



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:39 AM BST

PDB ID : 6P4U
Title : The structure of condensation and adenylation domains of teixobactin-producing nonribosomal peptide synthetase Txo1 serine module in complex with Mg and AMP
Authors : Tan, K.; Zhou, M.; Jedrzejczak, R.; Babnigg, G.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-05-28
Resolution : 2.10 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 : 2.13.1
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) : 2.13.1

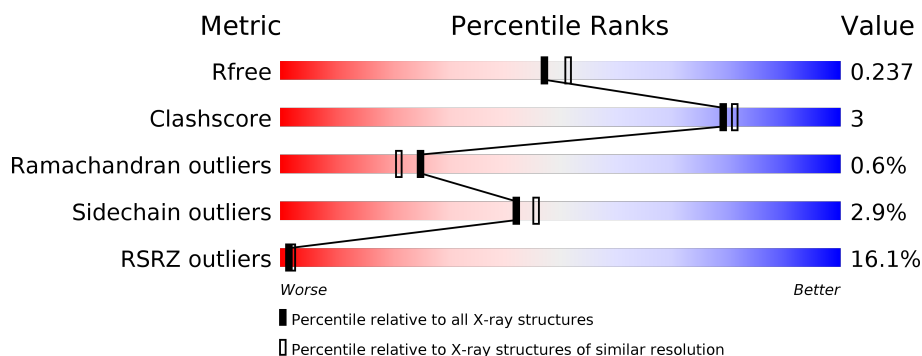
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	<div> <div>16%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	3117	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6725 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.

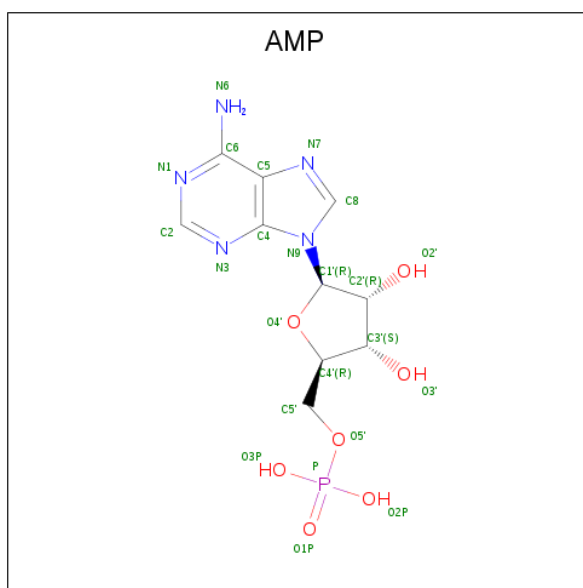
- Molecule 1 is a protein called Txo1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	843	6439	4062	1167	1188	22	0	5	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 (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

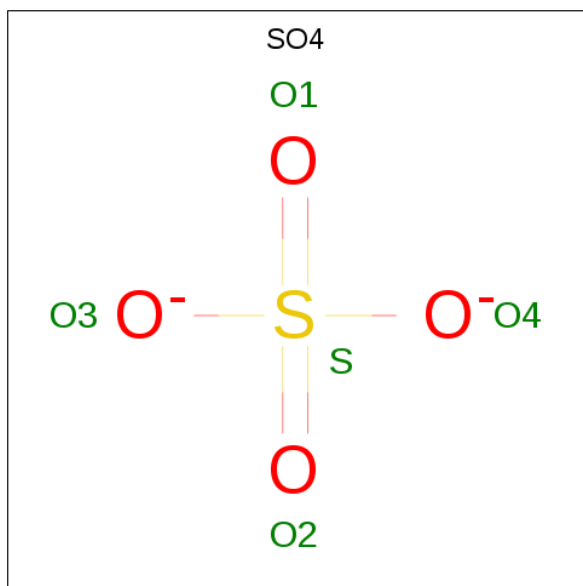


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	23	10	5	7	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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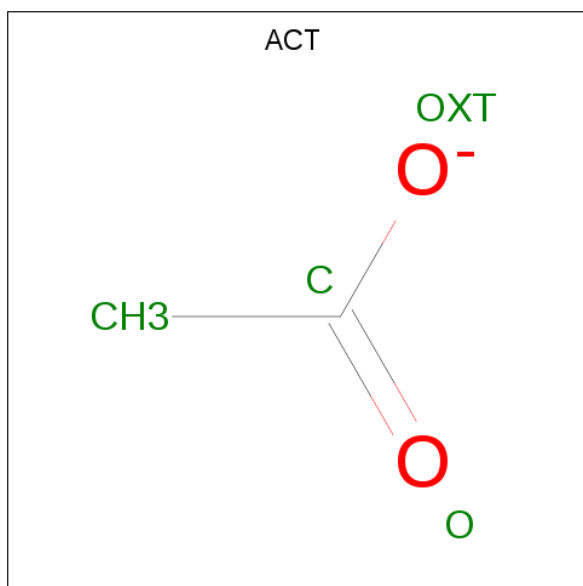
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

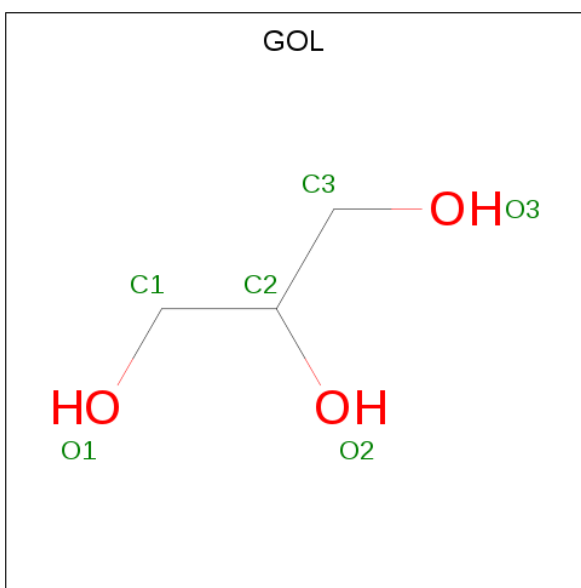
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



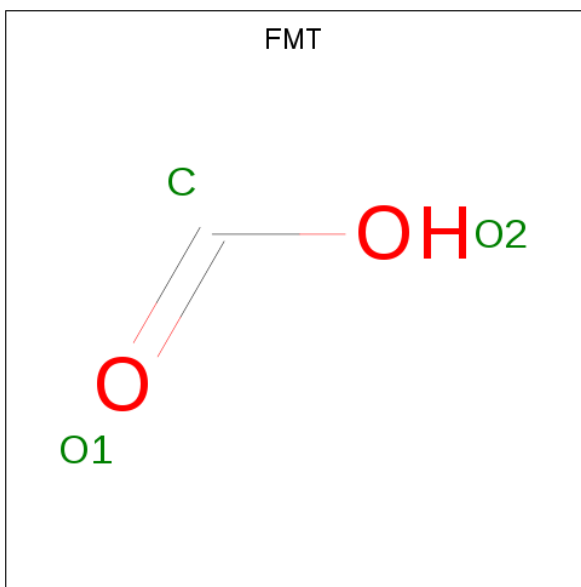
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	1	2		

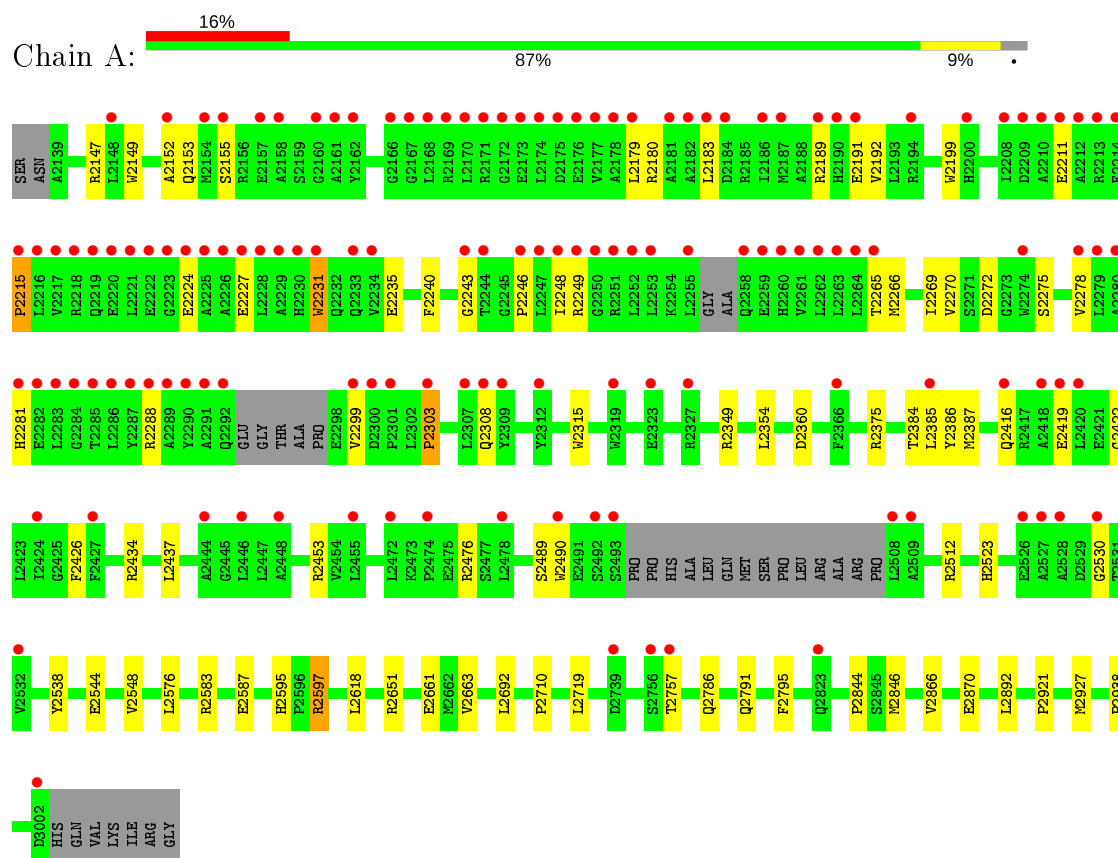
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	157	Total 157	O 157	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 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	154.23 Å 90.83 Å 98.46 Å 90.00° 106.10° 90.00°	Depositor
Resolution (Å)	46.08 – 2.10 46.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (46.08-2.10) 87.5 (46.08-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.208 , 0.237 0.208 , 0.237	Depositor DCC
R_{free} test set	3670 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	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	0.96	EDS
Total number of atoms	6725	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, MG, CL, FMT, SO4, ACT, 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	0.23	0/6585	0.42	0/8977

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	6439	0	6199	36	0
2	A	23	0	12	0	0
3	A	1	0	0	0	0
4	A	85	0	0	1	0
5	A	1	0	0	0	0
6	A	4	0	3	0	0
7	A	12	0	16	0	0
8	A	3	0	1	0	0
9	A	157	0	0	0	0
All	All	6725	0	6231	36	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 (36) 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:2189:ARG:NH2	1:A:2303:PRO:O	2.22	0.72
1:A:2384:THR:HG23	1:A:2386:TYR:H	1.70	0.56
1:A:2248:ILE:HG12	1:A:2266:MET:HG2	1.88	0.55
1:A:2618:LEU:HD11	1:A:2663:VAL:HB	1.89	0.54
1:A:2235:GLU:OE2	1:A:2265:THR:OG1	2.23	0.51
1:A:2538:TYR:CG	1:A:2548:VAL:HG21	2.47	0.49
1:A:2269:ILE:HG23	1:A:2270:VAL:HG13	1.94	0.49
1:A:2618:LEU:HD21	1:A:2663:VAL:HG21	1.95	0.49
1:A:2661:GLU:HB3	1:A:2719:LEU:HG	1.95	0.48
1:A:2215:PRO:HG3	1:A:2246:PRO:HG3	1.95	0.48
1:A:2360:ASP:HB3	1:A:2538:TYR:CZ	2.49	0.48
1:A:2419:GLU:N	1:A:2419:GLU:OE1	2.43	0.48
1:A:2384:THR:HG22	1:A:2387:MET:HG3	1.96	0.47
1:A:2315:TRP:NE1	4:A:3119:SO4:O2	2.36	0.47
1:A:2583:ARG:HA	1:A:2587:GLU:HB2	1.98	0.46
1:A:2272:ASP:H	1:A:2275:SER:HB2	1.80	0.46
1:A:2921:PRO:HB3	1:A:2927:MET:HG2	1.97	0.46
1:A:2489:SER:OG	1:A:2523:HIS:ND1	2.48	0.46
1:A:2375:ARG:NH2	1:A:2530:GLY:O	2.39	0.45
1:A:2349:ARG:NH1	1:A:2544:GLU:OE2	2.41	0.45
1:A:2227:GLU:O	1:A:2231:TRP:HB2	2.16	0.45
1:A:2179:LEU:O	1:A:2183:LEU:N	2.48	0.45
1:A:2434:ARG:O	1:A:2453:ARG:NH2	2.49	0.45
1:A:2866:VAL:HG13	1:A:2892:LEU:HD13	1.99	0.45
1:A:2576:LEU:HD21	1:A:2938:PRO:HA	1.98	0.45
1:A:2278:VAL:HG11	1:A:2422:GLY:HA2	2.00	0.44
1:A:2147:ARG:NE	1:A:2354:LEU:HD11	2.33	0.43
1:A:2692:LEU:HD21	1:A:2710:PRO:HB3	2.00	0.43
1:A:2152:ALA:O	1:A:2155:SER:OG	2.36	0.41
1:A:2385:LEU:HB3	1:A:2490:TRP:CZ2	2.55	0.41
1:A:2191:GLU:HB2	1:A:2308:GLN:CD	2.40	0.41
1:A:2240:PHE:HE1	1:A:2249:ARG:HD2	1.85	0.41
1:A:2211:GLU:OE2	1:A:2211:GLU:N	2.42	0.41
1:A:2595:HIS:H	1:A:2597:ARG:HH11	1.67	0.41
1:A:2149:TRP:O	1:A:2153:GLN:HG2	2.22	0.40
1:A:2844:PRO:HD2	1:A:2870:GLU:HB2	2.03	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	840/873 (96%)	812 (97%)	23 (3%)	5 (1%)	25	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2303	PRO
1	A	2224	GLU
1	A	2243	GLY
1	A	2299	VAL
1	A	2215	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	634/700 (91%)	615 (97%)	19 (3%)	41	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2180	ARG
1	A	2192	VAL
1	A	2199	TRP
1	A	2231	TRP
1	A	2281	HIS
1	A	2288	ARG

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Mol	Chain	Res	Type
1	A	2416	GLN
1	A	2426	PHE
1	A	2437	LEU
1	A	2476	ARG
1	A	2512	ARG
1	A	2597	ARG
1	A	2651	ARG
1	A	2757	THR
1	A	2786	GLN
1	A	2791	GLN
1	A	2795	PHE
1	A	2846[A]	MET
1	A	2846[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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
4	SO4	A	3115	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3112	-	4,4,4	0.14	0	6,6,6	0.05	0
6	ACT	A	3121	-	1,3,3	6.43	1 (100%)	0,3,3	0.00	-
4	SO4	A	3114	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3117	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3119	-	4,4,4	0.14	0	6,6,6	0.05	0
7	GOL	A	3122	-	5,5,5	0.91	0	5,5,5	0.99	0
4	SO4	A	3118	-	4,4,4	0.14	0	6,6,6	0.05	0
8	FMT	A	3124	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	A	3103	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3105	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3109	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3111	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3106	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3107	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3113	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3104	-	4,4,4	0.14	0	6,6,6	0.05	0
2	AMP	A	3101	3	22,25,25	0.88	1 (4%)	25,38,38	1.21	2 (8%)
4	SO4	A	3108	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	3110	-	4,4,4	0.14	0	6,6,6	0.05	0
7	GOL	A	3123	-	5,5,5	0.92	0	5,5,5	0.98	0
4	SO4	A	3116	-	4,4,4	0.14	0	6,6,6	0.05	0

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
7	GOL	A	3122	-	-	0/4/4/4	-
7	GOL	A	3123	-	-	2/4/4/4	-
2	AMP	A	3101	3	-	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)
6	A	3121	ACT	CH3-C	6.43	1.56	1.48
2	A	3101	AMP	C5-C4	2.52	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3101	AMP	N3-C2-N1	-3.17	123.72	128.68
2	A	3101	AMP	C4-C5-N7	-2.63	106.65	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

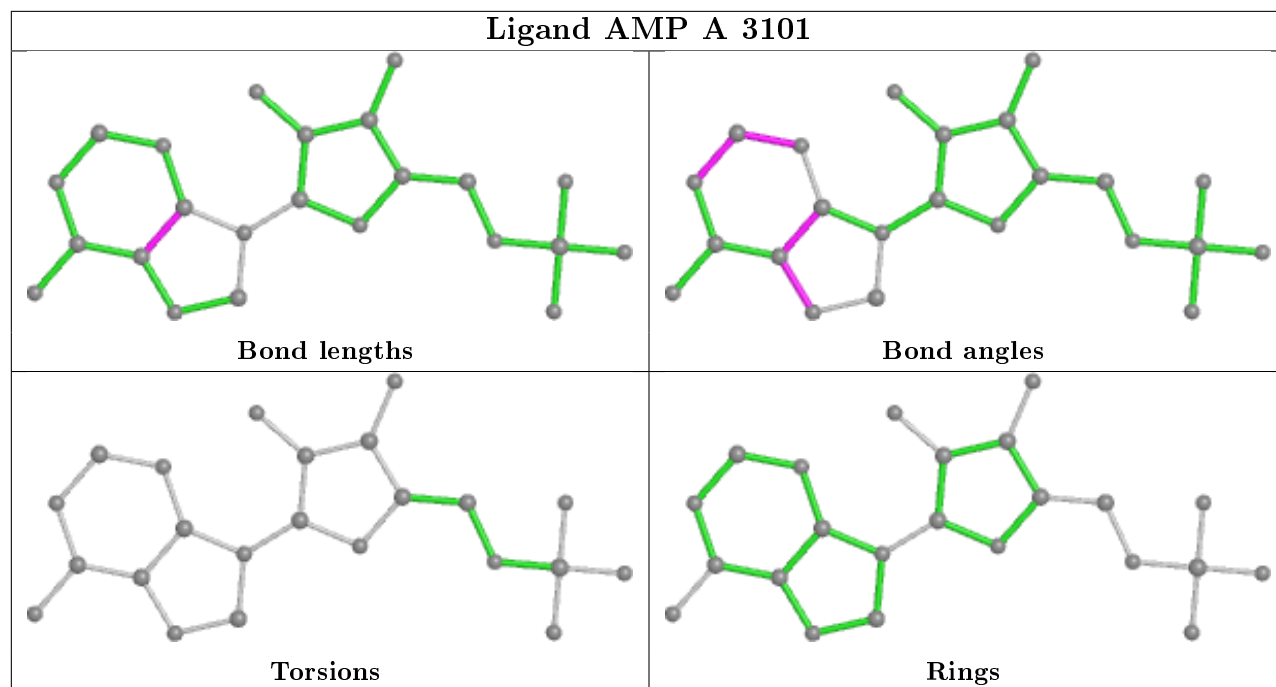
Mol	Chain	Res	Type	Atoms
7	A	3123	GOL	O1-C1-C2-C3
7	A	3123	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3119	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	843/873 (96%)	0.90	136 (16%) 1 2	38, 69, 173, 249	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2179	LEU	15.2
1	A	2252	LEU	13.0
1	A	2177	VAL	11.7
1	A	2174	LEU	11.6
1	A	2221	LEU	10.5
1	A	2225	ALA	9.8
1	A	2261	VAL	9.6
1	A	2213	ARG	9.0
1	A	2286	LEU	8.8
1	A	2226	ALA	8.6
1	A	2253	LEU	8.4
1	A	2216	LEU	8.3
1	A	2287	TYR	8.1
1	A	2264	LEU	7.6
1	A	2756	SER	7.5
1	A	2231	TRP	7.4
1	A	2528	ALA	7.4
1	A	2255	LEU	7.4
1	A	2167	GLY	7.3
1	A	2175	ASP	7.2
1	A	2250	GLY	7.1
1	A	2279	LEU	6.7
1	A	2228	LEU	6.7
1	A	2260	HIS	6.7
1	A	2218	ARG	6.6
1	A	2247	LEU	6.6
1	A	2170	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	2263	LEU	6.2
1	A	2183	LEU	6.2
1	A	2158	ALA	6.1
1	A	2224	GLU	6.0
1	A	2215	PRO	5.5
1	A	2217	VAL	5.4
1	A	2229	ALA	5.4
1	A	2757	THR	5.4
1	A	2223	GLY	5.4
1	A	2289	ALA	5.4
1	A	2194	ARG	5.3
1	A	2178	ALA	5.2
1	A	2244	THR	5.2
1	A	2291	ALA	5.0
1	A	2227	GLU	5.0
1	A	2284	GLY	5.0
1	A	2210	ALA	5.0
1	A	2166	GLY	5.0
1	A	2262	LEU	4.9
1	A	2222	GLU	4.8
1	A	2220	GLU	4.7
1	A	2280	ALA	4.6
1	A	2492	SER	4.6
1	A	2190	HIS	4.5
1	A	2208	ILE	4.4
1	A	2152	ALA	4.4
1	A	2292	GLN	4.4
1	A	2307	LEU	4.4
1	A	2283	LEU	4.3
1	A	2219	GLN	4.2
1	A	2508	LEU	4.0
1	A	2234	VAL	3.9
1	A	2154	MET	3.9
1	A	2173	GLU	3.8
1	A	2171	ARG	3.7
1	A	2186	ILE	3.7
1	A	2301	PRO	3.7
1	A	2527	ALA	3.6
1	A	2160	GLY	3.5
1	A	2169	ARG	3.4
1	A	2455	LEU	3.4
1	A	2259	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2474	PRO	3.4
1	A	2168	LEU	3.4
1	A	2212	ALA	3.3
1	A	2249	ARG	3.3
1	A	2532	VAL	3.3
1	A	2181	ALA	3.3
1	A	2290	TYR	3.2
1	A	2200	HIS	3.2
1	A	2288	ARG	3.2
1	A	2299	VAL	3.1
1	A	2176	GLU	3.1
1	A	2448	ALA	3.0
1	A	2187	MET	3.0
1	A	2420	LEU	3.0
1	A	2248	ILE	3.0
1	A	2274	TRP	3.0
1	A	2312	TYR	3.0
1	A	2319	TRP	2.9
1	A	2251	ARG	2.8
1	A	2282	GLU	2.8
1	A	2161	ALA	2.8
1	A	2366	PHE	2.8
1	A	2189	ARG	2.7
1	A	2243	GLY	2.7
1	A	2182	ALA	2.7
1	A	2444	ALA	2.7
1	A	2308	GLN	2.6
1	A	2509	ALA	2.6
1	A	2172	GLY	2.6
1	A	2211	GLU	2.6
1	A	2214	PHE	2.5
1	A	2490	TRP	2.5
1	A	2191	GLU	2.5
1	A	3002	ASP	2.5
1	A	2285	THR	2.5
1	A	2446	LEU	2.5
1	A	2472	LEU	2.5
1	A	2278	VAL	2.5
1	A	2162	TYR	2.5
1	A	2530	GLY	2.5
1	A	2148	LEU	2.4
1	A	2300	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2478	LEU	2.4
1	A	2418	ALA	2.4
1	A	2281	HIS	2.4
1	A	2258	GLN	2.4
1	A	2823	GLN	2.4
1	A	2246	PRO	2.3
1	A	2265	THR	2.3
1	A	2230	HIS	2.3
1	A	2157	GLU	2.3
1	A	2184	ASP	2.3
1	A	2323	GLU	2.3
1	A	2303	PRO	2.3
1	A	2327	ARG	2.3
1	A	2419	GLU	2.2
1	A	2424	ILE	2.2
1	A	2155	SER	2.2
1	A	2233	GLN	2.2
1	A	2385	LEU	2.2
1	A	2739	ASP	2.2
1	A	2416	GLN	2.2
1	A	2427	PHE	2.1
1	A	2493	SER	2.1
1	A	2209	ASP	2.1
1	A	2309	TYR	2.1
1	A	2526	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

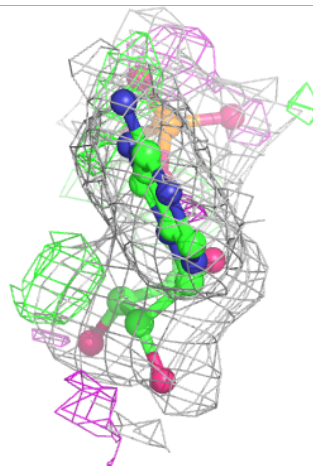
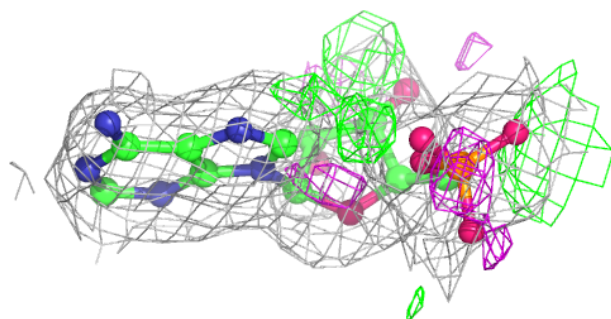
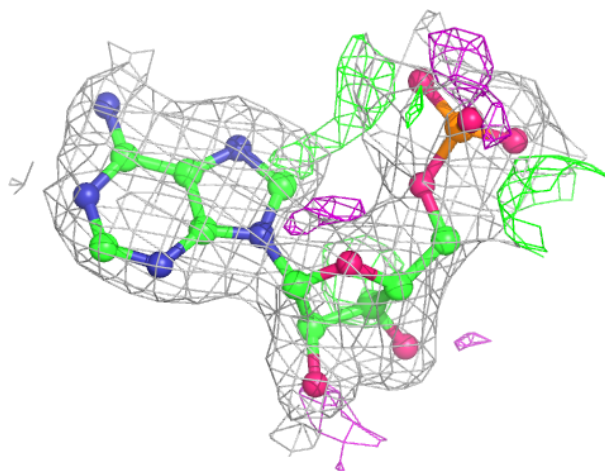
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	3117	5/5	0.53	0.40	152,154,155,156	5
4	SO4	A	3119	5/5	0.65	0.30	106,107,109,113	5
4	SO4	A	3112	5/5	0.70	0.26	173,175,176,177	0
4	SO4	A	3118	5/5	0.72	0.28	146,149,150,152	5
4	SO4	A	3114	5/5	0.73	0.29	125,128,130,133	5
4	SO4	A	3113	5/5	0.76	0.28	210,210,211,212	0
8	FMT	A	3124	3/3	0.77	0.16	84,84,84,87	0
7	GOL	A	3123	6/6	0.78	0.15	83,87,87,90	0
4	SO4	A	3106	5/5	0.80	0.17	128,130,134,140	0
4	SO4	A	3110	5/5	0.81	0.30	189,189,190,190	0
4	SO4	A	3103	5/5	0.83	0.14	90,99,107,108	0
4	SO4	A	3116	5/5	0.83	0.23	113,113,114,115	5
5	CL	A	3120	1/1	0.84	0.05	96,96,96,96	0
7	GOL	A	3122	6/6	0.84	0.24	65,73,83,86	0
4	SO4	A	3115	5/5	0.85	0.14	152,153,155,156	5
4	SO4	A	3111	5/5	0.85	0.13	172,172,173,174	0
4	SO4	A	3108	5/5	0.89	0.13	153,155,156,157	0
6	ACT	A	3121	4/4	0.90	0.14	89,92,94,98	0
4	SO4	A	3107	5/5	0.90	0.15	110,110,111,114	5
2	AMP	A	3101	23/23	0.92	0.13	57,68,86,87	0
4	SO4	A	3105	5/5	0.93	0.11	141,142,144,145	0
4	SO4	A	3109	5/5	0.93	0.18	141,143,143,146	5
3	MG	A	3102	1/1	0.95	0.13	39,39,39,39	0
4	SO4	A	3104	5/5	0.95	0.15	128,129,129,132	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.