Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2021 – 08:02 am BST

PDB ID	:	7A1C
Title	:	LdtMT2 with covalent adduct derived from N-Thio-beta-lactam 1a
Authors	:	Schnell, R.; Steiner, E.M.
Deposited on	:	2020-08-12
Resolution	:	1.77 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 following versions of software and data (see references (i)) were used in the production of this report:

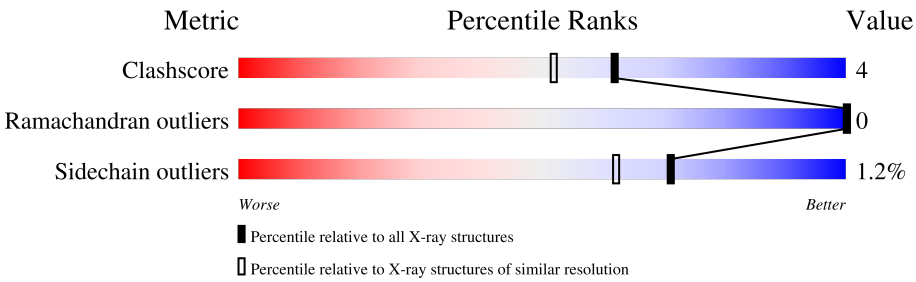
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 1.77 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))
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	87% 10% • •
1	B	261	89% 10% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4644 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.

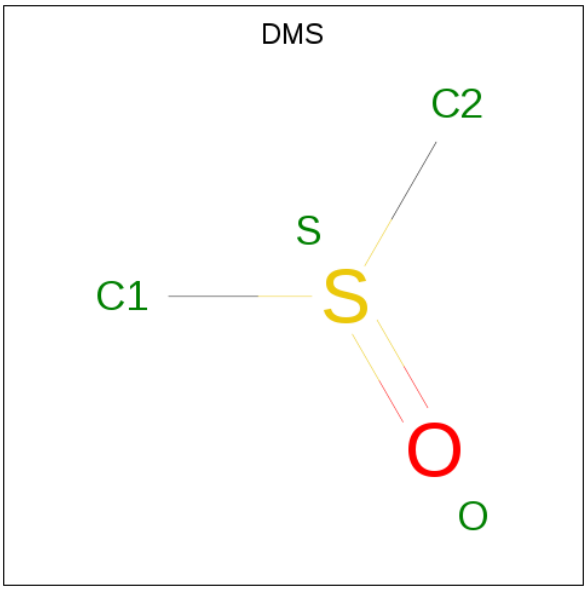
- Molecule 1 is a protein called L,D-transpeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	1993	1255	345	384	9	0	4	0
1	B	259	1998	1258	346	386	8	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	SER	-	expression tag	UNP I6Y9J2
A	149	MET	-	expression tag	UNP I6Y9J2
B	148	SER	-	expression tag	UNP I6Y9J2
B	149	MET	-	expression tag	UNP I6Y9J2

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	4	2	1	1	0	0
			Total	C	O	S		
2	A	1	4	2	1	1	0	0
			Total	C	O	S		
2	B	1	4	2	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	318	318	318	0	0
			Total	O		
3	B	323	323	323	0	0

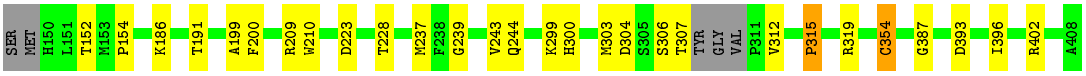
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

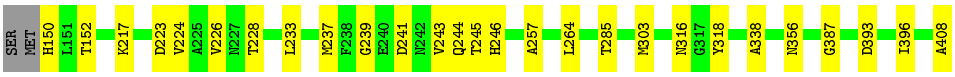
- Molecule 1: L,D-transpeptidase 2

Chain A:



- Molecule 1: L,D-transpeptidase 2

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.21Å 75.38Å 68.35Å 90.00° 111.55° 90.00°	Depositor
Resolution (Å)	39.70 – 1.77	Depositor
% Data completeness (in resolution range)	95.4 (39.70-1.77)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.179 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4644	wwPDB-VP
Average B, all atoms ($Å^2$)	24.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SCH, DMS

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	0.61	0/2050	0.76	1/2797 (0.0%)
1	B	0.55	0/2048	0.70	1/2799 (0.0%)
All	All	0.58	0/4098	0.73	2/5596 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	PRO	N-CA-C	6.59	129.23	112.10
1	B	241	ASP	CB-CG-OD1	5.36	123.12	118.30

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	1993	0	1901	19	0
1	B	1998	0	1893	15	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0
3	A	318	0	0	3	2
3	B	323	0	0	1	2
All	All	4644	0	3812	34	3

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 4.

All (34) 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:299:LYS:O	1:A:299:LYS:HD2	1.91	0.71
1:A:186:LYS:NZ	3:A:603:HOH:O	2.25	0.69
1:A:300:HIS:ND1	3:A:602:HOH:O	2.25	0.68
1:B:224:VAL:HB	1:B:245:THR:HG22	1.79	0.64
1:B:150:HIS:HB3	1:B:237:MET:CE	2.27	0.64
1:B:408:ALA:O	3:B:602:HOH:O	2.17	0.57
1:B:226:VAL:HB	1:B:243:VAL:HG22	1.87	0.56
1:A:154:PRO:HG2	1:A:243:VAL:HG23	1.89	0.55
1:A:387:GLY:HA3	1:A:396:ILE:HG13	1.89	0.55
1:B:223:ASP:OD1	1:B:246:HIS:ND1	2.23	0.54
1:B:226:VAL:HB	1:B:243:VAL:CG2	2.37	0.54
1:A:303:MET:HE3	1:A:354:SCH:SG	2.49	0.53
1:A:402:ARG:NH1	3:A:609:HOH:O	2.44	0.51
1:A:154:PRO:HG2	1:A:243:VAL:CG2	2.41	0.51
1:B:387:GLY:HA3	1:B:396:ILE:HG13	1.94	0.50
1:A:303:MET:CE	1:A:354:SCH:SG	3.00	0.49
1:A:228:THR:O	1:A:239:GLY:HA3	2.13	0.48
1:B:257:ALA:HB2	1:B:264:LEU:HD13	1.95	0.47
1:A:152:THR:HG21	1:A:237[A]:MET:HE3	1.98	0.45
1:A:304:ASP:OD1	1:A:306:SER:OG	2.27	0.45
1:A:191:THR:HB	1:A:223:ASP:HB2	1.99	0.45
1:A:312:VAL:HG22	1:A:319:ARG:HB2	1.99	0.44
1:B:150:HIS:HB3	1:B:237:MET:SD	2.58	0.44
1:B:228:THR:O	1:B:239:GLY:HA3	2.17	0.44
1:B:152:THR:CG2	1:B:233:LEU:HD12	2.48	0.43
1:A:199:ALA:O	1:A:210:TRP:HA	2.18	0.43
1:B:244:GLN:HG2	1:B:245:THR:N	2.33	0.43
1:A:200:PHE:HA	1:A:209:ARG:O	2.19	0.42
1:A:307:THR:O	1:A:307:THR:OG1	2.37	0.42
1:A:312:VAL:CG2	1:A:319:ARG:HB2	2.49	0.42
1:B:303:MET:HG2	1:B:318:TYR:CE1	2.54	0.42
1:A:237[A]:MET:HE2	1:A:237[A]:MET:HB3	1.93	0.41
1:B:285:THR:HG21	1:B:316[B]:ASN:OD1	2.21	0.41
1:B:338:ALA:HB3	1:B:356:ASN:HB3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:637:HOH:O	3:B:882:HOH:O[1_655]	2.15	0.05
3:A:831:HOH:O	3:B:890:HOH:O[1_556]	2.17	0.03
3:A:857:HOH:O	3:A:895:HOH:O[1_655]	2.18	0.02

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	255/261 (98%)	250 (98%)	5 (2%)	0	100	100
1	B	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
All	All	512/522 (98%)	500 (98%)	12 (2%)	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	A	213/213 (100%)	210 (99%)	3 (1%)	67	56
1	B	212/213 (100%)	210 (99%)	2 (1%)	78	72
All	All	425/426 (100%)	420 (99%)	5 (1%)	71	62

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

Mol	Chain	Res	Type
1	A	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	315	PRO
1	A	393	ASP
1	B	217	LYS
1	B	393	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	316	ASN
1	B	214	HIS
1	B	260	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SCH	B	354	1	6,7,8	0.60	0	3,7,9	1.23	0
1	SCH	A	354	1	6,7,8	0.70	0	3,7,9	2.03	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCH	B	354	1	-	0/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCH	A	354	1	-	0/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	SCH	CE-SD-SG	2.87	112.50	102.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	354	SCH	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DMS	B	501	-	3,3,3	0.71	0	3,3,3	0.75	0
2	DMS	A	501	-	3,3,3	0.53	0	3,3,3	0.22	0
2	DMS	A	502	-	3,3,3	0.40	0	3,3,3	1.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.