Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 08:44 AM EDT

PDB ID	:	4LA5
Title	:	Crystal structure of 2-methylisoborneol synthase from Streptomyces coelicolor A3(2)
Authors	:	Koksal, M.; Christianson, D.W.
Deposited on	:	2013-06-19
Resolution	:	1.85 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:

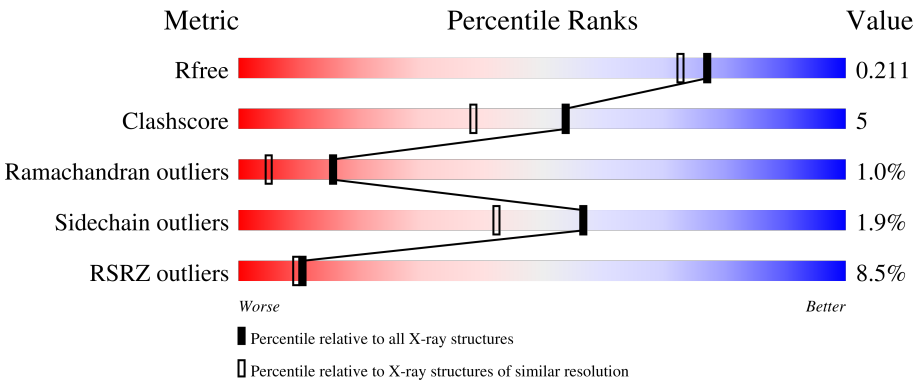
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.85 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	A	461	6% 53% 14% • 31%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2679 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 2-methylisoborneol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2534	1600	458	463	13	0	2	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9F1Y6
A	-19	GLY	-	expression tag	UNP Q9F1Y6
A	-18	SER	-	expression tag	UNP Q9F1Y6
A	-17	SER	-	expression tag	UNP Q9F1Y6
A	-16	HIS	-	expression tag	UNP Q9F1Y6
A	-15	HIS	-	expression tag	UNP Q9F1Y6
A	-14	HIS	-	expression tag	UNP Q9F1Y6
A	-13	HIS	-	expression tag	UNP Q9F1Y6
A	-12	HIS	-	expression tag	UNP Q9F1Y6
A	-11	HIS	-	expression tag	UNP Q9F1Y6
A	-10	SER	-	expression tag	UNP Q9F1Y6
A	-9	SER	-	expression tag	UNP Q9F1Y6
A	-8	GLY	-	expression tag	UNP Q9F1Y6
A	-7	LEU	-	expression tag	UNP Q9F1Y6
A	-6	VAL	-	expression tag	UNP Q9F1Y6
A	-5	PRO	-	expression tag	UNP Q9F1Y6
A	-4	ARG	-	expression tag	UNP Q9F1Y6
A	-3	GLY	-	expression tag	UNP Q9F1Y6
A	-2	SER	-	expression tag	UNP Q9F1Y6
A	-1	HIS	-	expression tag	UNP Q9F1Y6
A	0	MET	-	expression tag	UNP Q9F1Y6

- Molecule 2 is water.

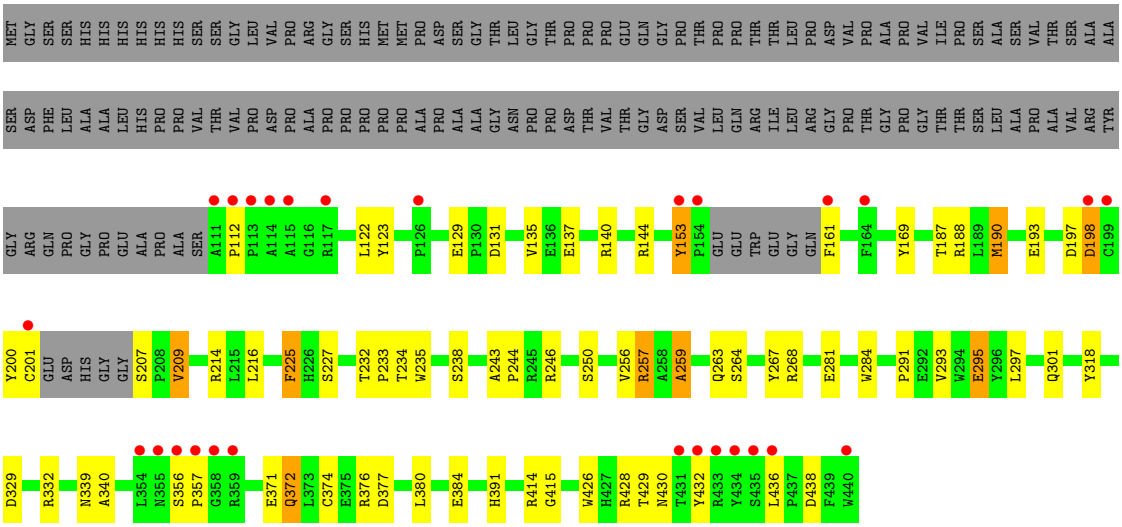
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	145	145	145	0	0

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: 2-methylisoborneol synthase

Chain A: 6% 53% 14% • 31%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.45Å 99.45Å 104.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 1.85 49.73 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.73-1.85) 93.9 (49.73-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.214 0.182 , 0.211	Depositor DCC
R_{free} test set	1983 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2679	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.65	33/2623 (1.3%)	1.31	21/3584 (0.6%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	GLU	CG-CD	9.27	1.65	1.51
1	A	193	GLU	CD-OE2	9.02	1.35	1.25
1	A	295	GLU	CG-CD	8.94	1.65	1.51
1	A	268	ARG	CB-CG	7.96	1.74	1.52
1	A	332	ARG	CZ-NH1	7.33	1.42	1.33
1	A	372	GLN	CB-CG	7.32	1.72	1.52
1	A	384	GLU	CG-CD	7.32	1.62	1.51
1	A	372	GLN	CG-CD	7.28	1.67	1.51
1	A	259	ALA	CA-CB	6.95	1.67	1.52
1	A	256	VAL	CB-CG2	6.93	1.67	1.52
1	A	267	TYR	CD1-CE1	6.93	1.49	1.39
1	A	238	SER	CB-OG	6.80	1.51	1.42
1	A	188	ARG	CB-CG	6.66	1.70	1.52
1	A	235	TRP	CG-CD1	6.50	1.45	1.36
1	A	264	SER	CB-OG	6.34	1.50	1.42
1	A	246	ARG	CG-CD	6.21	1.67	1.51
1	A	250	SER	CA-CB	6.10	1.62	1.52
1	A	144	ARG	CG-CD	6.01	1.67	1.51
1	A	384	GLU	CD-OE2	5.98	1.32	1.25
1	A	293	VAL	CB-CG2	5.87	1.65	1.52
1	A	193	GLU	CB-CG	5.79	1.63	1.52
1	A	137	GLU	CG-CD	5.63	1.60	1.51
1	A	281	GLU	CG-CD	5.40	1.60	1.51
1	A	284	TRP	CE3-CZ3	5.39	1.47	1.38
1	A	426	TRP	CG-CD1	5.28	1.44	1.36
1	A	318	TYR	CD2-CE2	5.21	1.47	1.39
1	A	371	GLU	CB-CG	5.20	1.62	1.52
1	A	415	GLY	CA-C	5.18	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	TYR	CE1-CZ	5.12	1.45	1.38
1	A	187	THR	CA-CB	5.08	1.66	1.53
1	A	295	GLU	CD-OE1	5.07	1.31	1.25
1	A	340	ALA	CA-CB	5.05	1.63	1.52
1	A	384	GLU	CB-CG	5.05	1.61	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	A	188	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	A	257[A]	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	257[B]	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	257[A]	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	257[B]	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	332	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	140	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	A	144	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	268	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	214	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	225	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	225	PHE	CB-CG-CD1	5.98	124.99	120.80
1	A	329	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	193	GLU	CG-CD-OE2	5.86	130.01	118.30
1	A	332	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	216	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	198	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	209	VAL	C-N-CA	-5.29	111.20	122.30
1	A	190	MET	CA-CB-CG	-5.15	104.54	113.30
1	A	193	GLU	OE1-CD-OE2	-5.11	117.17	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2534	0	2404	26	0
2	A	145	0	0	3	0
All	All	2679	0	2404	26	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 5.

All (26) 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:257[A]:ARG:NH2	2:A:598:HOH:O	1.57	1.29
1:A:374:CYS:SG	1:A:377:ASP:OD2	2.22	0.97
1:A:257[A]:ARG:CZ	2:A:598:HOH:O	2.03	0.88
1:A:112:PRO:HG3	1:A:438:ASP:HB2	1.79	0.63
1:A:153:TYR:CE2	1:A:161:PHE:HB2	2.37	0.59
1:A:429:THR:O	1:A:432:TYR:HD2	1.88	0.56
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.75	0.52
1:A:259:ALA:HB1	1:A:263:GLN:HB2	1.92	0.51
1:A:190:MET:O	1:A:190:MET:HG3	2.11	0.48
1:A:414:ARG:HG3	2:A:569:HOH:O	2.12	0.48
1:A:243:ALA:N	1:A:244:PRO:CD	2.77	0.47
1:A:301:GLN:HA	1:A:339:ASN:OD1	2.16	0.46
1:A:197:ASP:O	1:A:201:CYS:HB2	2.16	0.45
1:A:428:ARG:HG2	1:A:428:ARG:NH1	2.32	0.45
1:A:232:THR:HB	1:A:233:PRO:HD3	2.00	0.44
1:A:291:PRO:HB2	1:A:295:GLU:HB2	2.00	0.42
1:A:376:ARG:O	1:A:380:LEU:HG	2.19	0.42
1:A:225:PHE:CZ	1:A:227:SER:HB2	2.56	0.41
1:A:131:ASP:O	1:A:135:VAL:HG23	2.21	0.41
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.21	0.41
1:A:243:ALA:HB3	1:A:244:PRO:HD3	2.03	0.41
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.98	0.41
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.87	0.41
1:A:207:SER:OG	1:A:209:VAL:HG23	2.21	0.40
1:A:122:LEU:C	1:A:122:LEU:HD23	2.41	0.40
1:A:123:TYR:CE2	1:A:391:HIS:CE1	3.10	0.40

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	A	315/461 (68%)	304 (96%)	8 (2%)	3 (1%)	15 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	357	PRO
1	A	356	SER

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	262/372 (70%)	257 (98%)	5 (2%)	57 42

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	TYR
1	A	169	TYR
1	A	198	ASP
1	A	234	THR
1	A	430	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	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, 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	319/461 (69%)	0.26	27 (8%) 10 9	17, 32, 70, 108	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	PRO	7.4
1	A	112	PRO	7.3
1	A	111	ALA	7.0
1	A	432	TYR	6.1
1	A	114	ALA	5.9
1	A	431	THR	5.7
1	A	113	PRO	5.6
1	A	358	GLY	5.5
1	A	115	ALA	5.4
1	A	356	SER	4.9
1	A	355	ASN	4.9
1	A	434	TYR	4.5
1	A	433	ARG	4.2
1	A	117	ARG	4.0
1	A	153	TYR	3.9
1	A	201	CYS	3.8
1	A	154	PRO	3.6
1	A	435	SER	3.5
1	A	198	ASP	2.8
1	A	164	PHE	2.7
1	A	440	TRP	2.5
1	A	359	ARG	2.4
1	A	161	PHE	2.3
1	A	126	PRO	2.2
1	A	354	LEU	2.2
1	A	199	CYS	2.2
1	A	436	LEU	2.1

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.