



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:32 PM BST

PDB ID : 5Y0T
Title : Crystal structure of Thermotoga maritima TmcAL bound with alpha-thio
ATP(Form II)
Authors : Yamashita, S.; Tomita, K.
Deposited on : 2017-07-18
Resolution : 1.90 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

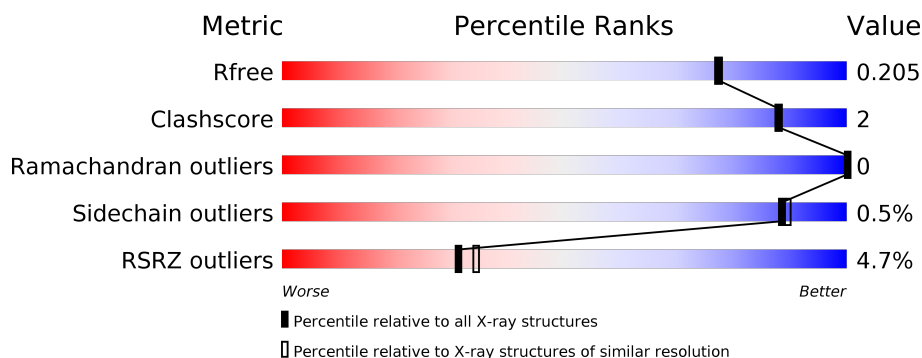
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	425	<div> <div style="width: 92%;"></div> <div style="width: 5%;"></div> <div style="width: 3%;"></div> </div> <div> <div style="width: 92%;"></div> <div style="width: 5%;"></div> <div style="width: 3%;"></div> </div>
1	B	425	<div> <div style="width: 6%;"></div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> <div style="width: 7%;"></div> </div> <div> <div style="width: 6%;"></div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> <div style="width: 7%;"></div> </div>
1	C	425	<div> <div style="width: 0%;"></div> <div style="width: 93%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div> <div> <div style="width: 0%;"></div> <div style="width: 93%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div>
1	D	425	<div> <div style="width: 11%;"></div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 11%;"></div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div>

2 Entry composition [i](#)

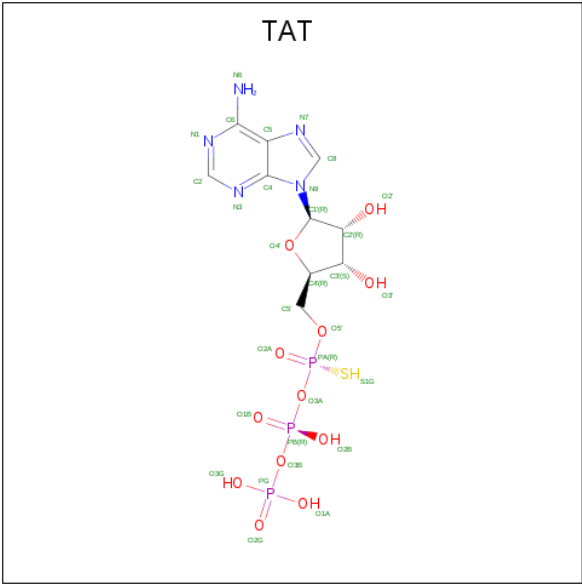
There are 5 unique types of molecules in this entry. The entry contains 14432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thermotoga maritima TmcAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3388	2178	585	607	18			
1	B	414	Total	C	N	O	S	0	0	0
			3387	2177	585	607	18			
1	C	412	Total	C	N	O	S	0	0	0
			3379	2173	583	605	18			
1	D	414	Total	C	N	O	S	0	0	0
			3387	2177	585	607	18			

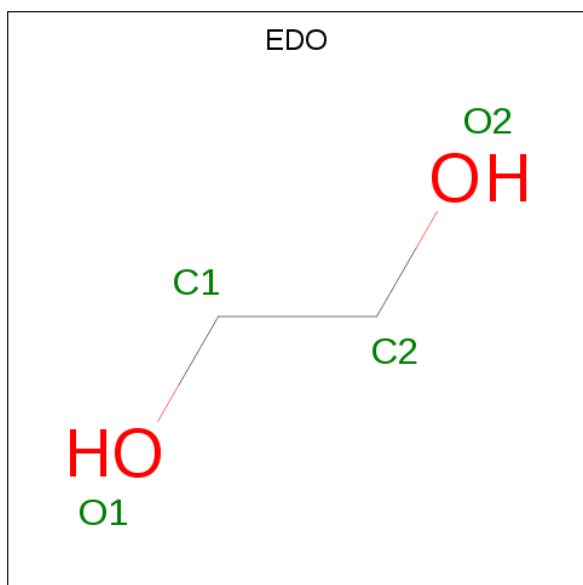
- Molecule 2 is ADENOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: TAT) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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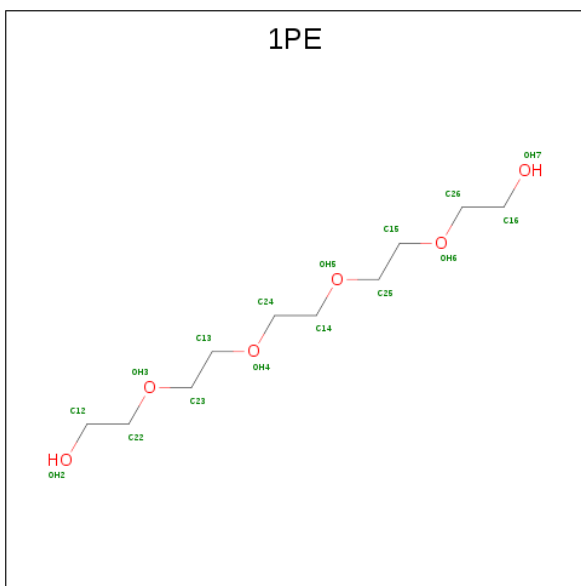
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- 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		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total	O	0	0
			237	237		
5	B	124	Total	O	0	0
			124	124		
5	C	203	Total	O	0	0
			203	203		
5	D	151	Total	O	0	0
			151	151		

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.

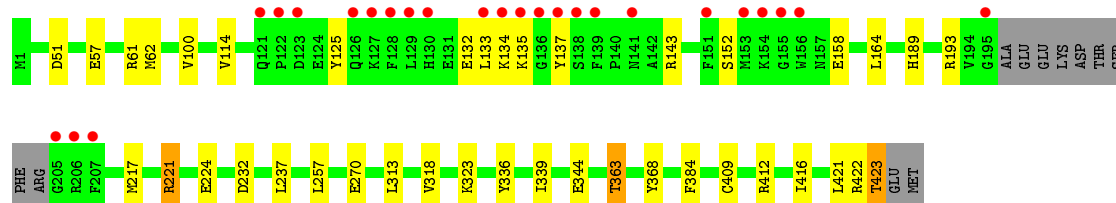
• Molecule 1: *Thermotoga maritima* TmcAL

Chain A: 



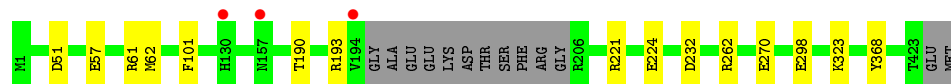
• Molecule 1: *Thermotoga maritima* TmcAL

Chain B: 




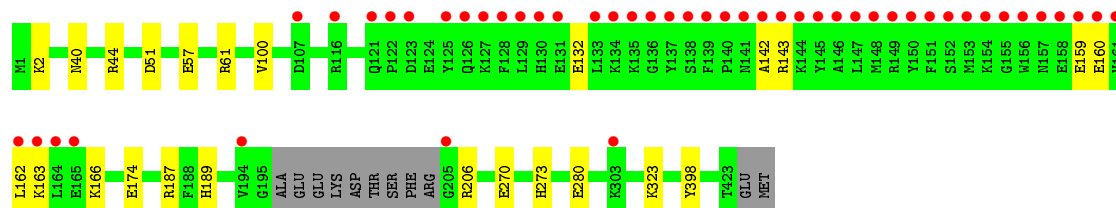
• Molecule 1: *Thermotoga maritima* TmcAL

Chain C: 



• Molecule 1: *Thermotoga maritima* TmcAL

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.62Å 97.81Å 144.60Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	47.57 – 1.90 49.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.57-1.90) 98.1 (49.87-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.170 , 0.203 0.174 , 0.205	Depositor DCC
R_{free} test set	8550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14432	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: TAT, CSD, CME, EDO, 1PE

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	0.42	0/3441	0.52	0/4621
1	B	0.34	0/3440	0.49	0/4619
1	C	0.40	0/3432	0.53	1/4609 (0.0%)
1	D	0.36	0/3440	0.50	1/4619 (0.0%)
All	All	0.38	0/13753	0.51	2/18468 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	51	ASP	CB-CG-OD1	5.61	123.34	118.30

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	3388	0	3400	12	0
1	B	3387	0	3398	22	0
1	C	3379	0	3392	8	0
1	D	3387	0	3398	14	0
2	A	31	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	14	1	0
2	C	31	0	14	1	0
2	D	31	0	14	1	0
3	A	12	0	18	0	0
3	B	12	0	18	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
4	D	16	0	22	2	0
5	A	237	0	0	0	0
5	B	124	0	0	0	0
5	C	203	0	0	0	0
5	D	151	0	0	1	0
All	All	14432	0	13720	56	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 (56) 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:B:57:GLU:OE2	1:B:61:ARG:NH1	2.21	0.73
1:D:44:ARG:HH22	4:D:1003:1PE:H241	1.57	0.69
1:D:206:ARG:NH1	5:D:1102:HOH:O	2.29	0.66
1:C:57:GLU:OE2	1:C:61:ARG:NH1	2.29	0.66
1:B:339:ILE:HD12	1:B:363:THR:HG23	1.77	0.65
1:B:270:GLU:O	1:B:323:LYS:HE2	2.05	0.57
1:B:51:ASP:OD2	1:B:412:ARG:NH1	2.37	0.57
1:D:163:LYS:HA	1:D:166:LYS:HE3	1.88	0.55
1:B:344:GLU:HG3	1:B:422:ARG:HA	1.88	0.53
1:D:160:GLU:HA	1:D:163:LYS:HZ3	1.73	0.53
1:D:44:ARG:NH2	4:D:1003:1PE:H241	2.24	0.53
1:A:123:ASP:O	1:A:127:LYS:HG2	2.09	0.52
1:B:114:VAL:HG11	1:B:164:LEU:HD11	1.91	0.52
1:B:152:SER:OG	1:B:158:GLU:OE1	2.28	0.52
1:B:134:LYS:HG2	1:B:135:LYS:H	1.77	0.49
1:B:344:GLU:HB2	1:B:423:THR:HG22	1.95	0.49
1:C:270:GLU:O	1:C:323:LYS:HE2	2.13	0.49
1:B:412:ARG:CZ	1:B:416:ILE:HD11	2.43	0.49
1:C:62:MET:HE1	1:C:232:ASP:HB2	1.94	0.49
1:A:352:LEU:HD11	1:A:356:LYS:HE2	1.94	0.48
1:C:221:ARG:HD2	1:C:224:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLU:OE2	1:D:61:ARG:NH2	2.47	0.48
1:B:221:ARG:HD2	1:B:224:GLU:OE2	2.14	0.47
1:B:61:ARG:HG2	1:B:421:LEU:HD11	1.96	0.47
1:A:374:LYS:NZ	1:C:298:GLU:O	2.47	0.47
1:B:257:LEU:HD23	1:B:318:VAL:HG11	1.96	0.47
1:A:1:MET:HB2	1:A:31:ASP:OD1	2.15	0.46
1:B:132:GLU:O	1:B:137:TYR:HB2	2.15	0.46
1:C:101:PHE:CE2	1:C:190:THR:HG22	2.50	0.46
1:D:143:ARG:NH1	1:D:174:GLU:OE2	2.48	0.46
1:B:336:TYR:HB3	1:B:384:PHE:CE2	2.51	0.46
1:B:62:MET:CE	1:B:232:ASP:HB2	2.46	0.45
1:D:100:VAL:HG22	1:D:189:HIS:HB2	1.98	0.45
1:B:62:MET:HE1	1:B:232:ASP:HB2	1.99	0.45
1:B:100:VAL:HG22	1:B:189:HIS:HB2	2.00	0.44
1:D:2:LYS:HD2	1:D:187:ARG:HH22	1.82	0.44
1:A:336:TYR:HB3	1:A:384:PHE:CE2	2.52	0.44
1:B:125:TYR:OH	1:B:143:ARG:HG3	2.18	0.44
1:D:132:GLU:HB3	1:D:142:ALA:HA	2.00	0.43
1:B:193:ARG:HA	2:B:1001:TAT:C2	2.49	0.43
1:A:270:GLU:HG3	1:A:280:GLU:HG2	2.00	0.43
1:C:193:ARG:HA	2:C:1001:TAT:C2	2.49	0.42
1:B:217:MET:HE1	1:B:237:LEU:HD11	2.00	0.42
1:D:40:ASN:HB3	1:D:398:TYR:CD2	2.54	0.42
1:A:273:HIS:HA	1:A:323:LYS:HG2	2.02	0.42
1:C:221:ARG:NH1	1:C:224:GLU:OE1	2.53	0.42
1:A:221:ARG:NH2	1:A:224:GLU:OE1	2.49	0.41
1:A:62:MET:HE1	1:A:232:ASP:HB2	2.00	0.41
1:A:36:VAL:HG22	1:A:70:LEU:HB2	2.02	0.41
2:D:1001:TAT:O1B	2:D:1001:TAT:H8	2.20	0.41
1:D:270:GLU:HG2	1:D:280:GLU:HG2	2.01	0.41
1:B:133:LEU:HA	1:B:133:LEU:HD23	1.91	0.41
1:D:159:GLU:HG3	1:D:162:LEU:HD12	2.02	0.41
1:D:273:HIS:HA	1:D:323:LYS:HG2	2.03	0.41
1:A:345:LYS:H	1:A:423:THR:HG21	1.85	0.40
1:A:134:LYS:HB3	1:A:134:LYS:HE2	1.96	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	408/425 (96%)	404 (99%)	4 (1%)	0	100	100
1	B	408/425 (96%)	402 (98%)	6 (2%)	0	100	100
1	C	406/425 (96%)	401 (99%)	5 (1%)	0	100	100
1	D	408/425 (96%)	404 (99%)	4 (1%)	0	100	100
All	All	1630/1700 (96%)	1611 (99%)	19 (1%)	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	364/374 (97%)	364 (100%)	0	100	100
1	B	364/374 (97%)	359 (99%)	5 (1%)	67	65
1	C	364/374 (97%)	362 (100%)	2 (0%)	88	89
1	D	364/374 (97%)	364 (100%)	0	100	100
All	All	1456/1496 (97%)	1449 (100%)	7 (0%)	88	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	ARG
1	B	313	LEU

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Mol	Chain	Res	Type
1	B	363	THR
1	B	368	TYR
1	B	423	THR
1	C	262	ARG
1	C	368	TYR

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	D	409	1	8,9,10	0.84	0	5,9,11	0.70	0
1	CSD	B	42	1	3,7,8	0.94	0	1,8,10	1.05	0
1	CSD	C	42	1	3,7,8	0.83	0	1,8,10	0.04	0
1	CSD	A	42	1	3,7,8	0.73	0	1,8,10	0.14	0
1	CSD	D	42	1	3,7,8	0.90	0	1,8,10	0.78	0
1	CME	A	409	1	8,9,10	0.92	0	5,9,11	0.59	0
1	CME	C	409	1	8,9,10	0.98	0	5,9,11	1.06	0
1	CME	B	409	1	8,9,10	1.06	1 (12%)	5,9,11	1.13	1 (20%)

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
1	CME	D	409	1	-	0/5/8/10	-
1	CSD	B	42	1	-	1/2/6/8	-
1	CSD	C	42	1	-	1/2/6/8	-
1	CSD	A	42	1	-	1/2/6/8	-
1	CSD	D	42	1	-	1/2/6/8	-
1	CME	A	409	1	-	0/5/8/10	-
1	CME	C	409	1	-	0/5/8/10	-
1	CME	B	409	1	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	CME	CB-SG	-2.23	1.74	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	CME	CB-SG-SD	2.02	109.06	103.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	42	CSD	CA-CB-SG-OD1
1	C	42	CSD	CA-CB-SG-OD1
1	A	42	CSD	CA-CB-SG-OD1
1	D	42	CSD	CA-CB-SG-OD1
1	B	409	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	B	1004	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	B	1002	-	3,3,3	0.43	0	2,2,2	0.48	0
4	1PE	D	1003	-	15,15,15	0.61	0	14,14,14	0.24	0
2	TAT	A	1001	-	24,33,33	1.00	2 (8%)	29,52,52	1.28	3 (10%)
2	TAT	B	1001	-	24,33,33	1.14	2 (8%)	29,52,52	1.32	5 (17%)
2	TAT	C	1001	-	24,33,33	1.05	2 (8%)	29,52,52	1.30	3 (10%)
2	TAT	D	1001	-	24,33,33	1.11	2 (8%)	29,52,52	1.38	5 (17%)
3	EDO	C	1002	-	3,3,3	0.50	0	2,2,2	0.28	0
3	EDO	A	1002	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	A	1003	-	3,3,3	0.62	0	2,2,2	0.29	0
3	EDO	B	1003	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	D	1002	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	C	1003	-	3,3,3	0.36	0	2,2,2	0.53	0
3	EDO	A	1004	-	3,3,3	0.52	0	2,2,2	0.38	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	B	1004	-	-	0/1/1/1	-
3	EDO	B	1002	-	-	0/1/1/1	-
4	1PE	D	1003	-	-	7/13/13/13	-
2	TAT	A	1001	-	-	0/14/38/38	0/3/3/3
2	TAT	B	1001	-	-	0/14/38/38	0/3/3/3
2	TAT	C	1001	-	-	0/14/38/38	0/3/3/3
2	TAT	D	1001	-	-	0/14/38/38	0/3/3/3
3	EDO	C	1002	-	-	0/1/1/1	-
3	EDO	A	1002	-	-	0/1/1/1	-
3	EDO	A	1003	-	-	1/1/1/1	-
3	EDO	B	1003	-	-	1/1/1/1	-
3	EDO	D	1002	-	-	0/1/1/1	-
3	EDO	C	1003	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1004	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	TAT	PA-O5'	3.54	1.63	1.57
2	C	1001	TAT	C5-C4	2.43	1.47	1.40
2	D	1001	TAT	C5-C4	2.39	1.47	1.40
2	C	1001	TAT	PA-O5'	2.36	1.61	1.57
2	A	1001	TAT	C5-C4	2.32	1.47	1.40
2	B	1001	TAT	C5-C4	2.22	1.46	1.40
2	D	1001	TAT	PA-O5'	2.15	1.61	1.57
2	A	1001	TAT	PA-O5'	2.14	1.61	1.57

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	TAT	N3-C2-N1	-3.73	122.86	128.68
2	B	1001	TAT	N3-C2-N1	-3.35	123.44	128.68
2	A	1001	TAT	N3-C2-N1	-3.32	123.50	128.68
2	D	1001	TAT	N3-C2-N1	-3.06	123.89	128.68
2	D	1001	TAT	PB-O3B-PG	-2.99	122.58	132.83
2	D	1001	TAT	C4-C5-N7	-2.72	106.57	109.40
2	A	1001	TAT	C4-C5-N7	-2.51	106.79	109.40
2	B	1001	TAT	C1'-N9-C4	-2.48	122.28	126.64
2	C	1001	TAT	C4-C5-N7	-2.38	106.92	109.40
2	C	1001	TAT	C2-N1-C6	2.32	122.72	118.75
2	A	1001	TAT	O3G-PG-O1A	2.25	116.24	107.64
2	B	1001	TAT	C2-N1-C6	2.23	122.56	118.75
2	D	1001	TAT	O5'-PA-O2A	-2.22	106.24	114.42
2	B	1001	TAT	C4-C5-N7	-2.09	107.22	109.40
2	D	1001	TAT	O3G-PG-O1A	2.07	115.53	107.64
2	B	1001	TAT	PB-O3B-PG	-2.01	125.93	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1003	1PE	OH4-C13-C23-OH3
4	D	1003	1PE	OH5-C14-C24-OH4
4	D	1003	1PE	OH6-C15-C25-OH5

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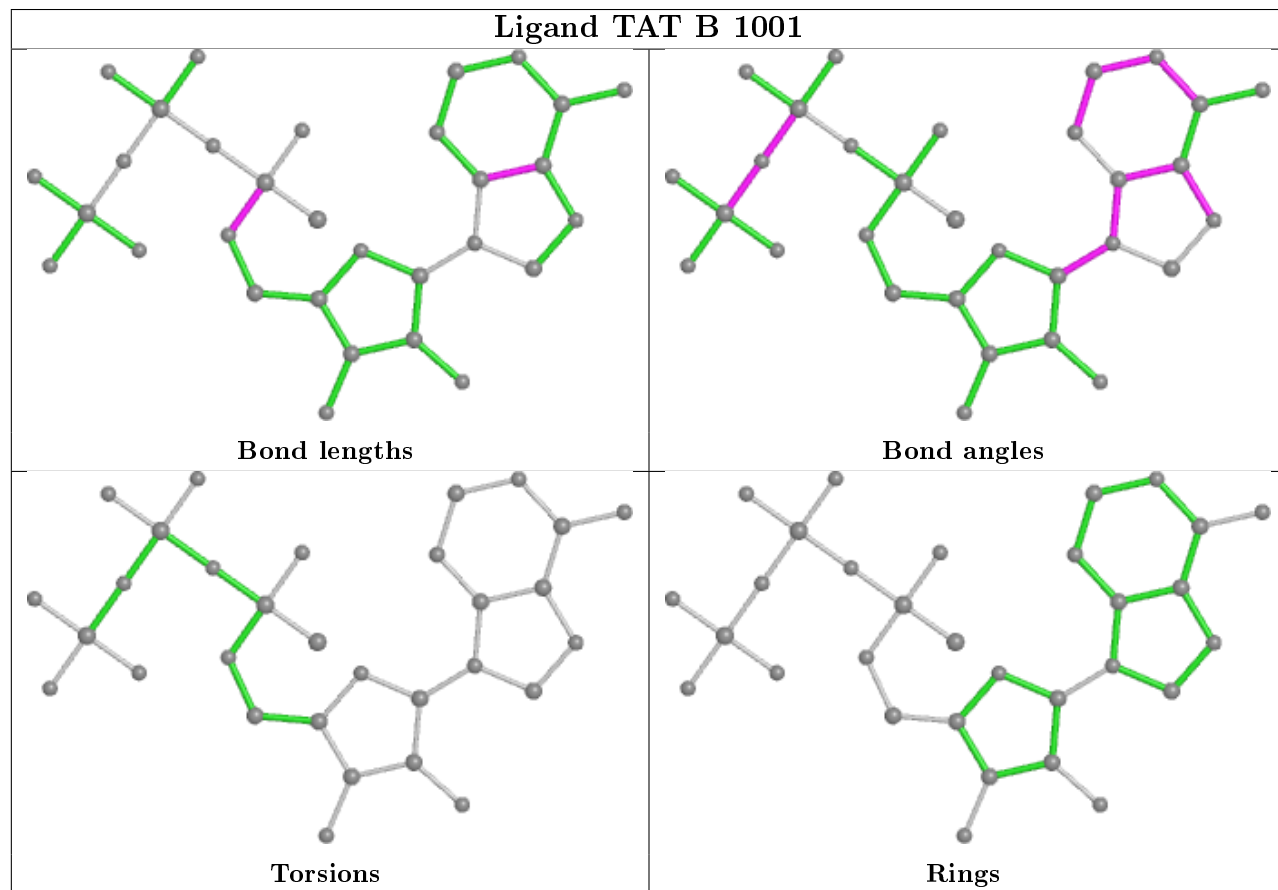
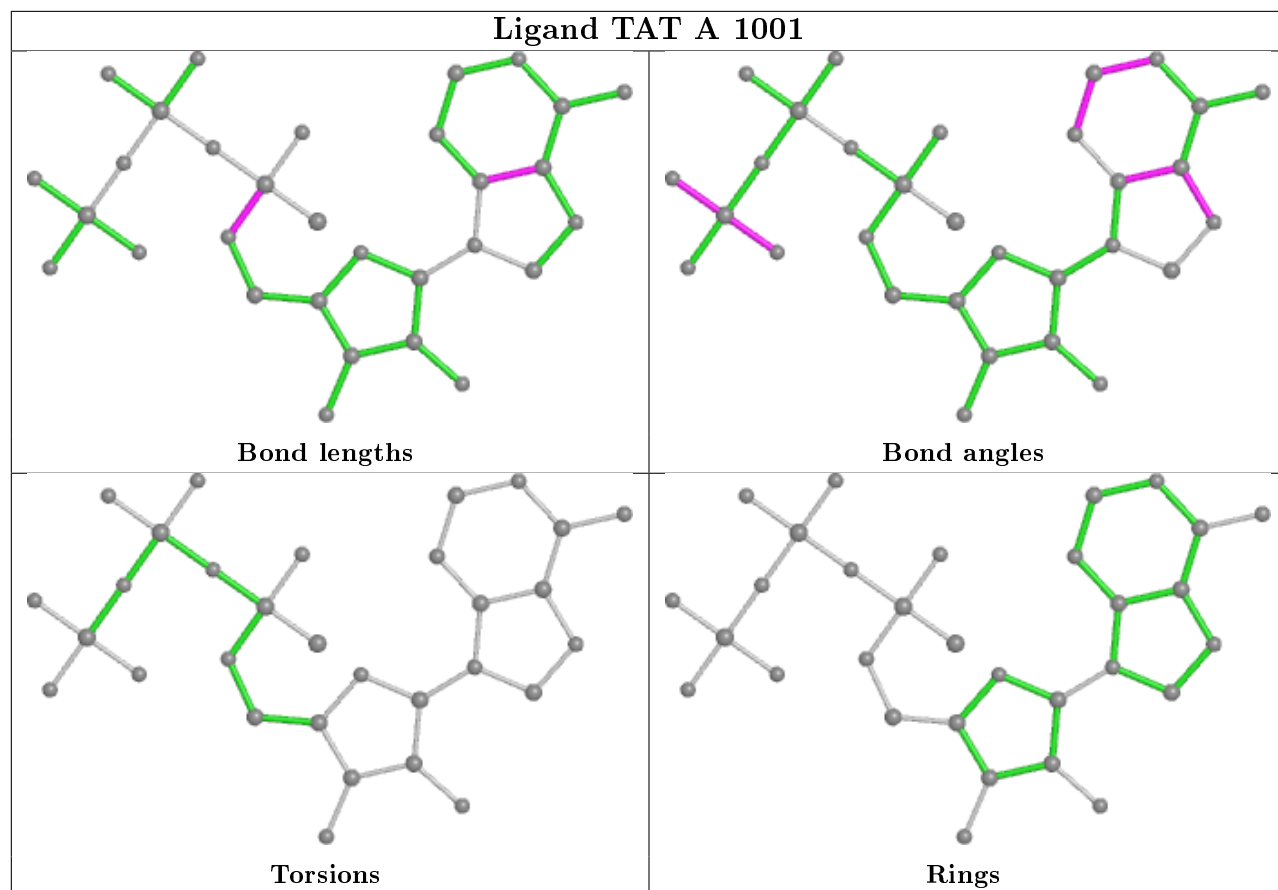
Mol	Chain	Res	Type	Atoms
4	D	1003	1PE	OH2-C12-C22-OH3
4	D	1003	1PE	C16-C26-OH6-C15
4	D	1003	1PE	OH7-C16-C26-OH6
3	A	1003	EDO	O1-C1-C2-O2
4	D	1003	1PE	C23-C13-OH4-C24
3	B	1003	EDO	O1-C1-C2-O2

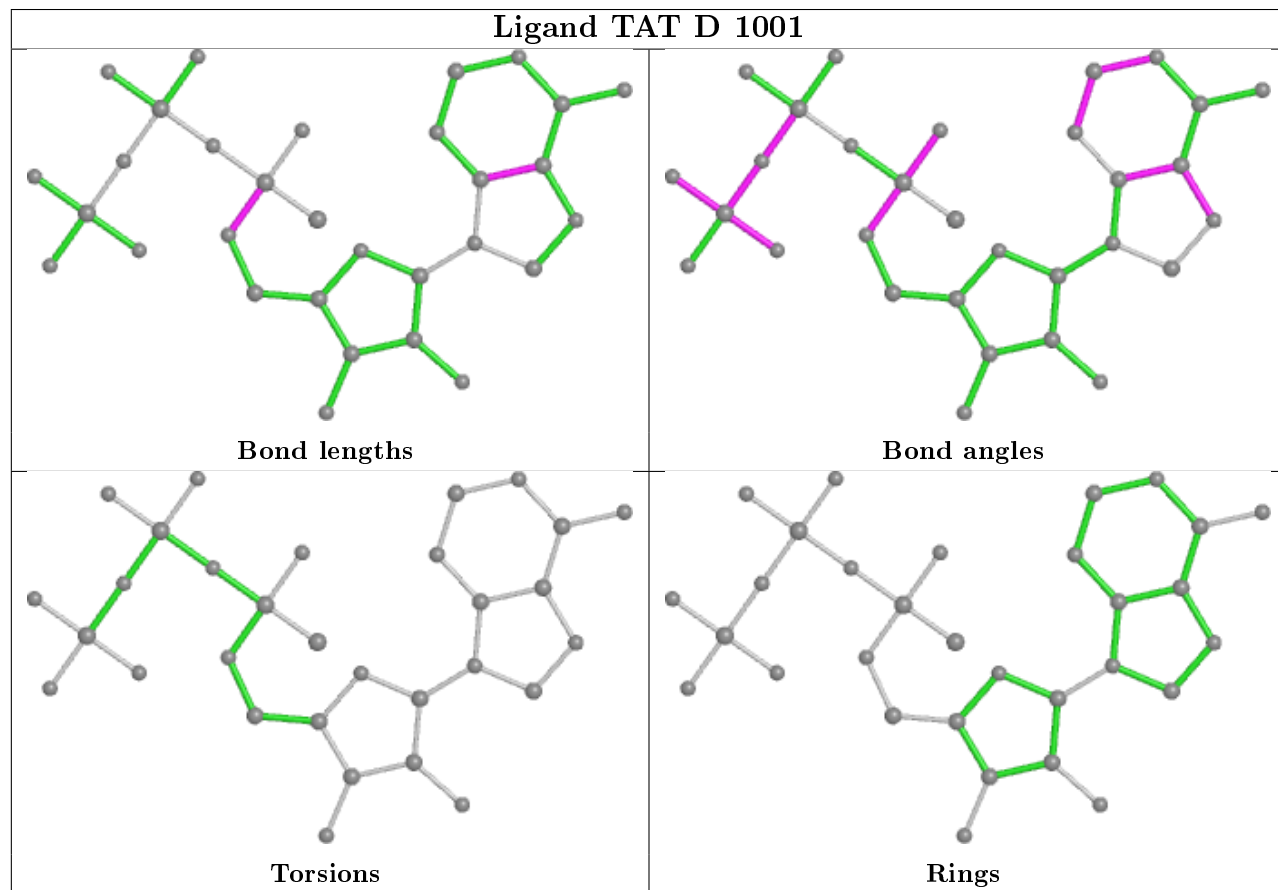
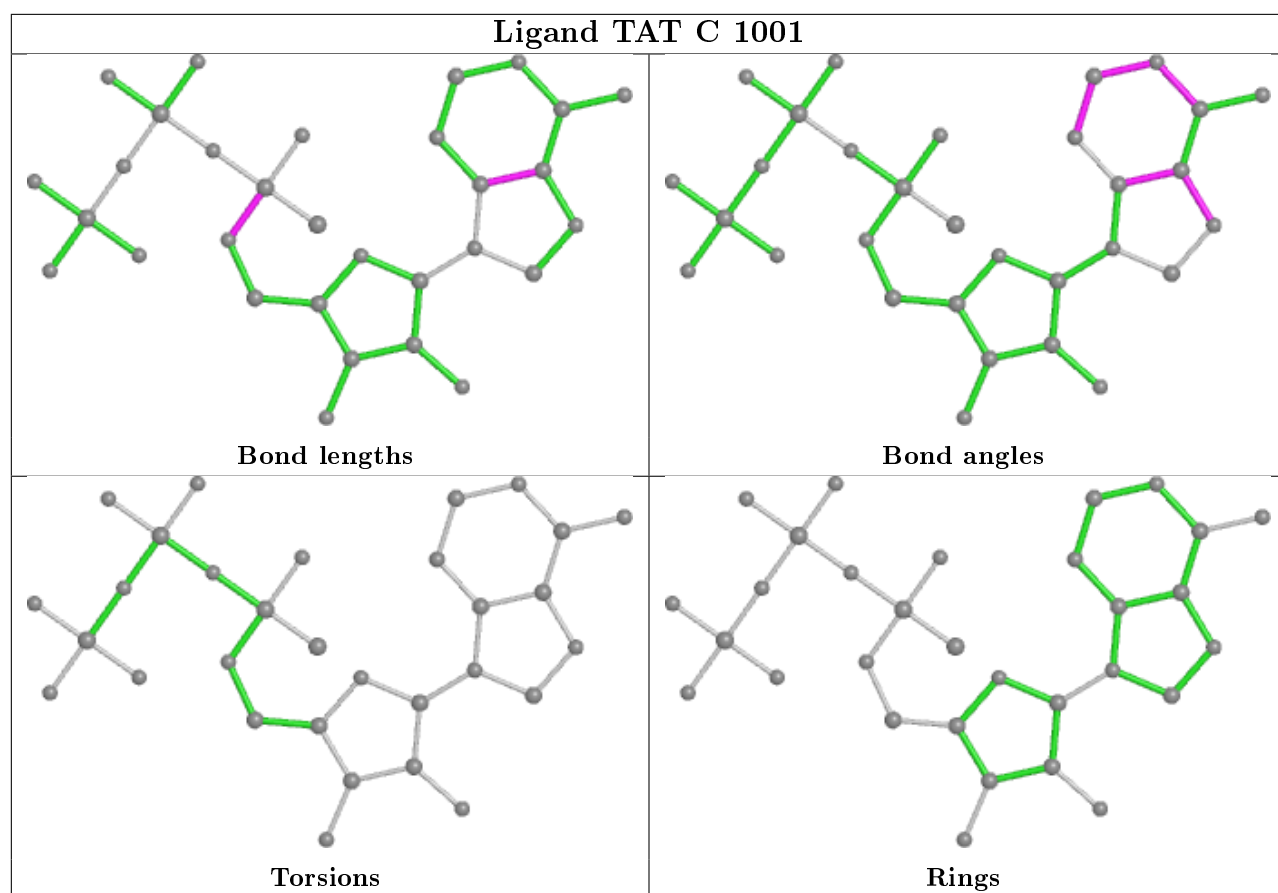
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1003	1PE	2	0
2	B	1001	TAT	1	0
2	C	1001	TAT	1	0
2	D	1001	TAT	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	412/425 (96%)	-0.31	2 (0%) 91 92	17, 26, 53, 89	0
1	B	412/425 (96%)	0.07	25 (6%) 21 24	21, 35, 80, 110	0
1	C	410/425 (96%)	-0.33	3 (0%) 87 88	18, 27, 53, 75	0
1	D	412/425 (96%)	0.43	48 (11%) 4 5	19, 33, 120, 163	0
All	All	1646/1700 (96%)	-0.03	78 (4%) 31 34	17, 31, 73, 163	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	TRP	12.5
1	D	155	GLY	11.6
1	D	162	LEU	10.5
1	D	153	MET	9.5
1	D	154	LYS	8.8
1	D	137	TYR	8.8
1	D	130	HIS	7.6
1	B	205	GLY	7.2
1	D	145	TYR	7.1
1	D	152	SER	6.7
1	B	133	LEU	6.7
1	D	151	PHE	6.5
1	D	157	ASN	6.3
1	D	161	VAL	6.3
1	D	150	TYR	6.2
1	A	196	ALA	6.2
1	D	127	LYS	5.9
1	B	130	HIS	5.6
1	D	136	GLY	5.5
1	D	147	LEU	5.4
1	D	146	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	138	SER	5.0
1	B	137	TYR	4.9
1	D	141	ASN	4.8
1	D	133	LEU	4.4
1	D	148	MET	4.4
1	B	156	TRP	4.4
1	B	139	PHE	4.4
1	D	205	GLY	4.3
1	D	125	TYR	4.3
1	B	195	GLY	4.2
1	D	135	LYS	4.2
1	D	143	ARG	4.1
1	D	121	GLN	4.1
1	B	135	LYS	4.0
1	B	127	LYS	4.0
1	D	140	PRO	3.9
1	B	123	ASP	3.8
1	D	129	LEU	3.8
1	B	134	LYS	3.7
1	D	158	GLU	3.7
1	D	159	GLU	3.7
1	B	206	ARG	3.7
1	B	126	GLN	3.7
1	D	164	LEU	3.7
1	D	126	GLN	3.6
1	D	122	PRO	3.5
1	D	128	PHE	3.5
1	D	165	GLU	3.4
1	D	160	GLU	3.4
1	B	154	LYS	3.4
1	D	134	LYS	3.3
1	B	136	GLY	3.3
1	D	139	PHE	3.2
1	D	149	ARG	3.1
1	B	155	GLY	3.0
1	B	141	ASN	3.0
1	D	142	ALA	3.0
1	B	151	PHE	2.9
1	B	122	PRO	2.8
1	D	163	LYS	2.8
1	D	303	LYS	2.8
1	D	116	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	2.5
1	B	121	GLN	2.4
1	B	138	SER	2.3
1	D	194	VAL	2.3
1	D	107	ASP	2.3
1	B	207	PHE	2.2
1	B	128	PHE	2.2
1	C	194	VAL	2.2
1	C	157	ASN	2.2
1	A	423	THR	2.2
1	D	144	LYS	2.1
1	D	123	ASP	2.1
1	B	153	MET	2.1
1	D	131	GLU	2.1
1	C	130	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	B	409	10/11	0.91	0.14	27,43,86,87	0
1	CSD	A	42	8/9	0.94	0.08	18,23,41,46	0
1	CME	C	409	10/11	0.95	0.10	22,33,66,67	0
1	CSD	B	42	8/9	0.95	0.10	25,31,43,51	0
1	CSD	C	42	8/9	0.96	0.09	16,21,37,48	0
1	CSD	D	42	8/9	0.97	0.10	24,25,43,50	0
1	CME	D	409	10/11	0.98	0.11	22,25,29,30	0
1	CME	A	409	10/11	0.98	0.11	21,26,37,41	0

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,

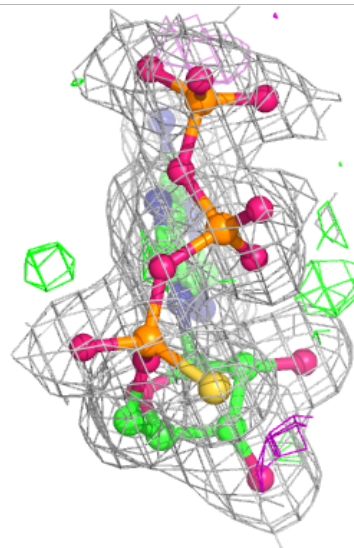
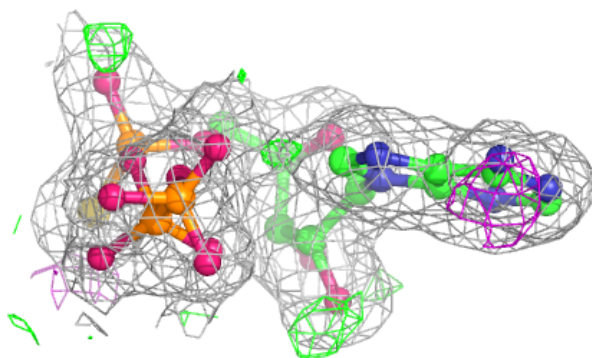
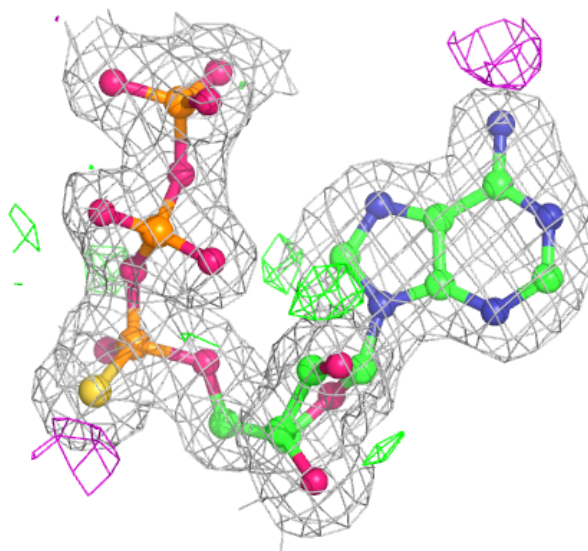
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1PE	D	1003	16/16	0.52	0.20	70,84,88,89	0
3	EDO	C	1002	4/4	0.84	0.17	44,44,48,52	0
3	EDO	B	1002	4/4	0.86	0.14	36,38,46,56	0
3	EDO	C	1003	4/4	0.88	0.15	44,48,51,55	0
3	EDO	A	1003	4/4	0.90	0.09	30,33,34,45	0
3	EDO	D	1002	4/4	0.91	0.15	36,40,46,52	0
3	EDO	B	1003	4/4	0.92	0.10	52,57,58,60	0
3	EDO	B	1004	4/4	0.93	0.17	48,49,55,55	0
3	EDO	A	1002	4/4	0.93	0.11	49,50,53,53	0
2	TAT	A	1001	31/31	0.97	0.08	20,26,31,34	0
2	TAT	D	1001	31/31	0.97	0.08	27,33,40,42	0
2	TAT	C	1001	31/31	0.98	0.09	19,24,30,35	0
2	TAT	B	1001	31/31	0.98	0.09	25,30,36,37	0
3	EDO	A	1004	4/4	0.99	0.14	24,24,27,28	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.

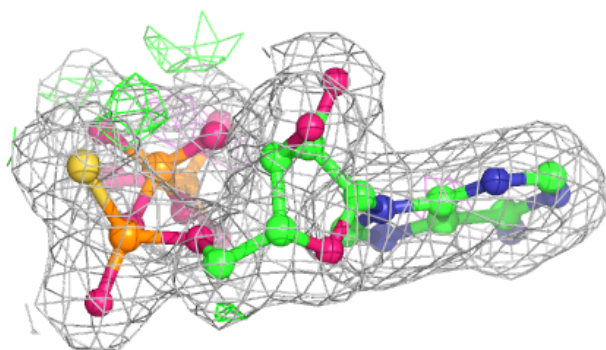
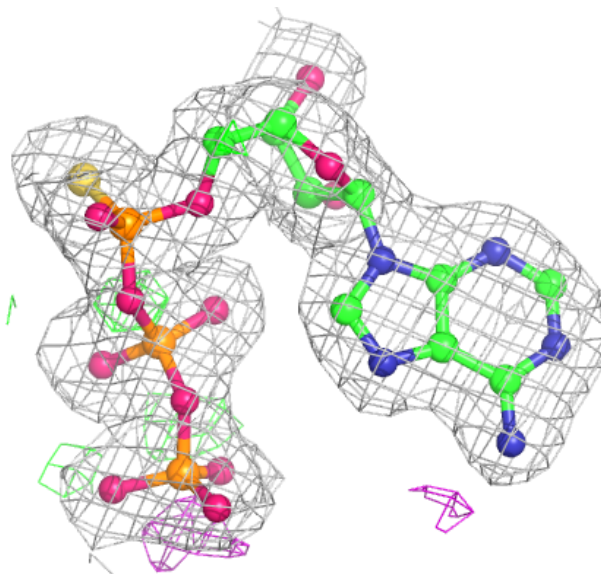
Electron density around TAT A 1001:

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



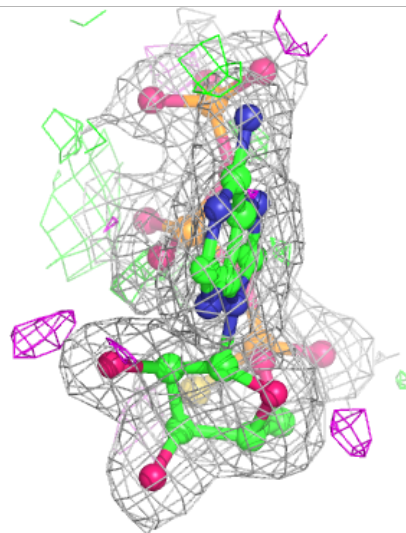
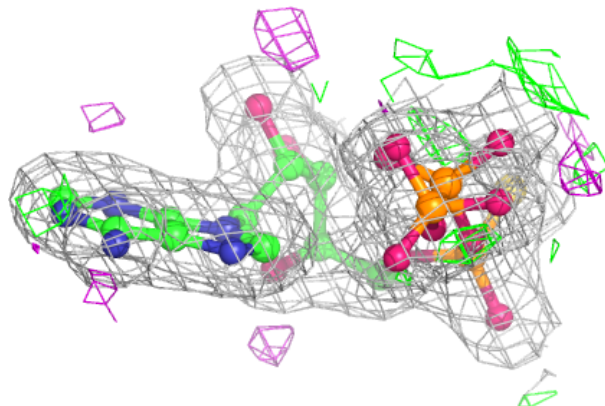
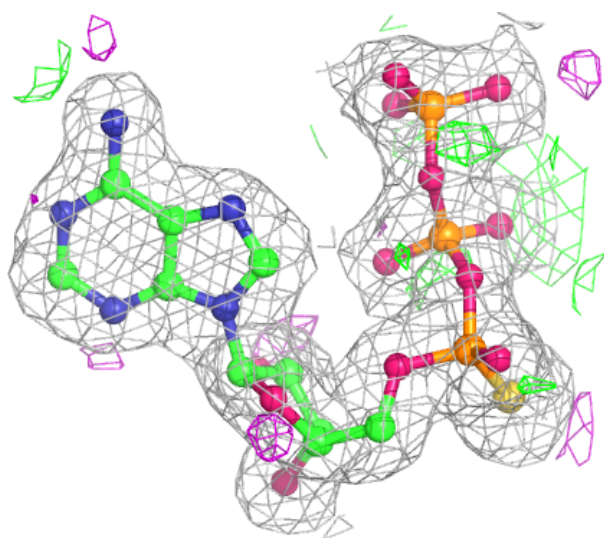
Electron density around TAT D 1001:

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



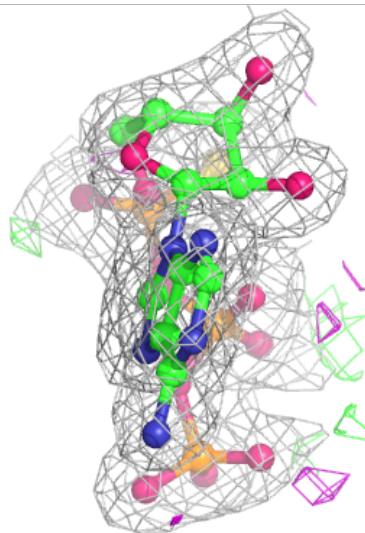
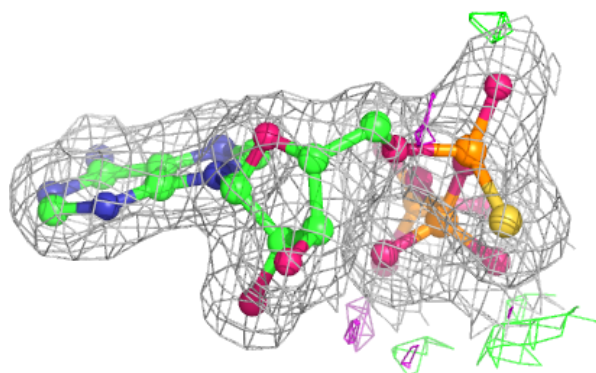
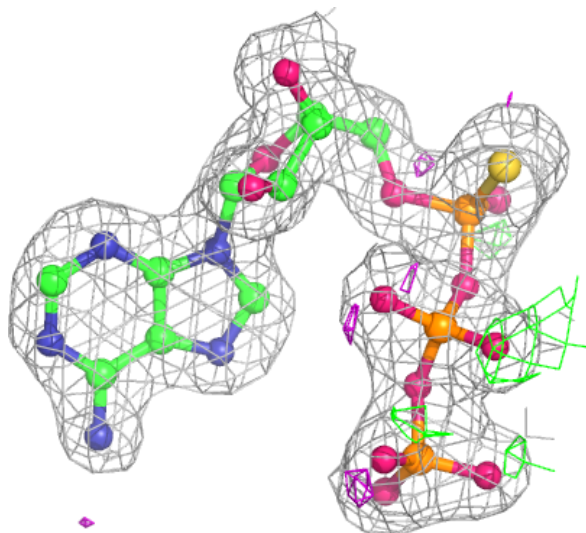
Electron density around TAT C 1001:

$2mF_o-DF_c$ (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.