



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:35 PM UTC

PDB ID : 6OZV / pdb_00006ozv
Title : The structure of condensation and adenylation domains of teixobactin-producing nonribosomal peptide synthetase Txo1 serine module in complex with AMP
Authors : Tan, K.; Zhou, M.; Jedrzejczak, R.; Babnigg, G.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-05-16
Resolution : 2.18 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](#) ①) 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

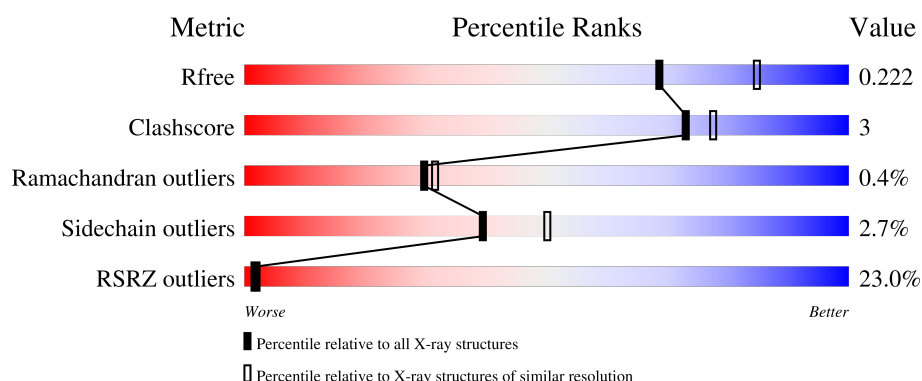
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	873	22% 87% 9% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6706 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.

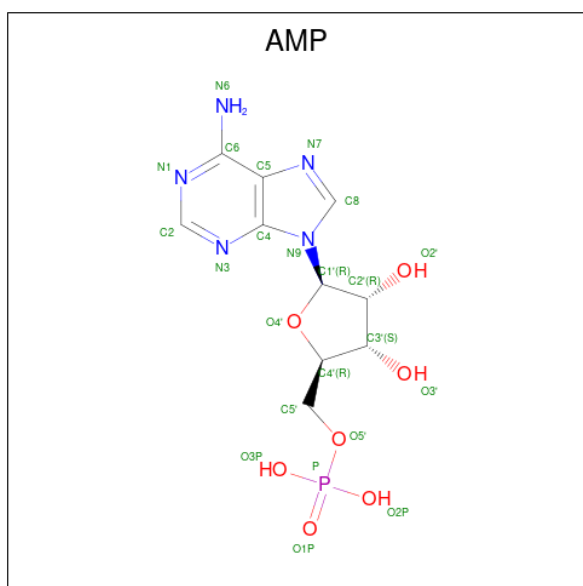
- Molecule 1 is a protein called Txo1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	838	6380	4030	1159	1170	21	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

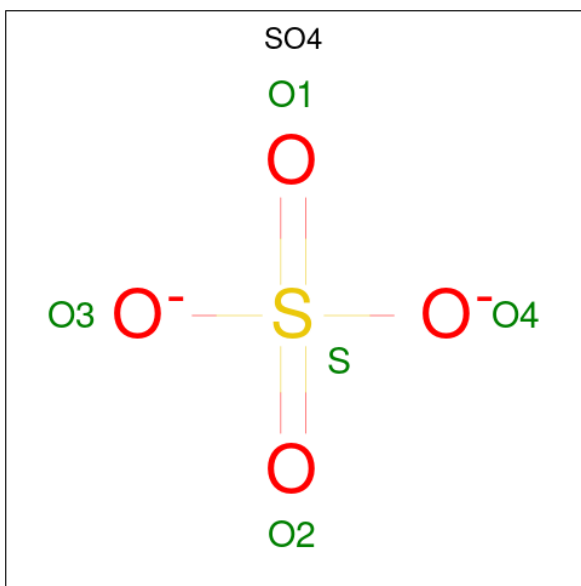
Chain	Residue	Modelled	Actual	Comment	Reference
A	2137	SER	-	expression tag	UNP A0A0B5GUD2
A	2138	ASN	-	expression tag	UNP A0A0B5GUD2
A	2139	ALA	-	expression tag	UNP A0A0B5GUD2

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



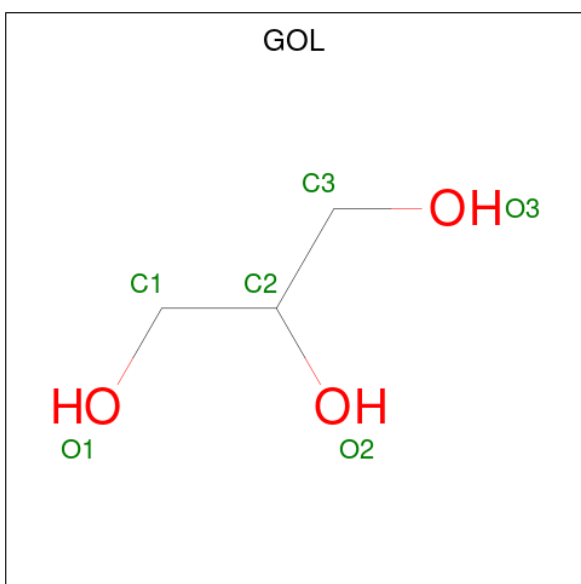
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	23	10	5	7	1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

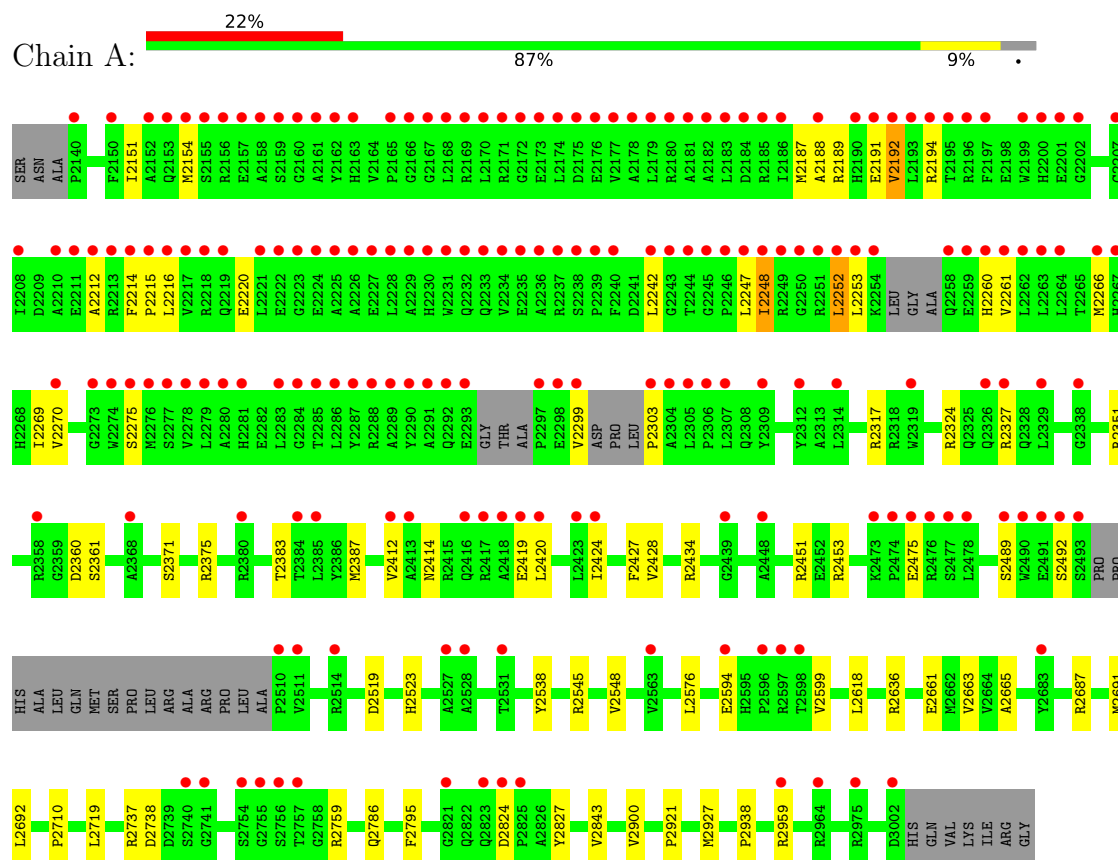
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	276	Total	O	0	1
			277	277		

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 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: Txo1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.67Å 90.86Å 98.18Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	47.02 – 2.18 47.02 – 2.18	Depositor EDS
% Data completeness (in resolution range)	84.1 (47.02-2.18) 84.1 (47.02-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.190 , 0.217 0.195 , 0.222	Depositor DCC
R_{free} test set	2811 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	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	6706	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: GOL, AMP, SO4

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	0.11	0/6529	0.31	0/8900

There are no bond length outliers.

There are no bond angle outliers.

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	6380	0	6170	40	0
2	A	23	0	12	0	0
3	A	20	0	0	1	0
4	A	6	0	8	1	0
5	A	277	0	0	0	0
All	All	6706	0	6190	40	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 3.

All (40) 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:2489:SER:HG	1:A:2523:HIS:HD1	1.37	0.70
1:A:2194:ARG:HD3	1:A:2212:ALA:HB2	1.73	0.69
1:A:2189:ARG:NH2	1:A:2303:PRO:O	2.29	0.66
1:A:2269:ILE:HG23	1:A:2270:VAL:HG13	1.84	0.60
1:A:2252:LEU:HD21	1:A:2260:HIS:HB3	1.83	0.59
1:A:2275:SER:HB3	1:A:2424:ILE:HG23	1.84	0.59
1:A:2187:MET:HB3	1:A:2212:ALA:HB1	1.85	0.59
1:A:2434:ARG:O	1:A:2453:ARG:NH2	2.33	0.58
1:A:2636:ARG:NH1	3:A:3103:SO4:O4	2.36	0.57
1:A:2687:ARG:HG3	1:A:2691:MET:HE2	1.87	0.56
1:A:2665:ALA:HB2	1:A:2719:LEU:HD11	1.88	0.55
1:A:2191:GLU:OE1	1:A:2191:GLU:N	2.38	0.54
1:A:2187:MET:HE2	1:A:2248:ILE:HG23	1.90	0.53
1:A:2188:ALA:HA	1:A:2194:ARG:HE	1.74	0.52
1:A:2360:ASP:HB3	1:A:2538:TYR:CZ	2.45	0.52
1:A:2248:ILE:HB	1:A:2266:MET:HG2	1.93	0.51
1:A:2242:LEU:HA	1:A:2247:LEU:HD21	1.92	0.51
1:A:2843:VAL:HG13	4:A:3106:GOL:H32	1.93	0.51
1:A:2538:TYR:CG	1:A:2548:VAL:HG21	2.46	0.50
1:A:2759:ARG:HA	1:A:2759:ARG:HE	1.74	0.50
1:A:2252:LEU:CD2	1:A:2260:HIS:HB3	2.41	0.50
1:A:2618:LEU:HD11	1:A:2663:VAL:HB	1.94	0.48
1:A:2220:GLU:HA	1:A:2253:LEU:HB2	1.94	0.48
1:A:2383:THR:HG22	1:A:2451:ARG:HB2	1.96	0.48
1:A:2661:GLU:HB3	1:A:2719:LEU:HG	1.97	0.47
1:A:2489:SER:OG	1:A:2523:HIS:ND1	2.36	0.47
1:A:2419:GLU:N	1:A:2419:GLU:OE1	2.49	0.46
1:A:2324:ARG:HG3	1:A:2327:ARG:HH22	1.81	0.46
1:A:2351:ARG:HH22	1:A:2519:ASP:CG	2.23	0.46
1:A:2151:ILE:HA	1:A:2154:MET:HE2	1.98	0.45
1:A:2824:ASP:HB3	1:A:2827:TYR:HB3	1.98	0.45
1:A:2192:VAL:HG13	1:A:2270:VAL:HB	2.00	0.44
1:A:2361:SER:O	1:A:2545:ARG:NH2	2.50	0.44
1:A:2576:LEU:HD21	1:A:2938:PRO:HA	2.00	0.44
1:A:2414:ASN:HB3	1:A:2427:PHE:O	2.18	0.43
1:A:2692:LEU:HD21	1:A:2710:PRO:HB3	2.00	0.43
1:A:2214:PHE:HA	1:A:2215:PRO:HD3	1.90	0.42
1:A:2383:THR:HB	1:A:2387:MET:HB2	2.01	0.42
1:A:2921:PRO:HB3	1:A:2927:MET:HG2	2.00	0.42
1:A:2371:SER:O	1:A:2375:ARG:HG3	2.20	0.41

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	829/873 (95%)	797 (96%)	29 (4%)	3 (0%)	30	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2475	GLU
1	A	2261	VAL
1	A	2900	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	630/700 (90%)	613 (97%)	17 (3%)	39	50

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2192	VAL
1	A	2216	LEU
1	A	2248	ILE
1	A	2252	LEU
1	A	2299	VAL
1	A	2317	ARG
1	A	2412	VAL
1	A	2420	LEU

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Mol	Chain	Res	Type
1	A	2428	VAL
1	A	2492	SER
1	A	2594	GLU
1	A	2599	VAL
1	A	2737	ARG
1	A	2738	ASP
1	A	2786	GLN
1	A	2795	PHE
1	A	2959	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2786	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
4	GOL	A	3106	-	5,5,5	0.89	0	5,5,5	1.08	0
3	SO4	A	3102	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	3105	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	A	3103	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	3104	-	4,4,4	0.23	0	6,6,6	0.11	0
2	AMP	A	3101	-	25,25,25	1.44	4 (16%)	37,38,38	1.87	8 (21%)

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
4	GOL	A	3106	-	-	0/4/4/4	-
2	AMP	A	3101	-	-	3/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3101	AMP	C5-C4	4.81	1.47	1.39
2	A	3101	AMP	C5-C6	2.82	1.48	1.41
2	A	3101	AMP	C8-N7	2.44	1.36	1.31
2	A	3101	AMP	C5-N7	-2.18	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3101	AMP	C5-C4-N3	-5.76	118.78	126.72
2	A	3101	AMP	N3-C4-N9	4.51	134.83	127.17
2	A	3101	AMP	C2-N3-C4	3.70	120.87	111.83
2	A	3101	AMP	C4-C5-N7	-3.50	106.58	110.58
2	A	3101	AMP	N3-C2-N1	-3.20	123.74	128.58
2	A	3101	AMP	C4-N9-C8	2.63	108.50	105.74
2	A	3101	AMP	C5-N7-C8	2.51	107.39	103.45
2	A	3101	AMP	C6-C5-N7	2.21	136.35	132.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3101	AMP	C5'-O5'-P-O1P

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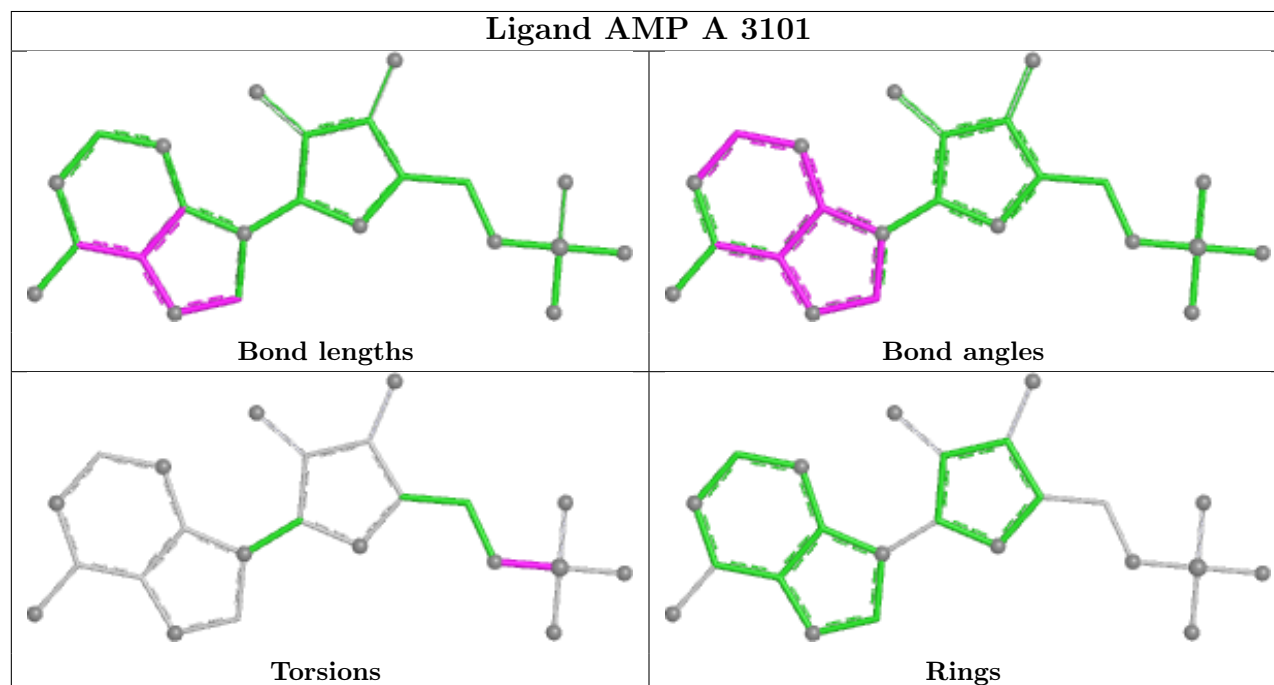
Mol	Chain	Res	Type	Atoms
2	A	3101	AMP	C5'-O5'-P-O3P
2	A	3101	AMP	C5'-O5'-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3106	GOL	1	0
3	A	3103	SO4	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	838/873 (95%)	0.91	193 (23%) 2 2	19, 48, 147, 203	1 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2158	ALA	8.9
1	A	2299	VAL	7.6
1	A	2279	LEU	7.3
1	A	2290	TYR	7.1
1	A	2157	GLU	6.8
1	A	2303	PRO	6.7
1	A	2177	VAL	6.4
1	A	2168	LEU	6.2
1	A	2253	LEU	6.1
1	A	2244	THR	6.1
1	A	2159	SER	6.0
1	A	2140	PRO	6.0
1	A	2174	LEU	5.8
1	A	2186	ILE	5.6
1	A	2293	GLU	5.6
1	A	2160	GLY	5.5
1	A	2167	GLY	5.5
1	A	2286	LEU	5.4
1	A	2178	ALA	5.3
1	A	2252	LEU	5.3
1	A	2208	ILE	5.3
1	A	2173	GLU	5.3
1	A	2179	LEU	5.2
1	A	2284	GLY	5.2
1	A	2289	ALA	5.2
1	A	2280	ALA	5.1
1	A	2217	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	2231	TRP	5.1
1	A	2170	LEU	5.1
1	A	2228	LEU	5.1
1	A	2224	GLU	5.0
1	A	2262	LEU	5.0
1	A	2234	VAL	4.9
1	A	2596	PRO	4.9
1	A	2418	ALA	4.8
1	A	2304	ALA	4.8
1	A	2192	VAL	4.7
1	A	2307	LEU	4.7
1	A	2155	SER	4.6
1	A	2258	GLN	4.6
1	A	2221	LEU	4.6
1	A	2212	ALA	4.6
1	A	2153	GLN	4.6
1	A	2297	PRO	4.5
1	A	2183	LEU	4.5
1	A	2152	ALA	4.5
1	A	2263	LEU	4.5
1	A	2181	ALA	4.4
1	A	2492	SER	4.4
1	A	2200	HIS	4.4
1	A	2214	PHE	4.3
1	A	2210	ALA	4.3
1	A	2291	ALA	4.2
1	A	2242	LEU	4.2
1	A	2264	LEU	4.2
1	A	2243	GLY	4.2
1	A	2171	ARG	4.2
1	A	2182	ALA	4.2
1	A	2755	GLY	4.2
1	A	2247	LEU	4.2
1	A	2287	TYR	4.1
1	A	2172	GLY	4.1
1	A	2225	ALA	4.1
1	A	2207	CYS	4.1
1	A	2259	GLU	4.1
1	A	2757	THR	4.0
1	A	2245	GLY	4.0
1	A	2211	GLU	4.0
1	A	2227	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2238	SER	4.0
1	A	2161	ALA	4.0
1	A	2230	HIS	4.0
1	A	2169	ARG	4.0
1	A	2261	VAL	4.0
1	A	2288	ARG	4.0
1	A	2305	LEU	3.9
1	A	2254	LYS	3.9
1	A	2473	LYS	3.9
1	A	2248	ILE	3.9
1	A	2226	ALA	3.9
1	A	2213	ARG	3.9
1	A	2229	ALA	3.8
1	A	2528	ALA	3.8
1	A	2423	LEU	3.8
1	A	2239	PRO	3.8
1	A	2219	GLN	3.8
1	A	2740	SER	3.8
1	A	2193	LEU	3.8
1	A	2201	GLU	3.8
1	A	2493	SER	3.7
1	A	2199	TRP	3.7
1	A	2298	GLU	3.6
1	A	2314	LEU	3.6
1	A	2188	ALA	3.6
1	A	2474	PRO	3.6
1	A	2236	ALA	3.6
1	A	2156	ARG	3.6
1	A	2154	MET	3.5
1	A	2420	LEU	3.5
1	A	2202	GLY	3.4
1	A	2285	THR	3.4
1	A	2306	PRO	3.4
1	A	2191	GLU	3.4
1	A	2511	VAL	3.4
1	A	2240	PHE	3.4
1	A	2190	HIS	3.3
1	A	2309	TYR	3.3
1	A	2754	SER	3.3
1	A	2490	TRP	3.3
1	A	3002	ASP	3.3
1	A	2216	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2246	PRO	3.3
1	A	2165	PRO	3.2
1	A	2412	VAL	3.2
1	A	2166	GLY	3.2
1	A	2222	GLU	3.2
1	A	2163	HIS	3.2
1	A	2475	GLU	3.1
1	A	2195	THR	3.1
1	A	2510	PRO	3.0
1	A	2424	ILE	3.0
1	A	2273	GLY	3.0
1	A	2185	ARG	3.0
1	A	2194	ARG	3.0
1	A	2756	SER	3.0
1	A	2419	GLU	3.0
1	A	2476	ARG	2.9
1	A	2283	LEU	2.9
1	A	2598	THR	2.9
1	A	2249	ARG	2.9
1	A	2250	GLY	2.9
1	A	2180	ARG	2.9
1	A	2448	ALA	2.9
1	A	2184	ASP	2.8
1	A	2270	VAL	2.8
1	A	2281	HIS	2.8
1	A	2235	GLU	2.7
1	A	2150	PHE	2.7
1	A	2597	ARG	2.7
1	A	2232	GLN	2.7
1	A	2275	SER	2.7
1	A	2197	PHE	2.7
1	A	2825	PRO	2.7
1	A	2162	TYR	2.7
1	A	2278	VAL	2.7
1	A	2417	ARG	2.6
1	A	2260	HIS	2.6
1	A	2233	GLN	2.6
1	A	2439	GLY	2.5
1	A	2489	SER	2.5
1	A	2292	GLN	2.5
1	A	2823	GLN	2.5
1	A	2267	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2176	GLU	2.5
1	A	2531	THR	2.5
1	A	2821	GLY	2.5
1	A	2385	LEU	2.4
1	A	2218	ARG	2.4
1	A	2478	LEU	2.4
1	A	2251	ARG	2.4
1	A	2312	TYR	2.4
1	A	2413	ALA	2.4
1	A	2959	ARG	2.4
1	A	2975	ARG	2.4
1	A	2277	SER	2.4
1	A	2319	TRP	2.4
1	A	2266	MET	2.3
1	A	2276	MET	2.3
1	A	2380	ARG	2.3
1	A	2491	GLU	2.3
1	A	2741	GLY	2.3
1	A	2824	ASP	2.3
1	A	2416	GLN	2.3
1	A	2215	PRO	2.2
1	A	2527	ALA	2.2
1	A	2326	GLN	2.2
1	A	2237	ARG	2.2
1	A	2329	LEU	2.2
1	A	2175	ASP	2.2
1	A	2477	SER	2.2
1	A	2274	TRP	2.2
1	A	2327	ARG	2.1
1	A	2514	ARG	2.1
1	A	2964	ARG	2.1
1	A	2338	GLY	2.1
1	A	2594	GLU	2.1
1	A	2683	TYR	2.1
1	A	2563	VAL	2.1
1	A	2368	ALA	2.1
1	A	2196	ARG	2.0
1	A	2384	THR	2.0
1	A	2358	ARG	2.0
1	A	2223	GLY	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](#)

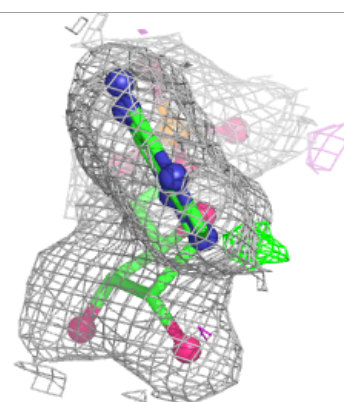
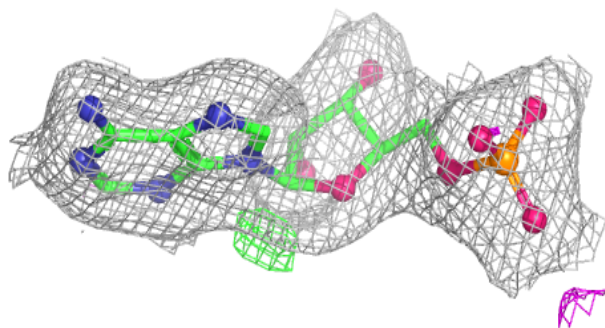
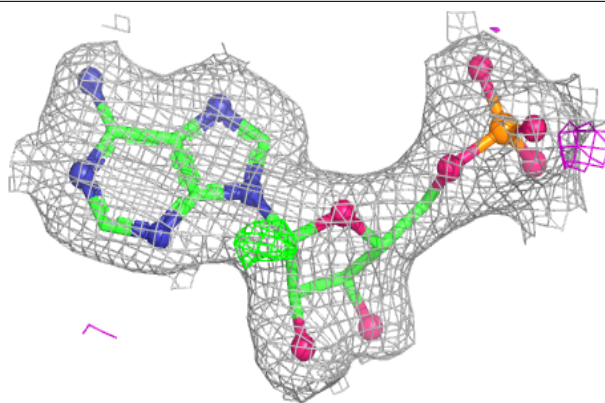
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	3104	5/5	0.66	0.12	131,132,133,133	0
3	SO4	A	3103	5/5	0.87	0.11	95,97,99,101	0
4	GOL	A	3106	6/6	0.87	0.15	39,48,57,63	0
3	SO4	A	3105	5/5	0.90	0.14	97,108,112,113	0
3	SO4	A	3102	5/5	0.97	0.11	34,38,43,50	0
2	AMP	A	3101	23/23	0.98	0.05	23,27,32,34	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 3101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.