



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:46 AM UTC

PDB ID : 2ASY / pdb_00002asy
Title : Solution Structure of ydhR protein from Escherichia coli
Authors : Revington, M.; Semesi, A.; Yee, A.; Shaw, G.S.; Ontario Centre for Structural Proteomics (OCSF)
Deposited on : 2005-08-24

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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

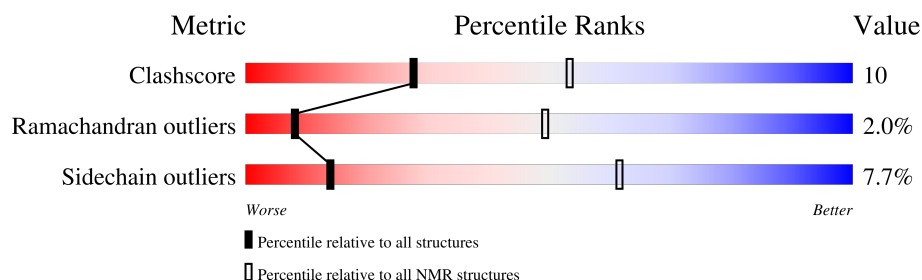
1 Overall quality at a glance

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	123	 64% 17% • 18%
1	B	123	 61% 20% • 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:1-A:101, B:1-B:101 (202)	0.77	15

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. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 8, 9, 10, 11, 12, 13, 15, 16, 17, 19, 20
2	2, 7, 18
3	6, 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3171 atoms, of which 1575 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein ydhR precursor.

Mol	Chain	Residues	Atoms						Trace
1	A	101	Total	C	H	N	O	S	0
			1584	514	786	131	151	2	
1	B	101	Total	C	H	N	O	S	0
			1587	514	789	131	151	2	

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	cloning artifact	UNP P77225
A	-20	GLY	-	cloning artifact	UNP P77225
A	-19	THR	-	cloning artifact	UNP P77225
A	-18	SER	-	cloning artifact	UNP P77225
A	-17	HIS	-	cloning artifact	UNP P77225
A	-16	HIS	-	cloning artifact	UNP P77225
A	-15	HIS	-	cloning artifact	UNP P77225
A	-14	HIS	-	cloning artifact	UNP P77225
A	-13	HIS	-	cloning artifact	UNP P77225
A	-12	HIS	-	cloning artifact	UNP P77225
A	-11	SER	-	cloning artifact	UNP P77225
A	-10	SER	-	cloning artifact	UNP P77225
A	-9	GLY	-	cloning artifact	UNP P77225
A	-8	ARG	-	cloning artifact	UNP P77225
A	-7	GLU	-	cloning artifact	UNP P77225
A	-6	ASN	-	cloning artifact	UNP P77225
A	-5	LEU	-	cloning artifact	UNP P77225
A	-4	TYR	-	cloning artifact	UNP P77225
A	-3	PHE	-	cloning artifact	UNP P77225
A	-2	GLN	-	cloning artifact	UNP P77225
A	-1	GLY	-	cloning artifact	UNP P77225
A	0	HIS	-	cloning artifact	UNP P77225
B	-21	MET	-	cloning artifact	UNP P77225
B	-20	GLY	-	cloning artifact	UNP P77225
B	-19	THR	-	cloning artifact	UNP P77225
B	-18	SER	-	cloning artifact	UNP P77225
B	-17	HIS	-	cloning artifact	UNP P77225
B	-16	HIS	-	cloning artifact	UNP P77225
B	-15	HIS	-	cloning artifact	UNP P77225

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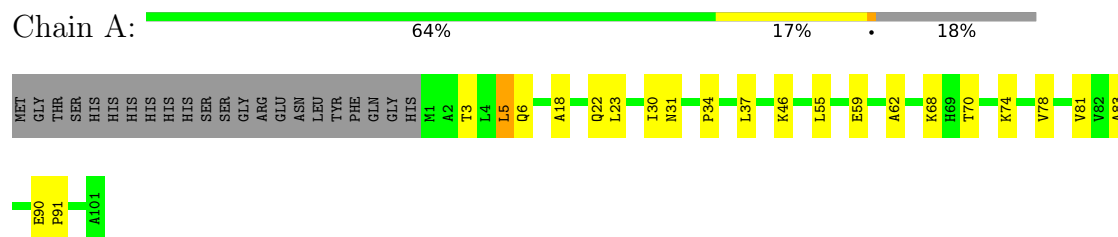
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	cloning artifact	UNP P77225
B	-13	HIS	-	cloning artifact	UNP P77225
B	-12	HIS	-	cloning artifact	UNP P77225
B	-11	SER	-	cloning artifact	UNP P77225
B	-10	SER	-	cloning artifact	UNP P77225
B	-9	GLY	-	cloning artifact	UNP P77225
B	-8	ARG	-	cloning artifact	UNP P77225
B	-7	GLU	-	cloning artifact	UNP P77225
B	-6	ASN	-	cloning artifact	UNP P77225
B	-5	LEU	-	cloning artifact	UNP P77225
B	-4	TYR	-	cloning artifact	UNP P77225
B	-3	PHE	-	cloning artifact	UNP P77225
B	-2	GLN	-	cloning artifact	UNP P77225
B	-1	GLY	-	cloning artifact	UNP P77225
B	0	HIS	-	cloning artifact	UNP P77225

4 Residue-property plots [i](#)

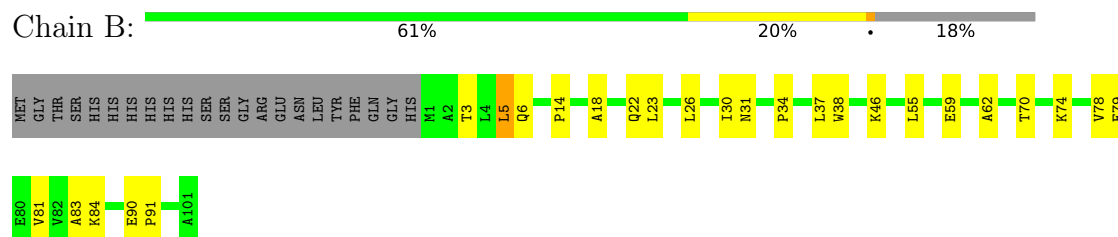
4.1 Average score per residue in the NMR ensemble

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: Protein ydhR precursor



- Molecule 1: Protein ydhR precursor

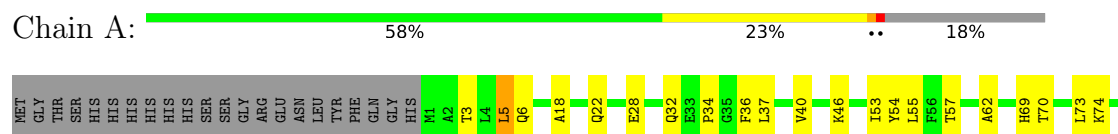


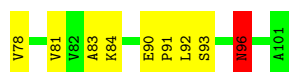
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein ydhR precursor





- Molecule 1: Protein ydhR precursor

Chain B: 56% 24% 18%



4.2.2 Score per residue for model 2

- Molecule 1: Protein ydhR precursor

Chain A: 58% 21% 18%



- Molecule 1: Protein ydhR precursor

Chain B: 58% 22% 18%



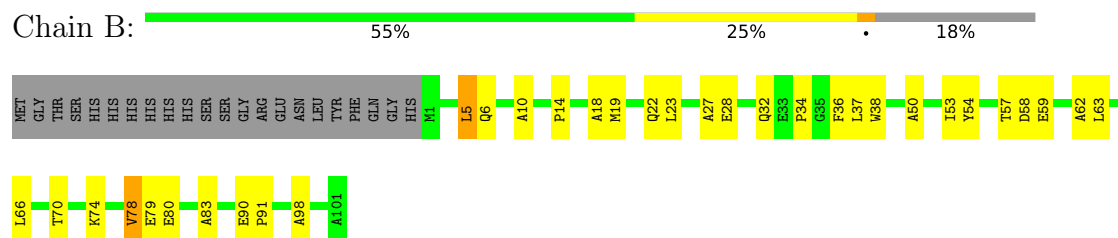
4.2.3 Score per residue for model 3

- Molecule 1: Protein ydhR precursor

Chain A: 56% 24% 18%

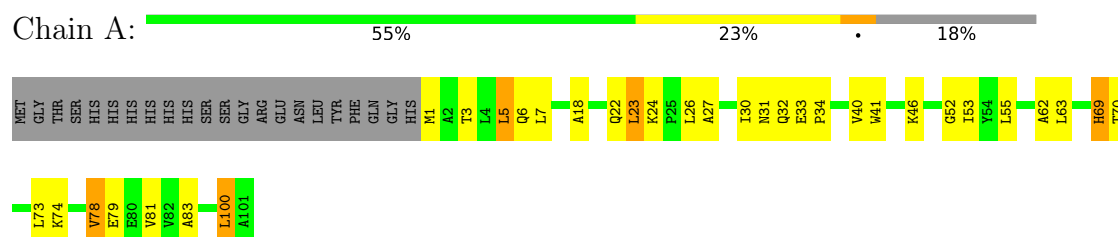


- Molecule 1: Protein ydhR precursor

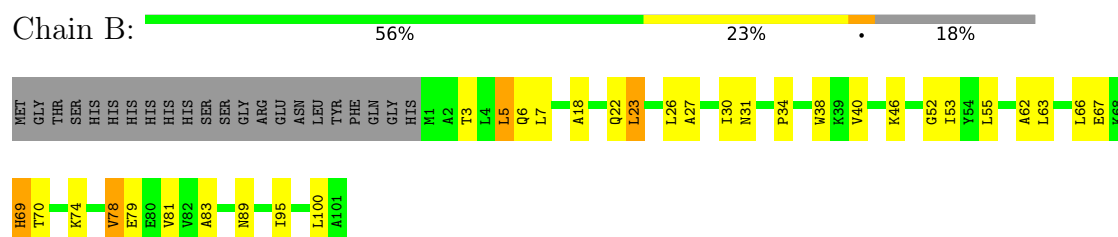


4.2.4 Score per residue for model 4

- Molecule 1: Protein ydhR precursor

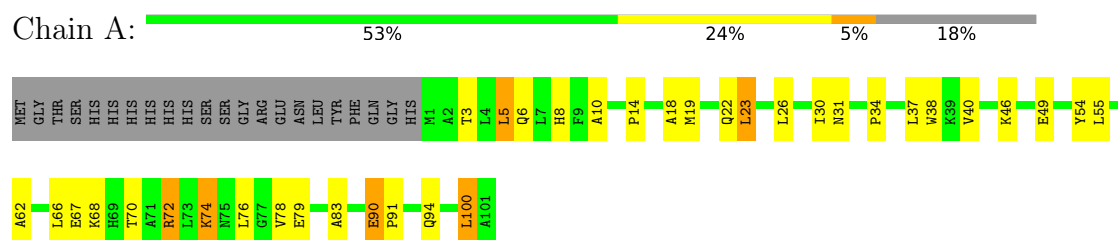


- Molecule 1: Protein ydhR precursor

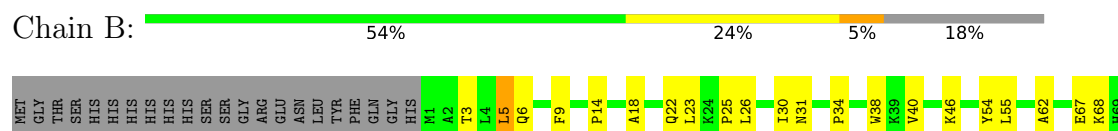


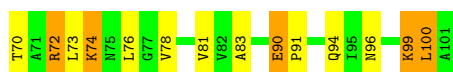
4.2.5 Score per residue for model 5

- Molecule 1: Protein ydhR precursor



- Molecule 1: Protein ydhR precursor



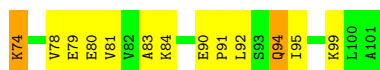


4.2.6 Score per residue for model 6

- Molecule 1: Protein ydhR precursor

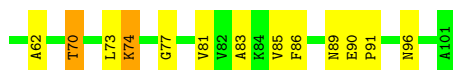


- Molecule 1: Protein ydhR precursor

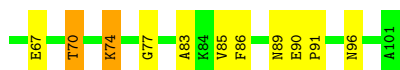


4.2.7 Score per residue for model 7

- Molecule 1: Protein ydhR precursor

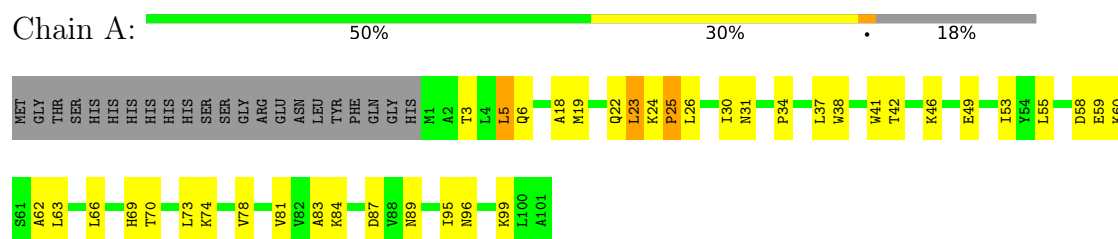


- Molecule 1: Protein ydhR precursor

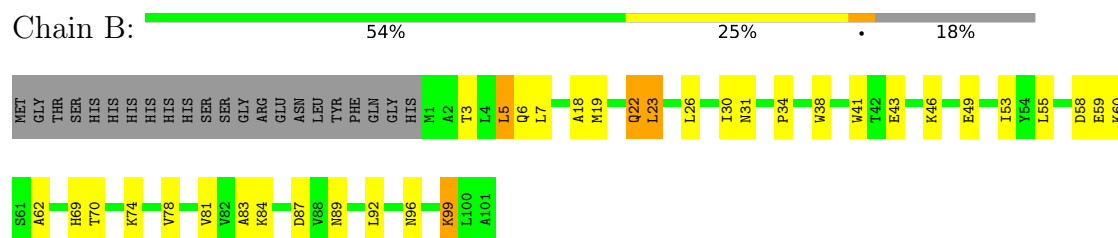


4.2.8 Score per residue for model 8

- Molecule 1: Protein ydhR precursor

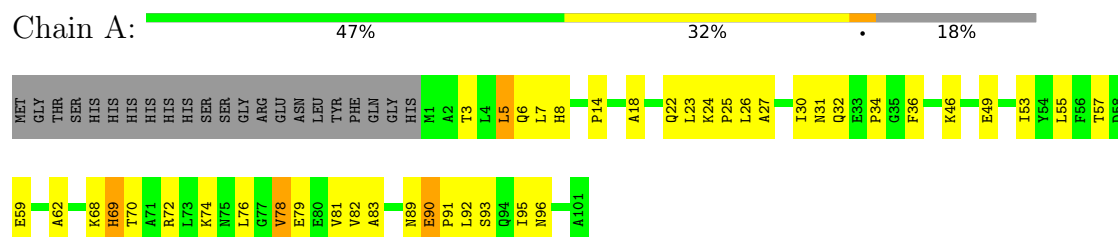


- Molecule 1: Protein ydhR precursor

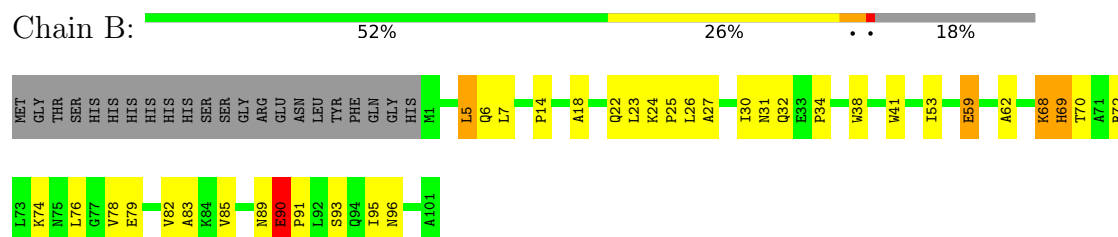


4.2.9 Score per residue for model 9

- Molecule 1: Protein ydhR precursor

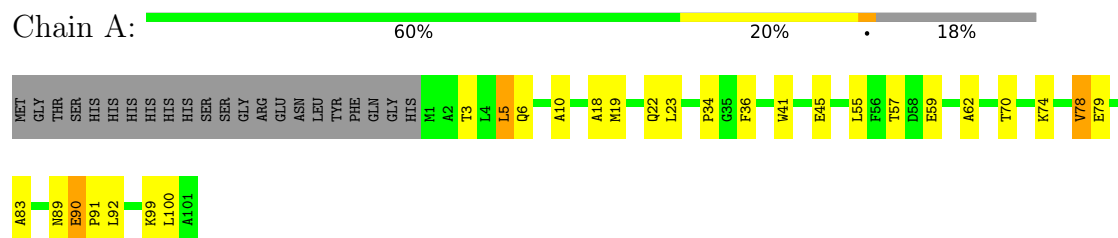


- Molecule 1: Protein ydhR precursor

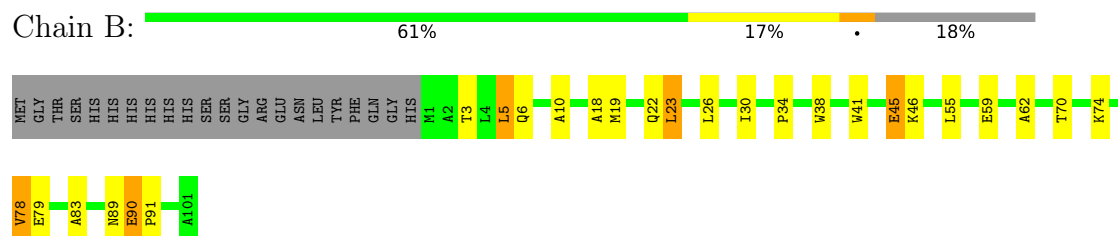


4.2.10 Score per residue for model 10

- Molecule 1: Protein ydhR precursor

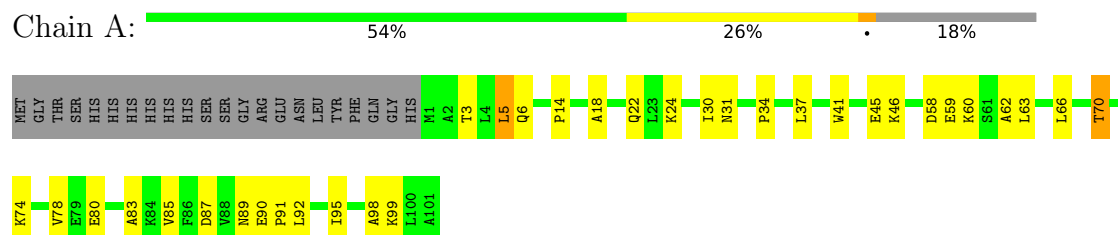


- Molecule 1: Protein ydhR precursor

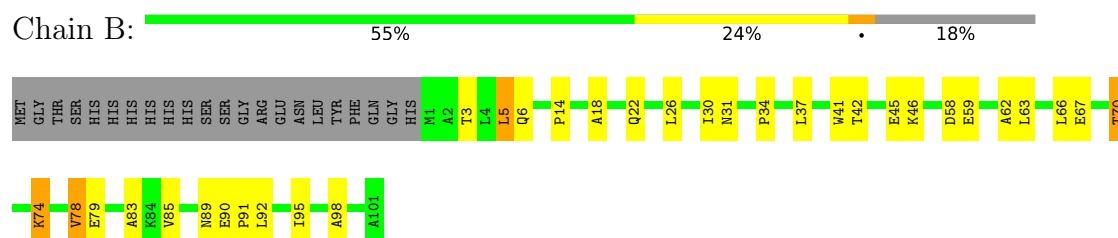


4.2.11 Score per residue for model 11

- Molecule 1: Protein ydhR precursor

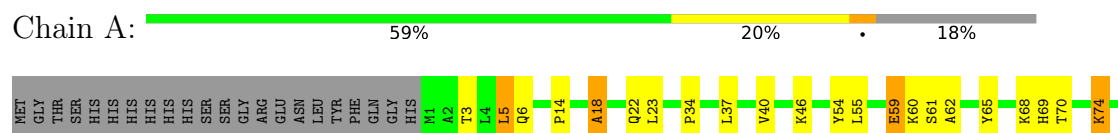


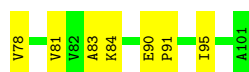
- Molecule 1: Protein ydhR precursor



4.2.12 Score per residue for model 12

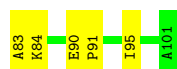
- Molecule 1: Protein ydhR precursor





- Molecule 1: Protein ydhR precursor

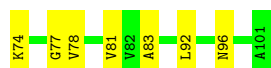
Chain B:



4.2.13 Score per residue for model 13

- Molecule 1: Protein ydhR precursor

Chain A:



- Molecule 1: Protein ydhR precursor

Chain B:



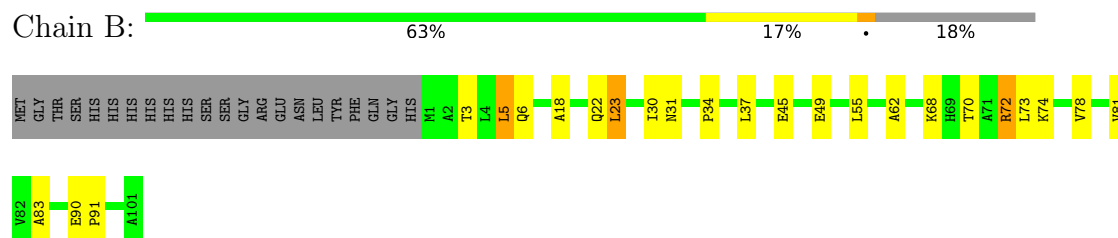
4.2.14 Score per residue for model 14

- Molecule 1: Protein ydhR precursor

Chain A:

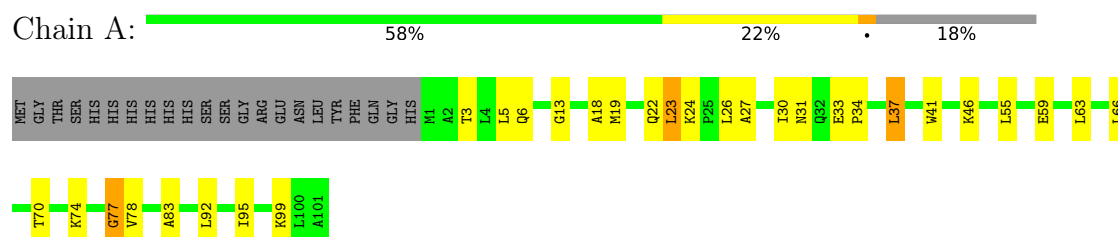


- Molecule 1: Protein ydhR precursor

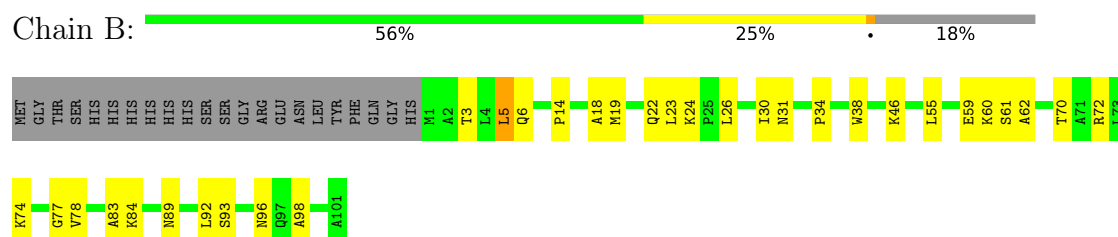


4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Protein ydhR precursor

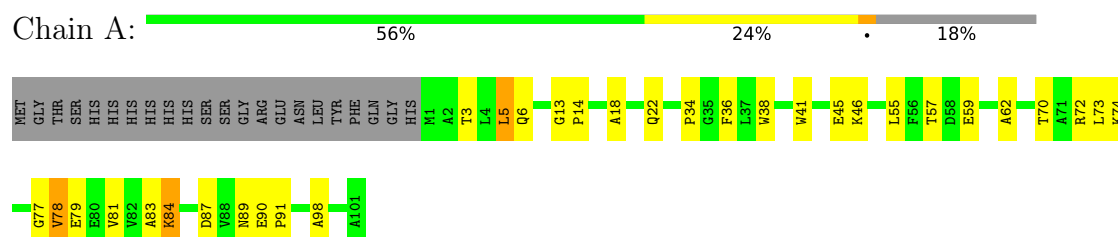


- Molecule 1: Protein ydhR precursor

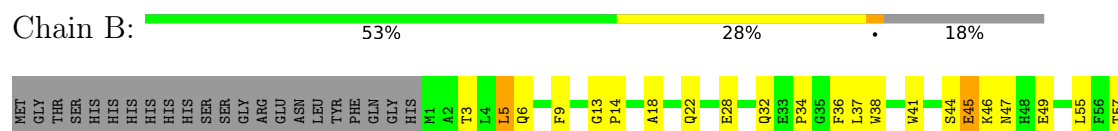


4.2.16 Score per residue for model 16

- Molecule 1: Protein ydhR precursor



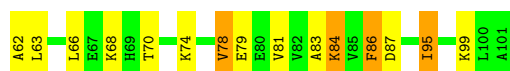
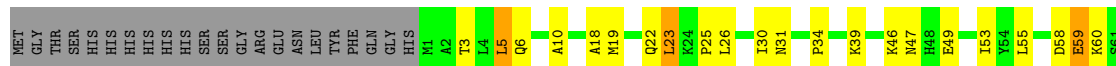
- Molecule 1: Protein ydhR precursor



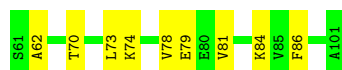


4.2.17 Score per residue for model 17

- Molecule 1: Protein ydhR precursor



- Molecule 1: Protein ydhR precursor

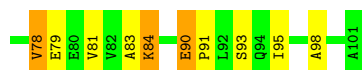


4.2.18 Score per residue for model 18

- Molecule 1: Protein ydhR precursor

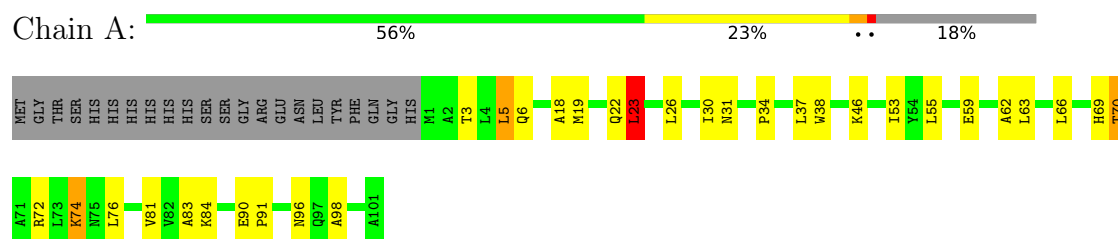


- Molecule 1: Protein ydhR precursor

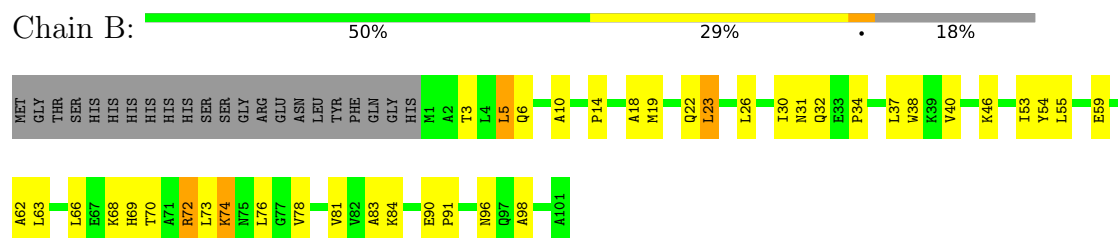


4.2.19 Score per residue for model 19

- Molecule 1: Protein ydhR precursor

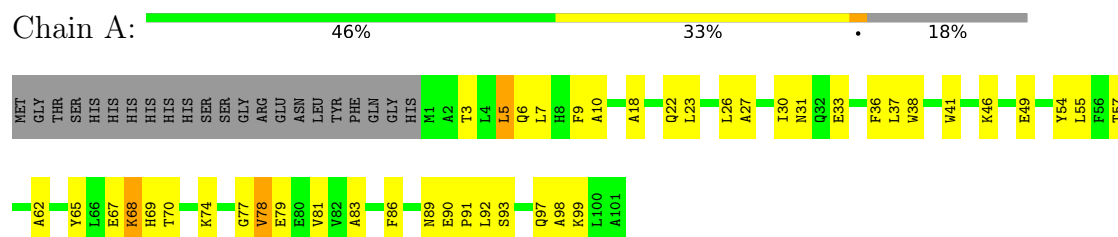


- Molecule 1: Protein ydhR precursor

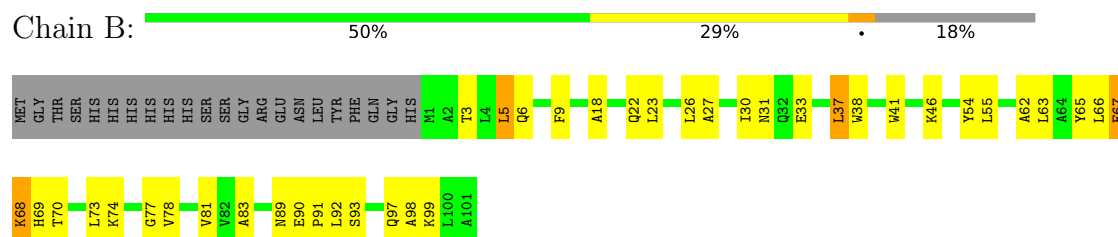


4.2.20 Score per residue for model 20

- Molecule 1: Protein ydhR precursor



- Molecule 1: Protein ydhR precursor



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing, torsion angle dynamics, molecular dynamics, refinement in presence of solvent*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	2.032.3
CNS	structure solution	1.1

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	1.19±0.03	1±1/816 (0.1± 0.1%)	1.07±0.03	1±1/1103 (0.1± 0.1%)
1	B	1.20±0.03	1±1/816 (0.1± 0.1%)	1.06±0.02	1±0/1103 (0.1± 0.0%)
All	All	1.19	34/32640 (0.1%)	1.07	26/44120 (0.1%)

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	B	0.0±0.0	0.1±0.3
All	All	0	2

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	B	14	PRO	N-CA	-7.04	1.40	1.46	5	11
1	A	95	ILE	CA-CB	6.38	1.61	1.54	12	4
1	A	14	PRO	N-CA	-6.31	1.41	1.46	5	9
1	A	18	ALA	C-O	-5.43	1.17	1.24	12	1
1	B	90	GLU	CA-C	5.28	1.59	1.52	9	1
1	B	95	ILE	CA-CB	5.28	1.61	1.54	12	2
1	A	50	ALA	C-N	-5.24	1.28	1.33	3	2
1	B	50	ALA	C-N	-5.18	1.28	1.33	3	2
1	A	86	PHE	N-CA	-5.17	1.39	1.45	20	1
1	B	23	LEU	C-O	-5.02	1.18	1.24	10	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	B	86	PHE	CA-CB-CG	6.93	120.73	113.80	17	1
1	A	77	GLY	N-CA-C	6.16	115.81	110.21	15	3
1	A	96	ASN	CA-CB-CG	6.12	118.72	112.60	1	1
1	A	95	ILE	N-CA-C	-6.11	107.03	112.90	3	3
1	B	77	GLY	N-CA-C	6.07	115.73	110.21	15	3
1	B	96	ASN	CA-CB-CG	5.92	118.52	112.60	2	1
1	B	58	ASP	CA-CB-CG	5.88	118.48	112.60	3	2
1	A	69	HIS	CA-CB-CG	5.71	119.50	113.80	1	2
1	A	23	LEU	N-CA-C	-5.46	105.40	111.36	19	1
1	B	69	HIS	CA-CB-CG	5.40	119.20	113.80	1	1
1	A	94	GLN	N-CA-C	-5.35	107.12	113.97	5	2
1	B	90	GLU	N-CA-C	5.33	121.60	109.81	9	1
1	B	95	ILE	N-CA-C	-5.17	107.71	112.83	18	1
1	B	94	GLN	N-CA-C	-5.12	107.58	113.88	6	2
1	A	86	PHE	CA-CB-CG	5.09	118.89	113.80	17	1
1	B	23	LEU	N-CA-C	-5.03	105.50	111.69	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	72	ARG	Sidechain	2

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	798	786	788	17±4
1	B	798	789	788	18±4
All	All	31920	31500	31520	613

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:GLN:O	1:B:83:ALA:HA	0.67	1.90	15	19
1:A:6:GLN:O	1:A:83:ALA:HA	0.64	1.93	4	20
1:A:5:LEU:HD13	1:A:62:ALA:HB1	0.60	1.71	4	18
1:A:86:PHE:CD1	1:B:42:THR:HG21	0.60	2.31	17	1
1:B:69:HIS:HB2	1:B:81:VAL:HG21	0.60	1.74	20	2
1:B:23:LEU:O	1:B:27:ALA:HB2	0.60	1.96	18	8
1:B:18:ALA:HA	1:B:22:GLN:HB2	0.59	1.75	19	19
1:B:10:ALA:HB3	1:B:78:VAL:HG11	0.58	1.75	3	4
1:B:5:LEU:HD13	1:B:62:ALA:HB1	0.58	1.73	4	19
1:A:23:LEU:O	1:A:27:ALA:HB2	0.58	1.99	18	7
1:A:70:THR:O	1:A:74:LYS:HG2	0.58	1.98	20	20
1:A:89:ASN:O	1:B:41:TRP:HB2	0.58	1.99	16	6
1:B:70:THR:O	1:B:74:LYS:HG2	0.57	1.99	20	20
1:A:100:LEU:HD23	1:B:38:TRP:CZ2	0.57	2.35	5	2
1:A:18:ALA:HA	1:A:22:GLN:HB2	0.55	1.77	19	19
1:A:41:TRP:HB2	1:B:89:ASN:O	0.54	2.01	16	5
1:A:63:LEU:O	1:A:66:LEU:HG	0.54	2.02	6	8
1:A:99:LYS:HB2	1:B:38:TRP:CD1	0.54	2.38	20	3
1:B:19:MET:O	1:B:23:LEU:HB2	0.53	2.03	19	3
1:A:90:GLU:N	1:A:91:PRO:HD2	0.53	2.19	18	13
1:A:96:ASN:HB2	1:B:38:TRP:CB	0.53	2.34	7	1
1:A:53:ILE:HG13	1:B:53:ILE:HG13	0.52	1.80	4	6
1:B:40:VAL:HB	1:B:54:TYR:CD1	0.52	2.39	5	6
1:A:49:GLU:HG2	1:A:50:ALA:N	0.52	2.18	13	1
1:B:78:VAL:HG12	1:B:79:GLU:HG3	0.52	1.79	17	1
1:A:10:ALA:HB3	1:A:78:VAL:HG11	0.52	1.79	3	4
1:B:28:GLU:O	1:B:32:GLN:HA	0.52	2.05	1	3
1:A:93:SER:HA	1:A:96:ASN:OD1	0.52	2.05	9	1
1:A:24:LYS:HB3	1:B:95:ILE:HD11	0.52	1.81	11	2
1:A:37:LEU:O	1:B:98:ALA:HB3	0.52	2.05	19	7
1:A:3:THR:O	1:A:55:LEU:HA	0.51	2.04	12	18
1:B:3:THR:O	1:B:55:LEU:HA	0.51	2.05	12	17
1:A:92:LEU:HD11	1:B:23:LEU:HB2	0.51	1.81	15	1
1:A:19:MET:O	1:A:23:LEU:HB2	0.51	2.05	19	4
1:A:70:THR:HG23	1:A:74:LYS:HE3	0.51	1.81	11	1
1:A:7:LEU:HD11	1:A:69:HIS:CE1	0.51	2.41	4	1
1:A:38:TRP:CB	1:B:96:ASN:HB2	0.51	2.36	7	1
1:B:90:GLU:N	1:B:91:PRO:HD2	0.51	2.21	18	13
1:B:26:LEU:O	1:B:30:ILE:HG13	0.50	2.06	9	13
1:A:70:THR:OG1	1:A:81:VAL:HG12	0.50	2.07	19	4
1:A:38:TRP:CD1	1:B:99:LYS:HB3	0.50	2.41	8	2
1:A:58:ASP:OD1	1:A:60:LYS:HG2	0.50	2.07	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:SER:HA	1:B:96:ASN:OD1	0.50	2.07	2	2
1:B:73:LEU:HD21	1:B:81:VAL:HG23	0.50	1.82	6	7
1:A:93:SER:HA	1:A:96:ASN:HB3	0.50	1.84	2	1
1:B:59:GLU:HB3	1:B:85:VAL:HG11	0.50	1.84	7	4
1:A:98:ALA:HB3	1:B:37:LEU:O	0.50	2.06	19	6
1:A:70:THR:HG22	1:A:74:LYS:HE3	0.50	1.83	17	3
1:A:23:LEU:HB3	1:B:92:LEU:HD21	0.50	1.84	8	1
1:B:58:ASP:OD1	1:B:60:LYS:HG2	0.50	2.06	8	2
1:A:36:PHE:CD1	1:A:57:THR:HB	0.49	2.42	2	9
1:A:40:VAL:HB	1:A:54:TYR:CD1	0.49	2.42	5	5
1:A:38:TRP:CZ2	1:B:100:LEU:HD23	0.49	2.43	5	1
1:A:59:GLU:HB3	1:A:85:VAL:HG11	0.49	1.83	7	3
1:B:38:TRP:CZ3	1:B:54:TYR:HA	0.49	2.42	20	2
1:B:9:PHE:CD1	1:B:81:VAL:HG22	0.49	2.43	6	3
1:A:26:LEU:O	1:A:30:ILE:HG13	0.49	2.08	9	10
1:A:45:GLU:OE2	1:A:46:LYS:HE3	0.48	2.08	18	1
1:A:87:ASP:O	1:B:42:THR:HG23	0.48	2.08	11	1
1:A:78:VAL:HG13	1:A:79:GLU:H	0.48	1.69	17	7
1:A:87:ASP:HB3	1:B:43:GLU:O	0.47	2.09	8	1
1:A:87:ASP:OD1	1:B:44:SER:HA	0.47	2.09	17	1
1:B:19:MET:HA	1:B:23:LEU:HG	0.47	1.86	15	1
1:B:93:SER:O	1:B:97:GLN:HG3	0.47	2.09	20	1
1:A:73:LEU:HD21	1:A:81:VAL:HG23	0.47	1.86	8	7
1:B:70:THR:OG1	1:B:81:VAL:HG12	0.47	2.08	4	4
1:B:70:THR:HG22	1:B:74:LYS:HE3	0.47	1.86	15	5
1:A:31:ASN:OD1	1:A:33:GLU:HB3	0.47	2.10	18	1
1:A:92:LEU:HD11	1:B:19:MET:O	0.47	2.10	1	3
1:A:30:ILE:HD12	1:A:31:ASN:N	0.47	2.25	8	11
1:B:30:ILE:HD12	1:B:31:ASN:N	0.47	2.24	9	12
1:A:3:THR:HG21	1:A:59:GLU:HB3	0.47	1.85	11	3
1:A:72:ARG:O	1:A:76:LEU:HG	0.47	2.10	5	3
1:A:38:TRP:CZ3	1:A:54:TYR:HA	0.46	2.45	20	2
1:B:63:LEU:O	1:B:66:LEU:HG	0.46	2.10	4	6
1:B:90:GLU:HA	1:B:93:SER:OG	0.46	2.10	18	1
1:A:38:TRP:CB	1:B:96:ASN:HA	0.46	2.40	13	3
1:A:86:PHE:HB3	1:B:49:GLU:OE2	0.46	2.10	7	1
1:A:93:SER:O	1:A:97:GLN:HG3	0.46	2.10	20	1
1:B:7:LEU:HD11	1:B:69:HIS:NE2	0.46	2.24	9	2
1:A:96:ASN:HB2	1:B:38:TRP:HB2	0.46	1.87	7	1
1:A:6:GLN:NE2	1:A:84:LYS:HB2	0.46	2.26	17	2
1:B:40:VAL:HG21	1:B:52:GLY:N	0.46	2.26	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD11	1:A:69:HIS:NE2	0.46	2.26	9	2
1:B:6:GLN:OE1	1:B:84:LYS:HB2	0.46	2.11	13	1
1:B:7:LEU:HD11	1:B:69:HIS:CE1	0.46	2.46	4	1
1:A:74:LYS:HB3	1:A:80:GLU:OE1	0.46	2.11	11	1
1:B:6:GLN:NE2	1:B:84:LYS:HB2	0.46	2.26	18	4
1:B:38:TRP:CZ2	1:B:55:LEU:HD13	0.46	2.45	16	2
1:A:84:LYS:HD3	1:B:49:GLU:OE2	0.46	2.11	8	1
1:A:23:LEU:HD23	1:B:92:LEU:HD13	0.46	1.88	13	1
1:B:30:ILE:O	1:B:72:ARG:HD3	0.46	2.11	14	1
1:A:93:SER:O	1:A:96:ASN:HB3	0.46	2.11	1	1
1:B:19:MET:HA	1:B:23:LEU:HB2	0.46	1.87	18	2
1:B:46:LYS:HD3	1:B:46:LYS:H	0.45	1.70	7	2
1:A:96:ASN:HA	1:B:38:TRP:CB	0.45	2.41	19	3
1:B:3:THR:HG21	1:B:59:GLU:HB3	0.45	1.87	11	1
1:A:19:MET:O	1:B:92:LEU:HD11	0.45	2.11	15	1
1:B:31:ASN:O	1:B:68:LYS:HG3	0.45	2.11	1	1
1:B:78:VAL:HG13	1:B:79:GLU:H	0.45	1.71	9	10
1:B:13:GLY:O	1:B:77:GLY:HA2	0.45	2.12	16	2
1:A:19:MET:HA	1:A:23:LEU:HB2	0.45	1.88	5	4
1:B:89:ASN:C	1:B:91:PRO:HD2	0.45	2.36	10	3
1:B:31:ASN:OD1	1:B:33:GLU:HG3	0.45	2.12	18	1
1:B:70:THR:CG2	1:B:74:LYS:HE3	0.45	2.42	14	2
1:B:72:ARG:O	1:B:76:LEU:HG	0.45	2.12	9	3
1:A:31:ASN:HB3	1:A:33:GLU:CD	0.45	2.37	6	1
1:A:49:GLU:OE2	1:B:84:LYS:HD3	0.45	2.11	8	1
1:A:41:TRP:C	1:B:89:ASN:HB3	0.45	2.37	15	3
1:A:99:LYS:HB3	1:B:38:TRP:CD1	0.45	2.47	17	2
1:A:31:ASN:O	1:A:68:LYS:HB3	0.45	2.12	3	1
1:A:69:HIS:HB2	1:A:81:VAL:HG21	0.44	1.87	2	2
1:B:96:ASN:HD22	1:B:96:ASN:C	0.44	2.21	2	1
1:B:6:GLN:HG2	1:B:53:ILE:HD12	0.44	1.89	3	1
1:A:41:TRP:HE1	1:B:96:ASN:CG	0.44	2.20	8	1
1:B:45:GLU:H	1:B:45:GLU:CD	0.44	2.21	16	2
1:B:36:PHE:CD1	1:B:57:THR:HB	0.44	2.48	7	5
1:A:95:ILE:HD12	1:A:95:ILE:N	0.44	2.28	17	1
1:A:70:THR:CG2	1:A:74:LYS:HE3	0.44	2.42	14	3
1:A:40:VAL:HG21	1:A:52:GLY:N	0.44	2.27	4	1
1:B:66:LEU:O	1:B:70:THR:HB	0.44	2.12	19	2
1:A:66:LEU:HD12	1:A:67:GLU:N	0.43	2.27	5	1
1:A:49:GLU:OE2	1:B:86:PHE:HB3	0.43	2.13	7	1
1:A:38:TRP:HB2	1:B:96:ASN:HB2	0.43	1.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LYS:H	1:A:46:LYS:HD3	0.43	1.72	7	1
1:B:22:GLN:HE21	1:B:22:GLN:HA	0.43	1.73	8	1
1:A:7:LEU:HA	1:A:82:VAL:O	0.43	2.14	9	1
1:A:38:TRP:CD1	1:B:99:LYS:HB2	0.43	2.48	20	2
1:B:93:SER:O	1:B:96:ASN:HB3	0.43	2.13	15	2
1:A:66:LEU:O	1:A:70:THR:HB	0.43	2.13	19	1
1:A:70:THR:CG2	1:A:74:LYS:HE2	0.43	2.43	19	1
1:A:28:GLU:O	1:A:32:GLN:HA	0.43	2.14	3	2
1:A:8:HIS:HD2	1:A:49:GLU:CD	0.43	2.22	9	2
1:A:92:LEU:HD21	1:B:19:MET:O	0.43	2.14	10	1
1:B:61:SER:O	1:B:65:TYR:HB2	0.43	2.14	12	1
1:A:9:PHE:HB3	1:A:81:VAL:HA	0.43	1.91	20	1
1:B:68:LYS:N	1:B:68:LYS:HE3	0.42	2.29	9	1
1:A:61:SER:O	1:A:65:TYR:HB2	0.42	2.13	12	1
1:B:73:LEU:HD11	1:B:80:GLU:HA	0.42	1.89	6	1
1:A:38:TRP:CZ2	1:A:55:LEU:HD13	0.42	2.49	5	2
1:B:9:PHE:HB3	1:B:81:VAL:HA	0.42	1.90	16	1
1:A:78:VAL:HG22	1:A:79:GLU:HG3	0.42	1.92	4	1
1:B:7:LEU:HA	1:B:82:VAL:O	0.42	2.14	9	1
1:A:31:ASN:C	1:A:33:GLU:H	0.42	2.22	4	1
1:A:89:ASN:C	1:A:91:PRO:HD2	0.42	2.39	10	2
1:B:47:ASN:ND2	1:B:49:GLU:HB3	0.42	2.30	16	1
1:A:13:GLY:O	1:A:77:GLY:HA2	0.42	2.14	15	3
1:A:65:TYR:HA	1:A:68:LYS:HD2	0.42	1.92	20	1
1:B:59:GLU:OE1	1:B:60:LYS:HG2	0.42	2.15	2	2
1:A:73:LEU:HD11	1:A:80:GLU:HA	0.42	1.92	6	1
1:A:41:TRP:HE1	1:B:96:ASN:ND2	0.42	2.13	15	1
1:A:87:ASP:N	1:B:44:SER:HB3	0.42	2.30	16	1
1:B:66:LEU:HD12	1:B:67:GLU:N	0.42	2.30	20	1
1:A:96:ASN:CG	1:B:41:TRP:HE1	0.41	2.22	8	1
1:A:68:LYS:N	1:A:68:LYS:HE2	0.41	2.30	6	1
1:B:67:GLU:HA	1:B:70:THR:HB	0.41	1.92	5	1
1:B:94:GLN:HB3	1:B:95:ILE:HD12	0.41	1.92	6	1
1:A:100:LEU:HD21	1:B:38:TRP:CE2	0.41	2.50	10	1
1:B:24:LYS:HB2	1:B:25:PRO:HD3	0.41	1.91	13	1
1:B:60:LYS:HG3	1:B:61:SER:N	0.41	2.31	15	1
1:A:31:ASN:ND2	1:A:33:GLU:HB3	0.41	2.30	4	1
1:A:22:GLN:O	1:A:25:PRO:HD2	0.41	2.15	17	1
1:A:70:THR:HG22	1:A:74:LYS:HE2	0.41	1.92	5	1
1:B:83:ALA:C	1:B:84:LYS:HD2	0.41	2.40	6	1
1:A:24:LYS:HB2	1:A:25:PRO:HD3	0.41	1.93	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:59:GLU:O	1:B:62:ALA:HB3	0.41	2.16	8	1
1:A:47:ASN:ND2	1:A:49:GLU:HB3	0.41	2.31	17	1
1:A:63:LEU:H	1:A:63:LEU:HD23	0.41	1.75	4	1
1:A:84:LYS:HG2	1:B:49:GLU:OE1	0.41	2.16	14	1
1:B:37:LEU:HB2	1:B:55:LEU:HB3	0.41	1.93	20	1
1:A:53:ILE:HG13	1:B:53:ILE:CG1	0.41	2.45	4	1
1:A:59:GLU:OE1	1:A:60:LYS:HG2	0.41	2.16	12	1
1:B:65:TYR:HA	1:B:68:LYS:HD2	0.41	1.93	20	1
1:A:89:ASN:HB3	1:B:41:TRP:C	0.41	2.41	8	1
1:B:67:GLU:HA	1:B:70:THR:HG22	0.40	1.91	11	1
1:A:42:THR:HG23	1:B:87:ASP:O	0.40	2.16	8	1
1:B:32:GLN:OE1	1:B:68:LYS:HD2	0.40	2.15	19	1
1:A:10:ALA:HA	1:A:49:GLU:OE1	0.40	2.17	20	1
1:A:59:GLU:O	1:A:62:ALA:HB3	0.40	2.17	8	1
1:B:62:ALA:O	1:B:65:TYR:HB3	0.40	2.17	6	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	99/123 (80%)	83±2 (84±2%)	14±2 (14±2%)	2±1 (2±1%)	7	47
1	B	99/123 (80%)	83±2 (84±2%)	14±2 (14±2%)	2±1 (2±1%)	9	52
All	All	3960/4920 (80%)	3313 (84%)	568 (14%)	79 (2%)	8	49

All 11 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	34	PRO	17
1	A	78	VAL	16
1	B	34	PRO	16
1	B	78	VAL	13
1	A	25	PRO	5
1	A	90	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	90	GLU	3
1	B	25	PRO	3
1	A	32	GLN	1
1	A	14	PRO	1
1	B	14	PRO	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	83/102 (81%)	76±2 (92±2%)	7±2 (8±2%)	13	61
1	B	83/102 (81%)	77±2 (92±2%)	6±2 (8±2%)	14	62
All	All	3320/4080 (81%)	3063 (92%)	257 (8%)	14	61

All 50 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	5	LEU	20
1	B	5	LEU	20
1	A	46	LYS	16
1	B	46	LYS	15
1	A	59	GLU	13
1	B	59	GLU	13
1	A	68	LYS	8
1	A	23	LEU	8
1	A	37	LEU	8
1	B	23	LEU	7
1	B	74	LYS	7
1	B	37	LEU	7
1	A	84	LYS	6
1	B	70	THR	6
1	B	84	LYS	6
1	A	33	GLU	6
1	A	45	GLU	6
1	A	74	LYS	6
1	B	45	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	68	LYS	5
1	A	70	THR	5
1	B	33	GLU	4
1	A	72	ARG	4
1	B	72	ARG	4
1	B	90	GLU	4
1	A	92	LEU	4
1	B	32	GLN	3
1	A	69	HIS	3
1	B	67	GLU	3
1	B	69	HIS	3
1	B	92	LEU	3
1	A	96	ASN	2
1	A	1	MET	2
1	A	100	LEU	2
1	B	100	LEU	2
1	A	90	GLU	2
1	B	99	LYS	2
1	A	32	GLN	2
1	A	24	LYS	2
1	B	24	LYS	2
1	A	99	LYS	2
1	B	96	ASN	1
1	A	80	GLU	1
1	B	80	GLU	1
1	B	22	GLN	1
1	B	41	TRP	1
1	A	39	LYS	1
1	A	95	ILE	1
1	B	39	LYS	1
1	A	67	GLU	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 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