



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:14 AM UTC

PDB ID : 1DK2 / pdb_00001dk2
Title : REFINED SOLUTION STRUCTURE OF THE N-TERMINAL DOMAIN OF
DNA POLYMERASE BETA
Authors : Maciejewski, M.W.; Prasad, R.; Liu, D.-J.; Wilson, S.H.; Mullen, G.P.
Deposited on : 1999-12-06

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

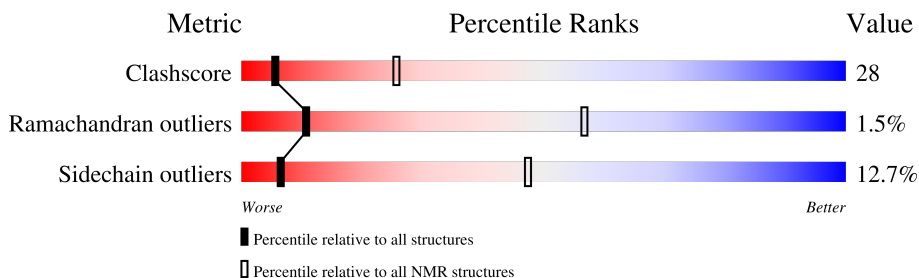
1 Overall quality at a glance

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	86	

2 Ensemble composition and analysis i

This entry contains 25 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 10 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:13-A:79 (67)	0.45	20

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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1380 atoms, of which 713 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA POLYMERASE BETA.

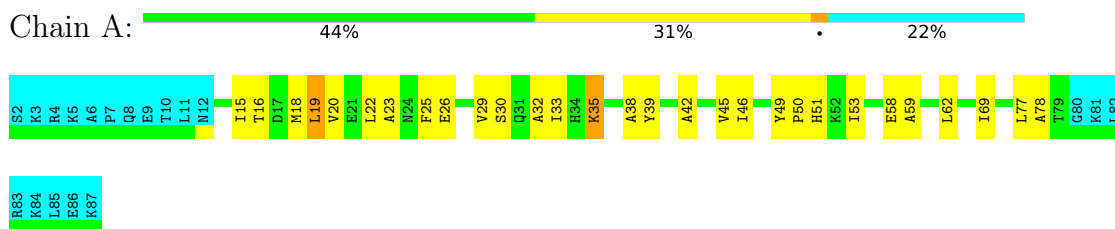
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1380	425	713	120	121	1	0

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: DNA POLYMERASE BETA

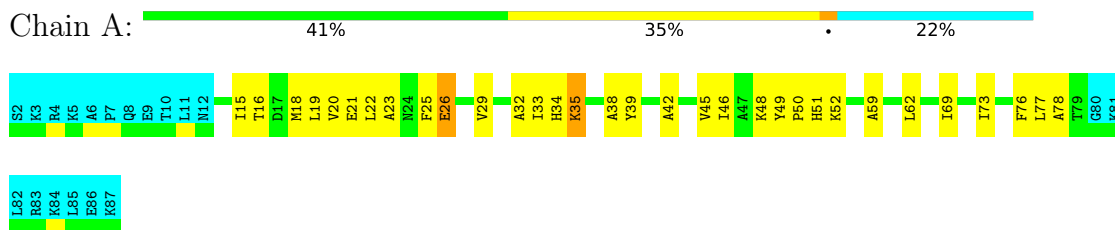


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

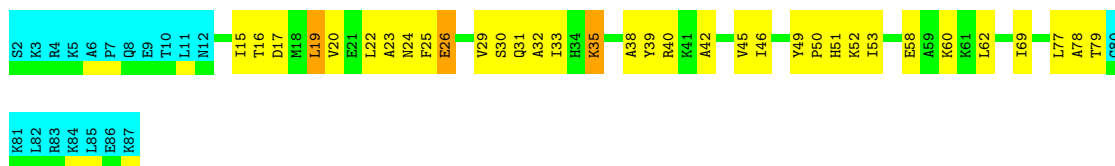
- Molecule 1: DNA POLYMERASE BETA



4.2.2 Score per residue for model 2

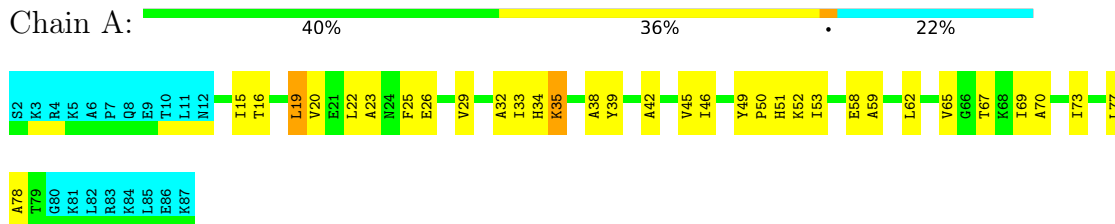
- Molecule 1: DNA POLYMERASE BETA





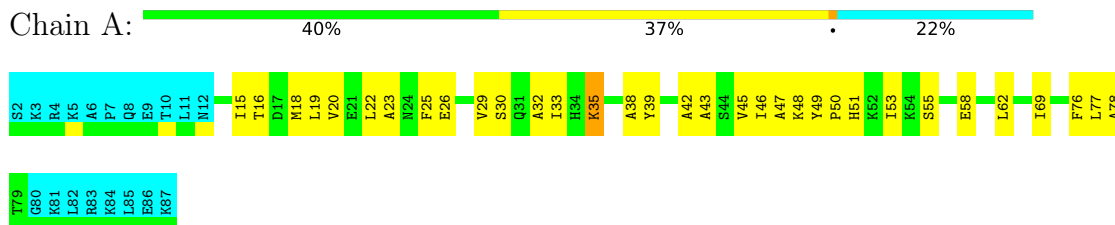
4.2.3 Score per residue for model 3

- Molecule 1: DNA POLYMERASE BETA



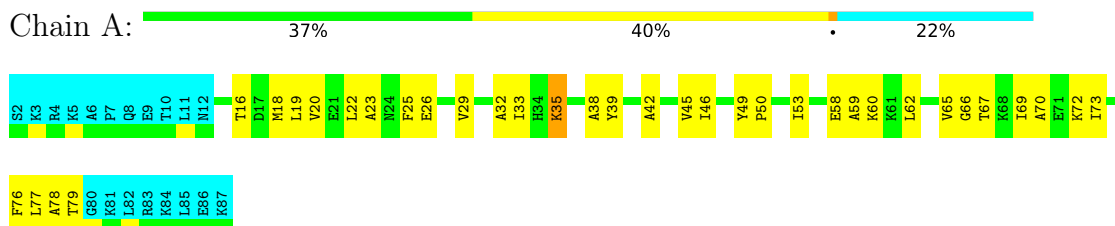
4.2.4 Score per residue for model 4

- Molecule 1: DNA POLYMERASE BETA



4.2.5 Score per residue for model 5

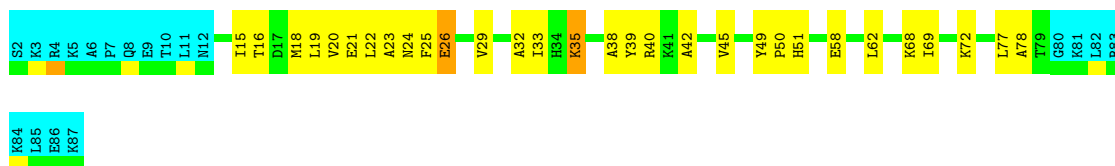
- Molecule 1: DNA POLYMERASE BETA



4.2.6 Score per residue for model 6

- Molecule 1: DNA POLYMERASE BETA

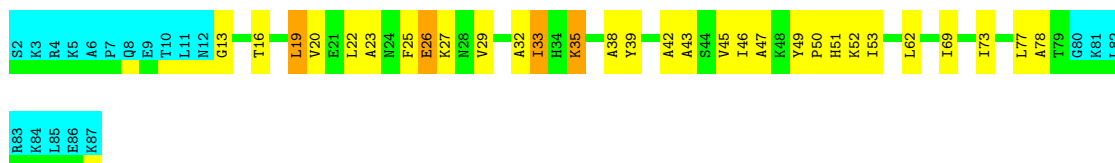




4.2.7 Score per residue for model 7

- Molecule 1: DNA POLYMERASE BETA

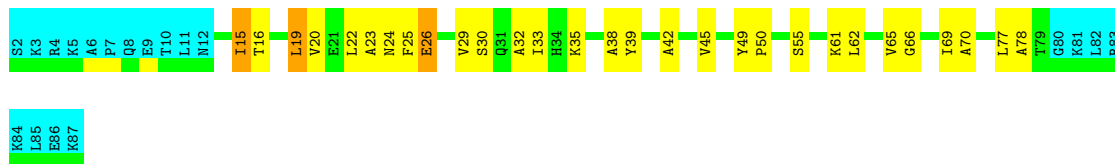
Chain A: 43% 30% 5% 22%



4.2.8 Score per residue for model 8

- Molecule 1: DNA POLYMERASE BETA

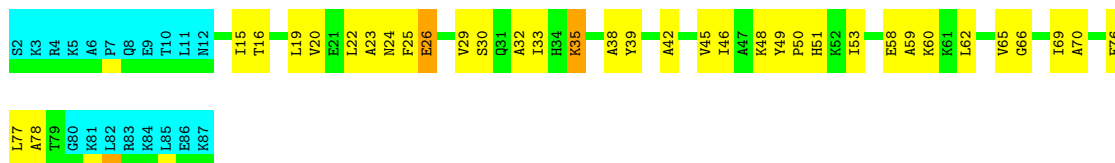
Chain A: 44% 30% • 22%



4.2.9 Score per residue for model 9

- Molecule 1: DNA POLYMERASE BETA

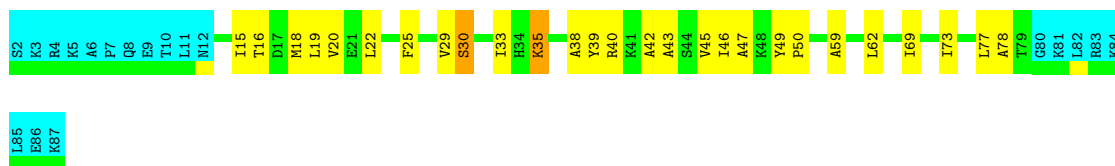
Chain A: 37% 38% • 22%



4.2.10 Score per residue for model 10

- Molecule 1: DNA POLYMERASE BETA

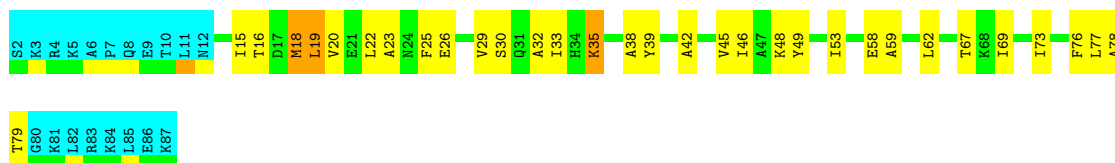
Chain A: 47% 29% • 22%



4.2.11 Score per residue for model 11

- Molecule 1: DNA POLYMERASE BETA

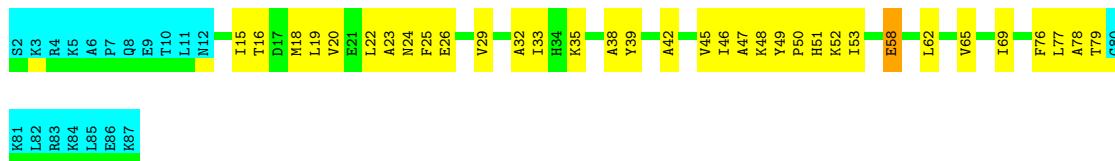
Chain A: 41% 34% 22%



4.2.12 Score per residue for model 12

- Molecule 1: DNA POLYMERASE BETA

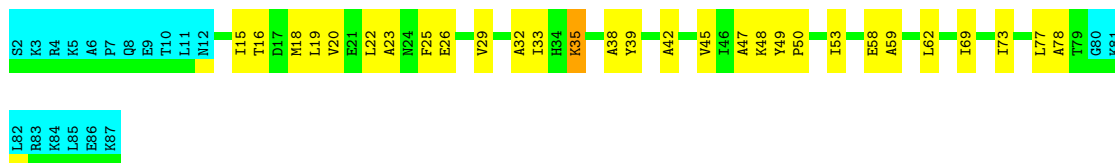
Chain A: 38% 38% 22%



4.2.13 Score per residue for model 13

- Molecule 1: DNA POLYMERASE BETA

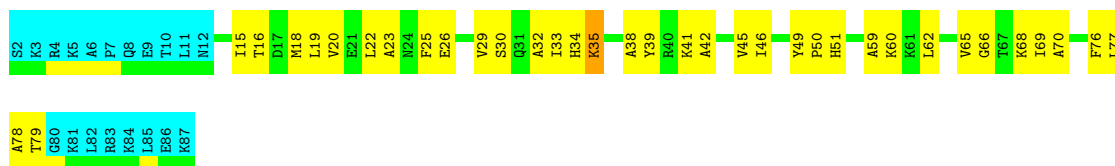
Chain A: 44% 33% 22%



4.2.14 Score per residue for model 14

- Molecule 1: DNA POLYMERASE BETA

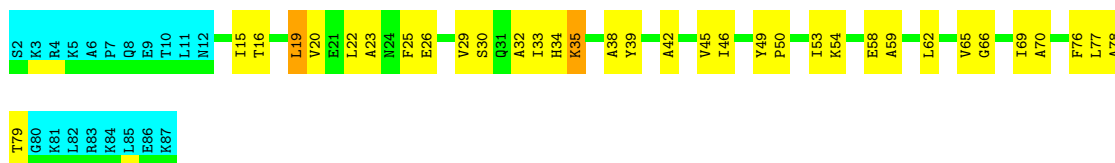
Chain A: 36% 41% 22%



4.2.15 Score per residue for model 15

- Molecule 1: DNA POLYMERASE BETA

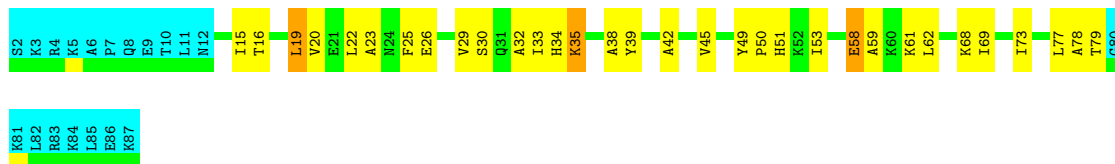
Chain A: 38% 37% 22%



4.2.16 Score per residue for model 16

- Molecule 1: DNA POLYMERASE BETA

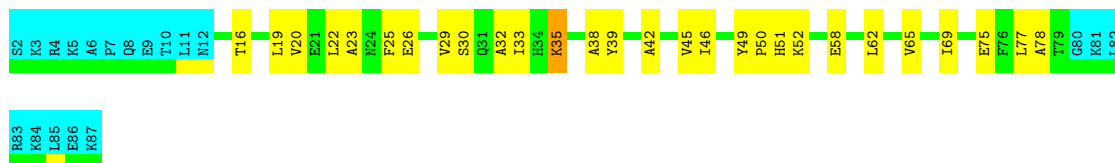
Chain A: 41% 34% 22%



4.2.17 Score per residue for model 17

- Molecule 1: DNA POLYMERASE BETA

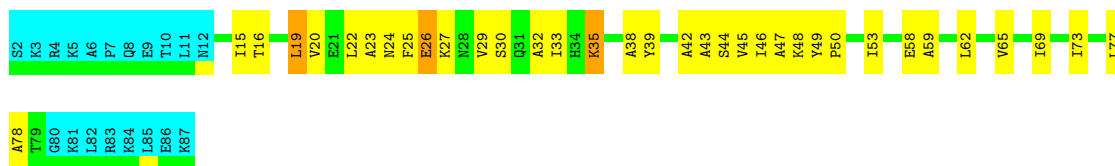
Chain A: 45% 31% 22%



4.2.18 Score per residue for model 18

- Molecule 1: DNA POLYMERASE BETA

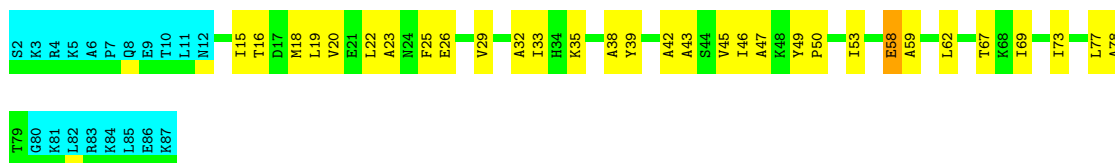
Chain A: 37% 37% 22%



4.2.19 Score per residue for model 19

- Molecule 1: DNA POLYMERASE BETA

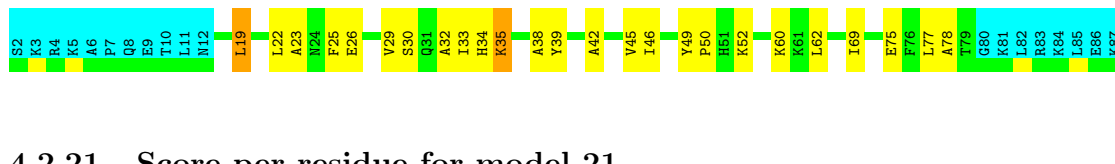
Chain A: 42% 35% 22%



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: DNA POLYMERASE BETA

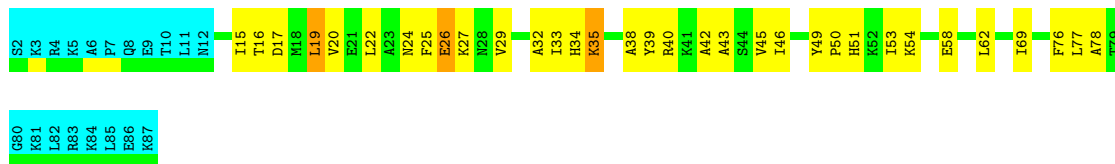
Chain A: 49% 27% 22%



4.2.21 Score per residue for model 21

- Molecule 1: DNA POLYMERASE BETA

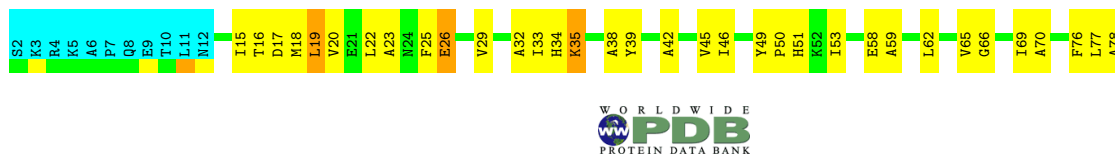
Chain A: 40% 35% 22%



4.2.22 Score per residue for model 22

- Molecule 1: DNA POLYMERASE BETA

Chain A: 38% 36% 22%



T79
G80
K81
L82
R83
K84
L85
E86
K87

4.2.23 Score per residue for model 23

- Molecule 1: DNA POLYMERASE BETA

Chain A:  40% 36% 22%

S2 K3 R4 K5 A6 P7 O8 E9 T10 L11 M12 I15 T16 D17 M18 L19 V20 E21 L22 A23 N24 F25 E26 V29 V30 Q31 A32 I33 H34 K35 A38 Y39 A42 A43 S44 V45 I46 A47 K48 Y49 P50 H51 K52 A59 K60 K61 L62 K68 I69 I73 L77 A78

T79
G80
K81
L82
R83
K84
L85
E86
K87

4.2.24 Score per residue for model 24

- Molecule 1: DNA POLYMERASE BETA

Chain A:  47% 27% 5% 22%

S2 K3 R4 K5 A6 P7 O8 E9 T10 L11 M12 I15 L19 V20 E21 A23 N24 F25 E26 V29 A32 I33 K35 A38 Y39 A42 V45 I46 Y49 P50 I53 K54 S55 E58 L62 I69 F76 L77 A78 T79 G80 K81 L82 R83 K84

L85
E86
K87

4.2.25 Score per residue for model 25

- Molecule 1: DNA POLYMERASE BETA

Chain A:  41% 35% 22%

S2 K3 R4 P7 O8 E9 T10 L11 M12 I15 T16 D17 M18 V20 E21 L22 A23 N24 F25 E26 V29 V30 Q31 A32 I33 H34 K35 A38 Y39 A42 A43 S44 V45 I46 A47 K48 Y49 I53 R54 S55 E58 A59 L62 I69 I73 L77 A78

T79
G80
K81
L82
R83
K84
L85
E86
K87

5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS AND SIMULATED ANNEALING*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *THE SELECTION UTILIZED THE LOWEST ENERGY STRUCTURES WITH NO NOE VIOLATIONS EXCEEDING 0.3 ANGSTROMS AND NO DIHEDRAL VIOLATIONS EXCEEDING 0.3 DEGREES..*

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

Software name	Classification	Version
DYANA	structure solution	1.5
X-PLOR	refinement	4.0

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	512	536	536	29±3
All	All	12800	13400	13400	724

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ALA:HB1	1:A:69:ILE:HD11	1.01	1.32	10	22
1:A:22:LEU:HD11	1:A:39:TYR:CG	0.89	2.02	17	21
1:A:22:LEU:HD11	1:A:39:TYR:CD1	0.78	2.14	25	23
1:A:22:LEU:HD21	1:A:39:TYR:CE2	0.78	2.14	9	5
1:A:15:ILE:HG22	1:A:19:LEU:CD1	0.77	2.10	10	20
1:A:38:ALA:HB1	1:A:69:ILE:CD1	0.76	2.10	3	22
1:A:45:VAL:HG11	1:A:65:VAL:HG23	0.76	1.57	15	8
1:A:42:ALA:CB	1:A:69:ILE:HG21	0.75	2.11	11	24
1:A:15:ILE:O	1:A:19:LEU:HD12	0.75	1.82	16	10
1:A:42:ALA:HB2	1:A:69:ILE:HG21	0.75	1.58	3	18
1:A:22:LEU:HD21	1:A:39:TYR:CD2	0.74	2.18	23	16
1:A:38:ALA:CB	1:A:69:ILE:HD11	0.73	2.12	25	18
1:A:45:VAL:HG22	1:A:62:LEU:HD13	0.72	1.59	8	1
1:A:19:LEU:HD22	1:A:42:ALA:HB3	0.70	1.61	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:THR:O	1:A:20:VAL:HG23	0.68	1.89	21	22
1:A:45:VAL:HG11	1:A:65:VAL:CG2	0.68	2.18	8	8
1:A:53:ILE:HD12	1:A:73:ILE:HG21	0.67	1.64	7	1
1:A:22:LEU:HD11	1:A:39:TYR:CE1	0.67	2.24	21	2
1:A:26:GLU:O	1:A:32:ALA:HB3	0.67	1.88	6	24
1:A:19:LEU:HD23	1:A:39:TYR:CD2	0.66	2.25	2	1
1:A:22:LEU:HD12	1:A:26:GLU:OE1	0.65	1.90	15	2
1:A:53:ILE:HG23	1:A:58:GLU:CB	0.64	2.22	13	10
1:A:45:VAL:HG21	1:A:62:LEU:HB3	0.64	1.69	25	16
1:A:15:ILE:HG22	1:A:19:LEU:HD12	0.63	1.68	23	7
1:A:45:VAL:HG11	1:A:65:VAL:HG22	0.63	1.69	8	2
1:A:15:ILE:HG22	1:A:19:LEU:HD11	0.63	1.70	1	12
1:A:16:THR:CB	1:A:47:ALA:HB2	0.63	2.24	4	3
1:A:53:ILE:HG23	1:A:58:GLU:HB3	0.62	1.72	25	15
1:A:18:MET:O	1:A:22:LEU:HD23	0.61	1.96	25	12
1:A:16:THR:OG1	1:A:47:ALA:HB2	0.61	1.95	25	7
1:A:59:ALA:HB2	1:A:73:ILE:HG21	0.59	1.74	19	10
1:A:66:GLY:O	1:A:70:ALA:HB2	0.59	1.98	5	6
1:A:43:ALA:O	1:A:47:ALA:HB3	0.58	1.99	4	6
1:A:19:LEU:O	1:A:23:ALA:HB2	0.57	1.99	12	23
1:A:16:THR:HG21	1:A:47:ALA:HB2	0.57	1.76	7	1
1:A:42:ALA:HB3	1:A:69:ILE:HG21	0.57	1.76	9	3
1:A:19:LEU:HB3	1:A:43:ALA:HB2	0.57	1.77	21	3
1:A:59:ALA:HA	1:A:62:LEU:HD12	0.56	1.77	14	5
1:A:39:TYR:CD2	1:A:69:ILE:HD12	0.56	2.36	17	2
1:A:35:LYS:O	1:A:38:ALA:HB3	0.56	2.00	16	25
1:A:16:THR:HB	1:A:47:ALA:HB2	0.55	1.77	4	2
1:A:22:LEU:HD11	1:A:39:TYR:CD2	0.55	2.34	2	6
1:A:22:LEU:HD12	1:A:22:LEU:C	0.55	2.26	1	21
1:A:15:ILE:HG21	1:A:73:ILE:HD12	0.55	1.79	3	1
1:A:49:TYR:CZ	1:A:62:LEU:HD21	0.53	2.38	25	14
1:A:77:LEU:N	1:A:77:LEU:HD22	0.53	2.19	14	25
1:A:22:LEU:HD11	1:A:39:TYR:CE2	0.53	2.39	10	2
1:A:16:THR:HG23	1:A:43:ALA:HB1	0.53	1.81	7	1
1:A:53:ILE:HG23	1:A:58:GLU:HB2	0.52	1.81	16	1
1:A:38:ALA:HB1	1:A:69:ILE:CG1	0.52	2.35	16	17
1:A:39:TYR:CD1	1:A:69:ILE:HD12	0.51	2.41	10	1
1:A:22:LEU:HD11	1:A:39:TYR:CZ	0.51	2.41	10	4
1:A:60:LYS:CG	1:A:70:ALA:HB1	0.51	2.35	9	2
1:A:19:LEU:CB	1:A:43:ALA:HB2	0.49	2.36	21	1
1:A:49:TYR:CE1	1:A:62:LEU:HD22	0.49	2.43	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HG22	1:A:58:GLU:HB3	0.48	1.83	4	1
1:A:25:PHE:O	1:A:29:VAL:HG23	0.48	2.08	1	25
1:A:60:LYS:HG3	1:A:70:ALA:HB1	0.48	1.85	14	2
1:A:59:ALA:CB	1:A:73:ILE:HG21	0.48	2.39	25	1
1:A:18:MET:O	1:A:22:LEU:HD22	0.47	2.08	10	1
1:A:34:HIS:CD2	1:A:35:LYS:CD	0.47	2.97	22	8
1:A:22:LEU:CD1	1:A:39:TYR:CE2	0.46	2.99	8	2
1:A:49:TYR:CE1	1:A:62:LEU:CD2	0.45	2.99	4	20
1:A:39:TYR:CE2	1:A:69:ILE:CD1	0.45	3.00	17	2
1:A:27:LYS:HD2	1:A:33:ILE:HD11	0.45	1.88	7	1
1:A:15:ILE:HG22	1:A:19:LEU:HD13	0.45	1.84	12	2
1:A:19:LEU:O	1:A:22:LEU:HD23	0.45	2.11	10	1
1:A:22:LEU:CD1	1:A:39:TYR:CD1	0.45	3.00	1	10
1:A:39:TYR:CE2	1:A:69:ILE:HD12	0.45	2.47	17	2
1:A:22:LEU:HD12	1:A:23:ALA:N	0.45	2.27	16	5
1:A:65:VAL:HG12	1:A:70:ALA:HB2	0.44	1.89	3	1
1:A:15:ILE:HG23	1:A:76:PHE:CD2	0.44	2.47	24	1
1:A:19:LEU:HD23	1:A:39:TYR:HD2	0.43	1.71	17	4
1:A:49:TYR:CD1	1:A:50:PRO:HD2	0.43	2.48	15	17
1:A:34:HIS:CD2	1:A:35:LYS:HD3	0.43	2.49	21	5
1:A:22:LEU:CD2	1:A:39:TYR:CE2	0.43	2.99	2	1
1:A:59:ALA:O	1:A:65:VAL:HG21	0.43	2.13	14	5
1:A:60:LYS:HB2	1:A:70:ALA:HB1	0.43	1.89	5	1
1:A:45:VAL:HG13	1:A:46:ILE:N	0.43	2.29	7	15
1:A:53:ILE:HD12	1:A:73:ILE:CG2	0.42	2.41	7	1
1:A:45:VAL:HG13	1:A:46:ILE:HG13	0.42	1.91	9	5
1:A:50:PRO:C	1:A:51:HIS:CG	0.42	2.98	3	13
1:A:77:LEU:N	1:A:77:LEU:CD2	0.42	2.83	21	17
1:A:39:TYR:CE1	1:A:69:ILE:CD1	0.41	3.03	8	1
1:A:42:ALA:HA	1:A:65:VAL:HG22	0.41	1.92	12	1
1:A:53:ILE:HD13	1:A:59:ALA:HB2	0.41	1.90	18	1
1:A:42:ALA:O	1:A:46:ILE:HD12	0.41	2.16	9	1
1:A:26:GLU:CG	1:A:35:LYS:CG	0.41	2.99	22	1
1:A:32:ALA:HB1	1:A:35:LYS:HE3	0.40	1.92	17	2
1:A:45:VAL:CG2	1:A:62:LEU:HD13	0.40	2.38	8	1
1:A:29:VAL:HG12	1:A:30:SER:N	0.40	2.31	9	4
1:A:32:ALA:HB1	1:A:35:LYS:HD2	0.40	1.92	12	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	67/86 (78%)	60±1 (90±2%)	6±1 (9±2%)	1±0 (1±0%)	11	57
All	All	1675/2150 (78%)	1503 (90%)	147 (9%)	25 (1%)	11	57

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	78	ALA	25

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	52/69 (75%)	45±2 (87±4%)	7±2 (13±4%)	6	47
All	All	1300/1725 (75%)	1135 (87%)	165 (13%)	6	47

All 28 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	33	ILE	25
1	A	35	LYS	22
1	A	19	LEU	13
1	A	26	GLU	11
1	A	30	SER	11
1	A	76	PHE	10
1	A	24	ASN	8
1	A	48	LYS	7
1	A	79	THR	6
1	A	58	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	52	LYS	5
1	A	21	GLU	4
1	A	40	ARG	4
1	A	67	THR	4
1	A	55	SER	4
1	A	68	LYS	4
1	A	17	ASP	3
1	A	60	LYS	3
1	A	72	LYS	2
1	A	61	LYS	2
1	A	54	LYS	2
1	A	75	GLU	2
1	A	27	LYS	2
1	A	31	GLN	1
1	A	15	ILE	1
1	A	18	MET	1
1	A	41	LYS	1
1	A	44	SER	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

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided