Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 01:36 am BST

PDB ID	:	1CEW
Title	:	THE 2.0 ANGSTROMS X-RAY CRYSTAL STRUCTURE OF CHICKEN EGG WHITE CYSTATIN AND ITS POSSIBLE MODE OF INTERACTION WITH CYSTEINE PROTEINASES
Authors	:	Bode, W.; Musil, D.; Huber, R.
Deposited on	:	1993-04-21
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 following versions of software and data (see references (i)) were used in the production of this report:

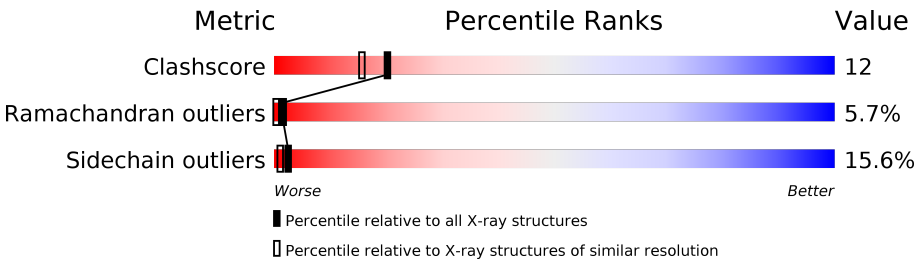
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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 (#Entries)	Similar resolution (#Entries, resolution range(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 on 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	I	108	42% 32% 19% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 977 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 CYSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	108	854	535	147	166	6	45	0	0

- Molecule 2 is water.

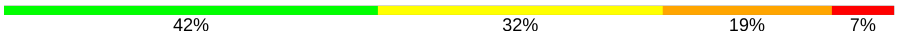
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	I	123	123	123	0	0

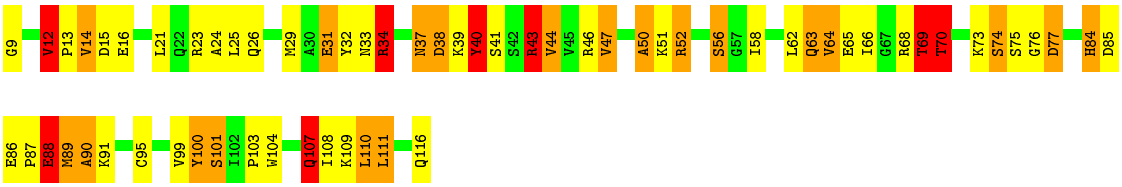
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CYSTATIN

Chain I: 



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	47.90Å 47.90Å 87.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	977	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	wwPDB-VP

5 Model quality (i)

5.1 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 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	I	1.08	2/869 (0.2%)	2.02	29/1173 (2.5%)

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 outliers	#Planarity outliers
1	I	0	29

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	104	TRP	NE1-CE2	-7.79	1.27	1.37
1	I	89	MET	N-CA	7.26	1.60	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	43	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	I	23	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	I	38	ASP	CB-CG-OD1	8.35	125.81	118.30
1	I	88	GLU	N-CA-CB	-8.29	95.68	110.60
1	I	34	ARG	CB-CA-C	-8.04	94.32	110.40
1	I	84	HIS	CA-CB-CG	-8.02	99.97	113.60
1	I	77	ASP	CB-CG-OD1	7.79	125.31	118.30
1	I	89	MET	N-CA-CB	7.79	124.63	110.60
1	I	69	THR	CA-CB-CG2	6.95	122.13	112.40
1	I	65	GLU	CB-CA-C	-6.80	96.80	110.40
1	I	107	GLN	CB-CG-CD	-6.45	94.83	111.60
1	I	52	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	I	77	ASP	N-CA-CB	-6.29	99.28	110.60
1	I	88	GLU	O-C-N	-6.28	112.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	47	VAL	CG1-CB-CG2	-6.15	101.06	110.90
1	I	89	MET	CA-CB-CG	6.09	123.65	113.30
1	I	34	ARG	O-C-N	-5.84	113.35	122.70
1	I	46	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	I	88	GLU	CA-C-N	5.69	129.71	117.20
1	I	44	VAL	CB-CA-C	-5.64	100.69	111.40
1	I	88	GLU	CA-C-O	-5.63	108.27	120.10
1	I	14	VAL	CB-CA-C	-5.53	100.89	111.40
1	I	40	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	I	88	GLU	CB-CA-C	5.36	121.12	110.40
1	I	88	GLU	C-N-CA	5.31	134.98	121.70
1	I	24	ALA	CB-CA-C	-5.10	102.45	110.10
1	I	76	GLY	C-N-CA	5.09	134.43	121.70
1	I	116	GLN	CB-CA-C	-5.09	100.22	110.40
1	I	23	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	100	TYR	Sidechain
1	I	101	SER	Mainchain
1	I	103	PRO	Mainchain
1	I	107	GLN	Mainchain
1	I	108	ILE	Mainchain
1	I	109	LYS	Mainchain
1	I	110	LEU	Mainchain
1	I	12	VAL	Mainchain
1	I	16	GLU	Mainchain
1	I	26	GLN	Mainchain
1	I	32	TYR	Sidechain
1	I	33	ASN	Mainchain
1	I	34	ARG	Mainchain
1	I	37	ASN	Mainchain
1	I	40	TYR	Mainchain
1	I	43	ARG	Sidechain
1	I	47	VAL	Mainchain
1	I	50	ALA	Mainchain
1	I	51	LYS	Mainchain
1	I	56	SER	Mainchain
1	I	58	ILE	Mainchain
1	I	63	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	I	70	THR	Mainchain
1	I	74	SER	Mainchain
1	I	85	ASP	Mainchain
1	I	88	GLU	Mainchain,Peptide
1	I	9	GLY	Mainchain
1	I	90	ALA	Mainchain

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	H(model)	H(added)	Clashes	Symm-Clashes
1	I	854	0	844	20	4
2	I	123	0	0	4	5
All	All	977	0	844	20	6

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 12.

All (20) 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:I:38:ASP:OD2	1:I:68:ARG:HD2	1.85	0.76
1:I:14:VAL:HG22	1:I:52:ARG:HG2	1.79	0.65
1:I:25:LEU:HD11	1:I:64:VAL:HG21	1.82	0.61
1:I:99:VAL:HG22	1:I:110:LEU:HD12	1.82	0.61
1:I:69:THR:HA	2:I:1084:HOH:O	2.01	0.60
1:I:29:MET:HA	1:I:29:MET:HE2	1.84	0.58
1:I:64:VAL:HG12	1:I:66:ILE:HG13	1.85	0.58
1:I:100:TYR:HB2	1:I:111:LEU:HD22	1.85	0.58
1:I:15:ASP:HB2	2:I:1090:HOH:O	2.05	0.55
1:I:29:MET:HA	1:I:29:MET:CE	2.37	0.54
1:I:43:ARG:HD2	2:I:1011:HOH:O	2.07	0.53
1:I:44:VAL:HG13	1:I:64:VAL:HG13	1.92	0.51
1:I:66:ILE:HD12	1:I:95:CYS:SG	2.52	0.49
1:I:31:GLU:HA	1:I:34:ARG:HD2	1.95	0.48
1:I:63:GLN:HB3	1:I:63:GLN:HE21	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:LEU:HD11	1:I:50:ALA:HB1	2.00	0.43
1:I:12:VAL:HA	1:I:13:PRO:HD3	1.76	0.43
1:I:70:THR:HG21	2:I:1107:HOH:O	2.18	0.43
1:I:38:ASP:CG	1:I:68:ARG:HH11	2.23	0.42
1:I:39:LYS:HE3	1:I:40:TYR:CZ	2.55	0.41

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1103:HOH:O	2:I:1104:HOH:O[5_674]	0.63	1.57
1:I:15:ASP:OD2	1:I:91:LYS:NZ[2_665]	1.37	0.83
1:I:74:SER:OG	2:I:1020:HOH:O[3_674]	1.52	0.68
2:I:1102:HOH:O	2:I:1102:HOH:O[5_674]	1.54	0.66
1:I:91:LYS:CE	2:I:1090:HOH:O[3_564]	1.56	0.64
1:I:91:LYS:NZ	2:I:1090:HOH:O[3_564]	2.05	0.15

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	I	106/108 (98%)	92 (87%)	8 (8%)	6 (6%)	1 0

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	86	GLU
1	I	87	PRO
1	I	89	MET
1	I	90	ALA
1	I	56	SER
1	I	73	LYS

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	I	96/96 (100%)	81 (84%)	15 (16%)	2 1

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

Mol	Chain	Res	Type
1	I	12	VAL
1	I	31	GLU
1	I	37	ASN
1	I	41	SER
1	I	62	LEU
1	I	64	VAL
1	I	69	THR
1	I	70	THR
1	I	75	SER
1	I	77	ASP
1	I	84	HIS
1	I	88	GLU
1	I	101	SER
1	I	107	GLN
1	I	111	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	37	ASN
1	I	63	GLN
1	I	107	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.