



Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 07:07 pm GMT

PDB ID : 1IML
Title : CYSTEINE RICH INTESTINAL PROTEIN, NMR, 48 STRUCTURES
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Deposited on : 1995-12-23

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 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
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

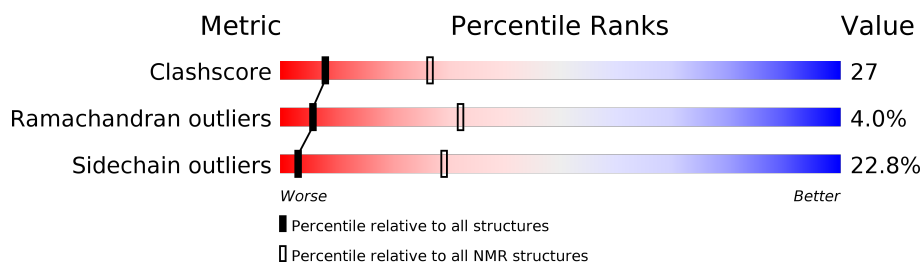
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	76	

2 Ensemble composition and analysis

This entry contains 48 models. Model 28 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:1-A:58 (58)	0.43	28

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 8 clusters and 11 single-model clusters were found.

Cluster number	Models
1	1, 8, 9, 10, 11, 18, 19, 25, 28, 35
2	3, 4, 5, 6, 7, 13, 23, 24
3	12, 15, 17, 31, 36
4	2, 20, 22, 34
5	21, 27, 29
6	26, 32, 33
7	38, 45
8	16, 30
Single-model clusters	14; 37; 39; 40; 41; 42; 43; 44; 46; 47; 48

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1150 atoms, of which 560 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYSTEINE RICH INTESTINAL PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1148	368	560	107	105	8	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

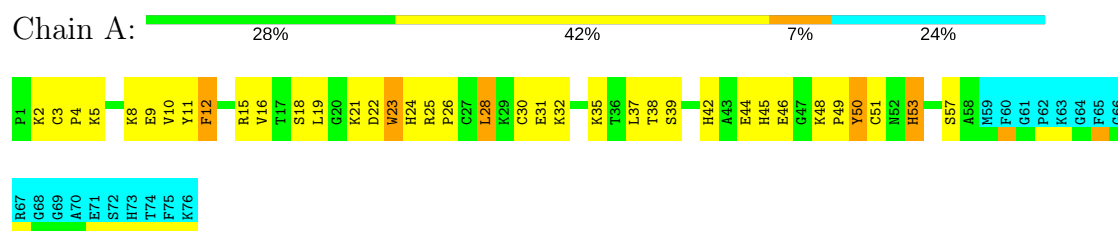
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: CYSTEINE RICH INTESTINAL PROTEIN

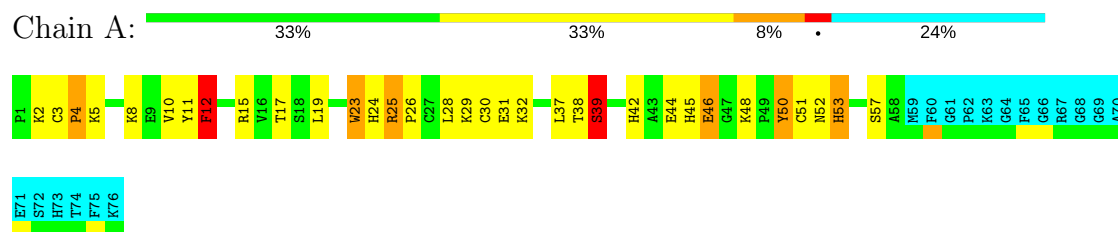


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

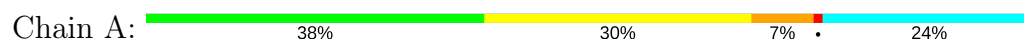
4.2.1 Score per residue for model 1

• Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.2 Score per residue for model 2

• Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

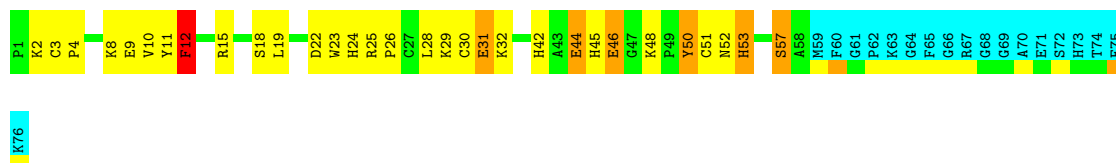




4.2.3 Score per residue for model 3

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

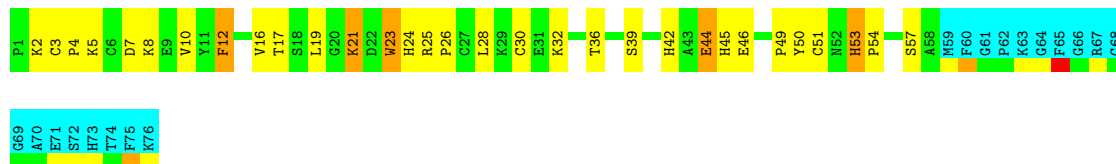
Chain A: 36% 32% 8% 24%



4.2.4 Score per residue for model 4

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

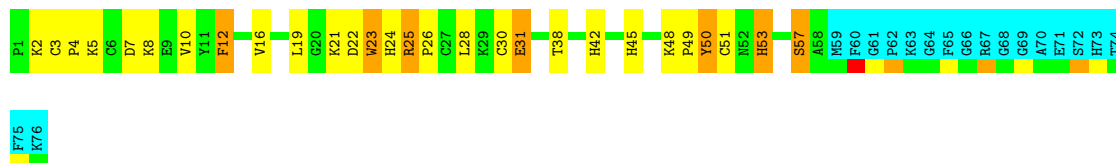
Chain A: 36% 34% 7% 24%



4.2.5 Score per residue for model 5

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

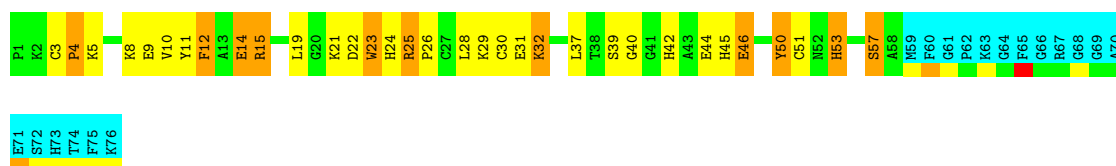
Chain A: 39% 28% 9% 24%



4.2.6 Score per residue for model 6

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

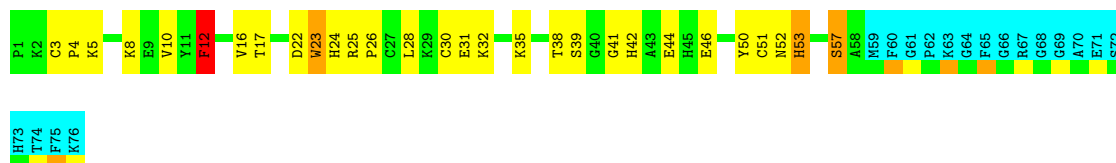
Chain A: 33% 29% 14% 24%



4.2.7 Score per residue for model 7

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

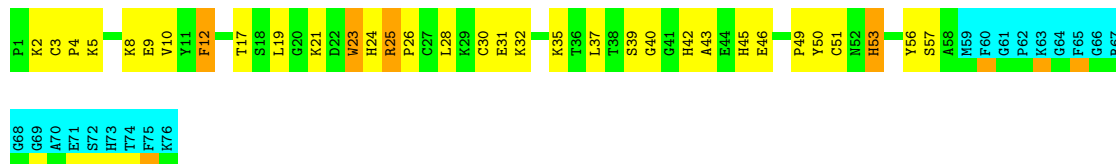
Chain A: 38% 33% • • 24%



4.2.8 Score per residue for model 8

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

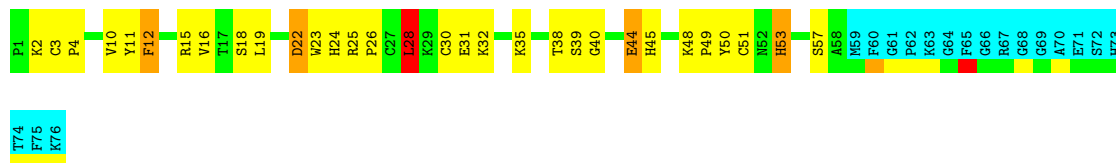
Chain A: 33% 38% 5% 24%



4.2.9 Score per residue for model 9

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

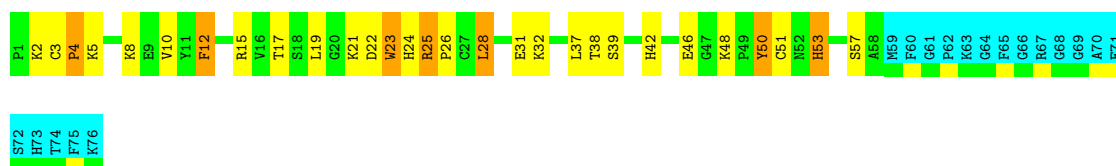
Chain A: 36% 34% 5% • 24%

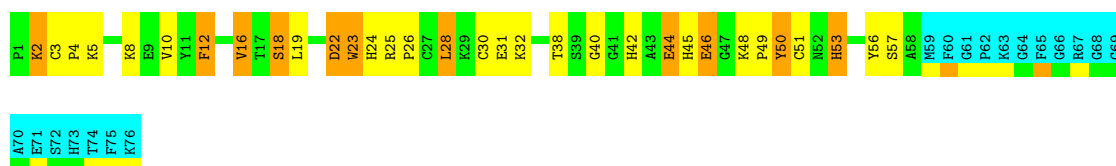


4.2.10 Score per residue for model 10

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

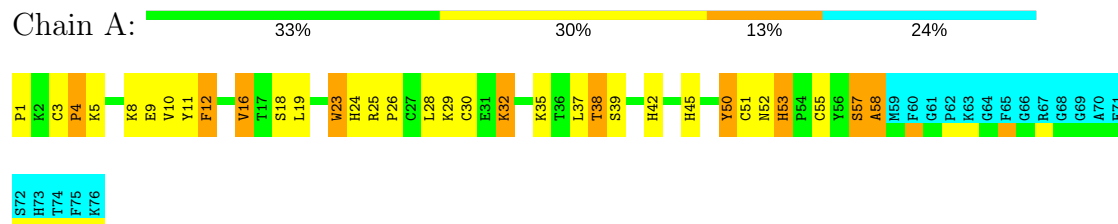
Chain A: 38% 29% 9% 24%





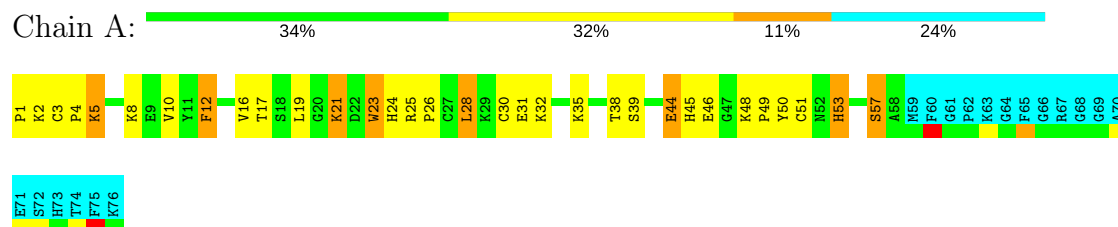
4.2.15 Score per residue for model 15

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



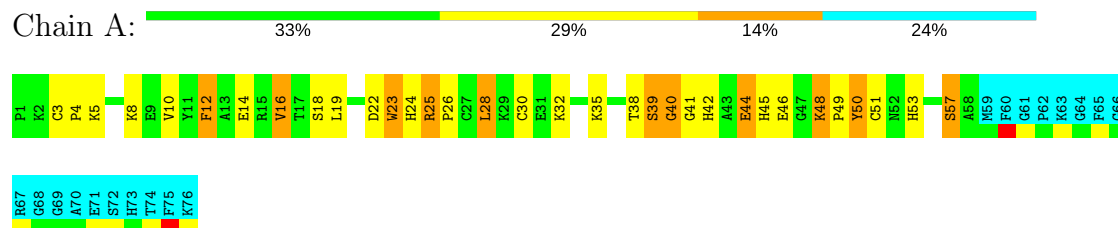
4.2.16 Score per residue for model 16

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.17 Score per residue for model 17

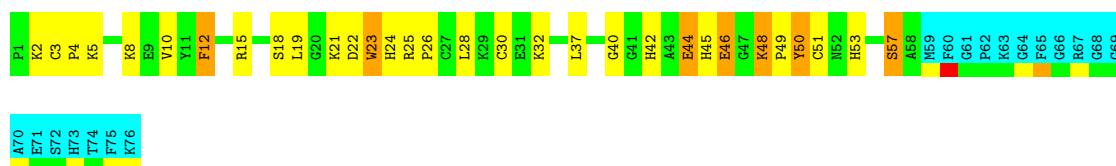
- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.18 Score per residue for model 18

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

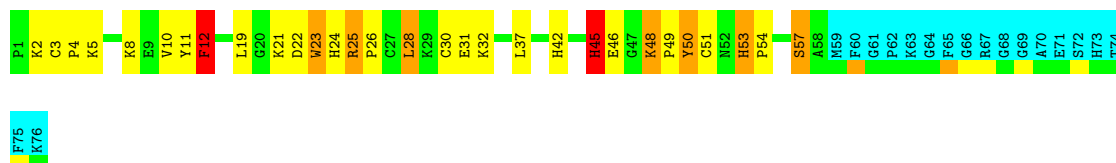




4.2.19 Score per residue for model 19

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

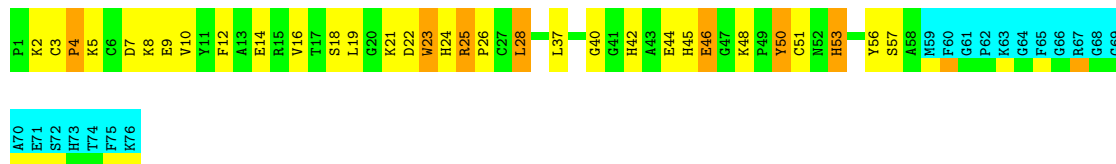
Chain A: 37% 28% 9% • 24%



4.2.20 Score per residue for model 20

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

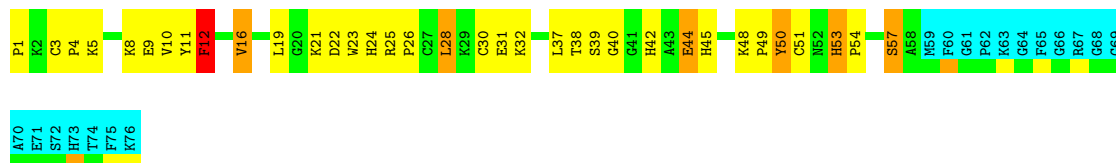
Chain A: 34% 33% 9% 24%



4.2.21 Score per residue for model 21

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

Chain A: 30% 37% 8% • 24%



4.2.22 Score per residue for model 22

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

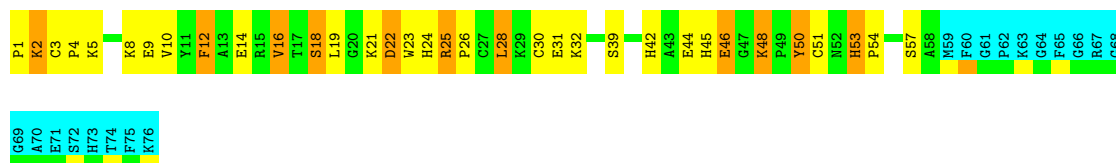
Chain A: 38% 32% 5% • 24%



4.2.23 Score per residue for model 23

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

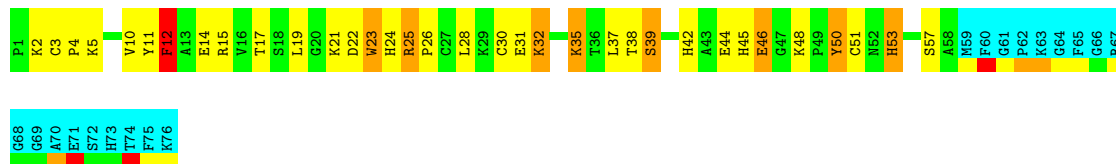
Chain A: 32% 30% 14% 24%



4.2.24 Score per residue for model 24

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

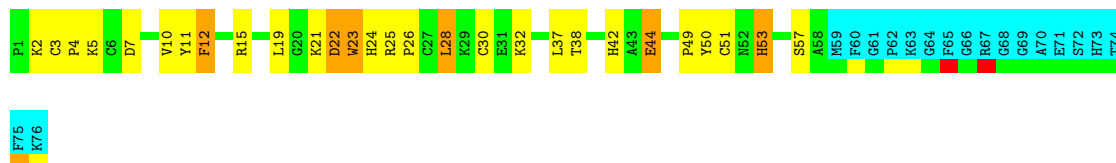
Chain A: 32% 33% 11% 24%



4.2.25 Score per residue for model 25

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

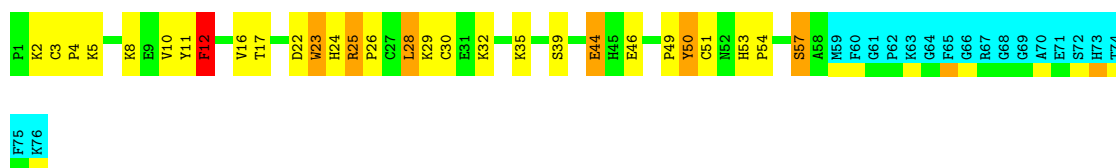
Chain A: 39% 29% 8% 24%



4.2.26 Score per residue for model 26

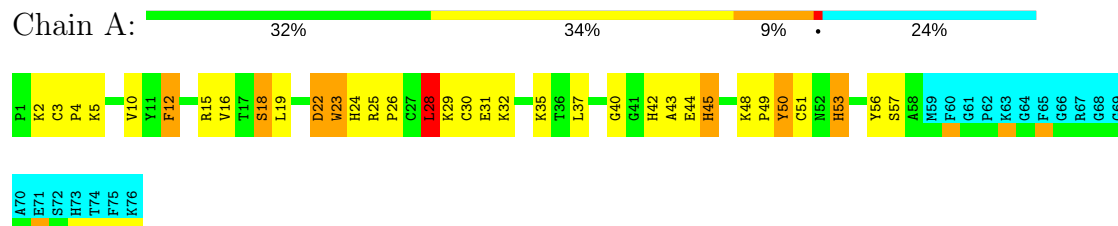
- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

Chain A: 38% 29% 8% 24%



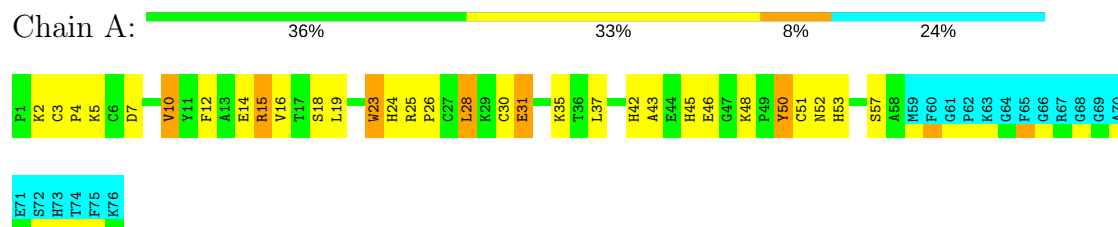
4.2.27 Score per residue for model 27

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



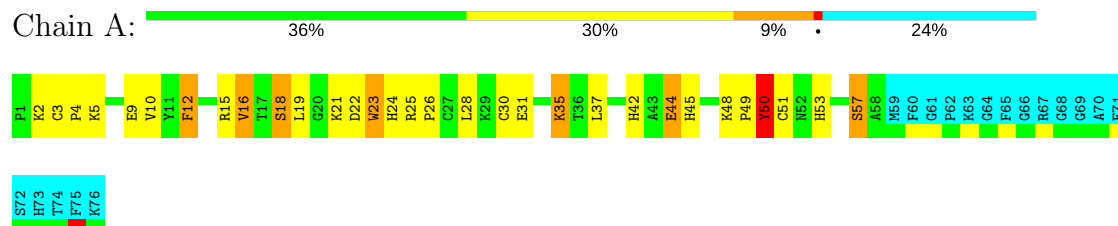
4.2.28 Score per residue for model 28 (medoid)

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.29 Score per residue for model 29

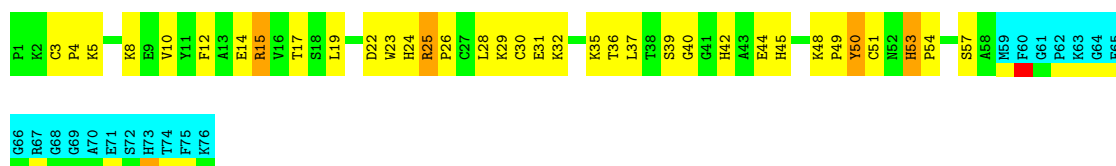
- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.30 Score per residue for model 30

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

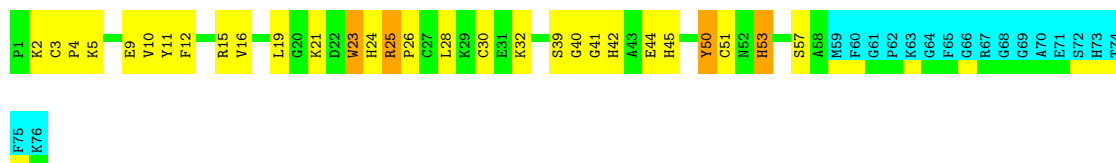




4.2.31 Score per residue for model 31

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

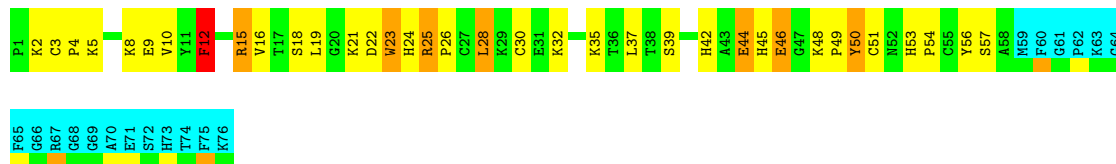
Chain A: 38% 33% 5% 24%



4.2.32 Score per residue for model 32

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

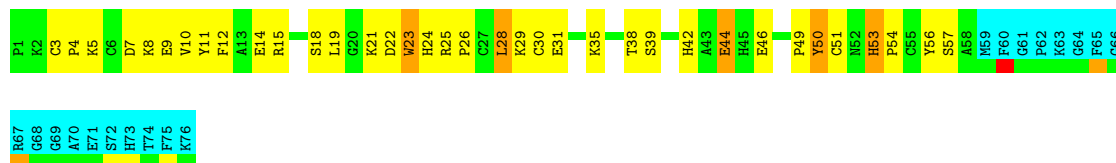
Chain A: 29% 37% 9% 24%



4.2.33 Score per residue for model 33

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

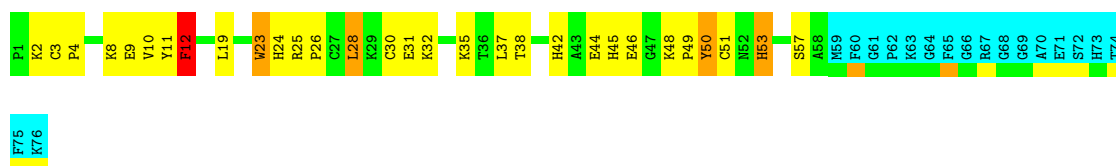
Chain A: 29% 41% 7% 24%



4.2.34 Score per residue for model 34

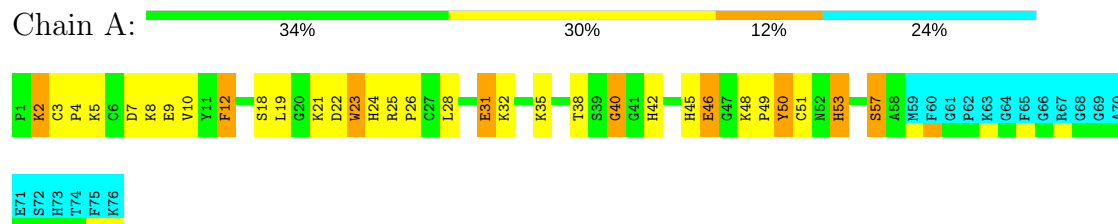
- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

Chain A: 37% 33% 5% 24%



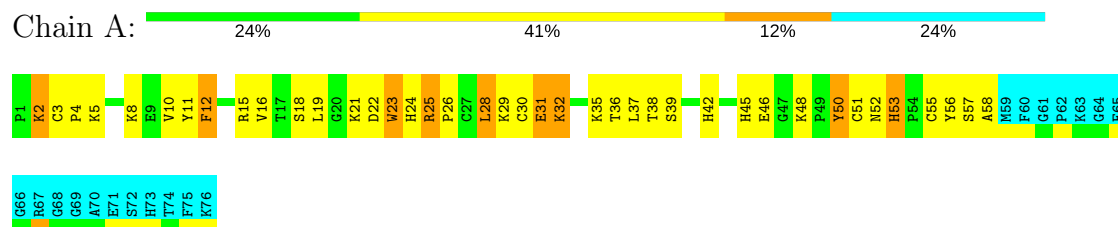
4.2.35 Score per residue for model 35

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



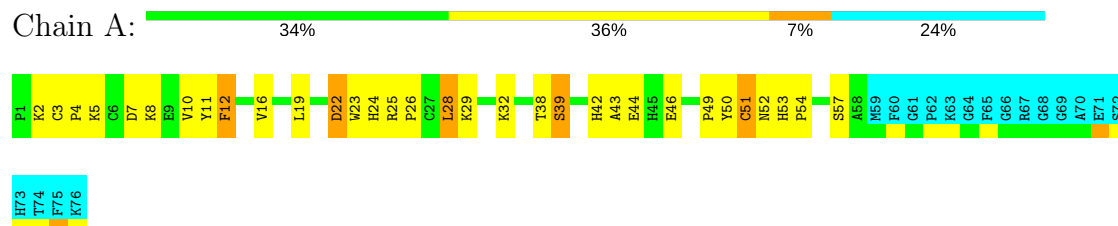
4.2.36 Score per residue for model 36

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.37 Score per residue for model 37

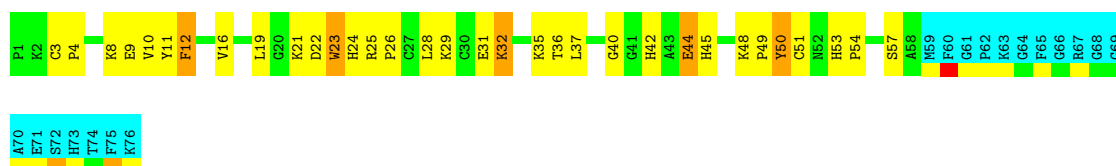
- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN



4.2.38 Score per residue for model 38

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

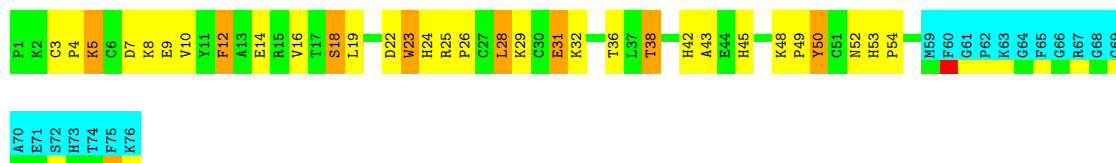




4.2.39 Score per residue for model 39

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

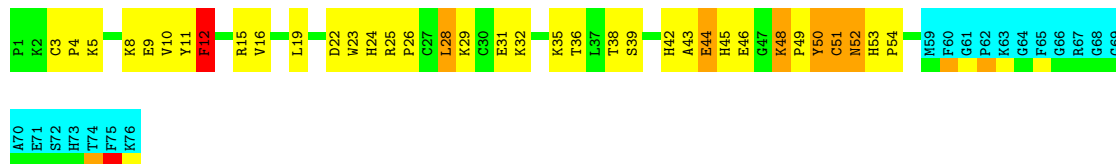
Chain A: 34% 32% 11% 24%



4.2.40 Score per residue for model 40

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

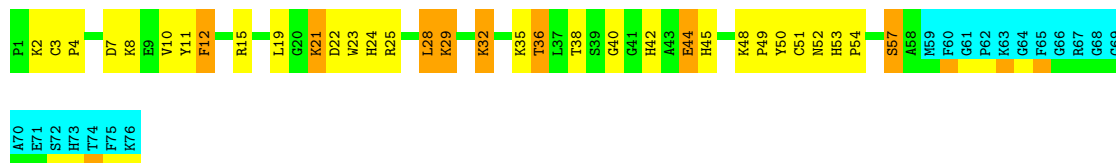
Chain A: 29% 38% 8% 24%



4.2.41 Score per residue for model 41

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

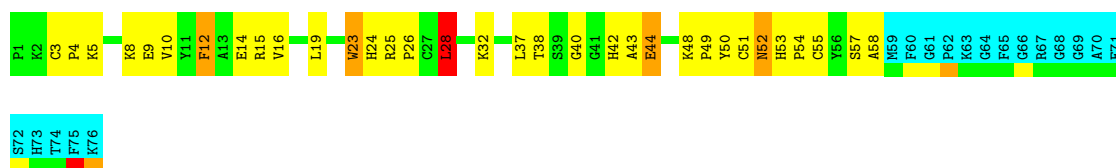
Chain A: 33% 33% 11% 24%



4.2.42 Score per residue for model 42

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

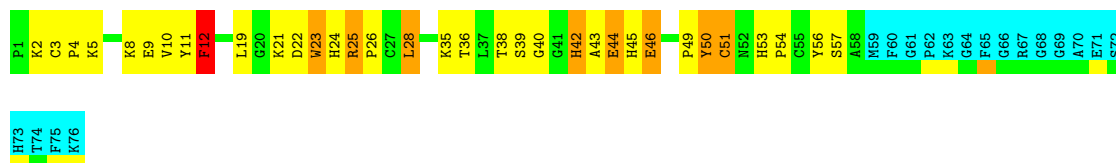
Chain A: 33% 37% 5% 24%



4.2.43 Score per residue for model 43

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

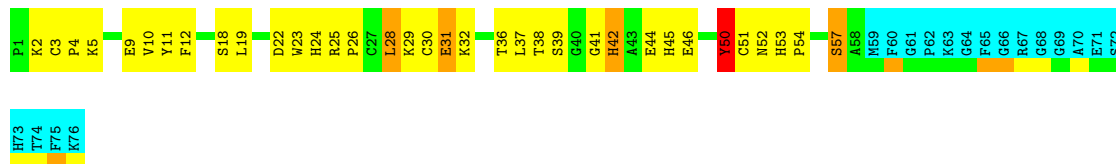
Chain A: 32% 33% 11% • 24%



4.2.44 Score per residue for model 44

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

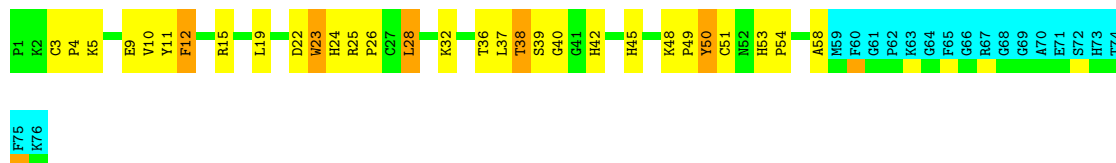
Chain A: 30% 39% 5% • 24%



4.2.45 Score per residue for model 45

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

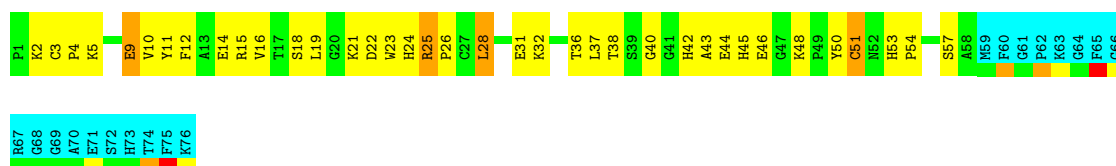
Chain A: 37% 33% 7% 24%



4.2.46 Score per residue for model 46

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

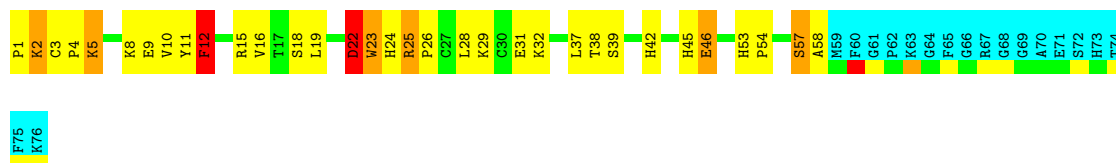
Chain A: 28% 43% 5% 24%



4.2.47 Score per residue for model 47

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

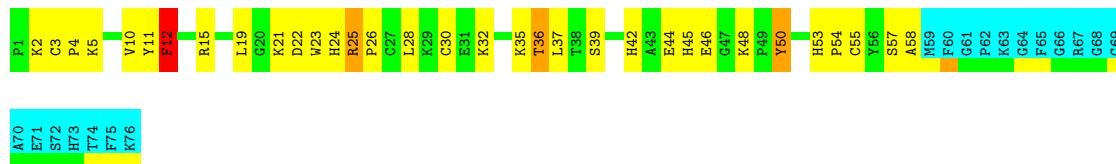
Chain A: 33% 33% 8% 24%



4.2.48 Score per residue for model 48

- Molecule 1: CYSTEINE RICH INTESTINAL PROTEIN

Chain A: 33% 38% 24%



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 48 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DSPACE	refinement	

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

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.58±0.01	0±0/468 (0.0±0.0%)	0.92±0.01	1±0/630 (0.2±0.0%)
All	All	0.58	0/22464 (0.0%)	0.92	46/30240 (0.2%)

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	5.3±2.3
All	All	0	256

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	12	PHE	CB-CG-CD2	-6.24	116.43	120.80	40	32
1	A	12	PHE	CB-CG-CD1	-5.61	116.87	120.80	25	14

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	50	TYR	Mainchain	45
1	A	51	CYS	Mainchain	37
1	A	23	TRP	Mainchain	37
1	A	30	CYS	Mainchain	31

Continued on next page...

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	53	HIS	Mainchain	30
1	A	12	PHE	Mainchain	28
1	A	22	ASP	Mainchain	16
1	A	16	VAL	Mainchain	9
1	A	18	SER	Mainchain	3
1	A	40	GLY	Mainchain	3
1	A	41	GLY	Mainchain	3
1	A	11	TYR	Mainchain	2
1	A	52	ASN	Mainchain	2
1	A	58	ALA	Mainchain	2
1	A	10	VAL	Mainchain	1
1	A	44	GLU	Mainchain	1
1	A	45	HIS	Mainchain	1
1	A	15	ARG	Mainchain	1
1	A	14	GLU	Mainchain	1
1	A	32	LYS	Mainchain	1
1	A	38	THR	Mainchain	1
1	A	39	SER	Mainchain	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	453	432	430	24±5
All	All	21840	20736	20640	1137

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD11	1:A:42:HIS:CE1	0.87	2.05	15	28
1:A:28:LEU:HD21	1:A:42:HIS:CD2	0.86	2.05	46	14
1:A:28:LEU:HD21	1:A:42:HIS:NE2	0.85	1.86	41	23
1:A:16:VAL:HG21	1:A:28:LEU:HD22	0.83	1.49	17	21
1:A:10:VAL:HG22	1:A:24:HIS:CD2	0.82	2.10	48	48

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:HG22	1:A:24:HIS:NE2	0.82	1.89	45	48
1:A:28:LEU:HD21	1:A:42:HIS:CE1	0.79	2.12	14	11
1:A:37:LEU:HD13	1:A:42:HIS:CG	0.78	2.14	44	2
1:A:10:VAL:HG12	1:A:15:ARG:HG2	0.74	1.58	28	1
1:A:43:ALA:HB2	1:A:52:ASN:ND2	0.74	1.98	40	2
1:A:19:LEU:HD23	1:A:44:GLU:OE2	0.73	1.83	9	1
1:A:37:LEU:HD13	1:A:42:HIS:CB	0.72	2.14	20	21
1:A:37:LEU:HD13	1:A:42:HIS:HB2	0.72	1.60	12	17
1:A:43:ALA:HB2	1:A:52:ASN:OD1	0.70	1.86	39	1
1:A:16:VAL:CG2	1:A:28:LEU:HD22	0.69	2.18	39	14
1:A:19:LEU:HD23	1:A:44:GLU:HG2	0.69	1.62	27	5
1:A:37:LEU:HD22	1:A:42:HIS:HB3	0.69	1.65	44	3
1:A:28:LEU:HD21	1:A:42:HIS:CG	0.67	2.24	46	1
1:A:28:LEU:HD11	1:A:42:HIS:NE2	0.66	2.05	48	4
1:A:10:VAL:HG12	1:A:15:ARG:HB3	0.65	1.68	30	4
1:A:19:LEU:HD23	1:A:44:GLU:CD	0.65	2.12	9	1
1:A:28:LEU:HD23	1:A:37:LEU:O	0.65	1.91	25	2
1:A:10:VAL:HG12	1:A:15:ARG:CB	0.64	2.24	45	4
1:A:19:LEU:N	1:A:19:LEU:HD22	0.62	2.10	14	23
1:A:19:LEU:HD22	1:A:19:LEU:N	0.61	2.10	46	14
1:A:38:THR:HG22	1:A:39:SER:OG	0.61	1.95	7	1
1:A:37:LEU:HD13	1:A:42:HIS:HB3	0.61	1.72	48	5
1:A:38:THR:HG22	1:A:40:GLY:H	0.61	1.55	17	1
1:A:10:VAL:HG12	1:A:15:ARG:CG	0.60	2.27	28	1
1:A:28:LEU:HD11	1:A:42:HIS:HE1	0.59	1.55	32	4
1:A:10:VAL:HG13	1:A:14:GLU:O	0.59	1.98	33	3
1:A:54:PRO:O	1:A:58:ALA:HB2	0.58	1.99	47	1
1:A:55:CYS:O	1:A:58:ALA:HB3	0.58	1.98	15	4
1:A:35:LYS:HE3	1:A:37:LEU:HD23	0.58	1.76	29	1
1:A:38:THR:HG23	1:A:40:GLY:H	0.56	1.60	14	3
1:A:19:LEU:HD23	1:A:44:GLU:OE1	0.55	2.01	24	1
1:A:18:SER:OG	1:A:19:LEU:HD13	0.55	2.02	3	1
1:A:43:ALA:HB3	1:A:51:CYS:O	0.54	2.03	40	4
1:A:19:LEU:HD21	1:A:43:ALA:HA	0.53	1.80	27	1
1:A:10:VAL:HG11	1:A:23:TRP:O	0.53	2.04	13	32
1:A:25:ARG:HH12	1:A:36:THR:HG21	0.53	1.63	4	1
1:A:19:LEU:HD21	1:A:44:GLU:OE1	0.52	2.04	18	1
1:A:19:LEU:HD23	1:A:44:GLU:CG	0.52	2.34	3	2
1:A:43:ALA:HB2	1:A:52:ASN:HD22	0.52	1.64	28	1
1:A:38:THR:HG22	1:A:39:SER:N	0.52	2.19	1	5
1:A:31:GLU:HG3	1:A:50:TYR:CE2	0.52	2.39	22	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:SER:OG	1:A:42:HIS:HE1	0.51	1.88	33	2
1:A:25:ARG:NH1	1:A:36:THR:HG21	0.51	2.20	4	1
1:A:4:PRO:HG2	1:A:23:TRP:CZ2	0.51	2.41	40	40
1:A:43:ALA:HB1	1:A:56:TYR:CE1	0.51	2.40	43	1
1:A:25:ARG:N	1:A:26:PRO:HD2	0.51	2.21	24	31
1:A:23:TRP:CD2	1:A:28:LEU:HD12	0.51	2.41	9	2
1:A:45:HIS:CD2	1:A:50:TYR:CE1	0.50	3.00	32	4
1:A:4:PRO:HG2	1:A:23:TRP:CE2	0.50	2.41	40	28
1:A:11:TYR:CE2	1:A:12:PHE:CE1	0.50	3.00	45	1
1:A:11:TYR:CE2	1:A:12:PHE:CZ	0.50	3.00	40	2
1:A:28:LEU:HD12	1:A:49:PRO:HG3	0.50	1.84	2	2
1:A:45:HIS:CE1	1:A:56:TYR:CD1	0.50	3.00	27	2
1:A:11:TYR:CZ	1:A:12:PHE:CZ	0.50	3.00	40	1
1:A:23:TRP:CZ3	1:A:49:PRO:HD3	0.50	2.42	34	7
1:A:11:TYR:CD1	1:A:12:PHE:N	0.50	2.80	21	4
1:A:45:HIS:ND1	1:A:50:TYR:CD1	0.49	2.80	43	6
1:A:4:PRO:HB2	1:A:23:TRP:CZ3	0.49	2.43	41	8
1:A:11:TYR:CD2	1:A:12:PHE:N	0.49	2.80	43	1
1:A:45:HIS:NE2	1:A:46:GLU:HG3	0.49	2.23	36	1
1:A:31:GLU:HB2	1:A:50:TYR:CZ	0.49	2.43	21	1
1:A:45:HIS:CE1	1:A:48:LYS:HB2	0.49	2.43	14	3
1:A:11:TYR:CZ	1:A:12:PHE:CE1	0.49	3.00	19	2
1:A:53:HIS:CE1	1:A:57:SER:HB2	0.49	2.43	33	19
1:A:4:PRO:HD2	1:A:23:TRP:CD2	0.49	2.43	47	1
1:A:45:HIS:CE1	1:A:50:TYR:CG	0.49	3.00	43	1
1:A:11:TYR:CZ	1:A:14:GLU:HG3	0.48	2.42	33	2
1:A:4:PRO:HD2	1:A:23:TRP:CE3	0.48	2.44	18	42
1:A:4:PRO:HG2	1:A:23:TRP:CH2	0.48	2.44	19	47
1:A:4:PRO:HB2	1:A:23:TRP:CH2	0.48	2.43	47	1
1:A:53:HIS:ND1	1:A:57:SER:HB2	0.48	2.23	20	4
1:A:10:VAL:HG22	1:A:24:HIS:CE1	0.48	2.43	38	46
1:A:12:PHE:CZ	1:A:15:ARG:NH2	0.48	2.82	32	1
1:A:45:HIS:CE1	1:A:50:TYR:CD1	0.48	3.02	43	2
1:A:11:TYR:CG	1:A:12:PHE:N	0.48	2.82	43	1
1:A:23:TRP:CZ2	1:A:44:GLU:HG2	0.48	2.44	20	1
1:A:45:HIS:CD2	1:A:46:GLU:HG3	0.48	2.44	36	1
1:A:31:GLU:HB2	1:A:50:TYR:CE2	0.47	2.44	6	4
1:A:3:CYS:HB2	1:A:24:HIS:CE1	0.47	2.44	1	48
1:A:23:TRP:CH2	1:A:49:PRO:HD3	0.47	2.44	41	2
1:A:38:THR:HG23	1:A:39:SER:HB3	0.47	1.85	16	1
1:A:25:ARG:HB3	1:A:26:PRO:HD3	0.47	1.87	3	29

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:SER:HB3	1:A:42:HIS:CE1	0.47	2.45	23	3
1:A:53:HIS:CE1	1:A:57:SER:HB3	0.47	2.45	37	4
1:A:19:LEU:CD2	1:A:44:GLU:HG2	0.47	2.40	17	2
1:A:42:HIS:CE1	1:A:49:PRO:HB3	0.47	2.44	37	2
1:A:23:TRP:CZ3	1:A:49:PRO:HG3	0.46	2.45	11	2
1:A:44:GLU:HA	1:A:49:PRO:HA	0.46	1.87	32	6
1:A:4:PRO:HG2	1:A:23:TRP:CZ3	0.46	2.46	46	22
1:A:25:ARG:CG	1:A:26:PRO:HD3	0.46	2.39	32	3
1:A:35:LYS:HB2	1:A:35:LYS:NZ	0.46	2.26	24	1
1:A:4:PRO:HG3	1:A:21:LYS:HG3	0.46	1.88	41	1
1:A:45:HIS:CE1	1:A:56:TYR:CE1	0.46	3.04	43	1
1:A:37:LEU:HD12	1:A:49:PRO:HB2	0.46	1.88	25	1
1:A:45:HIS:NE2	1:A:48:LYS:HG2	0.46	2.25	16	1
1:A:31:GLU:HB3	1:A:50:TYR:CE2	0.46	2.46	39	6
1:A:11:TYR:CE1	1:A:14:GLU:HG3	0.46	2.45	13	1
1:A:29:LYS:HB3	1:A:29:LYS:NZ	0.46	2.26	41	1
1:A:1:PRO:HA	1:A:22:ASP:HB2	0.46	1.88	47	1
1:A:45:HIS:CE1	1:A:48:LYS:CG	0.45	3.00	13	1
1:A:23:TRP:CH2	1:A:44:GLU:HG3	0.45	2.46	25	2
1:A:25:ARG:N	1:A:26:PRO:CD	0.45	2.80	31	41
1:A:28:LEU:HD21	1:A:42:HIS:HE2	0.45	1.71	33	1
1:A:53:HIS:CE1	1:A:57:SER:CB	0.45	3.00	9	34
1:A:31:GLU:CB	1:A:50:TYR:CE2	0.45	3.00	36	2
1:A:18:SER:CB	1:A:42:HIS:CE1	0.45	3.00	46	5
1:A:53:HIS:CB	1:A:54:PRO:HA	0.45	2.42	47	19
1:A:23:TRP:CD2	1:A:28:LEU:CD1	0.45	3.00	44	5
1:A:31:GLU:CG	1:A:50:TYR:CE2	0.45	3.00	46	5
1:A:25:ARG:CB	1:A:26:PRO:HD3	0.45	2.42	48	2
1:A:25:ARG:HD3	1:A:26:PRO:HD3	0.45	1.88	24	2
1:A:21:LYS:HG2	1:A:22:ASP:N	0.45	2.27	10	1
1:A:53:HIS:ND1	1:A:57:SER:CB	0.45	2.80	2	1
1:A:48:LYS:HG3	1:A:50:TYR:CE1	0.45	2.47	18	2
1:A:45:HIS:NE2	1:A:46:GLU:CG	0.45	2.80	36	1
1:A:38:THR:CG2	1:A:39:SER:N	0.45	2.80	1	3
1:A:11:TYR:CZ	1:A:14:GLU:CG	0.45	3.00	13	2
1:A:11:TYR:CE1	1:A:14:GLU:CG	0.45	3.00	13	1
1:A:45:HIS:CE1	1:A:48:LYS:CB	0.45	3.00	40	3
1:A:2:LYS:N	1:A:2:LYS:CD	0.45	2.80	23	1
1:A:19:LEU:N	1:A:19:LEU:CD2	0.45	2.80	41	6
1:A:53:HIS:CG	1:A:57:SER:HB2	0.45	2.47	2	1
1:A:19:LEU:CD2	1:A:19:LEU:N	0.44	2.80	46	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ALA:CB	1:A:56:TYR:CD2	0.44	3.00	13	2
1:A:2:LYS:CD	1:A:2:LYS:N	0.44	2.80	36	1
1:A:37:LEU:CD1	1:A:49:PRO:HB2	0.44	2.43	27	5
1:A:25:ARG:HB2	1:A:26:PRO:HD3	0.44	1.89	27	3
1:A:18:SER:CB	1:A:42:HIS:NE2	0.44	2.80	36	1
1:A:4:PRO:HG2	1:A:23:TRP:CD2	0.44	2.48	40	3
1:A:43:ALA:CB	1:A:56:TYR:CD1	0.44	3.00	43	1
1:A:48:LYS:HD2	1:A:48:LYS:N	0.44	2.28	38	1
1:A:18:SER:C	1:A:19:LEU:HD22	0.44	2.33	23	5
1:A:5:LYS:CE	1:A:49:PRO:HD2	0.44	2.42	17	1
1:A:38:THR:HG22	1:A:39:SER:H	0.44	1.72	33	4
1:A:53:HIS:HB3	1:A:54:PRO:HA	0.44	1.90	48	15
1:A:31:GLU:CB	1:A:50:TYR:CE1	0.44	3.00	44	1
1:A:2:LYS:HG2	1:A:9:GLU:HB3	0.44	1.90	46	1
1:A:19:LEU:HD23	1:A:44:GLU:HG3	0.44	1.88	29	1
1:A:1:PRO:HB2	1:A:22:ASP:HB2	0.44	1.90	23	1
1:A:5:LYS:HB2	1:A:23:TRP:CZ3	0.43	2.48	47	2
1:A:5:LYS:N	1:A:23:TRP:CZ3	0.43	2.86	47	1
1:A:45:HIS:NE2	1:A:48:LYS:HB2	0.43	2.28	13	1
1:A:2:LYS:HG2	1:A:21:LYS:NZ	0.43	2.28	35	1
1:A:5:LYS:HE3	1:A:48:LYS:HD3	0.43	1.89	16	1
1:A:28:LEU:HA	1:A:49:PRO:HG2	0.43	1.89	19	1
1:A:45:HIS:CD2	1:A:46:GLU:CG	0.43	3.01	36	1
1:A:31:GLU:HB2	1:A:50:TYR:CE1	0.43	2.49	44	1
1:A:32:LYS:CG	1:A:50:TYR:CE2	0.43	3.01	41	1
1:A:36:THR:HG22	1:A:37:LEU:H	0.43	1.73	48	2
1:A:50:TYR:N	1:A:50:TYR:CD1	0.43	2.87	48	1
1:A:45:HIS:CG	1:A:46:GLU:N	0.43	2.87	3	7
1:A:16:VAL:HG11	1:A:25:ARG:HD3	0.43	1.90	46	1
1:A:19:LEU:CD2	1:A:44:GLU:HB2	0.43	2.44	34	2
1:A:18:SER:HB3	1:A:42:HIS:NE2	0.43	2.28	23	1
1:A:2:LYS:N	1:A:2:LYS:HD2	0.43	2.29	14	1
1:A:25:ARG:NH1	1:A:36:THR:CG2	0.43	2.82	4	1
1:A:11:TYR:CE1	1:A:12:PHE:CE2	0.43	3.07	24	1
1:A:25:ARG:CD	1:A:26:PRO:HD3	0.42	2.44	24	2
1:A:45:HIS:CE1	1:A:50:TYR:HH	0.42	2.32	29	1
1:A:31:GLU:HG2	1:A:50:TYR:CE2	0.42	2.49	46	1
1:A:18:SER:HB2	1:A:23:TRP:NE1	0.42	2.30	23	4
1:A:16:VAL:HG12	1:A:39:SER:OG	0.42	2.14	17	1
1:A:16:VAL:HG21	1:A:28:LEU:CB	0.42	2.44	42	1
1:A:1:PRO:HD3	1:A:21:LYS:NZ	0.42	2.30	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLU:CB	1:A:49:PRO:HA	0.42	2.45	33	9
1:A:18:SER:OG	1:A:19:LEU:HD22	0.42	2.15	36	3
1:A:45:HIS:CE1	1:A:48:LYS:HB3	0.42	2.50	16	1
1:A:38:THR:HG23	1:A:40:GLY:N	0.42	2.30	11	1
1:A:5:LYS:HD3	1:A:49:PRO:HD2	0.42	1.92	17	1
1:A:44:GLU:HB2	1:A:49:PRO:HA	0.42	1.92	33	1
1:A:44:GLU:HG3	1:A:49:PRO:N	0.41	2.31	41	1
1:A:53:HIS:CE1	1:A:57:SER:HG	0.41	2.33	46	1
1:A:44:GLU:CA	1:A:49:PRO:HA	0.41	2.45	32	2
1:A:19:LEU:HG	1:A:44:GLU:HB3	0.41	1.92	38	1
1:A:19:LEU:N	1:A:19:LEU:CD1	0.41	2.84	25	2
1:A:18:SER:HG	1:A:42:HIS:CE1	0.41	2.33	3	2
1:A:2:LYS:HD3	1:A:2:LYS:N	0.41	2.30	23	1
1:A:19:LEU:HG	1:A:44:GLU:HG2	0.41	1.92	6	1
1:A:16:VAL:HG21	1:A:28:LEU:HB2	0.41	1.91	42	1
1:A:14:GLU:HA	1:A:25:ARG:HG2	0.41	1.92	24	1
1:A:31:GLU:HB3	1:A:50:TYR:CZ	0.41	2.49	27	2
1:A:10:VAL:CG2	1:A:24:HIS:NE2	0.41	2.80	37	4
1:A:23:TRP:CG	1:A:28:LEU:HD13	0.41	2.50	39	1
1:A:5:LYS:HD2	1:A:49:PRO:HD2	0.41	1.92	5	1
1:A:19:LEU:HB3	1:A:21:LYS:NZ	0.41	2.31	4	1
1:A:32:LYS:HE2	1:A:50:TYR:CD2	0.41	2.51	38	1
1:A:28:LEU:CD1	1:A:42:HIS:CE1	0.41	3.00	42	1
1:A:29:LYS:HG3	1:A:36:THR:HA	0.41	1.93	30	2
1:A:32:LYS:HE2	1:A:58:ALA:HB2	0.40	1.92	45	1
1:A:11:TYR:CE2	1:A:12:PHE:CE2	0.40	3.09	40	1
1:A:45:HIS:HB2	1:A:48:LYS:HG3	0.40	1.93	17	1
1:A:48:LYS:HB3	1:A:50:TYR:CE1	0.40	2.52	23	1
1:A:45:HIS:ND1	1:A:45:HIS:N	0.40	2.69	19	1
1:A:32:LYS:HB2	1:A:50:TYR:CE1	0.40	2.51	15	1
1:A:25:ARG:HG3	1:A:26:PRO:HD3	0.40	1.93	17	1
1:A:10:VAL:CG1	1:A:15:ARG:CB	0.40	3.00	6	1
1:A:38:THR:CG2	1:A:39:SER:H	0.40	2.29	1	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	57/76 (75%)	45±3 (78±5%)	10±2 (18±4%)	2±1 (4±2%)	6	32
All	All	2736/3648 (75%)	2136 (78%)	491 (18%)	109 (4%)	6	32

All 13 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	28	LEU	31
1	A	46	GLU	20
1	A	40	GLY	16
1	A	39	SER	13
1	A	12	PHE	9
1	A	51	CYS	8
1	A	38	THR	4
1	A	30	CYS	2
1	A	42	HIS	2
1	A	36	THR	1
1	A	22	ASP	1
1	A	41	GLY	1
1	A	2	LYS	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	50/62 (81%)	39±2 (77±5%)	11±2 (23±5%)	3	29
All	All	2400/2976 (81%)	1853 (77%)	547 (23%)	3	29

All 31 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	32	LYS	41
1	A	5	LYS	40
1	A	2	LYS	34
1	A	8	LYS	34

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Mol	Chain	Res	Type	Models (Total)
1	A	44	GLU	30
1	A	48	LYS	28
1	A	21	LYS	26
1	A	22	ASP	25
1	A	15	ARG	25
1	A	9	GLU	24
1	A	35	LYS	23
1	A	25	ARG	22
1	A	31	GLU	18
1	A	46	GLU	17
1	A	29	LYS	17
1	A	57	SER	17
1	A	38	THR	14
1	A	11	TYR	14
1	A	12	PHE	13
1	A	7	ASP	13
1	A	17	THR	10
1	A	39	SER	9
1	A	14	GLU	9
1	A	28	LEU	9
1	A	52	ASN	8
1	A	36	THR	8
1	A	18	SER	6
1	A	4	PRO	5
1	A	50	TYR	4
1	A	1	PRO	2
1	A	45	HIS	2

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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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