Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:02 am BST

PDB ID	:	2Z2N
Title	:	Crystal Structure of selenomethionine substituted virginiamycin B lyase from Staphylococcus aureus
Authors	:	Korczynska, M.; Berghuis, A.M.
Deposited on	:	2007-05-25
Resolution	:	1.65 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

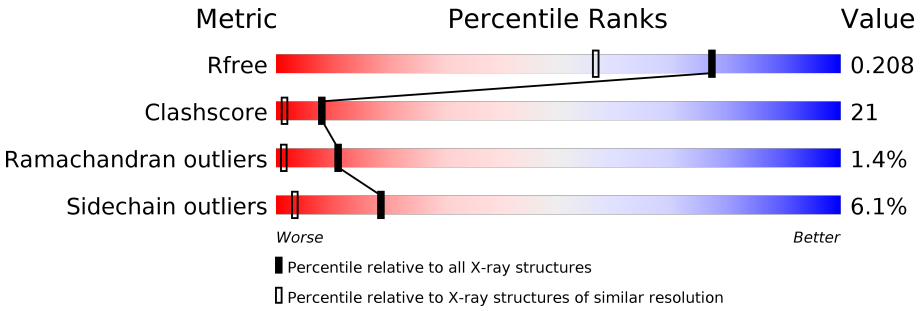
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 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%

Mol	Chain	Length	Quality of chain
1	A	299	66% 26%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2523 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 virginiamycin B lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	Se	0	10	0
			2312	1475	378	448	6	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	THR	PRO	SEE REMARK 999	UNP Q53744
A	212	SER	LEU	SEE REMARK 999	UNP Q53744

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

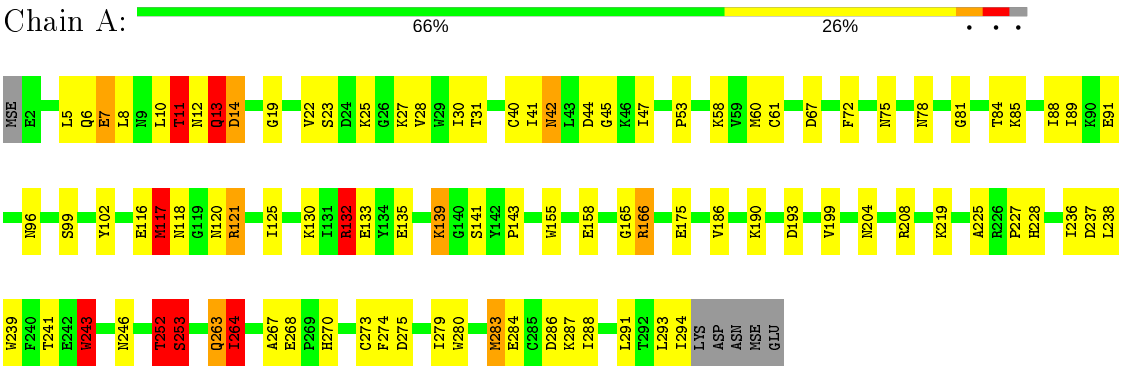
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total	O	0	0
			210	210		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: virginiamycin B lyase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.97Å 34.75Å 86.60Å 90.00° 117.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 19.17 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-1.65) 93.3 (19.17-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.156 , 0.203 0.160 , 0.208	Depositor DCC
R_{free} test set	2747 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2523	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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

5.1 Standard geometry

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

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	1.16	4/2392 (0.2%)	1.14	17/3246 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	VAL	CB-CG2	-7.73	1.36	1.52
1	A	190	LYS	CE-NZ	7.01	1.66	1.49
1	A	121	ARG	CB-CG	-6.77	1.34	1.52
1	A	102	TYR	CE2-CZ	-5.01	1.32	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	121	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	A	243	TRP	CA-CB-CG	7.76	128.44	113.70
1	A	166	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	11	THR	N-CA-C	7.46	131.16	111.00
1	A	283	MSE	CA-CB-CG	7.34	125.78	113.30
1	A	132	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	166	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	252	THR	C-N-CA	-6.32	105.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	117[A]	MSE	CG-SE-CE	-5.68	86.41	98.90
1	A	117[B]	MSE	CG-SE-CE	-5.68	86.41	98.90
1	A	237	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	208	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	252	THR	N-CA-C	-5.53	96.07	111.00
1	A	238	LEU	CB-CG-CD1	5.35	120.09	111.00
1	A	264	ILE	CB-CA-C	5.26	122.12	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LEU	Peptide
1	A	252	THR	Peptide
1	A	253	SER	Peptide

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	2312	0	2298	98	0
2	A	1	0	0	0	0
3	A	210	0	0	16	0
All	All	2523	0	2298	98	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 21.

All (98) 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:13:GLN:HG2	3:A:480:HOH:O	1.63	0.99
1:A:243:TRP:CZ3	3:A:498:HOH:O	2.24	0.91
1:A:117[B]:MSE:HE3	3:A:478:HOH:O	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117[B]:MSE:HG3	1:A:143:PRO:O	1.74	0.86
1:A:263:GLN:O	1:A:264:ILE:HB	1.72	0.86
1:A:118:ASN:HB3	3:A:483:HOH:O	1.76	0.85
1:A:246:ASN:ND2	1:A:267:ALA:HB3	1.92	0.84
1:A:252:THR:O	1:A:253:SER:HB3	1.77	0.78
1:A:22:VAL:HG22	1:A:28[A]:VAL:HG12	1.66	0.76
1:A:12[B]:ASN:HD22	1:A:13:GLN:N	1.82	0.76
1:A:42:ASN:ND2	1:A:44:ASP:OD1	2.21	0.73
1:A:243:TRP:CE3	3:A:498:HOH:O	2.42	0.70
1:A:219[B]:LYS:HD2	3:A:406:HOH:O	1.93	0.69
1:A:27:LYS:CG	1:A:40[B]:CYS:SG	2.82	0.67
1:A:45:GLY:O	1:A:47:ILE:HD12	1.96	0.66
1:A:27:LYS:HG2	1:A:40[B]:CYS:SG	2.37	0.64
1:A:283:MSE:HG3	1:A:287:LYS:HB2	1.80	0.63
1:A:60:MSE:HG3	1:A:75:ASN:HB2	1.80	0.62
1:A:139:LYS:HD2	3:A:426:HOH:O	1.99	0.61
1:A:28[A]:VAL:HG23	1:A:41:ILE:HD12	1.81	0.61
1:A:246:ASN:HD22	1:A:267:ALA:HB3	1.65	0.60
1:A:23:SER:HB2	1:A:25:LYS:HG2	1.83	0.59
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.67	0.58
1:A:121:ARG:HD3	1:A:135:GLU:OE1	2.05	0.57
1:A:13:GLN:CG	3:A:480:HOH:O	2.34	0.57
1:A:239:TRP:CD1	1:A:279:ILE:HD11	2.40	0.56
1:A:13:GLN:O	1:A:286:ASP:OD2	2.21	0.56
1:A:246:ASN:HD21	1:A:267:ALA:N	2.03	0.56
1:A:28[A]:VAL:CG2	1:A:41:ILE:HD12	2.34	0.56
1:A:117[B]:MSE:CE	3:A:478:HOH:O	2.43	0.55
1:A:23:SER:CB	1:A:25:LYS:HG2	2.37	0.55
1:A:293:LEU:O	1:A:294:ILE:CG1	2.55	0.55
1:A:11:THR:HG23	1:A:286:ASP:CB	2.37	0.55
1:A:228:HIS:ND1	3:A:421:HOH:O	2.31	0.54
1:A:204:ASN:HD21	1:A:225:ALA:H	1.55	0.54
1:A:22:VAL:HG23	1:A:273[B]:CYS:SG	2.48	0.54
1:A:120:ASN:HD21	1:A:141:SER:H	1.56	0.54
1:A:270:HIS:HE1	1:A:284:GLU:OE2	1.92	0.52
1:A:78:ASN:ND2	1:A:99:SER:H	2.07	0.52
1:A:268:GLU:O	1:A:268:GLU:CG	2.58	0.52
1:A:27:LYS:CE	1:A:40[B]:CYS:SG	2.98	0.52
1:A:263:GLN:HA	3:A:500:HOH:O	2.09	0.51
1:A:139:LYS:N	1:A:139:LYS:HD2	2.25	0.51
1:A:13:GLN:HA	1:A:13:GLN:NE2	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:OD1	1:A:275:ASP:C	2.49	0.51
1:A:132:ARG:CG	1:A:132:ARG:HH11	2.23	0.51
1:A:274:PHE:HD1	1:A:279:ILE:HD13	1.76	0.51
1:A:246:ASN:HD21	1:A:268:GLU:H	1.59	0.50
1:A:30:ILE:HG21	1:A:288:ILE:HD11	1.92	0.50
1:A:27:LYS:HG3	1:A:40[B]:CYS:SG	2.51	0.50
1:A:120:ASN:ND2	1:A:141:SER:H	2.10	0.50
1:A:246:ASN:ND2	1:A:267:ALA:CB	2.70	0.50
1:A:44:ASP:OD1	1:A:44:ASP:C	2.50	0.49
1:A:31[A]:THR:HG21	1:A:60:MSE:O	2.12	0.49
1:A:72:PHE:CZ	1:A:81:GLY:HA3	2.48	0.49
1:A:42:ASN:HD21	1:A:44:ASP:CG	2.16	0.49
1:A:53:PRO:HG2	1:A:91:GLU:CD	2.33	0.49
1:A:5:LEU:HD13	1:A:291:LEU:HD13	1.94	0.48
1:A:27:LYS:HE3	1:A:40[B]:CYS:SG	2.53	0.48
1:A:84:THR:HG23	1:A:88:ILE:O	2.13	0.48
1:A:132:ARG:NH1	1:A:132:ARG:HG2	2.28	0.48
1:A:155:TRP:CZ2	1:A:166:ARG:HD3	2.48	0.48
1:A:58:LYS:HD3	1:A:75:ASN:HD22	1.78	0.48
1:A:60:MSE:HE2	1:A:60:MSE:HA	1.95	0.48
1:A:204:ASN:HB3	1:A:219[B]:LYS:HE3	1.95	0.47
1:A:246:ASN:HD21	1:A:267:ALA:CA	2.28	0.47
1:A:219[A]:LYS:HE2	3:A:314:HOH:O	2.14	0.47
1:A:19:GLY:H	1:A:31[A]:THR:HG22	1.78	0.47
1:A:11:THR:O	1:A:11:THR:HG22	2.16	0.46
1:A:42:ASN:ND2	1:A:44:ASP:CG	2.70	0.46
1:A:139:LYS:CD	3:A:426:HOH:O	2.59	0.46
1:A:28[B]:VAL:HG21	1:A:280:TRP:CZ3	2.51	0.45
1:A:61:CYS:SG	3:A:430:HOH:O	2.27	0.45
1:A:246:ASN:ND2	1:A:267:ALA:N	2.65	0.45
1:A:125:ILE:HA	1:A:130:LYS:O	2.17	0.45
1:A:14:ASP:O	1:A:14:ASP:OD1	2.35	0.44
1:A:263:GLN:O	1:A:264:ILE:CB	2.56	0.44
1:A:293:LEU:O	1:A:294:ILE:HG13	2.17	0.44
1:A:116:GLU:OE2	1:A:133:GLU:OE2	2.37	0.43
1:A:236:ILE:CD1	1:A:253:SER:HA	2.48	0.43
1:A:27:LYS:NZ	3:A:454:HOH:O	2.50	0.43
1:A:274:PHE:HD1	1:A:279:ILE:CD1	2.32	0.43
1:A:227:PRO:HA	1:A:241:THR:O	2.19	0.42
1:A:7:GLU:HG2	1:A:287:LYS:HD3	2.00	0.42
1:A:12[B]:ASN:ND2	1:A:13:GLN:N	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HE2	1:A:27:LYS:CB	2.49	0.42
1:A:117[A]:MSE:HE3	1:A:117[A]:MSE:HB2	1.70	0.42
1:A:158:GLU:OE2	1:A:175:GLU:OE2	2.38	0.42
1:A:96:ASN:O	1:A:99:SER:OG	2.38	0.41
1:A:252:THR:O	1:A:252:THR:HG23	2.20	0.41
1:A:274:PHE:CD1	1:A:279:ILE:HD13	2.55	0.41
1:A:155:TRP:HA	1:A:165:GLY:O	2.21	0.41
1:A:293:LEU:O	1:A:294:ILE:HG12	2.20	0.41
1:A:246:ASN:HD21	1:A:268:GLU:N	2.17	0.41
1:A:75:ASN:ND2	3:A:372:HOH:O	2.54	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	301/299 (101%)	285 (95%)	12 (4%)	4 (1%)	12 1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	264	ILE
1	A	13	GLN
1	A	186	VAL

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	256/247 (104%)	240 (94%)	16 (6%)	18 3

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	GLU
1	A	8	LEU
1	A	11	THR
1	A	13	GLN
1	A	14	ASP
1	A	42	ASN
1	A	67	ASP
1	A	85	LYS
1	A	89	ILE
1	A	117[A]	MSE
1	A	117[B]	MSE
1	A	132	ARG
1	A	139	LYS
1	A	243	TRP
1	A	263	GLN

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	9	ASN
1	A	32	GLN
1	A	75	ASN
1	A	78	ASN
1	A	118	ASN
1	A	120	ASN
1	A	160	GLN
1	A	162	ASN
1	A	204	ASN
1	A	246	ASN
1	A	254	ASN
1	A	270	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.