



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:09 PM BST

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

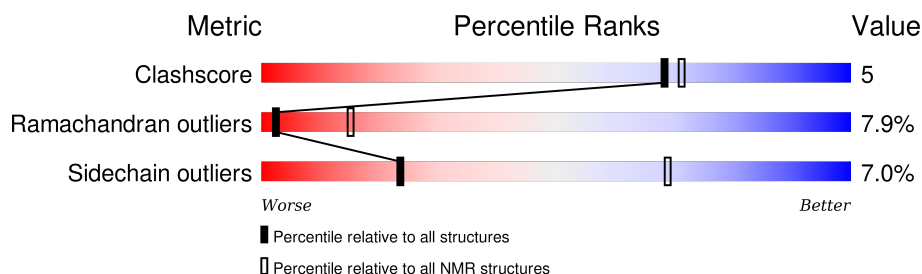
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	191	 71% 13% • 6% 9%

2 Ensemble composition and analysis

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

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
1	A	173	Total	C	H	N	O	S	0
			2656	812	1331	239	270	4	

There are 4 discrepancies between the modelled and reference sequences:

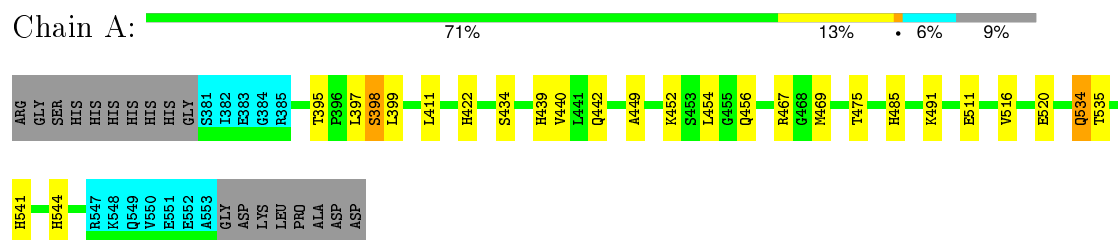
Chain	Residue	Modelled	Actual	Comment	Reference
A	381	SER	VAL	CONFLICT	UNP P0A6Y8
A	382	ILE	LEU	CONFLICT	UNP P0A6Y8
A	383	GLU	THR	CONFLICT	UNP P0A6Y8
A	385	ARG	ASP	CONFLICT	UNP P0A6Y8

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

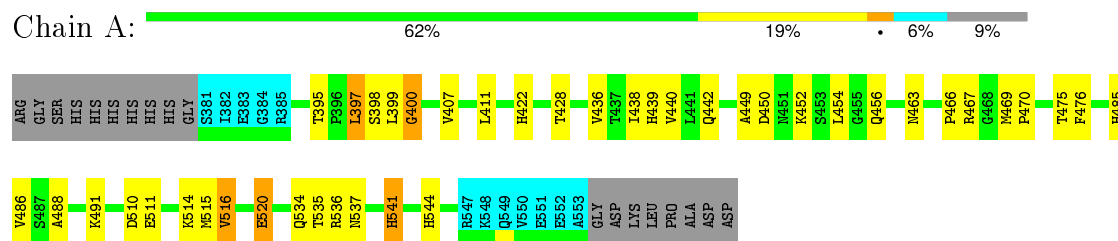


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

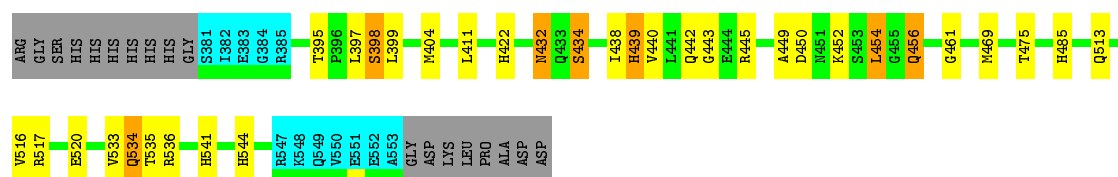
- Molecule 1: DNAK



4.2.2 Score per residue for model 2

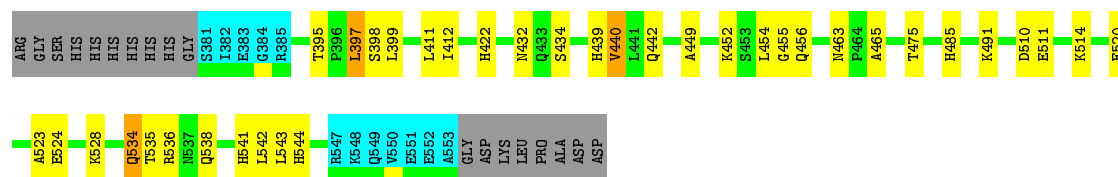
- Molecule 1: DNAK





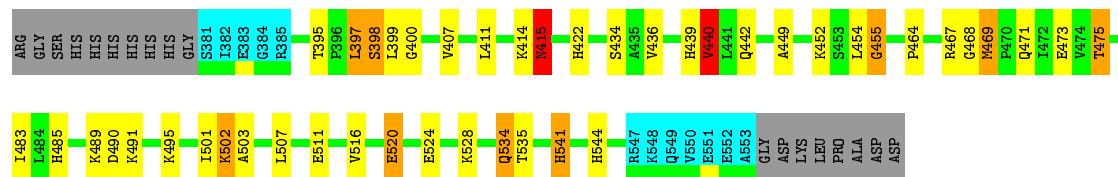
4.2.3 Score per residue for model 3

- Molecule 1: DNAK



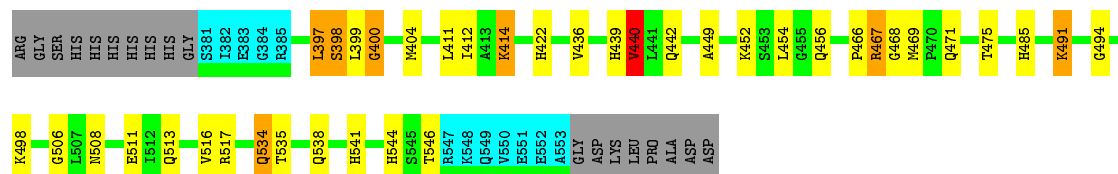
4.2.4 Score per residue for model 4

- Molecule 1: DNAK



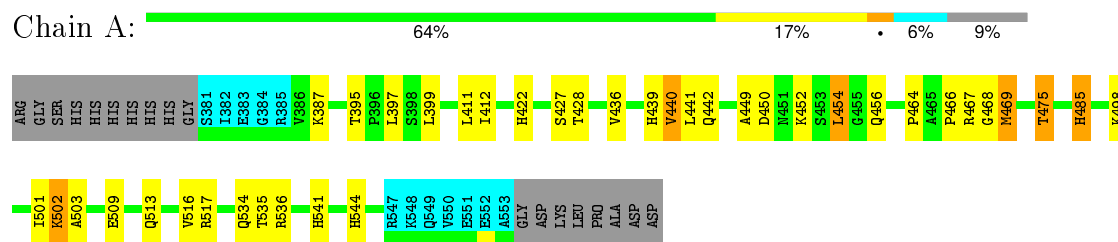
4.2.5 Score per residue for model 5

- Molecule 1: DNAK



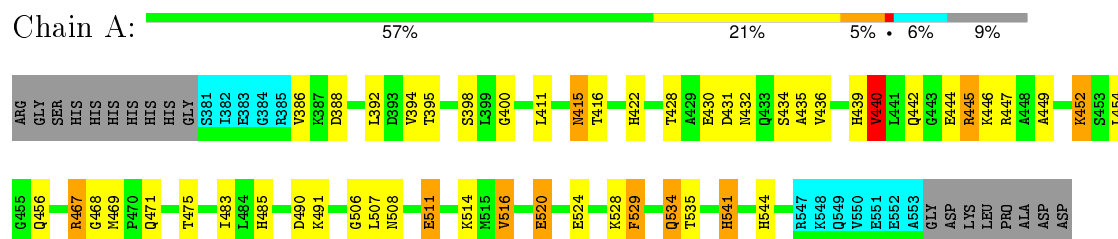
4.2.6 Score per residue for model 6

- Molecule 1: DNAK



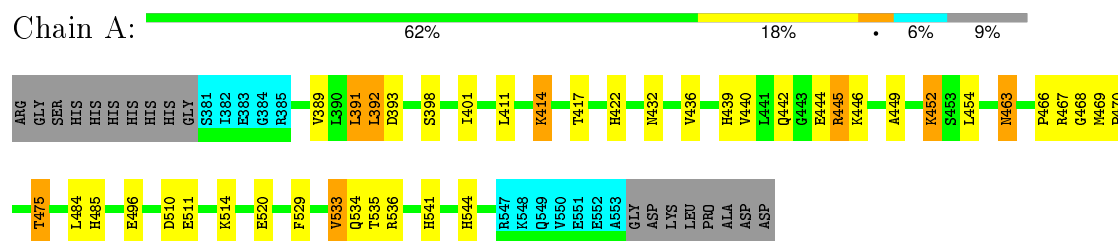
4.2.7 Score per residue for model 7

- Molecule 1: DNAK



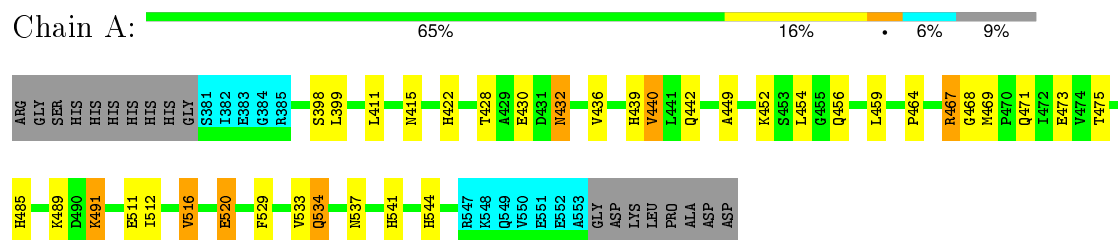
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: DNAK



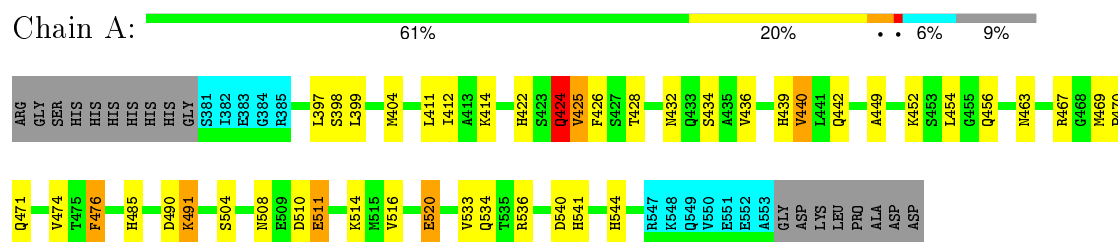
4.2.9 Score per residue for model 9

- Molecule 1: DNAK



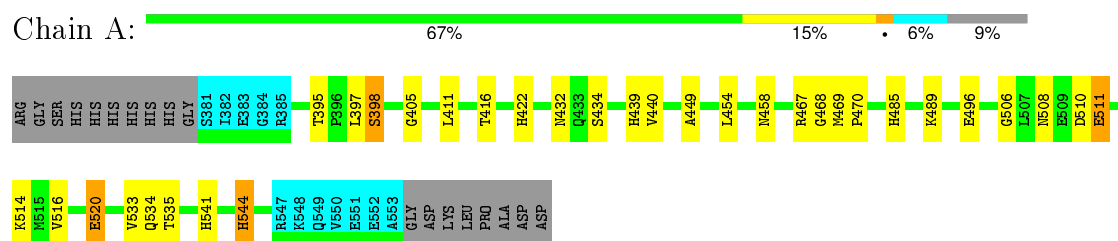
4.2.10 Score per residue for model 10

- Molecule 1: DNAK



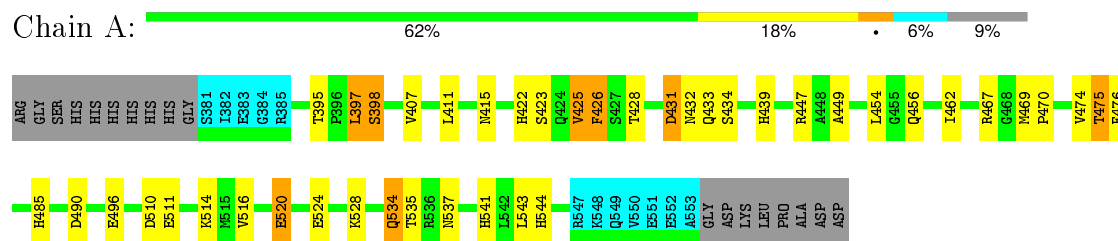
4.2.11 Score per residue for model 11

- Molecule 1: DNAK



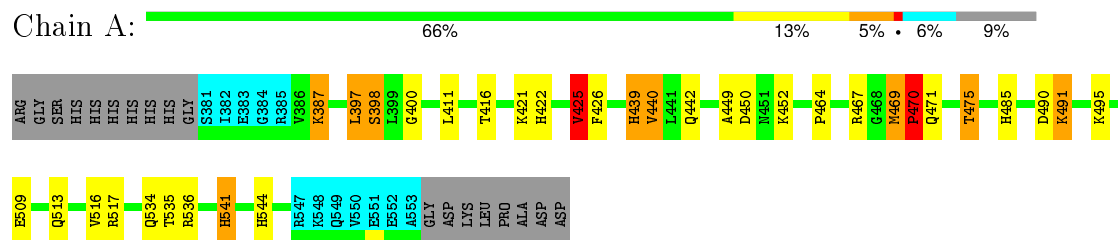
4.2.12 Score per residue for model 12

- Molecule 1: DNAK



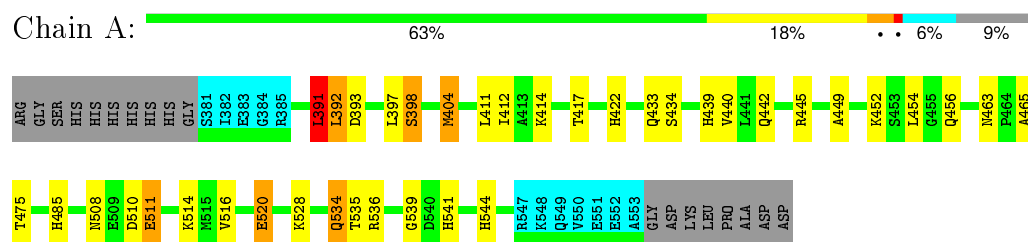
4.2.13 Score per residue for model 13

- Molecule 1: DNAK



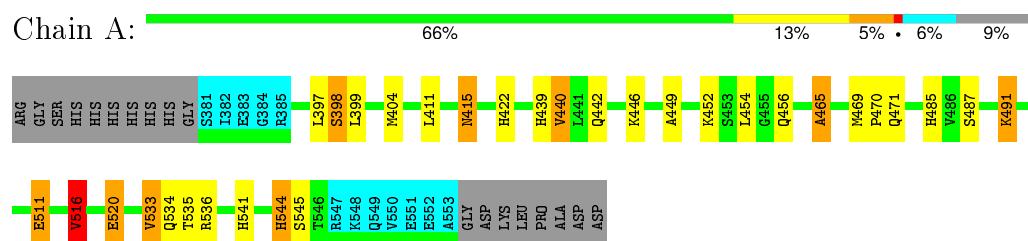
4.2.14 Score per residue for model 14

- Molecule 1: DNAK



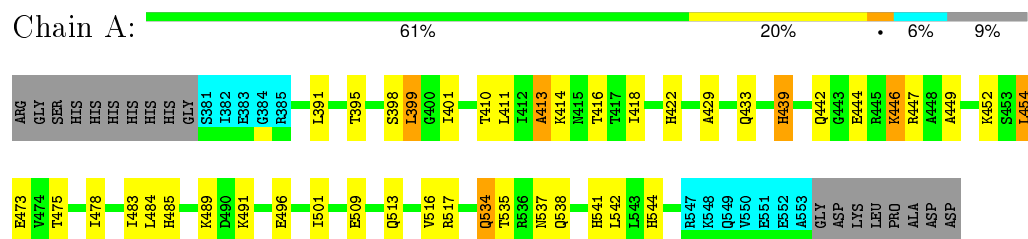
4.2.15 Score per residue for model 15

- Molecule 1: DNAK



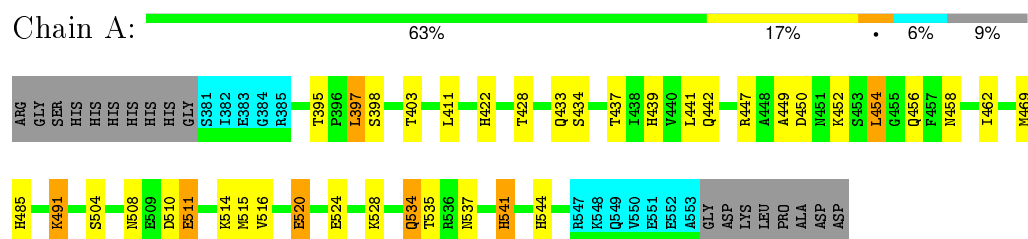
4.2.16 Score per residue for model 16

- Molecule 1: DNAK



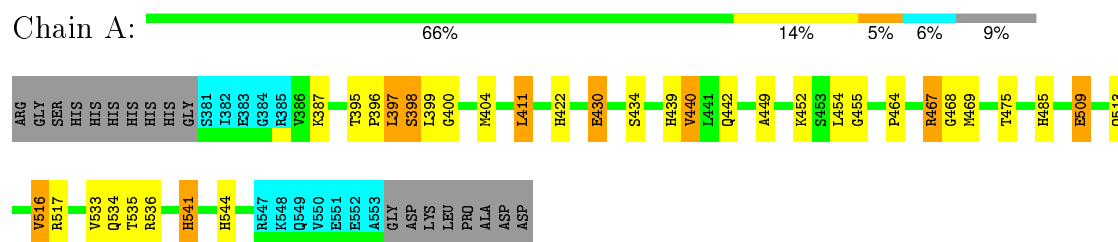
4.2.17 Score per residue for model 17

- Molecule 1: DNAK



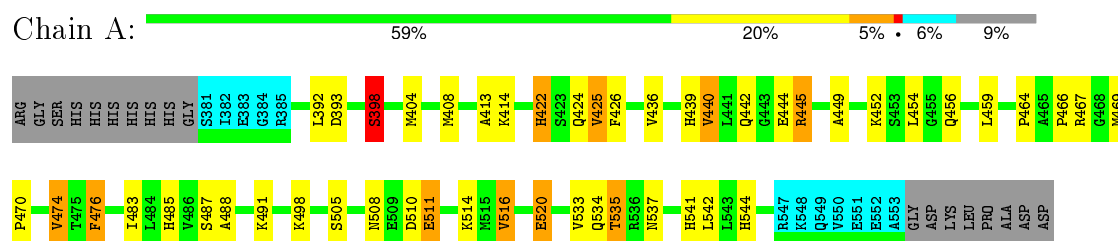
4.2.18 Score per residue for model 18

- Molecule 1: DNAK



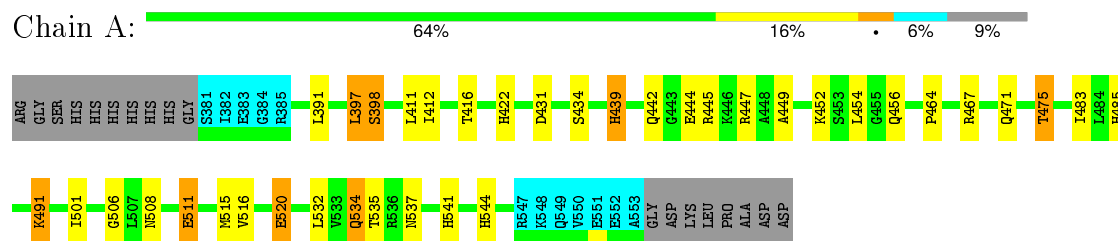
4.2.19 Score per residue for model 19

- Molecule 1: DNAK



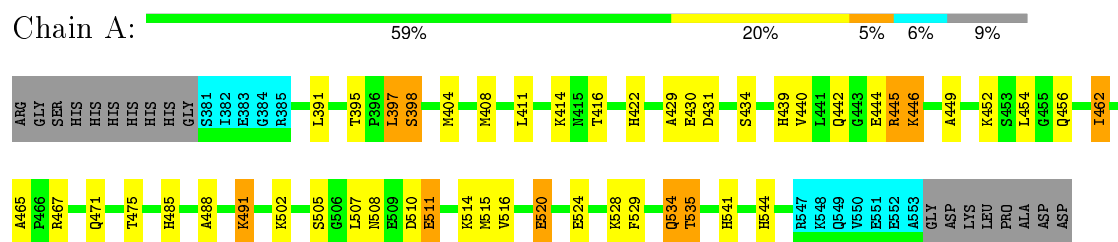
4.2.20 Score per residue for model 20

- Molecule 1: DNAK



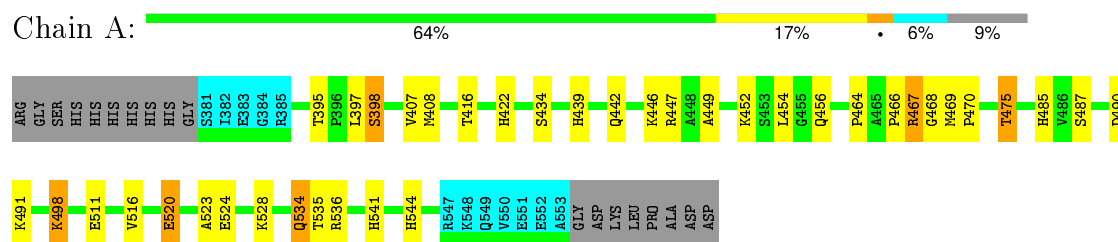
4.2.21 Score per residue for model 21

- Molecule 1: DNAK



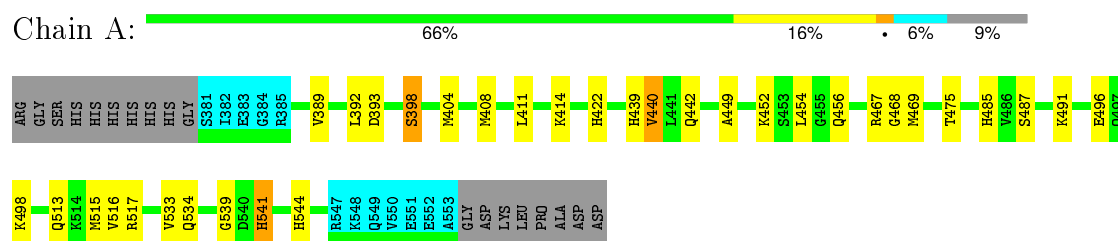
4.2.22 Score per residue for model 22

- Molecule 1: DNAK



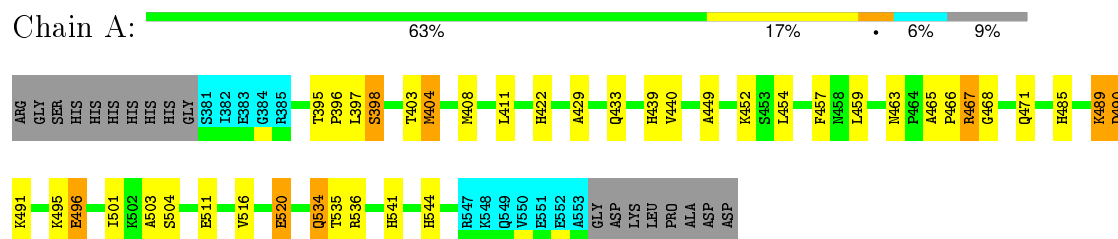
4.2.23 Score per residue for model 23

- Molecule 1: DNAK



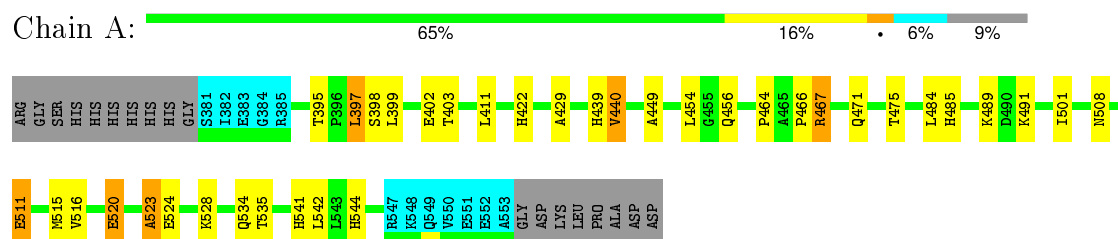
4.2.24 Score per residue for model 24

- Molecule 1: DNAK



4.2.25 Score per residue for model 25

- Molecule 1: DNAK



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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(°)	Ideal(°)	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(°)	Ideal(°)	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(°)	Ideal(°)	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 ⓘ

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:CA	1:A:528:LYS:HB2	1.07	1.79	17	3
1:A:524:GLU:O	1:A:528:LYS:CB	1.07	2.00	17	4
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:471:GLN:HB3	1:A:491:LYS:HG2	0.55	1.78	21	1
1:A:501:ILE:O	1:A:502:LYS:HB2	0.55	2.01	6	2
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:524:GLU:OE1	1:A:528:LYS:HG2	0.52	2.04	17	2
1:A:471:GLN:CB	1:A:491:LYS:CB	0.52	2.87	21	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:399:LEU:HB2	1:A:410:THR:HG22	0.40	1.92	16	1
1:A:471:GLN:CB	1:A:491:LYS:CG	0.40	3.00	10	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	15
All	All	4025/4775 (84%)	2814 (70%)	895 (22%)	316 (8%)	2	15

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	467	ARG	18
1	A	397	LEU	18
1	A	456	GLN	15
1	A	468	GLY	12
1	A	536	ARG	11
1	A	470	PRO	9
1	A	464	PRO	9
1	A	404	MET	9
1	A	541	HIS	7
1	A	537	ASN	7
1	A	466	PRO	6
1	A	434	SER	6
1	A	432	ASN	6
1	A	446	LYS	6
1	A	463	ASN	6
1	A	445	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	533	VAL	5
1	A	447	ARG	5
1	A	506	GLY	5
1	A	425	VAL	4
1	A	426	PHE	4
1	A	504	SER	3
1	A	538	GLN	3
1	A	431	ASP	3
1	A	415	ASN	3
1	A	503	ALA	3
1	A	523	ALA	3
1	A	433	GLN	3
1	A	429	ALA	3
1	A	539	GLY	2
1	A	400	GLY	2
1	A	544	HIS	2
1	A	458	ASN	2
1	A	476	PHE	2
1	A	505	SER	2
1	A	391	LEU	2
1	A	455	GLY	2
1	A	502	LYS	2
1	A	427	SER	1
1	A	386	VAL	1
1	A	413	ALA	1
1	A	396	PRO	1
1	A	393	ASP	1
1	A	388	ASP	1
1	A	424	GLN	1
1	A	461	GLY	1
1	A	457	PHE	1
1	A	405	GLY	1
1	A	465	ALA	1
1	A	543	LEU	1
1	A	540	ASP	1
1	A	394	VAL	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	137/161 (85%)	127±3 (93±2%)	10±3 (7±2%)	23	69
All	All	3425/4025 (85%)	3185 (93%)	240 (7%)	23	69

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	416	THR	7
1	A	428	THR	7
1	A	414	LYS	6
1	A	496	GLU	5
1	A	412	ILE	5
1	A	490	ASP	5
1	A	432	ASN	4
1	A	501	ILE	4
1	A	542	LEU	4
1	A	407	VAL	4
1	A	476	PHE	4
1	A	439	HIS	4
1	A	408	MET	4
1	A	391	LEU	4
1	A	454	LEU	4
1	A	483	ILE	4
1	A	507	LEU	3
1	A	395	THR	3
1	A	434	SER	3
1	A	398	SER	3
1	A	484	LEU	3
1	A	403	THR	3
1	A	392	LEU	3
1	A	411	LEU	3
1	A	535	THR	3
1	A	462	ILE	3
1	A	456	GLN	3
1	A	489	LYS	3
1	A	459	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	498	LYS	2
1	A	404	MET	2
1	A	529	PHE	2
1	A	533	VAL	2
1	A	452	LYS	2
1	A	417	THR	2
1	A	512	ILE	1
1	A	418	ILE	1
1	A	425	VAL	1
1	A	470	PRO	1
1	A	433	GLN	1
1	A	467	ARG	1
1	A	430	GLU	1
1	A	515	MET	1
1	A	444	GLU	1
1	A	545	SER	1
1	A	401	ILE	1
1	A	502	LYS	1
1	A	424	GLN	1
1	A	415	ASN	1
1	A	478	ILE	1
1	A	532	LEU	1
1	A	441	LEU	1
1	A	486	VAL	1
1	A	469	MET	1
1	A	509	GLU	1
1	A	422	HIS	1
1	A	543	LEU	1
1	A	421	LYS	1
1	A	528	LYS	1
1	A	387	LYS	1
1	A	546	THR	1
1	A	431	ASP	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 [i](#)

There are no carbohydrates 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