



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 05:36 AM UTC

PDB ID : 1MNT / pdb_00001mnt
Title : SOLUTION STRUCTURE OF DIMERIC MNT REPRESSOR (1-76)
Authors : Burgering, M.J.M.; Boelens, R.; Gilbert, D.E.; Breg, J.N.; Knight, K.L.; Sauer, R.T.; Kaptein, R.
Deposited on : 1994-06-28

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

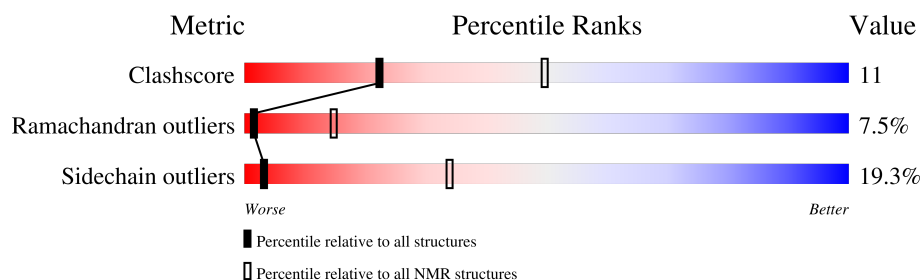
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	76	
1	B	76	

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 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:4-A:24, A:28-A:41, B:5-B:42 (73)	0.51	4

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 4 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1064 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MNT REPRESSOR.

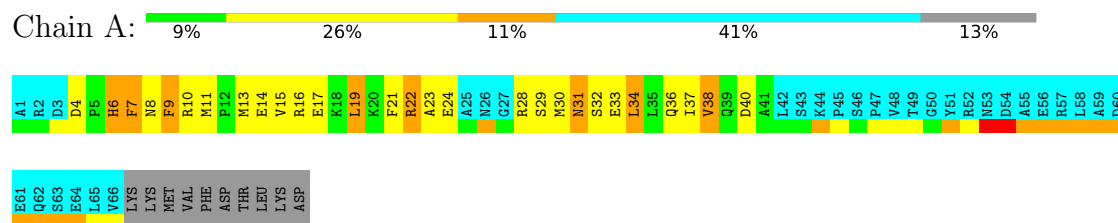
Mol	Chain	Residues	Atoms					Trace
1	A	66	Total	C	N	O	S	0
			532	326	99	104	3	
1	B	66	Total	C	N	O	S	0
			532	326	99	104	3	

4 Residue-property plots [i](#)

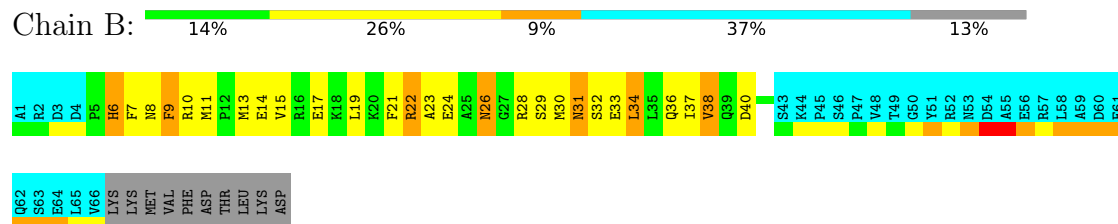
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: MNT REPRESSOR



• Molecule 1: MNT REPRESSOR

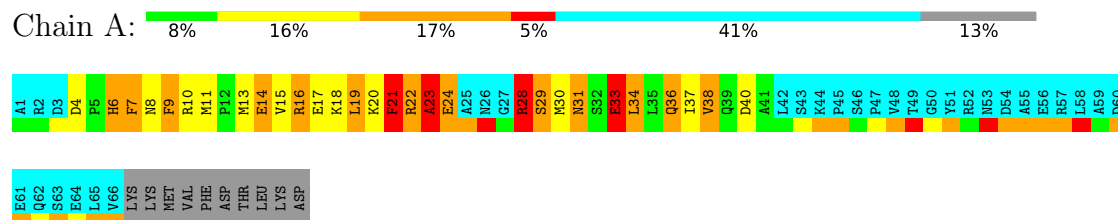


4.2 Scores per residue for each member of the ensemble

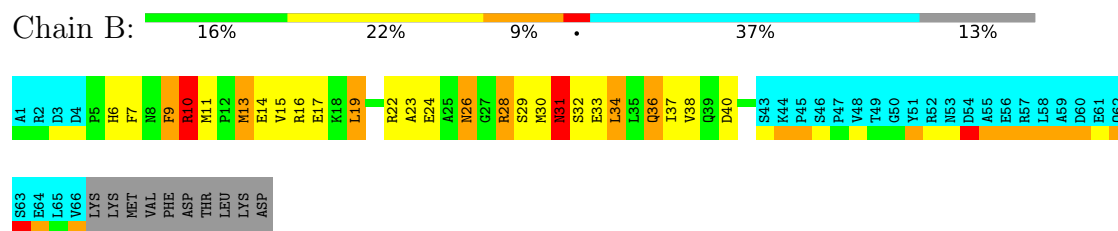
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: MNT REPRESSOR

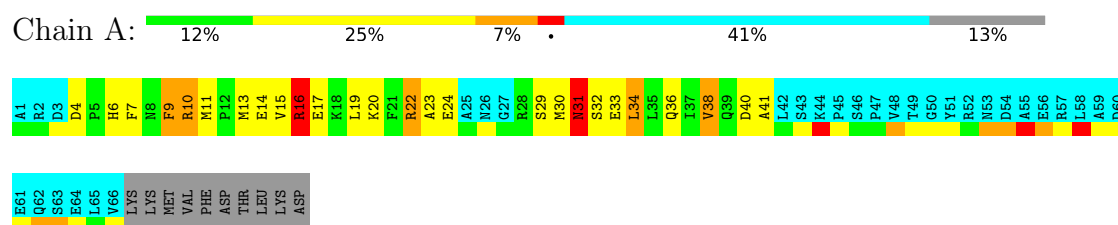


- Molecule 1: MNT REPRESSOR

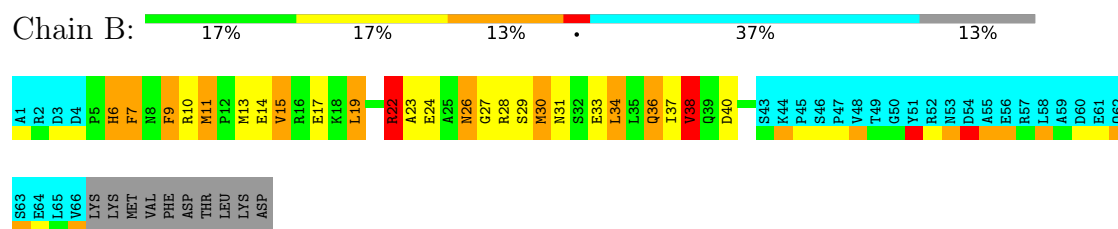


4.2.2 Score per residue for model 2

- Molecule 1: MNT REPRESSOR

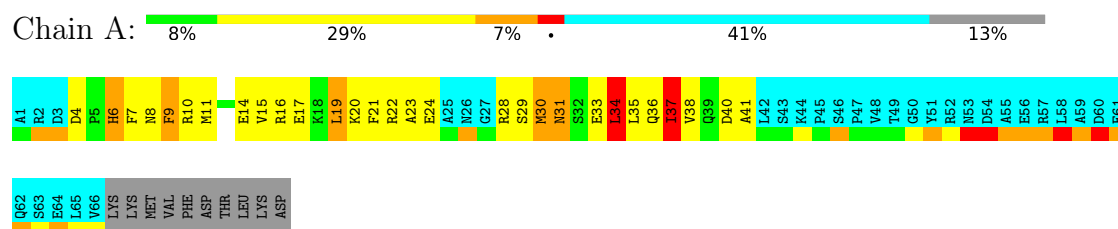


- Molecule 1: MNT REPRESSOR

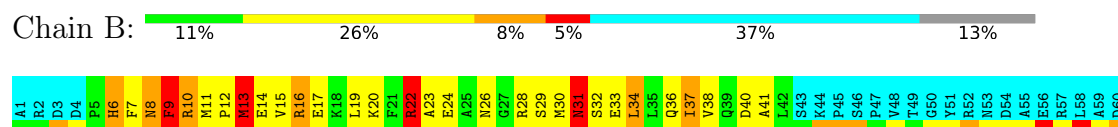


4.2.3 Score per residue for model 3

- Molecule 1: MNT REPRESSOR



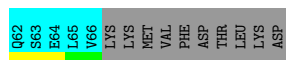
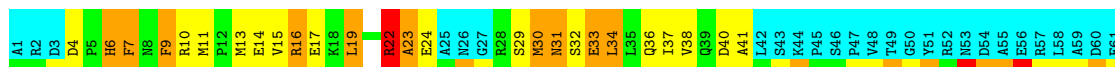
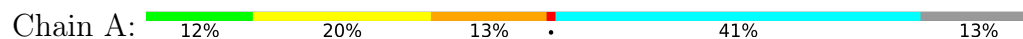
- Molecule 1: MNT REPRESSOR



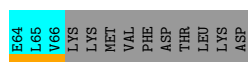
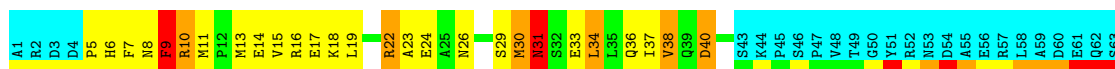
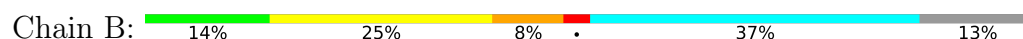


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: MNT REPRESSOR

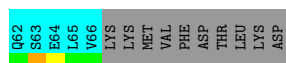
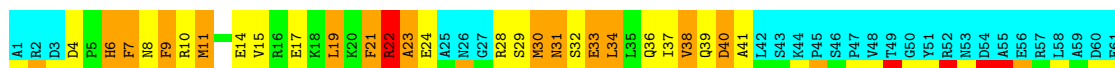


- Molecule 1: MNT REPRESSOR

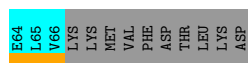
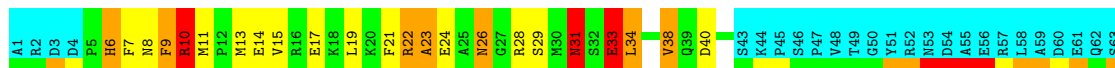
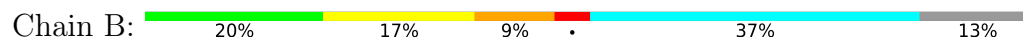


4.2.5 Score per residue for model 5

- Molecule 1: MNT REPRESSOR



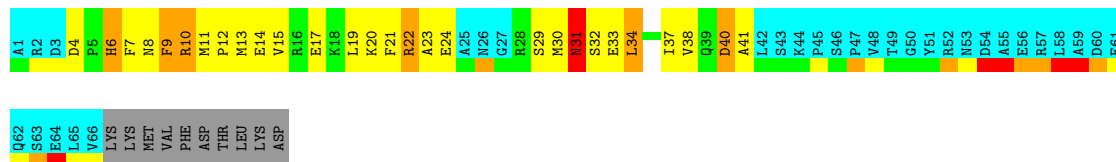
- Molecule 1: MNT REPRESSOR



4.2.6 Score per residue for model 6

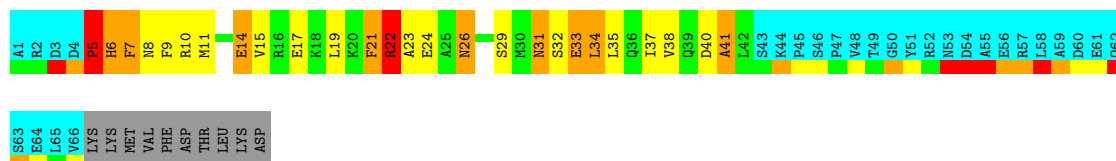
• Molecule 1: MNT REPRESSOR

Chain A: 9% 28% 8% 41% 13%



• Molecule 1: MNT REPRESSOR

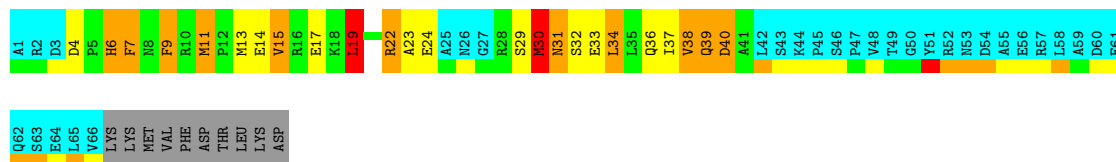
Chain B: 16% 20% 12% 37% 13%



4.2.7 Score per residue for model 7

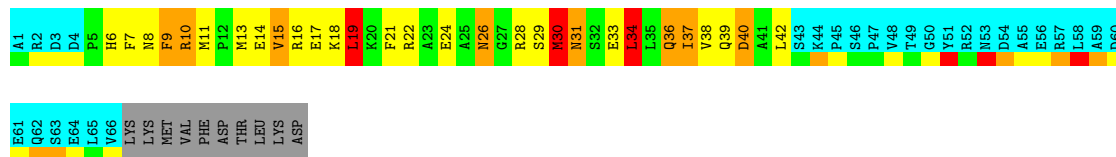
• Molecule 1: MNT REPRESSOR

Chain A: 14% 14% 14% 41% 13%



• Molecule 1: MNT REPRESSOR

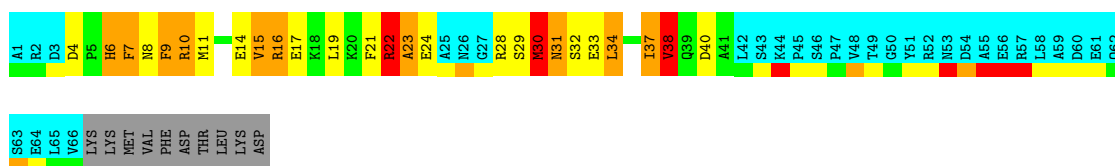
Chain B: 12% 24% 11% 37% 13%



4.2.8 Score per residue for model 8

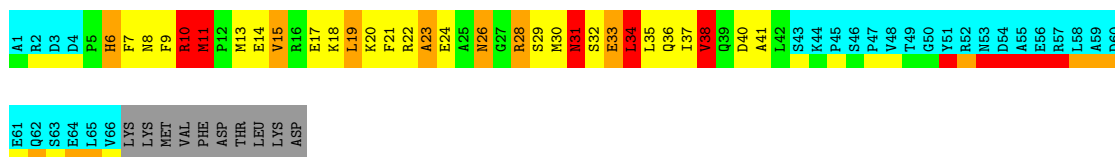
• Molecule 1: MNT REPRESSOR

Chain A: 12% 17% 13% 41% 13%



- Molecule 1: MNT REPRESSOR

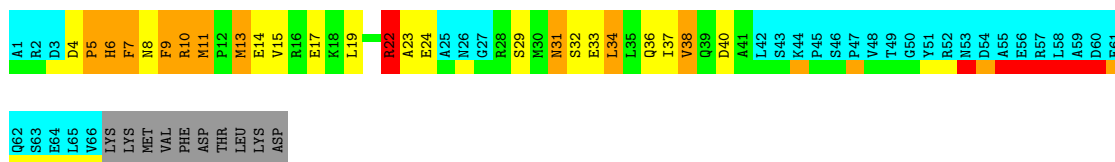
Chain B: 9% 25% 9% 7% 37% 13%



4.2.9 Score per residue for model 9

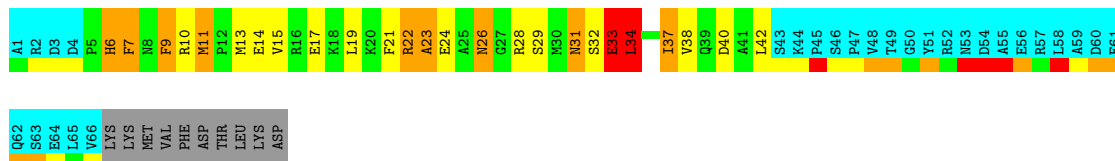
- Molecule 1: MNT REPRESSOR

Chain A: 13% 18% 13% . 41% 13%



- Molecule 1: MNT REPRESSOR

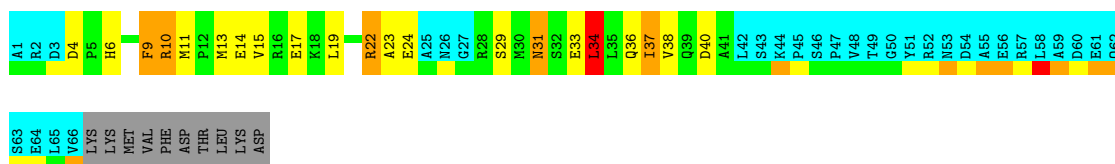
Chain B: 17% 18% 12% . 37% 13%



4.2.10 Score per residue for model 10

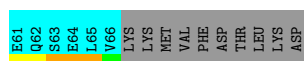
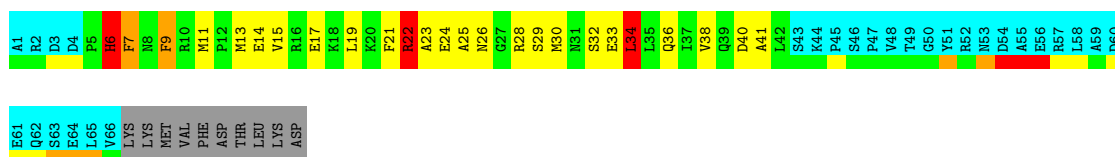
- Molecule 1: MNT REPRESSOR

Chain A: 18% 20% 7% . 41% 13%



- Molecule 1: MNT REPRESSOR

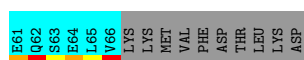
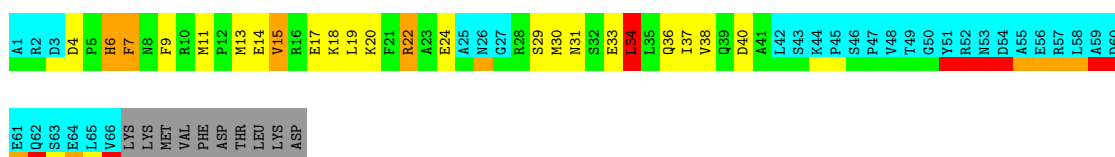
Chain B: 



4.2.11 Score per residue for model 11

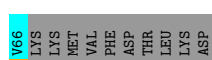
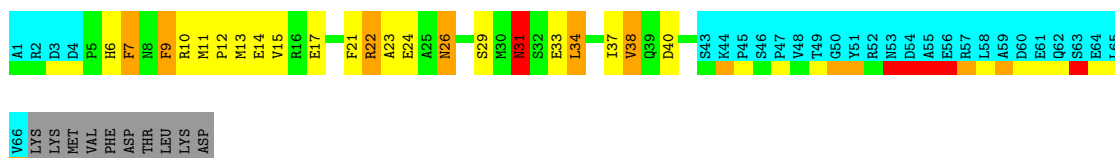
- Molecule 1: MNT REPRESSOR

Chain A: 



- Molecule 1: MNT REPRESSOR

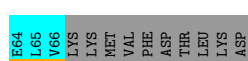
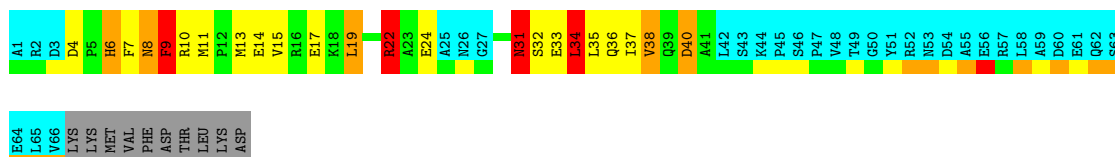
Chain B: 



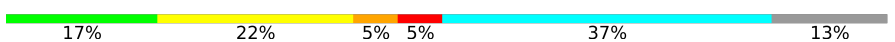
4.2.12 Score per residue for model 12

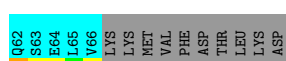
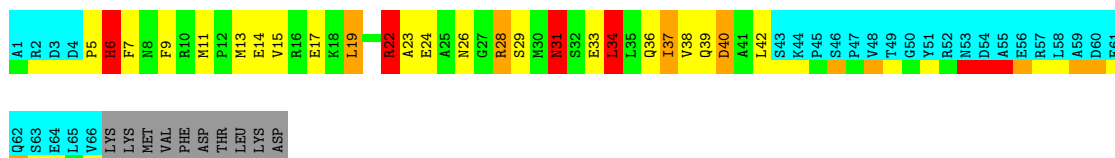
- Molecule 1: MNT REPRESSOR

Chain A: 



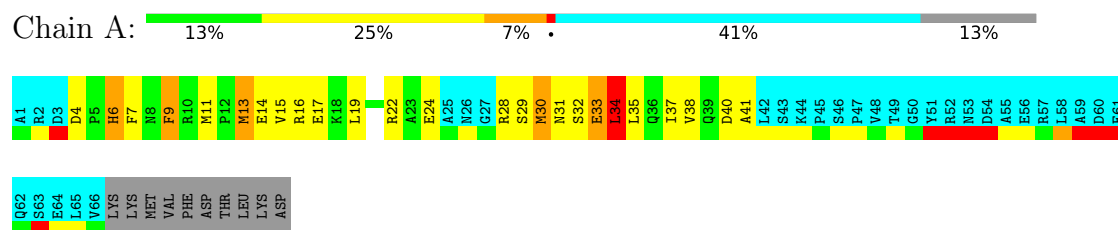
- Molecule 1: MNT REPRESSOR

Chain B: 

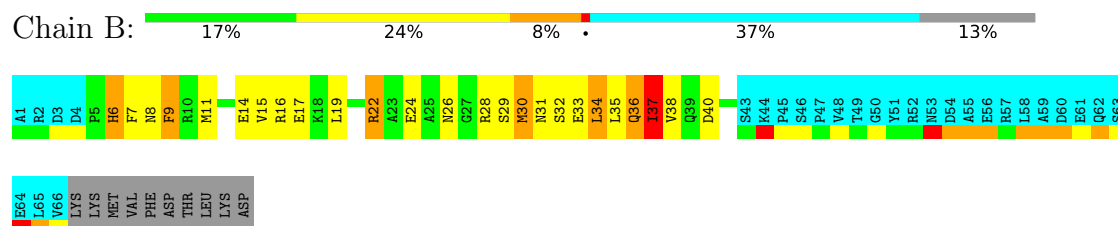


4.2.13 Score per residue for model 13

- Molecule 1: MNT REPRESSOR

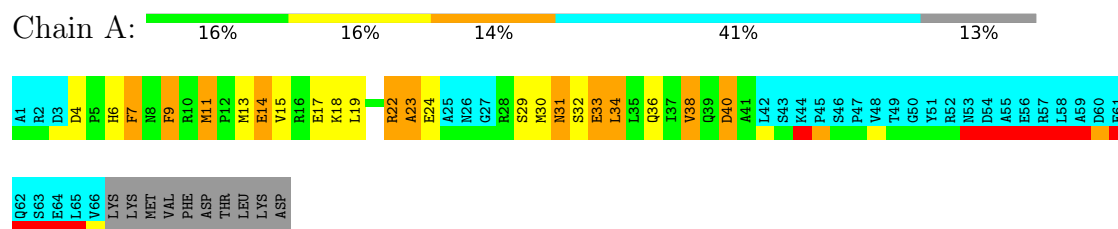


- Molecule 1: MNT REPRESSOR

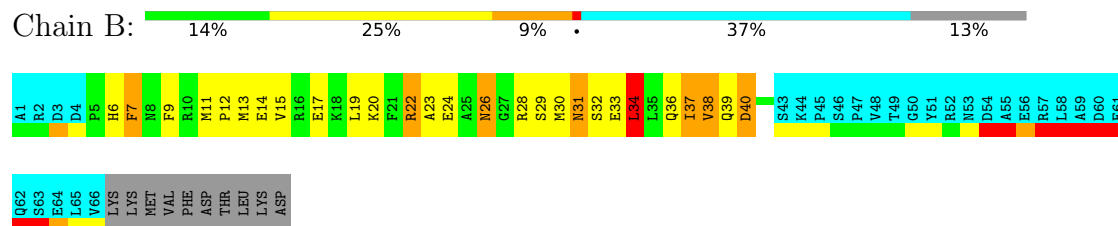


4.2.14 Score per residue for model 14

- Molecule 1: MNT REPRESSOR

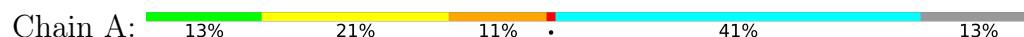


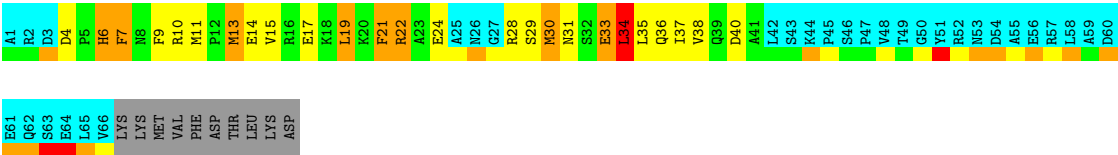
- Molecule 1: MNT REPRESSOR



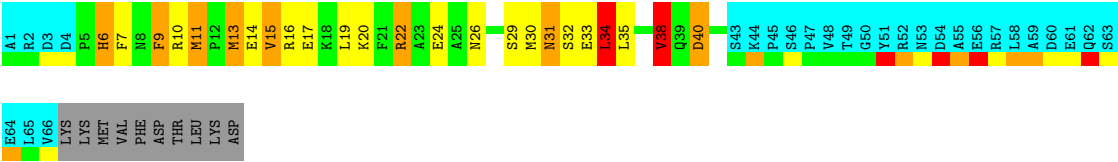
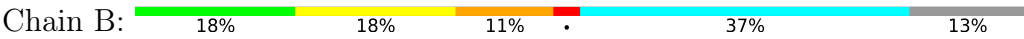
4.2.15 Score per residue for model 15

- Molecule 1: MNT REPRESSOR





● Molecule 1: MNT REPRESSOR



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

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	1.94±0.02	9±1/303 (2.8± 0.3%)	2.48±0.07	18±3/405 (4.4± 0.8%)
1	B	1.92±0.02	8±1/320 (2.4± 0.2%)	2.45±0.07	19±4/427 (4.4± 0.9%)
All	All	1.93	242/9345 (2.6%)	2.47	551/12480 (4.4%)

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	5.1±2.1
1	B	0.0±0.0	4.5±1.5
All	All	0	145

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	ARG	CA-C	6.74	1.61	1.52	15	10
1	B	11	MET	CA-C	6.38	1.58	1.52	8	2
1	B	40	ASP	CG-OD1	6.19	1.37	1.25	3	7
1	A	33	GLU	CD-OE1	6.18	1.37	1.25	12	8
1	A	14	GLU	CD-OE2	6.14	1.37	1.25	12	6
1	B	14	GLU	CD-OE2	6.13	1.37	1.25	14	8
1	B	40	ASP	CG-OD2	6.13	1.36	1.25	6	8
1	A	14	GLU	CD-OE1	6.12	1.36	1.25	5	9
1	A	24	GLU	CD-OE1	6.10	1.36	1.25	14	13
1	B	14	GLU	CD-OE1	6.08	1.36	1.25	9	7
1	B	17	GLU	CD-OE1	6.07	1.36	1.25	15	13
1	A	40	ASP	CG-OD1	6.05	1.36	1.25	5	8
1	A	17	GLU	CD-OE1	6.04	1.36	1.25	5	10
1	B	24	GLU	CD-OE1	6.01	1.36	1.25	2	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	4	ASP	CG-OD1	6.01	1.36	1.25	11	10
1	A	4	ASP	CG-OD2	6.01	1.36	1.25	14	5
1	A	33	GLU	CD-OE2	5.94	1.36	1.25	8	7
1	A	24	GLU	CD-OE2	5.93	1.36	1.25	13	2
1	B	33	GLU	CD-OE2	5.93	1.36	1.25	2	9
1	A	17	GLU	CD-OE2	5.89	1.36	1.25	6	5
1	B	33	GLU	CD-OE1	5.89	1.36	1.25	13	6
1	B	17	GLU	CD-OE2	5.86	1.36	1.25	1	2
1	A	21	PHE	N-CA	5.82	1.53	1.46	1	1
1	B	26	ASN	CA-C	5.82	1.58	1.52	2	1
1	B	24	GLU	CD-OE2	5.81	1.36	1.25	11	1
1	A	40	ASP	CG-OD2	5.81	1.36	1.25	8	7
1	B	31	ASN	CA-C	5.78	1.60	1.52	3	11
1	A	31	ASN	CA-C	5.75	1.60	1.52	9	12
1	B	22	ARG	CA-C	5.68	1.60	1.52	13	9
1	A	33	GLU	N-CA	5.50	1.52	1.46	2	1
1	B	33	GLU	N-CA	5.41	1.52	1.46	4	2
1	A	6	HIS	CE1-NE2	5.39	1.38	1.32	9	2
1	A	6	HIS	ND1-CE1	5.31	1.37	1.32	4	9
1	B	6	HIS	ND1-CE1	5.22	1.37	1.32	3	10
1	A	23	ALA	CA-C	5.19	1.59	1.52	1	2
1	B	6	HIS	CE1-NE2	5.16	1.37	1.32	10	2
1	B	28	ARG	CZ-NH2	-5.16	1.26	1.33	12	1
1	B	28	ARG	CA-C	5.09	1.58	1.52	1	1
1	A	22	ARG	CZ-NH2	-5.01	1.26	1.33	3	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	6	HIS	ND1-CE1-NE2	11.95	120.35	108.40	8	15
1	B	6	HIS	ND1-CE1-NE2	11.90	120.30	108.40	9	15
1	B	6	HIS	CB-CG-CD2	-11.75	115.93	131.20	12	4
1	A	6	HIS	CB-CG-CD2	-11.21	116.63	131.20	9	4
1	B	34	LEU	CB-CA-C	10.84	129.10	110.68	10	4
1	A	4	ASP	CA-CB-CG	10.60	123.19	112.60	8	14
1	A	34	LEU	CB-CA-C	10.51	130.85	110.46	15	5
1	A	21	PHE	CA-CB-CG	10.38	124.18	113.80	1	2
1	B	40	ASP	CA-CB-CG	10.30	122.91	112.60	7	10
1	B	6	HIS	CE1-NE2-CD2	-9.71	99.29	109.00	3	15
1	A	6	HIS	CE1-NE2-CD2	-9.68	99.32	109.00	8	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	26	ASN	CA-CB-CG	9.45	122.05	112.60	15	15
1	B	6	HIS	CA-CB-CG	9.38	123.18	113.80	10	4
1	A	33	GLU	CB-CG-CD	9.34	128.48	112.60	13	3
1	B	32	SER	N-CA-C	9.12	120.91	110.97	15	7
1	A	28	ARG	CB-CA-C	9.06	125.33	110.74	1	5
1	A	38	VAL	CA-CB-CG1	8.94	125.61	110.40	8	15
1	A	32	SER	N-CA-C	8.91	120.69	110.97	2	5
1	B	30	MET	N-CA-C	8.79	123.76	112.34	10	6
1	A	23	ALA	CB-CA-C	8.67	127.67	110.42	1	1
1	A	40	ASP	CA-CB-CG	8.63	121.23	112.60	6	7
1	B	33	GLU	N-CA-C	8.53	120.35	111.14	8	7
1	B	38	VAL	CA-CB-CG1	8.40	124.69	110.40	14	15
1	B	23	ALA	N-CA-C	8.23	119.94	110.97	4	2
1	A	30	MET	N-CA-C	7.78	121.70	111.75	15	7
1	A	33	GLU	N-CA-C	7.69	119.35	110.97	5	11
1	A	6	HIS	CA-CB-CG	7.60	121.40	113.80	9	3
1	A	24	GLU	N-CA-C	7.59	119.34	111.14	8	14
1	A	8	ASN	CA-CB-CG	7.58	120.18	112.60	5	5
1	B	33	GLU	CB-CA-C	-7.33	99.67	110.96	10	8
1	B	24	GLU	N-CA-C	7.31	119.32	111.36	3	14
1	A	37	ILE	CA-C-O	-7.30	113.11	120.85	5	8
1	B	18	LYS	CB-CA-C	7.27	123.21	110.85	4	3
1	A	7	PHE	CA-CB-CG	7.23	121.03	113.80	5	9
1	B	28	ARG	CB-CA-C	7.09	124.33	109.79	1	9
1	A	40	ASP	N-CA-CB	7.05	122.40	110.49	13	2
1	A	9	PHE	O-C-N	-6.99	113.90	123.12	10	3
1	A	19	LEU	CB-CA-C	6.94	122.65	110.85	7	4
1	A	31	ASN	CA-CB-CG	6.92	119.52	112.60	9	2
1	A	18	LYS	CB-CA-C	6.89	122.56	110.85	11	3
1	B	9	PHE	O-C-N	-6.85	114.08	123.12	5	4
1	B	8	ASN	CA-CB-CG	6.85	119.45	112.60	13	7
1	B	33	GLU	CB-CG-CD	6.83	124.20	112.60	14	3
1	A	40	ASP	N-CA-C	6.82	119.56	111.71	12	7
1	A	34	LEU	CA-C-O	-6.81	113.27	120.63	12	6
1	A	13	MET	N-CA-C	6.80	119.53	111.71	4	10
1	A	33	GLU	CB-CA-C	-6.78	100.18	110.90	3	11
1	B	28	ARG	CG-CD-NE	6.78	126.92	112.00	1	1
1	B	7	PHE	CA-CB-CG	6.78	120.58	113.80	10	6
1	B	5	PRO	N-CA-C	6.70	126.26	112.47	6	1
1	B	19	LEU	CB-CA-C	6.60	122.06	110.85	7	2
1	B	40	ASP	N-CA-C	6.56	119.26	111.33	8	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	13	MET	N-CA-C	6.50	118.36	111.28	11	11
1	B	34	LEU	CA-C-O	-6.44	113.68	120.63	12	7
1	B	18	LYS	N-CA-C	6.42	118.36	111.36	7	3
1	B	41	ALA	N-CA-C	6.39	120.56	113.21	6	2
1	B	10	ARG	CB-CA-C	6.39	123.13	110.42	8	1
1	B	17	GLU	N-CA-CB	-6.37	100.41	110.22	14	1
1	B	40	ASP	CB-CA-C	6.33	121.45	110.68	7	2
1	B	21	PHE	CA-C-O	-6.32	111.47	120.51	6	6
1	B	26	ASN	CB-CA-C	6.31	119.99	110.08	2	3
1	A	39	GLN	CA-C-O	-6.31	114.13	121.07	5	1
1	B	22	ARG	CB-CA-C	6.30	122.96	110.42	15	3
1	A	37	ILE	N-CA-C	6.28	116.45	110.42	11	2
1	A	14	GLU	N-CA-C	6.27	117.77	111.07	1	8
1	A	37	ILE	CA-C-N	6.23	128.53	120.56	8	1
1	A	37	ILE	C-N-CA	6.23	128.53	120.56	8	1
1	A	10	ARG	N-CA-CB	6.19	121.02	110.50	2	1
1	B	14	GLU	N-CA-C	6.18	117.69	111.07	6	6
1	B	5	PRO	CA-N-CD	-6.18	103.35	112.00	6	1
1	A	21	PHE	CA-C-O	-6.17	114.54	120.90	15	3
1	B	6	HIS	CG-ND1-CE1	-6.09	98.95	109.30	9	15
1	B	10	ARG	N-CA-CB	6.09	120.85	110.50	5	5
1	B	22	ARG	N-CA-CB	-6.09	100.20	110.49	3	3
1	B	31	ASN	CA-CB-CG	6.08	118.69	112.60	12	2
1	B	22	ARG	CA-CB-CG	6.06	126.21	114.10	3	1
1	A	6	HIS	CG-ND1-CE1	-6.02	99.06	109.30	7	15
1	A	36	GLN	CB-CA-C	5.95	120.97	110.85	1	2
1	B	40	ASP	N-CA-CB	5.95	119.47	109.78	12	5
1	B	37	ILE	CA-C-O	-5.93	114.06	120.47	14	6
1	A	18	LYS	N-CA-C	5.89	117.78	111.36	11	1
1	A	28	ARG	CG-CD-NE	5.87	124.91	112.00	3	2
1	A	40	ASP	CB-CA-C	5.84	121.43	110.63	12	2
1	A	9	PHE	CB-CA-C	5.82	119.36	109.53	12	1
1	A	41	ALA	N-CA-C	5.81	119.18	111.75	2	3
1	A	19	LEU	N-CA-C	5.77	117.25	111.07	15	1
1	A	39	GLN	N-CA-CB	-5.77	101.64	110.12	7	1
1	A	6	HIS	N-CA-C	5.77	118.17	109.23	9	1
1	B	37	ILE	CA-C-N	5.77	127.94	120.56	2	2
1	B	37	ILE	C-N-CA	5.77	127.94	120.56	2	2
1	A	21	PHE	N-CA-C	5.75	119.99	112.92	1	1
1	A	22	ARG	CB-CA-C	5.72	121.80	110.42	14	5
1	B	15	VAL	CA-CB-CG2	5.65	120.00	110.40	8	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	ASP	CB-CA-C	5.59	117.91	110.81	13	1
1	B	36	GLN	CB-CA-C	5.58	120.04	110.79	13	2
1	A	10	ARG	N-CA-C	5.51	118.01	110.24	3	1
1	B	28	ARG	O-C-N	-5.45	116.06	123.15	1	2
1	B	37	ILE	N-CA-C	5.39	117.83	111.09	13	3
1	B	35	LEU	N-CA-C	5.38	116.84	110.97	13	2
1	A	30	MET	O-C-N	-5.38	115.93	122.11	3	1
1	B	33	GLU	N-CA-CB	5.38	117.78	109.98	7	3
1	A	16	ARG	N-CA-C	5.34	119.35	112.41	2	1
1	A	22	ARG	N-CA-CB	-5.33	101.47	110.49	3	2
1	A	35	LEU	N-CA-CB	5.33	117.71	109.98	13	1
1	A	35	LEU	N-CA-C	5.32	116.76	111.07	3	3
1	B	28	ARG	CB-CG-CD	5.30	123.50	111.30	1	1
1	B	39	GLN	OE1-CD-NE2	-5.25	117.35	122.60	14	1
1	A	29	SER	CA-C-O	-5.22	115.11	120.54	1	1
1	B	21	PHE	CA-CB-CG	5.22	119.02	113.80	9	1
1	B	11	MET	O-C-N	-5.22	117.10	121.54	8	1
1	A	34	LEU	CB-CG-CD2	5.21	126.32	110.70	10	1
1	A	6	HIS	ND1-CG-CD2	5.18	111.28	106.10	9	1
1	A	15	VAL	CA-CB-CG2	5.17	119.18	110.40	11	2
1	B	41	ALA	CB-CA-C	5.16	119.46	110.79	3	1
1	B	9	PHE	CB-CA-C	5.15	120.01	109.76	3	1
1	A	33	GLU	N-CA-CB	5.13	117.50	110.07	1	1
1	B	26	ASN	OD1-CG-ND2	-5.12	117.47	122.60	3	1
1	A	19	LEU	N-CA-CB	-5.11	102.60	110.16	12	1
1	A	28	ARG	O-C-N	-5.09	116.62	123.23	3	1
1	B	12	PRO	CB-CA-C	5.08	117.74	111.23	3	1
1	B	36	GLN	CB-CG-CD	5.08	121.23	112.60	7	1
1	A	41	ALA	CB-CA-C	5.06	120.39	110.67	13	1
1	A	23	ALA	O-C-N	-5.05	115.88	122.59	1	1
1	A	15	VAL	N-CA-C	5.03	115.25	110.42	8	1
1	B	39	GLN	CA-C-O	-5.03	115.52	120.90	12	1
1	B	5	PRO	CB-CA-C	5.01	119.83	111.56	6	1

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	31	ASN	Peptide	15
1	B	29	SER	Peptide	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	29	SER	Peptide	14
1	B	31	ASN	Peptide	13
1	A	6	HIS	Peptide,Sidechain	12
1	A	9	PHE	Peptide,Sidechain	10
1	B	6	HIS	Peptide,Sidechain	10
1	B	9	PHE	Peptide,Sidechain	9
1	B	22	ARG	Mainchain	7
1	A	22	ARG	Mainchain	6
1	A	10	ARG	Peptide	3
1	A	16	ARG	Peptide,Mainchain	2
1	B	38	VAL	Peptide	2
1	B	5	PRO	Peptide	2
1	B	42	LEU	Peptide	2
1	B	12	PRO	Peptide	2
1	A	21	PHE	Peptide,Mainchain	1
1	A	23	ALA	Peptide	1
1	A	28	ARG	Peptide	1
1	A	11	MET	Peptide	1
1	A	40	ASP	Peptide	1
1	A	41	ALA	Peptide	1
1	B	41	ALA	Peptide	1
1	A	39	GLN	Peptide	1
1	B	10	ARG	Peptide	1
1	B	11	MET	Peptide	1
1	A	5	PRO	Peptide	1
1	A	8	ASN	Peptide	1
1	B	28	ARG	Sidechain	1
1	B	26	ASN	Peptide	1
1	B	20	LYS	Peptide	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	297	0	295	10±3
1	B	314	0	316	9±3
All	All	9165	0	9165	209

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:PHE:CD2	1:B:11:MET:HE3	0.75	2.17	15	4
1:A:7:PHE:CZ	1:B:34:LEU:HD12	0.73	2.19	6	11
1:A:34:LEU:HD12	1:B:7:PHE:CZ	0.73	2.19	3	10
1:B:9:PHE:CD2	1:B:11:MET:HE2	0.70	2.21	4	6
1:A:9:PHE:CD2	1:A:11:MET:HE3	0.70	2.22	13	6
1:A:9:PHE:CD2	1:A:11:MET:HE2	0.69	2.22	4	6
1:A:19:LEU:HB3	1:A:30:MET:CE	0.63	2.23	8	4
1:A:34:LEU:HD23	1:B:7:PHE:CZ	0.62	2.28	12	5
1:A:9:PHE:HD2	1:A:11:MET:HE3	0.59	1.57	10	1
1:A:9:PHE:CD2	1:B:34:LEU:HD13	0.59	2.33	11	11
1:A:19:LEU:HD13	1:A:34:LEU:HD22	0.58	1.76	13	2
1:A:34:LEU:HD13	1:B:9:PHE:CD2	0.57	2.34	9	10
1:A:19:LEU:HG	1:A:30:MET:SD	0.57	2.40	5	1
1:B:19:LEU:HG	1:B:30:MET:SD	0.55	2.40	2	1
1:A:11:MET:SD	1:A:19:LEU:HD23	0.55	2.42	1	3
1:A:19:LEU:HD21	1:A:34:LEU:HG	0.55	1.78	6	6
1:A:34:LEU:HD13	1:B:9:PHE:CG	0.53	2.38	1	10
1:A:9:PHE:CG	1:B:34:LEU:HD13	0.53	2.38	6	10
1:A:7:PHE:CZ	1:B:34:LEU:HD23	0.53	2.38	12	3
1:B:11:MET:SD	1:B:19:LEU:HD23	0.53	2.44	4	3
1:A:19:LEU:HD21	1:A:34:LEU:HD22	0.53	1.81	12	3
1:A:34:LEU:HD22	1:B:9:PHE:CE2	0.53	2.38	6	1
1:B:19:LEU:HD22	1:B:30:MET:SD	0.53	2.44	7	1
1:B:9:PHE:CD2	1:B:11:MET:SD	0.52	3.02	8	3
1:B:19:LEU:HD13	1:B:34:LEU:HD22	0.52	1.81	12	1
1:A:19:LEU:HD22	1:A:30:MET:SD	0.52	2.44	7	1
1:A:38:VAL:HG13	1:B:19:LEU:HD12	0.52	1.82	8	1
1:A:19:LEU:HB3	1:A:30:MET:HE3	0.51	1.81	15	2
1:A:19:LEU:CD2	1:A:34:LEU:HD22	0.51	2.35	12	3
1:A:16:ARG:HG2	1:A:30:MET:HE1	0.51	1.82	4	3
1:A:22:ARG:O	1:A:24:GLU:N	0.51	2.43	1	1
1:A:9:PHE:CD2	1:A:11:MET:SD	0.50	3.04	7	2
1:B:19:LEU:HB3	1:B:30:MET:CE	0.50	2.37	7	3
1:B:19:LEU:HB3	1:B:30:MET:HE1	0.50	1.84	7	1
1:B:19:LEU:HB3	1:B:30:MET:HE3	0.50	1.83	13	1
1:A:16:ARG:CB	1:A:30:MET:HE1	0.49	2.37	2	1
1:A:20:LYS:HB2	1:A:30:MET:SD	0.49	2.48	1	2
1:B:19:LEU:HD21	1:B:34:LEU:HD22	0.48	1.86	14	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:LEU:HD21	1:B:34:LEU:HG	0.48	1.85	5	2
1:B:19:LEU:HD21	1:B:34:LEU:CD2	0.47	2.40	4	2
1:B:19:LEU:CD2	1:B:34:LEU:HD22	0.47	2.39	14	2
1:B:34:LEU:HD22	1:B:38:VAL:HG21	0.47	1.87	2	1
1:B:16:ARG:HG2	1:B:30:MET:HE1	0.47	1.87	4	2
1:A:19:LEU:HB3	1:A:30:MET:SD	0.47	2.50	8	1
1:B:19:LEU:HD22	1:B:34:LEU:HB2	0.46	1.88	12	1
1:A:34:LEU:HD13	1:B:9:PHE:CE2	0.46	2.46	8	1
1:B:19:LEU:C	1:B:30:MET:HE3	0.46	2.35	3	3
1:A:19:LEU:HD21	1:A:34:LEU:CG	0.45	2.41	6	1
1:B:38:VAL:HA	1:B:41:ALA:HB3	0.45	1.88	8	1
1:A:34:LEU:HD22	1:A:38:VAL:HG21	0.44	1.88	5	2
1:A:11:MET:HB2	1:B:35:LEU:HD21	0.44	1.88	6	1
1:A:34:LEU:O	1:A:38:VAL:HG23	0.43	2.13	1	6
1:A:22:ARG:HH21	1:A:37:ILE:HD11	0.43	1.74	4	1
1:A:19:LEU:CD2	1:A:34:LEU:HG	0.43	2.44	6	1
1:A:23:ALA:HB2	1:A:33:GLU:HB3	0.43	1.90	1	1
1:B:10:ARG:C	1:B:11:MET:SD	0.43	3.01	8	1
1:B:21:PHE:O	1:B:25:ALA:HB3	0.43	2.14	10	1
1:A:9:PHE:HD2	1:A:34:LEU:HD11	0.43	1.72	3	1
1:A:19:LEU:C	1:A:30:MET:HE3	0.43	2.39	1	2
1:B:20:LYS:N	1:B:30:MET:HE3	0.43	2.29	3	1
1:A:30:MET:SD	1:A:34:LEU:HB2	0.43	2.54	5	2
1:B:23:ALA:HB2	1:B:33:GLU:CB	0.43	2.44	8	3
1:B:28:ARG:HE	1:B:33:GLU:HG2	0.42	1.74	8	1
1:A:23:ALA:HB2	1:A:33:GLU:CB	0.42	2.44	5	3
1:B:28:ARG:HE	1:B:36:GLN:HB3	0.42	1.73	1	1
1:A:34:LEU:HD13	1:B:9:PHE:CD1	0.42	2.50	4	1
1:A:19:LEU:HD21	1:A:34:LEU:CD2	0.42	2.45	2	1
1:A:7:PHE:CE2	1:B:34:LEU:HD23	0.42	2.50	12	1
1:A:9:PHE:HD2	1:A:11:MET:HE2	0.42	1.69	2	1
1:A:37:ILE:O	1:A:41:ALA:HB2	0.42	2.15	3	1
1:A:9:PHE:CE2	1:B:34:LEU:HD22	0.42	2.50	15	1
1:A:19:LEU:HD22	1:A:34:LEU:HB2	0.42	1.92	15	1
1:B:34:LEU:O	1:B:38:VAL:HG23	0.41	2.15	4	2
1:B:13:MET:HA	1:B:13:MET:HE2	0.41	1.91	1	1
1:A:19:LEU:HD22	1:B:38:VAL:CG1	0.41	2.45	5	1
1:B:21:PHE:O	1:B:22:ARG:C	0.41	2.63	6	1
1:A:9:PHE:CE1	1:B:35:LEU:HG	0.41	2.51	15	1
1:A:34:LEU:HB3	1:B:9:PHE:CE1	0.41	2.50	7	1
1:A:21:PHE:O	1:A:22:ARG:C	0.40	2.64	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:PHE:HD2	1:B:11:MET:HE2	0.40	1.72	7	1
1:A:9:PHE:CD2	1:A:11:MET:CE	0.40	3.04	14	1
1:A:19:LEU:HD11	1:B:38:VAL:HG11	0.40	1.94	15	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	35/76 (46%)	27±1 (78±4%)	5±1 (14±4%)	3±1 (8±3%)	1	13
1	B	38/76 (50%)	30±2 (78±5%)	6±2 (15±5%)	3±1 (7±2%)	2	17
All	All	1095/2280 (48%)	851 (78%)	162 (15%)	82 (7%)	1	15

All 15 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	22	ARG	15
1	A	22	ARG	14
1	A	23	ALA	11
1	B	23	ALA	10
1	A	10	ARG	8
1	B	10	ARG	8
1	A	32	SER	5
1	B	32	SER	2
1	B	5	PRO	2
1	A	8	ASN	2
1	B	27	GLY	1
1	A	21	PHE	1
1	B	8	ASN	1
1	A	12	PRO	1
1	A	5	PRO	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	33/68 (49%)	27±1 (82±4%)	6±1 (18±4%)	4	37
1	B	34/68 (50%)	27±2 (79±5%)	7±2 (21±5%)	3	31
All	All	1005/2040 (49%)	811 (81%)	194 (19%)	3	34

All 40 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	15	VAL	15
1	A	34	LEU	15
1	B	15	VAL	15
1	B	34	LEU	15
1	A	36	GLN	11
1	B	36	GLN	10
1	B	26	ASN	8
1	B	31	ASN	8
1	B	37	ILE	7
1	A	37	ILE	6
1	A	16	ARG	5
1	B	16	ARG	5
1	B	19	LEU	5
1	B	40	ASP	5
1	A	13	MET	4
1	B	10	ARG	4
1	B	13	MET	4
1	B	11	MET	4
1	A	11	MET	4
1	A	33	GLU	3
1	A	20	LYS	3
1	A	31	ASN	3
1	A	30	MET	3
1	B	33	GLU	3
1	A	10	ARG	3
1	A	40	ASP	3
1	B	38	VAL	3
1	A	14	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	28	ARG	2
1	B	30	MET	2
1	A	19	LEU	2
1	A	38	VAL	2
1	B	20	LYS	2
1	B	6	HIS	2
1	A	21	PHE	1
1	B	22	ARG	1
1	B	14	GLU	1
1	B	39	GLN	1
1	B	42	LEU	1
1	B	28	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided