



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:57 PM BST

PDB ID : 1MX7
Title : Two homologous rat cellular retinol-binding proteins differ in local structure and flexibility
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Deposited on : 2002-10-01

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

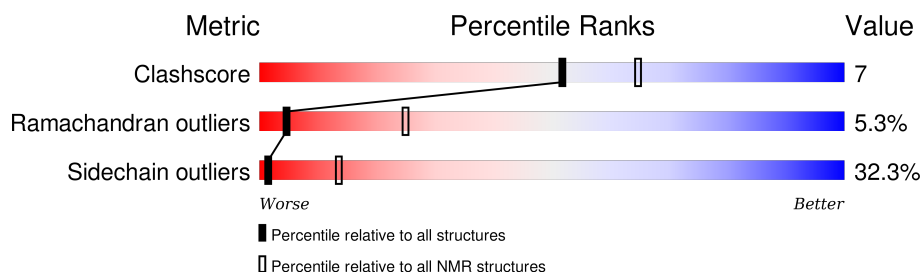
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	134	<div> <div>53%</div> <div>46%</div> <div>.</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 22 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: *closest to the average*.

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:3-A:134 (132)	0.65	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 and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2182 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELLULAR RETINOL-BINDING PROTEIN I, APO.

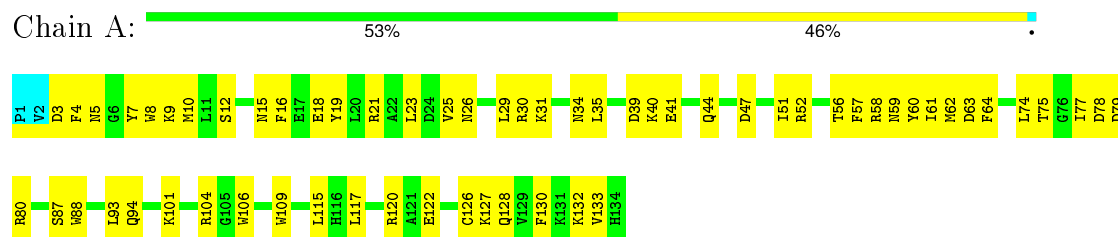
Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2182	695	1080	189	210	8	

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: CELLULAR RETINOL-BINDING PROTEIN I, APO

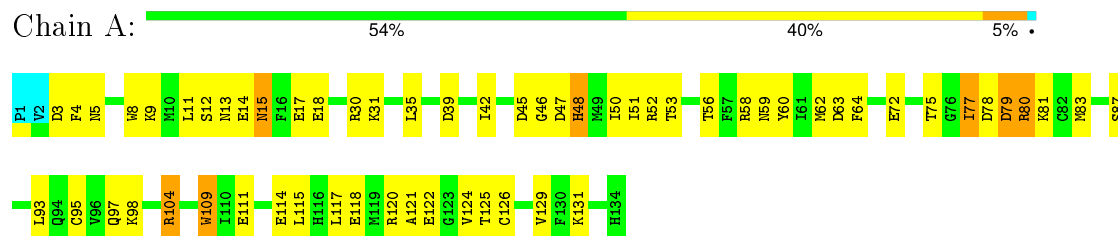


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

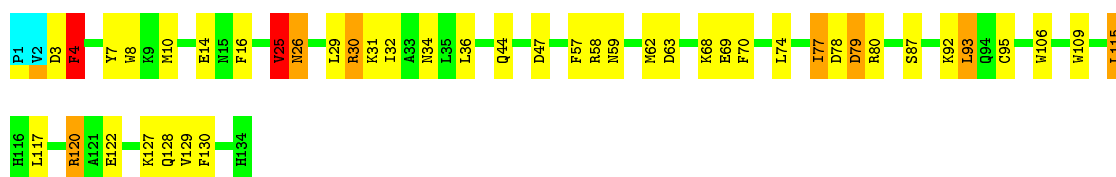
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



4.2.2 Score per residue for model 2

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO

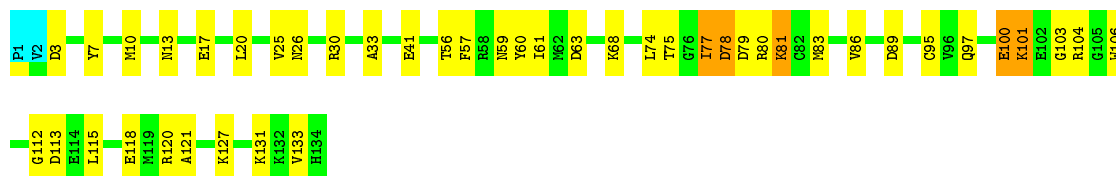




4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO

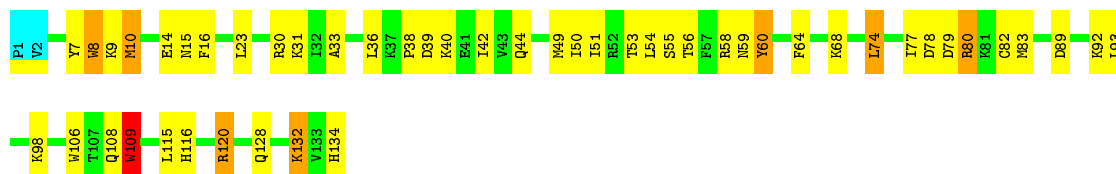
Chain A: 66% 29% ..



4.2.4 Score per residue for model 4

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO

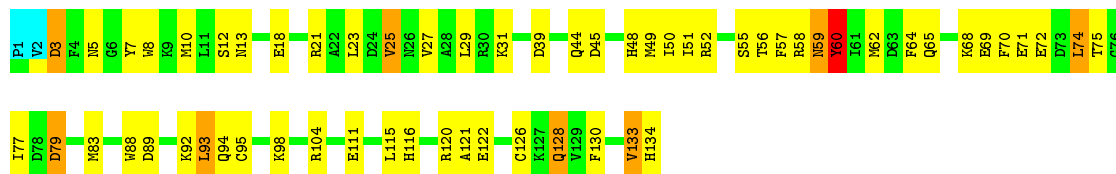
Chain A: 62% 31% 5% ..



4.2.5 Score per residue for model 5

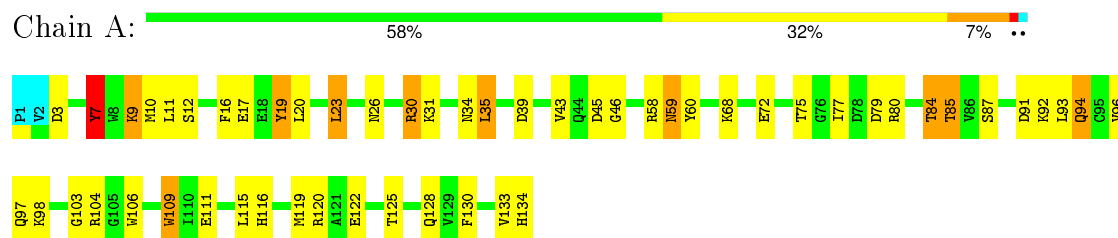
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO

Chain A: 54% 38% 6% ..



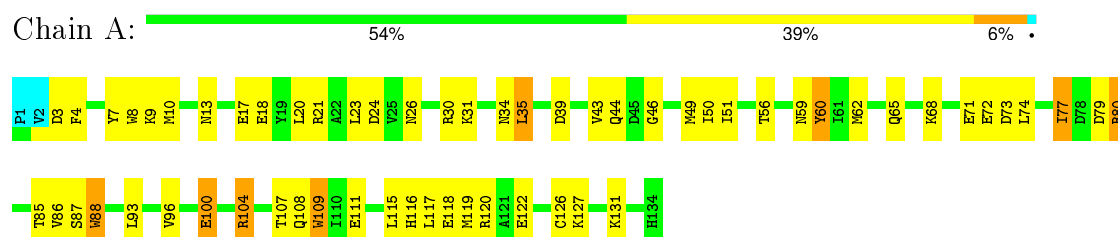
4.2.6 Score per residue for model 6

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



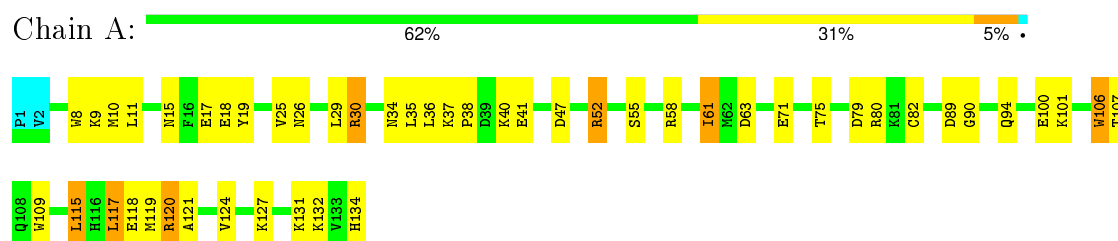
4.2.7 Score per residue for model 7

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



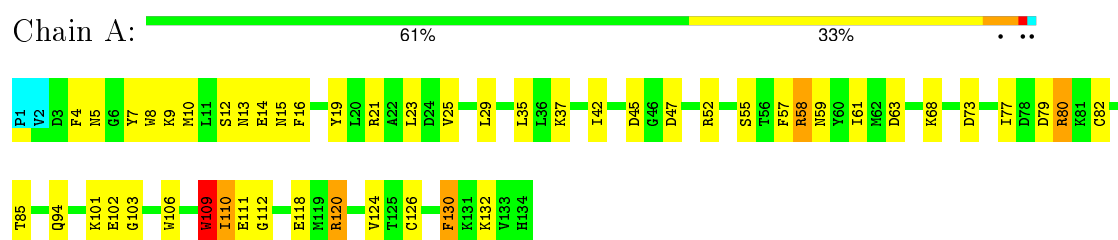
4.2.8 Score per residue for model 8

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



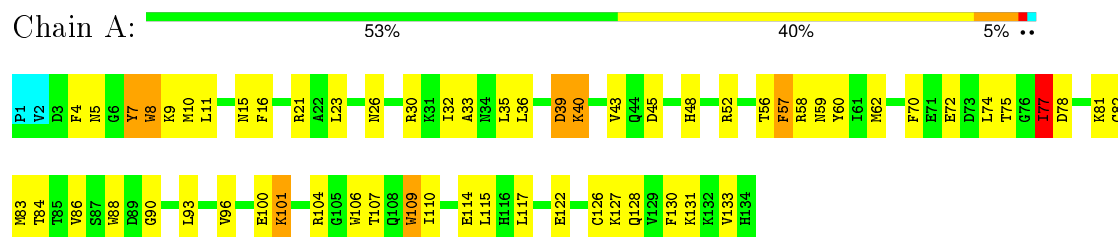
4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



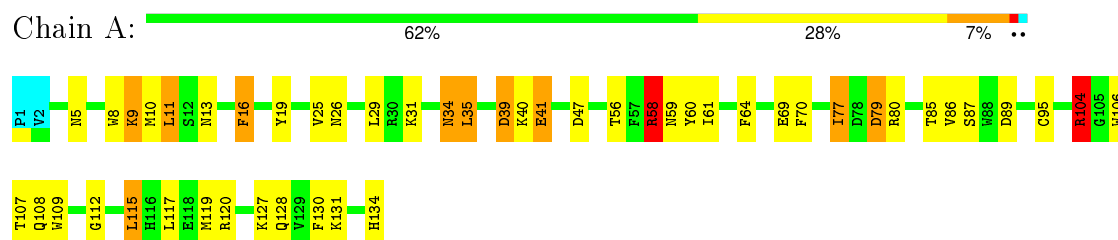
4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



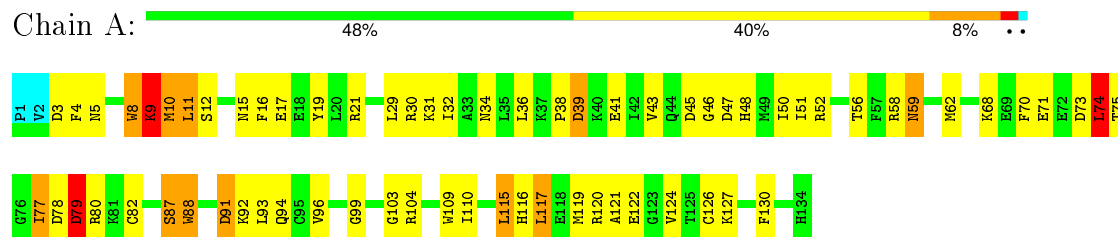
4.2.11 Score per residue for model 11

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



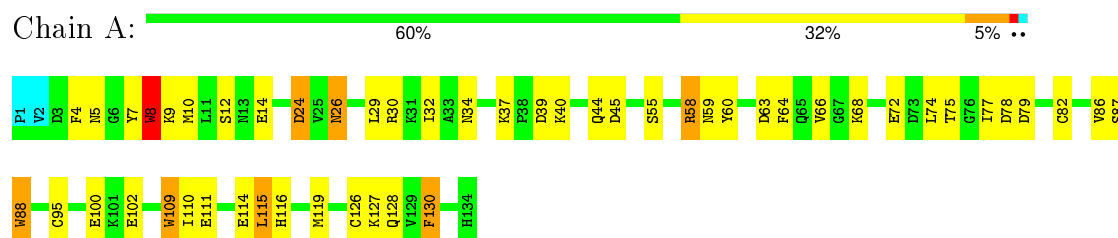
4.2.12 Score per residue for model 12

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



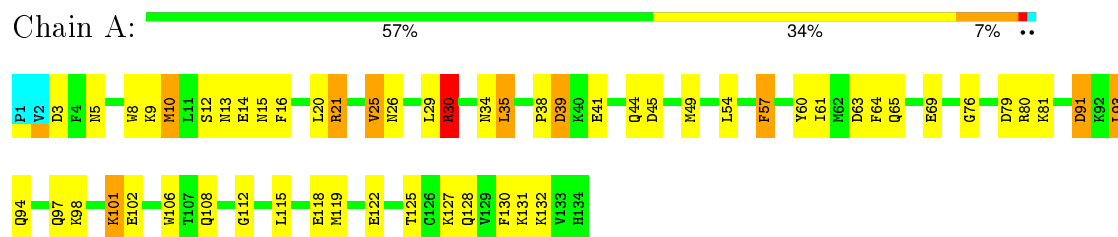
4.2.13 Score per residue for model 13

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



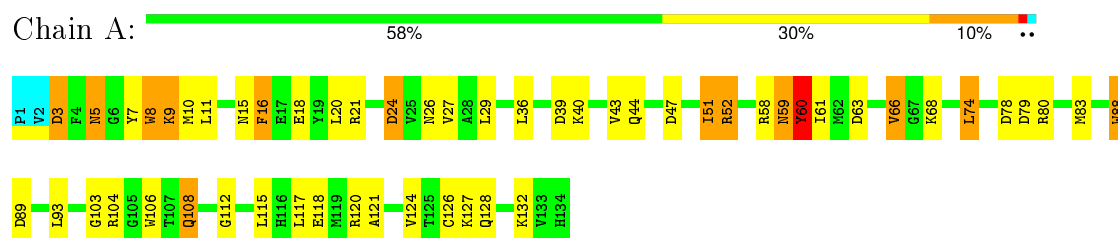
4.2.14 Score per residue for model 14

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



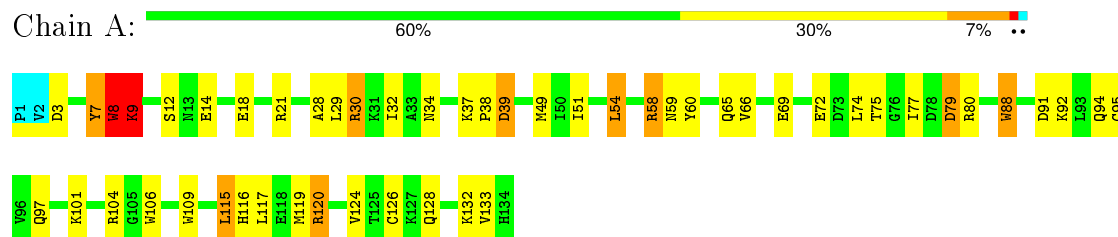
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



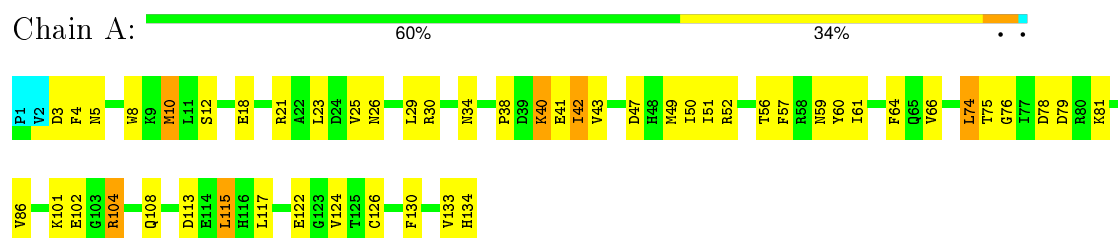
4.2.16 Score per residue for model 16

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



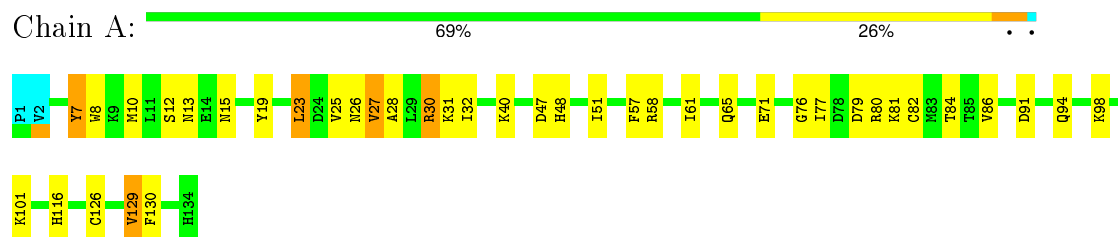
4.2.17 Score per residue for model 17

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



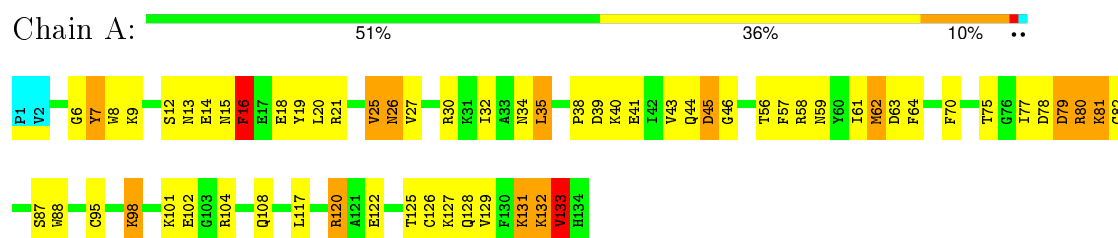
4.2.18 Score per residue for model 18

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



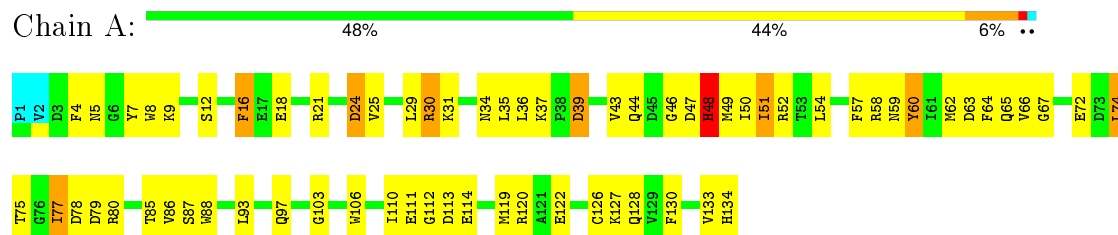
4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



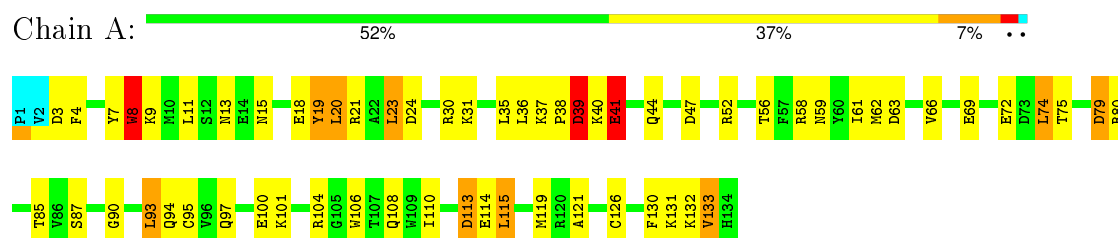
4.2.20 Score per residue for model 20

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



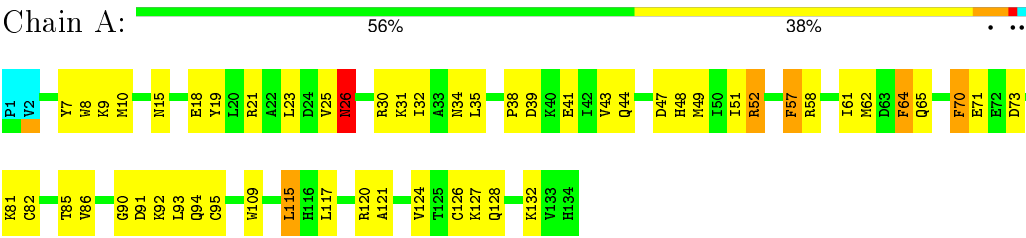
4.2.21 Score per residue for model 21

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



4.2.22 Score per residue for model 22

● Molecule 1: CELLULAR RETINOL-BINDING PROTEIN I, APO



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing*.

Of the 25 calculated structures, 22 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
TINKER	structure solution	3.3
TINKER	refinement	3.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5579
Number of chemical shift lists	1
Total number of shifts	1634
Number of shifts mapped to atoms	1634
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	0.54±0.01	0±0/1108 (0.0±0.0%)	1.27±0.05	5±3/1486 (0.4±0.2%)
All	All	0.54	0/24376 (0.0%)	1.27	116/32692 (0.4%)

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	60	TYR	CB-CG-CD1	10.57	127.34	121.00	5	4
1	A	21	ARG	NE-CZ-NH1	10.13	125.37	120.30	15	5
1	A	30	ARG	NE-CZ-NH1	8.45	124.52	120.30	10	7
1	A	104	ARG	NE-CZ-NH1	8.35	124.47	120.30	12	4
1	A	52	ARG	NE-CZ-NH1	8.32	124.46	120.30	22	3
1	A	120	ARG	NE-CZ-NH1	8.01	124.31	120.30	15	5
1	A	8	TRP	CD1-CG-CD2	-7.50	100.30	106.30	10	3
1	A	30	ARG	NE-CZ-NH2	-7.41	116.59	120.30	2	7
1	A	58	ARG	NE-CZ-NH2	-7.23	116.69	120.30	11	5
1	A	64	PHE	CB-CG-CD1	7.20	125.84	120.80	1	2
1	A	120	ARG	NE-CZ-NH2	-7.11	116.75	120.30	22	7
1	A	16	PHE	CB-CG-CD1	6.96	125.67	120.80	19	5
1	A	88	TRP	CG-CD2-CE3	6.90	140.11	133.90	16	1
1	A	80	ARG	NE-CZ-NH1	6.74	123.67	120.30	21	7
1	A	7	TYR	CB-CG-CD1	-6.68	116.99	121.00	13	3
1	A	60	TYR	CB-CG-CD2	-6.67	117.00	121.00	5	3
1	A	8	TRP	CG-CD2-CE3	6.63	139.87	133.90	16	2
1	A	88	TRP	CE2-CD2-CG	-6.54	102.07	107.30	19	2
1	A	8	TRP	CE2-CD2-CG	6.51	112.51	107.30	10	1
1	A	58	ARG	NE-CZ-NH1	6.49	123.55	120.30	16	2
1	A	52	ARG	NE-CZ-NH2	-6.33	117.13	120.30	20	4
1	A	7	TYR	CB-CG-CD2	-6.22	117.27	121.00	9	3
1	A	45	ASP	CB-CG-OD2	6.15	123.83	118.30	19	3
1	A	104	ARG	NE-CZ-NH2	-6.14	117.23	120.30	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	TRP	CB-CG-CD1	6.02	134.83	127.00	13	1
1	A	89	ASP	CB-CG-OD1	6.01	123.71	118.30	11	2
1	A	21	ARG	NE-CZ-NH2	5.90	123.25	120.30	19	2
1	A	39	ASP	CB-CG-OD1	5.89	123.60	118.30	21	1
1	A	16	PHE	CB-CG-CD2	-5.65	116.85	120.80	15	2
1	A	109	TRP	CD1-CG-CD2	-5.61	101.81	106.30	4	2
1	A	64	PHE	O-C-N	5.58	131.62	122.70	22	1
1	A	38	PRO	CA-N-CD	-5.45	103.88	111.50	21	3
1	A	70	PHE	CB-CG-CD1	-5.44	116.99	120.80	10	1
1	A	79	ASP	CB-CG-OD1	5.39	123.15	118.30	19	1
1	A	109	TRP	CD1-NE1-CE2	5.37	113.84	109.00	10	1
1	A	8	TRP	CB-CA-C	-5.26	99.88	110.40	21	1
1	A	47	ASP	CB-CG-OD1	5.22	123.00	118.30	21	1
1	A	19	TYR	CB-CG-CD1	5.22	124.13	121.00	9	1
1	A	80	ARG	NE-CZ-NH2	-5.21	117.69	120.30	1	1
1	A	4	PHE	CB-CG-CD2	5.17	124.42	120.80	7	1
1	A	88	TRP	CD1-NE1-CE2	-5.17	104.35	109.00	16	1
1	A	64	PHE	CB-CG-CD2	-5.15	117.19	120.80	4	1
1	A	63	ASP	CB-CG-OD1	5.11	122.90	118.30	15	1
1	A	38	PRO	N-CD-CG	-5.00	95.69	103.20	4	1

There are no chirality outliers.

There are no planarity outliers.

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	1088	1062	1059	15±6
All	All	23936	23364	23298	331

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:LEU:HG	1:A:133:VAL:HG11	0.90	1.43	21	1
1:A:64:PHE:CD2	1:A:86:VAL:HG11	0.77	2.15	22	1
1:A:117:LEU:HD21	1:A:119:MET:CE	0.75	2.11	12	1
1:A:25:VAL:HG11	1:A:29:LEU:HD22	0.72	1.61	17	1
1:A:77:ILE:O	1:A:77:ILE:HD12	0.71	1.85	20	1
1:A:115:LEU:CG	1:A:133:VAL:HG11	0.70	2.16	21	1
1:A:115:LEU:HD12	1:A:116:HIS:N	0.69	2.03	16	2
1:A:8:TRP:CE2	1:A:40:LYS:HB2	0.68	2.23	18	1
1:A:8:TRP:CE3	1:A:130:PHE:CE2	0.67	2.83	13	1
1:A:8:TRP:NE1	1:A:42:ILE:HD12	0.65	2.07	9	1
1:A:8:TRP:CG	1:A:9:LYS:N	0.65	2.64	16	1
1:A:8:TRP:CE2	1:A:115:LEU:HD22	0.64	2.28	7	1
1:A:74:LEU:HD13	1:A:74:LEU:O	0.64	1.93	20	2
1:A:74:LEU:HD12	1:A:77:ILE:HG22	0.64	1.67	2	1
1:A:19:TYR:CE1	1:A:23:LEU:HD11	0.63	2.28	6	2
1:A:76:GLY:C	1:A:77:ILE:HD13	0.63	2.14	18	1
1:A:29:LEU:HD13	1:A:29:LEU:O	0.62	1.94	11	1
1:A:121:ALA:O	1:A:124:VAL:HG22	0.62	1.94	8	4
1:A:8:TRP:CZ3	1:A:39:ASP:CB	0.62	2.83	21	3
1:A:115:LEU:HD23	1:A:130:PHE:CG	0.61	2.29	6	1
1:A:8:TRP:CD2	1:A:130:PHE:CD2	0.60	2.88	13	1
1:A:8:TRP:HA	1:A:132:LYS:HB3	0.60	1.72	19	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.60	2.11	7	1
1:A:76:GLY:O	1:A:77:ILE:HD13	0.60	1.95	18	1
1:A:117:LEU:HD21	1:A:119:MET:HE1	0.59	1.73	12	1
1:A:7:TYR:O	1:A:133:VAL:HG12	0.59	1.98	16	1
1:A:20:LEU:HD12	1:A:30:ARG:HG2	0.59	1.73	14	1
1:A:77:ILE:HD13	1:A:77:ILE:N	0.59	2.12	1	3
1:A:8:TRP:CD2	1:A:115:LEU:CD1	0.59	2.85	17	1
1:A:60:TYR:OH	1:A:74:LEU:HD11	0.59	1.98	4	1
1:A:8:TRP:CD2	1:A:115:LEU:HD22	0.58	2.33	7	1
1:A:74:LEU:HD13	1:A:74:LEU:C	0.58	2.19	12	1
1:A:115:LEU:HG	1:A:130:PHE:CE2	0.58	2.33	13	1
1:A:93:LEU:HD13	1:A:94:GLN:N	0.58	2.14	6	1
1:A:34:ASN:O	1:A:35:LEU:HD12	0.57	1.99	6	1
1:A:115:LEU:C	1:A:115:LEU:HD12	0.57	2.19	12	1
1:A:8:TRP:CD1	1:A:40:LYS:C	0.57	2.78	21	2
1:A:8:TRP:CE3	1:A:115:LEU:HD12	0.57	2.35	8	2
1:A:8:TRP:CE3	1:A:39:ASP:HB3	0.57	2.35	20	1
1:A:8:TRP:CZ3	1:A:41:GLU:CG	0.57	2.88	11	2
1:A:8:TRP:CZ3	1:A:39:ASP:HB3	0.56	2.34	15	3
1:A:59:ASN:O	1:A:61:ILE:HD12	0.56	2.01	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:HG2	1:A:61:ILE:HD12	0.56	1.77	15	1
1:A:106:TRP:CE3	1:A:117:LEU:HD11	0.56	2.35	11	2
1:A:32:ILE:HG21	1:A:57:PHE:CE2	0.56	2.36	22	1
1:A:72:GLU:OE2	1:A:74:LEU:HD23	0.56	2.01	21	1
1:A:64:PHE:CD2	1:A:86:VAL:HG21	0.55	2.35	11	2
1:A:26:ASN:ND2	1:A:26:ASN:N	0.55	2.53	2	2
1:A:32:ILE:HD13	1:A:32:ILE:N	0.55	2.16	10	1
1:A:108:GLN:CD	1:A:115:LEU:HD21	0.55	2.21	15	1
1:A:74:LEU:HD12	1:A:77:ILE:CG2	0.55	2.31	2	1
1:A:59:ASN:HD22	1:A:59:ASN:N	0.55	1.98	5	1
1:A:19:TYR:CD2	1:A:20:LEU:HD23	0.54	2.37	6	1
1:A:64:PHE:HD2	1:A:86:VAL:HG11	0.54	1.62	22	1
1:A:8:TRP:CD2	1:A:115:LEU:HD12	0.54	2.38	22	1
1:A:54:LEU:N	1:A:54:LEU:HD22	0.54	2.16	4	1
1:A:117:LEU:C	1:A:117:LEU:HD23	0.54	2.23	15	2
1:A:4:PHE:CD1	1:A:110:ILE:CD1	0.54	2.89	12	1
1:A:88:TRP:CD1	1:A:91:ASP:HA	0.53	2.38	12	1
1:A:8:TRP:CH2	1:A:41:GLU:HB2	0.53	2.39	19	1
1:A:50:ILE:N	1:A:50:ILE:HD12	0.53	2.19	12	1
1:A:8:TRP:CD1	1:A:39:ASP:CB	0.53	2.92	11	2
1:A:8:TRP:CE3	1:A:41:GLU:HA	0.53	2.38	19	2
1:A:29:LEU:O	1:A:29:LEU:HD23	0.53	2.03	8	1
1:A:58:ARG:HG2	1:A:77:ILE:HD11	0.53	1.80	12	1
1:A:110:ILE:HG23	1:A:114:GLU:O	0.53	2.04	10	1
1:A:8:TRP:C	1:A:8:TRP:CD1	0.52	2.83	13	2
1:A:8:TRP:CZ2	1:A:130:PHE:CE1	0.52	2.97	13	1
1:A:50:ILE:C	1:A:51:ILE:HD13	0.52	2.25	5	1
1:A:29:LEU:HD13	1:A:29:LEU:C	0.52	2.25	11	1
1:A:16:PHE:CE2	1:A:33:ALA:HB1	0.52	2.40	4	1
1:A:8:TRP:CZ3	1:A:130:PHE:CZ	0.51	2.98	13	1
1:A:8:TRP:CD2	1:A:115:LEU:CD2	0.51	2.94	7	1
1:A:8:TRP:CE3	1:A:115:LEU:CD1	0.51	2.93	17	1
1:A:117:LEU:HD23	1:A:117:LEU:O	0.51	2.06	22	1
1:A:50:ILE:C	1:A:51:ILE:HD12	0.51	2.26	7	1
1:A:8:TRP:CZ3	1:A:39:ASP:HB2	0.51	2.40	21	1
1:A:8:TRP:CE3	1:A:39:ASP:HB2	0.51	2.41	10	1
1:A:8:TRP:CE2	1:A:115:LEU:HD21	0.51	2.41	1	1
1:A:25:VAL:HG22	1:A:26:ASN:N	0.50	2.21	19	1
1:A:49:MET:CE	1:A:93:LEU:HD11	0.50	2.36	5	1
1:A:8:TRP:CD1	1:A:39:ASP:HB3	0.50	2.41	11	1
1:A:64:PHE:CD1	1:A:70:PHE:CD2	0.50	3.00	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG12	1:A:26:ASN:N	0.50	2.21	3	1
1:A:49:MET:HE2	1:A:93:LEU:HD21	0.50	1.83	20	1
1:A:8:TRP:CD1	1:A:39:ASP:HB2	0.50	2.42	19	1
1:A:8:TRP:CE3	1:A:40:LYS:HB3	0.50	2.41	13	1
1:A:109:TRP:C	1:A:109:TRP:CD1	0.50	2.86	4	6
1:A:53:THR:C	1:A:54:LEU:HD22	0.50	2.27	4	1
1:A:20:LEU:HD12	1:A:30:ARG:HA	0.49	1.83	6	2
1:A:8:TRP:CH2	1:A:130:PHE:CZ	0.49	3.00	13	1
1:A:8:TRP:CZ3	1:A:41:GLU:HG3	0.49	2.42	19	2
1:A:108:GLN:NE2	1:A:117:LEU:HD13	0.49	2.21	7	2
1:A:4:PHE:CE1	1:A:93:LEU:HD12	0.49	2.42	2	1
1:A:7:TYR:CB	1:A:133:VAL:CG1	0.49	2.90	10	1
1:A:109:TRP:CD1	1:A:109:TRP:C	0.49	2.86	13	2
1:A:8:TRP:CH2	1:A:41:GLU:HG3	0.49	2.43	19	2
1:A:8:TRP:CE3	1:A:115:LEU:HG	0.49	2.42	1	1
1:A:74:LEU:HD22	1:A:77:ILE:CD1	0.49	2.38	7	1
1:A:8:TRP:CH2	1:A:40:LYS:HE3	0.49	2.43	13	1
1:A:120:ARG:HG3	1:A:125:THR:HG23	0.49	1.84	19	1
1:A:8:TRP:CZ2	1:A:130:PHE:CZ	0.49	3.01	18	1
1:A:75:THR:N	1:A:79:ASP:HA	0.49	2.23	20	1
1:A:48:HIS:CD2	1:A:66:VAL:HB	0.49	2.43	20	1
1:A:84:THR:HG23	1:A:85:THR:N	0.49	2.22	6	1
1:A:8:TRP:CD1	1:A:9:LYS:N	0.48	2.81	16	2
1:A:117:LEU:HD23	1:A:118:GLU:N	0.48	2.22	15	1
1:A:133:VAL:O	1:A:133:VAL:HG13	0.48	2.08	19	1
1:A:48:HIS:CE1	1:A:50:ILE:HD11	0.48	2.42	1	1
1:A:106:TRP:CD1	1:A:119:MET:CG	0.48	2.97	21	1
1:A:8:TRP:CE3	1:A:39:ASP:CB	0.48	2.97	10	2
1:A:8:TRP:CZ3	1:A:132:LYS:HG2	0.48	2.43	4	1
1:A:8:TRP:CE3	1:A:115:LEU:CD2	0.48	2.96	7	1
1:A:8:TRP:CD1	1:A:41:GLU:HA	0.48	2.44	21	1
1:A:25:VAL:O	1:A:25:VAL:HG22	0.48	2.08	22	1
1:A:8:TRP:NE1	1:A:40:LYS:O	0.48	2.47	21	1
1:A:8:TRP:NE1	1:A:39:ASP:CB	0.48	2.77	12	4
1:A:19:TYR:CZ	1:A:119:MET:HE1	0.48	2.44	6	1
1:A:66:VAL:HG21	1:A:88:TRP:CD1	0.48	2.43	15	1
1:A:48:HIS:HE1	1:A:50:ILE:HD11	0.48	1.68	1	1
1:A:70:PHE:CD1	1:A:70:PHE:N	0.48	2.82	22	1
1:A:115:LEU:HD23	1:A:130:PHE:CB	0.48	2.38	6	1
1:A:7:TYR:O	1:A:133:VAL:HG23	0.47	2.08	6	1
1:A:7:TYR:N	1:A:7:TYR:CD1	0.47	2.81	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TRP:CZ2	1:A:115:LEU:HD21	0.47	2.45	1	1
1:A:8:TRP:CG	1:A:130:PHE:CD2	0.47	3.03	13	1
1:A:20:LEU:HD11	1:A:33:ALA:CB	0.47	2.40	3	1
1:A:8:TRP:CZ3	1:A:115:LEU:HG	0.47	2.44	1	1
1:A:60:TYR:C	1:A:61:ILE:HD12	0.47	2.30	14	1
1:A:80:ARG:CD	1:A:104:ARG:CZ	0.47	2.92	19	1
1:A:8:TRP:CD2	1:A:39:ASP:HB2	0.47	2.45	10	1
1:A:49:MET:C	1:A:50:ILE:HD12	0.47	2.30	20	2
1:A:8:TRP:CD2	1:A:130:PHE:CE2	0.47	3.03	13	1
1:A:35:LEU:HD23	1:A:35:LEU:N	0.47	2.25	10	1
1:A:88:TRP:C	1:A:88:TRP:CD1	0.47	2.87	13	1
1:A:8:TRP:CE2	1:A:115:LEU:HD12	0.46	2.45	5	2
1:A:61:ILE:HD12	1:A:61:ILE:N	0.46	2.25	9	1
1:A:51:ILE:HD13	1:A:51:ILE:N	0.46	2.25	18	1
1:A:19:TYR:CZ	1:A:23:LEU:HD11	0.46	2.46	18	1
1:A:35:LEU:HD12	1:A:35:LEU:C	0.46	2.31	9	1
1:A:60:TYR:CG	1:A:60:TYR:O	0.46	2.68	7	1
1:A:77:ILE:C	1:A:77:ILE:HD12	0.46	2.30	20	1
1:A:8:TRP:CH2	1:A:130:PHE:CE1	0.46	3.04	18	1
1:A:133:VAL:HG13	1:A:134:HIS:N	0.46	2.25	20	1
1:A:47:ASP:CB	1:A:65:GLN:HB3	0.46	2.40	20	2
1:A:8:TRP:CH2	1:A:42:ILE:HG13	0.46	2.46	17	1
1:A:8:TRP:CD1	1:A:130:PHE:CB	0.45	2.99	13	1
1:A:8:TRP:CE3	1:A:8:TRP:O	0.45	2.69	21	1
1:A:28:ALA:O	1:A:32:ILE:HD13	0.45	2.11	16	1
1:A:66:VAL:CG1	1:A:67:GLY:N	0.45	2.79	20	1
1:A:8:TRP:CZ3	1:A:41:GLU:CB	0.45	2.99	19	1
1:A:8:TRP:CZ3	1:A:41:GLU:HA	0.45	2.46	19	1
1:A:8:TRP:CH2	1:A:115:LEU:HD11	0.45	2.46	2	2
1:A:7:TYR:CB	1:A:133:VAL:HG12	0.45	2.42	10	1
1:A:8:TRP:CD1	1:A:41:GLU:N	0.45	2.84	21	1
1:A:47:ASP:O	1:A:48:HIS:CB	0.45	2.63	20	1
1:A:26:ASN:N	1:A:26:ASN:HD22	0.45	2.08	2	1
1:A:115:LEU:O	1:A:129:VAL:HG22	0.45	2.12	1	1
1:A:8:TRP:CZ3	1:A:41:GLU:HB2	0.45	2.47	12	1
1:A:9:LYS:O	1:A:11:LEU:N	0.45	2.50	12	1
1:A:64:PHE:CE1	1:A:70:PHE:CE1	0.45	3.04	19	1
1:A:75:THR:O	1:A:79:ASP:N	0.45	2.50	20	2
1:A:133:VAL:CG1	1:A:134:HIS:N	0.45	2.79	20	1
1:A:20:LEU:HD12	1:A:30:ARG:HG3	0.45	1.88	7	1
1:A:132:LYS:O	1:A:133:VAL:CB	0.45	2.64	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD21	1:A:77:ILE:HG22	0.45	1.88	5	1
1:A:25:VAL:HG22	1:A:78:ASP:HA	0.45	1.89	3	1
1:A:8:TRP:NE1	1:A:39:ASP:HB2	0.45	2.27	12	1
1:A:8:TRP:CD2	1:A:39:ASP:CB	0.44	3.00	20	1
1:A:8:TRP:CD1	1:A:8:TRP:N	0.44	2.83	15	2
1:A:40:LYS:HB2	1:A:130:PHE:CE2	0.44	2.47	17	1
1:A:8:TRP:CD2	1:A:40:LYS:HB3	0.44	2.48	13	1
1:A:116:HIS:CE1	1:A:129:VAL:HG12	0.44	2.47	18	1
1:A:25:VAL:CG2	1:A:29:LEU:HD23	0.44	2.42	5	1
1:A:77:ILE:N	1:A:77:ILE:CD1	0.44	2.80	10	2
1:A:51:ILE:N	1:A:51:ILE:CD1	0.44	2.81	15	1
1:A:75:THR:O	1:A:75:THR:HG23	0.44	2.13	19	1
1:A:49:MET:HE3	1:A:86:VAL:HG11	0.44	1.90	20	1
1:A:25:VAL:HG21	1:A:29:LEU:HD23	0.44	1.89	14	1
1:A:8:TRP:CD1	1:A:130:PHE:HB3	0.43	2.48	13	1
1:A:32:ILE:HG21	1:A:57:PHE:CZ	0.43	2.48	2	1
1:A:115:LEU:CG	1:A:130:PHE:CE2	0.43	3.01	13	1
1:A:4:PHE:CZ	1:A:110:ILE:HD12	0.43	2.48	20	1
1:A:29:LEU:CD1	1:A:29:LEU:C	0.43	2.87	11	1
1:A:117:LEU:O	1:A:117:LEU:HD23	0.43	2.13	8	1
1:A:51:ILE:CD1	1:A:51:ILE:N	0.43	2.81	20	2
1:A:59:ASN:N	1:A:59:ASN:ND2	0.43	2.66	5	2
1:A:80:ARG:HD2	1:A:104:ARG:CZ	0.43	2.43	19	1
1:A:8:TRP:CZ2	1:A:39:ASP:HB2	0.43	2.48	16	1
1:A:8:TRP:HA	1:A:132:LYS:CB	0.43	2.42	19	1
1:A:43:VAL:HG12	1:A:50:ILE:HD12	0.43	1.88	17	1
1:A:25:VAL:CG2	1:A:78:ASP:HA	0.43	2.43	3	1
1:A:56:THR:O	1:A:56:THR:HG22	0.43	2.14	4	1
1:A:32:ILE:HD13	1:A:57:PHE:CZ	0.43	2.48	18	1
1:A:8:TRP:CE2	1:A:130:PHE:CD1	0.43	3.06	13	1
1:A:49:MET:O	1:A:64:PHE:N	0.43	2.51	20	1
1:A:8:TRP:CZ3	1:A:10:MET:HB3	0.43	2.49	18	1
1:A:77:ILE:HG22	1:A:78:ASP:N	0.43	2.29	4	1
1:A:20:LEU:HD12	1:A:30:ARG:CA	0.43	2.44	6	1
1:A:8:TRP:CE3	1:A:9:LYS:N	0.43	2.87	15	1
1:A:133:VAL:O	1:A:133:VAL:HG22	0.43	2.14	21	1
1:A:25:VAL:HG13	1:A:78:ASP:HA	0.43	1.90	2	1
1:A:8:TRP:CZ3	1:A:42:ILE:HD11	0.42	2.49	1	1
1:A:49:MET:SD	1:A:51:ILE:HD11	0.42	2.54	16	1
1:A:59:ASN:HB3	1:A:61:ILE:CD1	0.42	2.43	11	1
1:A:74:LEU:HD22	1:A:75:THR:N	0.42	2.28	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TRP:CA	1:A:132:LYS:HB3	0.42	2.43	19	1
1:A:48:HIS:CD2	1:A:48:HIS:N	0.42	2.86	20	1
1:A:7:TYR:HA	1:A:8:TRP:CE3	0.42	2.49	19	1
1:A:46:GLY:O	1:A:65:GLN:NE2	0.42	2.53	20	1
1:A:106:TRP:N	1:A:106:TRP:CD1	0.42	2.88	8	1
1:A:77:ILE:HD12	1:A:77:ILE:N	0.42	2.29	7	1
1:A:16:PHE:HE2	1:A:33:ALA:HB1	0.42	1.73	10	1
1:A:4:PHE:CE1	1:A:110:ILE:HD12	0.42	2.49	12	1
1:A:132:LYS:C	1:A:133:VAL:HG12	0.42	2.34	21	1
1:A:77:ILE:HG22	1:A:77:ILE:O	0.42	2.14	3	1
1:A:64:PHE:CE2	1:A:86:VAL:HG21	0.42	2.48	11	1
1:A:109:TRP:CD1	1:A:110:ILE:N	0.42	2.88	9	1
1:A:8:TRP:CH2	1:A:39:ASP:HB2	0.42	2.50	21	1
1:A:84:THR:CG2	1:A:85:THR:N	0.42	2.83	6	1
1:A:39:ASP:N	1:A:39:ASP:OD1	0.42	2.53	21	1
1:A:13:ASN:N	1:A:13:ASN:OD1	0.42	2.52	21	1
1:A:23:LEU:HD13	1:A:78:ASP:HB3	0.42	1.90	4	1
1:A:132:LYS:O	1:A:133:VAL:HG12	0.42	2.15	21	2
1:A:52:ARG:HA	1:A:61:ILE:HG22	0.42	1.91	8	1
1:A:20:LEU:CD1	1:A:30:ARG:HG3	0.42	2.44	21	1
1:A:7:TYR:HB3	1:A:133:VAL:CG1	0.42	2.44	10	1
1:A:7:TYR:O	1:A:133:VAL:N	0.42	2.53	19	1
1:A:8:TRP:O	1:A:40:LYS:N	0.42	2.53	18	1
1:A:92:LYS:HD3	1:A:109:TRP:CE3	0.42	2.50	12	1
1:A:128:GLN:NE2	1:A:130:PHE:CZ	0.42	2.88	5	1
1:A:18:GLU:HB3	1:A:124:VAL:HG11	0.41	1.90	16	1
1:A:29:LEU:HD23	1:A:29:LEU:C	0.41	2.35	8	1
1:A:8:TRP:NE1	1:A:40:LYS:CB	0.41	2.83	18	1
1:A:130:PHE:CD1	1:A:130:PHE:N	0.41	2.88	9	1
1:A:8:TRP:CZ3	1:A:40:LYS:HG2	0.41	2.50	13	1
1:A:125:THR:HG22	1:A:125:THR:O	0.41	2.15	14	1
1:A:8:TRP:CZ2	1:A:40:LYS:HB2	0.41	2.49	18	1
1:A:60:TYR:O	1:A:60:TYR:CD1	0.41	2.73	15	1
1:A:34:ASN:CG	1:A:35:LEU:N	0.41	2.74	11	1
1:A:10:MET:HA	1:A:130:PHE:CD1	0.41	2.50	14	1
1:A:4:PHE:CE2	1:A:93:LEU:CD1	0.41	3.03	21	1
1:A:19:TYR:CD2	1:A:20:LEU:CD2	0.41	3.03	6	1
1:A:8:TRP:NE1	1:A:39:ASP:HB3	0.41	2.30	14	1
1:A:4:PHE:CE1	1:A:110:ILE:CD1	0.41	3.04	12	1
1:A:51:ILE:N	1:A:51:ILE:HD13	0.41	2.31	5	1
1:A:108:GLN:NE2	1:A:115:LEU:HD13	0.41	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLY:C	1:A:65:GLN:NE2	0.41	2.74	20	1
1:A:27:VAL:CG1	1:A:28:ALA:N	0.41	2.82	18	1
1:A:20:LEU:HD22	1:A:25:VAL:HG11	0.41	1.93	19	1
1:A:8:TRP:CH2	1:A:42:ILE:CD1	0.41	3.04	1	1
1:A:11:LEU:HD11	1:A:131:LYS:CG	0.41	2.45	11	1
1:A:23:LEU:HD21	1:A:104:ARG:NH2	0.41	2.30	17	1
1:A:4:PHE:CZ	1:A:93:LEU:HD13	0.41	2.50	10	1
1:A:8:TRP:N	1:A:40:LYS:O	0.41	2.51	18	1
1:A:8:TRP:CE2	1:A:40:LYS:CB	0.41	3.01	18	1
1:A:8:TRP:CZ3	1:A:132:LYS:HB2	0.41	2.51	22	1
1:A:17:GLU:OE2	1:A:34:ASN:ND2	0.41	2.54	8	1
1:A:113:ASP:N	1:A:113:ASP:OD1	0.41	2.54	21	1
1:A:77:ILE:HG23	1:A:77:ILE:O	0.41	2.15	2	1
1:A:60:TYR:CD1	1:A:60:TYR:O	0.41	2.74	5	1
1:A:72:GLU:OE1	1:A:74:LEU:HD23	0.41	2.16	5	1
1:A:134:HIS:CD2	1:A:134:HIS:C	0.41	2.94	17	1
1:A:10:MET:HE2	1:A:130:PHE:CZ	0.40	2.51	9	1
1:A:61:ILE:HG22	1:A:62:MET:N	0.40	2.31	21	1
1:A:24:ASP:N	1:A:24:ASP:OD1	0.40	2.54	20	1
1:A:54:LEU:N	1:A:54:LEU:CD2	0.40	2.85	4	1
1:A:49:MET:HE1	1:A:93:LEU:HD11	0.40	1.92	14	1
1:A:91:ASP:N	1:A:91:ASP:OD1	0.40	2.55	12	1
1:A:49:MET:N	1:A:64:PHE:O	0.40	2.54	17	1
1:A:92:LYS:HD3	1:A:109:TRP:CZ3	0.40	2.51	12	1
1:A:9:LYS:HD3	1:A:132:LYS:CG	0.40	2.46	19	1
1:A:101:LYS:N	1:A:101:LYS:CD	0.40	2.85	3	1
1:A:48:HIS:CE1	1:A:50:ILE:CG1	0.40	3.05	1	1
1:A:79:ASP:OD1	1:A:79:ASP:N	0.40	2.55	20	1
1:A:73:ASP:OD1	1:A:73:ASP:N	0.40	2.55	12	1
1:A:131:LYS:HD2	1:A:131:LYS:C	0.40	2.37	19	1
1:A:106:TRP:CD1	1:A:119:MET:HG2	0.40	2.51	21	1
1:A:59:ASN:N	1:A:59:ASN:OD1	0.40	2.55	21	1
1:A:47:ASP:C	1:A:48:HIS:CD2	0.40	2.95	20	1
1:A:3:ASP:O	1:A:5:ASN:N	0.40	2.55	15	1
1:A:61:ILE:CG2	1:A:62:MET:N	0.40	2.85	19	1
1:A:16:PHE:CD1	1:A:16:PHE:N	0.40	2.89	19	1
1:A:8:TRP:CD1	1:A:41:GLU:CA	0.40	3.05	21	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	131/134 (98%)	102±4 (78±3%)	22±3 (17±2%)	7±2 (5±2%)	4	25
All	All	2882/2948 (98%)	2250 (78%)	478 (17%)	154 (5%)	4	25

All 54 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	79	ASP	16
1	A	9	LYS	8
1	A	103	GLY	6
1	A	77	ILE	6
1	A	112	GLY	6
1	A	25	VAL	5
1	A	57	PHE	5
1	A	46	GLY	5
1	A	38	PRO	4
1	A	100	GLU	4
1	A	90	GLY	4
1	A	15	ASN	4
1	A	4	PHE	4
1	A	121	ALA	4
1	A	101	LYS	4
1	A	26	ASN	4
1	A	133	VAL	3
1	A	58	ARG	3
1	A	10	MET	3
1	A	74	LEU	3
1	A	78	ASP	3
1	A	104	ARG	3
1	A	76	GLY	3
1	A	59	ASN	2
1	A	48	HIS	2
1	A	81	LYS	2
1	A	80	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	56	THR	2
1	A	24	ASP	2
1	A	69	GLU	2
1	A	34	ASN	2
1	A	8	TRP	2
1	A	35	LEU	2
1	A	3	ASP	2
1	A	98	LYS	2
1	A	5	ASN	2
1	A	87	SER	1
1	A	49	MET	1
1	A	75	THR	1
1	A	71	GLU	1
1	A	39	ASP	1
1	A	72	GLU	1
1	A	13	ASN	1
1	A	41	GLU	1
1	A	97	GLN	1
1	A	84	THR	1
1	A	6	GLY	1
1	A	54	LEU	1
1	A	45	ASP	1
1	A	99	GLY	1
1	A	7	TYR	1
1	A	61	ILE	1
1	A	91	ASP	1
1	A	66	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	118/120 (98%)	80±5 (68±4%)	38±5 (32±4%)	1	13
All	All	2596/2640 (98%)	1757 (68%)	839 (32%)	1	13

All 117 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	59	ASN	15
1	A	126	CYS	15
1	A	10	MET	15
1	A	58	ARG	13
1	A	39	ASP	13
1	A	128	GLN	13
1	A	127	LYS	13
1	A	115	LEU	13
1	A	12	SER	12
1	A	9	LYS	12
1	A	31	LYS	12
1	A	80	ARG	12
1	A	60	TYR	12
1	A	74	LEU	11
1	A	122	GLU	11
1	A	79	ASP	11
1	A	30	ARG	11
1	A	26	ASN	11
1	A	106	TRP	10
1	A	35	LEU	10
1	A	94	GLN	10
1	A	109	TRP	10
1	A	68	LYS	10
1	A	87	SER	10
1	A	93	LEU	10
1	A	3	ASP	10
1	A	7	TYR	10
1	A	63	ASP	10
1	A	95	CYS	10
1	A	120	ARG	10
1	A	44	GLN	10
1	A	18	GLU	10
1	A	75	THR	9
1	A	5	ASN	9
1	A	82	CYS	9
1	A	34	ASN	9
1	A	62	MET	9
1	A	47	ASP	9
1	A	15	ASN	9
1	A	23	LEU	8
1	A	36	LEU	8
1	A	131	LYS	8
1	A	88	TRP	8

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Mol	Chain	Res	Type	Models (Total)
1	A	13	ASN	8
1	A	130	PHE	8
1	A	11	LEU	8
1	A	101	LYS	8
1	A	16	PHE	8
1	A	81	LYS	8
1	A	56	THR	8
1	A	77	ILE	8
1	A	43	VAL	8
1	A	14	GLU	8
1	A	21	ARG	8
1	A	132	LYS	7
1	A	29	LEU	7
1	A	104	ARG	7
1	A	41	GLU	7
1	A	85	THR	7
1	A	119	MET	7
1	A	19	TYR	7
1	A	111	GLU	7
1	A	40	LYS	7
1	A	48	HIS	6
1	A	83	MET	6
1	A	52	ARG	6
1	A	78	ASP	6
1	A	117	LEU	6
1	A	37	LYS	6
1	A	118	GLU	6
1	A	72	GLU	6
1	A	92	LYS	6
1	A	45	ASP	6
1	A	57	PHE	6
1	A	97	GLN	6
1	A	98	LYS	6
1	A	51	ILE	6
1	A	55	SER	5
1	A	24	ASP	5
1	A	65	GLN	5
1	A	91	ASP	5
1	A	108	GLN	5
1	A	116	HIS	5
1	A	25	VAL	5
1	A	71	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	86	VAL	5
1	A	134	HIS	5
1	A	102	GLU	5
1	A	17	GLU	5
1	A	70	PHE	4
1	A	107	THR	4
1	A	27	VAL	4
1	A	96	VAL	4
1	A	114	GLU	4
1	A	66	VAL	4
1	A	133	VAL	4
1	A	100	GLU	4
1	A	89	ASP	4
1	A	69	GLU	4
1	A	8	TRP	4
1	A	113	ASP	4
1	A	61	ILE	3
1	A	110	ILE	3
1	A	54	LEU	3
1	A	129	VAL	3
1	A	124	VAL	3
1	A	32	ILE	3
1	A	73	ASP	3
1	A	20	LEU	2
1	A	42	ILE	2
1	A	4	PHE	2
1	A	125	THR	2
1	A	38	PRO	2
1	A	84	THR	2
1	A	53	THR	1
1	A	49	MET	1
1	A	64	PHE	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

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5579

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1634
Number of shifts mapped to atoms	1634
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	17

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	134	-0.15 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	124	0.08 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	134	0.21 ± 0.13	None needed (< 0.5 ppm)
^{15}N	126	-4.58 ± 0.29	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1453 atoms were assigned a chemical shift out of a possible 1698. 20 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	646/658 (98%)	257/263 (98%)	264/264 (100%)	125/131 (95%)
Sidechain	758/890 (85%)	474/519 (91%)	270/326 (83%)	14/45 (31%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	49/150 (33%)	46/78 (59%)	0/62 (0%)	3/10 (30%)
Overall	1453/1698 (86%)	777/860 (90%)	534/652 (82%)	142/186 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1476 atoms were assigned a chemical shift out of a possible 1721. 21 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	654/666 (98%)	260/266 (98%)	268/268 (100%)	126/132 (95%)
Sidechain	773/905 (85%)	483/528 (91%)	276/332 (83%)	14/45 (31%)
Aromatic	49/150 (33%)	46/78 (59%)	0/62 (0%)	3/10 (30%)
Overall	1476/1721 (86%)	789/872 (90%)	544/662 (82%)	143/187 (76%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	80	ARG	NE	121.90	92.63 – 76.73	23.4
1	A	120	ARG	NE	119.80	92.63 – 76.73	22.1
1	A	108	GLN	HE22	3.60	9.27 – 4.77	-7.6
1	A	108	GLN	HE21	3.83	9.53 – 4.93	-7.4
1	A	116	HIS	HB2	0.80	4.91 – 1.31	-6.4
1	A	116	HIS	HB3	0.55	5.00 – 1.10	-6.4
1	A	95	CYS	HB3	-0.02	5.25 – 0.55	-6.2
1	A	95	CYS	HB2	0.26	5.20 – 0.70	-6.0
1	A	108	GLN	NE2	101.40	120.91 – 102.81	-5.8
1	A	132	LYS	HG3	-0.21	2.76 – -0.04	-5.6
1	A	13	ASN	HD22	4.45	9.59 – 4.69	-5.5
1	A	40	LYS	HD3	0.34	2.75 – 0.45	-5.5
1	A	5	ASN	ND2	125.20	124.24 – 101.34	5.4
1	A	40	LYS	HE3	1.90	3.86 – 1.96	-5.3
1	A	93	LEU	HB2	-0.13	3.32 – -0.08	-5.1
1	A	84	THR	HB	2.49	5.82 – 2.52	-5.1
1	A	128	GLN	HE22	4.77	9.27 – 4.77	-5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

