



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 12:59 PM EST

PDB ID : 5G1V
Title : Linalool Dehydratase Isomerase: Selenomethionine Derivative
Authors : Chambers, S.; Hau, A.; Man, H.; Omar, M.; Turkenburg, J.P.; Grogan, G.
Deposited on : 2016-03-30
Resolution : 2.68 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

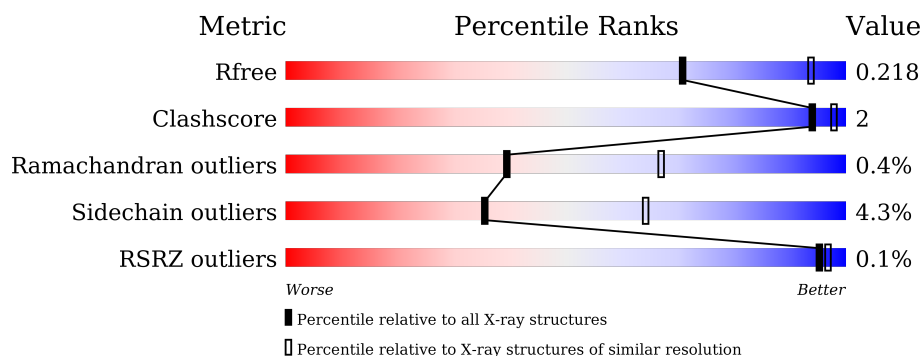
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	372	<div> <div>90%</div> <div>6% ..</div> </div>
1	B	372	<div> <div>90%</div> <div>6% ...</div> </div>
1	C	372	<div> <div>90%</div> <div>6% ..</div> </div>
1	D	372	<div> <div>91%</div> <div>5% ..</div> </div>
1	E	372	<div> <div>90%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15049 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 LINALOOL DEHYDRATASE ISOMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2875	1859	480	523	4	9			
1	B	363	Total	C	N	O	S	Se	0	0	0
			2877	1860	479	525	4	9			
1	C	363	Total	C	N	O	S	Se	0	0	0
			2891	1868	482	528	4	9			
1	D	362	Total	C	N	O	S	Se	0	0	0
			2866	1855	475	523	4	9			
1	E	362	Total	C	N	O	S	Se	0	0	0
			2885	1864	485	523	4	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP E1XUJ2
B	1	MSE	-	EXPRESSION TAG	UNP E1XUJ2
C	1	MSE	-	EXPRESSION TAG	UNP E1XUJ2
D	1	MSE	-	EXPRESSION TAG	UNP E1XUJ2
E	1	MSE	-	EXPRESSION TAG	UNP E1XUJ2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	131	Total	O	0	0
			131	131		
2	C	147	Total	O	0	0
			147	147		
2	D	123	Total	O	0	0
			123	123		
2	E	131	Total	O	0	0
			131	131		

LEU
ALA
GLY
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.51Å 106.72Å 222.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.41 – 2.68 96.25 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (111.41-2.68) 99.8 (96.25-2.68)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.168 , 0.203 0.180 , 0.218	Depositor DCC
R_{free} test set	3290 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	1.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15049	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.72	0/2952	0.87	7/4003 (0.2%)
1	B	0.72	1/2954 (0.0%)	0.89	10/4007 (0.2%)
1	C	0.73	0/2968	0.85	4/4023 (0.1%)
1	D	0.72	0/2943	0.85	5/3993 (0.1%)
1	E	0.72	0/2962	0.87	9/4015 (0.2%)
All	All	0.72	1/14779 (0.0%)	0.87	35/20041 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	GLU	CD-OE2	-5.25	1.19	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	8	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	D	8	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	B	8	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	8	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	E	8	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	D	8	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	8	ARG	CG-CD-NE	-6.84	97.43	111.80
1	E	155	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	219	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	214	LEU	CB-CG-CD2	6.54	122.11	111.00
1	E	214	LEU	CB-CG-CD2	6.42	121.91	111.00
1	C	327	SER	O-C-N	6.36	132.87	122.70
1	B	219	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	8	ARG	CG-CD-NE	-6.23	98.71	111.80
1	A	8	ARG	CG-CD-NE	-6.10	99.00	111.80
1	C	61	GLN	CA-CB-CG	6.09	126.81	113.40
1	B	155	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	61	GLN	CA-CB-CG	6.00	126.59	113.40
1	B	61	GLN	CA-CB-CG	5.98	126.55	113.40
1	E	273	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	D	61	GLN	CA-CB-CG	5.87	126.31	113.40
1	E	61	GLN	CA-CB-CG	5.59	125.70	113.40
1	D	248	MSE	CA-CB-CG	-5.58	103.81	113.30
1	B	39	ASP	C-N-CA	5.40	135.21	121.70
1	B	8	ARG	CG-CD-NE	-5.36	100.55	111.80
1	C	248	MSE	CA-CB-CG	-5.32	104.25	113.30
1	E	248	MSE	CA-CB-CG	-5.31	104.28	113.30
1	C	179	GLN	CB-CA-C	-5.22	99.97	110.40
1	B	4	LEU	N-CA-C	5.14	124.87	111.00
1	A	331	ALA	N-CA-C	-5.07	97.31	111.00
1	A	193	ARG	CG-CD-NE	-5.04	101.23	111.80
1	B	279	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	E	179	GLN	CB-CA-C	-5.00	100.39	110.40

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	2875	0	2767	11	0
1	B	2877	0	2758	8	0
1	C	2891	0	2786	14	0
1	D	2866	0	2744	9	0
1	E	2885	0	2782	13	0
2	A	123	0	0	3	0
2	B	131	0	0	2	0
2	C	147	0	0	6	0
2	D	123	0	0	1	0
2	E	131	0	0	5	0
All	All	15049	0	13837	52	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 2.

All (52) 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:E:121:LYS:HG2	1:E:122:GLU:HG2	1.35	1.06
1:A:172:GLU:OE2	2:A:2034:HOH:O	1.82	0.95
1:D:329:VAL:O	2:D:2116:HOH:O	1.83	0.94
1:E:121:LYS:HG2	1:E:122:GLU:CG	2.12	0.77
1:E:121:LYS:C	1:E:122:GLU:HG2	2.05	0.77
1:E:125:MSE:HE2	2:E:2032:HOH:O	1.89	0.72
1:A:216:ASP:OD2	1:A:219:ARG:NH1	2.24	0.70
1:C:121:LYS:O	2:C:2054:HOH:O	2.10	0.69
1:A:337:HIS:HB3	2:A:2118:HOH:O	1.96	0.66
1:B:291:GLY:HA3	1:D:330:SER:OG	1.98	0.63
1:C:125:MSE:HE2	2:C:2036:HOH:O	2.02	0.59
1:D:79:ALA:HB3	1:D:362:MSE:HE1	1.86	0.58
1:C:121:LYS:HG3	1:C:122:GLU:HG2	1.87	0.56
1:E:121:LYS:CG	1:E:122:GLU:HG2	2.22	0.56
1:C:8:ARG:HD2	2:C:2001:HOH:O	2.06	0.55
1:E:193:ARG:NH2	1:E:362:MSE:O	2.39	0.55
1:D:193:ARG:NH2	1:D:362:MSE:O	2.39	0.55
1:A:193:ARG:NH2	1:A:362:MSE:O	2.38	0.55
1:C:8:ARG:NH2	1:C:314:ASP:OD1	2.39	0.55
1:A:125:MSE:HE1	2:A:2032:HOH:O	2.08	0.54
1:C:193:ARG:NH2	1:C:362:MSE:O	2.41	0.53
1:C:121:LYS:C	1:C:122:GLU:HG2	2.28	0.53
1:C:250:HIS:HD2	1:C:306:GLU:OE2	1.91	0.53
1:A:219:ARG:HD2	1:A:237:ILE:HD13	1.92	0.52
1:D:250:HIS:HD2	1:D:306:GLU:OE2	1.92	0.52
1:E:174:ASP:N	2:E:2069:HOH:O	2.42	0.52
1:E:250:HIS:HD2	1:E:306:GLU:OE2	1.93	0.52
1:B:121:LYS:C	1:B:122:GLU:HG2	2.28	0.52
1:B:250:HIS:HD2	1:B:306:GLU:OE2	1.93	0.51
1:C:155:ARG:HG2	2:C:2072:HOH:O	2.09	0.51
1:A:250:HIS:HD2	1:A:306:GLU:OE2	1.94	0.51
1:C:337:HIS:HB3	2:C:2142:HOH:O	2.11	0.51
1:B:125:MSE:HE2	2:B:2038:HOH:O	2.10	0.50
1:A:91:HIS:CE1	1:D:227:HIS:CD2	3.00	0.50
1:E:327:SER:HB3	2:E:2122:HOH:O	2.12	0.49
1:C:125:MSE:HE1	2:C:2034:HOH:O	2.14	0.46
1:E:8:ARG:NH2	1:E:314:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ARG:NH2	1:D:314:ASP:OD1	2.49	0.45
1:C:121:LYS:HG3	1:C:122:GLU:CG	2.45	0.45
1:B:8:ARG:NH2	1:B:314:ASP:OD1	2.50	0.45
1:A:227:HIS:CD2	1:C:91:HIS:CE1	3.06	0.44
1:E:266:GLN:HB2	2:E:2094:HOH:O	2.17	0.44
1:D:79:ALA:CB	1:D:362:MSE:HE1	2.46	0.44
1:E:8:ARG:HD2	2:E:2002:HOH:O	2.17	0.44
1:B:125:MSE:HE1	2:B:2036:HOH:O	2.19	0.43
1:B:325:LYS:N	1:B:326:PRO:CD	2.83	0.41
1:B:214:LEU:HD11	1:B:226:TYR:HB2	2.01	0.41
1:E:325:LYS:N	1:E:326:PRO:CD	2.83	0.41
1:A:8:ARG:NH2	1:A:314:ASP:OD1	2.51	0.41
1:A:39:ASP:HA	1:A:45:TYR:CE1	2.56	0.41
1:D:18:GLN:HE21	1:D:24:VAL:HA	1.86	0.41
1:C:18:GLN:HE21	1:C:25:THR:H	1.69	0.40

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	360/372 (97%)	350 (97%)	8 (2%)	2 (1%)	30	56
1	B	361/372 (97%)	350 (97%)	11 (3%)	0	100	100
1	C	361/372 (97%)	352 (98%)	7 (2%)	2 (1%)	30	56
1	D	360/372 (97%)	351 (98%)	8 (2%)	1 (0%)	46	73
1	E	360/372 (97%)	351 (98%)	6 (2%)	3 (1%)	24	49
All	All	1802/1860 (97%)	1754 (97%)	40 (2%)	8 (0%)	39	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	174	ASP
1	A	212	LYS
1	C	122	GLU
1	D	212	LYS
1	E	212	LYS
1	A	330	SER
1	C	212	LYS
1	E	122	GLU

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	293/293 (100%)	280 (96%)	13 (4%)	35	63
1	B	292/293 (100%)	278 (95%)	14 (5%)	31	59
1	C	296/293 (101%)	284 (96%)	12 (4%)	37	66
1	D	290/293 (99%)	280 (97%)	10 (3%)	44	73
1	E	294/293 (100%)	280 (95%)	14 (5%)	31	59
All	All	1465/1465 (100%)	1402 (96%)	63 (4%)	35	64

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	8	ARG
1	A	46	SER
1	A	61	GLN
1	A	80	LEU
1	A	98	SER
1	A	121	LYS
1	A	179	GLN
1	A	204	ARG
1	A	214	LEU
1	A	219	ARG
1	A	240	TYR

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Mol	Chain	Res	Type
1	A	330	SER
1	B	4	LEU
1	B	8	ARG
1	B	40	PHE
1	B	46	SER
1	B	61	GLN
1	B	80	LEU
1	B	98	SER
1	B	122	GLU
1	B	179	GLN
1	B	214	LEU
1	B	218	GLU
1	B	240	TYR
1	B	327	SER
1	B	330	SER
1	C	4	LEU
1	C	8	ARG
1	C	46	SER
1	C	61	GLN
1	C	80	LEU
1	C	98	SER
1	C	122	GLU
1	C	179	GLN
1	C	214	LEU
1	C	240	TYR
1	C	328	ILE
1	C	330	SER
1	D	4	LEU
1	D	8	ARG
1	D	46	SER
1	D	61	GLN
1	D	98	SER
1	D	121	LYS
1	D	179	GLN
1	D	214	LEU
1	D	240	TYR
1	D	330	SER
1	E	4	LEU
1	E	8	ARG
1	E	46	SER
1	E	61	GLN
1	E	80	LEU

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Mol	Chain	Res	Type
1	E	98	SER
1	E	121	LYS
1	E	122	GLU
1	E	155	ARG
1	E	179	GLN
1	E	204	ARG
1	E	214	LEU
1	E	240	TYR
1	E	330	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	61	GLN
1	A	211	GLN
1	A	227	HIS
1	A	250	HIS
1	A	310	GLN
1	B	18	GLN
1	B	61	GLN
1	B	211	GLN
1	B	227	HIS
1	B	250	HIS
1	B	310	GLN
1	C	18	GLN
1	C	61	GLN
1	C	211	GLN
1	C	227	HIS
1	C	250	HIS
1	D	18	GLN
1	D	61	GLN
1	D	211	GLN
1	D	227	HIS
1	D	250	HIS
1	D	310	GLN
1	E	18	GLN
1	E	58	HIS
1	E	61	GLN
1	E	227	HIS
1	E	250	HIS
1	E	310	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	353/372 (94%)	-0.31	0 100 100	18, 26, 44, 64	0
1	B	354/372 (95%)	-0.31	1 (0%) 94 95	17, 25, 44, 70	0
1	C	354/372 (95%)	-0.39	0 100 100	16, 25, 42, 66	0
1	D	353/372 (94%)	-0.26	0 100 100	16, 26, 40, 54	0
1	E	353/372 (94%)	-0.33	1 (0%) 94 95	16, 27, 43, 67	0
All	All	1767/1860 (95%)	-0.32	2 (0%) 95 97	16, 26, 43, 70	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	PRO	2.2
1	E	4	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.