



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:53 pm BST

PDB ID : 5Y0P
Title : Crystal structure of Bacillus subtilis TmcAL bound with alpha-thio ATP
Authors : Yamashita, S.; Tomita, K.
Deposited on : 2017-07-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

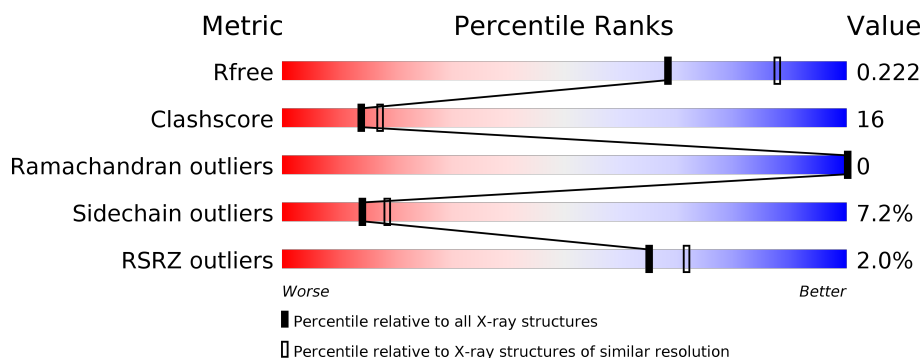
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	434	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>• 8%</div> </div> </div>
1	B	434	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6539 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 UPF0348 protein B4417_3650.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3205	2047	553	593	12			
1	B	401	Total	C	N	O	S	0	0	0
			3205	2047	553	593	12			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP A0A164SIT4
A	-17	GLY	-	expression tag	UNP A0A164SIT4
A	-16	SER	-	expression tag	UNP A0A164SIT4
A	-15	SER	-	expression tag	UNP A0A164SIT4
A	-14	HIS	-	expression tag	UNP A0A164SIT4
A	-13	HIS	-	expression tag	UNP A0A164SIT4
A	-12	HIS	-	expression tag	UNP A0A164SIT4
A	-11	HIS	-	expression tag	UNP A0A164SIT4
A	-10	HIS	-	expression tag	UNP A0A164SIT4
A	-9	HIS	-	expression tag	UNP A0A164SIT4
A	-8	SER	-	expression tag	UNP A0A164SIT4
A	-7	SER	-	expression tag	UNP A0A164SIT4
A	-6	GLY	-	expression tag	UNP A0A164SIT4
A	-5	LEU	-	expression tag	UNP A0A164SIT4
A	-4	VAL	-	expression tag	UNP A0A164SIT4
A	-3	PRO	-	expression tag	UNP A0A164SIT4
A	-2	ARG	-	expression tag	UNP A0A164SIT4
A	-1	GLY	-	expression tag	UNP A0A164SIT4
A	0	SER	-	expression tag	UNP A0A164SIT4
B	-18	MET	-	expression tag	UNP A0A164SIT4
B	-17	GLY	-	expression tag	UNP A0A164SIT4
B	-16	SER	-	expression tag	UNP A0A164SIT4
B	-15	SER	-	expression tag	UNP A0A164SIT4
B	-14	HIS	-	expression tag	UNP A0A164SIT4
B	-13	HIS	-	expression tag	UNP A0A164SIT4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A164SIT4
B	-11	HIS	-	expression tag	UNP A0A164SIT4
B	-10	HIS	-	expression tag	UNP A0A164SIT4
B	-9	HIS	-	expression tag	UNP A0A164SIT4
B	-8	SER	-	expression tag	UNP A0A164SIT4
B	-7	SER	-	expression tag	UNP A0A164SIT4
B	-6	GLY	-	expression tag	UNP A0A164SIT4
B	-5	LEU	-	expression tag	UNP A0A164SIT4
B	-4	VAL	-	expression tag	UNP A0A164SIT4
B	-3	PRO	-	expression tag	UNP A0A164SIT4
B	-2	ARG	-	expression tag	UNP A0A164SIT4
B	-1	GLY	-	expression tag	UNP A0A164SIT4
B	0	SER	-	expression tag	UNP A0A164SIT4

- # TAT

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

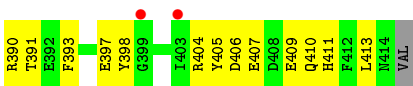
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	28	Total 28	O 28	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:
-
- 29% 57% 32% 8%
- MET GLY SER HIS HIS HIS HIS HIS SER SER SER GLY LEU VAL PRO ARG GLY SER M1 K2 A3 V8 E9 Y10 F13 H14 N15 G16 H17 L18 A24 K25 L26 Q27 Q27 T28 D31 V36 K37 S38 G39 Q43 R44 G45 E46 P47 N50 R55 T56 K57 V58

- Chain B:
-
- 29%
- 58%
- 32%
- 8%
- MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
M1
V8
E9
Y10
M11
P12
F13
H14
M15
E20
D31
V36
K37
S38
G39
R44
P47
A48
V49
V50
S51
K52
W53
A54
R55
T56
K57
M58
A59
L60
Q61
D65
L66
W67



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.00Å 68.00Å 211.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.30 48.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.91-2.30) 99.8 (48.91-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, R_{free}	0.200 , 0.225 0.206 , 0.222	Depositor DCC
R_{free} test set	2223 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.476 for k,h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
Outliers	0 of 44459 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAT

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	0/3274	0.57	0/4423
1	B	0.37	0/3274	0.60	1/4423 (0.0%)
All	All	0.38	0/6548	0.58	1/8846 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	165	LEU	CA-CB-CG	5.79	128.62	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ASP	Peptide
1	B	409	GLU	Peptide

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	3205	0	3232	100	0
1	B	3205	0	3232	108	0
2	A	31	0	14	3	0
2	B	31	0	14	2	0
3	A	39	0	0	4	0
3	B	28	0	0	4	0
All	All	6539	0	6492	203	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 16.

All (203) 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:404:ARG:HE	1:A:413:LEU:HD12	1.37	0.90
1:B:11:ASN:O	1:B:211:ARG:NH1	2.09	0.83
1:B:220:GLU:HA	1:B:223:LEU:HD23	1.61	0.82
1:B:44:ARG:NH2	2:B:1001:TAT:O1B	2.16	0.79
1:B:379:ARG:NH2	1:B:398:TYR:OH	2.21	0.74
1:B:109:PRO:HB2	1:B:156:LEU:HD22	1.70	0.74
1:A:107:ILE:HD13	1:A:183:TYR:HA	1.70	0.72
1:A:285:ARG:NH2	3:A:1103:HOH:O	2.23	0.72
1:B:49:VAL:HG12	1:B:50:VAL:HG23	1.73	0.70
1:B:60:LEU:O	3:B:1101:HOH:O	2.08	0.70
1:A:121:LYS:NZ	3:A:1104:HOH:O	2.24	0.69
1:B:15:ASN:ND2	1:B:203:HIS:O	2.19	0.69
1:B:102:SER:HA	1:B:162:ASN:HB3	1.74	0.68
1:B:103:GLU:OE2	1:B:162:ASN:ND2	2.23	0.68
1:B:151:HIS:ND1	1:B:151:HIS:O	2.28	0.67
1:A:188:ILE:HD11	1:A:203:HIS:NE2	2.10	0.67
1:A:285:ARG:O	3:A:1101:HOH:O	2.13	0.67
1:A:103:GLU:OE1	1:A:163:ASN:ND2	2.21	0.66
1:B:31:ASP:O	1:B:343:LYS:NZ	2.25	0.65
1:B:303:THR:HG23	1:B:306:ARG:HB2	1.80	0.64
1:A:57:LYS:HG2	1:A:403:ILE:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	1:B:120:HIS:ND1	2.27	0.64
1:B:109:PRO:O	1:B:113:THR:OG1	2.12	0.64
1:B:157:ASP:HB2	1:B:160:LYS:HG2	1.78	0.64
1:A:16:GLY:HA3	1:A:204:ILE:HG21	1.80	0.64
1:B:52:LYS:NZ	1:B:397:GLU:OE2	2.28	0.63
1:B:38:SER:O	1:B:55:ARG:NH2	2.29	0.63
1:B:397:GLU:OE1	3:B:1102:HOH:O	2.16	0.63
1:A:255:LYS:NZ	1:B:387:GLU:OE1	2.31	0.62
1:B:162:ASN:HA	1:B:165:LEU:HG	1.80	0.62
1:A:125:ASN:HA	1:A:128:ILE:HD12	1.81	0.62
1:B:10:TYR:O	1:B:55:ARG:HD2	2.00	0.61
1:A:73:LEU:O	1:A:77:GLN:NE2	2.28	0.61
1:A:374:ASP:OD2	3:A:1102:HOH:O	2.16	0.60
1:A:329:ASN:ND2	1:A:331:LYS:O	2.36	0.59
1:A:269:VAL:HG11	1:A:314:ILE:HG12	1.85	0.59
1:B:212:LYS:HA	1:B:215:ILE:HD12	1.84	0.59
1:B:301:ARG:O	1:B:306:ARG:NH1	2.36	0.59
1:A:326:LEU:HD21	1:A:369:PRO:HB2	1.86	0.57
1:A:132:LEU:HD21	1:A:138:TYR:HA	1.84	0.57
1:B:341:THR:HB	1:B:407:GLU:HG2	1.86	0.57
1:A:105:GLY:HA2	1:A:185:THR:HA	1.85	0.57
1:A:229:ALA:HA	1:A:232:ARG:HD2	1.87	0.56
1:B:124:LEU:HD21	1:B:149:ILE:HD11	1.87	0.56
1:B:8:VAL:O	1:B:37:MET:HA	2.05	0.56
1:A:171:THR:O	1:A:175:THR:HG23	2.06	0.55
1:A:39:GLY:O	1:A:55:ARG:NH2	2.30	0.55
1:B:211:ARG:HA	1:B:214:MET:HE2	1.89	0.55
1:B:387:GLU:OE2	1:B:390:ARG:NH1	2.39	0.55
1:A:188:ILE:CD1	1:A:203:HIS:NE2	2.68	0.55
1:B:406:ASP:N	1:B:411:HIS:O	2.37	0.55
1:A:220:GLU:OE1	1:A:220:GLU:N	2.40	0.55
1:A:10:TYR:O	1:A:55:ARG:HD2	2.07	0.54
1:A:285:ARG:CZ	1:B:379:ARG:HG2	2.38	0.54
1:B:290:TYR:O	1:B:294:MET:HG2	2.07	0.54
1:B:8:VAL:HG23	1:B:37:MET:HG3	1.90	0.54
1:A:336:ARG:NH2	1:A:397:GLU:OE2	2.40	0.54
1:A:187:ARG:HH21	2:A:1001:TAT:H8	1.72	0.53
1:A:405:TYR:CE1	1:A:410:GLN:HA	2.42	0.53
1:B:103:GLU:HG3	1:B:160:LYS:HB3	1.91	0.53
1:A:107:ILE:HG12	1:A:184:THR:HG22	1.92	0.52
1:B:298:LYS:HG3	1:B:304:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:SER:HG	1:B:184:THR:HG1	1.58	0.52
1:B:50:VAL:CG1	1:B:54:ALA:HB3	2.39	0.52
1:A:117:ILE:HG22	1:A:121:LYS:HE2	1.92	0.52
1:A:154:SER:N	1:A:155:ALA:HA	2.24	0.52
1:B:128:ILE:HG13	1:B:145:ALA:CB	2.40	0.52
1:B:203:HIS:CG	1:B:204:ILE:H	2.28	0.52
1:B:158:LEU:HD23	1:B:163:ASN:HB3	1.91	0.51
1:A:276:LEU:HD22	1:A:302:TYR:CE1	2.44	0.51
1:B:222:CYS:O	1:B:225:PHE:N	2.39	0.51
1:B:50:VAL:HG22	1:B:237:TYR:CG	2.45	0.51
1:B:127:ARG:O	1:B:131:GLU:HG2	2.11	0.51
1:A:158:LEU:HB3	1:A:164:ILE:HD11	1.92	0.51
1:B:107:ILE:HG23	1:B:184:THR:HG22	1.93	0.51
1:A:159:SER:OG	1:A:160:LYS:N	2.45	0.50
1:B:305:THR:O	1:B:309:ARG:HG3	2.11	0.50
1:A:334:TYR:OH	1:A:374:ASP:OD2	2.22	0.50
1:B:15:ASN:ND2	1:B:224:ARG:O	2.44	0.50
1:B:231:ALA:HA	1:B:234:LEU:HD12	1.93	0.50
1:A:302:TYR:CD2	1:A:306:ARG:HD3	2.47	0.50
1:A:385:ILE:O	1:A:390:ARG:HB2	2.12	0.50
1:A:47:PRO:HD2	1:A:247:PRO:HG3	1.94	0.50
1:B:298:LYS:HG3	1:B:304:TRP:CZ2	2.47	0.50
1:B:58:MET:HG2	1:B:230:SER:HA	1.94	0.49
1:A:50:VAL:HG22	1:A:237:TYR:CD2	2.47	0.49
1:B:10:TYR:OH	1:B:20:HIS:HE1	1.96	0.49
1:A:214:MET:HG2	1:A:219:LEU:HD13	1.93	0.49
1:A:391:THR:OG1	1:B:255:LYS:NZ	2.46	0.49
1:B:202:ASN:N	1:B:224:ARG:O	2.46	0.49
1:B:36:VAL:HG22	1:B:70:LEU:HB2	1.94	0.49
1:A:73:LEU:HD22	1:A:326:LEU:HB3	1.94	0.48
1:B:10:TYR:CD2	1:B:13:PHE:HD1	2.32	0.48
1:B:145:ALA:O	1:B:148:SER:OG	2.21	0.48
1:B:47:PRO:HD2	1:B:247:PRO:HG3	1.96	0.48
1:A:36:VAL:HG22	1:A:70:LEU:HB2	1.94	0.48
1:B:107:ILE:HD13	1:B:183:TYR:HA	1.95	0.48
1:A:126:ASP:O	1:A:129:LYS:HB3	2.13	0.47
1:A:290:TYR:O	1:A:294:MET:HG2	2.14	0.47
1:A:406:ASP:HB3	1:A:411:HIS:HB2	1.96	0.47
1:B:267:GLN:HG3	1:B:268:GLN:OE1	2.15	0.47
1:A:28:THR:HG22	1:A:183:TYR:CG	2.50	0.47
1:A:288:SER:HB3	1:B:387:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:O	1:B:61:GLN:HG3	2.15	0.47
1:A:401:ALA:HB1	1:A:402:PRO:HD2	1.97	0.47
1:A:140:ALA:O	1:A:144:ILE:HG13	2.15	0.47
1:A:15:ASN:O	1:A:18:LEU:HB3	2.15	0.46
1:A:228:ALA:O	1:A:232:ARG:HG3	2.14	0.46
1:A:272:VAL:O	1:A:320:LYS:NZ	2.36	0.46
1:B:1:MET:N	3:B:1111:HOH:O	2.46	0.46
1:A:16:GLY:CA	1:A:204:ILE:HG21	2.45	0.46
1:A:363:LEU:HD11	1:A:397:GLU:HG3	1.97	0.46
1:A:3:ALA:HB3	1:A:95:CYS:HA	1.97	0.46
1:B:238:ARG:HD2	1:B:244:TRP:CE2	2.51	0.46
1:A:121:LYS:HD3	1:A:121:LYS:HA	1.74	0.46
1:A:215:ILE:C	1:A:217:GLN:H	2.18	0.46
1:B:123:ILE:HD12	1:B:123:ILE:H	1.80	0.45
1:B:336:ARG:NH1	1:B:361:SER:O	2.49	0.45
1:B:342:LYS:HD2	1:B:406:ASP:OD1	2.16	0.45
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.17	0.45
1:B:10:TYR:HB3	1:B:13:PHE:HB2	1.98	0.45
1:B:211:ARG:O	1:B:215:ILE:HG13	2.17	0.45
1:B:53:TRP:O	1:B:56:THR:HB	2.16	0.45
1:A:24:ALA:HA	1:A:99:PHE:CD1	2.52	0.45
1:A:266:LEU:HD23	1:A:277:GLU:HB2	1.99	0.45
1:B:157:ASP:OD2	1:B:157:ASP:N	2.29	0.45
1:B:298:LYS:HE3	1:B:304:TRP:CE2	2.52	0.45
1:A:76:VAL:HG12	1:A:309:ARG:HG2	1.98	0.45
1:A:138:TYR:HB3	1:A:139:PRO:HD3	1.98	0.44
1:A:187:ARG:NH2	2:A:1001:TAT:O1B	2.49	0.44
1:B:50:VAL:HG22	1:B:237:TYR:CD2	2.53	0.44
1:B:73:LEU:HD12	1:B:323:MET:SD	2.57	0.44
1:A:212:LYS:HA	1:A:215:ILE:HD12	1.99	0.44
1:A:45:GLY:O	1:A:308:GLN:HG2	2.18	0.44
1:A:387:GLU:HG3	1:A:388:PRO:HA	1.99	0.44
1:A:169:TYR:O	1:A:173:ILE:HG13	2.18	0.44
1:B:188:ILE:O	1:B:204:ILE:HD13	2.18	0.44
1:A:14:HIS:HE2	1:A:207:ALA:HB2	1.82	0.43
1:A:277:GLU:OE2	1:A:278:HIS:NE2	2.51	0.43
1:A:43:GLN:O	1:A:309:ARG:NH1	2.50	0.43
1:B:227:PRO:HG2	1:B:230:SER:OG	2.18	0.43
1:B:303:THR:OG1	1:B:304:TRP:N	2.51	0.43
1:A:187:ARG:HA	2:A:1001:TAT:C2	2.48	0.43
1:A:236:ALA:O	1:A:240:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.86	0.43
1:A:127:ARG:NH2	1:A:131:GLU:OE2	2.52	0.43
1:A:362:LYS:HB3	1:A:362:LYS:HE3	1.81	0.43
1:B:126:ASP:O	1:B:130:GLU:HB2	2.18	0.43
1:A:383:LEU:HB2	1:A:384:PRO:HD3	2.00	0.43
1:A:210:ILE:HG21	1:A:226:LEU:HD11	1.99	0.43
1:B:374:ASP:OD1	3:B:1103:HOH:O	2.20	0.43
1:B:50:VAL:HG13	1:B:237:TYR:CD1	2.54	0.43
1:A:396:GLN:O	1:A:400:HIS:N	2.28	0.43
2:B:1001:TAT:O2B	2:B:1001:TAT:H8	2.19	0.43
1:B:151:HIS:CG	1:B:151:HIS:O	2.71	0.43
1:B:68:ILE:HG23	1:B:336:ARG:O	2.19	0.43
1:A:114:ALA:HA	1:A:167:TYR:HE1	1.84	0.42
1:B:104:ASN:ND2	1:B:106:ASP:H	2.17	0.42
1:B:39:GLY:O	1:B:52:LYS:HB3	2.19	0.42
1:A:14:HIS:HA	1:A:227:PRO:HD2	2.01	0.42
1:A:383:LEU:HD11	1:B:256:TYR:HD1	1.84	0.42
1:B:78:LYS:HB3	1:B:78:LYS:HE2	1.81	0.42
1:B:332:ALA:O	1:B:357:VAL:HG11	2.19	0.42
1:B:382:SER:HB3	1:B:393:PHE:CD1	2.55	0.42
1:B:14:HIS:HA	1:B:226:LEU:HD23	2.02	0.42
1:B:270:TYR:CE2	1:B:323:MET:HG2	2.55	0.41
1:A:117:ILE:HD13	1:A:146:PHE:CZ	2.55	0.41
1:A:298:LYS:HA	1:A:307:LEU:HD11	2.01	0.41
1:B:173:ILE:O	1:B:177:GLY:N	2.53	0.41
1:B:214:MET:HA	1:B:218:ASN:O	2.20	0.41
1:B:387:GLU:OE1	1:B:391:THR:OG1	2.36	0.41
1:A:149:ILE:HG12	1:A:149:ILE:H	1.46	0.41
1:B:405:TYR:HE1	1:B:410:GLN:HA	1.85	0.41
1:A:8:VAL:O	1:A:37:MET:HA	2.20	0.41
1:B:270:TYR:CZ	1:B:323:MET:HG2	2.56	0.41
1:B:78:LYS:HG2	1:B:78:LYS:H	1.47	0.41
1:A:146:PHE:HA	1:A:146:PHE:HD1	1.75	0.41
1:A:28:THR:HG22	1:A:183:TYR:CD2	2.56	0.41
1:A:219:LEU:N	1:A:220:GLU:OE1	2.54	0.41
1:A:414:ASN:OD1	1:A:414:ASN:N	2.54	0.41
1:A:127:ARG:HD2	1:A:127:ARG:HA	1.77	0.41
1:A:154:SER:H	1:A:155:ALA:HA	1.84	0.41
1:B:107:ILE:O	1:B:110:PHE:HB2	2.21	0.41
1:B:128:ILE:O	1:B:132:LEU:HG	2.20	0.41
1:B:258:LEU:HD21	1:B:314:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:O	1:A:184:THR:OG1	2.23	0.41
1:A:113:THR:O	1:A:117:ILE:HG13	2.21	0.41
1:A:250:TYR:HB3	1:A:315:LEU:HD11	2.02	0.41
1:B:102:SER:O	1:B:186:ALA:HA	2.20	0.41
1:B:165:LEU:HD12	1:B:166:GLY:N	2.36	0.41
1:B:48:ALA:O	1:B:245:HIS:HB2	2.21	0.41
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.78	0.40
1:B:138:TYR:HB3	1:B:139:PRO:HD3	2.03	0.40
1:B:65:ASP:O	1:B:344:GLY:HA3	2.22	0.40
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.96	0.40
1:A:216:GLY:C	1:A:218:ASN:H	2.24	0.40
1:A:288:SER:CB	1:B:387:GLU:HG2	2.52	0.40
1:B:238:ARG:HD2	1:B:244:TRP:NE1	2.36	0.40
1:B:293:PHE:O	1:B:297:LEU:HG	2.22	0.40
1:A:116:LEU:O	1:A:120:HIS:HB2	2.22	0.40
1:A:269:VAL:O	1:A:320:LYS:HE3	2.22	0.40
1:B:152:THR:OG1	1:B:153:GLU:N	2.55	0.40
1:B:385:ILE:HG22	1:B:386:GLU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	397/434 (92%)	383 (96%)	14 (4%)	0	100	100
1	B	397/434 (92%)	377 (95%)	20 (5%)	0	100	100
All	All	794/868 (92%)	760 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	345/373 (92%)	314 (91%)	31 (9%)	9	11
1	B	345/373 (92%)	326 (94%)	19 (6%)	21	30
All	All	690/746 (92%)	640 (93%)	50 (7%)	14	18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	26	LEU
1	A	31	ASP
1	A	46	GLU
1	A	50	VAL
1	A	102	SER
1	A	108	LYS
1	A	116	LEU
1	A	127	ARG
1	A	146	PHE
1	A	149	ILE
1	A	175	THR
1	A	187	ARG
1	A	188	ILE
1	A	209	SER
1	A	249	SER
1	A	252	SER
1	A	259	SER
1	A	260	THR
1	A	261	VAL
1	A	282	ARG
1	A	285	ARG
1	A	288	SER
1	A	299	THR
1	A	303	THR
1	A	308	GLN
1	A	325	LYS

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Mol	Chain	Res	Type
1	A	336	ARG
1	A	400	HIS
1	A	411	HIS
1	A	414	ASN
1	B	20	HIS
1	B	66	LEU
1	B	78	LYS
1	B	104	ASN
1	B	107	ILE
1	B	149	ILE
1	B	154	SER
1	B	157	ASP
1	B	185	THR
1	B	223	LEU
1	B	246	THR
1	B	264	ARG
1	B	289	SER
1	B	303	THR
1	B	348	LEU
1	B	353	LYS
1	B	387	GLU
1	B	404	ARG
1	B	413	LEU

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

Mol	Chain	Res	Type
1	B	20	HIS
1	B	104	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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
2	TAT	A	1001	-	24,33,33	0.96	1 (4%)	29,52,52	1.55	5 (17%)
2	TAT	B	1001	-	24,33,33	0.98	1 (4%)	29,52,52	1.74	5 (17%)

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	TAT	A	1001	-	-	0/14/38/38	0/3/3/3
2	TAT	B	1001	-	-	1/14/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	TAT	C5-C4	2.41	1.47	1.40
2	A	1001	TAT	C5-C4	2.35	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	TAT	PB-O3B-PG	-4.61	116.99	132.83
2	B	1001	TAT	N3-C2-N1	-3.67	122.94	128.68
2	B	1001	TAT	O5'-PA-O2A	-3.49	101.57	114.42
2	A	1001	TAT	PB-O3B-PG	-3.37	121.25	132.83
2	A	1001	TAT	C4-C5-N7	-3.14	106.12	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	TAT	O5'-PA-O2A	-3.12	102.93	114.42
2	A	1001	TAT	N3-C2-N1	-2.72	124.42	128.68
2	B	1001	TAT	C2-N1-C6	2.43	122.91	118.75
2	A	1001	TAT	O3A-PA-O5'	2.32	109.68	101.37
2	B	1001	TAT	C4-C5-N7	-2.24	107.07	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

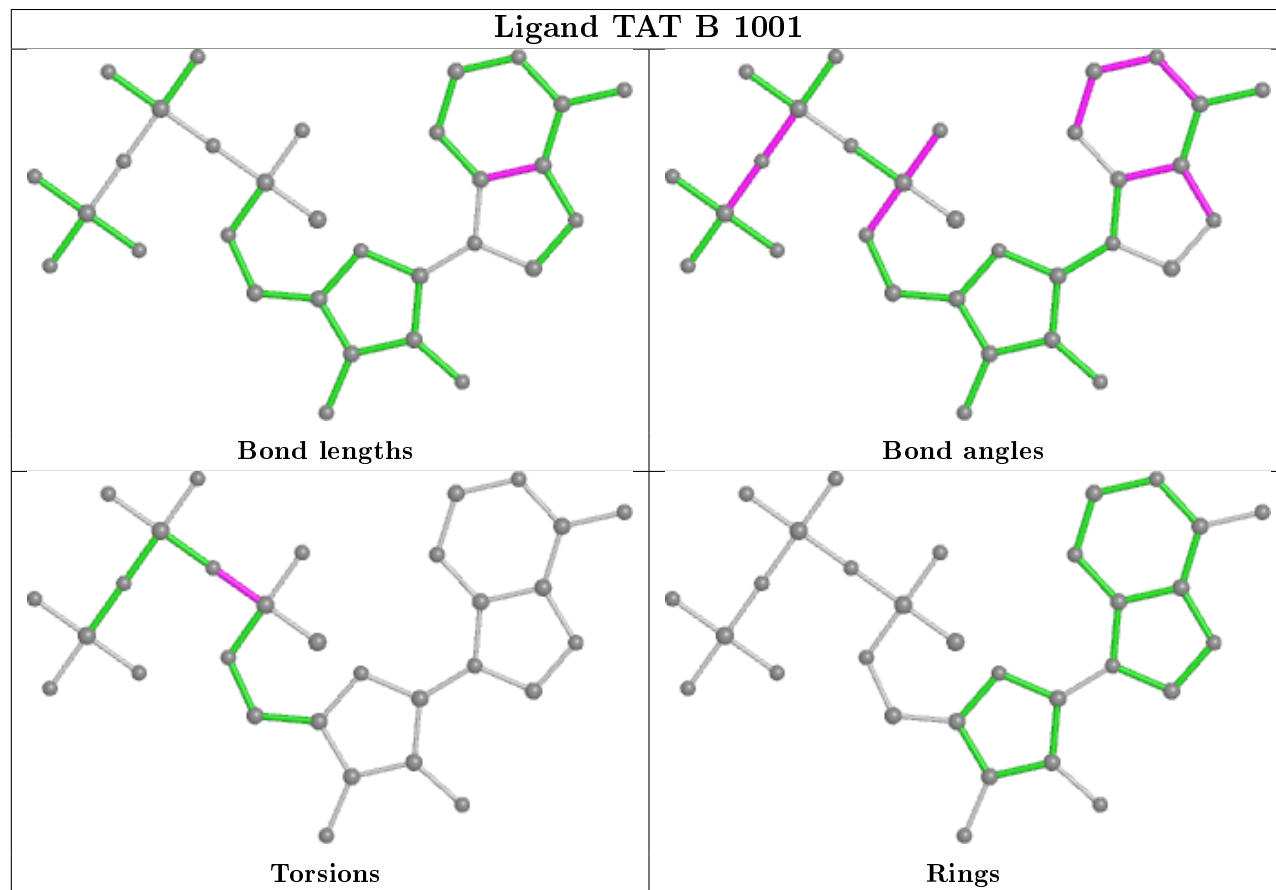
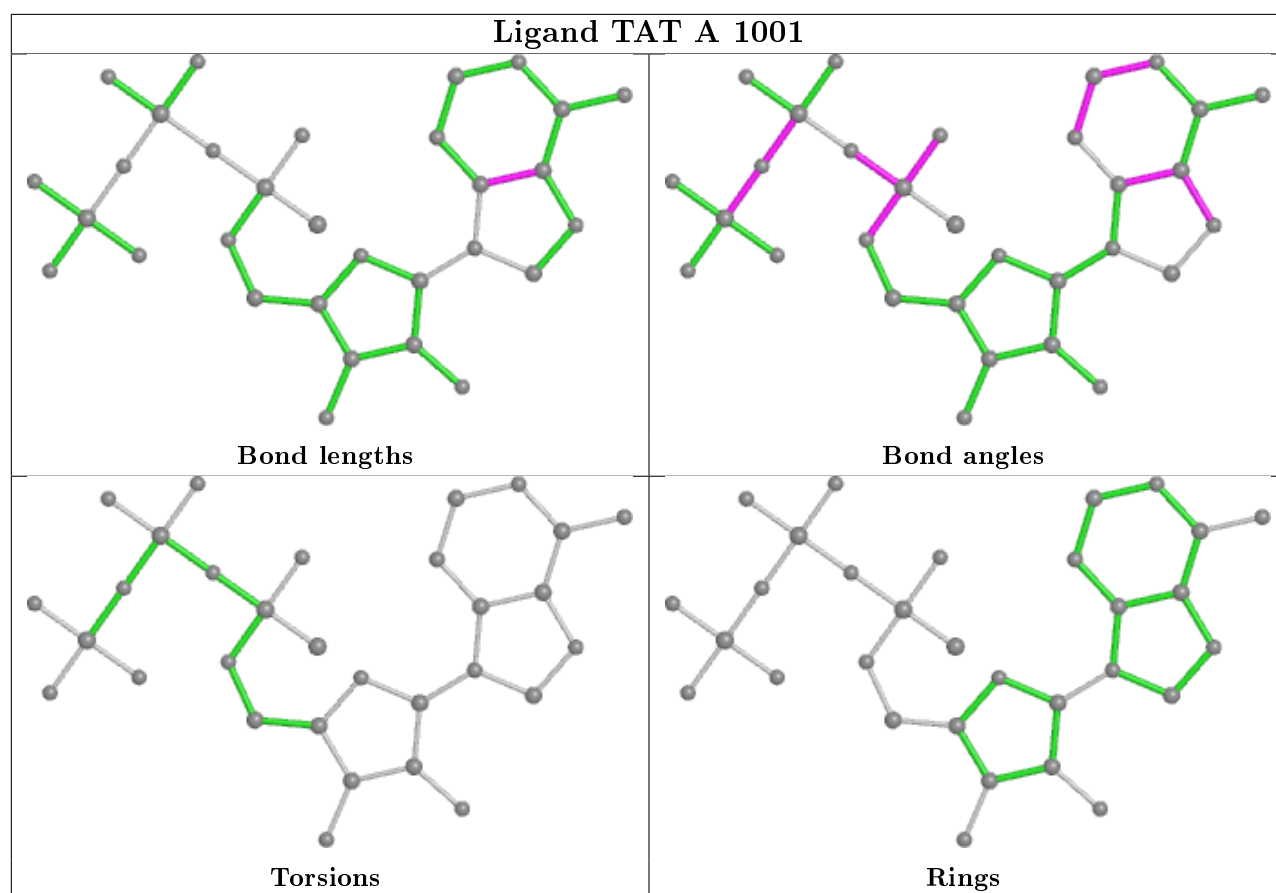
Mol	Chain	Res	Type	Atoms
2	B	1001	TAT	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TAT	3	0
2	B	1001	TAT	2	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	401/434 (92%)	-0.04	9 (2%) 62 69	38, 67, 108, 157	0
1	B	401/434 (92%)	-0.13	7 (1%) 70 76	37, 64, 97, 164	0
All	All	802/868 (92%)	-0.09	16 (1%) 65 71	37, 66, 105, 164	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ALA	9.9
1	A	154	SER	4.7
1	B	122	HIS	4.7
1	A	204	ILE	4.4
1	B	188	ILE	4.4
1	B	403	ILE	3.3
1	A	188	ILE	3.1
1	B	149	ILE	3.1
1	A	225	PHE	3.1
1	B	399	GLY	3.0
1	B	215	ILE	2.8
1	B	156	LEU	2.7
1	A	222	CYS	2.6
1	A	244	TRP	2.4
1	A	156	LEU	2.2
1	A	64	VAL	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

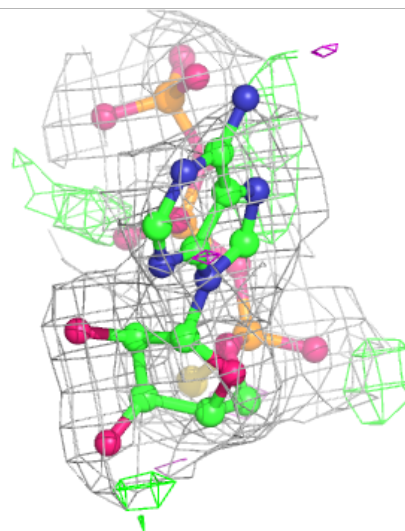
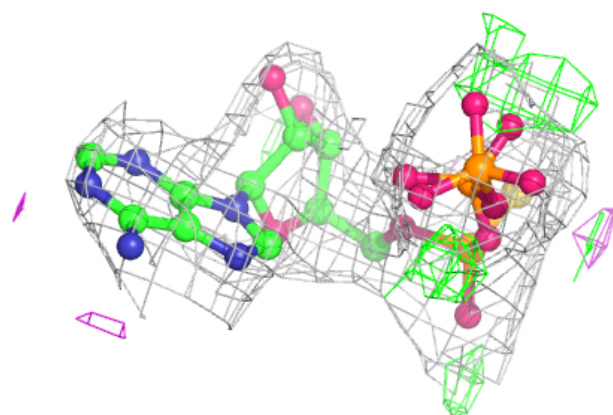
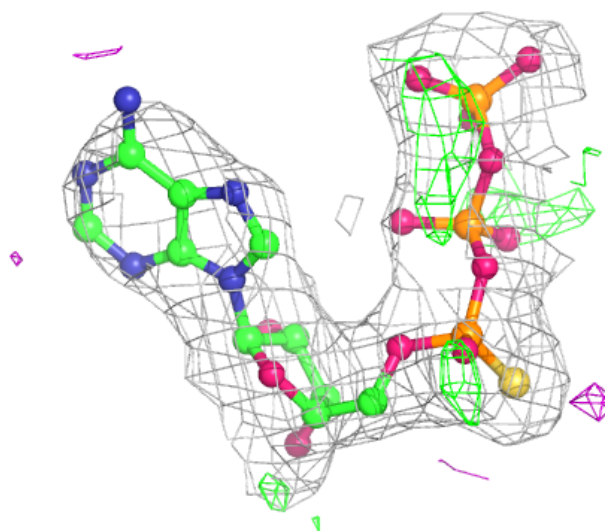
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TAT	A	1001	31/31	0.96	0.15	48,71,86,91	0
2	TAT	B	1001	31/31	0.96	0.12	44,57,115,116	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.

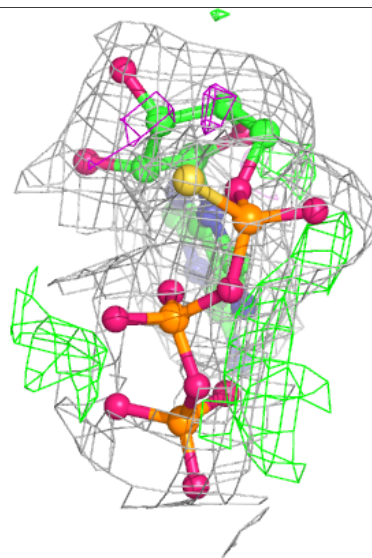
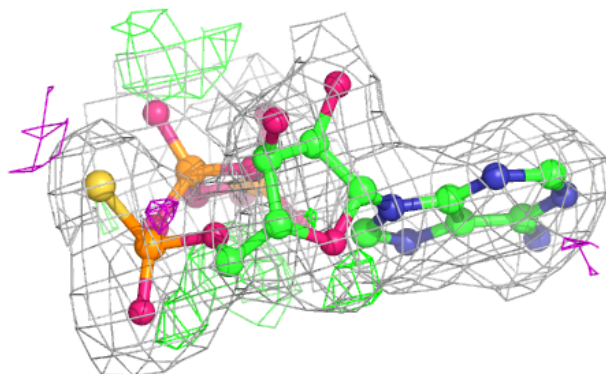
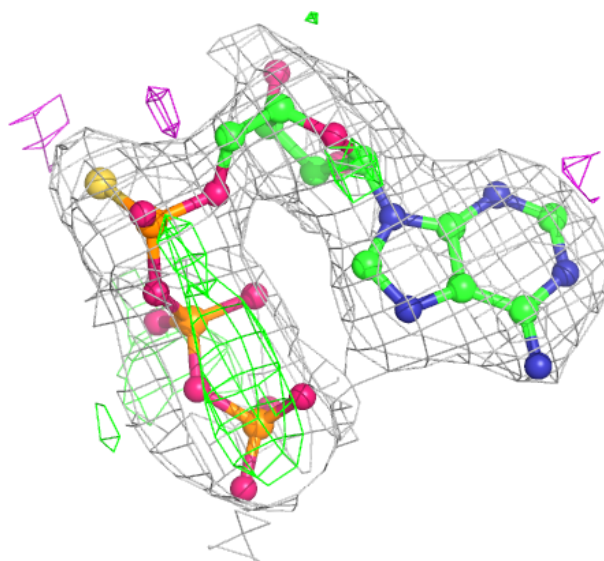
Electron density around TAT A 1001:

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



Electron density around TAT B 1001:

$2mF_o-DF_c$ (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.