Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 PM GMT

PDB ID	:	7CEI
Title	:	THE ENDONUCLEASE DOMAIN OF COLICIN E7 IN COMPLEX WITH ITS INHIBITOR IM7 PROTEIN
Authors	:	Ko, T.P.; Liao, C.C.; Ku, W.Y.; Chak, K.F.; Yuan, H.S.
Deposited on	:	1998-09-17
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
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:

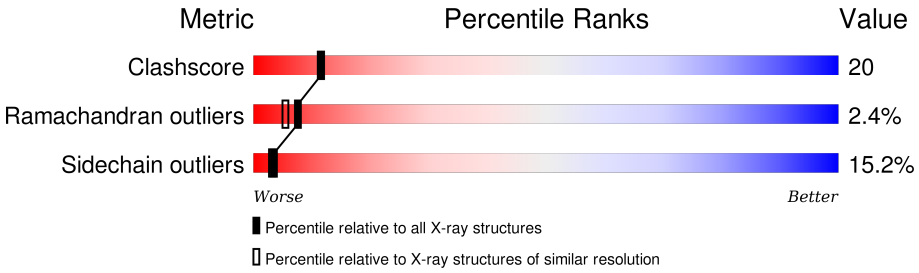
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	62% 34% .
2	B	206	31% 23% 7% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1887 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 PROTEIN (COLICIN E7 IMMUNITY PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			698	440	112	145	1			

- Molecule 2 is a protein called PROTEIN (COLICIN E7 IMMUNITY PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	0
			1026	637	197	190	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	76	Total	O	0	0
			76	76		

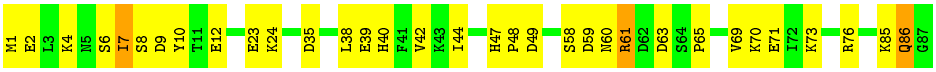
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

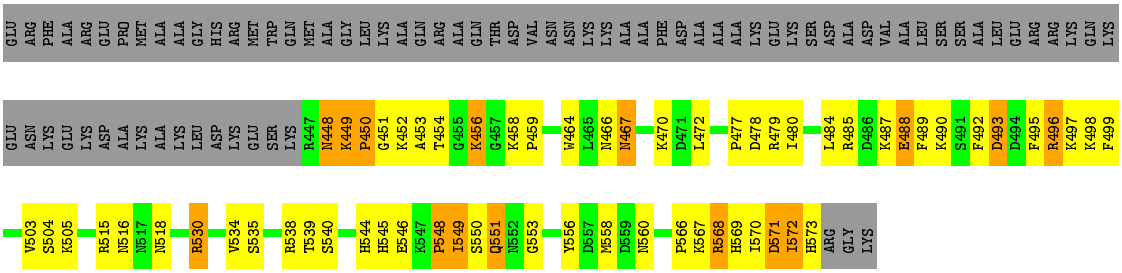
- Molecule 1: PROTEIN (COLICIN E7 IMMUNITY PROTEIN)

Chain A:



- Molecule 2: PROTEIN (COLICIN E7 IMMUNITY PROTEIN)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	65.44Å 76.02Å 119.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	76.8 (40.00-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.203 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1887	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/711	0.53	0/960
2	B	0.32	0/1048	0.49	0/1403
All	All	0.32	0/1759	0.51	0/2363

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	698	0	674	21	0
2	B	1026	0	1027	52	0
3	B	1	0	0	0	0
4	A	86	0	0	1	0
4	B	76	0	0	2	0
All	All	1887	0	1701	70	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 20.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	4:A:833:HOH:O	1.73	0.88
1:A:35:ASP:O	1:A:39:GLU:HG3	1.74	0.87
2:B:448:ASN:HA	2:B:449:LYS:HE3	1.57	0.87
2:B:549:ILE:H	2:B:549:ILE:HD12	1.44	0.82
1:A:61:ARG:HD3	1:A:71:GLU:OE1	1.85	0.76
2:B:496:ARG:HD2	4:B:857:HOH:O	1.85	0.75
1:A:63:ASP:OD2	2:B:515:ARG:HG3	1.90	0.71
2:B:472:LEU:HB2	2:B:568:ARG:HD3	1.75	0.69
2:B:477:PRO:HB2	2:B:480:ILE:HG12	1.75	0.68
2:B:472:LEU:CB	2:B:568:ARG:HD3	2.25	0.67
2:B:549:ILE:HA	2:B:553:GLY:HA2	1.75	0.67
2:B:489:PHE:HB2	2:B:556:TYR:HE2	1.59	0.67
1:A:23:GLU:HG2	2:B:516:ASN:HD21	1.61	0.66
2:B:496:ARG:HG3	2:B:497:LYS:N	2.11	0.64
2:B:493:ASP:HA	2:B:496:ARG:HG2	1.82	0.61
2:B:459:PRO:HA	2:B:478:ASP:OD2	1.99	0.61
2:B:453:ALA:HA	2:B:556:TYR:HB3	1.83	0.60
1:A:58:SER:HB3	1:A:60:ASN:ND2	2.16	0.60
2:B:451:GLY:O	2:B:488:GLU:HA	2.01	0.60
2:B:534:VAL:HG13	2:B:538:ARG:O	2.02	0.60
2:B:546:GLU:HB2	2:B:560:ASN:OD1	2.03	0.59
2:B:567:LYS:O	2:B:571:ASP:HB2	2.03	0.59
2:B:449:LYS:HD2	2:B:449:LYS:H	1.67	0.59
2:B:530:ARG:HB3	2:B:530:ARG:HH11	1.69	0.58
2:B:530:ARG:HG3	4:B:836:HOH:O	2.04	0.56
2:B:548:PRO:HG2	2:B:551:GLN:HG3	1.88	0.56
1:A:1:MET:HG3	1:A:2:GLU:N	2.21	0.55
2:B:448:ASN:CA	2:B:449:LYS:HE3	2.34	0.55
2:B:489:PHE:HB2	2:B:556:TYR:CE2	2.41	0.55
2:B:530:ARG:HB3	2:B:530:ARG:NH1	2.22	0.55
1:A:40:HIS:O	1:A:44:ILE:HG12	2.07	0.54
2:B:452:LYS:HA	2:B:487:LYS:O	2.08	0.53
2:B:544:HIS:ND1	2:B:545:HIS:N	2.57	0.51
1:A:58:SER:HB3	1:A:60:ASN:HD21	1.75	0.51
1:A:6:SER:HB3	1:A:9:ASP:OD2	2.10	0.51
1:A:7:ILE:HG21	1:A:76:ARG:NE	2.25	0.51
2:B:569:HIS:O	2:B:573:HIS:CD2	2.65	0.50
1:A:65:PRO:O	1:A:69:VAL:HG23	2.12	0.50
2:B:450:PRO:HA	2:B:489:PHE:O	2.11	0.50
1:A:7:ILE:HG21	1:A:76:ARG:CZ	2.42	0.50
1:A:12:GLU:OE2	1:A:73:LYS:HD2	2.12	0.49
2:B:453:ALA:HB3	2:B:484:LEU:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:O	1:A:42:VAL:HG23	2.12	0.48
2:B:479:ARG:HG3	2:B:479:ARG:HH11	1.78	0.48
2:B:472:LEU:HB3	2:B:568:ARG:HD3	1.96	0.48
2:B:566:PRO:O	2:B:570:ILE:HD12	2.13	0.48
1:A:4:LYS:HB2	1:A:10:TYR:CE2	2.50	0.47
2:B:449:LYS:CD	2:B:449:LYS:N	2.78	0.47
1:A:23:GLU:HG2	2:B:516:ASN:ND2	2.30	0.47
2:B:454:THR:O	2:B:558:MET:N	2.42	0.46
2:B:535:SER:OG	2:B:570:ILE:HD13	2.15	0.46
2:B:456:LYS:HA	2:B:485:ARG:HH21	1.79	0.46
2:B:459:PRO:CA	2:B:478:ASP:OD2	2.64	0.45
2:B:569:HIS:CE1	2:B:573:HIS:HE2	2.33	0.45
2:B:568:ARG:O	2:B:572:ILE:HG12	2.16	0.45
2:B:569:HIS:O	2:B:573:HIS:HD2	2.00	0.45
2:B:467:ASN:HA	2:B:467:ASN:HD22	1.62	0.44
2:B:544:HIS:CG	2:B:545:HIS:N	2.86	0.44
2:B:492:PHE:O	2:B:495:PHE:HB3	2.18	0.44
2:B:556:TYR:CD1	2:B:556:TYR:N	2.87	0.43
1:A:1:MET:CG	1:A:2:GLU:N	2.82	0.43
2:B:534:VAL:CG1	2:B:539:THR:HG22	2.49	0.43
2:B:479:ARG:HG3	2:B:479:ARG:NH1	2.34	0.42
1:A:86:GLN:HA	1:A:86:GLN:OE1	2.18	0.42
2:B:534:VAL:HG11	2:B:539:THR:HG22	2.02	0.41
2:B:535:SER:HB3	2:B:566:PRO:HB2	2.02	0.41
2:B:449:LYS:N	2:B:449:LYS:HD2	2.32	0.41
1:A:47:HIS:ND1	1:A:49:ASP:HB2	2.36	0.41
2:B:499:PHE:O	2:B:503:VAL:HG23	2.20	0.41
1:A:47:HIS:ND1	1:A:48:PRO:HD2	2.36	0.41

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	Percentiles
1	A	85/87 (98%)	85 (100%)	0	0	100 100
2	B	125/206 (61%)	109 (87%)	11 (9%)	5 (4%)	4 2
All	All	210/293 (72%)	194 (92%)	11 (5%)	5 (2%)	7 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	466	ASN
2	B	450	PRO
2	B	464	TRP
2	B	548	PRO
2	B	572	ILE

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	Percentiles
1	A	77/77 (100%)	69 (90%)	8 (10%)	9 10
2	B	114/174 (66%)	93 (82%)	21 (18%)	2 1
All	All	191/251 (76%)	162 (85%)	29 (15%)	3 3

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	SER
1	A	24	LYS
1	A	59	ASP
1	A	61	ARG
1	A	70	LYS
1	A	85	LYS
1	A	86	GLN
2	B	448	ASN
2	B	449	LYS
2	B	456	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	458	LYS
2	B	467	ASN
2	B	470	LYS
2	B	488	GLU
2	B	490	LYS
2	B	493	ASP
2	B	496	ARG
2	B	498	LYS
2	B	504	SER
2	B	505	LYS
2	B	518	ASN
2	B	530	ARG
2	B	540	SER
2	B	549	ILE
2	B	550	SER
2	B	551	GLN
2	B	568	ARG
2	B	571	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	60	ASN
2	B	462	ASN
2	B	467	ASN
2	B	512	GLN
2	B	516	ASN
2	B	518	ASN
2	B	532	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.