



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 11:25 AM UTC

PDB ID : 1G4D / pdb_00001g4d
Title : NMR STRUCTURE OF THE MU BACTERIOPHAGE REPRESSOR DNA-BINDING DOMAIN/DNA COMPLEX
Authors : Wojciak, J.M.; Iwahara, J.; Clubb, R.T.
Deposited on : 2000-10-26

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

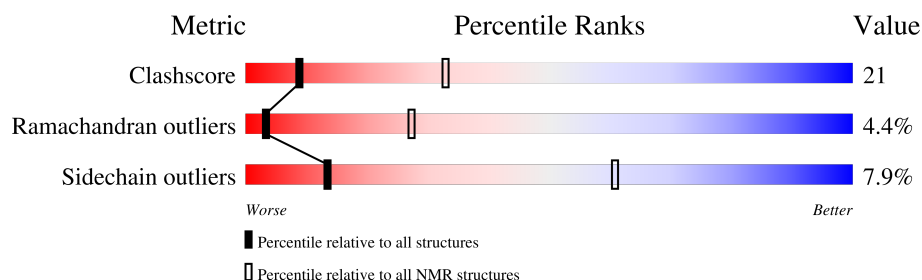
1 Overall quality at a glance

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	B	16	
2	C	16	
3	A	69	

2 Ensemble composition and analysis

This entry contains 25 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:79 (67)	0.46	16

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 12, 13, 21, 22, 23
2	6, 7, 10, 14, 16, 17
3	1, 8, 11, 18, 19, 20
4	9, 24
5	3, 25
Single-model clusters	5; 15

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2076 atoms, of which 894 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	B	16	Total	C	H	N	O	P	0
			506	156	183	51	100	16	

- Molecule 2 is a DNA chain called 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
2	C	16	Total	C	H	N	O	P	0
			512	158	179	67	92	16	

- Molecule 3 is a protein called REPRESSOR PROTEIN C.

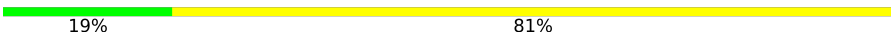
Mol	Chain	Residues	Atoms						Trace
3	A	69	Total	C	H	N	O	S	0
			1058	328	532	95	98	5	

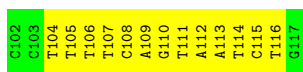
4 Residue-property plots

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: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',

Chain B: 



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',

Chain C: 



- Molecule 3: REPRESSOR PROTEIN C

Chain A: 

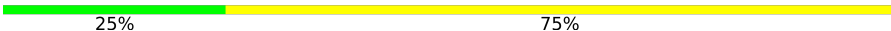


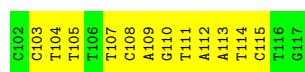
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',

Chain B: 



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



4.2.2 Score per residue for model 2

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



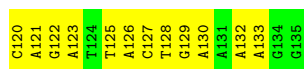
4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C



4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



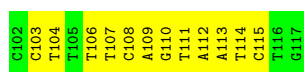
- Molecule 3: REPRESSOR PROTEIN C



4.2.7 Score per residue for model 7

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C



4.2.8 Score per residue for model 8

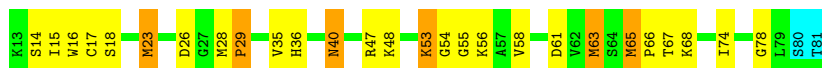
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



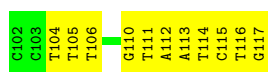
- Molecule 3: REPRESSOR PROTEIN C



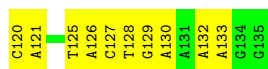
4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,

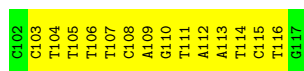


- Molecule 3: REPRESSOR PROTEIN C



4.2.10 Score per residue for model 10

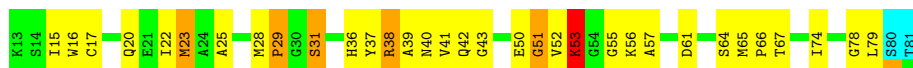
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



4.2.11 Score per residue for model 11

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



- Molecule 3: REPRESSOR PROTEIN C



4.2.12 Score per residue for model 12

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



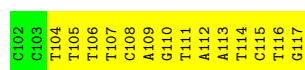
- Molecule 3: REPRESSOR PROTEIN C



4.2.13 Score per residue for model 13

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C

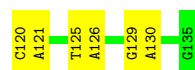


4.2.14 Score per residue for model 14

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



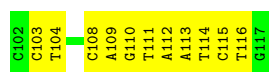
- Molecule 3: REPRESSOR PROTEIN C



4.2.15 Score per residue for model 15

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C



4.2.16 Score per residue for model 16 (medoid)

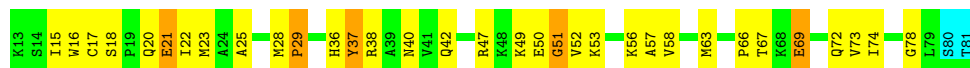
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C



4.2.17 Score per residue for model 17

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',

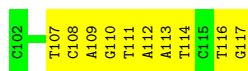


- Molecule 3: REPRESSOR PROTEIN C



4.2.18 Score per residue for model 18

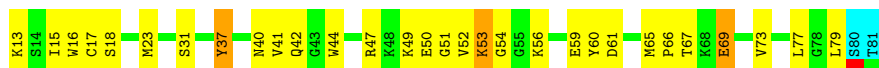
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



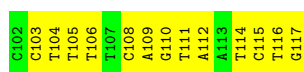
- Molecule 3: REPRESSOR PROTEIN C



4.2.19 Score per residue for model 19

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',

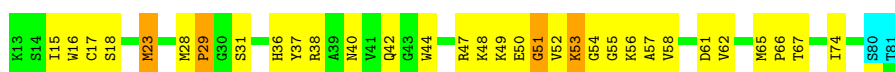




- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,

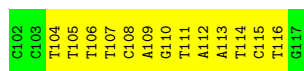


- Molecule 3: REPRESSOR PROTEIN C

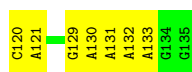


4.2.20 Score per residue for model 20

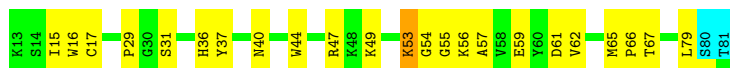
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



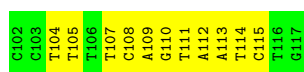
- Molecule 3: REPRESSOR PROTEIN C



4.2.21 Score per residue for model 21

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,





- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,

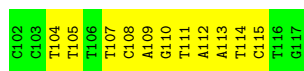


- Molecule 3: REPRESSOR PROTEIN C



4.2.22 Score per residue for model 22

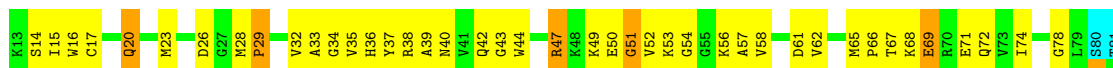
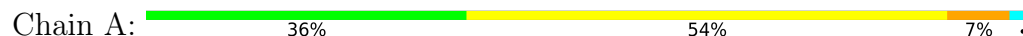
- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3 ,



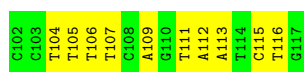
- Molecule 3: REPRESSOR PROTEIN C



4.2.23 Score per residue for model 23

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3 ,

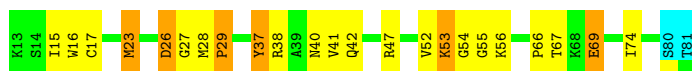




- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',

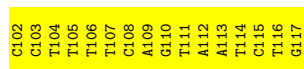


- Molecule 3: REPRESSOR PROTEIN C



4.2.24 Score per residue for model 24

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



- Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



- Molecule 3: REPRESSOR PROTEIN C



4.2.25 Score per residue for model 25

- Molecule 1: 5'-D(P*CP*CP*TP*TP*TP*TP*CP*AP*GP*TP*AP*AP*TP*CP*TP*G)-3',



C102
C103
T104
T105
T106
T107
C108
A109
G110
T111
A112
A113
T114
C115
T116
G117

● Molecule 2: 5'-D(P*CP*AP*GP*AP*TP*TP*AP*CP*TP*GP*AP*AP*AP*AP*GP*G)-3',



C120
A121
T125
A126
G129
A130
A131
A132
A133
G134
G135

● Molecule 3: REPRESSOR PROTEIN C



K13
S14
I15
W16
C17
M23
M28
P29
H36
Y37
M40
W44
R47
K48
K49
E50
G51
V52
K53
G54
G55
K56
A57
V58
E59
Y60
D61
S64
M65
P66
T67
R68
E69
I74
S80
T81

5 Refinement protocol and experimental data overview ⓘ

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

Of the ? calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	
X-PLOR	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	0.55±0.00	0±0/359 (0.0± 0.0%)	1.16±0.00	0±0/551 (0.0± 0.0%)
2	C	0.52±0.01	0±0/375 (0.0± 0.0%)	1.07±0.00	0±0/577 (0.0± 0.0%)
3	A	1.48±0.01	0±0/523 (0.0± 0.0%)	1.19±0.02	0±0/703 (0.0± 0.1%)
All	All	1.04	0/31425 (0.0%)	1.14	3/45775 (0.0%)

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
3	A	76	HIS	N-CA-C	-5.50	105.29	111.28	11	1
3	A	27	GLY	N-CA-C	-5.16	108.87	115.42	5	1
3	A	77	LEU	N-CA-C	-5.14	105.75	111.36	11	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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	B	323	183	184	9±2
2	C	333	179	180	8±2
3	A	512	520	517	29±4
All	All	29200	22050	22025	1071

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:44:TRP:CE3	3:A:65:MET:HE1	0.90	2.02	20	6
3:A:65:MET:SD	3:A:65:MET:N	0.65	2.69	18	9
3:A:44:TRP:CZ3	3:A:65:MET:HE1	0.65	2.26	21	2
3:A:16:TRP:CD1	3:A:47:ARG:HH21	0.63	2.12	17	17
3:A:16:TRP:CD1	3:A:47:ARG:NH2	0.61	2.68	23	6
3:A:79:LEU:HD12	3:A:79:LEU:N	0.61	2.10	20	2
3:A:38:ARG:NH1	3:A:42:GLN:NE2	0.61	2.49	10	2
2:C:120:DC:H2''	2:C:121:DA:O5'	0.61	1.96	12	25
2:C:129:DG:H2''	2:C:130:DA:O5'	0.61	1.95	12	25
2:C:125:DT:H2''	2:C:126:DA:O5'	0.61	1.96	16	21
2:C:120:DC:H6	2:C:120:DC:O5'	0.60	1.79	8	16
3:A:15:ILE:C	3:A:16:TRP:CD1	0.59	2.81	8	25
3:A:54:GLY:O	3:A:56:LYS:N	0.59	2.34	5	7
3:A:38:ARG:CZ	3:A:42:GLN:HE21	0.59	2.10	17	1
1:B:110:DG:N2	3:A:56:LYS:HZ2	0.59	1.95	17	2
3:A:44:TRP:CE3	3:A:65:MET:HE3	0.58	2.32	18	7
3:A:38:ARG:NH1	3:A:42:GLN:HE21	0.58	1.96	10	2
1:B:110:DG:N2	3:A:56:LYS:NZ	0.58	2.51	17	2
1:B:110:DG:N3	3:A:56:LYS:NZ	0.58	2.52	16	4
1:B:102:DC:H6	1:B:102:DC:O5'	0.56	1.84	8	4
1:B:111:DT:H2''	1:B:112:DA:O5'	0.56	2.01	25	22
3:A:20:GLN:NE2	3:A:23:MET:CE	0.56	2.69	10	1
3:A:50:GLU:O	3:A:52:VAL:N	0.56	2.39	16	21
3:A:79:LEU:CD1	3:A:79:LEU:N	0.56	2.69	5	1
1:B:113:DA:H2''	1:B:114:DT:O5'	0.56	2.01	4	18
3:A:37:TYR:O	3:A:40:ASN:ND2	0.56	2.39	2	20
3:A:36:HIS:O	3:A:40:ASN:ND2	0.55	2.39	12	20
3:A:16:TRP:NE1	3:A:47:ARG:HH21	0.55	1.99	1	7
3:A:59:GLU:OE1	3:A:59:GLU:N	0.55	2.38	3	3
3:A:69:GLU:OE1	3:A:69:GLU:N	0.55	2.40	5	15
3:A:63:MET:N	3:A:63:MET:SD	0.55	2.79	6	2
3:A:26:ASP:O	3:A:28:MET:N	0.55	2.40	7	3
3:A:79:LEU:N	3:A:79:LEU:CD1	0.55	2.70	2	2
1:B:109:DA:C2	2:C:129:DG:N2	0.55	2.74	3	4
3:A:38:ARG:NH2	3:A:69:GLU:OE2	0.54	2.41	13	2
1:B:112:DA:C6	1:B:113:DA:C6	0.54	2.95	3	5
3:A:40:ASN:OD1	3:A:41:VAL:N	0.54	2.40	18	7
3:A:20:GLN:N	3:A:20:GLN:CD	0.54	2.65	22	1
3:A:79:LEU:N	3:A:79:LEU:HD12	0.54	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:55:GLY:C	3:A:57:ALA:N	0.54	2.65	5	6
3:A:50:GLU:C	3:A:52:VAL:H	0.54	2.11	18	3
3:A:37:TYR:O	3:A:40:ASN:OD1	0.53	2.27	24	1
3:A:59:GLU:N	3:A:59:GLU:CD	0.53	2.65	18	4
3:A:59:GLU:N	3:A:59:GLU:OE1	0.53	2.42	18	1
1:B:104:DT:H2''	1:B:105:DT:O5'	0.53	2.03	20	16
3:A:15:ILE:HG22	3:A:16:TRP:N	0.53	2.18	7	25
3:A:16:TRP:CE2	3:A:61:ASP:OD1	0.53	2.62	22	1
1:B:110:DG:H2''	1:B:111:DT:O5'	0.53	2.04	6	19
3:A:16:TRP:CD1	3:A:16:TRP:N	0.53	2.76	8	23
3:A:54:GLY:C	3:A:56:LYS:H	0.53	2.12	1	20
1:B:112:DA:N3	3:A:53:LYS:NZ	0.53	2.57	10	2
3:A:22:ILE:CG2	3:A:28:MET:SD	0.53	2.97	16	2
3:A:66:PRO:O	3:A:69:GLU:N	0.52	2.43	17	1
2:C:122:DG:C6	2:C:123:DA:C6	0.52	2.98	3	6
3:A:53:LYS:O	3:A:55:GLY:N	0.52	2.42	12	8
3:A:21:GLU:N	3:A:21:GLU:OE1	0.52	2.41	17	2
3:A:61:ASP:O	3:A:65:MET:SD	0.52	2.68	18	6
3:A:38:ARG:HH11	3:A:42:GLN:HE21	0.52	1.47	10	1
2:C:122:DG:C4	2:C:123:DA:C8	0.52	2.98	13	1
3:A:20:GLN:NE2	3:A:32:VAL:HG22	0.52	2.19	22	1
2:C:125:DT:C4	2:C:126:DA:C6	0.52	2.98	4	5
2:C:131:DA:H2''	2:C:132:DA:O5'	0.52	2.04	5	3
3:A:38:ARG:HE	3:A:42:GLN:NE2	0.52	2.03	4	2
2:C:129:DG:P	3:A:36:HIS:HE2	0.52	2.26	20	6
3:A:54:GLY:C	3:A:56:LYS:N	0.52	2.68	5	7
3:A:66:PRO:O	3:A:67:THR:C	0.52	2.52	17	25
3:A:16:TRP:CE2	3:A:47:ARG:NH2	0.52	2.77	15	3
1:B:107:DT:H2''	1:B:108:DC:O5'	0.52	2.04	25	19
2:C:132:DA:H2''	2:C:133:DA:O5'	0.51	2.05	20	13
2:C:125:DT:C4	2:C:126:DA:N6	0.51	2.78	14	3
3:A:26:ASP:C	3:A:28:MET:N	0.51	2.68	7	3
3:A:50:GLU:O	3:A:51:GLY:C	0.51	2.53	22	16
3:A:69:GLU:OE1	3:A:72:GLN:NE2	0.51	2.43	14	2
3:A:39:ALA:O	3:A:43:GLY:N	0.51	2.44	22	7
3:A:40:ASN:CG	3:A:41:VAL:N	0.51	2.67	4	7
1:B:105:DT:H2'	1:B:106:DT:H72	0.51	1.81	24	5
3:A:31:SER:OG	3:A:34:GLY:N	0.51	2.42	24	1
3:A:26:ASP:C	3:A:28:MET:H	0.51	2.14	23	7
1:B:116:DT:H2''	1:B:117:DG:O5'	0.51	2.06	4	10
3:A:50:GLU:C	3:A:52:VAL:N	0.50	2.69	5	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:23:MET:C	3:A:23:MET:SD	0.50	2.94	24	11
2:C:128:DT:O2	3:A:56:LYS:CE	0.50	2.59	10	4
3:A:42:GLN:NE2	3:A:44:TRP:HE1	0.50	2.04	18	2
1:B:103:DC:H2''	1:B:104:DT:O5'	0.50	2.07	3	8
3:A:28:MET:HE1	3:A:69:GLU:OE1	0.50	2.07	24	3
3:A:74:ILE:O	3:A:78:GLY:N	0.50	2.41	14	11
1:B:112:DA:C2	1:B:113:DA:C2	0.50	3.00	18	4
3:A:49:LYS:NZ	3:A:59:GLU:CD	0.49	2.70	20	2
3:A:15:ILE:CG2	3:A:16:TRP:N	0.49	2.75	17	25
2:C:126:DA:C5	2:C:127:DC:N4	0.49	2.80	7	1
2:C:126:DA:C4	2:C:127:DC:C5	0.49	3.00	16	1
3:A:20:GLN:HE22	3:A:32:VAL:HG22	0.49	1.68	22	1
3:A:16:TRP:C	3:A:17:CYS:SG	0.49	2.95	7	22
1:B:105:DT:C7	3:A:31:SER:OG	0.49	2.61	13	3
1:B:115:DC:H2''	1:B:116:DT:O5'	0.49	2.07	6	6
1:B:108:DC:H2''	1:B:109:DA:O5'	0.49	2.07	15	13
2:C:124:DT:H2''	2:C:125:DT:O5'	0.49	2.07	24	2
3:A:28:MET:SD	3:A:28:MET:N	0.49	2.86	9	1
3:A:55:GLY:C	3:A:57:ALA:H	0.49	2.15	5	6
2:C:128:DT:O2	3:A:56:LYS:NZ	0.49	2.46	17	3
3:A:38:ARG:CZ	3:A:69:GLU:OE2	0.49	2.61	24	1
1:B:114:DT:H2''	1:B:115:DC:O5'	0.48	2.07	22	17
3:A:79:LEU:HD22	3:A:79:LEU:N	0.48	2.22	6	1
3:A:17:CYS:SG	3:A:62:VAL:CG2	0.48	3.01	21	5
3:A:29:PRO:C	3:A:31:SER:H	0.48	2.16	20	1
3:A:56:LYS:O	3:A:58:VAL:HG13	0.48	2.08	11	1
3:A:22:ILE:O	3:A:25:ALA:N	0.48	2.42	21	5
3:A:38:ARG:HH21	3:A:42:GLN:HE22	0.48	1.50	19	4
3:A:14:SER:C	3:A:15:ILE:HD12	0.48	2.33	6	2
3:A:71:GLU:CD	3:A:72:GLN:N	0.47	2.72	22	1
1:B:103:DC:H2'	1:B:104:DT:H72	0.47	1.86	4	1
3:A:38:ARG:HH11	3:A:42:GLN:NE2	0.47	2.07	10	1
1:B:102:DC:H2''	1:B:103:DC:O5'	0.47	2.10	4	2
3:A:53:LYS:C	3:A:55:GLY:H	0.47	2.17	8	11
1:B:108:DC:C4	1:B:109:DA:N6	0.47	2.82	19	1
3:A:20:GLN:NE2	3:A:20:GLN:CA	0.47	2.76	22	1
2:C:129:DG:OP2	3:A:36:HIS:NE2	0.47	2.46	1	1
3:A:27:GLY:O	3:A:38:ARG:NH1	0.47	2.45	15	1
3:A:22:ILE:C	3:A:24:ALA:N	0.47	2.70	15	3
2:C:130:DA:OP2	3:A:36:HIS:CG	0.47	2.68	15	1
1:B:106:DT:H2''	1:B:107:DT:O5'	0.47	2.10	25	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:122:DG:C5	2:C:123:DA:N7	0.46	2.83	13	1
2:C:130:DA:H2''	2:C:131:DA:O5'	0.46	2.10	22	6
3:A:65:MET:O	3:A:66:PRO:C	0.46	2.59	13	17
3:A:55:GLY:O	3:A:57:ALA:N	0.46	2.48	5	1
1:B:109:DA:C2	2:C:129:DG:C2	0.46	3.04	12	1
3:A:58:VAL:O	3:A:58:VAL:HG13	0.46	2.11	22	3
3:A:36:HIS:O	3:A:40:ASN:CG	0.45	2.59	1	3
3:A:15:ILE:C	3:A:16:TRP:CG	0.45	2.95	4	5
3:A:28:MET:O	3:A:29:PRO:O	0.45	2.34	22	12
2:C:122:DG:H2''	2:C:123:DA:O5'	0.45	2.11	22	8
3:A:16:TRP:CZ2	3:A:47:ARG:NH2	0.45	2.84	15	2
1:B:105:DT:H2''	1:B:106:DT:O5'	0.45	2.12	5	1
3:A:23:MET:O	3:A:29:PRO:O	0.45	2.35	22	4
2:C:127:DC:H2''	2:C:128:DT:O5'	0.45	2.11	3	3
3:A:21:GLU:CD	3:A:21:GLU:N	0.45	2.75	5	1
2:C:122:DG:C6	2:C:123:DA:C5	0.45	3.05	13	2
3:A:44:TRP:CZ3	3:A:65:MET:HE3	0.45	2.46	7	1
3:A:58:VAL:O	3:A:58:VAL:HG23	0.45	2.12	5	2
3:A:56:LYS:O	3:A:57:ALA:C	0.45	2.60	16	2
1:B:112:DA:C2	2:C:126:DA:C2	0.45	3.05	10	1
2:C:122:DG:C2	2:C:123:DA:C4	0.45	3.05	13	1
1:B:113:DA:C1'	3:A:53:LYS:NZ	0.45	2.80	16	2
3:A:49:LYS:NZ	3:A:59:GLU:OE2	0.45	2.50	21	1
3:A:52:VAL:O	3:A:53:LYS:O	0.45	2.35	10	8
3:A:36:HIS:ND1	3:A:60:TYR:OH	0.44	2.46	9	1
3:A:60:TYR:CD1	3:A:60:TYR:N	0.44	2.86	18	1
1:B:112:DA:H2''	1:B:113:DA:O5'	0.44	2.12	20	3
3:A:15:ILE:O	3:A:61:ASP:OD1	0.44	2.34	22	4
3:A:69:GLU:OE1	3:A:69:GLU:CA	0.44	2.65	25	13
1:B:113:DA:C4	3:A:53:LYS:NZ	0.44	2.84	10	1
2:C:128:DT:OP1	3:A:20:GLN:NE2	0.44	2.50	9	1
1:B:112:DA:C2	3:A:53:LYS:NZ	0.44	2.78	10	1
1:B:112:DA:N6	2:C:124:DT:O4	0.44	2.50	21	2
3:A:49:LYS:O	3:A:57:ALA:O	0.44	2.36	17	5
1:B:113:DA:N3	3:A:53:LYS:NZ	0.44	2.51	6	1
2:C:128:DT:C4	2:C:129:DG:C6	0.44	3.06	19	1
3:A:49:LYS:O	3:A:50:GLU:OE1	0.44	2.36	22	1
3:A:48:LYS:O	3:A:50:GLU:OE2	0.43	2.36	3	1
3:A:49:LYS:O	3:A:50:GLU:OE2	0.43	2.36	3	2
2:C:130:DA:OP2	3:A:36:HIS:ND1	0.43	2.51	15	1
3:A:71:GLU:C	3:A:71:GLU:OE1	0.43	2.61	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:38:ARG:NH1	3:A:38:ARG:CG	0.43	2.79	10	1
3:A:26:ASP:C	3:A:72:GLN:OE1	0.43	2.62	14	1
3:A:14:SER:OG	3:A:61:ASP:OD1	0.43	2.35	22	1
2:C:125:DT:O4	2:C:126:DA:N6	0.43	2.51	4	3
3:A:44:TRP:CD1	3:A:44:TRP:N	0.43	2.86	15	1
3:A:28:MET:HE2	3:A:69:GLU:OE1	0.43	2.12	1	1
3:A:69:GLU:N	3:A:69:GLU:CD	0.43	2.76	22	4
3:A:26:ASP:O	3:A:72:GLN:OE1	0.43	2.36	14	1
3:A:49:LYS:HZ3	3:A:59:GLU:CD	0.43	2.22	20	1
3:A:49:LYS:CB	3:A:49:LYS:NZ	0.43	2.82	2	1
3:A:26:ASP:N	3:A:26:ASP:OD1	0.43	2.48	9	1
3:A:73:VAL:O	3:A:77:LEU:N	0.43	2.44	15	2
2:C:129:DG:P	3:A:36:HIS:NE2	0.43	2.92	20	1
3:A:16:TRP:CE3	3:A:47:ARG:CB	0.43	3.02	2	1
3:A:22:ILE:O	3:A:23:MET:C	0.43	2.62	24	3
3:A:14:SER:OG	3:A:15:ILE:N	0.43	2.52	14	3
2:C:122:DG:C6	2:C:123:DA:N6	0.43	2.86	11	1
3:A:16:TRP:NE1	3:A:47:ARG:NH2	0.43	2.66	5	2
3:A:40:ASN:OD1	3:A:41:VAL:HG23	0.43	2.14	2	1
3:A:28:MET:O	3:A:29:PRO:C	0.43	2.62	12	5
3:A:79:LEU:N	3:A:79:LEU:CD2	0.43	2.82	6	1
2:C:126:DA:O4'	3:A:53:LYS:NZ	0.43	2.52	11	1
3:A:68:LYS:O	3:A:71:GLU:OE2	0.43	2.37	22	1
3:A:27:GLY:O	3:A:69:GLU:OE2	0.42	2.36	1	1
3:A:36:HIS:O	3:A:40:ASN:OD1	0.42	2.37	1	2
3:A:49:LYS:CD	3:A:59:GLU:OE1	0.42	2.67	5	1
3:A:35:VAL:O	3:A:36:HIS:C	0.42	2.62	8	2
2:C:126:DA:C4	2:C:127:DC:C4	0.42	3.06	7	2
2:C:122:DG:N1	2:C:123:DA:C5	0.42	2.87	13	1
3:A:50:GLU:O	3:A:52:VAL:O	0.42	2.37	19	1
3:A:38:ARG:HH21	3:A:42:GLN:NE2	0.42	2.13	22	1
3:A:71:GLU:CD	3:A:71:GLU:C	0.42	2.87	22	1
3:A:73:VAL:O	3:A:74:ILE:C	0.42	2.63	13	1
1:B:112:DA:N1	1:B:113:DA:C6	0.42	2.88	3	1
1:B:113:DA:C5	1:B:114:DT:C4	0.42	3.08	4	1
2:C:126:DA:C6	2:C:127:DC:N4	0.42	2.88	7	1
3:A:21:GLU:N	3:A:21:GLU:CD	0.42	2.77	16	1
2:C:126:DA:C5	2:C:127:DC:C4	0.42	3.07	5	2
3:A:69:GLU:O	3:A:73:VAL:HG23	0.42	2.15	16	1
3:A:61:ASP:O	3:A:64:SER:OG	0.42	2.36	10	3
2:C:122:DG:O6	2:C:123:DA:N6	0.42	2.53	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:121:DA:H2''	2:C:122:DG:O5'	0.42	2.15	16	2
3:A:31:SER:O	3:A:32:VAL:C	0.41	2.62	21	2
2:C:128:DT:H2''	2:C:129:DG:O5'	0.41	2.15	19	1
3:A:40:ASN:OD1	3:A:40:ASN:C	0.41	2.63	4	2
2:C:133:DA:H2''	2:C:134:DG:O5'	0.41	2.16	6	4
1:B:104:DT:H71	1:B:104:DT:OP2	0.41	2.15	11	1
3:A:38:ARG:CZ	3:A:42:GLN:NE2	0.41	2.83	17	1
3:A:48:LYS:NZ	3:A:55:GLY:O	0.41	2.48	21	1
3:A:61:ASP:OD1	3:A:61:ASP:C	0.41	2.63	20	2
3:A:58:VAL:O	3:A:58:VAL:CG1	0.41	2.68	22	1
1:B:112:DA:C2	1:B:113:DA:C4	0.41	3.09	3	1
3:A:37:TYR:O	3:A:38:ARG:C	0.41	2.63	23	1
3:A:46:LYS:CB	3:A:46:LYS:NZ	0.41	2.84	7	1
3:A:53:LYS:C	3:A:55:GLY:N	0.41	2.79	11	2
2:C:127:DC:H2''	2:C:128:DT:O4'	0.41	2.16	9	1
3:A:42:GLN:OE1	3:A:44:TRP:NE1	0.41	2.42	9	1
3:A:33:ALA:O	3:A:34:GLY:C	0.41	2.64	22	1
2:C:128:DT:O2	3:A:56:LYS:CD	0.41	2.68	23	1
3:A:58:VAL:O	3:A:58:VAL:CG2	0.41	2.69	5	1
3:A:56:LYS:HZ3	3:A:56:LYS:HB2	0.41	1.75	15	1
3:A:16:TRP:O	3:A:17:CYS:SG	0.40	2.79	7	1
3:A:18:SER:O	3:A:19:PRO:C	0.40	2.64	13	1
3:A:49:LYS:O	3:A:57:ALA:HB3	0.40	2.15	16	1
3:A:23:MET:SD	3:A:23:MET:C	0.40	3.04	19	1
3:A:35:VAL:C	3:A:37:TYR:N	0.40	2.78	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	66/69 (96%)	57±2 (86±3%)	6±2 (10±3%)	3±1 (4±1%)	3	27
All	All	1650/1725 (96%)	1415 (86%)	162 (10%)	73 (4%)	3	27

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	51	GLY	20
3	A	29	PRO	18
3	A	53	LYS	17
3	A	37	TYR	10
3	A	27	GLY	3
3	A	26	ASP	2
3	A	54	GLY	2
3	A	55	GLY	1

6.3.2 Protein sidechains [i](#)

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	
3	A	53/55 (96%)	49±2 (92±3%)	4±2 (8±3%)	13	61
All	All	1325/1375 (96%)	1220 (92%)	105 (8%)	13	61

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)
3	A	23	MET	23
3	A	69	GLU	15
3	A	18	SER	8
3	A	65	MET	6
3	A	48	LYS	4
3	A	53	LYS	4
3	A	13	LYS	4
3	A	31	SER	4
3	A	63	MET	4
3	A	40	ASN	3
3	A	46	LYS	3
3	A	20	GLN	3
3	A	21	GLU	3
3	A	49	LYS	2
3	A	47	ARG	2
3	A	59	GLU	2
3	A	58	VAL	2
3	A	68	LYS	2

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Mol	Chain	Res	Type	Models (Total)
3	A	79	LEU	2
3	A	64	SER	2
3	A	26	ASP	1
3	A	45	THR	1
3	A	70	ARG	1
3	A	28	MET	1
3	A	38	ARG	1
3	A	56	LYS	1
3	A	35	VAL	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