

wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 09:03 AM EDT

PDB ID	:	4 FJQ
Title	:	Crystal Structure of an alpha-Bisabolol synthase
Authors	:	Jianxu, L.; Peng, Z.
Deposited on	:	2012-06-12
Resolution	:	2.00 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 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:

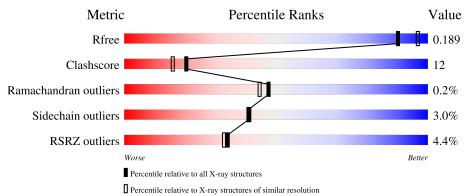
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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% 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		
			4%		
1	А	563	71%	20%	• 7%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4547 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 Amorpha-4,11-diene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	521	Total 4268	C 2762	N 698	0 791	S 17	0	0	0

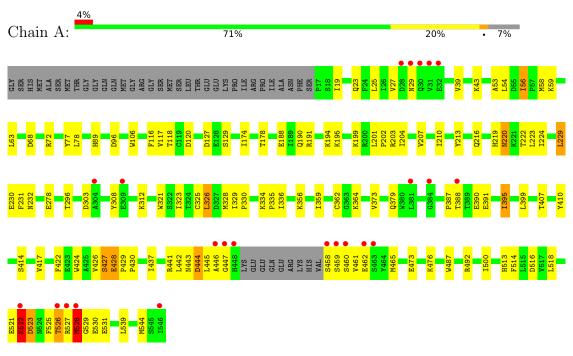
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	279	Total O 279 279	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 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: Amorpha-4,11-diene synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	52.00Å 77.33Å 68.78Å	Depositor
a, b, c, α , β , γ	90.00° 102.50° 90.00°	Depositor
Resolution (Å)	39.22 - 2.00	Depositor
Resolution (A)	39.22 - 2.00	EDS
% Data completeness	93.5 (39.22-2.00)	Depositor
(in resolution range)	96.9 (39.22-2.00)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
D D	0.181 , 0.223	Depositor
R, R_{free}	0.187 , 0.189	DCC
R_{free} test set	1754 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 52.3	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	0.95	EDS
Total number of atoms	4547	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.

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		Bo	nd lengths	Bond angles		
Mol Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.82	26/4362~(0.6%)	0.65	10/5904~(0.2%)	

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(A)	Ideal(Å)
1	А	427	SER	CB-OG	-14.72	1.23	1.42
1	А	426	VAL	CB-CG2	-11.01	1.29	1.52
1	А	529	GLY	C-O	-9.87	1.07	1.23
1	А	443	ASN	C-O	-8.94	1.06	1.23
1	А	426	VAL	C-O	-8.29	1.07	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	427	SER	CA-CB-OG	-10.43	83.05	111.20
1	А	531	GLU	OE1-CD-OE2	-7.71	114.05	123.30
1	А	444	ASP	CB-CG-OD1	7.57	125.11	118.30
1	А	523	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	А	530	GLU	OE1-CD-OE2	6.13	130.66	123.30

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.

Mo	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4268	0	4272	106	0



Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	279	0	0	9	0
All	All	4547	0	4272	106	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 12.

The worst 5 of 106 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:19:ILE:HD11	1:A:528:MET:HE1	1.42	0.99
1:A:188:GLU:OE1	1:A:191:ARG:HD3	1.67	0.95
1:A:118:THR:HG23	1:A:120:ASP:H	1.35	0.91
1:A:56:ILE:HD11	1:A:58:MET:HB2	1.53	0.90
1:A:232:ASN:HD21	1:A:544:MET:H	1.24	0.85

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	517/563~(92%)	507~(98%)	9~(2%)	1 (0%)	47 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	528	MET

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	467/507~(92%)	453~(97%)	14 (3%)	41 41

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	395	ILE
1	А	473	GLU
1	А	528	MET
1	А	522	LYS
1	А	526	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such side chains are listed below:

Mol	Chain	Res	Type
1	А	232	ASN
1	А	235	GLN
1	А	513	HIS
1	А	379	GLN
1	А	125	HIS

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	<RSRZ $>$	#RS	\mathbf{RZ} >	-2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	521/563~(92%)	-0.09	23~(4%)	34	33	12, 24, 52, 71	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	528	MET	7.0
1	А	462	GLU	5.1
1	А	459	SER	4.1
1	А	546	ILE	4.1
1	А	460	SER	3.6

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.

