



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:37 PM BST

PDB ID : 2K5X
Title : Chemical shift structure of COLICIN E9 DNASE domain with its cognate immunity protein IM9
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Deposited on : 2008-07-01

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:

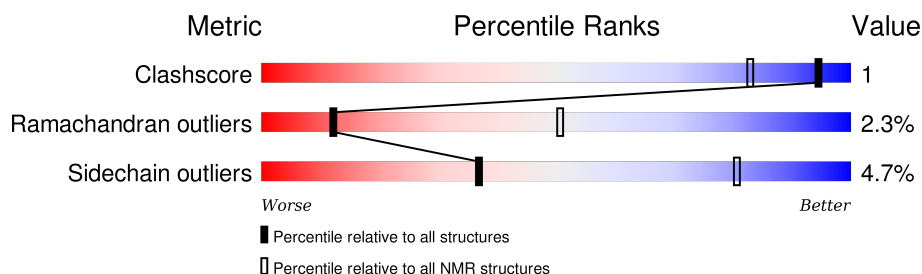
Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal 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 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	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	86	<div> <div style="width: 69%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div>69% 26% 6%</div> </div>
2	B	134	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div>72% 25% •</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2148 atoms, of which 411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Colicin-E9 immunity protein.

Mol	Chain	Residues	Atoms						Trace
1	A	86	Total	C	H	N	O	S	0
			816	418	143	108	144	3	

- Molecule 2 is a protein called Colicin-E9.

Mol	Chain	Residues	Atoms						Trace
2	B	134	Total	C	H	N	O	S	0
			1332	661	268	197	204	2	

There is a discrepancy between the modelled and reference sequences:

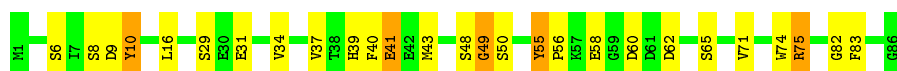
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP P09883

4 Residue-property plots

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: Colicin-E9 immunity protein

Chain A: 



- Molecule 2: Colicin-E9

Chain B: 



5 Refinement protocol and experimental data overview ⓘ

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

Of the 500 calculated structures, 1 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
CHESHIRE	geometry optimization	

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	1.64	5/686 (0.7%)	2.13	30/926 (3.2%)
2	B	1.62	8/1088 (0.7%)	2.08	35/1457 (2.4%)
All	All	1.62	13/1774 (0.7%)	2.10	65/2383 (2.7%)

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	2
2	B	0	2
All	All	0	4

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	TYR	CD2-CE2	-6.04	1.30	1.39
2	B	46	GLU	CD-OE2	-5.58	1.19	1.25
1	A	74	TRP	CG-CD2	-5.55	1.34	1.43
2	B	58	TRP	CG-CD1	5.53	1.44	1.36
1	A	58	GLU	CD-OE2	-5.27	1.19	1.25
2	B	63	LYS	CA-CB	-5.23	1.42	1.53
1	A	31	GLU	CD-OE2	-5.22	1.20	1.25
2	B	108	SER	CB-OG	5.21	1.49	1.42
1	A	65	SER	CA-CB	5.17	1.60	1.52
2	B	3	SER	CA-CB	5.12	1.60	1.52
2	B	77	SER	CA-CB	5.10	1.60	1.52
2	B	124	PRO	CA-CB	-5.06	1.43	1.53
2	B	2	GLU	CD-OE2	-5.03	1.20	1.25

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	114	TYR	CB-CG-CD2	-13.98	112.61	121.00
2	B	114	TYR	CG-CD1-CE1	-11.99	111.71	121.30
1	A	74	TRP	NE1-CE2-CZ2	-11.78	117.44	130.40
1	A	74	TRP	CE2-CD2-CG	-11.75	97.90	107.30
2	B	22	TRP	CE2-CD2-CG	-11.52	98.09	107.30
1	A	74	TRP	CD1-CG-CD2	9.91	114.23	106.30
2	B	22	TRP	NE1-CE2-CD2	9.58	116.88	107.30
2	B	5	ARG	NE-CZ-NH1	9.52	125.06	120.30
2	B	22	TRP	CD1-CG-CD2	8.77	113.31	106.30
2	B	126	ARG	NE-CZ-NH2	8.47	124.53	120.30
2	B	44	ASP	CB-CG-OD1	8.35	125.82	118.30
1	A	74	TRP	NE1-CE2-CD2	8.25	115.55	107.30
2	B	22	TRP	NE1-CE2-CZ2	-7.92	121.69	130.40
2	B	114	TYR	CD1-CG-CD2	7.78	126.46	117.90
1	A	55	TYR	CD1-CE1-CZ	-7.45	113.10	119.80
1	A	10	TYR	CG-CD1-CE1	7.43	127.24	121.30
1	A	40	PHE	CB-CG-CD2	-7.04	115.88	120.80
2	B	71	LEU	CB-CG-CD2	-7.03	99.06	111.00
1	A	83	PHE	CB-CG-CD1	-6.75	116.07	120.80
2	B	129	ASP	CB-CG-OD2	6.54	124.18	118.30
2	B	32	ALA	CB-CA-C	-6.43	100.45	110.10
1	A	37	VAL	CA-CB-CG1	6.43	120.55	110.90
2	B	53	PHE	CB-CG-CD2	-6.42	116.30	120.80
2	B	26	ALA	O-C-N	-6.24	112.59	123.20
2	B	22	TRP	CG-CD2-CE3	6.18	139.47	133.90
1	A	31	GLU	O-C-N	-6.17	112.83	122.70
2	B	126	ARG	NE-CZ-NH1	-6.13	117.23	120.30
2	B	54	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	62	ASP	O-C-N	-5.97	113.14	122.70
1	A	55	TYR	N-CA-CB	5.96	121.33	110.60
2	B	29	ASP	CB-CG-OD1	-5.95	112.95	118.30
2	B	44	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	9	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	16	LEU	CA-CB-CG	5.88	128.84	115.30
2	B	58	TRP	NE1-CE2-CD2	5.87	113.17	107.30
2	B	58	TRP	CB-CG-CD1	-5.81	119.45	127.00
1	A	71	VAL	CA-CB-CG1	5.79	119.58	110.90
1	A	9	ASP	CB-CG-OD1	-5.77	113.11	118.30
2	B	37	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	75	ARG	CA-CB-CG	5.70	125.93	113.40
2	B	71	LEU	CB-CG-CD1	5.62	120.55	111.00
2	B	50	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	A	55	TYR	CG-CD1-CE1	5.58	125.76	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	SER	N-CA-CB	-5.54	102.19	110.50
2	B	132	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	28	LYS	O-C-N	-5.48	113.93	122.70
1	A	75	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	58	TRP	CB-CG-CD2	5.39	133.61	126.60
2	B	54	ARG	CD-NE-CZ	5.26	130.96	123.60
2	B	22	TRP	CD1-NE1-CE2	-5.25	104.27	109.00
1	A	74	TRP	CD1-NE1-CE2	-5.20	104.32	109.00
1	A	56	PRO	CA-C-N	-5.19	105.79	117.20
1	A	65	SER	N-CA-CB	-5.19	102.72	110.50
1	A	10	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
2	B	29	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	58	TRP	NE1-CE2-CZ2	-5.13	124.76	130.40
2	B	108	SER	CA-C-N	5.12	128.47	117.20
1	A	60	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	29	SER	O-C-N	5.12	130.88	122.70
1	A	6	SER	CA-CB-OG	5.08	124.92	111.20
2	B	37	ARG	CB-CG-CD	5.06	124.76	111.60
1	A	62	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	A	34	VAL	CA-CB-CG1	5.05	118.48	110.90
2	B	45	LYS	CA-CB-CG	5.03	124.47	113.40
1	A	83	PHE	CG-CD1-CE1	-5.00	115.30	120.80

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
2	B	96	ARG	Sidechain
1	A	55	TYR	Sidechain
2	B	47	PHE	Sidechain
1	A	10	TYR	Sidechain

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	673	143	635	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	B	1064	268	1060	3
All	All	1737	411	1695	5

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:116:MET:HA	2:B:119:ILE:HD12	0.65	1.67
1:A:41:GLU:HG3	1:A:49:GLY:HA3	0.56	1.76
1:A:75:ARG:HH21	1:A:82:GLY:N	0.44	2.09
2:B:55:LYS:O	2:B:59:GLU:HG3	0.44	2.11
2:B:42:LEU:HD22	2:B:47:PHE:CZ	0.41	2.51

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	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	12	49
2	B	132/134 (99%)	111 (84%)	18 (14%)	3 (2%)	12	51
All	All	216/220 (98%)	185 (86%)	26 (12%)	5 (2%)	12	51

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	73	PRO
1	A	49	GLY
1	A	8	SER
2	B	85	PRO
2	B	29	ASP

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	76/76 (100%)	72 (95%)	4 (5%)	33	77
2	B	117/117 (100%)	112 (96%)	5 (4%)	40	83
All	All	193/193 (100%)	184 (95%)	9 (5%)	37	80

All 9 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	124	PRO
1	A	50	SER
2	B	117	ASP
1	A	41	GLU
2	B	20	ASP
2	B	73	PRO
1	A	43	MET
2	B	79	VAL
1	A	39	HIS

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 [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