



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2022 – 06:06 pm BST

PDB ID : 7YWK  
Title : Crystal structure of an engineered TycA variant, TycApPLA, in complex with AMP  
Authors : Mittl, P.; Camus, A.; Truong, G.; Markert, G.; Hilvert, D.  
Deposited on : 2022-02-14  
Resolution : 1.39 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.30  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.30

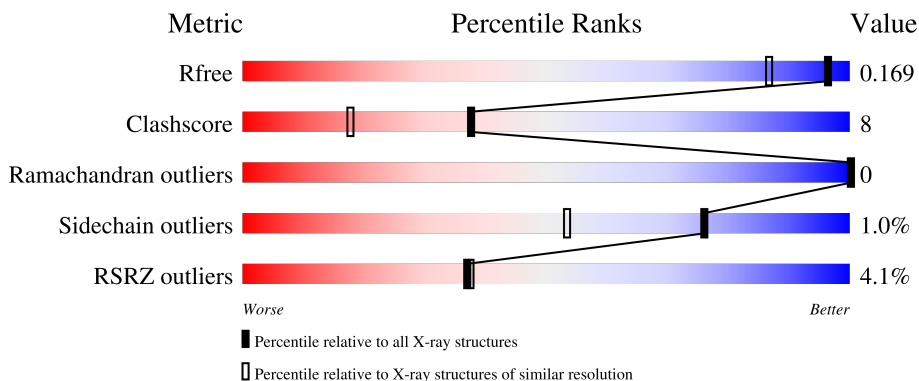
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.39 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	427	 4% 84% 8% 6%
1	B	427	 4% 85% 8% 7%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8117 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 Tyrocidine synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3288	2093	549	634	12	0	21	0
1	B	399	3277	2082	546	637	12	0	22	0

There are 32 discrepancies between the modelled and reference sequences:

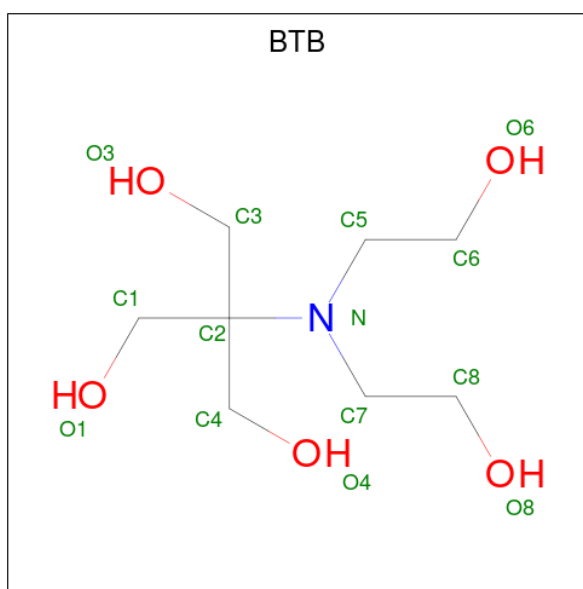
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP P09095
A	3	HIS	-	expression tag	UNP P09095
A	4	HIS	-	expression tag	UNP P09095
A	5	HIS	-	expression tag	UNP P09095
A	6	HIS	-	expression tag	UNP P09095
A	7	HIS	-	expression tag	UNP P09095
A	8	SER	-	expression tag	UNP P09095
A	9	GLY	-	expression tag	UNP P09095
A	10	ARG	-	expression tag	UNP P09095
A	11	SER	-	expression tag	UNP P09095
A	12	VAL	-	expression tag	UNP P09095
A	233	ALA	ASP	conflict	UNP P09095
A	237	SER	TRP	conflict	UNP P09095
A	323	LEU	PRO	conflict	UNP P09095
A	328	CYS	ILE	conflict	UNP P09095
A	329	SER	CYS	conflict	UNP P09095
B	2	HIS	-	expression tag	UNP P09095
B	3	HIS	-	expression tag	UNP P09095
B	4	HIS	-	expression tag	UNP P09095
B	5	HIS	-	expression tag	UNP P09095
B	6	HIS	-	expression tag	UNP P09095
B	7	HIS	-	expression tag	UNP P09095
B	8	SER	-	expression tag	UNP P09095
B	9	GLY	-	expression tag	UNP P09095
B	10	ARG	-	expression tag	UNP P09095

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	SER	-	expression tag	UNP P09095
B	12	VAL	-	expression tag	UNP P09095
B	233	ALA	ASP	conflict	UNP P09095
B	237	SER	TRP	conflict	UNP P09095
B	323	LEU	PRO	conflict	UNP P09095
B	328	CYS	ILE	conflict	UNP P09095
B	329	SER	CYS	conflict	UNP P09095

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

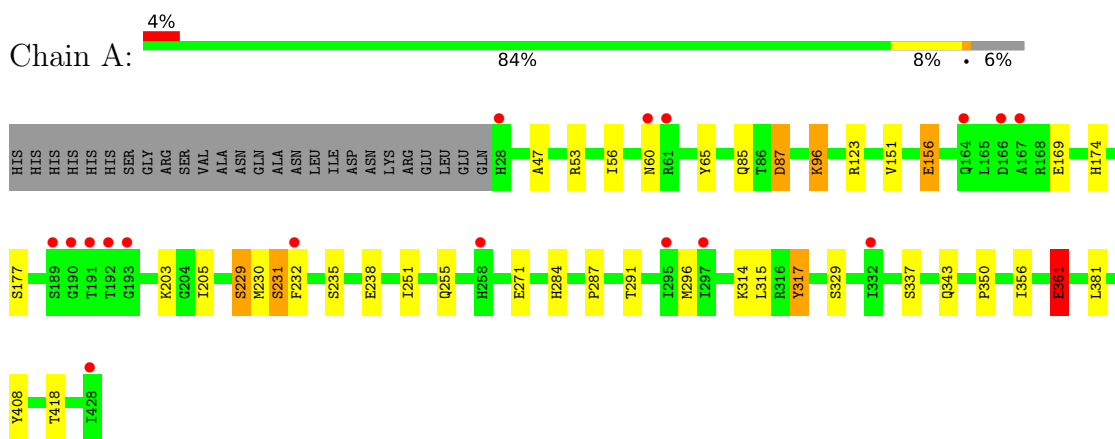
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	791	Total	O	0	0
			791	791		
6	B	675	Total	O	0	0
			675	675		

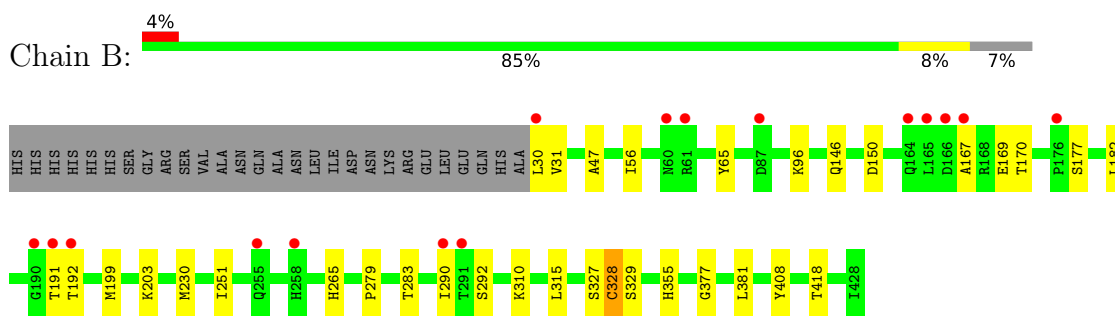
### 3 Residue-property plots [i](#)

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: Tyrocidine synthase 1



- Molecule 1: Tyrocidine synthase 1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.89Å 60.62Å 250.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.29 – 1.39 43.29 – 1.39	Depositor EDS
% Data completeness (in resolution range)	88.5 (43.29-1.39) 88.5 (43.29-1.39)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.38Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.119 , 0.169 0.119 , 0.169	Depositor DCC
$R_{free}$ test set	8220 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.034 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BTB, AMP, SO4, CL

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	0.89	4/3353 (0.1%)	0.95	4/4550 (0.1%)
1	B	0.80	1/3340 (0.0%)	0.92	0/4533
All	All	0.85	5/6693 (0.1%)	0.93	4/9083 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLU	CD-OE2	13.74	1.40	1.25
1	A	271	GLU	CD-OE2	-9.53	1.15	1.25
1	A	238	GLU	CD-OE1	-8.89	1.15	1.25
1	A	361	GLU	CD-OE1	6.82	1.33	1.25
1	B	292	SER	CB-OG	5.02	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	317	TYR	CB-CG-CD2	-6.27	117.23	121.00
1	A	317	TYR	CB-CG-CD1	5.40	124.24	121.00
1	A	53	ARG	NE-CZ-NH1	-5.15	117.72	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	THR	Peptide
1	A	317	TYR	Sidechain

## 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	3288	0	3276	61	0
1	B	3277	0	3262	35	0
2	A	14	0	19	6	0
2	B	14	0	19	1	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	791	0	0	46	1
6	B	675	0	0	18	2
All	All	8117	0	6600	103	3

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 (103) 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:418:THR:HG22	6:A:1109:HOH:O	1.14	1.32
1:A:296:MET:HG3	6:A:834:HOH:O	1.23	1.31
1:A:169[B]:GLU:HG3	6:A:1114:HOH:O	1.29	1.30
1:B:96:LYS:HG2	1:B:230[B]:MET:SD	1.76	1.25
2:A:501:BTB:H41	6:A:1041:HOH:O	1.08	1.23
1:A:156:GLU:HG3	6:A:867:HOH:O	1.43	1.14
1:B:290[A]:ILE:HG22	1:B:290[A]:ILE:O	1.43	1.08
1:B:355:HIS:HD2	6:B:967:HOH:O	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:MET:CG	6:A:834:HOH:O	1.86	1.03
1:A:296:MET:SD	6:A:834:HOH:O	2.17	0.99
1:B:96:LYS:CG	1:B:230[B]:MET:SD	2.56	0.93
1:B:31:VAL:N	6:B:601:HOH:O	2.02	0.93
1:A:232[B]:PHE:CD2	6:A:1366:HOH:O	2.21	0.92
1:B:146[A]:GLN:NE2	1:B:150[A]:ASP:OD1	2.05	0.90
1:A:87:ASP:HB2	6:A:603:HOH:O	1.71	0.89
1:A:205[B]:ILE:HD12	1:A:205[B]:ILE:H	1.37	0.88
1:B:290[A]:ILE:O	1:B:290[A]:ILE:CG2	2.21	0.88
1:A:205[B]:ILE:HD11	6:A:739:HOH:O	1.73	0.88
1:A:232[B]:PHE:CE2	6:A:1174:HOH:O	2.26	0.86
1:B:329[A]:SER:CB	6:B:652:HOH:O	2.23	0.85
1:B:418[A]:THR:HG23	6:B:870:HOH:O	1.77	0.83
1:A:123:ARG:HG3	1:A:151[A]:VAL:HG12	1.60	0.82
1:A:205[B]:ILE:HD12	1:A:205[B]:ILE:N	1.94	0.81
2:A:501:BTB:C4	6:A:1041:HOH:O	1.77	0.81
1:A:205[B]:ILE:CD1	6:A:739:HOH:O	2.29	0.80
1:B:329[A]:SER:CA	6:B:652:HOH:O	2.30	0.80
1:B:279:PRO:O	1:B:283[B]:THR:HG23	1.82	0.78
1:A:232[B]:PHE:CD2	6:A:1174:HOH:O	2.36	0.77
1:A:156:GLU:CG	6:A:867:HOH:O	2.15	0.77
1:A:329[B]:SER:CB	6:A:601:HOH:O	2.29	0.76
1:B:329[A]:SER:HB3	6:B:652:HOH:O	1.85	0.75
1:B:30:LEU:C	6:B:601:HOH:O	2.26	0.73
1:A:350:PRO:HB3	1:A:356[B]:ILE:HG12	1.71	0.73
1:A:229:SER:HB3	1:A:232[A]:PHE:CD1	2.24	0.72
1:B:329[A]:SER:HA	6:B:652:HOH:O	1.89	0.70
1:A:87:ASP:OD2	6:A:603:HOH:O	2.10	0.70
1:A:255:GLN:HG2	6:A:1098:HOH:O	1.91	0.69
1:A:87:ASP:CB	6:A:603:HOH:O	2.33	0.68
1:A:96[B]:LYS:HD3	6:A:815:HOH:O	1.95	0.67
2:A:501:BTB:C3	6:A:1041:HOH:O	2.43	0.67
1:B:327:SER:O	1:B:328[B]:CYS:HB2	1.96	0.65
1:A:232[B]:PHE:HD2	6:A:1366:HOH:O	1.70	0.65
1:A:329[B]:SER:HB3	6:A:601:HOH:O	1.92	0.65
1:B:310[A]:LYS:HE3	6:B:1162:HOH:O	1.96	0.65
1:B:355:HIS:CD2	6:B:967:HOH:O	2.23	0.65
1:A:287:PRO:HB3	1:A:314:LYS:HD2	1.80	0.63
1:B:329[B]:SER:HB2	6:B:762:HOH:O	1.99	0.62
1:A:232[A]:PHE:CE1	6:A:617:HOH:O	2.51	0.62
1:B:146[A]:GLN:HE21	1:B:150[A]:ASP:CG	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205[B]:ILE:H	1:A:205[B]:ILE:CD1	2.10	0.60
1:A:229:SER:HB3	1:A:232[A]:PHE:CE1	2.37	0.60
1:A:203:LYS:HG3	6:A:785:HOH:O	2.00	0.60
1:A:229:SER:CB	1:A:232[A]:PHE:CD1	2.85	0.60
2:A:501:BTB:H32	6:A:1041:HOH:O	2.01	0.59
1:A:337:SER:HB3	6:A:1224:HOH:O	2.02	0.59
1:A:203:LYS:CG	6:A:785:HOH:O	2.51	0.58
1:B:182:LEU:HD11	1:B:199:MET:HB3	1.85	0.58
1:A:329[B]:SER:HA	6:A:849:HOH:O	2.02	0.58
1:A:229:SER:HB2	6:A:1100:HOH:O	2.04	0.57
1:A:229:SER:CB	1:A:232[A]:PHE:HD1	2.18	0.57
1:A:96[A]:LYS:NZ	6:A:607:HOH:O	2.29	0.56
1:B:191:THR:HG23	1:B:192:THR:HG23	1.88	0.56
1:A:123:ARG:CG	1:A:151[A]:VAL:HG12	2.33	0.55
1:A:231[A]:SER:HB3	6:A:640:HOH:O	2.05	0.55
1:A:85:GLN:NE2	6:A:611:HOH:O	2.40	0.55
1:A:343[A]:GLN:OE1	6:A:604:HOH:O	2.18	0.54
1:B:96:LYS:HG3	1:B:230[A]:MET:HG2	1.92	0.51
1:A:361:GLU:H	1:A:361:GLU:CD	2.12	0.51
1:B:203:LYS:HG3	6:B:722:HOH:O	2.10	0.51
1:B:31:VAL:CA	6:B:601:HOH:O	2.55	0.50
1:B:203:LYS:CG	6:B:722:HOH:O	2.60	0.50
1:A:381[A]:LEU:HD11	1:A:408:TYR:HB2	1.94	0.50
1:A:418:THR:CG2	6:A:1109:HOH:O	2.01	0.50
1:A:174:HIS:HE1	6:A:1091:HOH:O	1.96	0.49
1:A:314:LYS:HE3	6:A:1070:HOH:O	2.11	0.49
1:B:56:ILE:HD11	1:B:251:ILE:HD11	1.97	0.47
2:A:501:BTB:C2	6:A:1041:HOH:O	2.31	0.47
1:A:96[B]:LYS:CD	6:A:815:HOH:O	2.56	0.47
1:A:329[B]:SER:OG	6:A:605:HOH:O	2.21	0.46
1:B:265:HIS:HE1	6:B:706:HOH:O	1.99	0.46
1:A:284:HIS:HE1	6:A:1156:HOH:O	1.98	0.46
1:B:381[A]:LEU:HD11	1:B:408:TYR:HB2	1.98	0.46
1:B:177:SER:HB2	6:B:836:HOH:O	2.17	0.45
1:A:156:GLU:CD	6:A:867:HOH:O	2.51	0.44
1:A:56:ILE:HD11	1:A:251:ILE:HD11	2.00	0.43
1:B:169[B]:GLU:HG3	1:B:170:THR:N	2.33	0.43
1:B:47:ALA:HA	1:B:65:TYR:HB3	2.02	0.42
1:A:229:SER:OG	1:A:232[A]:PHE:CD1	2.72	0.42
1:B:96:LYS:CG	1:B:230[A]:MET:HG2	2.49	0.42
2:B:501:BTB:H12	2:B:501:BTB:H72	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96[A]:LYS:HG3	1:A:230[A]:MET:HG3	2.00	0.42
1:A:350:PRO:HB3	1:A:356[B]:ILE:CG1	2.43	0.41
1:A:230[B]:MET:SD	1:A:235[B]:SER:OG	2.78	0.41
1:B:377:GLY:HA2	1:B:381[B]:LEU:HD11	2.02	0.41
1:A:232[A]:PHE:CZ	6:A:617:HOH:O	2.73	0.41
1:B:31:VAL:HA	6:B:601:HOH:O	2.18	0.41
1:A:60:ASN:HB3	6:A:1130:HOH:O	2.19	0.41
1:A:177:SER:HB3	6:A:856:HOH:O	2.21	0.41
1:A:229:SER:HA	6:A:1100:HOH:O	2.21	0.41
1:B:167:ALA:HB3	6:B:869:HOH:O	2.21	0.40
1:A:47:ALA:HA	1:A:65:TYR:HB3	2.02	0.40
1:A:96[A]:LYS:CG	1:A:230[A]:MET:HG3	2.52	0.40
2:A:501:BTB:H11	2:A:501:BTB:H72	1.98	0.40

All (3) 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)
6:B:623:HOH:O	6:B:965:HOH:O[1_565]	1.90	0.30
6:A:622:HOH:O	6:A:853:HOH:O[1_655]	2.06	0.14
6:B:748:HOH:O	6:B:846:HOH:O[4_565]	2.15	0.05

## 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	420/427 (98%)	412 (98%)	8 (2%)	0	100	100
1	B	419/427 (98%)	410 (98%)	9 (2%)	0	100	100
All	All	839/854 (98%)	822 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	362/365 (99%)	355 (98%)	7 (2%)	57	25
1	B	362/365 (99%)	359 (99%)	3 (1%)	81	62
All	All	724/730 (99%)	714 (99%)	10 (1%)	76	40

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96[A]	LYS
1	A	96[B]	LYS
1	A	229	SER
1	A	231[A]	SER
1	A	231[B]	SER
1	A	315	LEU
1	A	361	GLU
1	B	315	LEU
1	B	328[A]	CYS
1	B	328[B]	CYS

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	149	HIS
1	A	174	HIS
1	A	265	HIS
1	B	85	GLN
1	B	100	ASN
1	B	265	HIS
1	B	355	HIS

### 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	502	-	22,25,25	0.83	1 (4%)	25,38,38	0.94	1 (4%)
2	BTB	A	501	-	13,13,13	1.87	4 (30%)	7,16,16	1.02	1 (14%)
2	BTB	B	501	-	13,13,13	1.81	2 (15%)	7,16,16	1.21	1 (14%)
5	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.21	0
5	SO4	A	504	-	4,4,4	0.29	0	6,6,6	0.20	0
3	AMP	B	502	-	22,25,25	0.86	2 (9%)	25,38,38	1.02	3 (12%)

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
2	BTB	B	501	-	-	1/21/21/21	-
2	BTB	A	501	-	-	0/21/21/21	-
3	AMP	A	502	-	-	0/6/26/26	0/3/3/3
3	AMP	B	502	-	-	0/6/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	BTB	C7-N	5.12	1.55	1.48
2	A	501	BTB	C7-N	4.04	1.53	1.48
2	A	501	BTB	C2-N	3.52	1.55	1.48
2	A	501	BTB	C4-C2	2.42	1.56	1.53
2	A	501	BTB	C1-C2	2.17	1.56	1.53
3	B	502	AMP	C8-N7	-2.11	1.30	1.34
3	A	502	AMP	C2-N3	2.10	1.35	1.32
2	B	501	BTB	C2-N	-2.04	1.44	1.48
3	B	502	AMP	P-O2P	-2.03	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	AMP	O2P-P-O5'	2.75	114.04	106.73
2	B	501	BTB	O4-C4-C2	2.70	118.82	111.44
3	B	502	AMP	O3P-P-O5'	-2.23	100.81	106.73
3	B	502	AMP	C5-C6-N6	2.18	123.66	120.35
2	A	501	BTB	O4-C4-C2	2.07	117.10	111.44
3	A	502	AMP	O3P-P-O2P	2.03	115.39	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	BTB	C3-C2-C4-O4

There are no ring outliers.

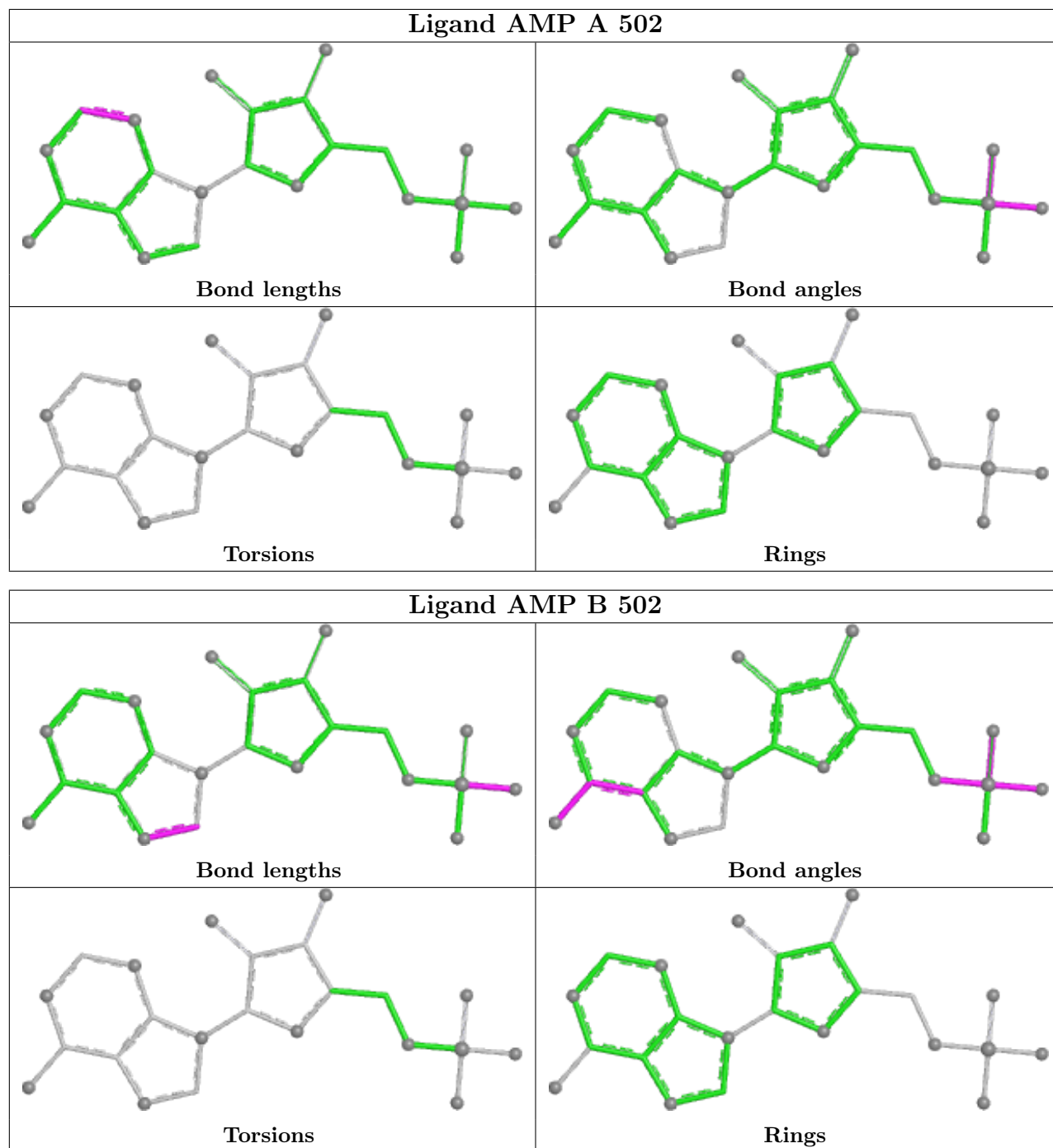
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BTB	6	0
2	B	501	BTB	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	401/427 (93%)	0.21	17 (4%) 36 37	10, 15, 32, 98	0
1	B	399/427 (93%)	0.15	16 (4%) 38 39	12, 18, 38, 97	0
All	All	800/854 (93%)	0.18	33 (4%) 37 37	10, 16, 36, 98	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	THR	11.5
1	B	165	LEU	8.7
1	A	191	THR	8.3
1	B	192	THR	7.5
1	A	28	HIS	6.9
1	B	191	THR	5.9
1	B	166	ASP	5.9
1	A	190	GLY	5.7
1	B	164	GLN	5.5
1	B	30	LEU	4.5
1	B	190	GLY	4.0
1	A	166	ASP	3.6
1	B	258	HIS	3.2
1	B	176	PRO	3.0
1	A	428	ILE	2.9
1	A	193	GLY	2.9
1	A	332	ILE	2.9
1	B	290[A]	ILE	2.9
1	A	232[A]	PHE	2.7
1	A	60	ASN	2.6
1	A	258	HIS	2.6
1	B	291	THR	2.5
1	B	255	GLN	2.5
1	B	87	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	164	GLN	2.4
1	B	61	ARG	2.3
1	A	297	ILE	2.3
1	A	167	ALA	2.3
1	B	167	ALA	2.2
1	B	60	ASN	2.1
1	A	61	ARG	2.1
1	A	295	ILE	2.1
1	A	189	SER	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](#)

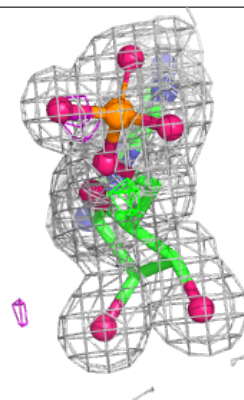
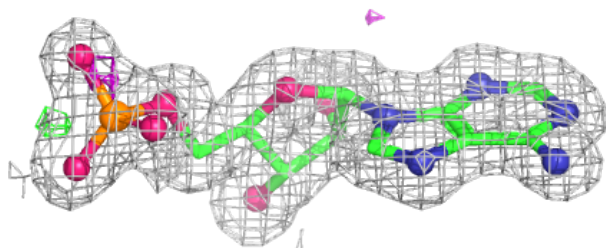
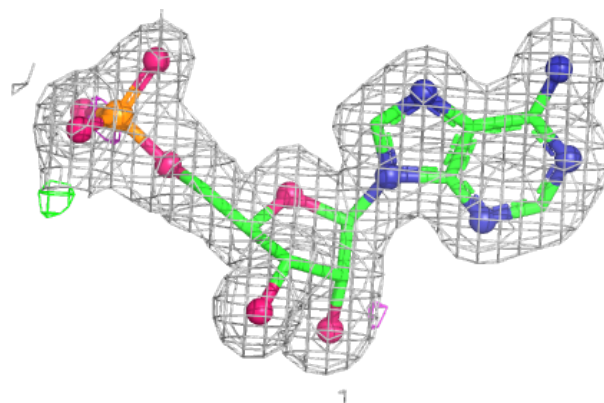
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BTB	B	501	14/14	0.90	0.11	17,26,34,36	0
2	BTB	A	501	14/14	0.92	0.09	14,18,25,26	0
3	AMP	B	502	23/23	0.95	0.06	14,17,25,38	0
3	AMP	A	502	23/23	0.97	0.06	11,13,17,22	0
4	CL	A	503	1/1	0.97	0.06	54,54,54,54	0
5	SO4	A	504	5/5	0.99	0.14	25,26,28,37	0
5	SO4	B	504	5/5	0.99	0.10	23,27,31,42	0
4	CL	B	503	1/1	1.00	0.04	24,24,24,24	0

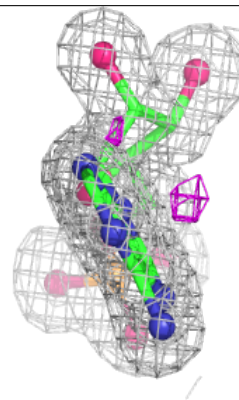
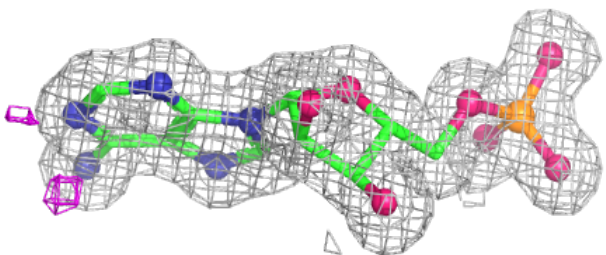
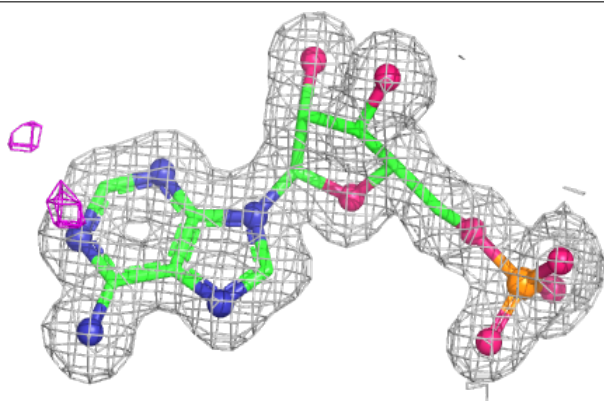
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AMP B 502:**

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

**Electron density around AMP A 502:**

$2mF_o-DF_c$  (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.