



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 03:07 PM EST

PDB ID : 7L3P
Title : Crystal Structure of Acetyl-CoA synthetase in complex with adenosine-5'-ethylphosphate and Co-enzyme A from *Coccidioides immitis* RS
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-12-18
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	:	2.16
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)	:	2.16

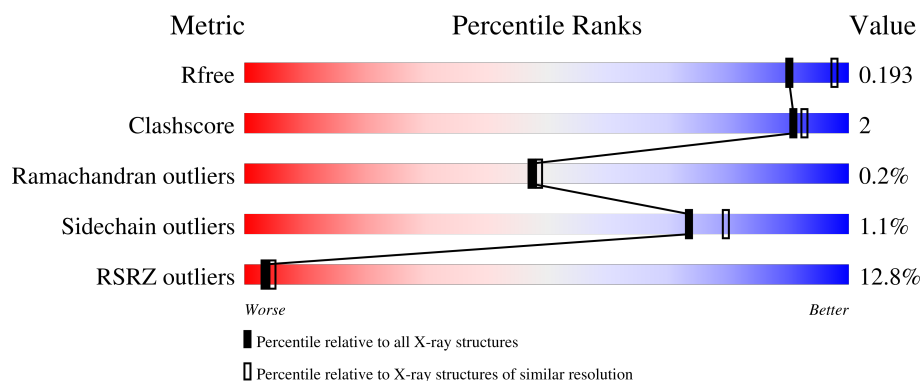
1 Overall quality at a glance

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 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	706	<div> <div>11%</div> <div>80%</div> <div>5%</div> <div>16%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4995 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.

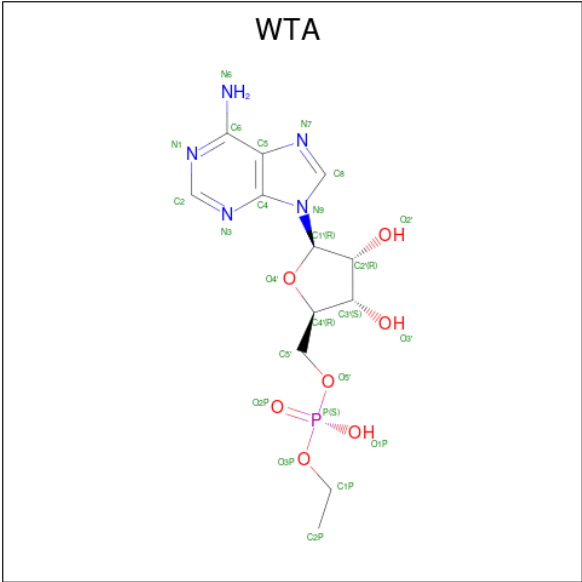
- Molecule 1 is a protein called Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	9	0
			4636	2977	798	842	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP J3KJC6
A	-14	HIS	-	expression tag	UNP J3KJC6
A	-13	HIS	-	expression tag	UNP J3KJC6
A	-12	HIS	-	expression tag	UNP J3KJC6
A	-11	HIS	-	expression tag	UNP J3KJC6
A	-10	HIS	-	expression tag	UNP J3KJC6
A	-9	HIS	-	expression tag	UNP J3KJC6
A	-8	HIS	-	expression tag	UNP J3KJC6
A	-7	HIS	-	expression tag	UNP J3KJC6
A	-6	GLU	-	expression tag	UNP J3KJC6
A	-5	ASN	-	expression tag	UNP J3KJC6
A	-4	LEU	-	expression tag	UNP J3KJC6
A	-3	TYR	-	expression tag	UNP J3KJC6
A	-2	PHE	-	expression tag	UNP J3KJC6
A	-1	GLN	-	expression tag	UNP J3KJC6
A	0	GLY	-	expression tag	UNP J3KJC6

- Molecule 2 is 5'-O-[(S)-ethoxy(hydroxy)phosphoryl]adenosine (three-letter code: WTA) (formula: C₁₂H₁₈N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	11	5	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



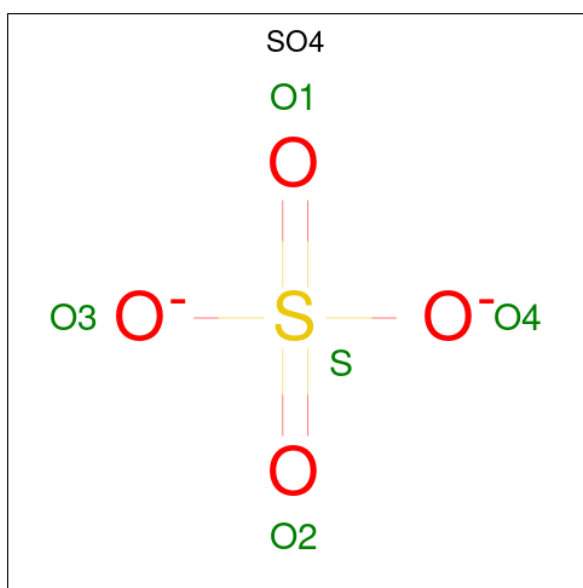
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- 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		

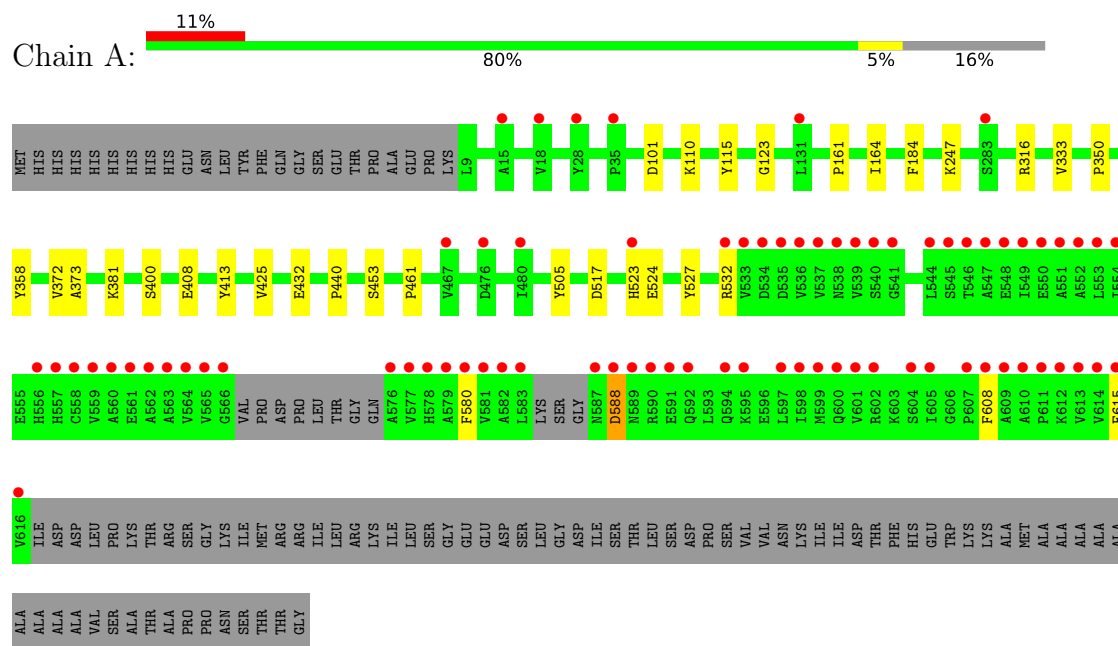
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	1
			298	298		

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: Acetyl-coenzyme A synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	107.57Å 107.57Å 116.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.58 – 2.10 49.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.58-2.10) 100.0 (49.38-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX V1.19RC4-4035	Depositor
R, R_{free}	0.160 , 0.195 0.158 , 0.193	Depositor DCC
R_{free} test set	2006 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WTA, SO4, EDO

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	0.38	0/4795	0.57	0/6533

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

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	4636	0	4435	16	0
2	A	24	0	0	0	0
3	A	32	0	48	0	0
4	A	5	0	0	0	0
5	A	298	0	0	2	0
All	All	4995	0	4483	16	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 2.

All (16) 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:381:LYS:HE3	1:A:408:GLU:HG2	1.79	0.65
1:A:580:PHE:HA	1:A:615:PHE:HB2	1.80	0.63
1:A:588:ASP:O	5:A:801:HOH:O	2.16	0.62
1:A:523:HIS:CE1	1:A:524:GLU:HG3	2.41	0.56
1:A:110:LYS:NZ	5:A:808:HOH:O	2.40	0.54
1:A:517:ASP:OD1	1:A:532:ARG:HD2	2.14	0.48
1:A:372:VAL:HG22	1:A:373:ALA:H	1.80	0.45
1:A:350:PRO:HB3	1:A:358:TYR:CE2	2.52	0.45
1:A:164:ILE:HG12	1:A:333:VAL:HG22	2.00	0.43
1:A:115:TYR:CD2	1:A:123:GLY:HA2	2.54	0.42
1:A:461:PRO:HG2	1:A:527:TYR:OH	2.20	0.42
1:A:115:TYR:CD1	1:A:161:PRO:HD3	2.55	0.40
1:A:184:PHE:CE1	1:A:608:PHE:HZ	2.38	0.40
1:A:425[B]:VAL:HA	1:A:440:PRO:HG2	2.03	0.40
1:A:372:VAL:O	1:A:400:SER:HA	2.21	0.40
1:A:432:GLU:HG2	1:A:505:TYR:CZ	2.57	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	599/706 (85%)	577 (96%)	21 (4%)	1 (0%)	47 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	SER

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	471/584 (81%)	466 (99%)	5 (1%)	73 79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ASP
1	A	247	LYS
1	A	316	ARG
1	A	413	TYR
1	A	588	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	538	ASN

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

10 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	$\# Z > 2$
3	EDO	A	704	-	3,3,3	0.49	0	2,2,2	0.13	0
3	EDO	A	709	-	3,3,3	0.43	0	2,2,2	0.11	0
4	SO4	A	710	-	4,4,4	0.15	0	6,6,6	0.16	0
3	EDO	A	707	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	A	706	-	3,3,3	0.60	0	2,2,2	0.21	0
3	EDO	A	703	-	3,3,3	0.52	0	2,2,2	0.37	0
3	EDO	A	708	-	3,3,3	0.55	0	2,2,2	0.33	0
2	WTA	A	701	-	23,26,27	1.00	3 (13%)	25,39,40	1.04	2 (8%)
3	EDO	A	702	-	3,3,3	0.58	0	2,2,2	0.16	0
3	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.43	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
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	A	707	-	-	1/1/1/1	-
3	EDO	A	706	-	-	1/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
2	WTA	A	701	-	-	2/9/29/30	0/3/3/3
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	WTA	P-O3P	2.18	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	WTA	C8-N7	-2.08	1.31	1.34
2	A	701	WTA	P-O5'	2.02	1.67	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	WTA	O1P-P-O2P	2.23	123.28	112.24
2	A	701	WTA	C5-C6-N6	2.03	123.43	120.35

There are no chirality outliers.

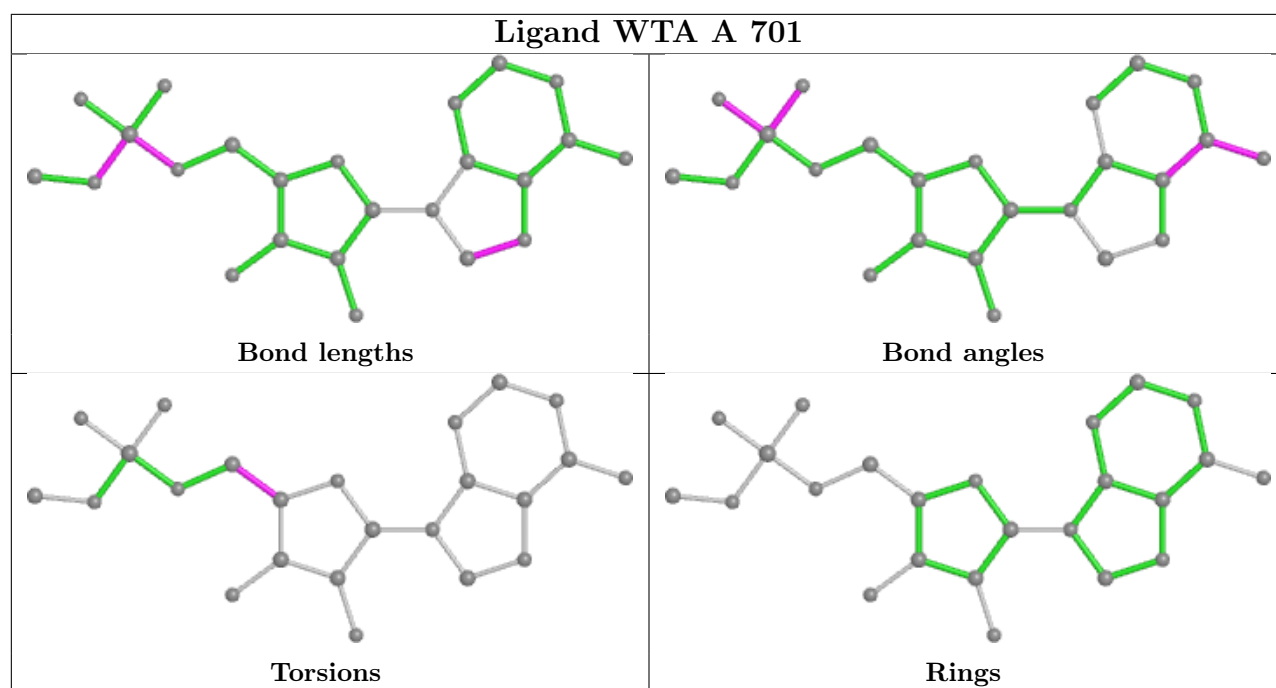
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	WTA	C3'-C4'-C5'-O5'
3	A	707	EDO	O1-C1-C2-O2
2	A	701	WTA	O4'-C4'-C5'-O5'
3	A	706	EDO	O1-C1-C2-O2
3	A	703	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	596/706 (84%)	0.72	76 (12%) 3 4	23, 46, 111, 130	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	PHE	11.1
1	A	613	VAL	9.1
1	A	610	ALA	7.9
1	A	581	VAL	7.6
1	A	611	PRO	6.7
1	A	615	PHE	6.6
1	A	538	ASN	6.5
1	A	577	VAL	6.4
1	A	536	VAL	6.4
1	A	565	VAL	6.4
1	A	579	ALA	6.3
1	A	576	ALA	6.0
1	A	537	VAL	5.9
1	A	560	ALA	5.6
1	A	616	VAL	5.5
1	A	609	ALA	5.5
1	A	562	ALA	5.4
1	A	578	HIS	5.4
1	A	554	ILE	5.3
1	A	597	LEU	5.1
1	A	467	VAL	5.0
1	A	559	VAL	4.8
1	A	541	GLY	4.8
1	A	614	VAL	4.8
1	A	558	CYS	4.8
1	A	533	VAL	4.7
1	A	598	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	582	ALA	4.4
1	A	547	ALA	4.4
1	A	601	VAL	4.2
1	A	539	VAL	4.1
1	A	546	THR	4.1
1	A	599	MET	4.1
1	A	566	GLY	4.0
1	A	608	PHE	4.0
1	A	563	ALA	3.9
1	A	564	VAL	3.8
1	A	283	SER	3.6
1	A	583	LEU	3.6
1	A	590	ARG	3.6
1	A	544	LEU	3.6
1	A	553	LEU	3.5
1	A	535	ASP	3.5
1	A	600	GLN	3.5
1	A	551	ALA	3.3
1	A	545	SER	3.2
1	A	556	HIS	3.1
1	A	552	ALA	3.0
1	A	480	ILE	3.0
1	A	561	GLU	3.0
1	A	612	LYS	3.0
1	A	35	PRO	3.0
1	A	523	HIS	2.9
1	A	592	GLN	2.8
1	A	28	TYR	2.8
1	A	607	PRO	2.7
1	A	549	ILE	2.7
1	A	550	GLU	2.6
1	A	595	LYS	2.6
1	A	532	ARG	2.6
1	A	534	ASP	2.5
1	A	591	GLU	2.5
1	A	476	ASP	2.5
1	A	540	SER	2.5
1	A	557	HIS	2.4
1	A	602	ARG	2.4
1	A	594	GLN	2.3
1	A	18	VAL	2.3
1	A	588	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	548	GLU	2.2
1	A	589	ASN	2.2
1	A	604	SER	2.2
1	A	131	LEU	2.1
1	A	605	ILE	2.1
1	A	587	ASN	2.0
1	A	15	ALA	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](#)

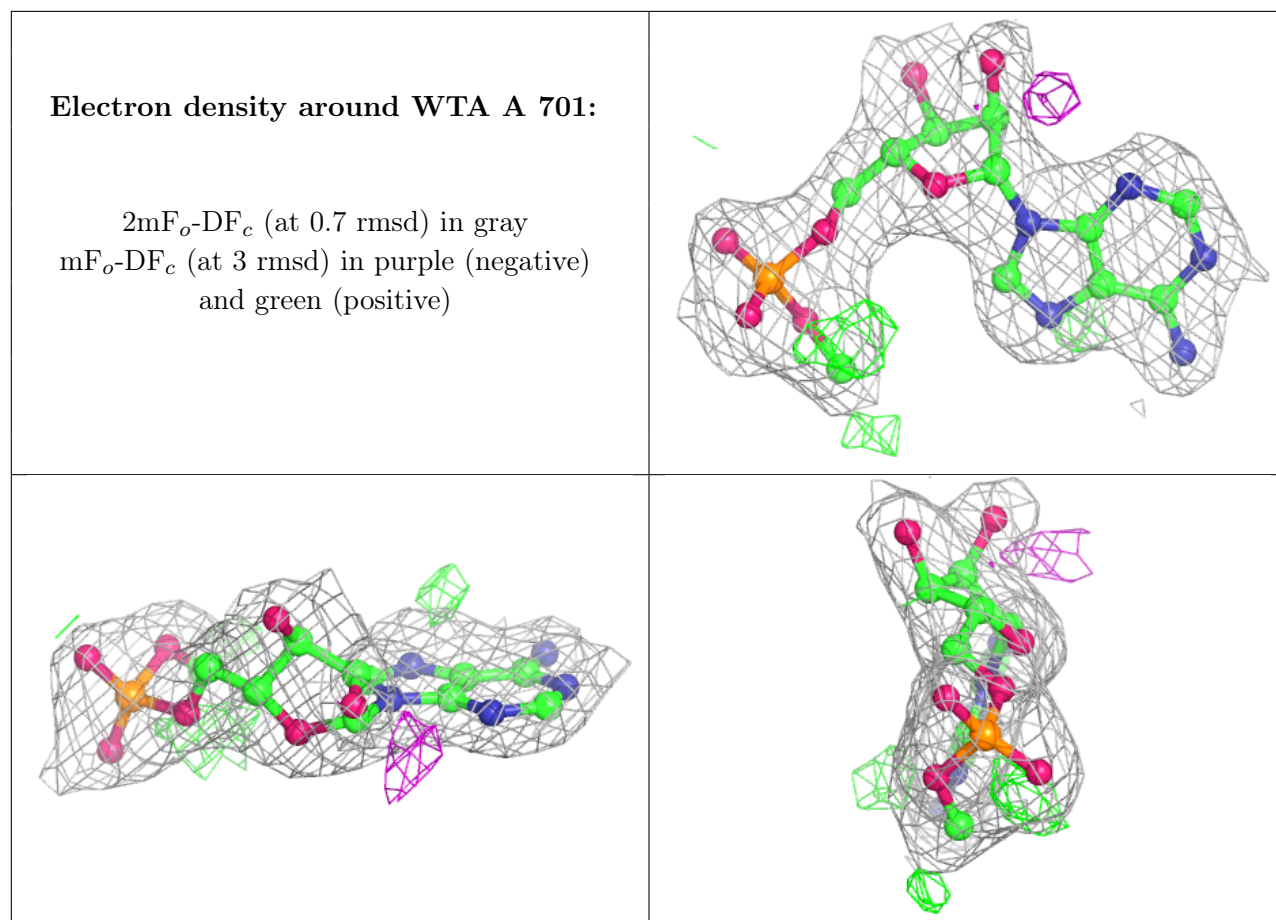
There are no monosaccharides in this entry.

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(Å ²)	Q<0.9
3	EDO	A	708	4/4	0.82	0.32	49,50,54,54	0
3	EDO	A	707	4/4	0.86	0.32	57,57,62,65	0
3	EDO	A	703	4/4	0.90	0.12	47,50,52,54	0
3	EDO	A	706	4/4	0.92	0.16	36,43,43,55	0
3	EDO	A	702	4/4	0.92	0.11	49,49,51,54	0
3	EDO	A	704	4/4	0.93	0.20	38,41,49,49	0
2	WTA	A	701	24/25	0.94	0.12	36,45,52,52	0
3	EDO	A	705	4/4	0.94	0.14	37,39,42,44	0
4	SO4	A	710	5/5	0.97	0.19	62,65,68,75	0
3	EDO	A	709	4/4	0.98	0.14	42,42,42,46	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.