecule 1: DNAK

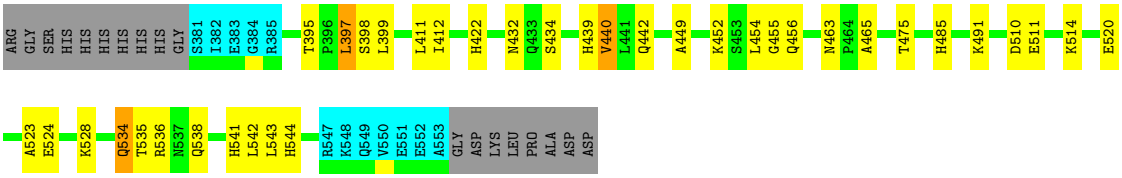
Chain A: 66% 14% • 6% 9%



4.2.3 Score per residue for model 3

- Molecule 1: DNAK

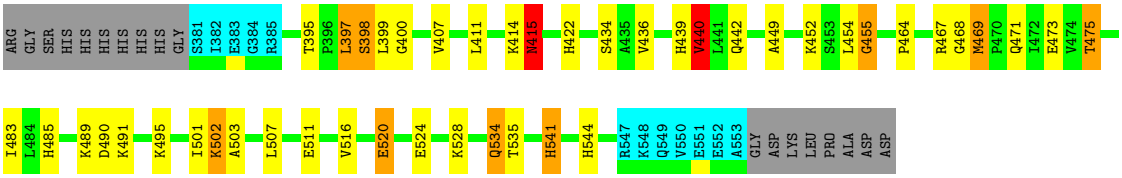
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: DNAK

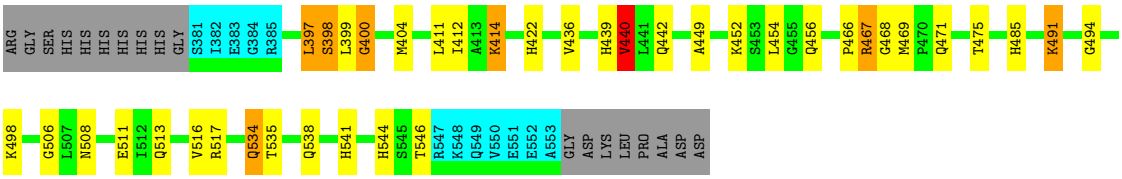
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: DNAK

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: DNAK

Chain A: 64% 17% • 6% 9%

ARG GLY SER HIS HIS HIS HIS HIS HIS GLY S381 I382 E383 G384 R385 V386 K387 T395 P396 L397 S398 L399 L411 I412 H422 S427 T428 V436 H439 V440 L441 Q442 A449 D450 N451 K452 S453 L454 G455 Q456 P464 A465 P466 R467 G468 M469 T475 H485 K498

I501 K502 A503 E509 Q513 V516 R517 Q534 T535 R536 H541 H544 R547 K548 Q549 V550 E551 E552 A553 GLY ASP LYS LEU PRO ALA ASP ASP

4.2.7 Score per residue for model 7

- Molecule 1: DNAK

Chain A: 57% 21% 5% • 6% 9%

ARG GLY SER HIS HIS HIS HIS HIS HIS GLY S381 I382 E383 G384 R385 V386 K387 D388 L392 D393 V394 T395 S398 L399 G400 L411 N415 T416 H422 T428 A429 E430 D431 N432 Q433 S434 A435 V436 H439 V440 L441 Q442 G443 E444 R445 K446 R447 A448 A449 K452 S453 L454

G455 Q456 R467 G468 M469 P470 Q471 T475 I483 L484 H485 D490 K491 G506 L507 N508 E511 K514 M515 V516 E520 E524 K528 F529 Q534 T535 H541 H544 R547 K548 Q549 V550 E551 E552 A553 GLY ASP LYS LEU PRO ALA ASP ASP

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: DNAK

Chain A: 62% 18% • 6% 9%

ARG GLY SER HIS HIS HIS HIS HIS HIS GLY S381 I382 E383 G384 R385 V389 L390 L391 L392 D393 S398 I401 L411 K414 T417 H422 N432 V436 H439 V440 L441 Q442 G443 E444 R445 K446 A449 K452 S453 L454 N463 P466 R467 G468 M469 P470

T475 L484 H485 E496 D510 E511 K514 E520 F529 V533 Q534 T535 R536 H541 H544 R547 K548 Q549 V550 E551 E552 A553 GLY ASP LYS LEU PRO ALA ASP ASP

4.2.9 Score per residue for model 9

- Molecule 1: DNAK

Chain A: 65% 16% • 6% 9%

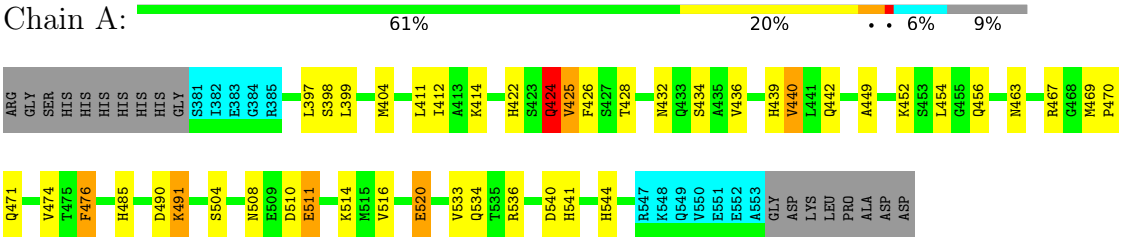
ARG GLY SER HIS HIS HIS HIS HIS HIS GLY S381 I382 E383 G384 R385 S398 L399 L411 N415 H422 T428 A429 E430 D431 N432 V436 H439 V440 L441 Q442 A449 K452 S453 L454 G455 Q456 L459 P464 R467 G468 M469 P470 Q471 I472 E473 V474 T475

H485 K489 D490 K491 E511 I512 V516 E520 F529 V533 Q534 N537 H541 H544 R547 K548 Q549 V550 E551 E552 A553 GLY ASP LYS LEU PRO ALA ASP ASP

4.2.10 Score per residue for model 10

- Molecule 1: DNAK

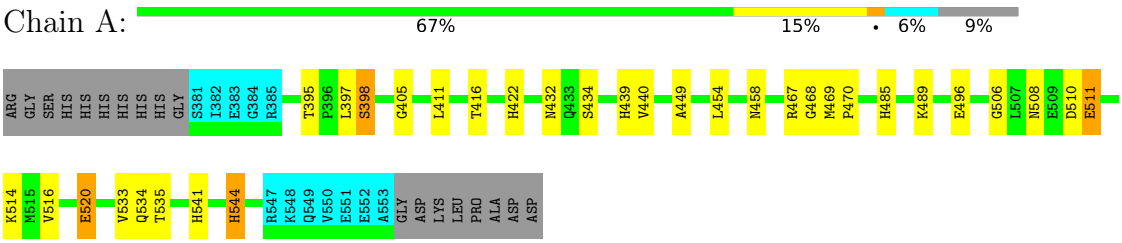
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: DNAK

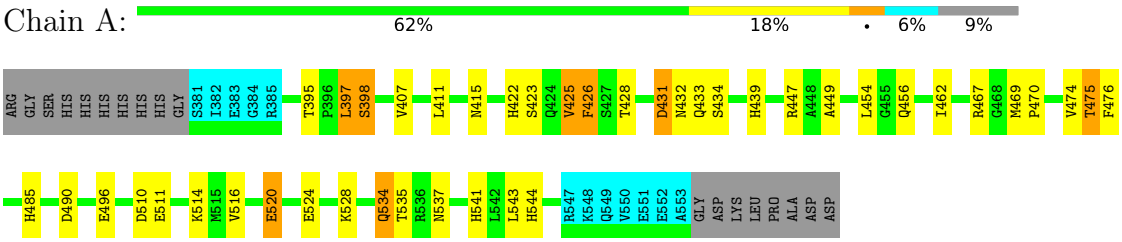
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: DNAK

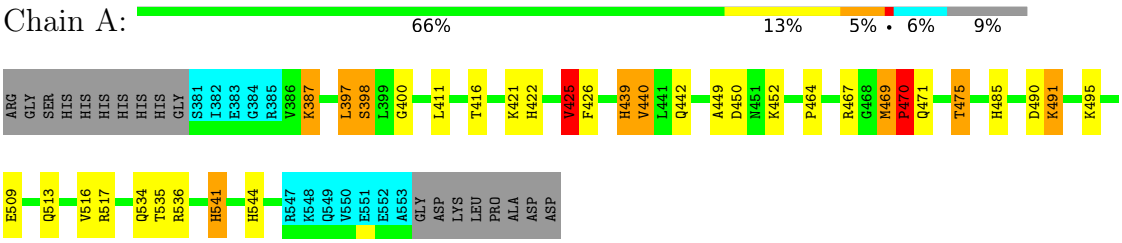
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: DNAK

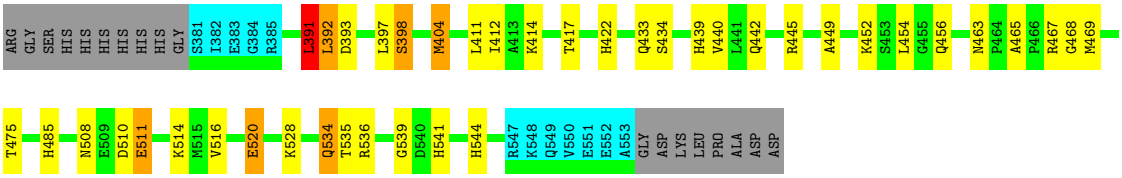
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: DNAK

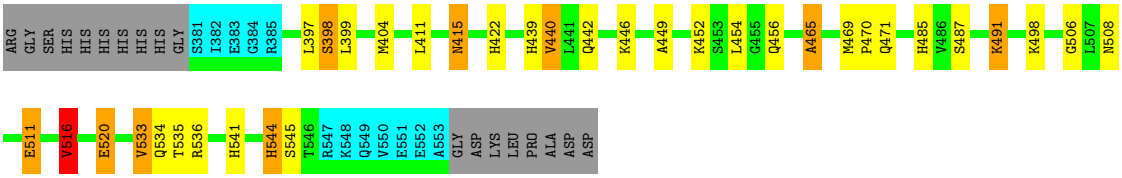
Chain A: 63% 18% • • 6% 9%



4.2.15 Score per residue for model 15

- Molecule 1: DNAK

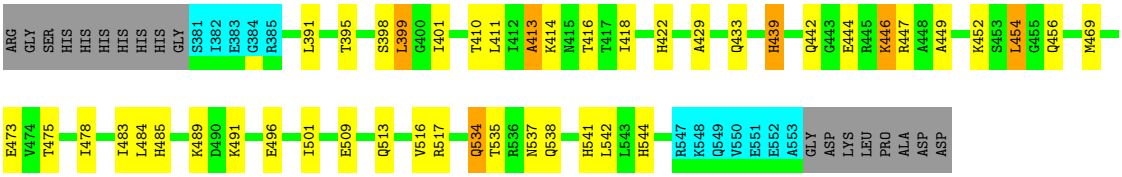
Chain A: 66% 13% 5% • 6% 9%



4.2.16 Score per residue for model 16

- Molecule 1: DNAK

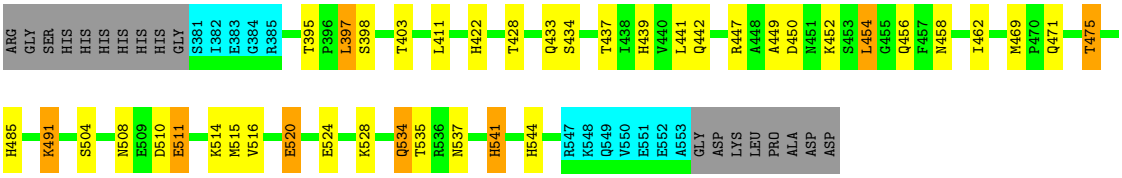
Chain A: 61% 20% • 6% 9%



4.2.17 Score per residue for model 17

- Molecule 1: DNAK

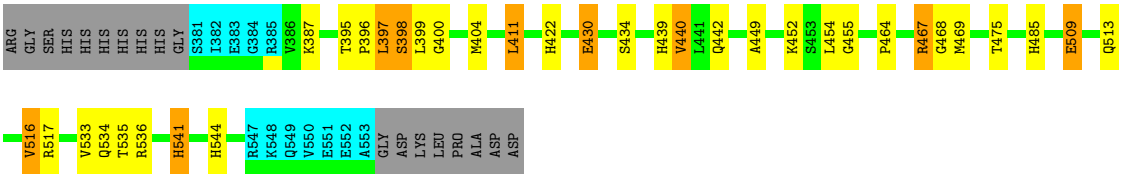
Chain A: 63% 17% • 6% 9%



4.2.18 Score per residue for model 18

- Molecule 1: DNAK

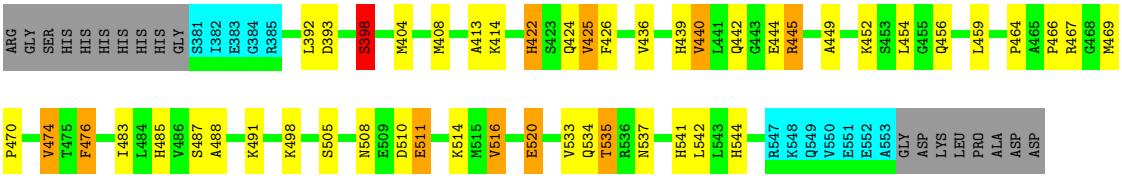
Chain A: 66% 14% 5% 6% 9%



4.2.19 Score per residue for model 19

- Molecule 1: DNAK

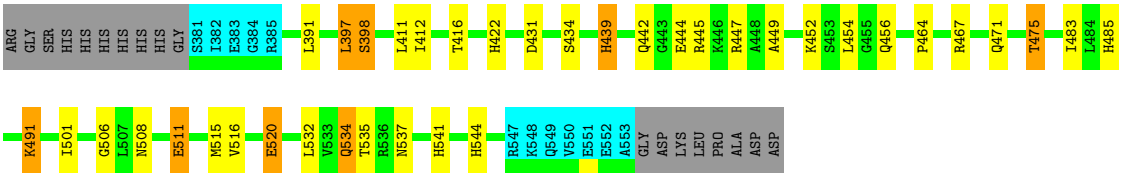
Chain A: 59% 20% 5% • 6% 9%



4.2.20 Score per residue for model 20

- Molecule 1: DNAK

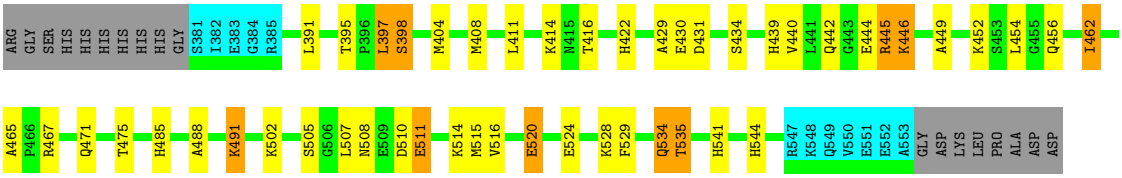
Chain A: 64% 16% • 6% 9%



4.2.21 Score per residue for model 21

- Molecule 1: DNAK

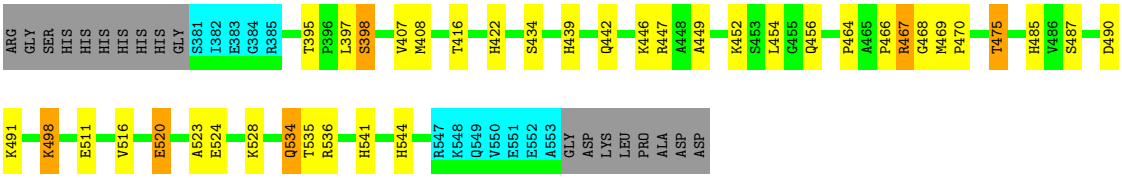
Chain A: 59% 20% 5% 6% 9%



4.2.22 Score per residue for model 22

- Molecule 1: DNAK

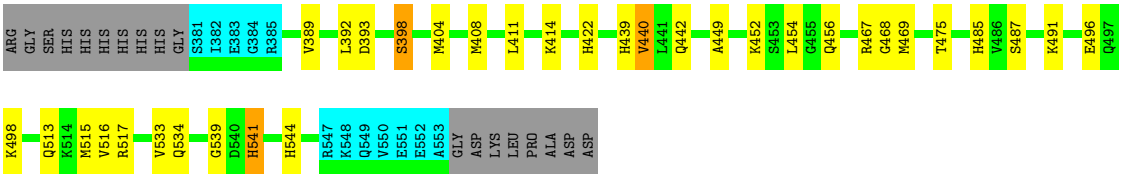
Chain A: 64% 17% • 6% 9%



4.2.23 Score per residue for model 23

- Molecule 1: DNAK

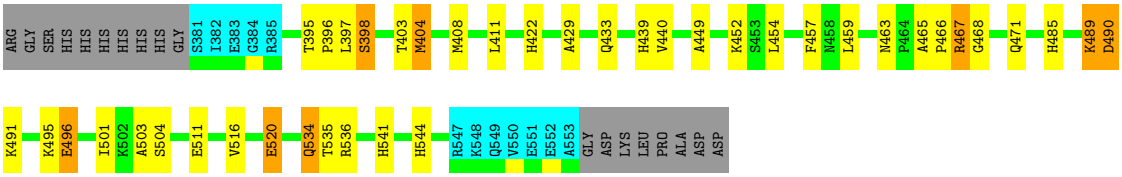
Chain A: 66% 16% • 6% 9%



4.2.24 Score per residue for model 24

- Molecule 1: DNAK

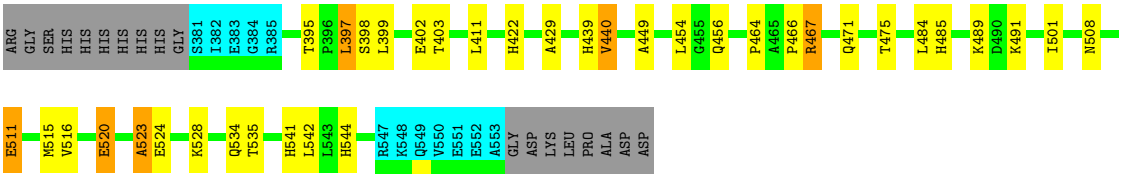
Chain A: 63% 17% • 6% 9%



4.2.25 Score per residue for model 25

- Molecule 1: DNAK

Chain A: 65% 16% • 6% 9%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY AND RESTRAINED MOLECULAR DYNAMICS WITH SIMULATED ANNEALING*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
Discover	refinement	
BIOSYM	structure solution	

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	0.57±0.01	0±0/1242 (0.0± 0.0%)	1.42±0.04	17±3/1678 (1.0± 0.2%)
All	All	0.57	0/31050 (0.0%)	1.42	415/41950 (1.0%)

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	0.7±0.6
All	All	0	17

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	434	SER	N-CA-CB	-13.48	90.29	110.50	4	5
1	A	439	HIS	CB-CA-C	13.01	136.42	110.40	13	1
1	A	454	LEU	CB-CA-C	10.43	130.03	110.20	4	24
1	A	439	HIS	CA-C-N	-10.26	94.62	117.20	13	2
1	A	520	GLU	N-CA-CB	10.10	128.78	110.60	8	18
1	A	392	LEU	CA-C-N	-9.73	95.80	117.20	23	4
1	A	449	ALA	N-CA-CB	9.45	123.33	110.10	7	25
1	A	411	LEU	N-CA-CB	9.32	129.04	110.40	17	21
1	A	516	VAL	CA-CB-CG2	8.93	124.30	110.90	15	3
1	A	511	GLU	N-CA-C	-8.82	87.18	111.00	20	18
1	A	438	ILE	N-CA-C	-8.16	88.97	111.00	2	2
1	A	440	VAL	N-CA-CB	-8.06	93.77	111.50	13	1
1	A	438	ILE	CB-CA-C	7.95	127.50	111.60	2	1
1	A	398	SER	N-CA-CB	7.59	121.89	110.50	20	13
1	A	391	LEU	N-CA-C	-7.38	91.07	111.00	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	516	VAL	N-CA-CB	7.10	127.12	111.50	15	2
1	A	534	GLN	N-CA-CB	6.89	123.01	110.60	7	15
1	A	440	VAL	CB-CA-C	6.79	124.30	111.40	10	10
1	A	389	VAL	CG1-CB-CG2	-6.63	100.28	110.90	8	2
1	A	433	GLN	N-CA-C	-6.55	93.30	111.00	16	1
1	A	456	GLN	CB-CA-C	6.52	123.44	110.40	1	2
1	A	439	HIS	CA-C-O	6.45	133.65	120.10	13	1
1	A	474	VAL	N-CA-CB	-6.38	97.46	111.50	12	1
1	A	440	VAL	CA-CB-CG1	6.35	120.42	110.90	2	6
1	A	440	VAL	CG1-CB-CG2	-6.33	100.78	110.90	4	2
1	A	474	VAL	CA-CB-CG2	6.29	120.34	110.90	19	2
1	A	408	MET	CG-SD-CE	-6.20	90.28	100.20	23	1
1	A	393	ASP	N-CA-C	-6.13	94.44	111.00	14	3
1	A	475	THR	CA-CB-CG2	-6.12	103.84	112.40	12	8
1	A	425	VAL	CA-CB-CG1	6.10	120.05	110.90	10	3
1	A	449	ALA	N-CA-C	-6.10	94.53	111.00	18	15
1	A	469	MET	CB-CA-C	6.08	122.56	110.40	13	1
1	A	423	SER	N-CA-CB	-6.02	101.46	110.50	12	1
1	A	450	ASP	N-CA-CB	-6.00	99.80	110.60	13	4
1	A	414	LYS	N-CA-CB	-5.99	99.81	110.60	8	3
1	A	496	GLU	N-CA-C	5.91	126.97	111.00	12	1
1	A	488	ALA	N-CA-CB	5.91	118.37	110.10	21	2
1	A	455	GLY	CA-C-N	-5.90	104.23	117.20	3	1
1	A	533	VAL	CG1-CB-CG2	-5.88	101.49	110.90	10	1
1	A	496	GLU	N-CA-CB	-5.86	100.05	110.60	12	1
1	A	415	ASN	N-CA-CB	5.81	121.06	110.60	4	5
1	A	392	LEU	CA-C-O	5.79	132.25	120.10	23	3
1	A	516	VAL	CB-CA-C	-5.78	100.41	111.40	15	1
1	A	454	LEU	N-CA-C	-5.78	95.40	111.00	17	9
1	A	426	PHE	N-CA-CB	5.75	120.94	110.60	12	1
1	A	392	LEU	O-C-N	5.73	131.87	122.70	23	1
1	A	439	HIS	N-CA-C	-5.66	95.71	111.00	17	3
1	A	485	HIS	CG-ND1-CE1	-5.63	98.38	105.70	20	25
1	A	544	HIS	CG-ND1-CE1	-5.62	98.40	105.70	12	25
1	A	422	HIS	CG-ND1-CE1	-5.60	98.42	105.70	24	25
1	A	541	HIS	CG-ND1-CE1	-5.60	98.42	105.70	15	25
1	A	534	GLN	N-CA-C	-5.58	95.94	111.00	25	1
1	A	533	VAL	CA-CB-CG1	5.55	119.23	110.90	15	1
1	A	437	THR	N-CA-C	-5.51	96.12	111.00	17	1
1	A	439	HIS	CG-ND1-CE1	-5.51	98.54	105.70	14	25
1	A	398	SER	CB-CA-C	5.44	120.44	110.10	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	470	PRO	CA-N-CD	-5.41	103.93	111.50	13	1
1	A	414	LYS	CB-CA-C	5.40	121.20	110.40	5	2
1	A	412	ILE	N-CA-C	-5.35	96.56	111.00	20	1
1	A	514	LYS	N-CA-CB	5.32	120.18	110.60	7	1
1	A	440	VAL	N-CA-C	-5.31	96.66	111.00	19	2
1	A	435	ALA	N-CA-CB	5.30	117.52	110.10	7	1
1	A	520	GLU	N-CA-C	-5.30	96.70	111.00	8	2
1	A	391	LEU	N-CA-CB	5.29	120.98	110.40	8	1
1	A	441	LEU	CB-CA-C	-5.29	100.15	110.20	6	1
1	A	455	GLY	N-CA-C	5.27	126.28	113.10	4	1
1	A	425	VAL	CG1-CB-CG2	-5.26	102.48	110.90	13	1
1	A	402	GLU	N-CA-CB	-5.26	101.13	110.60	25	1
1	A	529	PHE	CA-CB-CG	5.23	126.45	113.90	7	1
1	A	494	GLY	N-CA-C	-5.21	100.07	113.10	5	1
1	A	462	ILE	N-CA-C	-5.18	97.00	111.00	21	1
1	A	424	GLN	CB-CA-C	-5.17	100.05	110.40	10	1
1	A	459	LEU	N-CA-CB	-5.16	100.07	110.40	24	1
1	A	436	VAL	N-CA-C	-5.15	97.09	111.00	10	1
1	A	516	VAL	CG1-CB-CG2	-5.15	102.67	110.90	18	1
1	A	411	LEU	CB-CG-CD2	5.13	119.73	111.00	12	1
1	A	452	LYS	CB-CA-C	5.12	120.65	110.40	24	1
1	A	474	VAL	CA-CB-CG1	5.12	118.58	110.90	12	1
1	A	523	ALA	N-CA-CB	-5.11	102.95	110.10	25	1
1	A	399	LEU	CA-C-N	5.10	126.39	116.20	16	1
1	A	465	ALA	CB-CA-C	5.10	117.74	110.10	24	1
1	A	443	GLY	N-CA-C	-5.09	100.38	113.10	2	1
1	A	463	ASN	N-CA-CB	5.05	119.69	110.60	8	1
1	A	413	ALA	CB-CA-C	-5.04	102.54	110.10	16	1
1	A	469	MET	CA-C-N	5.03	131.19	117.10	6	1
1	A	396	PRO	N-CA-C	5.03	125.18	112.10	24	1
1	A	529	PHE	CB-CG-CD2	-5.02	117.29	120.80	7	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	395	THR	Peptide	12
1	A	465	ALA	Peptide	4
1	A	469	MET	Peptide	1

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	1228	1233	1233	12±6
All	All	30700	30825	30825	289

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:442:GLN:O	1:A:452:LYS:HB2	1.31	1.25	20	3
1:A:471:GLN:O	1:A:491:LYS:HB2	1.29	1.27	10	4
1:A:524:GLU:O	1:A:528:LYS:HB3	1.25	1.30	22	4
1:A:513:GLN:O	1:A:517:ARG:HB2	1.23	1.28	6	4
1:A:442:GLN:O	1:A:452:LYS:HB3	1.21	1.30	9	18
1:A:510:ASP:O	1:A:514:LYS:HB2	1.18	1.30	19	9
1:A:510:ASP:O	1:A:514:LYS:HB3	1.09	1.46	14	7
1:A:442:GLN:HB3	1:A:452:LYS:HB3	1.09	1.16	13	2
1:A:524:GLU:O	1:A:528:LYS:CB	1.07	2.00	17	4
1:A:524:GLU:CA	1:A:528:LYS:HB2	1.07	1.79	17	3
1:A:513:GLN:O	1:A:517:ARG:CB	1.03	2.05	2	4
1:A:442:GLN:O	1:A:452:LYS:CB	1.03	2.05	16	18
1:A:516:VAL:HA	1:A:520:GLU:HB2	1.01	1.31	22	16
1:A:487:SER:OG	1:A:498:LYS:HB3	0.99	1.55	23	3
1:A:510:ASP:O	1:A:514:LYS:CB	0.98	2.11	10	10
1:A:471:GLN:HB3	1:A:491:LYS:HB2	0.98	1.30	7	5
1:A:430:GLU:HA	1:A:467:ARG:HG2	0.96	1.35	9	3
1:A:444:GLU:O	1:A:445:ARG:CB	0.96	2.13	19	4
1:A:471:GLN:O	1:A:491:LYS:CB	0.92	2.17	10	4
1:A:524:GLU:HB3	1:A:528:LYS:CG	0.88	1.98	17	3
1:A:442:GLN:HB3	1:A:452:LYS:CB	0.88	1.98	13	2
1:A:431:ASP:N	1:A:467:ARG:HB2	0.88	1.82	12	1
1:A:466:PRO:O	1:A:467:ARG:CB	0.86	2.21	5	1
1:A:487:SER:OG	1:A:498:LYS:CB	0.86	2.24	15	3
1:A:524:GLU:HA	1:A:528:LYS:HB2	0.85	1.49	12	3
1:A:471:GLN:HB3	1:A:491:LYS:HB3	0.82	1.50	20	2
1:A:524:GLU:HB3	1:A:528:LYS:HG3	0.82	1.50	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:430:GLU:HB3	1:A:467:ARG:HD2	0.81	1.52	21	1
1:A:524:GLU:CB	1:A:528:LYS:HB2	0.79	2.08	22	3
1:A:446:LYS:O	1:A:447:ARG:HB3	0.79	1.77	16	1
1:A:444:GLU:HG2	1:A:509:GLU:HB3	0.78	1.55	16	1
1:A:524:GLU:HB3	1:A:528:LYS:CB	0.77	2.10	22	3
1:A:524:GLU:C	1:A:528:LYS:HB3	0.74	2.02	22	1
1:A:444:GLU:O	1:A:445:ARG:HB2	0.73	1.82	8	4
1:A:471:GLN:O	1:A:491:LYS:HB3	0.73	1.84	15	3
1:A:524:GLU:C	1:A:528:LYS:HB2	0.73	2.03	17	2
1:A:442:GLN:CB	1:A:452:LYS:HB3	0.72	2.09	13	1
1:A:442:GLN:O	1:A:452:LYS:CG	0.72	2.37	4	1
1:A:524:GLU:O	1:A:528:LYS:HB2	0.70	1.86	4	4
1:A:510:ASP:HB3	1:A:514:LYS:HB2	0.70	1.64	3	1
1:A:471:GLN:HB2	1:A:491:LYS:CB	0.68	2.18	10	1
1:A:466:PRO:O	1:A:467:ARG:HB2	0.68	1.87	5	1
1:A:524:GLU:CB	1:A:528:LYS:CB	0.68	2.72	22	2
1:A:471:GLN:CB	1:A:491:LYS:HB3	0.68	2.19	21	1
1:A:473:GLU:HG3	1:A:489:LYS:HB3	0.67	1.65	16	1
1:A:508:ASN:HB3	1:A:511:GLU:HB2	0.67	1.65	5	1
1:A:442:GLN:HB3	1:A:452:LYS:HB2	0.67	1.66	4	1
1:A:516:VAL:HA	1:A:520:GLU:CB	0.67	2.18	21	9
1:A:444:GLU:O	1:A:445:ARG:HB3	0.66	1.86	19	1
1:A:487:SER:HB3	1:A:498:LYS:HG2	0.66	1.65	19	1
1:A:524:GLU:C	1:A:528:LYS:CB	0.66	2.64	17	2
1:A:404:MET:HG3	1:A:536:ARG:HB2	0.66	1.66	14	1
1:A:524:GLU:CA	1:A:528:LYS:CB	0.65	2.75	22	2
1:A:429:ALA:O	1:A:467:ARG:HG3	0.64	1.92	25	1
1:A:404:MET:CG	1:A:536:ARG:HB2	0.63	2.23	14	1
1:A:473:GLU:O	1:A:489:LYS:HB3	0.62	1.95	4	2
1:A:487:SER:CB	1:A:498:LYS:HB3	0.62	2.24	15	2
1:A:524:GLU:HB3	1:A:528:LYS:HB2	0.61	1.71	12	2
1:A:471:GLN:HB2	1:A:491:LYS:HB3	0.61	1.72	21	2
1:A:471:GLN:CB	1:A:491:LYS:HB2	0.60	2.25	24	2
1:A:446:LYS:O	1:A:447:ARG:CB	0.60	2.45	16	1
1:A:466:PRO:O	1:A:467:ARG:HB3	0.60	1.97	24	2
1:A:431:ASP:H	1:A:467:ARG:HB2	0.58	1.58	12	1
1:A:471:GLN:HB3	1:A:491:LYS:CB	0.58	2.29	21	3
1:A:445:ARG:O	1:A:446:LYS:HB3	0.57	1.99	21	1
1:A:471:GLN:C	1:A:491:LYS:HB2	0.57	2.14	10	1
1:A:487:SER:OG	1:A:498:LYS:HB2	0.56	1.98	15	1
1:A:513:GLN:O	1:A:517:ARG:HB3	0.56	1.97	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:LYS:HB2	1:A:509:GLU:HB2	0.56	1.78	18	1
1:A:490:ASP:OD2	1:A:495:LYS:HB2	0.55	2.01	13	1
1:A:445:ARG:HB3	1:A:450:ASP:OD2	0.55	2.01	2	1
1:A:501:ILE:O	1:A:502:LYS:HB2	0.55	2.01	6	2
1:A:471:GLN:HB3	1:A:491:LYS:HG2	0.55	1.78	21	1
1:A:483:ILE:HG13	1:A:502:LYS:CB	0.53	2.33	4	1
1:A:483:ILE:HG13	1:A:502:LYS:HB3	0.52	1.81	4	1
1:A:471:GLN:CB	1:A:491:LYS:CB	0.52	2.87	21	2
1:A:524:GLU:OE1	1:A:528:LYS:HG2	0.52	2.04	17	2
1:A:508:ASN:HB3	1:A:511:GLU:CB	0.51	2.35	5	1
1:A:445:ARG:O	1:A:446:LYS:CB	0.51	2.58	21	1
1:A:400:GLY:O	1:A:440:VAL:HG13	0.51	2.05	1	2
1:A:508:ASN:O	1:A:511:GLU:HB3	0.50	2.06	14	11
1:A:516:VAL:CA	1:A:520:GLU:HB2	0.50	2.21	22	6
1:A:471:GLN:HB3	1:A:491:LYS:HG3	0.50	1.82	10	1
1:A:490:ASP:HB3	1:A:495:LYS:HB2	0.49	1.82	24	2
1:A:471:GLN:CB	1:A:491:LYS:HG3	0.49	2.38	10	1
1:A:517:ARG:HA	1:A:520:GLU:HB2	0.48	1.85	2	1
1:A:471:GLN:HB2	1:A:491:LYS:HB2	0.48	1.85	13	1
1:A:471:GLN:HB3	1:A:491:LYS:CG	0.47	2.38	21	1
1:A:398:SER:HA	1:A:413:ALA:HA	0.47	1.85	19	1
1:A:404:MET:HE3	1:A:536:ARG:HG3	0.47	1.85	14	1
1:A:400:GLY:O	1:A:440:VAL:HA	0.46	2.11	1	5
1:A:474:VAL:HG12	1:A:488:ALA:HA	0.45	1.88	19	1
1:A:529:PHE:O	1:A:533:VAL:HG23	0.45	2.11	8	2
1:A:489:LYS:HD2	1:A:496:GLU:HB3	0.45	1.89	24	1
1:A:513:GLN:O	1:A:517:ARG:N	0.45	2.50	5	3
1:A:515:MET:O	1:A:520:GLU:N	0.44	2.50	20	5
1:A:487:SER:CB	1:A:498:LYS:HG2	0.44	2.39	19	1
1:A:424:GLN:O	1:A:474:VAL:HG22	0.43	2.12	19	1
1:A:524:GLU:CA	1:A:528:LYS:HB3	0.43	2.41	22	1
1:A:471:GLN:HB2	1:A:491:LYS:CG	0.43	2.44	10	1
1:A:485:HIS:HD2	1:A:498:LYS:NZ	0.43	2.12	6	1
1:A:444:GLU:OE1	1:A:445:ARG:HB2	0.42	2.13	19	1
1:A:387:LYS:HB3	1:A:509:GLU:HG3	0.42	1.91	13	1
1:A:471:GLN:O	1:A:491:LYS:CG	0.41	2.68	13	1
1:A:442:GLN:CB	1:A:452:LYS:HB2	0.41	2.43	4	1
1:A:510:ASP:O	1:A:514:LYS:CG	0.41	2.69	1	1
1:A:387:LYS:CG	1:A:509:GLU:HG3	0.41	2.45	6	1
1:A:471:GLN:CB	1:A:491:LYS:CG	0.40	3.00	10	1
1:A:399:LEU:HB2	1:A:410:THR:HG22	0.40	1.92	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:404:MET:HG3	1:A:536:ARG:CB	0.40	2.43	14	1
1:A:401:ILE:HD13	1:A:440:VAL:HG13	0.40	1.92	8	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	161/191 (84%)	113±5 (70±3%)	36±5 (22±3%)	13±3 (8±2%)	2 14
All	All	4025/4775 (84%)	2814 (70%)	895 (22%)	316 (8%)	2 14

All 56 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	534	GLN	24
1	A	398	SER	22
1	A	535	THR	21
1	A	469	MET	19
1	A	397	LEU	18
1	A	467	ARG	18
1	A	456	GLN	15
1	A	468	GLY	12
1	A	536	ARG	11
1	A	470	PRO	9
1	A	404	MET	9
1	A	464	PRO	9
1	A	537	ASN	7
1	A	541	HIS	7
1	A	463	ASN	6
1	A	466	PRO	6
1	A	432	ASN	6
1	A	434	SER	6
1	A	445	ARG	6
1	A	446	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	506	GLY	5
1	A	447	ARG	5
1	A	533	VAL	5
1	A	425	VAL	4
1	A	426	PHE	4
1	A	523	ALA	3
1	A	538	GLN	3
1	A	415	ASN	3
1	A	503	ALA	3
1	A	431	ASP	3
1	A	504	SER	3
1	A	433	GLN	3
1	A	429	ALA	3
1	A	400	GLY	2
1	A	455	GLY	2
1	A	502	LYS	2
1	A	391	LEU	2
1	A	476	PHE	2
1	A	458	ASN	2
1	A	544	HIS	2
1	A	539	GLY	2
1	A	505	SER	2
1	A	461	GLY	1
1	A	543	LEU	1
1	A	427	SER	1
1	A	386	VAL	1
1	A	388	ASP	1
1	A	394	VAL	1
1	A	424	GLN	1
1	A	540	ASP	1
1	A	405	GLY	1
1	A	465	ALA	1
1	A	413	ALA	1
1	A	396	PRO	1
1	A	393	ASP	1
1	A	457	PHE	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	137/161 (85%)	127±3 (93±2%)	10±3 (7±2%)	19 67
All	All	3425/4025 (85%)	3185 (93%)	240 (7%)	19 67

All 69 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	475	THR	20
1	A	491	LYS	14
1	A	440	VAL	13
1	A	397	LEU	12
1	A	399	LEU	11
1	A	516	VAL	10
1	A	436	VAL	8
1	A	428	THR	7
1	A	416	THR	7
1	A	414	LYS	6
1	A	412	ILE	5
1	A	490	ASP	5
1	A	496	GLU	5
1	A	407	VAL	4
1	A	476	PHE	4
1	A	432	ASN	4
1	A	439	HIS	4
1	A	454	LEU	4
1	A	542	LEU	4
1	A	483	ILE	4
1	A	391	LEU	4
1	A	501	ILE	4
1	A	408	MET	4
1	A	456	GLN	3
1	A	507	LEU	3
1	A	395	THR	3
1	A	392	LEU	3
1	A	398	SER	3
1	A	484	LEU	3
1	A	434	SER	3
1	A	489	LYS	3
1	A	462	ILE	3
1	A	535	THR	3
1	A	411	LEU	3
1	A	403	THR	3
1	A	533	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	498	LYS	2
1	A	452	LYS	2
1	A	529	PHE	2
1	A	417	THR	2
1	A	459	LEU	2
1	A	404	MET	2
1	A	486	VAL	1
1	A	415	ASN	1
1	A	469	MET	1
1	A	546	THR	1
1	A	512	ILE	1
1	A	424	GLN	1
1	A	543	LEU	1
1	A	387	LYS	1
1	A	421	LYS	1
1	A	425	VAL	1
1	A	470	PRO	1
1	A	433	GLN	1
1	A	528	LYS	1
1	A	545	SER	1
1	A	401	ILE	1
1	A	418	ILE	1
1	A	478	ILE	1
1	A	441	LEU	1
1	A	430	GLU	1
1	A	509	GLU	1
1	A	422	HIS	1
1	A	431	ASP	1
1	A	444	GLU	1
1	A	532	LEU	1
1	A	502	LYS	1
1	A	467	ARG	1
1	A	515	MET	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