wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:06 AM GMT

PDB ID	:	3H6R
Title	:	Clitocypin, a beta-trefoil cysteine protease inhibitor
Authors	:	Renko, M.; Sabotic, J.; Brzin, J.; Turk, D.
Deposited on	:	2009-04-23
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

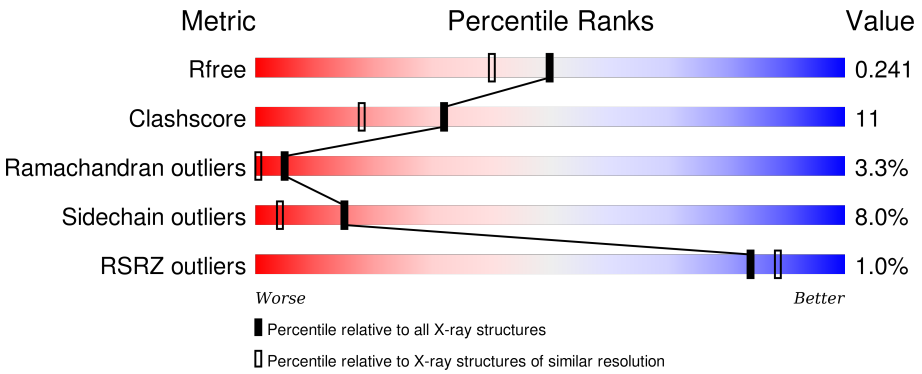
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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))
R_{free}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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.

Mol	Chain	Length	Quality of chain
1	A	152	2% 78% 15% 6% •
2	B	152	77% 17% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2666 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 Clitocypin analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1190	755	202	232	1	40	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	THR	ILE	VARIANT	UNP Q3Y9I4
A	35	GLN	ARG	VARIANT	UNP Q3Y9I4
A	42	SER	ASN	VARIANT	UNP Q3Y9I4
A	47	SER	PHE	VARIANT	UNP Q3Y9I4
A	58	SER	ALA	VARIANT	UNP Q3Y9I4
A	71	ALA	THR	VARIANT	UNP Q3Y9I4
A	81	GLN	GLU	VARIANT	UNP Q3Y9I4
A	117	VAL	ILE	VARIANT	UNP Q3Y9I4

- Molecule 2 is a protein called Clitocypin analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	152	1198	762	205	230	1	71	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	THR	ILE	VARIANT	UNP Q3Y9I4
B	35	GLN	ARG	VARIANT	UNP Q3Y9I4
B	38	GLN	LYS	VARIANT	UNP Q3Y9I4
B	49	ARG	GLN	VARIANT	UNP Q3Y9I4
B	71	ALA	THR	VARIANT	UNP Q3Y9I4
B	81	GLN	GLU	VARIANT	UNP Q3Y9I4
B	117	VAL	ILE	VARIANT	UNP Q3Y9I4

- Molecule 3 is water.

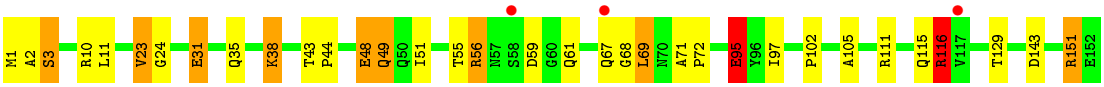
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	157	157	157	0	0
			Total	O		
3	B	121	121	121	0	0

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 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.

- Molecule 1: Clitocypin analog

Chain A:



- Molecule 2: Clitocypin analog

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.54Å 58.00Å 58.26Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 42.14 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.95) 99.0 (42.14-1.95)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.53 (at 1.95Å)	Xtriage
Refinement program	MAIN, REFMAC5	Depositor
R, R_{free}	0.186 , 0.241 0.186 , 0.241	Depositor DCC
R_{free} test set	1042 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.5	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 21085 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2666	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	A	1.15	2/1223 (0.2%)	1.10	5/1670 (0.3%)
2	B	1.14	1/1232 (0.1%)	1.11	7/1683 (0.4%)
All	All	1.14	3/2455 (0.1%)	1.10	12/3353 (0.4%)

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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	GLU	CB-CG	-8.73	1.35	1.52
1	A	105	ALA	CA-CB	5.60	1.64	1.52
2	B	76	GLY	C-O	-5.04	1.15	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NE-CZ-NH1	-9.03	115.78	120.30
2	B	74	GLU	N-CA-C	7.46	131.15	111.00
1	A	56	ARG	NE-CZ-NH1	-6.08	117.26	120.30
2	B	2	ALA	N-CA-C	-6.06	94.63	111.00
2	B	59	ASP	CB-CA-C	-6.01	98.38	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	79	TYR	Sidechain

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	A	1190	0	1140	23	0
2	B	1198	0	1145	24	2
3	A	157	0	0	5	0
3	B	121	0	0	5	1
All	All	2666	0	2285	47	2

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.

The worst 5 of 47 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)
2:B:49:ARG:HH21	2:B:49:ARG:HG3	1.28	0.98
1:A:43:THR:HB	1:A:44:PRO:HD2	1.51	0.91
2:B:8:THR:CG2	2:B:51:ILE:HG23	2.12	0.80
2:B:49:ARG:HG3	2:B:49:ARG:NH2	2.01	0.74
2:B:31:GLU:HG3	2:B:38:GLN:HG3	1.71	0.73

All (2) 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:B:67:GLN:NE2	3:B:219:HOH:O[2_645]	1.95	0.25
2:B:21:PRO:CB	2:B:72:PRO:CB[2_655]	2.09	0.11

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	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	6 1
2	B	150/152 (99%)	135 (90%)	9 (6%)	6 (4%)	4 0
All	All	300/304 (99%)	270 (90%)	20 (7%)	10 (3%)	5 0

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	116	ARG
2	B	71	ALA
1	A	68	GLY
2	B	74	GLU

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	126/126 (100%)	113 (90%)	13 (10%)	9 2
2	B	125/125 (100%)	118 (94%)	7 (6%)	26 11
All	All	251/251 (100%)	231 (92%)	20 (8%)	15 4

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU

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Mol	Chain	Res	Type
1	A	102	PRO
2	B	51	ILE
1	A	49	GLN
1	A	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	126	GLN
2	B	17	HIS
2	B	99	GLN
2	B	115	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	147/152 (96%)	-0.17	3 (2%) 68 75	15, 27, 46, 58	2 (1%)
2	B	144/152 (94%)	-0.22	0 100 100	16, 26, 46, 55	2 (1%)
All	All	291/304 (95%)	-0.19	3 (1%) 84 88	15, 26, 47, 58	4 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	3.3
1	A	67	GLN	2.6
1	A	58	SER	2.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.