



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:21 AM UTC

PDB ID : 5DZT / pdb_00005dzt
Title : Crystal structure of class II lanthipeptide synthetase CylM in complex with AMP
Authors : Dong, S.H.; Lukk, T.; Nair, S.K.
Deposited on : 2015-09-26
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

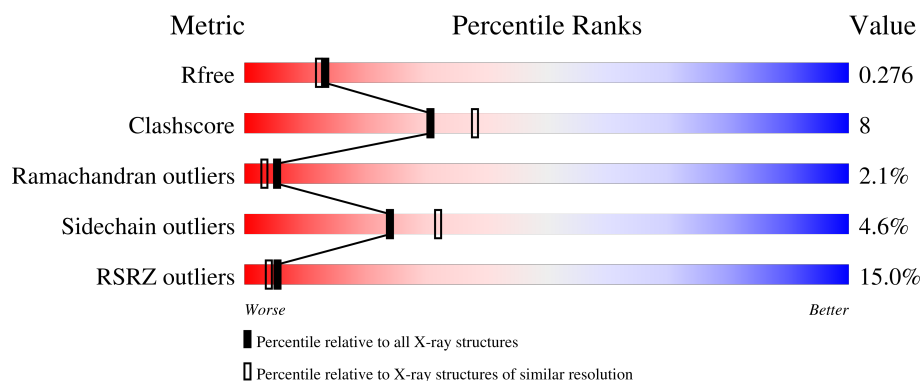
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	993	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7435 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.

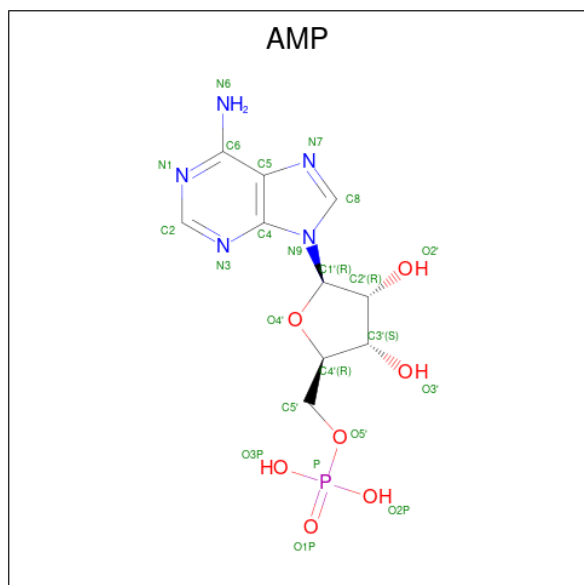
- Molecule 1 is a protein called CylM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	886	Total	C	N	O	S	0	0	0
			7251	4690	1174	1362	25			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total 160	O 160	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.19Å 90.70Å 246.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 25.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.4 (25.00-2.20) 87.3 (25.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.244 , 0.275 0.246 , 0.276	Depositor DCC
R_{free} test set	2636 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7435	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	4/7398 (0.1%)	0.91	6/9994 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	561	ASP	CG-OD2	8.09	1.40	1.25
1	A	561	ASP	CB-CG	7.04	1.69	1.52
1	A	561	ASP	CA-CB	5.67	1.64	1.53
1	A	561	ASP	CA-C	5.30	1.60	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	THR	CA-C-N	8.85	130.90	119.84
1	A	457	THR	C-N-CA	8.85	130.90	119.84
1	A	561	ASP	CB-CG-OD1	-7.29	101.63	118.40
1	A	561	ASP	N-CA-C	-6.67	104.86	112.87
1	A	459	ILE	N-CA-C	5.17	120.08	109.34
1	A	561	ASP	CB-CG-OD2	5.12	130.17	118.40

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	7251	0	7203	120	0
2	A	1	0	0	0	0
3	A	23	0	12	1	0
4	A	160	0	0	5	1
All	All	7435	0	7215	120	1

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 8.

All (120) 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:788:TRP:HB3	1:A:834:GLY:HA2	1.25	1.11
1:A:111:PHE:HE2	1:A:149:ILE:HD13	1.26	0.98
1:A:106:ASP:HB3	1:A:109:TYR:CE2	2.01	0.95
1:A:33:TRP:HE1	1:A:536:LYS:HG2	1.42	0.85
1:A:54:GLU:HB2	1:A:58:ASN:HD22	1.42	0.82
1:A:54:GLU:HB2	1:A:58:ASN:ND2	1.95	0.80
1:A:633:ASN:HA	1:A:949:LYS:HE2	1.64	0.78
1:A:111:PHE:CE2	1:A:149:ILE:HD13	2.15	0.78
1:A:518:MET:HE1	1:A:540:ASN:HB2	1.69	0.73
1:A:788:TRP:HB3	1:A:834:GLY:CA	2.15	0.71
1:A:393:ILE:HG23	1:A:399:VAL:HG21	1.74	0.69
1:A:394:MET:HE3	1:A:614:TRP:HB3	1.74	0.68
1:A:816:LEU:O	1:A:820:GLU:HG2	1.94	0.68
1:A:245:SER:HB3	1:A:264:THR:HB	1.76	0.67
1:A:393:ILE:HG22	1:A:394:MET:HE2	1.76	0.67
1:A:33:TRP:HE1	1:A:536:LYS:CG	2.09	0.66
1:A:393:ILE:CG2	1:A:394:MET:HE2	2.28	0.64
1:A:281:ASN:OD1	1:A:284:ARG:NH2	2.30	0.64
1:A:33:TRP:CD1	1:A:536:LYS:HZ1	2.17	0.62
1:A:152:THR:HG22	1:A:203:LEU:HD11	1.81	0.62
1:A:394:MET:HE1	1:A:399:VAL:HG11	1.81	0.62
1:A:111:PHE:HE2	1:A:149:ILE:CD1	2.07	0.61
1:A:897:ASP:O	1:A:901:THR:HG23	2.01	0.60
1:A:274:LYS:HE3	1:A:312:GLU:OE1	2.02	0.59
1:A:747:ILE:HG23	1:A:748:TYR:H	1.67	0.59
1:A:192:ASP:OD1	1:A:192:ASP:C	2.45	0.59
1:A:26:ASP:OD1	1:A:28:LYS:HB2	2.02	0.58
1:A:850:ILE:HG22	1:A:851:ASP:H	1.67	0.58
1:A:532:ILE:HG23	1:A:536:LYS:HE2	1.84	0.58
1:A:328:LYS:HE2	4:A:1133:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG22	1:A:394:MET:CE	2.34	0.57
1:A:792:HIS:O	1:A:795:ILE:HG22	2.05	0.56
1:A:260:VAL:HG21	3:A:1002:AMP:O3P	2.06	0.56
1:A:830:PHE:HB2	1:A:835:HIS:O	2.07	0.55
1:A:514:ARG:NH1	1:A:517:ASP:OD2	2.38	0.55
1:A:518:MET:CE	1:A:540:ASN:HB2	2.36	0.54
1:A:382:THR:HB	1:A:675:ASN:HD22	1.72	0.54
1:A:351:GLU:O	1:A:352:ASN:CG	2.51	0.54
1:A:623:ASN:HB3	1:A:626:LYS:HB2	1.91	0.53
1:A:550:LYS:HE3	1:A:584:VAL:HG13	1.91	0.53
1:A:33:TRP:NE1	1:A:536:LYS:HG2	2.18	0.53
1:A:393:ILE:HD13	1:A:478:MET:SD	2.48	0.53
1:A:160:LEU:HB2	1:A:161:HIS:HD2	1.75	0.53
1:A:787:ASP:OD1	1:A:793:ASN:ND2	2.43	0.51
1:A:7:VAL:HB	1:A:201:PRO:HB2	1.93	0.51
1:A:871:ASN:O	1:A:873:SER:N	2.42	0.51
1:A:666:ILE:O	1:A:674:VAL:HA	2.11	0.50
1:A:63:ILE:HG22	1:A:63:ILE:O	2.10	0.50
1:A:88:PHE:CE2	1:A:92:LEU:HD11	2.45	0.50
1:A:793:ASN:HD22	1:A:793:ASN:H	1.60	0.50
1:A:337:ILE:CG2	1:A:393:ILE:HG12	2.42	0.50
1:A:494:ALA:O	1:A:498:ASN:HB2	2.11	0.50
1:A:963:SER:HB2	1:A:969:GLY:HA2	1.94	0.50
1:A:351:GLU:O	1:A:352:ASN:CB	2.60	0.49
1:A:679:ILE:HG12	4:A:1148:HOH:O	2.12	0.49
1:A:63:ILE:HD12	1:A:536:LYS:HZ2	1.77	0.49
1:A:740:PHE:CZ	1:A:789:ILE:HD13	2.47	0.49
1:A:826:PRO:HG3	1:A:837:ILE:HG12	1.95	0.49
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.67	0.48
1:A:109:TYR:HB2	1:A:110:PRO:HD3	1.95	0.48
1:A:788:TRP:CZ2	1:A:991:PHE:CD2	3.01	0.48
1:A:139:ASN:O	1:A:143:ILE:HG12	2.14	0.48
1:A:59:PHE:O	1:A:63:ILE:HG12	2.14	0.48
1:A:694:MET:HA	1:A:699:PRO:HG2	1.96	0.47
1:A:567:PHE:HB3	1:A:576:LEU:HD22	1.96	0.47
1:A:197:TYR:HB3	1:A:204:MET:CE	2.44	0.47
1:A:638:LYS:HD3	1:A:945:LYS:HG2	1.97	0.47
1:A:798:VAL:HA	1:A:801:LEU:HD12	1.97	0.47
1:A:106:ASP:O	1:A:107:ALA:CB	2.62	0.46
1:A:250:GLN:C	1:A:252:ASP:H	2.23	0.46
1:A:269:LYS:HE2	4:A:1221:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:O	1:A:76:ILE:HG12	2.15	0.46
1:A:328:LYS:HD3	1:A:328:LYS:HA	1.56	0.46
1:A:698:LEU:N	1:A:699:PRO:HD2	2.31	0.46
1:A:747:ILE:HG23	1:A:748:TYR:N	2.31	0.45
1:A:33:TRP:CD1	1:A:536:LYS:NZ	2.82	0.45
1:A:533:GLU:O	1:A:537:VAL:HG23	2.16	0.45
1:A:796:ILE:HG23	1:A:815:SER:HB2	1.99	0.45
1:A:810:LYS:HA	1:A:813:LYS:HE2	1.98	0.45
1:A:197:TYR:HB3	1:A:204:MET:HE3	1.99	0.45
1:A:26:ASP:OD1	1:A:28:LYS:CB	2.65	0.45
1:A:518:MET:HG3	1:A:541:MET:SD	2.56	0.45
1:A:641:TYR:HB3	1:A:645:GLU:HG3	1.99	0.44
1:A:67:GLU:C	1:A:69:PHE:H	2.25	0.44
1:A:789:ILE:HB	1:A:835:HIS:CE1	2.52	0.44
1:A:29:ASN:ND2	1:A:65:PRO:HD3	2.32	0.44
1:A:30:LEU:O	1:A:34:LYS:HB2	2.17	0.44
1:A:159:ASP:CB	4:A:1179:HOH:O	2.66	0.44
1:A:729:TYR:CE1	1:A:765:VAL:HG11	2.52	0.44
1:A:847:PHE:C	1:A:849:ARG:H	2.25	0.44
1:A:457:THR:HA	1:A:458:PRO:HD3	1.86	0.44
1:A:640:ILE:HD11	1:A:938:LYS:HE3	2.00	0.44
1:A:848:ASN:O	1:A:850:ILE:HG13	2.17	0.44
1:A:613:VAL:HG11	1:A:679:ILE:HD12	2.00	0.43
1:A:63:ILE:HD12	1:A:536:LYS:NZ	2.33	0.43
1:A:316:ASP:CB	4:A:1132:HOH:O	2.67	0.43
1:A:725:LYS:HA	1:A:728:ILE:HG12	2.01	0.43
1:A:806:THR:C	1:A:808:ASP:H	2.27	0.42
1:A:871:ASN:C	1:A:873:SER:H	2.26	0.42
1:A:393:ILE:CD1	1:A:478:MET:SD	3.08	0.42
1:A:623:ASN:HA	1:A:624:PRO:HD2	1.93	0.42
1:A:875:CYS:HB3	1:A:911:CYS:SG	2.60	0.42
1:A:560:ILE:HD12	1:A:561:ASP:N	2.34	0.42
1:A:664:ARG:NH2	1:A:678:ASP:OD1	2.42	0.42
1:A:206:ILE:O	1:A:210:ARG:HG2	2.19	0.41
1:A:941:SER:O	1:A:945:LYS:HD3	2.19	0.41
1:A:211:MET:HE3	1:A:215:LEU:HD11	2.01	0.41
1:A:847:PHE:O	1:A:849:ARG:N	2.48	0.41
1:A:197:TYR:C	1:A:204:MET:HE3	2.45	0.41
1:A:637:ASN:O	1:A:638:LYS:HB2	2.19	0.41
1:A:680:LYS:HE3	1:A:680:LYS:HB2	1.83	0.41
1:A:803:SER:O	1:A:807:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HG2	1:A:85:TYR:CE2	2.55	0.41
1:A:13:ARG:NH2	1:A:530:ASN:OD1	2.52	0.41
1:A:711:ILE:HG22	1:A:712:THR:N	2.36	0.41
1:A:792:HIS:O	1:A:793:ASN:C	2.64	0.41
1:A:289:PHE:CE1	1:A:293:GLU:HG3	2.56	0.40
1:A:382:THR:HB	1:A:675:ASN:ND2	2.35	0.40
1:A:492:ILE:HG21	1:A:600:ILE:HD12	2.03	0.40
1:A:49:ILE:O	1:A:53:TYR:O	2.38	0.40

All (1) 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)
4:A:1124:HOH:O	4:A:1209:HOH:O[4_456]	1.96	0.24

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	874/993 (88%)	807 (92%)	49 (6%)	18 (2%)	5 3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
1	A	107	ALA
1	A	352	ASN
1	A	711	ILE
1	A	759	ASP
1	A	251	GLY
1	A	459	ILE
1	A	732	PRO

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Mol	Chain	Res	Type
1	A	736	ILE
1	A	872	ASN
1	A	23	GLU
1	A	98	SER
1	A	100	GLU
1	A	877	GLY
1	A	741	PHE
1	A	848	ASN
1	A	27	ILE
1	A	65	PRO

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	805/922 (87%)	768 (95%)	37 (5%)	24	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
1	A	67	GLU
1	A	74	VAL
1	A	83	SER
1	A	101	GLN
1	A	104	GLU
1	A	186	ARG
1	A	191	LYS
1	A	192	ASP
1	A	252	ASP
1	A	259	THR
1	A	324	GLU
1	A	362	ILE
1	A	364	ASP
1	A	382	THR
1	A	383	VAL

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Mol	Chain	Res	Type
1	A	393	ILE
1	A	395	VAL
1	A	536	LYS
1	A	551	VAL
1	A	560	ILE
1	A	633	ASN
1	A	644	LEU
1	A	679	ILE
1	A	712	THR
1	A	772	MET
1	A	789	ILE
1	A	804	GLU
1	A	822	LEU
1	A	831	ARG
1	A	837	ILE
1	A	850	ILE
1	A	860	ILE
1	A	871	ASN
1	A	901	THR
1	A	931	THR
1	A	948	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	161	HIS
1	A	250	GLN
1	A	365	ASN
1	A	372	ASN
1	A	634	GLN
1	A	693	ASN
1	A	793	ASN
1	A	835	HIS
1	A	923	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	AMP	A	1002	-	25,25,25	1.59	3 (12%)	37,38,38	1.99	10 (27%)

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
3	AMP	A	1002	-	-	0/10/26/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	AMP	C5-C4	5.79	1.49	1.39
3	A	1002	AMP	C5-C6	2.90	1.49	1.41
3	A	1002	AMP	C8-N7	2.53	1.36	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	AMP	C5-C4-N3	-4.81	120.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	AMP	N3-C4-N9	4.34	134.55	127.17
3	A	1002	AMP	N3-C2-N1	-3.63	123.09	128.58
3	A	1002	AMP	C2-N3-C4	3.58	120.57	111.83
3	A	1002	AMP	O5'-C5'-C4'	3.26	120.10	108.99
3	A	1002	AMP	C5'-C4'-C3'	-3.01	104.37	115.21
3	A	1002	AMP	C2-N1-C6	2.80	123.33	118.73
3	A	1002	AMP	C4-N9-C8	2.62	108.49	105.74
3	A	1002	AMP	C4-C5-N7	-2.26	108.00	110.58
3	A	1002	AMP	N6-C6-N1	2.17	123.20	118.38

There are no chirality outliers.

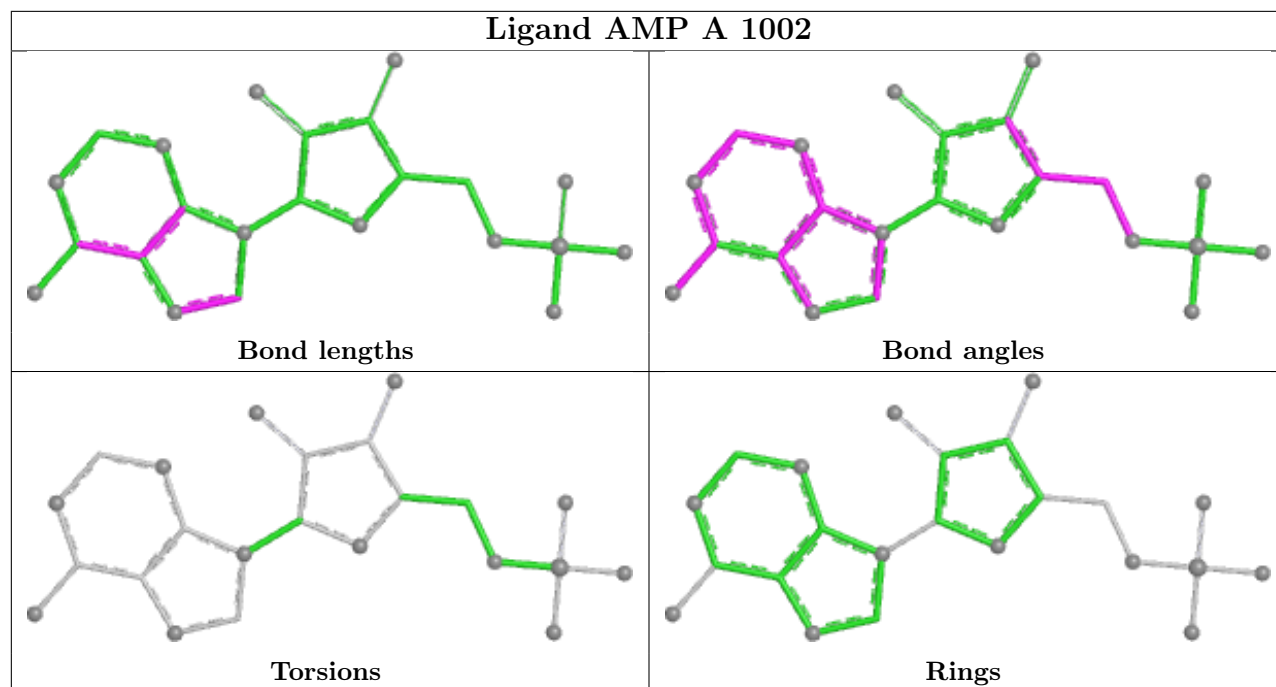
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	886/993 (89%)	0.77	133 (15%) 5 4	10, 41, 95, 144	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	LEU	8.8
1	A	103	LEU	8.4
1	A	105	VAL	7.0
1	A	66	ILE	6.0
1	A	636	SER	5.8
1	A	847	PHE	5.6
1	A	814	PHE	5.2
1	A	639	TYR	4.8
1	A	561	ASP	4.8
1	A	160	LEU	4.8
1	A	747	ILE	4.7
1	A	187	PHE	4.4
1	A	100	GLU	4.3
1	A	860	ILE	4.3
1	A	638	LYS	4.2
1	A	710	TYR	4.2
1	A	712	THR	4.1
1	A	104	GLU	4.1
1	A	772	MET	4.0
1	A	379	ASN	4.0
1	A	178	ARG	4.0
1	A	161	HIS	3.8
1	A	182	TYR	3.7
1	A	789	ILE	3.6
1	A	637	ASN	3.6
1	A	159	ASP	3.6
1	A	109	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	946	TYR	3.5
1	A	27	ILE	3.5
1	A	837	ILE	3.5
1	A	377	PHE	3.5
1	A	816	LEU	3.5
1	A	827	TYR	3.5
1	A	844	LEU	3.4
1	A	770	ALA	3.4
1	A	101	GLN	3.4
1	A	818	ILE	3.4
1	A	719	TYR	3.4
1	A	861	LYS	3.4
1	A	107	ALA	3.4
1	A	711	ILE	3.4
1	A	736	ILE	3.4
1	A	767	VAL	3.3
1	A	158	LEU	3.3
1	A	853	ALA	3.3
1	A	251	GLY	3.3
1	A	633	ASN	3.3
1	A	198	THR	3.3
1	A	33	TRP	3.3
1	A	799	LEU	3.3
1	A	856	LEU	3.3
1	A	858	HIS	3.2
1	A	802	LEU	3.2
1	A	819	PHE	3.1
1	A	387	TYR	3.1
1	A	828	PHE	3.1
1	A	758	ASN	3.1
1	A	849	ARG	3.1
1	A	787	ASP	3.1
1	A	179	PHE	3.0
1	A	760	ILE	3.0
1	A	992	GLU	2.9
1	A	30	LEU	2.9
1	A	857	LEU	2.9
1	A	716	LYS	2.9
1	A	715	HIS	2.9
1	A	805	ILE	2.9
1	A	63	ILE	2.8
1	A	181	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	720	VAL	2.8
1	A	5	ILE	2.8
1	A	835	HIS	2.8
1	A	106	ASP	2.7
1	A	798	VAL	2.7
1	A	817	GLU	2.7
1	A	822	LEU	2.7
1	A	811	TYR	2.7
1	A	885	THR	2.7
1	A	458	PRO	2.7
1	A	729	TYR	2.6
1	A	834	GLY	2.6
1	A	850	ILE	2.6
1	A	641	TYR	2.6
1	A	826	PRO	2.6
1	A	29	ASN	2.6
1	A	461	ASN	2.6
1	A	644	LEU	2.6
1	A	65	PRO	2.6
1	A	769	ILE	2.5
1	A	840	TYR	2.5
1	A	903	GLU	2.5
1	A	836	GLY	2.5
1	A	152	THR	2.5
1	A	859	LYS	2.5
1	A	737	LEU	2.4
1	A	713	LYS	2.4
1	A	250	GLN	2.4
1	A	762	SER	2.4
1	A	22	ASN	2.4
1	A	25	TYR	2.4
1	A	69	PHE	2.4
1	A	757	ASN	2.3
1	A	765	VAL	2.3
1	A	724	ILE	2.3
1	A	634	GLN	2.3
1	A	790	HIS	2.3
1	A	193	ILE	2.3
1	A	68	ASN	2.3
1	A	635	ASN	2.3
1	A	739	ALA	2.3
1	A	717	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	806	THR	2.2
1	A	851	ASP	2.2
1	A	845	SER	2.2
1	A	375	ILE	2.2
1	A	521	PHE	2.2
1	A	754	TYR	2.2
1	A	813	LYS	2.2
1	A	318	ILE	2.1
1	A	180	ILE	2.1
1	A	183	LEU	2.1
1	A	39	VAL	2.1
1	A	812	ARG	2.1
1	A	759	ASP	2.1
1	A	848	ASN	2.1
1	A	825	GLU	2.1
1	A	4	LEU	2.1
1	A	632	LYS	2.0
1	A	830	PHE	2.0
1	A	24	LYS	2.0
1	A	901	THR	2.0
1	A	348	LEU	2.0
1	A	756	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

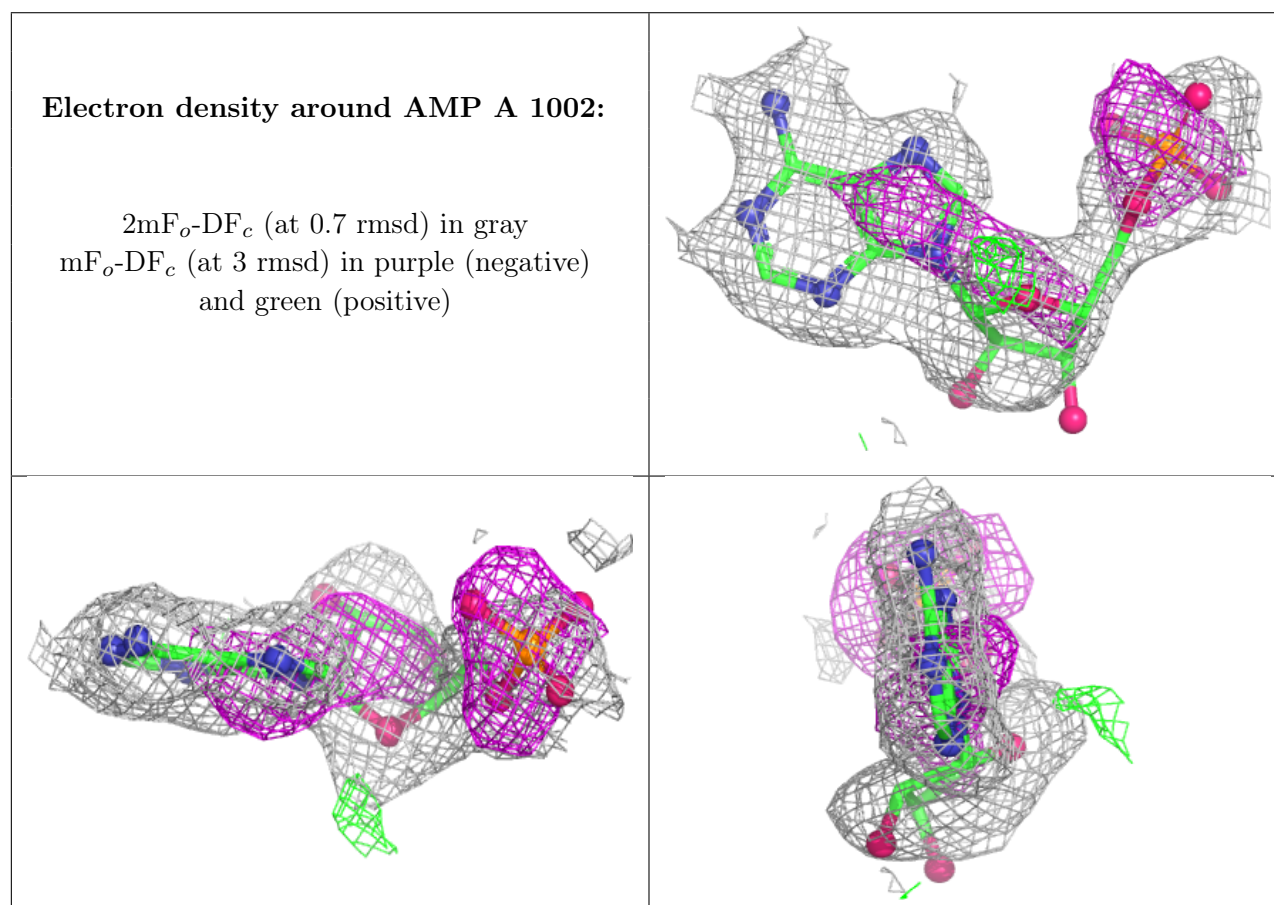
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	A	1002	23/23	0.72	0.16	26,47,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1001	1/1	0.98	0.03	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.