



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:30 pm GMT

PDB ID : 1ARQ
Title : RELAXATION MATRIX REFINEMENT OF THE SOLUTION STRUCTURE OF THE ARC REPRESSOR
Authors : Bonvin, A.M.J.J.; Vis, H.; Burgering, M.J.M.; Breg, J.N.; Boelens, R.; Kaptein, R.
Deposited on : 1993-08-24

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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

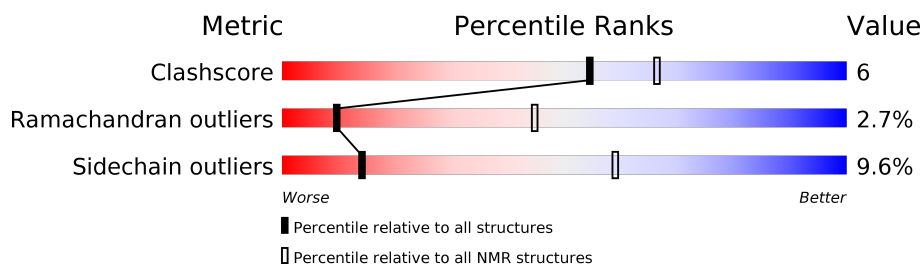
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	53	
1	B	53	

2 Ensemble composition and analysis

This entry contains 16 models. Model 2 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:8-A:46, B:8-B:46 (78)	0.33	2

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 870 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ARC REPRESSOR.

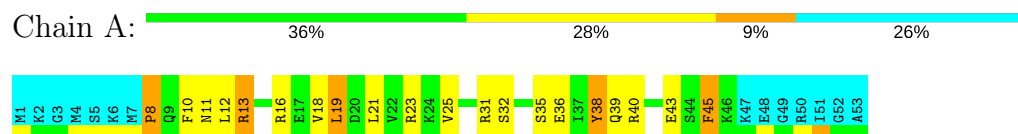
Mol	Chain	Residues	Atoms					Trace
1	A	53	Total	C	N	O	S	0
			435	271	82	78	4	
1	B	53	Total	C	N	O	S	0
			435	271	82	78	4	

4 Residue-property plots [i](#)

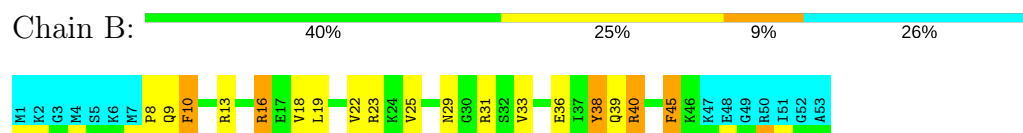
4.1 Average score per residue in the NMR ensemble

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: ARC REPRESSOR



• Molecule 1: ARC REPRESSOR

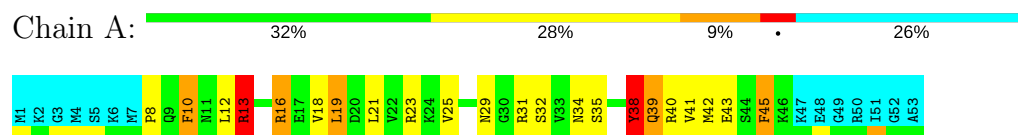


4.2 Scores per residue for each member of the ensemble

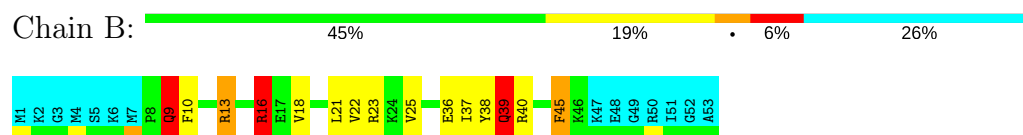
Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

• Molecule 1: ARC REPRESSOR

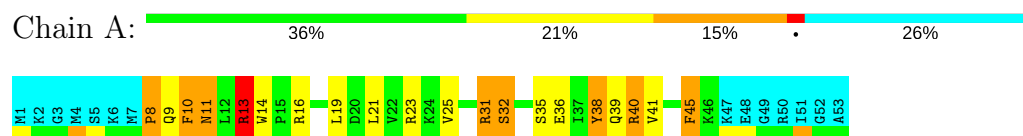


• Molecule 1: ARC REPRESSOR

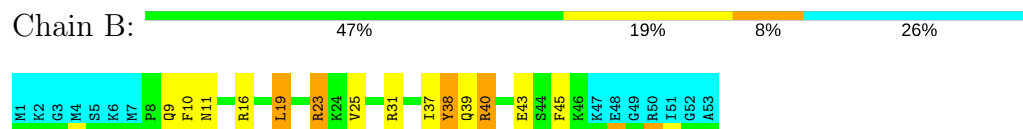


4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: ARC REPRESSOR

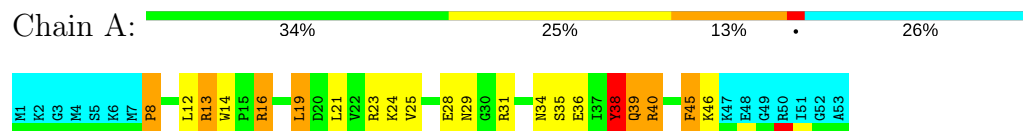


• Molecule 1: ARC REPRESSOR

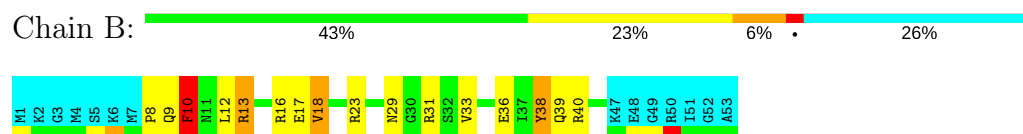


4.2.3 Score per residue for model 3

• Molecule 1: ARC REPRESSOR

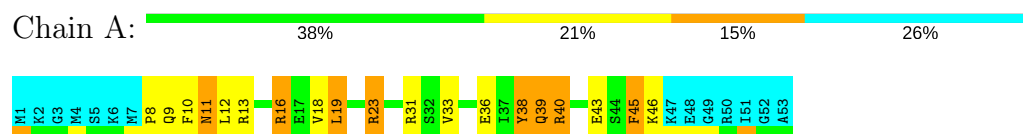


• Molecule 1: ARC REPRESSOR

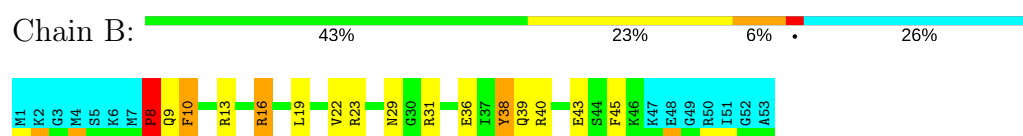


4.2.4 Score per residue for model 4

• Molecule 1: ARC REPRESSOR

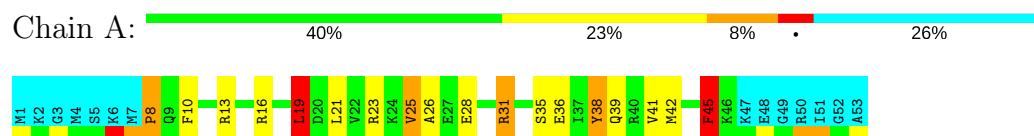


• Molecule 1: ARC REPRESSOR

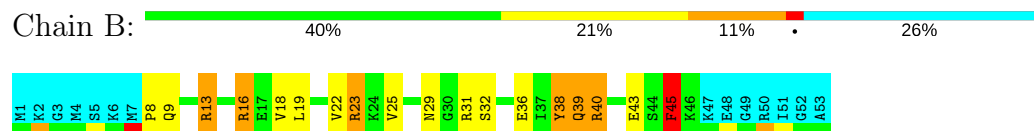


4.2.5 Score per residue for model 5

• Molecule 1: ARC REPRESSOR

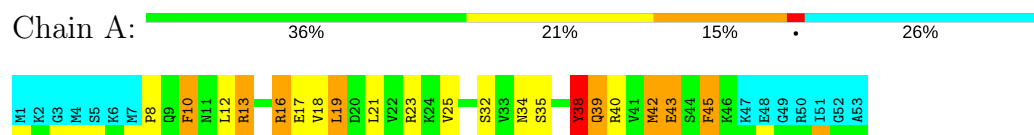


• Molecule 1: ARC REPRESSOR

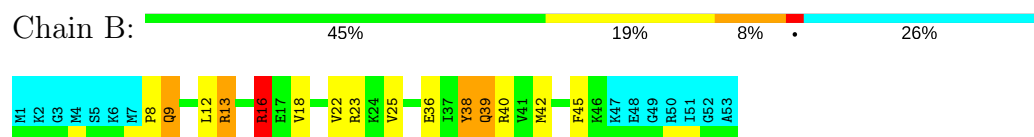


4.2.6 Score per residue for model 6

• Molecule 1: ARC REPRESSOR

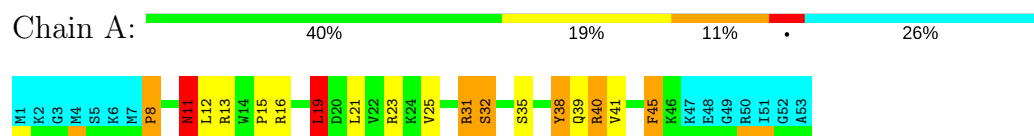


• Molecule 1: ARC REPRESSOR

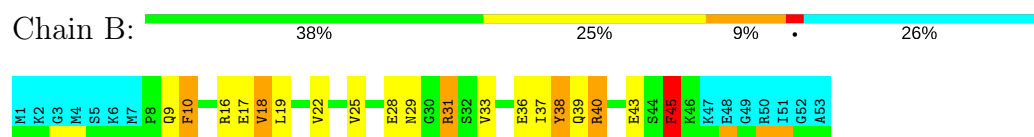


4.2.7 Score per residue for model 7

• Molecule 1: ARC REPRESSOR

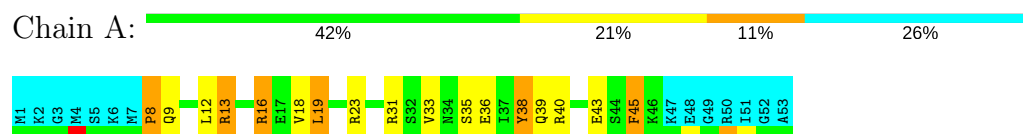


• Molecule 1: ARC REPRESSOR

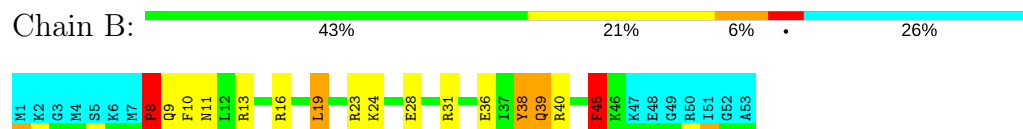


4.2.8 Score per residue for model 8

• Molecule 1: ARC REPRESSOR

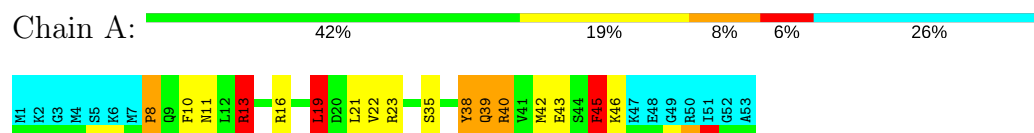


• Molecule 1: ARC REPRESSOR

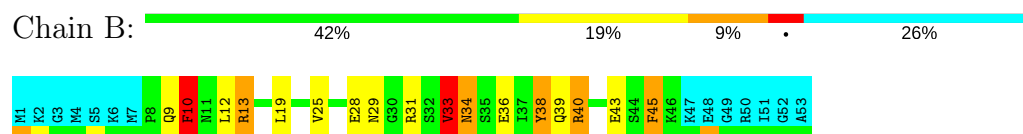


4.2.9 Score per residue for model 9

• Molecule 1: ARC REPRESSOR

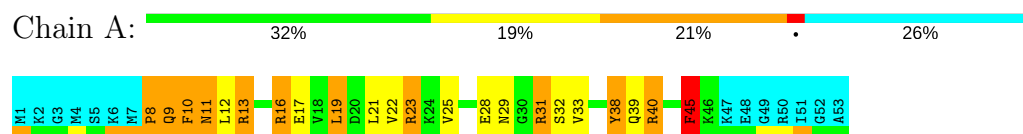


• Molecule 1: ARC REPRESSOR

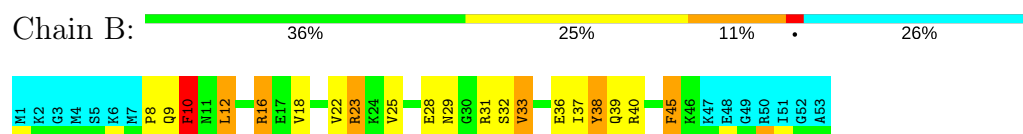


4.2.10 Score per residue for model 10

• Molecule 1: ARC REPRESSOR

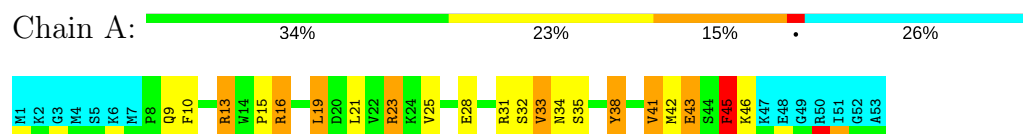


• Molecule 1: ARC REPRESSOR

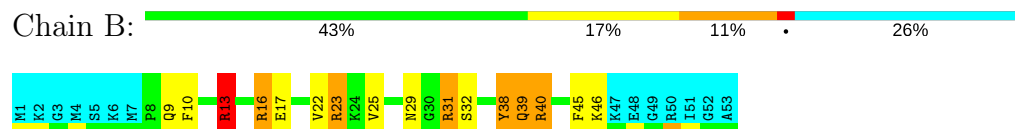


4.2.11 Score per residue for model 11

• Molecule 1: ARC REPRESSOR

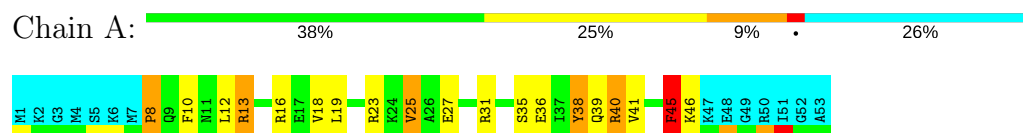


• Molecule 1: ARC REPRESSOR

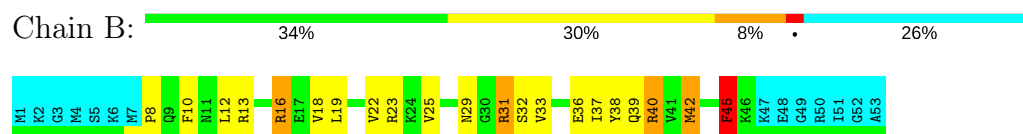


4.2.12 Score per residue for model 12

• Molecule 1: ARC REPRESSOR

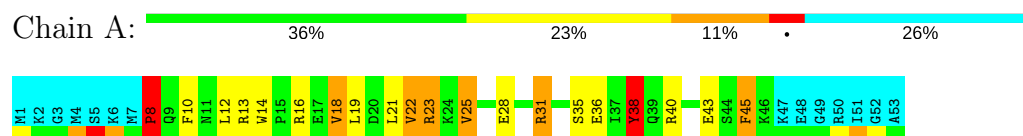


• Molecule 1: ARC REPRESSOR

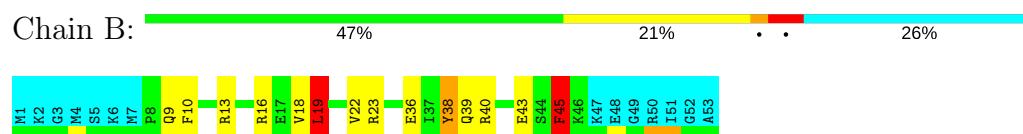


4.2.13 Score per residue for model 13

• Molecule 1: ARC REPRESSOR

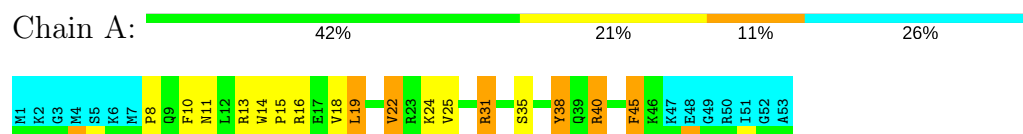


• Molecule 1: ARC REPRESSOR

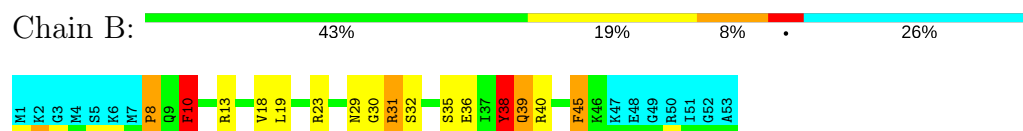


4.2.14 Score per residue for model 14

• Molecule 1: ARC REPRESSOR

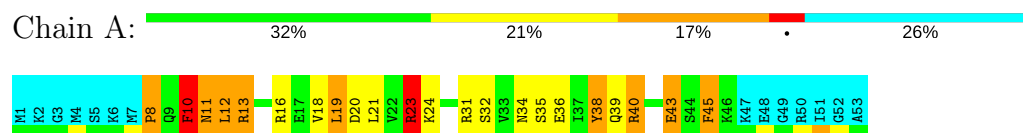


• Molecule 1: ARC REPRESSOR

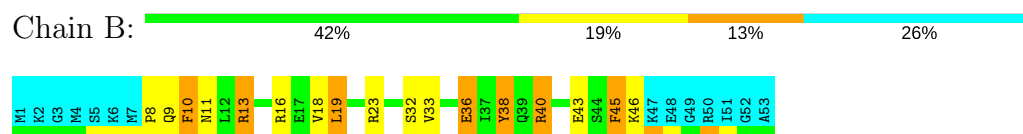


4.2.15 Score per residue for model 15

• Molecule 1: ARC REPRESSOR

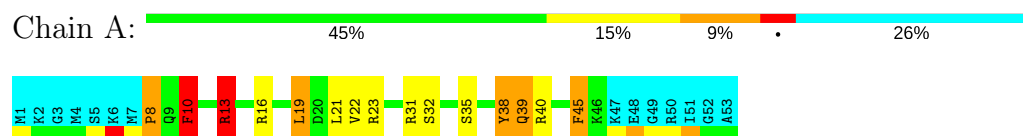


• Molecule 1: ARC REPRESSOR

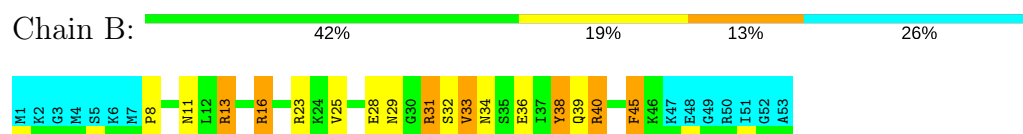


4.2.16 Score per residue for model 16

• Molecule 1: ARC REPRESSOR



• Molecule 1: ARC REPRESSOR



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 16 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
IRMA	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

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	1.01±0.03	0±0/339 (0.0±0.1%)	2.26±0.16	17±3/456 (3.7±0.6%)
1	B	0.88±0.02	0±0/339 (0.0±0.0%)	1.68±0.07	7±2/456 (1.6±0.3%)
All	All	0.95	1/10848 (0.0%)	2.00	383/14592 (2.6%)

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	0.8±0.4	6.1±0.9
1	B	0.0±0.0	5.2±1.2
All	All	13	182

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	10	PHE	CE2-CZ	5.03	1.47	1.37	16	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	A	38	TYR	CB-CG-CD1	-30.32	102.81	121.00	8	16
1	A	10	PHE	CB-CG-CD2	-28.79	100.65	120.80	15	13
1	A	45	PHE	CB-CG-CD2	-15.81	109.73	120.80	14	11
1	B	38	TYR	CB-CG-CD2	-15.65	111.61	121.00	12	2
1	B	45	PHE	CB-CG-CD2	-15.64	109.85	120.80	8	11
1	B	38	TYR	CB-CG-CD1	-14.53	112.28	121.00	7	15
1	B	10	PHE	CB-CG-CD2	-13.59	111.29	120.80	3	11
1	A	10	PHE	CB-CG-CD1	10.48	128.13	120.80	15	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	10	PHE	CB-CG-CD1	10.04	127.83	120.80	3	2
1	A	19	LEU	CB-CA-C	9.91	129.02	110.20	9	4
1	A	19	LEU	CB-CG-CD1	9.82	127.70	111.00	11	6
1	A	25	VAL	CA-CB-CG1	9.58	125.27	110.90	12	9
1	A	32	SER	N-CA-CB	8.38	123.06	110.50	2	4
1	A	38	TYR	CD1-CG-CD2	8.33	127.06	117.90	14	15
1	A	19	LEU	CA-CB-CG	-8.24	96.34	115.30	10	11
1	B	12	LEU	CB-CG-CD2	7.87	124.39	111.00	10	3
1	A	31	ARG	NE-CZ-NH1	7.79	124.20	120.30	4	6
1	A	35	SER	N-CA-CB	7.78	122.17	110.50	14	14
1	A	21	LEU	CB-CA-C	7.76	124.94	110.20	9	12
1	B	31	ARG	NE-CZ-NH1	7.57	124.08	120.30	12	5
1	B	19	LEU	CA-CB-CG	-7.55	97.93	115.30	9	4
1	A	12	LEU	CB-CG-CD2	7.46	123.68	111.00	1	6
1	B	13	ARG	NE-CZ-NH1	7.33	123.97	120.30	5	5
1	A	16	ARG	N-CA-CB	7.21	123.59	110.60	10	16
1	B	36	GLU	N-CA-CB	7.03	123.26	110.60	13	4
1	A	16	ARG	CB-CA-C	7.03	124.45	110.40	5	15
1	A	10	PHE	CD1-CG-CD2	6.99	127.39	118.30	15	1
1	B	23	ARG	NE-CZ-NH1	6.94	123.77	120.30	2	4
1	B	40	ARG	NE-CZ-NH1	6.93	123.77	120.30	16	3
1	A	13	ARG	NE-CZ-NH1	6.93	123.77	120.30	1	6
1	A	16	ARG	NE-CZ-NH1	6.88	123.74	120.30	4	5
1	A	40	ARG	N-CA-CB	6.80	122.84	110.60	13	1
1	A	38	TYR	CG-CD2-CE2	-6.79	115.87	121.30	14	8
1	B	16	ARG	N-CA-CB	-6.64	98.65	110.60	1	2
1	B	33	VAL	CA-CB-CG1	-6.59	101.01	110.90	16	1
1	A	28	GLU	N-CA-CB	6.58	122.45	110.60	5	2
1	A	19	LEU	N-CA-CB	-6.57	97.26	110.40	1	3
1	A	13	ARG	N-CA-CB	6.46	122.23	110.60	3	3
1	A	11	ASN	CB-CA-C	6.45	123.30	110.40	10	1
1	A	8	PRO	CA-C-N	-6.45	103.02	117.20	8	9
1	A	19	LEU	CB-CG-CD2	-6.43	100.06	111.00	12	2
1	B	38	TYR	CD1-CG-CD2	6.35	124.89	117.90	7	15
1	A	14	TRP	CB-CG-CD2	-6.35	118.35	126.60	14	3
1	B	16	ARG	NE-CZ-NH1	6.28	123.44	120.30	3	7
1	A	45	PHE	CB-CG-CD1	6.25	125.17	120.80	15	2
1	A	36	GLU	N-CA-CB	6.22	121.80	110.60	4	3
1	A	38	TYR	CB-CG-CD2	6.22	124.73	121.00	9	3
1	A	12	LEU	N-CA-CB	6.12	122.63	110.40	6	2
1	B	33	VAL	CG1-CB-CG2	-6.11	101.12	110.90	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	VAL	CG1-CB-CG2	-6.03	101.26	110.90	10	3
1	A	33	VAL	CG1-CB-CG2	-5.93	101.41	110.90	11	1
1	A	22	VAL	CA-CB-CG2	5.84	119.67	110.90	13	2
1	A	38	TYR	CG-CD1-CE1	-5.80	116.66	121.30	14	8
1	B	31	ARG	NE-CZ-NH2	-5.77	117.41	120.30	12	1
1	A	43	GLU	CA-CB-CG	5.75	126.06	113.40	6	2
1	A	42	MET	CA-C-N	-5.75	104.56	117.20	6	1
1	B	16	ARG	NE-CZ-NH2	-5.74	117.43	120.30	6	2
1	A	12	LEU	CB-CA-C	-5.68	99.41	110.20	7	1
1	A	14	TRP	CG-CD2-CE3	-5.66	128.80	133.90	2	1
1	A	40	ARG	NE-CZ-NH1	5.63	123.12	120.30	7	4
1	A	21	LEU	CB-CG-CD1	-5.61	101.47	111.00	9	1
1	B	19	LEU	CB-CG-CD1	-5.60	101.48	111.00	8	2
1	A	23	ARG	NE-CZ-NH1	5.57	123.08	120.30	13	2
1	B	8	PRO	CA-C-N	-5.56	104.98	117.20	8	1
1	A	45	PHE	N-CA-CB	5.49	120.48	110.60	10	3
1	B	38	TYR	CG-CD1-CE1	-5.48	116.92	121.30	13	7
1	A	43	GLU	N-CA-CB	5.44	120.40	110.60	15	2
1	A	36	GLU	CB-CA-C	5.39	121.19	110.40	5	2
1	A	40	ARG	CB-CA-C	5.33	121.06	110.40	3	3
1	A	42	MET	N-CA-C	5.33	125.39	111.00	6	1
1	B	9	GLN	CA-CB-CG	5.32	125.10	113.40	1	1
1	A	31	ARG	NE-CZ-NH2	-5.30	117.65	120.30	4	1
1	A	41	VAL	CG1-CB-CG2	-5.27	102.46	110.90	11	1
1	A	34	ASN	N-CA-CB	5.24	120.03	110.60	1	1
1	A	13	ARG	NE-CZ-NH2	-5.23	117.69	120.30	12	1
1	B	38	TYR	CG-CD2-CE2	-5.20	117.14	121.30	7	1
1	B	10	PHE	CB-CA-C	-5.15	100.09	110.40	10	1
1	B	39	GLN	N-CA-CB	5.12	119.82	110.60	1	1
1	A	27	GLU	N-CA-CB	5.11	119.79	110.60	12	1
1	A	16	ARG	CA-C-N	-5.03	106.13	117.20	2	1
1	A	11	ASN	CA-C-N	-5.03	106.15	117.20	10	1
1	B	19	LEU	CB-CA-C	5.00	119.71	110.20	15	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	16	ARG	CA	13

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	38	TYR	Sidechain	16
1	A	45	PHE	Sidechain	15
1	B	45	PHE	Sidechain	15
1	A	23	ARG	Mainchain	15
1	B	38	TYR	Sidechain	14
1	A	8	PRO	Mainchain	14
1	B	23	ARG	Mainchain	14
1	B	16	ARG	Mainchain,Sidechain	11
1	A	18	VAL	Mainchain	7
1	B	18	VAL	Mainchain	7
1	A	40	ARG	Mainchain	6
1	B	8	PRO	Mainchain	6
1	A	31	ARG	Mainchain,Sidechain	4
1	B	10	PHE	Sidechain,Mainchain	4
1	A	42	MET	Mainchain	4
1	B	40	ARG	Mainchain,Sidechain	4
1	A	10	PHE	Sidechain	3
1	B	19	LEU	Mainchain	3
1	A	17	GLU	Mainchain	2
1	A	32	SER	Mainchain	2
1	A	41	VAL	Mainchain	2
1	A	16	ARG	Mainchain	2
1	A	13	ARG	Sidechain	2
1	A	11	ASN	Mainchain	1
1	A	26	ALA	Mainchain	1
1	B	30	GLY	Mainchain	1
1	A	24	LYS	Mainchain	1
1	B	33	VAL	Mainchain,Peptide	1
1	A	19	LEU	Mainchain	1
1	B	31	ARG	Sidechain	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	332	0	331	5±2
1	B	332	0	331	6±2
All	All	10624	0	10592	132

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:GLN:HE22	1:B:40:ARG:CZ	0.69	2.00	1	9
1:A:11:ASN:HD21	1:B:9:GLN:HB2	0.67	1.49	2	3
1:A:39:GLN:HE22	1:A:40:ARG:CZ	0.66	2.04	4	6
1:A:31:ARG:NH1	1:A:39:GLN:HE22	0.61	1.93	12	4
1:B:39:GLN:HE21	1:B:40:ARG:NH2	0.58	1.96	7	3
1:A:11:ASN:HD21	1:B:9:GLN:NE2	0.58	1.96	10	1
1:A:31:ARG:CZ	1:A:39:GLN:HE22	0.57	2.13	2	3
1:A:25:VAL:O	1:A:28:GLU:HG2	0.57	2.00	10	2
1:B:31:ARG:CZ	1:B:39:GLN:HE22	0.57	2.13	3	2
1:A:9:GLN:HB2	1:B:11:ASN:HD21	0.57	1.60	8	1
1:A:13:ARG:CZ	1:B:34:ASN:HD22	0.56	2.13	9	2
1:B:33:VAL:HG12	1:B:34:ASN:H	0.56	1.60	9	1
1:A:19:LEU:HD13	1:B:10:PHE:CE2	0.56	2.35	11	3
1:B:29:ASN:HD22	1:B:31:ARG:CZ	0.56	2.13	12	4
1:B:39:GLN:HE21	1:B:40:ARG:NH1	0.55	2.00	3	1
1:A:10:PHE:O	1:B:11:ASN:HA	0.52	2.05	16	2
1:A:34:ASN:HD22	1:B:13:ARG:CZ	0.52	2.17	15	1
1:A:16:ARG:HB2	1:B:8:PRO:HG3	0.52	1.80	4	1
1:B:39:GLN:HE22	1:B:40:ARG:NH1	0.52	2.02	4	1
1:B:22:VAL:HG13	1:B:40:ARG:NH2	0.52	2.20	13	1
1:A:25:VAL:HG11	1:B:45:PHE:CE1	0.51	2.40	5	2
1:B:29:ASN:HD22	1:B:31:ARG:NH2	0.50	2.04	14	4
1:A:39:GLN:HE21	1:A:40:ARG:NH2	0.49	2.05	7	3
1:A:12:LEU:HD21	1:B:12:LEU:HD12	0.49	1.84	10	1
1:A:45:PHE:CZ	1:B:22:VAL:HG22	0.49	2.42	1	7
1:A:19:LEU:HD11	1:A:23:ARG:HH21	0.49	1.68	15	1
1:A:8:PRO:HD2	1:B:19:LEU:HD21	0.49	1.84	13	1
1:A:38:TYR:CE1	1:B:18:VAL:HG11	0.48	2.42	1	4
1:A:19:LEU:HD13	1:B:10:PHE:CE1	0.48	2.43	4	1
1:B:25:VAL:O	1:B:28:GLU:HG2	0.48	2.09	10	4
1:A:19:LEU:HD21	1:B:10:PHE:CE1	0.47	2.45	7	2
1:B:13:ARG:NE	1:B:13:ARG:H	0.47	2.07	15	2
1:B:33:VAL:O	1:B:37:ILE:HG12	0.46	2.10	10	1
1:A:19:LEU:HD12	1:A:19:LEU:C	0.46	2.31	9	1
1:B:31:ARG:NH2	1:B:40:ARG:HH21	0.46	2.07	9	1
1:B:24:LYS:O	1:B:28:GLU:HG3	0.46	2.11	8	1
1:A:16:ARG:HH12	1:A:23:ARG:NH2	0.46	2.09	10	1
1:A:16:ARG:HB2	1:B:8:PRO:HG2	0.45	1.88	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ASN:OD1	1:B:9:GLN:HB2	0.45	2.12	9	1
1:A:10:PHE:O	1:B:12:LEU:HD23	0.45	2.11	6	1
1:A:34:ASN:OD1	1:B:12:LEU:HB3	0.45	2.12	3	1
1:B:21:LEU:O	1:B:25:VAL:HG23	0.45	2.12	1	1
1:A:11:ASN:HD21	1:A:13:ARG:NH2	0.45	2.08	15	1
1:A:9:GLN:H	1:A:9:GLN:CD	0.44	2.15	10	1
1:A:34:ASN:HD22	1:B:13:ARG:NH1	0.44	2.10	15	1
1:B:43:GLU:HA	1:B:46:LYS:HD2	0.44	1.90	15	1
1:A:10:PHE:CE2	1:A:12:LEU:HD22	0.44	2.48	10	1
1:A:25:VAL:O	1:A:28:GLU:HB3	0.44	2.12	13	1
1:A:8:PRO:HB2	1:B:19:LEU:HD21	0.44	1.90	4	1
1:A:18:VAL:O	1:A:22:VAL:HG23	0.44	2.12	14	2
1:B:22:VAL:HG13	1:B:40:ARG:HH22	0.43	1.73	13	1
1:A:16:ARG:O	1:A:19:LEU:HB2	0.43	2.13	10	1
1:A:20:ASP:O	1:A:24:LYS:HG2	0.43	2.14	15	1
1:A:41:VAL:HG21	1:B:37:ILE:HG23	0.43	1.90	2	4
1:A:45:PHE:CE1	1:B:25:VAL:HG11	0.43	2.49	9	1
1:A:11:ASN:HD22	1:A:13:ARG:NH2	0.43	2.11	2	1
1:A:9:GLN:HB2	1:B:11:ASN:OD1	0.43	2.14	2	1
1:A:13:ARG:HB3	1:B:9:GLN:HB3	0.42	1.89	1	1
1:A:40:ARG:HD3	1:A:40:ARG:HA	0.42	1.79	9	1
1:A:34:ASN:ND2	1:B:13:ARG:HH11	0.42	2.13	11	1
1:A:13:ARG:NH2	1:B:9:GLN:HE21	0.42	2.12	6	2
1:A:42:MET:O	1:A:46:LYS:HG2	0.42	2.14	9	1
1:A:13:ARG:H	1:B:34:ASN:ND2	0.42	2.13	9	1
1:B:31:ARG:O	1:B:35:SER:HB3	0.42	2.15	14	1
1:A:34:ASN:HD22	1:B:13:ARG:HH11	0.42	1.58	11	1
1:B:13:ARG:H	1:B:13:ARG:NH1	0.42	2.13	11	1
1:B:31:ARG:HG3	1:B:36:GLU:HB2	0.42	1.91	16	1
1:A:34:ASN:ND2	1:B:13:ARG:H	0.41	2.14	6	1
1:A:12:LEU:O	1:B:9:GLN:HA	0.41	2.15	15	1
1:A:19:LEU:HD21	1:B:10:PHE:CE2	0.41	2.51	3	1
1:A:16:ARG:HH12	1:A:23:ARG:CZ	0.41	2.29	10	1
1:B:18:VAL:O	1:B:22:VAL:HG23	0.41	2.16	7	1
1:B:36:GLU:O	1:B:40:ARG:HD3	0.41	2.15	15	1
1:A:15:PRO:HD2	1:B:38:TYR:HE2	0.41	1.75	14	1
1:B:33:VAL:HG12	1:B:34:ASN:N	0.40	2.31	9	1
1:B:42:MET:O	1:B:45:PHE:HB2	0.40	2.17	12	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	39/53 (74%)	36±1 (92±3%)	2±1 (6±3%)	1±1 (2±2%)	11	48
1	B	39/53 (74%)	36±1 (93±3%)	2±1 (4±2%)	1±1 (3±2%)	9	42
All	All	1248/1696 (74%)	1152 (92%)	62 (5%)	34 (3%)	10	45

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	32	SER	7
1	B	8	PRO	6
1	B	33	VAL	5
1	A	46	LYS	4
1	A	33	VAL	4
1	A	32	SER	3
1	A	8	PRO	2
1	A	16	ARG	2
1	B	34	ASN	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	37/47 (79%)	34±1 (91±3%)	4±1 (9±3%)	14	59
1	B	37/47 (79%)	33±1 (90±4%)	4±1 (10±4%)	14	58
All	All	1184/1504 (79%)	1070 (90%)	114 (10%)	14	59

All 27 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	13	ARG	15
1	B	13	ARG	13
1	B	36	GLU	9
1	B	39	GLN	8
1	A	43	GLU	7
1	A	39	GLN	7
1	B	9	GLN	6
1	B	43	GLU	6
1	A	19	LEU	5
1	A	31	ARG	5
1	A	11	ASN	5
1	A	9	GLN	3
1	B	10	PHE	3
1	A	36	GLU	3
1	B	19	LEU	3
1	B	31	ARG	2
1	B	42	MET	2
1	A	10	PHE	2
1	B	17	GLU	2
1	B	29	ASN	1
1	A	24	LYS	1
1	A	32	SER	1
1	B	40	ARG	1
1	A	15	PRO	1
1	A	12	LEU	1
1	B	46	LYS	1
1	B	16	ARG	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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided