



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 03:27 AM EDT

PDB ID : 1P7C
Title : Crystal Structure of HSV1-TK complexed with TP5A
Authors : Gardberg, A.; Shuvalova, L.; Monnerjahn, C.; Konrad, M.; Lavie, A.
Deposited on : 2003-05-01
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

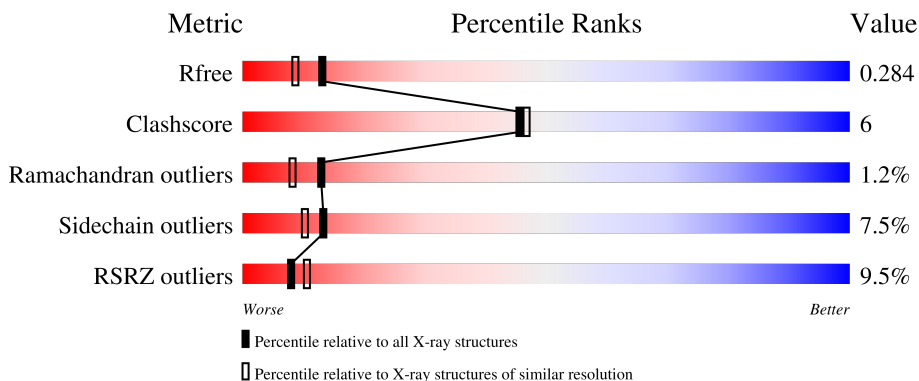
1 Overall quality at a glance

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	343	 8% 74% 12% • 12%
1	B	343	 9% 69% 20% • 7%

2 Entry composition [i](#)

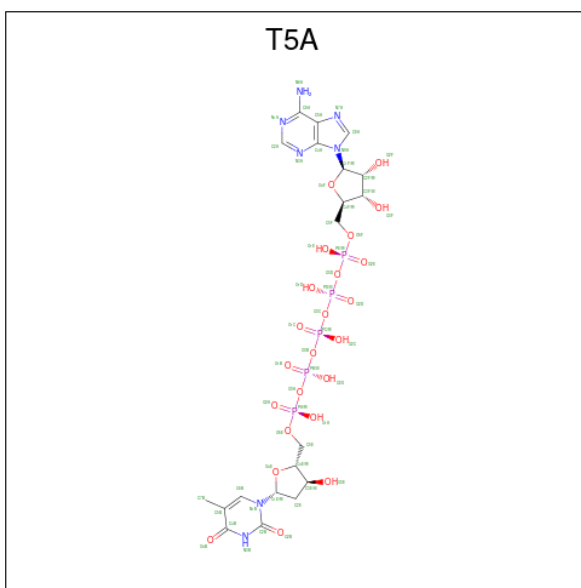
There are 5 unique types of molecules in this entry. The entry contains 5071 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	Total	C	N	O	S	0	0	0
			2261	1444	393	411	13			
1	B	318	Total	C	N	O	S	0	0	0
			2393	1526	416	435	16			

- Molecule 2 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (three-letter code: T5A) (formula: C₂₀H₃₀N₇O₂₃P₅).



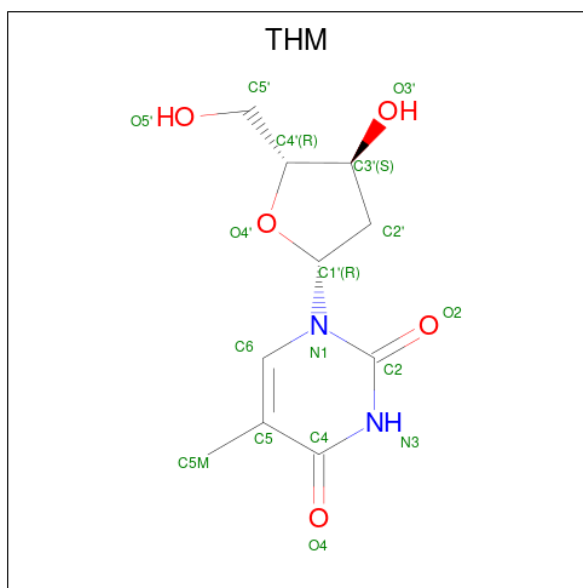
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			55	20	7	23	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is THYMIDINE (three-letter code: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	B	1	Total	C	N	O	0	0
			17	10	2	5		


- Molecule 5 is water.

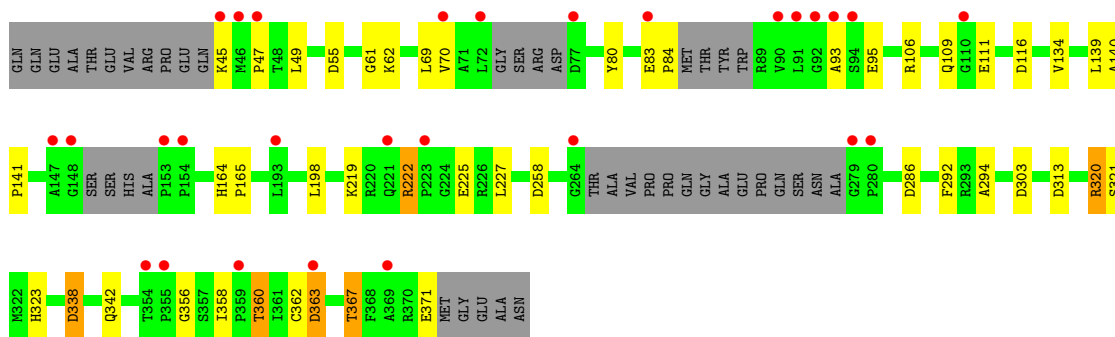
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	164	Total 164	O 164	0	0
5	B	176	Total 176	O 176	0	0

3 Residue-property plots [i](#)

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

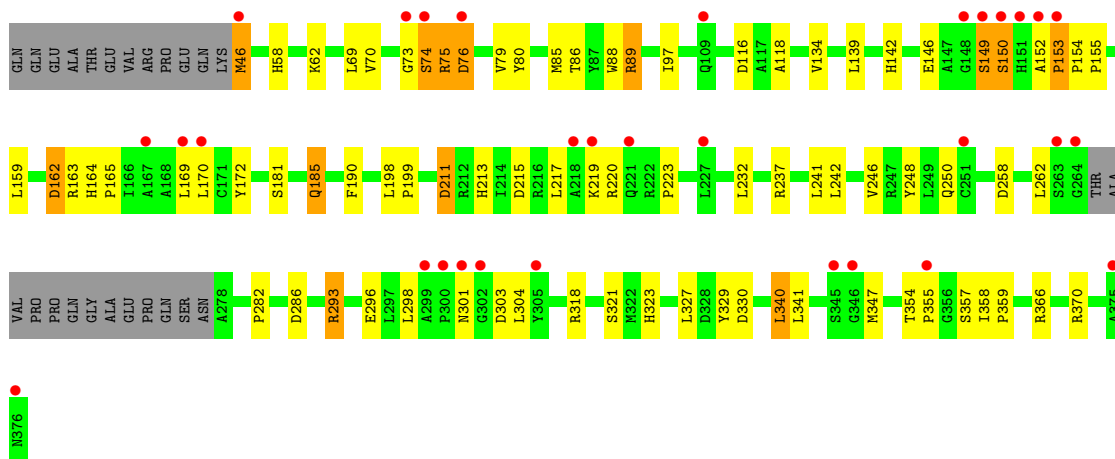
- Molecule 1: Thymidine kinase

Chain A: 



- Molecule 1: Thymidine kinase

Chain B: 



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.22Å 117.85Å 108.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.94 – 2.10 35.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.94-2.10) 97.0 (35.94-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.239 , 0.285 0.240 , 0.284	Depositor DCC
R_{free} test set	4142 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5071	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: SO4, T5A, THM

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	0.50	0/2311	0.80	10/3155 (0.3%)
1	B	0.52	0/2449	0.82	11/3347 (0.3%)
All	All	0.51	0/4760	0.81	21/6502 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CB-CG-OD2	7.90	125.41	118.30
1	B	116	ASP	CB-CG-OD2	7.74	125.26	118.30
1	A	303	ASP	CB-CG-OD2	7.46	125.02	118.30
1	B	303	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	318	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	286	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	116	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	318	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	215	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	211	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	76	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	258	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	162	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	338	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	320	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	320	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	330	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	363	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	286	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	258	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	313	ASP	CB-CG-OD2	5.12	122.91	118.30

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	2261	0	2258	18	1
1	B	2393	0	2384	41	0
2	A	55	0	25	1	0
3	B	5	0	0	0	0
4	B	17	0	14	1	0
5	A	164	0	0	4	1
5	B	176	0	0	4	1
All	All	5071	0	4681	60	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 6.

All (60) 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:89:ARG:HH11	1:B:89:ARG:HG3	1.28	0.99
1:B:149:SER:CB	1:B:347:MET:O	2.14	0.94
1:B:46:MET:HB2	5:B:523:HOH:O	1.70	0.89
1:B:185:GLN:HE21	1:B:185:GLN:H	1.24	0.82
1:B:89:ARG:HG3	1:B:89:ARG:NH1	1.94	0.78
1:B:69:LEU:HD22	1:B:340:LEU:HD13	1.67	0.76
1:A:83:GLU:OE2	1:A:84:PRO:HD2	1.85	0.74
1:B:85:MET:HE3	1:B:89:ARG:HG2	1.67	0.74
1:B:46:MET:SD	1:B:46:MET:N	2.62	0.73
1:A:62:LYS:HB2	5:A:637:HOH:O	1.88	0.73
1:B:85:MET:CE	1:B:89:ARG:HG2	2.21	0.70
1:B:370:ARG:NH2	5:B:531:HOH:O	2.30	0.65
1:A:61:GLY:N	2:A:503:T5A:O1D	2.28	0.64
1:A:47:PRO:HB2	1:A:358:ILE:HD13	1.78	0.63
1:A:222:ARG:HB2	1:A:225:GLU:HB2	1.84	0.60
1:A:70:VAL:HG21	1:A:80:TYR:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:HIS:HD2	1:B:172:TYR:OH	1.86	0.56
1:B:89:ARG:HD2	1:B:89:ARG:N	2.20	0.56
1:B:323:HIS:HE1	5:B:676:HOH:O	1.89	0.56
1:A:93:ALA:HB2	5:A:599:HOH:O	2.06	0.55
1:B:89:ARG:HD3	1:B:97:ILE:HD12	1.89	0.54
1:B:74:SER:O	1:B:76:ASP:N	2.33	0.53
1:B:70:VAL:HG21	1:B:80:TYR:HB2	1.91	0.52
1:A:356:GLY:O	1:A:360:THR:HG23	2.08	0.52
1:B:153:PRO:CB	1:B:154:PRO:CD	2.88	0.52
1:B:142:HIS:HD2	1:B:357:SER:OG	1.93	0.52
1:A:323:HIS:HE1	5:A:570:HOH:O	1.94	0.51
1:A:106:ARG:HD2	1:A:111:GLU:OE1	2.11	0.51
1:B:213:HIS:CE1	1:B:232:LEU:HD11	2.47	0.50
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.47	0.50
1:B:88:TRP:C	1:B:89:ARG:HD2	2.33	0.50
1:B:162:ASP:O	1:B:163:ARG:HB2	2.12	0.50
1:A:363:ASP:O	1:A:367:THR:OG1	2.28	0.49
1:B:262:LEU:HB3	1:B:293:ARG:HD3	1.94	0.49
1:B:223:PRO:HD3	5:B:677:HOH:O	2.12	0.48
1:B:73:GLY:O	1:B:74:SER:CB	2.61	0.47
1:B:246:VAL:O	1:B:250:GLN:HG3	2.13	0.47
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.49	0.47
1:B:149:SER:O	1:B:152:ALA:N	2.31	0.47
1:B:89:ARG:HH11	1:B:89:ARG:CG	2.08	0.47
1:B:75:ARG:O	1:B:366:ARG:NH2	2.48	0.47
4:B:501:THM:H5'2	4:B:501:THM:H6	1.98	0.45
1:A:47:PRO:HB2	1:A:358:ILE:CD1	2.44	0.45
1:A:356:GLY:O	1:A:360:THR:CG2	2.65	0.44
1:B:248:TYR:HB2	1:B:282:PRO:HG2	1.98	0.44
1:A:140:ALA:N	1:A:141:PRO:HD2	2.32	0.44
1:B:169:LEU:HD23	1:B:190:PHE:HD1	1.81	0.44
1:B:354:THR:HB	1:B:355:PRO:HD2	2.00	0.43
1:A:338:ASP:O	1:A:342:GLN:HG2	2.19	0.43
1:B:327:LEU:HD23	1:B:329:TYR:CZ	2.53	0.43
1:B:237:ARG:O	1:B:241:LEU:HG	2.19	0.43
1:B:198:LEU:HB3	1:B:199:PRO:CD	2.50	0.42
1:B:149:SER:O	1:B:150:SER:C	2.58	0.42
1:B:358:ILE:HB	1:B:359:PRO:HD3	2.00	0.42
1:B:79:VAL:CG2	1:B:159:LEU:HD23	2.50	0.42
1:B:169:LEU:O	1:B:190:PHE:HB3	2.20	0.41
1:B:118:ALA:HA	1:B:181:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.96	0.41
1:A:292:PHE:C	1:A:294:ALA:H	2.24	0.41
1:A:323:HIS:HD2	5:A:575:HOH:O	2.04	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)
5:B:653:HOH:O	5:B:653:HOH:O[3_555]	1.59	0.61
5:A:615:HOH:O	5:A:615:HOH:O[4_566]	1.84	0.36
1:A:320:ARG:NH2	1:A:320:ARG:NH2[4_566]	1.92	0.28

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	291/343 (85%)	280 (96%)	10 (3%)	1 (0%)	41	41
1	B	314/343 (92%)	294 (94%)	14 (4%)	6 (2%)	8	3
All	All	605/686 (88%)	574 (95%)	24 (4%)	7 (1%)	13	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	SER
1	B	149	SER
1	B	301	ASN
1	A	95	GLU
1	B	150	SER
1	B	75	ARG
1	B	153	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/275 (85%)	218 (94%)	15 (6%)	17	14
1	B	245/275 (89%)	224 (91%)	21 (9%)	10	7
All	All	478/550 (87%)	442 (92%)	36 (8%)	13	10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	49	LEU
1	A	69	LEU
1	A	109	GLN
1	A	134	VAL
1	A	139	LEU
1	A	198	LEU
1	A	219	LYS
1	A	222	ARG
1	A	227	LEU
1	A	321	SER
1	A	360	THR
1	A	362	CYS
1	A	367	THR
1	A	371	GLU
1	B	46	MET
1	B	62	LYS
1	B	86	THR
1	B	89	ARG
1	B	134	VAL
1	B	139	LEU
1	B	146	GLU
1	B	170	LEU
1	B	185	GLN
1	B	211	ASP
1	B	217	LEU
1	B	219	LYS

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Mol	Chain	Res	Type
1	B	220	ARG
1	B	242	LEU
1	B	293	ARG
1	B	296	GLU
1	B	298	LEU
1	B	304	LEU
1	B	321	SER
1	B	340	LEU
1	B	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	105	HIS
1	A	323	HIS
1	B	58	HIS
1	B	99	ASN
1	B	142	HIS
1	B	185	GLN
1	B	306	ASN
1	B	323	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](#)

3 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$
4	THM	B	501	-	18,18,18	1.42	3 (16%)	26,26,26	2.45	11 (42%)
2	T5A	A	503	-	48,59,59	1.31	5 (10%)	59,93,93	1.90	12 (20%)
3	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.37	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
4	THM	B	501	-	-	2/6/18/18	0/2/2/2
2	T5A	A	503	-	-	5/40/72/72	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	T5A	O4B-C4B	5.35	1.33	1.23
4	B	501	THM	C4-N3	-2.82	1.33	1.38
4	B	501	THM	C6-C5	2.82	1.39	1.34
2	A	503	T5A	C6B-C5B	2.58	1.38	1.34
2	A	503	T5A	C5A-C4A	-2.40	1.34	1.40
4	B	501	THM	C6-N1	-2.37	1.34	1.38
2	A	503	T5A	C4B-C5B	2.28	1.48	1.44
2	A	503	T5A	C4B-N3B	-2.25	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	T5A	N3A-C2A-N1A	-5.59	119.93	128.68
2	A	503	T5A	C1F-N9A-C4A	-5.06	117.74	126.64
2	A	503	T5A	C4B-N3B-C2B	-4.82	121.11	127.35
4	B	501	THM	C4-N3-C2	-4.78	121.16	127.35
4	B	501	THM	N3-C2-N1	4.60	120.99	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	T5A	C5B-C4B-N3B	4.59	119.23	115.31
4	B	501	THM	C5'-C4'-C3'	-4.46	103.55	114.81
4	B	501	THM	C5-C4-N3	4.00	118.72	115.31
2	A	503	T5A	N3B-C2B-N1B	3.97	120.16	114.89
2	A	503	T5A	C5B-C6B-N1B	-3.93	119.29	123.34
4	B	501	THM	O3'-C3'-C2'	-3.46	98.51	110.90
2	A	503	T5A	PC-O3B-PB	-3.46	120.97	132.83
4	B	501	THM	C5-C6-N1	-3.41	119.83	123.34
2	A	503	T5A	O4B-C4B-C5B	-3.38	120.99	124.90
4	B	501	THM	O4-C4-C5	-3.30	121.07	124.90
4	B	501	THM	C2'-C3'-C4'	3.05	109.12	102.76
4	B	501	THM	O2-C2-N1	-2.73	119.15	122.79
4	B	501	THM	C2'-C1'-N1	2.52	119.57	113.77
2	A	503	T5A	PD-O3C-PC	-2.38	124.66	132.83
2	A	503	T5A	O2C-PC-O1C	2.31	123.64	112.24
2	A	503	T5A	C7B-C5B-C4B	2.22	121.21	118.77
2	A	503	T5A	O2B-C2B-N1B	-2.17	119.90	122.79
4	B	501	THM	O4'-C4'-C5'	-2.04	104.80	109.21

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	THM	O4'-C4'-C5'-O5'
4	B	501	THM	C3'-C4'-C5'-O5'
2	A	503	T5A	PD-O3D-PE-O5F
2	A	503	T5A	C4F-C5F-O5F-PE
2	A	503	T5A	PB-O3A-PA-O5E
2	A	503	T5A	PB-O3A-PA-O1A
2	A	503	T5A	PD-O3D-PE-O2E

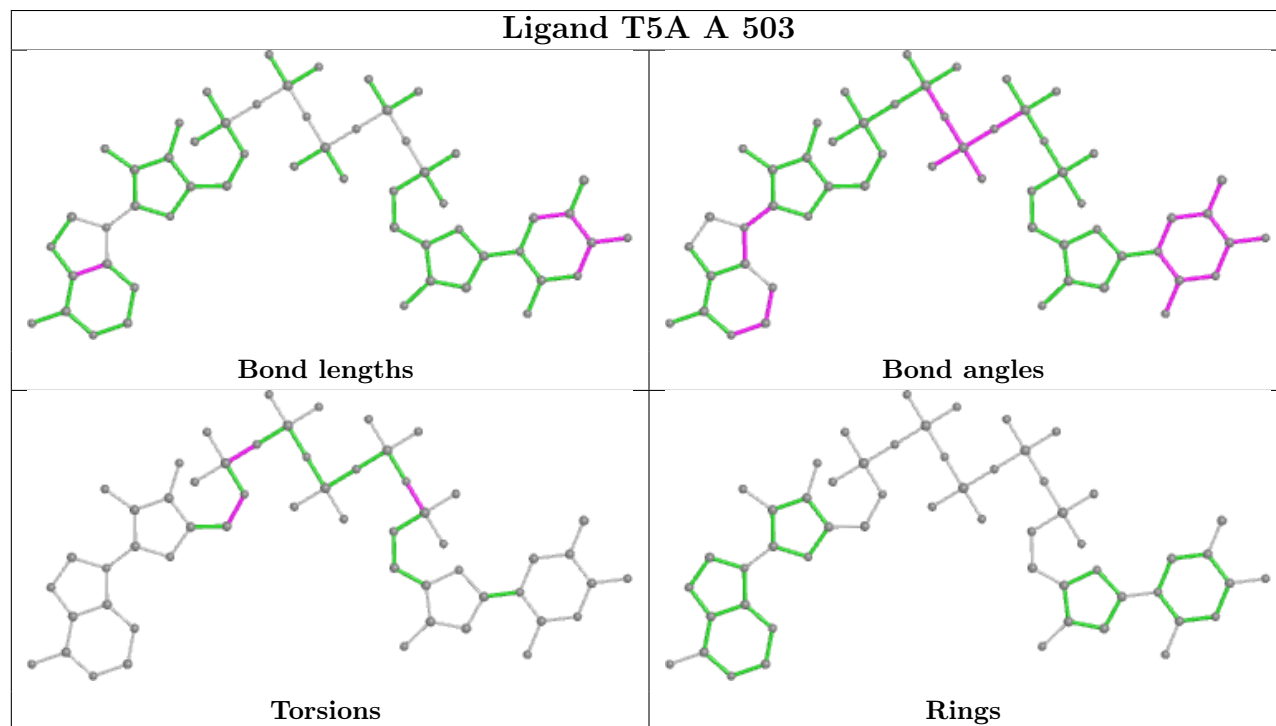
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	THM	1	0
2	A	503	T5A	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	301/343 (87%)	0.38	28 (9%) 8 11	14, 24, 52, 65	0
1	B	318/343 (92%)	0.49	31 (9%) 7 10	14, 24, 47, 55	0
All	All	619/686 (90%)	0.44	59 (9%) 8 10	14, 24, 50, 65	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	SER	8.5
1	B	148	GLY	7.2
1	B	300	PRO	6.4
1	A	72	LEU	6.0
1	B	263	SER	5.9
1	A	264	GLY	5.8
1	A	279	GLY	5.7
1	B	150	SER	5.5
1	A	148	GLY	5.4
1	A	94	SER	5.2
1	A	93	ALA	5.2
1	B	46	MET	4.8
1	B	264	GLY	4.7
1	B	299	ALA	4.3
1	B	151	HIS	4.2
1	B	74	SER	4.0
1	B	376	ASN	4.0
1	A	90	VAL	3.9
1	A	153	PRO	3.8
1	B	218	ALA	3.8
1	B	76	ASP	3.8
1	B	346	GLY	3.6
1	A	369	ALA	3.6
1	B	251	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	355	PRO	3.2
1	A	280	PRO	3.2
1	A	92	GLY	3.2
1	B	305	TYR	3.2
1	A	359	PRO	2.9
1	A	45	LYS	2.8
1	B	219	LYS	2.6
1	A	154	PRO	2.6
1	A	46	MET	2.6
1	A	223	PRO	2.6
1	A	147	ALA	2.5
1	B	152	ALA	2.5
1	B	167	ALA	2.5
1	B	375	ALA	2.5
1	B	169	LEU	2.4
1	A	83	GLU	2.4
1	A	91	LEU	2.4
1	A	355	PRO	2.4
1	B	153	PRO	2.4
1	A	70	VAL	2.3
1	A	363	ASP	2.3
1	A	193	LEU	2.3
1	B	302	GLY	2.3
1	A	221	GLN	2.3
1	A	110	GLY	2.3
1	A	47	PRO	2.2
1	B	301	ASN	2.2
1	B	345	SER	2.2
1	B	109	GLN	2.2
1	B	73	GLY	2.2
1	B	170	LEU	2.2
1	B	221	GLN	2.1
1	A	354	THR	2.1
1	A	77	ASP	2.1
1	B	227	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

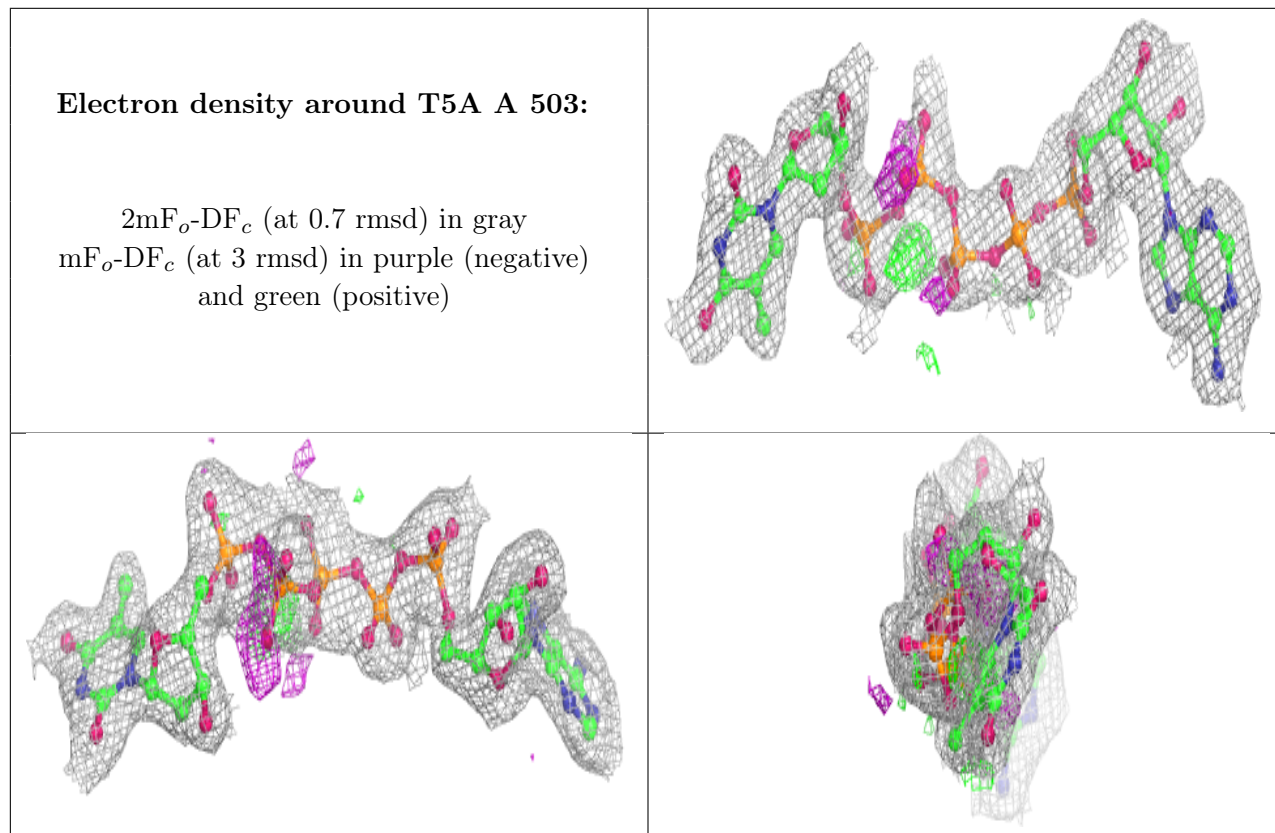
There are no monosaccharides in this entry.

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
2	T5A	A	503	55/55	0.92	0.12	16,30,46,49	0
4	THM	B	501	17/17	0.92	0.15	14,16,23,30	0
3	SO4	B	502	5/5	0.98	0.10	21,24,25,26	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.