

Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 - 05:47 am GMT

PDB ID	:	7QYD
Title	:	mosquitocidal Cry11Ba determined at pH 6.5 from naturally-occurring
		nanocrystals by Serial femtosecond crystallography
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Deposited on	:	2022-01-28
Resolution	:	2.40 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 (1)) were used in the production of this report:

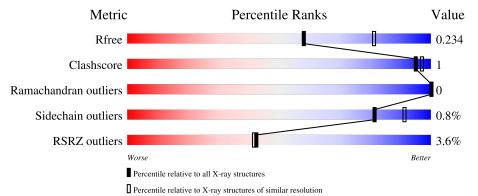
Refmac CCP4	: : : :	 1.13 2.36 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996)
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1 Overall quality 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 2.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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% 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	А	724	85%	·	12%
1	В	724	83%	•	13%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10706 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 Pesticidal crystal protein Cry11Ba.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	637	Total 5072	C 3260	1,	O 958	S 12	0	2	0
1	В	630	Total 5011	C 3218		O 950	S 11	0	2	0

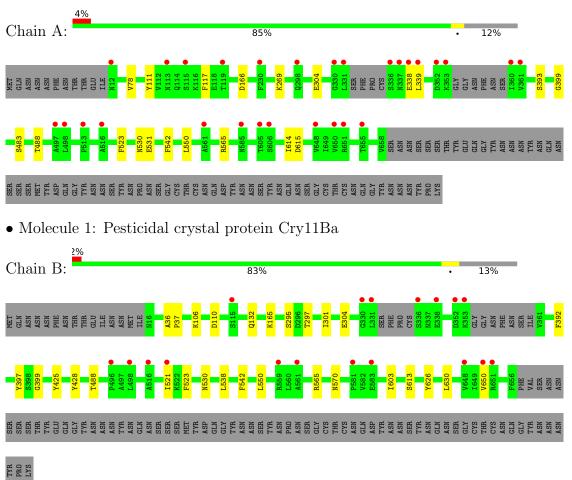
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	318	Total O 318 318	0	0
2	В	304	Total O 305 305	0	1



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 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: Pesticidal crystal protein Cry11Ba



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	168.25Å 158.53Å 57.53Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.10 - 2.40	Depositor
Resolution (A)	42.06 - 2.40	EDS
% Data completeness	99.9 (42.10-2.40)	Depositor
(in resolution range)	$100.0 \ (42.06-2.40)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.16 (at 2.39 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.183 , 0.231	Depositor
R, R_{free}	0.190 , 0.234	DCC
R_{free} test set	5991 reflections (9.81%)	wwPDB-VP
Wilson B-factor $(Å^2)$	40.2	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34,52.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10706	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 49.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8400e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		lengths	Bond angles		
	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.67	0/5199	0.72	0/7064	
1	В	0.67	0/5137	0.72	0/6981	
All	All	0.67	0/10336	0.72	0/14045	

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 (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	А	5072	0	5007	9	0
1	В	5011	0	4938	15	0
2	А	318	0	0	1	0
2	В	305	0	0	3	0
All	All	10706	0	9945	24	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 1.

All (24) 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:B:570:ASN:ND2	2:B:802:HOH:O	2.35	0.60	



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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:523:PHE:CD1	1:A:530:ASN:HB3	2.44	0.53
1:B:523:PHE:CD1	1:B:530:ASN:HB3	2.45	0.51
1:B:106:LYS:NZ	1:B:110:ASP:OD2	2.40	0.51
1:A:531:GLU:HA	1:A:614:ILE:O	2.12	0.50
1:A:488:THR:HB	1:A:542:PHE:HA	1.93	0.50
1:B:392:PHE:HB2	1:B:397:TYR:HB2	1.94	0.48
1:B:650:VAL:HG22	2:B:942:HOH:O	2.13	0.47
1:A:530:ASN:O	1:A:615:ASP:HA	2.15	0.47
1:A:111:TYR:CE2	1:A:117:PHE:HB2	2.51	0.46
1:A:78:VAL:HG11	2:A:852:HOH:O	2.15	0.45
1:A:338:GLU:HG2	1:A:339:LEU:HD22	1.98	0.45
1:B:538:LEU:HD22	1:B:603:ILE:HG22	1.98	0.45
1:B:304:GLU:HB2	1:B:399:GLY:HA2	1.98	0.45
1:A:304:GLU:HB2	1:A:399:GLY:HA2	1.98	0.45
1:B:488:THR:HB	1:B:542:PHE:HA	1.98	0.44
1:B:295:SER:HA	1:B:301:ILE:O	2.18	0.44
1:B:521:ILE:O	1:B:626:TYR:HA	2.18	0.43
1:B:165:LYS:NZ	2:B:822:HOH:O	2.51	0.42
1:B:550:LEU:HD23	1:B:550:LEU:HA	1.88	0.41
1:B:630:LEU:N	1:B:630:LEU:HD12	2.36	0.41
1:B:36:ALA:HB3	1:B:37:PRO:HD3	2.03	0.41
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.96	0.41
1:B:425:TYR:HB2	1:B:428:TYR:HB2	2.03	0.41

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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	А	633/724~(87%)	615 (97%)	18 (3%)	0	100 100
1	В	626/724~(86%)	611 (98%)	15 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percer	ntiles
All	All	1259/1448~(87%)	1226 (97%)	33~(3%)	0	100	100

There are no Ramachandran outliers to report.

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	А	557/635~(88%)	552~(99%)	5(1%)	78 90
1	В	550/635~(87%)	546 (99%)	4 (1%)	84 92
All	All	1107/1270~(87%)	1098 (99%)	9~(1%)	81 91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	166	ASP
1	А	269	LYS
1	А	393	SER
1	А	483	SER
1	А	565	ARG
1	В	132	GLN
1	В	297	THR
1	В	565	ARG
1	В	613	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	637/724~(87%)	-0.02	28 (4%) 34 33	32, 46, 84, 142	0
1	В	630/724~(87%)	-0.09	18 (2%) 51 50	31, 46, 78, 141	0
All	All	1267/1448~(87%)	-0.05	46 (3%) 42 42	31, 46, 81, 142	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	330	GLY	5.5
1	А	360	ILE	5.3
1	А	336	SER	5.1
1	В	330	GLY	4.8
1	А	651	ARG	4.6
1	А	352	ASP	4.4
1	А	650	VAL	4.3
1	А	337	ASN	4.1
1	В	352	ASP	4.0
1	А	115	SER	3.7
1	А	648	VAL	3.6
1	А	338	GLU	3.6
1	В	583	GLU	3.4
1	В	650	VAL	3.4
1	В	648	VAL	3.1
1	В	338	GLU	3.0
1	А	339	LEU	3.0
1	А	12	ASN	3.0
1	В	651	ARG	2.9
1	В	353	LYS	2.9
1	А	361	VAL	2.8
1	В	336	SER	2.7
1	А	298	GLN	2.7
1	А	119	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	А	353	LYS	2.7
1	В	521	ILE	2.6
1	В	331	LEU	2.5
1	В	561	ALA	2.4
1	В	115	SER	2.4
1	В	581	PRO	2.3
1	А	497	ALA	2.3
1	В	516	ALA	2.3
1	А	655	THR	2.3
1	В	559	ARG	2.2
1	А	113	ASN	2.2
1	А	230	PHE	2.2
1	А	331	LEU	2.2
1	А	516	ALA	2.2
1	А	513	PRO	2.2
1	А	605	THR	2.2
1	В	498	LEU	2.2
1	А	561	ALA	2.1
1	А	585	ASN	2.1
1	В	496	PRO	2.1
1	А	606	SER	2.0
1	А	498	LEU	2.0

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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 monosaccharides 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.

