



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:37 PM GMT

PDB ID : 4FJQ
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 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) : 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

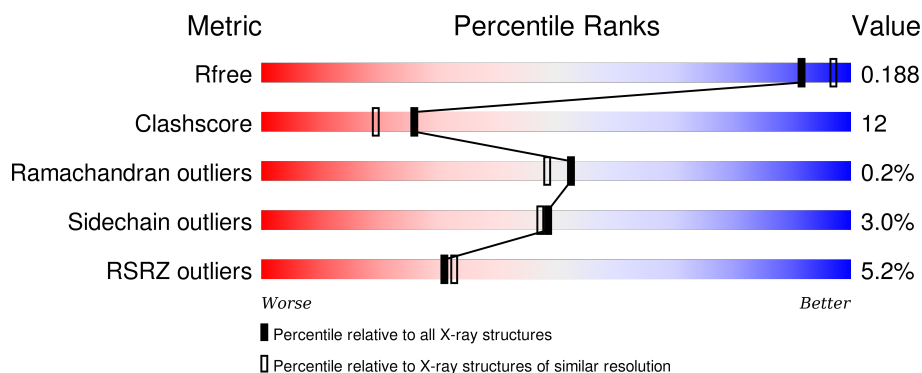
1 Overall quality at a glance

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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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 $\leq 5\%$. 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	563	<div> <div>5%</div> <div>71%</div> <div>20%</div> <div>7%</div> </div>

2 Entry composition

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	A	521	Total	C	N	O	S	0	0	0
			4268	2762	698	791	17			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.00 Å 77.33 Å 68.78 Å 90.00° 102.50° 90.00°	Depositor
Resolution (Å)	39.22 – 2.00 39.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.22-2.00) 96.9 (39.22-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.181 , 0.223 0.186 , 0.188	Depositor DCC
R_{free} test set	1755 reflections (5.02%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35019 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.82	26/4362 (0.6%)	0.65	10/5904 (0.2%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	SER	CB-OG	-14.72	1.23	1.42
1	A	426	VAL	CB-CG2	-11.01	1.29	1.52
1	A	529	GLY	C-O	-9.87	1.07	1.23
1	A	443	ASN	C-O	-8.94	1.06	1.23
1	A	426	VAL	C-O	-8.29	1.07	1.23
1	A	430	PRO	C-O	-8.21	1.06	1.23
1	A	531	GLU	CD-OE2	-8.15	1.16	1.25
1	A	430	PRO	CB-CG	-7.63	1.11	1.50
1	A	442	LEU	C-O	-7.53	1.09	1.23
1	A	531	GLU	CD-OE1	-7.34	1.17	1.25
1	A	429	PRO	CB-CG	-7.30	1.13	1.50
1	A	531	GLU	C-O	-7.24	1.09	1.23
1	A	428	GLU	CD-OE1	-7.01	1.18	1.25
1	A	528	MET	C-O	-6.76	1.10	1.23
1	A	530	GLU	CB-CG	-6.73	1.39	1.52
1	A	525	PHE	CD2-CE2	-6.54	1.26	1.39
1	A	428	GLU	C-O	-6.46	1.11	1.23
1	A	444	ASP	C-O	-6.20	1.11	1.23
1	A	522	LYS	CB-CG	-6.16	1.35	1.52
1	A	531	GLU	CB-CG	-5.98	1.40	1.52
1	A	525	PHE	CE1-CZ	-5.88	1.26	1.37
1	A	530	GLU	CA-CB	-5.69	1.41	1.53
1	A	447	GLY	C-O	-5.65	1.14	1.23
1	A	525	PHE	CD1-CE1	-5.47	1.28	1.39
1	A	446	ALA	C-O	-5.36	1.13	1.23
1	A	430	PRO	N-CD	-5.32	1.40	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	SER	CA-CB-OG	-10.43	83.05	111.20
1	A	531	GLU	OE1-CD-OE2	-7.71	114.05	123.30
1	A	444	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	523	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	530	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	A	445	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	442	LEU	CB-CG-CD2	5.76	120.79	111.00
1	A	531	GLU	CB-CA-C	5.53	121.45	110.40
1	A	522	LYS	CB-CG-CD	-5.10	98.33	111.60
1	A	444	ASP	CB-CG-OD2	-5.03	113.77	118.30

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	4268	0	4272	106	0
2	A	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.

All (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
1:A:461:VAL:HG11	1:A:476:LYS:HE3	1.63	0.78
1:A:106:TRP:CH2	1:A:117:VAL:HG11	2.19	0.78
1:A:96:ASP:OD2	1:A:118:THR:HG22	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:CD1	1:A:528:MET:HE1	2.17	0.72
1:A:207:VAL:HG12	1:A:231:PHE:CE1	2.25	0.72
1:A:424:TRP:O	1:A:427:SER:HB2	1.89	0.72
1:A:523:ASP:CG	1:A:526:THR:HG23	2.10	0.72
1:A:232:ASN:HD21	1:A:544:MET:N	1.86	0.72
1:A:462:GLU:HA	1:A:465:MET:CE	2.23	0.69
1:A:53:ALA:HA	1:A:59:LYS:HE2	1.74	0.69
1:A:462:GLU:HA	1:A:465:MET:HE3	1.76	0.68
1:A:513:HIS:HD2	2:A:637:HOH:O	1.77	0.67
1:A:308:TYR:CZ	1:A:312:LYS:HD2	2.29	0.66
1:A:459:SER:HA	1:A:462:GLU:OE1	1.96	0.65
1:A:216:GLN:O	1:A:219:HIS:HD2	1.80	0.65
1:A:458:SER:HB3	1:A:461:VAL:HB	1.78	0.64
1:A:207:VAL:HG11	1:A:539:LEU:HD12	1.79	0.63
1:A:19:ILE:HD11	1:A:528:MET:CE	2.24	0.62
1:A:174:ILE:O	1:A:178:THR:HG23	1.99	0.62
1:A:461:VAL:O	1:A:465:MET:HG3	2.01	0.61
1:A:308:TYR:CE2	1:A:312:LYS:HD2	2.35	0.61
1:A:414:SER:O	1:A:417:VAL:HG22	2.04	0.58
1:A:220:ASN:HD22	1:A:223:LEU:H	1.52	0.58
1:A:388:THR:HG22	1:A:390:GLU:H	1.69	0.57
1:A:521:GLU:O	1:A:522:LYS:CD	2.53	0.57
1:A:188:GLU:HA	1:A:191:ARG:HG2	1.87	0.56
1:A:521:GLU:O	1:A:522:LYS:HD2	2.05	0.56
1:A:199:LYS:NZ	1:A:487:TRP:CE2	2.74	0.56
1:A:356:LYS:CD	1:A:414:SER:HB3	2.36	0.55
1:A:96:ASP:OD2	1:A:118:THR:CG2	2.53	0.54
1:A:207:VAL:HG12	1:A:231:PHE:HE1	1.71	0.54
1:A:321:TRP:CG	1:A:364:LYS:HE3	2.42	0.54
1:A:527:ARG:O	1:A:528:MET:HB2	2.07	0.53
1:A:334:LYS:N	1:A:335:PRO:HD2	2.24	0.53
1:A:78:LEU:HD11	1:A:230:GLU:HG3	1.90	0.52
1:A:54:LEU:HD13	1:A:63:LEU:HD21	1.91	0.52
1:A:492:ARG:HD2	2:A:876:HOH:O	2.09	0.52
1:A:356:LYS:HD3	1:A:414:SER:HB3	1.90	0.52
1:A:444:ASP:HB3	1:A:460:SER:HB2	1.90	0.52
1:A:513:HIS:HE1	2:A:630:HOH:O	1.93	0.52
1:A:523:ASP:OD1	1:A:526:THR:HG23	2.09	0.51
1:A:203:ARG:O	1:A:207:VAL:HG13	2.11	0.51
1:A:190:GLN:HG3	1:A:194:LYS:HE3	1.92	0.51
1:A:188:GLU:CD	1:A:191:ARG:HD3	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:O	1:A:191:ARG:HG2	2.12	0.50
1:A:19:ILE:CD1	1:A:528:MET:CE	2.85	0.50
1:A:201:LEU:HD21	1:A:514:PHE:HD1	1.77	0.49
1:A:326:LEU:O	1:A:334:LYS:HE2	2.13	0.49
1:A:325:CYS:O	1:A:328:MET:HG2	2.13	0.49
1:A:387:PRO:HA	1:A:391:GLU:OE1	2.13	0.49
1:A:118:THR:HG23	1:A:120:ASP:N	2.16	0.48
1:A:220:ASN:HD21	1:A:222:THR:HB	1.77	0.48
1:A:127:ASP:HB3	1:A:129:SER:H	1.79	0.48
1:A:106:TRP:CH2	1:A:117:VAL:CG1	2.95	0.47
1:A:207:VAL:HG12	1:A:231:PHE:CZ	2.50	0.47
1:A:308:TYR:OH	1:A:379:GLN:NE2	2.46	0.47
1:A:459:SER:CA	1:A:462:GLU:OE1	2.62	0.47
1:A:27:VAL:CG1	1:A:29:ASN:HD21	2.27	0.47
1:A:77:TYR:HA	2:A:669:HOH:O	2.15	0.47
1:A:77:TYR:HB3	1:A:278:GLU:HG2	1.96	0.47
1:A:359:ILE:HD13	1:A:417:VAL:CG2	2.45	0.46
1:A:195:LYS:NZ	1:A:516:ASP:OD2	2.48	0.46
1:A:428:GLU:OE2	2:A:787:HOH:O	2.21	0.46
1:A:23:GLN:HB3	2:A:878:HOH:O	2.15	0.46
1:A:216:GLN:O	1:A:219:HIS:CD2	2.65	0.45
1:A:201:LEU:HB2	1:A:204:ILE:HD12	1.98	0.45
1:A:39:VAL:O	1:A:43:LYS:HG3	2.16	0.45
1:A:56:ILE:O	1:A:56:ILE:HG13	2.16	0.45
1:A:210:ILE:HG23	1:A:224:ILE:HD11	1.98	0.45
1:A:68:ASP:O	1:A:72:ARG:HG3	2.17	0.45
1:A:201:LEU:HA	1:A:202:PRO:HD3	1.86	0.44
1:A:220:ASN:ND2	1:A:223:LEU:H	2.15	0.44
1:A:329:ILE:HG22	1:A:330:PRO:O	2.17	0.44
1:A:296:THR:HB	2:A:732:HOH:O	2.17	0.44
1:A:521:GLU:C	1:A:522:LYS:CD	2.86	0.44
1:A:399:LEU:O	1:A:399:LEU:HD13	2.18	0.44
1:A:444:ASP:HB3	1:A:460:SER:CB	2.48	0.44
1:A:54:LEU:HD13	1:A:63:LEU:CD2	2.48	0.43
1:A:521:GLU:O	1:A:522:LYS:HD3	2.16	0.43
1:A:395:ILE:HG23	1:A:399:LEU:HB2	2.00	0.43
1:A:204:ILE:O	1:A:207:VAL:HG22	2.18	0.43
1:A:462:GLU:HA	1:A:465:MET:HE2	2.00	0.43
1:A:461:VAL:HG21	1:A:476:LYS:HE2	2.00	0.43
1:A:106:TRP:CZ3	1:A:117:VAL:HG11	2.54	0.42
1:A:323:ILE:O	1:A:326:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HD13	1:A:417:VAL:HG21	2.02	0.42
1:A:373:VAL:HG12	1:A:399:LEU:HD23	2.01	0.42
1:A:527:ARG:O	1:A:528:MET:CB	2.68	0.42
1:A:56:ILE:HD12	1:A:58:MET:H	1.84	0.42
1:A:458:SER:O	1:A:462:GLU:OE1	2.39	0.41
1:A:441:ARG:HD2	2:A:737:HOH:O	2.19	0.41
1:A:437:ILE:O	1:A:441:ARG:HG2	2.20	0.41
1:A:213:TYR:CE2	1:A:219:HIS:HB2	2.56	0.41
1:A:54:LEU:HD11	1:A:89:HIS:CD2	2.56	0.41
1:A:459:SER:C	1:A:462:GLU:OE1	2.59	0.41
1:A:229:LEU:HD13	2:A:806:HOH:O	2.19	0.41
1:A:522:LYS:HD2	1:A:522:LYS:HA	1.58	0.41
1:A:362:CYS:HB3	1:A:422:PHE:CD1	2.56	0.41
1:A:407:THR:O	1:A:410:TYR:HB2	2.20	0.41
1:A:336:ILE:HD12	1:A:336:ILE:N	2.36	0.41
1:A:54:LEU:HA	1:A:63:LEU:HD22	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	517/563 (92%)	507 (98%)	9 (2%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	MET

5.3.2 Protein sidechains ⓘ

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	467/507 (92%)	453 (97%)	14 (3%)	48 47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	56	ILE
1	A	116	PHE
1	A	220	ASN
1	A	229	LEU
1	A	303	ASP
1	A	326	LEU
1	A	395	ILE
1	A	473	GLU
1	A	500	ILE
1	A	518	LEU
1	A	522	LYS
1	A	526	THR
1	A	528	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	33	GLN
1	A	85	HIS
1	A	125	HIS
1	A	134	GLN
1	A	219	HIS
1	A	220	ASN
1	A	232	ASN
1	A	235	GLN
1	A	379	GLN
1	A	385	HIS

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Mol	Chain	Res	Type
1	A	513	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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	521/563 (92%)	-0.04	27 (5%) 31 33	12, 24, 52, 71	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	MET	7.1
1	A	462	GLU	5.2
1	A	546	ILE	4.3
1	A	459	SER	4.3
1	A	460	SER	3.7
1	A	447	GLY	3.7
1	A	32	GLU	3.7
1	A	463	SER	3.6
1	A	527	ARG	3.3
1	A	30	GLN	3.3
1	A	384	GLY	3.3
1	A	458	SER	3.3
1	A	304	ALA	3.2
1	A	448	HIS	3.2
1	A	526	THR	3.0
1	A	309	GLU	2.9
1	A	31	VAL	2.9
1	A	29	ASN	2.8
1	A	522	LYS	2.6
1	A	28	ASP	2.5
1	A	446	ALA	2.3
1	A	381	LEU	2.3
1	A	388	THR	2.2
1	A	386	ILE	2.1
1	A	34	GLY	2.1
1	A	468	TYR	2.1
1	A	390	GLU	2.0

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.