

Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 03:43 PM EDT

PDB ID : 1MZ8

Title : CRYSTAL STRUCTURES OF THE NUCLEASE DOMAIN OF COLE7/IM7

IN COMPLEX WITH A PHOSPHATE ION AND A ZINC ION

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Deposited on : 2002-10-07

Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

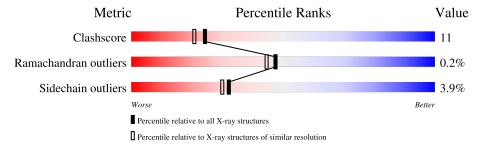
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.00 Å.

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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
Clashscore	141614	9178 (2.00-2.00)		
Ramachandran outliers	138981	9054 (2.00-2.00)		
Sidechain outliers	138945	9053 (2.00-2.00)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	87	83%	16%	•
1	С	87	75%	21%	•••
2	В	131	83%	15%	•
2	D	131	79%	18%	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4081 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Colicin E7 immunity protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	87	Total 698	C 440	• '	O 145	S 1	0	0	0
1	С	87	Total 698			O 145	S 1	0	0	0

• Molecule 2 is a protein called Colicin E7.

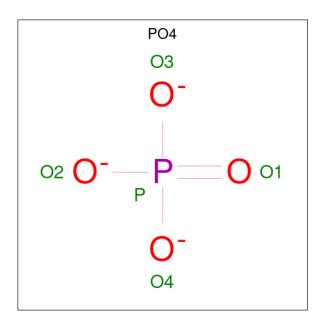
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	131	Total	С	N	О	S	0	0	0
2			1060	657	206	195	2			
2	D	130	Total	С	N	О	S	0	0	0
2		130	1051	651	204	194	2	0	0	U

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

$\bullet\,$ Molecule 5 is water.

Mol	Chain	Residues	Atoms	$\mathbf{ZeroOcc}$	AltConf
5	A	123	Total O 123 123	0	0
5	В	149	Total O 149 149	0	0
5	С	122	Total O 122 122	0	0
5	D	168	Total O 168 168	0	0

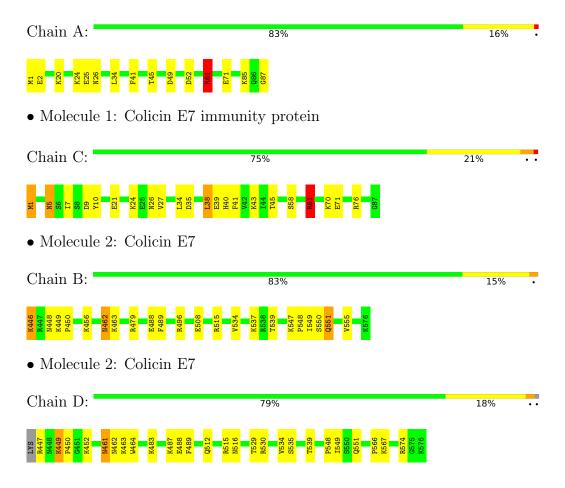


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Colicin E7 immunity protein





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 2	Depositor	
Cell constants	119.73Å 62.41Å 74.14Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	27.97 - 2.00	Depositor	
% Data completeness	93.6 (27.97-2.00)	Depositor	
(in resolution range)	30.0 (21.31 2.00)		
R_{merge}	(Not available)	Depositor	
R_{sym}	0.06	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.183 , 0.230	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4081	wwPDB-VP	
Average B, all atoms (Å ²)	29.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.75	0/711	0.86	2/960~(0.2%)	
1	С	0.72	0/711	0.84	2/960~(0.2%)	
2	В	0.61	0/1082	0.70	0/1444	
2	D	0.66	0/1073	0.69	0/1433	
All	All	0.68	0/3577	0.76	4/4797 (0.1%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	61	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	С	61	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	61	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	С	61	ARG	NE-CZ-NH1	8.07	124.33	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	698	0	674	8	0
1	С	698	0	674	20	0
2	В	1060	0	1069	29	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1051	0	1056	31	0
3	В	1	0	0	0	0
3	D	1	0	0	0	0
4	В	5	0	0	0	0
4	D	5	0	0	0	0
5	A	123	0	0	1	0
5	В	149	0	0	9	0
5	С	122	0	0	2	0
5	D	168	0	0	4	0
All	All	4081	0	3473	77	0

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 (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
2:D:452:LYS:HE3	2:D:488:GLU:HB3	1.59	0.85
2:B:446:LYS:N	2:B:449:LYS:HD3	1.94	0.80
2:B:549:ILE:HD13	2:B:555:VAL:HG23	1.65	0.78
2:B:515:ARG:CZ	2:D:515:ARG:CZ	2.64	0.76
1:C:26:ASN:HD21	2:D:516:ASN:HD22	1.32	0.76
1:A:85:LYS:HE2	1:A:87:GLY:OXT	1.89	0.71
2:D:534:VAL:HG22	2:D:539:THR:HA	1.72	0.71
2:D:464:TRP:H	2:D:512:GLN:HE22	1.41	0.69
1:C:5:ASN:HD22	1:C:5:ASN:N	1.91	0.68
2:B:496:ARG:HH11	2:B:496:ARG:HG2	1.57	0.68
1:A:41:PHE:O	1:A:45:THR:HG23	1.94	0.68
1:C:5:ASN:ND2	1:C:5:ASN:H	1.90	0.68
2:D:447:ARG:N	2:D:449:LYS:HZ2	1.94	0.65
2:B:548:PRO:HG2	2:B:551:GLN:HG2	1.78	0.64
2:B:534:VAL:HG22	2:B:539:THR:HA	1.82	0.62
1:C:5:ASN:N	1:C:5:ASN:ND2	2.45	0.62
1:A:61:ARG:HD3	1:A:71:GLU:OE1	1.99	0.62
2:D:548:PRO:HG2	2:D:551:GLN:HG2	1.81	0.61
2:B:496:ARG:HD3	5:B:793:HOH:O	2.00	0.60
1:C:26:ASN:ND2	2:D:516:ASN:HD22	1.98	0.60
2:D:452:LYS:CE	2:D:488:GLU:HB3	2.32	0.59
1:C:35:ASP:O	1:C:39:GLU:HG3	2.03	0.59
2:B:508:GLU:HG3	5:B:976:HOH:O	2.02	0.58
1:C:61:ARG:HD3	1:C:71:GLU:OE1	2.04	0.58



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Continued from prev		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap (Å)
2:B:515:ARG:CZ	2:D:515:ARG:NE	2.67	0.57
1:C:34:LEU:HG	1:C:38:LEU:HD22	1.85	0.57
2:D:461:ASN:ND2	2:D:463:LYS:H	2.03	0.56
2:B:496:ARG:HG2	2:B:496:ARG:NH1	2.20	0.56
2:B:548:PRO:HG2	2:B:551:GLN:CG	2.36	0.55
2:B:496:ARG:HD3	5:B:858:HOH:O	2.05	0.55
2:B:515:ARG:NH1	2:D:515:ARG:HD3	2.21	0.54
2:D:483:LYS:O	2:D:487:LYS:HE2	2.08	0.54
2:B:515:ARG:NH1	2:D:515:ARG:NE	2.56	0.53
1:A:20:LYS:HG3	1:C:27:VAL:HG21	1.91	0.53
1:A:2:GLU:HG2	5:A:871:HOH:O	2.09	0.52
2:B:515:ARG:NH1	2:D:515:ARG:CD	2.72	0.52
2:D:449:LYS:HD2	2:D:449:LYS:H	1.75	0.51
1:C:61:ARG:CD	1:C:71:GLU:OE1	2.58	0.51
2:B:446:LYS:HA	5:B:996:HOH:O	2.09	0.51
2:D:549:ILE:HG13	5:D:1053:HOH:O	2.11	0.50
2:D:515:ARG:NH1	5:D:984:HOH:O	2.40	0.50
1:C:41:PHE:O	1:C:45:THR:HG23	2.12	0.50
2:D:548:PRO:HG2	2:D:551:GLN:CG	2.41	0.50
2:B:479:ARG:NH2	2:B:508:GLU:HB2	2.27	0.49
1:C:7:ILE:HG21	1:C:76:ARG:CZ	2.43	0.49
2:B:456:LYS:HG3	5:B:1091:HOH:O	2.12	0.48
2:B:462:ASN:ND2	2:B:463:LYS:HG2	2.29	0.48
2:D:530:ARG:NH1	5:D:737:HOH:O	2.48	0.47
1:C:1:MET:HB3	5:C:820:HOH:O	2.14	0.47
2:D:534:VAL:CG1	2:D:535:SER:N	2.78	0.47
2:D:549:ILE:HG12	2:D:549:ILE:O	2.15	0.46
2:D:574:ARG:HD3	5:D:1067:HOH:O	2.16	0.46
2:B:450:PRO:HA	2:B:489:PHE:O	2.16	0.46
1:C:43:LYS:HD3	5:C:1134:HOH:O	2.17	0.45
2:B:549:ILE:HB	5:B:959:HOH:O	2.15	0.45
2:B:446:LYS:NZ	2:B:449:LYS:NZ	2.65	0.45
2:B:549:ILE:HD11	5:B:996:HOH:O	2.16	0.45
2:D:529:THR:HG21	2:D:566:PRO:HD3	1.99	0.45
1:A:24:LYS:HE2	1:C:21:GLU:OE1	2.16	0.45
2:D:447:ARG:N	2:D:449:LYS:HD2	2.32	0.44
2:D:450:PRO:HA	2:D:489:PHE:O	2.19	0.43
1:C:10:TYR:OH	1:C:40:HIS:HE1	2.02	0.43
2:D:449:LYS:HD2	2:D:449:LYS:N	2.34	0.43
2:B:547:LYS:HA	2:B:548:PRO:HD2	1.86	0.43
1:C:5:ASN:ND2	1:C:9:ASP:OD2	2.52	0.42



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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
2:D:462:ASN:O	2:D:463:LYS:HD3	2.19	0.42
2:B:446:LYS:NZ	2:B:449:LYS:HZ2	2.18	0.42
5:B:1114:HOH:O	1:C:70:LYS:HE2	2.20	0.42
1:A:25:GLU:HB3	1:A:34:LEU:HB2	2.02	0.42
1:A:49:ASP:HB3	1:A:52:ASP:HB2	2.02	0.41
2:B:496:ARG:NH1	2:B:496:ARG:CG	2.82	0.41
2:B:537:LYS:HE3	5:B:1121:HOH:O	2.19	0.41
1:C:26:ASN:ND2	2:D:516:ASN:ND2	2.68	0.41
2:D:463:LYS:HD3	2:D:463:LYS:HA	1.88	0.41
1:C:24:LYS:HD3	1:C:24:LYS:C	2.41	0.40
2:B:446:LYS:HE2	2:B:448:ASN:HB2	2.03	0.40
2:B:515:ARG:NE	2:D:515:ARG:CZ	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	ntiles
1	A	85/87~(98%)	84 (99%)	1 (1%)	0	100	100
1	\mathbf{C}	85/87 (98%)	85 (100%)	0	0	100	100
2	В	129/131 (98%)	125 (97%)	3 (2%)	1 (1%)	19	13
2	D	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
All	All	$427/436 \ (98\%)$	419 (98%)	7 (2%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	551	GLN



5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	entiles
1	A	77/77 (100%)	74 (96%)	3 (4%)	32	30
1	С	77/77 (100%)	72 (94%)	5 (6%)	17	12
2	В	117/117 (100%)	113 (97%)	4 (3%)	37	36
2	D	116/117 (99%)	113 (97%)	3 (3%)	46	48
All	All	387/388 (100%)	372 (96%)	15 (4%)	32	30

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	ASN
1	A	61	ARG
2	В	446	LYS
2	В	462	ASN
2	В	488	GLU
2	В	550	SER
1	С	1	MET
1	С	5	ASN
1	С	38	LEU
1	С	58	SER
1	С	61	ARG
2	D	449	LYS
2	D	461	ASN
2	D	567	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	462	ASN
2	В	518	ASN
1	С	5	ASN
1	С	26	ASN



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Mol	Chain	Res	Type
1	С	40	HIS
2	D	461	ASN
2	D	466	ASN
2	D	512	GLN
2	D	518	ASN
2	D	532	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal Tours Chaire Das		n Dog Link		Bond lengths			В	ond ang	gles	
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	В	601	3	4,4,4	1.97	2 (50%)	6,6,6	0.40	0
4	PO4	D	601	3	4,4,4	1.44	1 (25%)	6,6,6	0.44	0

All (3) bond length outliers are listed below:

I	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
	4	В	601	PO4	P-O3	-2.36	1.47	1.54



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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
4	D	601	PO4	P-O2	-2.04	1.48	1.54
4	В	601	PO4	P-O2	-2.03	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

