Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:25 am BST

PDB ID	:	5DZT
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 following versions of software and data (see references ⓘ) were used in the production of this report:

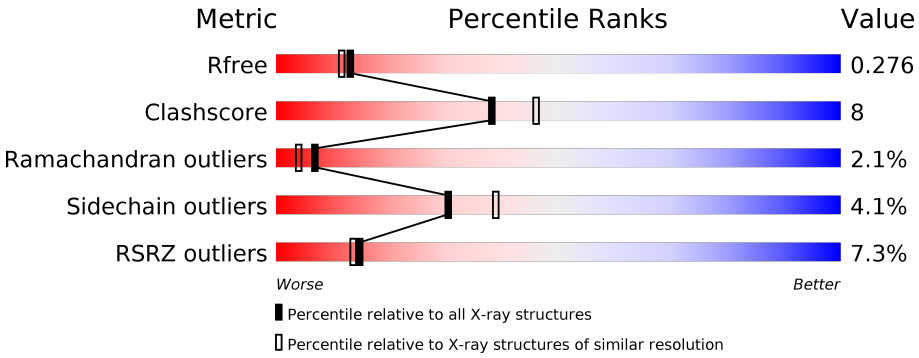
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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% 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	7% 71% 16% • 11%

2 Entry composition

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.

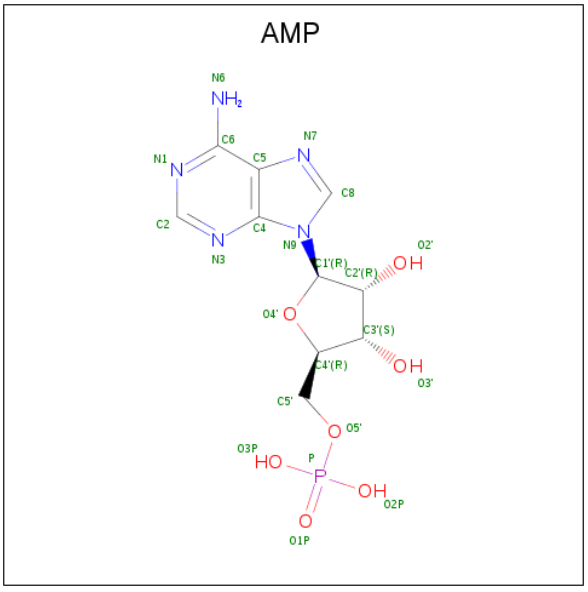
- Molecule 1 is a protein called CylM.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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.

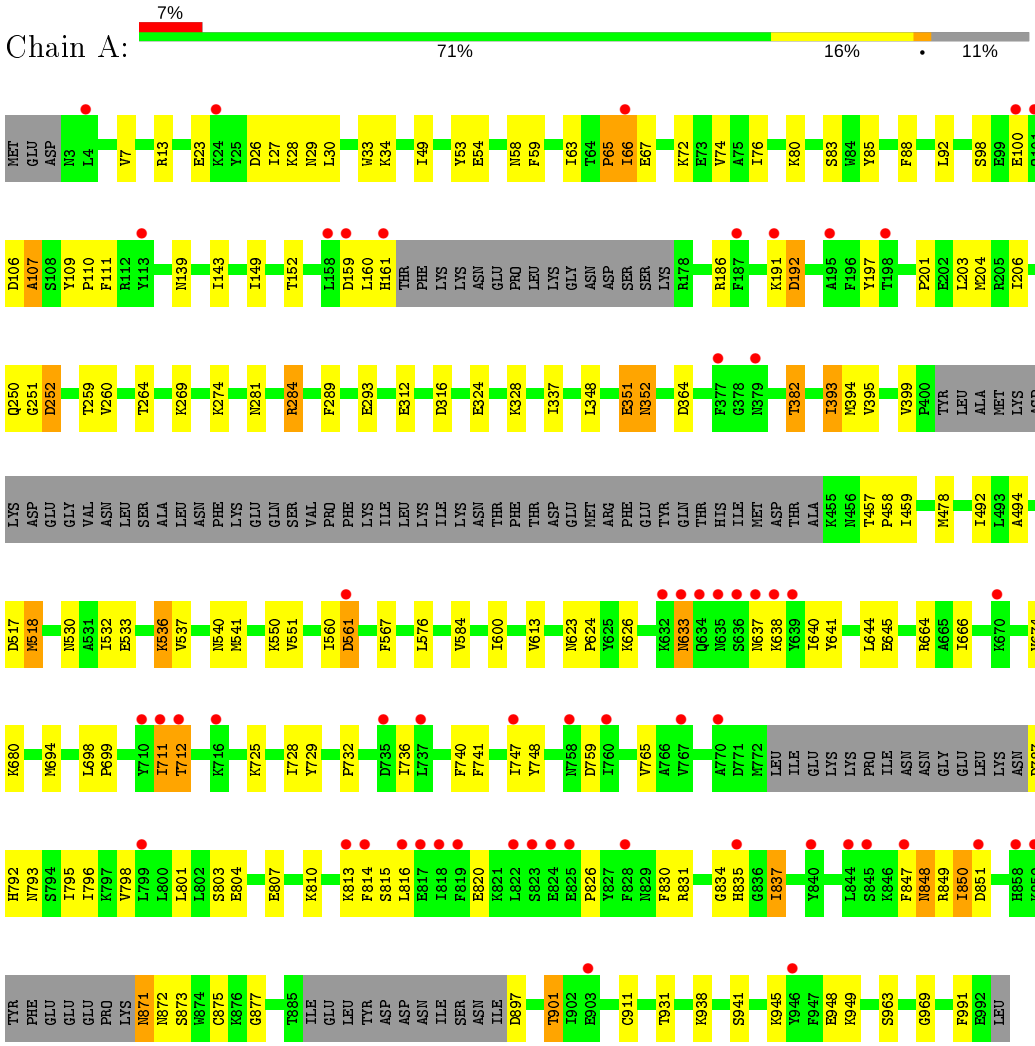
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		

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 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: CylM

Chain A:



4 Data and refinement statistics (i)

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 44.58 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.4 (25.00-2.20) 87.5 (44.58-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.08%)	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)	0.31 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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: AMP, ZN

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	0.48	2/7398 (0.0%)	0.66	3/9994 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	561	ASP	CB-CG	8.53	1.69	1.51
1	A	561	ASP	CG-OD2	6.68	1.40	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	561	ASP	CB-CG-OD1	-18.52	101.63	118.30
1	A	561	ASP	CB-CG-OD2	13.19	130.17	118.30
1	A	284	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	110	0
2	A	1	0	0	0	0
3	A	23	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	160	0	0	5	1
All	All	7435	0	7215	110	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 (110) 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:393:ILE:HG22	1:A:394:MET:HE3	1.62	0.78
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: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: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:33:TRP:HE1	1:A:536:LYS:CG	2.09	0.66
1:A:281:ASN:OD1	1:A:284:ARG:NH2	2.30	0.64
1:A:152:THR:HG22	1:A:203:LEU:HD11	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: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
1:A:393:ILE:HG22	1:A:394:MET:CE	2.34	0.57
1:A:518:MET:CE	1:A:540:ASN:HB2	2.36	0.56
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:192:ASP:OD1	1:A:192:ASP:C	2.45	0.55
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:382:THR:HB	1:A:675:ASN:HD22	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:393:ILE:HD13	1:A:478:MET:SD	2.48	0.53
1:A:33:TRP:NE1	1:A:536:LYS:HG2	2.18	0.53
1:A:160:LEU:HB2	1:A:161:HIS:HD2	1.75	0.53
1:A:63:ILE:HD12	1:A:536:LYS:HZ3	1.74	0.52
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:394:MET:HE2	1:A:399:VAL:HG21	1.92	0.50
1:A:63:ILE:O	1:A:63:ILE:HG22	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: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:351:GLU:O	1:A:352:ASN:CG	2.51	0.49
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.67	0.48
1:A:518:MET:HE3	1:A:540:ASN:HB2	1.94	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:269:LYS:HE2	4:A:1221:HOH:O	2.15	0.46
1:A:72:LYS:O	1:A:76:ILE:HG12	2.15	0.46
1:A:328:LYS:HA	1:A:328:LYS:HD3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:457:THR:HA	1:A:458:PRO:HD3	1.86	0.44
1:A:848:ASN:O	1:A:850:ILE:HG13	2.17	0.44
1:A:640:ILE:HD11	1:A:938:LYS:HE3	2.00	0.44
1:A:613:VAL:HG11	1:A:679:ILE:HD12	2.00	0.43
1:A:316:ASP:CB	4:A:1132:HOH:O	2.67	0.43
1:A:63:ILE:HD12	1:A:536:LYS:NZ	2.33	0.43
1:A:725:LYS:HA	1:A:728:ILE:HG12	2.01	0.43
1:A:393:ILE:CG2	1:A:394:MET:CE	2.97	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:250:GLN:C	1:A:252:ASP:H	2.23	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:847:PHE:O	1:A:849:ARG:N	2.48	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
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: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 (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	874/993 (88%)	807 (92%)	49 (6%)	18 (2%)	7 4

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
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%)	772 (96%)	33 (4%)	30 39

All (33) 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	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	351	GLU
1	A	364	ASP
1	A	382	THR
1	A	393	ILE
1	A	395	VAL
1	A	518	MET
1	A	536	LYS
1	A	551	VAL
1	A	633	ASN
1	A	644	LEU
1	A	679	ILE
1	A	712	THR
1	A	804	GLU
1	A	814	PHE
1	A	831	ARG
1	A	837	ILE
1	A	850	ILE
1	A	860	ILE
1	A	871	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	901	THR
1	A	931	THR
1	A	948	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	161	HIS
1	A	250	GLN
1	A	371	GLN
1	A	498	ASN
1	A	761	ASN
1	A	793	ASN
1	A	835	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 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	-	22,25,25	1.19	2 (9%)	25,38,38	1.76	6 (24%)

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	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	AMP	C5-C4	3.21	1.49	1.40
3	A	1002	AMP	O4'-C1'	3.13	1.45	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	AMP	N3-C2-N1	-3.57	123.09	128.68
3	A	1002	AMP	O5'-C5'-C4'	3.23	120.10	108.99
3	A	1002	AMP	C5'-C4'-C3'	-2.89	104.37	115.18
3	A	1002	AMP	C2-N1-C6	2.67	123.33	118.75
3	A	1002	AMP	P-O5'-C5'	-2.36	111.79	118.30
3	A	1002	AMP	N6-C6-N1	2.23	123.20	118.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

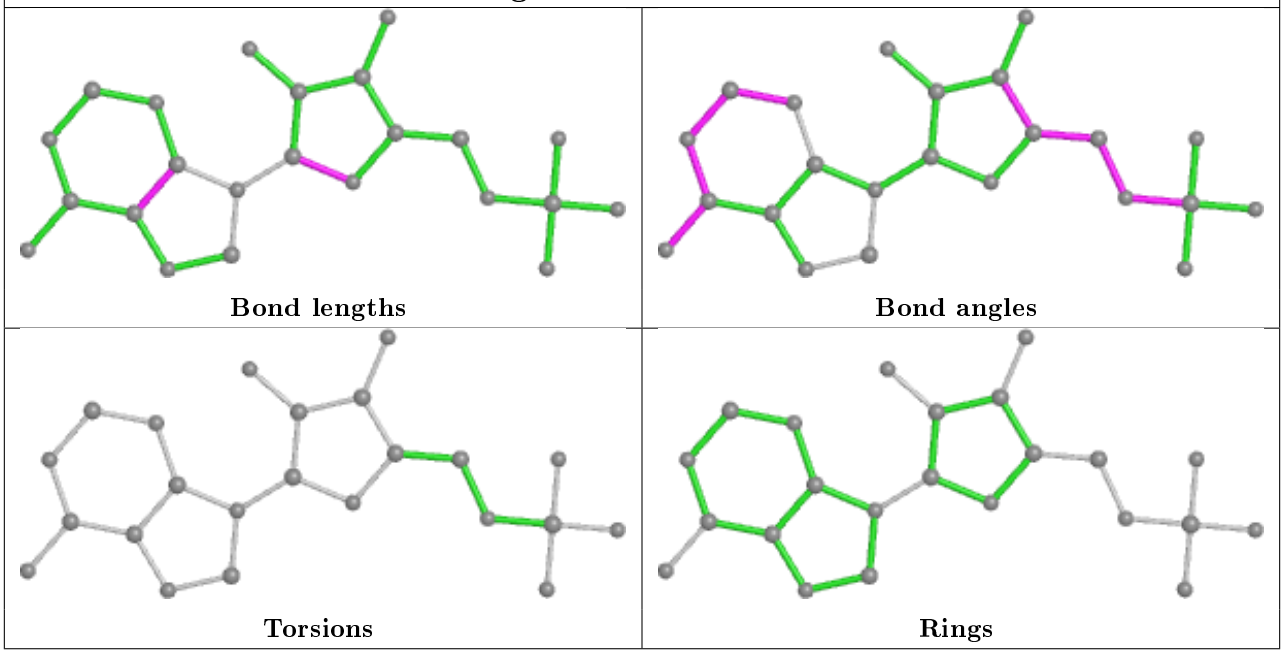
1 monomer is involved in 1 short contact:

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 then 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.

Ligand AMP A 1002



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

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, 95^{th} 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%)	0.32	65 (7%)	15	14	10, 41, 95, 144	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	LEU	14.6
1	A	100	GLU	13.9
1	A	102	LEU	11.1
1	A	636	SER	8.3
1	A	101	GLN	7.6
1	A	105	VAL	7.3
1	A	639	TYR	5.8
1	A	637	ASN	5.3
1	A	858	HIS	4.9
1	A	789	ILE	4.9
1	A	635	ASN	4.6
1	A	758	ASN	4.4
1	A	817	GLU	4.4
1	A	104	GLU	4.1
1	A	825	GLU	3.9
1	A	813	LYS	3.8
1	A	66	ILE	3.8
1	A	818	ILE	3.7
1	A	851	ASP	3.6
1	A	770	ALA	3.5
1	A	847	PHE	3.5
1	A	379	ASN	3.5
1	A	819	PHE	3.4
1	A	24	LYS	3.4
1	A	861	LYS	3.3
1	A	822	LEU	3.2
1	A	710	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	814	PHE	3.0
1	A	712	THR	3.0
1	A	824	GLU	3.0
1	A	760	ILE	3.0
1	A	191	LYS	2.9
1	A	844	LEU	2.9
1	A	840	TYR	2.9
1	A	737	LEU	2.9
1	A	845	SER	2.8
1	A	561	ASP	2.8
1	A	711	ILE	2.7
1	A	816	LEU	2.7
1	A	195	ALA	2.6
1	A	790	HIS	2.6
1	A	187	PHE	2.6
1	A	670	LYS	2.5
1	A	158	LEU	2.5
1	A	113	TYR	2.5
1	A	747	ILE	2.4
1	A	835	HIS	2.3
1	A	4	LEU	2.3
1	A	638	LYS	2.3
1	A	632	LYS	2.3
1	A	903	GLU	2.3
1	A	633	ASN	2.2
1	A	859	LYS	2.2
1	A	823	SER	2.2
1	A	198	THR	2.2
1	A	716	LYS	2.2
1	A	946	TYR	2.2
1	A	828	PHE	2.1
1	A	799	LEU	2.1
1	A	634	GLN	2.1
1	A	735	ASP	2.1
1	A	161	HIS	2.1
1	A	377	PHE	2.1
1	A	159	ASP	2.0
1	A	767	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

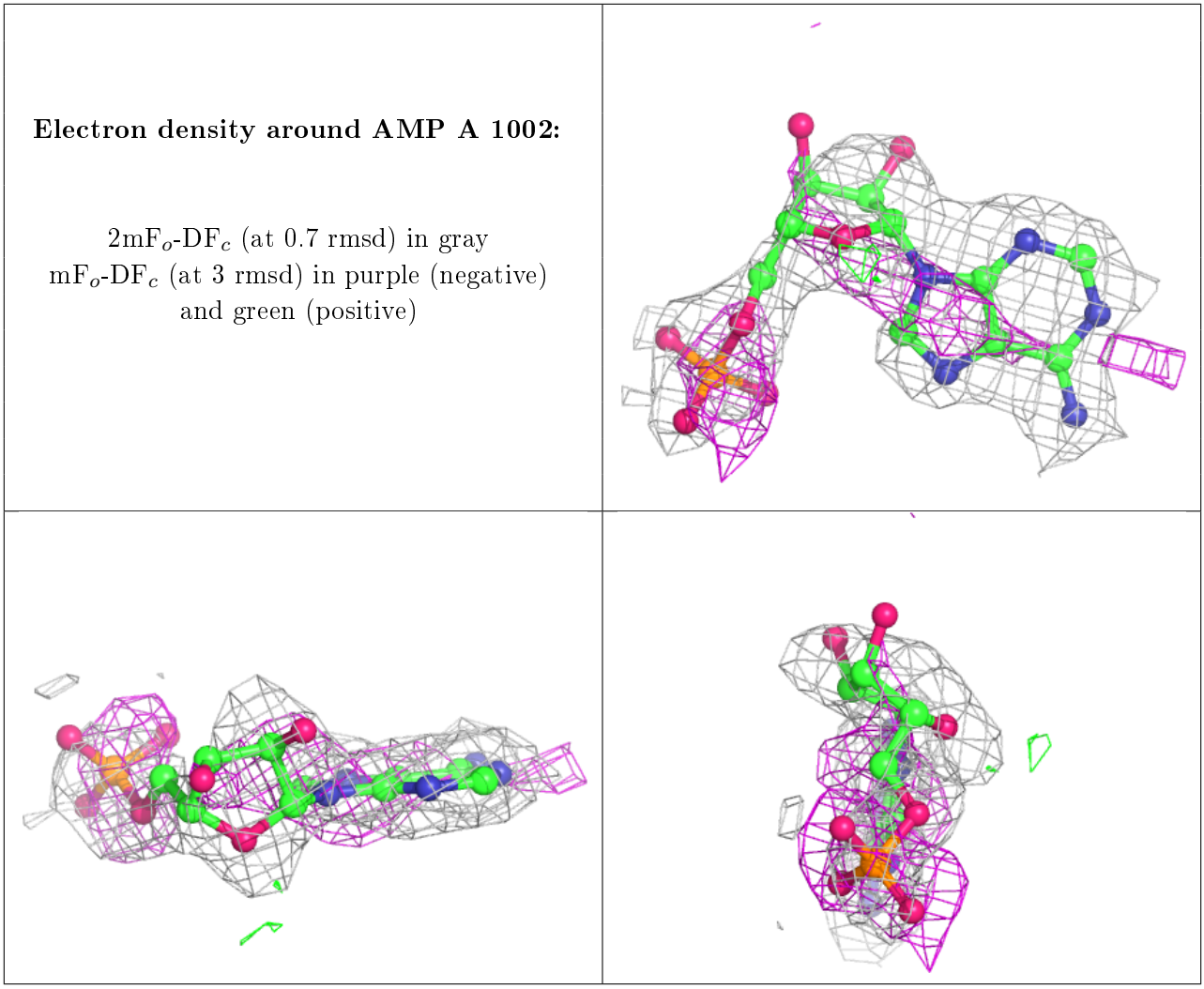
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AMP	A	1002	23/23	0.77	0.32	26,47,62,64	0
2	ZN	A	1001	1/1	0.98	0.07	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.

Electron density around AMP A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.