



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 11:36 PM EDT

PDB ID : 2WWH  
Title : Plasmodium falciparum thymidylate kinase in complex with AP5dT  
Authors : Whittingham, J.L.; Carrero-Lerida, J.; Brannigan, J.A.; Ruiz-Perez, L.M.; Silva, A.P.G.; Fogg, M.J.; Wilkinson, A.J.; Gilbert, I.H.; Wilson, K.S.; Gonzalez-Pacanowska, D.  
Deposited on : 2009-10-23  
Resolution : 2.70 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

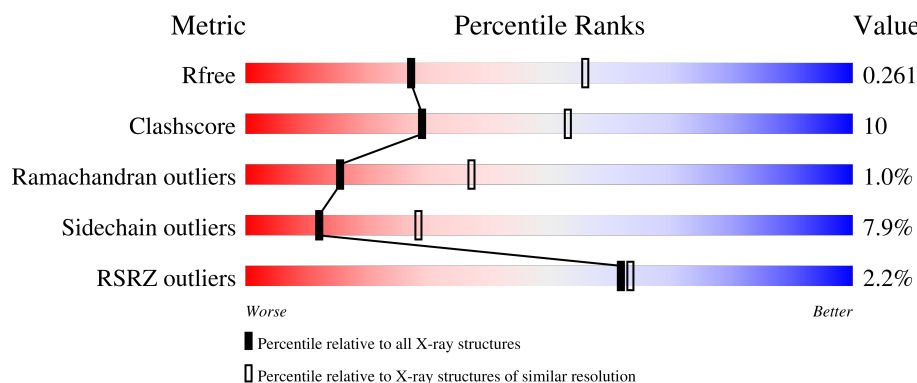
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	212	<div> <div>0%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	B	212	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	212	<div> <div>4%</div> <div>72%</div> <div>21%</div> <div>6%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

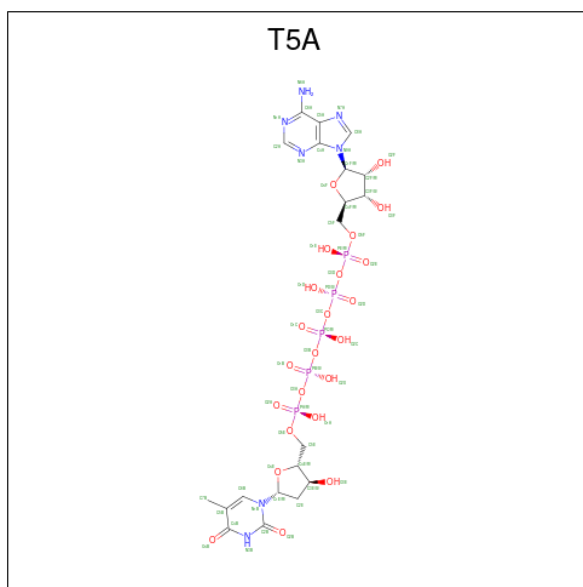
There are 4 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	31	1	0
			1759	1128	295	329	7			
1	B	210	Total	C	N	O	S	53	0	0
			1743	1119	289	328	7			
1	C	210	Total	C	N	O	S	60	1	0
			1749	1122	292	328	7			

- Molecule 2 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (three-letter code: T5A) (formula:  $C_{20}H_{30}N_7O_{23}P_5$ ).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Na 2	0	0
3	B	1	Total 1	Na 1	0	0
3	C	2	Total 2	Na 2	0	0

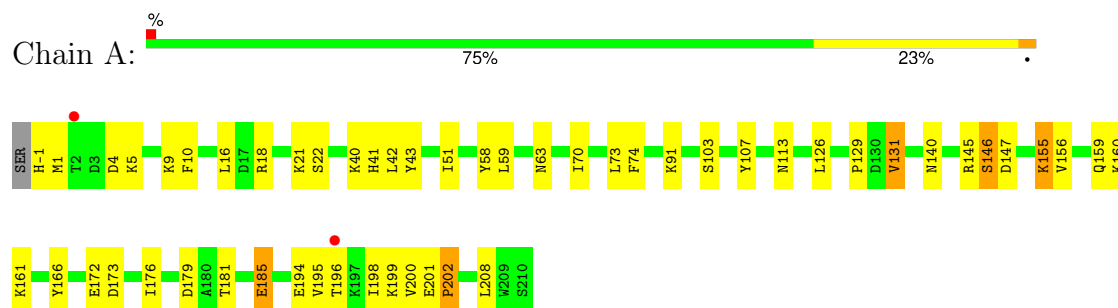
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	22	Total 22	O 22	0	0
4	C	15	Total 15	O 15	0	0

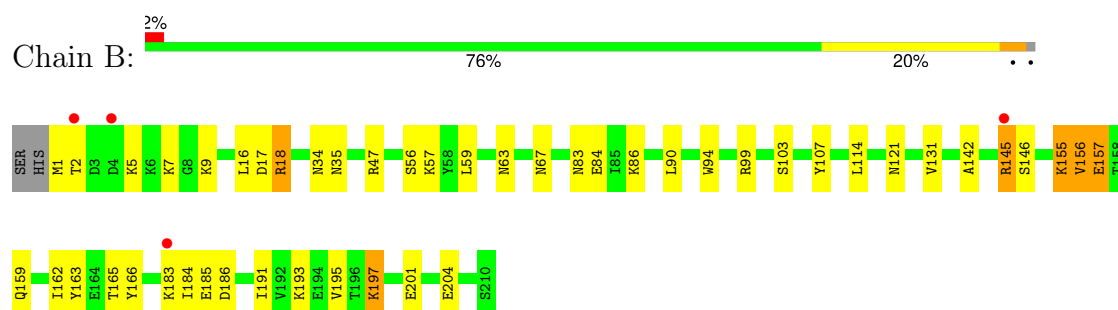
### 3 Residue-property plots [i](#)

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.

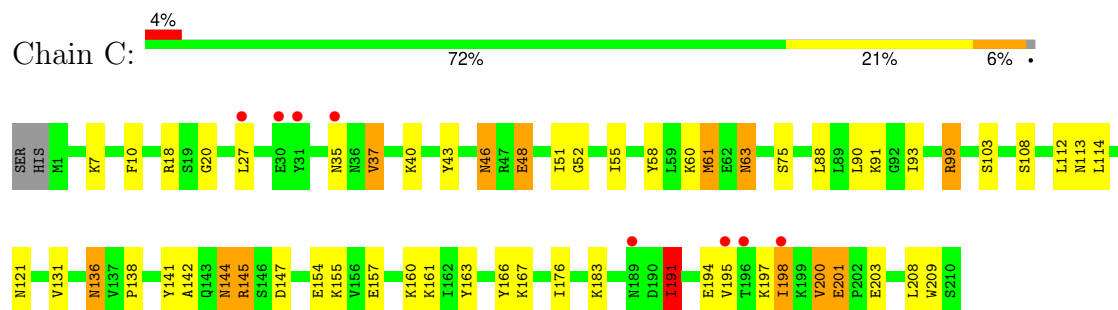
#### • Molecule 1: THYMIDILATE KINASE, PUTATIVE



#### • Molecule 1: THYMIDILATE KINASE, PUTATIVE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.54Å 109.54Å 119.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	94.92 – 2.70 37.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (94.92-2.70) 97.2 (37.13-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.270 0.186 , 0.261	Depositor DCC
$R_{free}$ test set	1163 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, T5A

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	0.91	3/1806 (0.2%)	0.84	4/2435 (0.2%)
1	B	0.83	6/1785 (0.3%)	0.76	3/2409 (0.1%)
1	C	0.91	8/1796 (0.4%)	0.89	6/2423 (0.2%)
All	All	0.88	17/5387 (0.3%)	0.83	13/7267 (0.2%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	GLU	CB-CG	-15.28	1.23	1.52
1	A	5	LYS	CD-CE	-14.55	1.14	1.51
1	C	157	GLU	CB-CG	-10.56	1.32	1.52
1	B	197	LYS	CG-CD	10.18	1.87	1.52
1	C	160	LYS	CG-CD	-10.13	1.18	1.52
1	B	201	GLU	CB-CG	9.66	1.70	1.52
1	C	37	VAL	CB-CG1	-9.50	1.32	1.52
1	B	185	GLU	CB-CG	-9.30	1.34	1.52
1	A	155	LYS	CG-CD	-9.27	1.21	1.52
1	B	193	LYS	CB-CG	-9.14	1.27	1.52
1	A	199	LYS	CA-CB	-7.79	1.36	1.53
1	C	183	LYS	CG-CD	6.88	1.75	1.52
1	B	157	GLU	CB-CG	-6.70	1.39	1.52
1	C	200	VAL	CA-CB	-6.28	1.41	1.54
1	B	155	LYS	CG-CD	6.04	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	LYS	CG-CD	-5.76	1.32	1.52
1	C	37	VAL	CB-CG2	-5.65	1.41	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	ILE	CG1-CB-CG2	-13.91	80.79	111.40
1	C	37	VAL	CG1-CB-CG2	9.20	125.61	110.90
1	C	183	LYS	CB-CG-CD	-7.83	91.24	111.60
1	A	199	LYS	CB-CA-C	6.87	124.15	110.40
1	B	197	LYS	CB-CG-CD	-6.87	93.74	111.60
1	B	201	GLU	CA-CB-CG	-6.51	99.07	113.40
1	B	155	LYS	CB-CG-CD	-6.42	94.91	111.60
1	C	161	LYS	CD-CE-NZ	-5.81	98.34	111.70
1	C	161	LYS	CG-CD-CE	-5.78	94.57	111.90
1	A	173	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	185	GLU	CB-CG-CD	5.49	129.02	114.20
1	C	160	LYS	CG-CD-CE	5.49	128.37	111.90
1	A	155	LYS	CB-CG-CD	5.48	125.86	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASP	Sidechain

## 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	1759	0	1733	32	0
1	B	1743	0	1715	25	0
1	C	1749	0	1724	42	0
2	A	55	0	25	5	0
2	B	55	0	25	4	0
2	C	55	0	25	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	63	0	0	2	0
4	B	22	0	0	1	0
4	C	15	0	0	1	0
All	All	5521	0	5247	99	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 10.

All (99) 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:C:18[B]:ARG:HH11	1:C:18[B]:ARG:HG2	0.88	1.05
1:C:18[B]:ARG:HG2	1:C:18[B]:ARG:NH1	1.69	0.96
1:C:18[B]:ARG:HH11	1:C:18[B]:ARG:CG	1.80	0.94
1:A:200:VAL:HG12	1:A:200:VAL:O	1.69	0.93
1:B:18:ARG:HB3	1:B:145:ARG:HG3	1.55	0.89
1:A:18[A]:ARG:NH2	1:A:147:ASP:HB2	1.88	0.88
1:C:63:ASN:C	1:C:63:ASN:HD22	1.82	0.83
1:B:17:ASP:H	1:B:159:GLN:HE22	1.23	0.82
1:B:18:ARG:HB3	1:B:145:ARG:CG	2.11	0.81
1:A:-1:HIS:C	1:A:1:MET:H1	1.90	0.75
1:C:58:TYR:HA	1:C:63:ASN:ND2	2.03	0.73
1:A:18[B]:ARG:HH22	1:A:146:SER:HB2	1.55	0.72
1:C:144:ASN:ND2	1:C:144:ASN:H	1.89	0.70
1:A:-1:HIS:C	1:A:1:MET:N	2.45	0.69
1:C:58:TYR:HA	1:C:63:ASN:HD21	1.58	0.69
1:A:-1:HIS:O	1:A:1:MET:N	2.22	0.68
1:C:46:ASN:HD22	1:C:46:ASN:C	1.97	0.68
1:A:-1:HIS:CA	1:A:1:MET:N	2.59	0.66
1:C:138:PRO:HG2	1:C:141:TYR:HB2	1.79	0.63
1:A:18[A]:ARG:HH22	1:A:147:ASP:HB2	1.63	0.61
1:B:99:ARG:HD3	1:B:103:SER:OG	2.01	0.60
1:B:18:ARG:HG2	1:B:145:ARG:HB3	1.84	0.60
1:B:107:TYR:CE1	2:B:211:T5A:HB22	2.36	0.60
1:B:121:ASN:HB3	1:C:121:ASN:HD22	1.68	0.59
1:A:200:VAL:O	1:A:200:VAL:CG1	2.40	0.57
1:C:176:ILE:HD13	1:C:194:GLU:HG2	1.85	0.57
1:B:16:LEU:HD11	1:B:163:TYR:HB2	1.86	0.57
1:C:63:ASN:C	1:C:63:ASN:ND2	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HB2	1:A:208:LEU:HD12	1.88	0.56
1:C:144:ASN:H	1:C:144:ASN:HD22	1.52	0.56
1:C:46:ASN:C	1:C:46:ASN:ND2	2.58	0.56
1:A:172:GLU:OE1	4:A:2052:HOH:O	2.18	0.55
1:A:107:TYR:CE1	2:A:211:T5A:HB22	2.41	0.54
1:C:51:ILE:HG13	4:C:2004:HOH:O	2.09	0.53
1:A:176:ILE:HD13	1:A:194:GLU:HG2	1.90	0.52
1:B:67:ASN:HB3	1:B:114:LEU:HD11	1.92	0.52
1:B:59:LEU:HD13	2:B:211:T5A:HB52	1.91	0.52
1:A:131:VAL:HG23	1:A:176:ILE:HD12	1.92	0.52
1:C:46:ASN:HD21	1:C:48:GLU:HB2	1.74	0.52
1:C:43:TYR:CD1	1:C:43:TYR:N	2.76	0.52
1:C:112:LEU:O	1:C:113:ASN:HB2	2.10	0.51
1:A:16:LEU:HB3	1:A:159:GLN:NE2	2.26	0.51
1:A:201:GLU:O	1:A:202:PRO:O	2.29	0.51
1:C:142:ALA:O	1:C:145:ARG:HG2	2.11	0.51
1:C:131:VAL:HG23	1:C:176:ILE:HD12	1.93	0.51
1:C:60:LYS:O	1:C:61:MET:HB2	2.10	0.50
1:C:191:ILE:O	1:C:195:VAL:HG23	2.11	0.50
1:A:21:LYS:NZ	2:A:211:T5A:O2X	2.42	0.50
1:C:18[B]:ARG:NH1	1:C:18[B]:ARG:CG	2.52	0.49
1:A:201:GLU:O	1:A:202:PRO:C	2.51	0.49
1:C:99:ARG:HG2	1:C:103:SER:OG	2.13	0.49
1:A:41:HIS:O	1:A:42:LEU:HD23	2.14	0.48
1:C:195:VAL:O	1:C:198:ILE:HG13	2.14	0.48
1:C:58:TYR:CA	1:C:63:ASN:HD21	2.23	0.48
1:B:145:ARG:HD2	1:B:145:ARG:HA	1.57	0.47
1:A:18[B]:ARG:HH22	1:A:146:SER:CB	2.25	0.47
1:A:59:LEU:HD13	2:A:211:T5A:HB51	1.96	0.47
1:A:156:VAL:O	1:A:160:LYS:HG3	2.15	0.47
1:A:10:PHE:HB3	1:A:129:PRO:HA	1.97	0.47
1:C:7:LYS:HG3	1:C:90:LEU:O	2.15	0.47
1:A:51:ILE:HG23	1:A:73:LEU:HD22	1.97	0.47
1:B:63:ASN:OD1	1:B:63:ASN:C	2.54	0.46
1:C:144:ASN:ND2	1:C:144:ASN:N	2.60	0.46
1:C:163:TYR:CE2	1:C:167:LYS:HE3	2.50	0.46
1:A:195:VAL:O	1:A:198:ILE:HG13	2.16	0.46
1:C:18[A]:ARG:NH2	1:C:147:ASP:HB2	2.31	0.46
1:C:144:ASN:HD22	1:C:144:ASN:N	2.14	0.46
1:A:63:ASN:OD1	1:A:63:ASN:C	2.54	0.45
1:B:142:ALA:O	1:B:145:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:HD22	1:B:83:ASN:H	1.65	0.45
1:A:58:TYR:CE2	1:A:70:ILE:HG12	2.51	0.45
1:A:179:ASP:OD1	1:A:181:THR:OG1	2.35	0.45
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.79	0.44
2:B:211:T5A:HB51	4:B:2001:HOH:O	2.17	0.44
1:C:46:ASN:ND2	1:C:48:GLU:H	2.16	0.44
1:C:208:LEU:HA	1:C:209:TRP:HA	1.64	0.44
1:C:91:LYS:HB2	1:C:93:ILE:HD12	2.01	0.43
1:C:52:GLY:HA2	1:C:55:ILE:HD12	2.00	0.43
1:B:107:TYR:CE1	1:B:162:ILE:HD13	2.53	0.43
1:C:108:SER:HB3	1:C:114:LEU:HD12	2.00	0.43
1:C:18[B]:ARG:HD3	1:C:145:ARG:HB2	2.01	0.43
1:B:5:LYS:O	1:B:7:LYS:HG3	2.19	0.42
1:B:34:ASN:C	1:B:35:ASN:HD22	2.23	0.42
1:B:9:LYS:HB2	1:B:94:TRP:CD2	2.53	0.42
1:B:156:VAL:HG12	1:B:157:GLU:N	2.34	0.42
1:A:91:LYS:HE3	4:A:2035:HOH:O	2.19	0.42
1:B:47:ARG:HD3	1:B:56:SER:HB2	2.02	0.42
1:B:191:ILE:O	1:B:195:VAL:HG23	2.20	0.42
1:C:40:LYS:HD3	1:C:88:LEU:HD11	2.01	0.42
1:A:43:TYR:CD1	1:A:43:TYR:N	2.88	0.41
1:B:183:LYS:HB2	1:B:186:ASP:OD2	2.20	0.41
1:B:107:TYR:CD1	2:B:211:T5A:HB22	2.55	0.41
1:C:131:VAL:CG2	1:C:176:ILE:HD12	2.50	0.41
1:C:136:ASN:C	1:C:136:ASN:HD22	2.24	0.41
1:C:20:GLY:HA2	2:C:211:T5A:O2E	2.21	0.41
1:B:34:ASN:C	1:B:35:ASN:ND2	2.74	0.41
1:A:74:PHE:CD1	2:A:211:T5A:C4B	3.04	0.40
1:C:18[B]:ARG:NH1	2:C:211:T5A:O1C	2.55	0.40
1:A:107:TYR:CD1	2:A:211:T5A:HB22	2.55	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	209/212 (99%)	197 (94%)	10 (5%)	2 (1%)	15	37
1	B	208/212 (98%)	197 (95%)	10 (5%)	1 (0%)	29	54
1	C	209/212 (99%)	194 (93%)	12 (6%)	3 (1%)	11	28
All	All	626/636 (98%)	588 (94%)	32 (5%)	6 (1%)	15	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	202	PRO
1	C	35	ASN
1	C	99	ARG
1	C	154	GLU
1	B	184	ILE

### 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	195/195 (100%)	182 (93%)	13 (7%)	16	37
1	B	193/195 (99%)	178 (92%)	15 (8%)	12	29
1	C	194/195 (100%)	176 (91%)	18 (9%)	9	21
All	All	582/585 (100%)	536 (92%)	46 (8%)	12	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	22	SER
1	A	40	LYS
1	A	103	SER

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Mol	Chain	Res	Type
1	A	113	ASN
1	A	131	VAL
1	A	140	ASN
1	A	145	ARG
1	A	155	LYS
1	A	161	LYS
1	A	166	TYR
1	A	185	GLU
1	A	196	THR
1	B	1	MET
1	B	2	THR
1	B	18	ARG
1	B	57	LYS
1	B	84	GLU
1	B	86	LYS
1	B	131	VAL
1	B	145	ARG
1	B	146	SER
1	B	155	LYS
1	B	156	VAL
1	B	165	THR
1	B	166	TYR
1	B	197	LYS
1	B	204	GLU
1	C	10	PHE
1	C	27	LEU
1	C	37	VAL
1	C	46	ASN
1	C	48	GLU
1	C	61	MET
1	C	63	ASN
1	C	75	SER
1	C	136	ASN
1	C	144	ASN
1	C	145	ARG
1	C	166	TYR
1	C	191	ILE
1	C	197	LYS
1	C	198	ILE
1	C	200	VAL
1	C	201	GLU
1	C	203	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	34	ASN
1	A	67	ASN
1	A	159	GLN
1	B	35	ASN
1	B	41	HIS
1	B	67	ASN
1	B	83	ASN
1	B	159	GLN
1	C	34	ASN
1	C	41	HIS
1	C	46	ASN
1	C	63	ASN
1	C	67	ASN
1	C	121	ASN
1	C	136	ASN
1	C	144	ASN
1	C	177	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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
2	T5A	B	211	3	55,59,59	1.49	9 (16%)	70,93,93	1.99	13 (18%)
2	T5A	C	211	3	55,59,59	1.83	12 (21%)	70,93,93	2.03	16 (22%)
2	T5A	A	211	3	55,59,59	1.49	8 (14%)	70,93,93	2.14	17 (24%)

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	T5A	B	211	3	-	4/40/72/72	0/5/5/5
2	T5A	C	211	3	-	9/40/72/72	0/5/5/5
2	T5A	A	211	3	-	8/40/72/72	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	211	T5A	PD-O3C	6.83	1.66	1.59
2	C	211	T5A	PC-O3C	5.97	1.65	1.59
2	A	211	T5A	PB-O3A	4.74	1.64	1.59
2	B	211	T5A	PC-O3C	4.48	1.64	1.59
2	A	211	T5A	PA-O3A	4.16	1.64	1.59
2	B	211	T5A	PD-O3C	4.08	1.63	1.59
2	A	211	T5A	PC-O3C	3.90	1.63	1.59
2	B	211	T5A	PA-O3A	3.68	1.63	1.59
2	C	211	T5A	PB-O3A	3.49	1.63	1.59
2	B	211	T5A	C4B-N3B	-3.23	1.32	1.38
2	C	211	T5A	PE-O3D	3.18	1.62	1.59
2	B	211	T5A	PE-O3D	3.03	1.62	1.59
2	C	211	T5A	O4F-C1F	3.02	1.44	1.40
2	A	211	T5A	PE-O3D	2.81	1.62	1.59
2	C	211	T5A	C6B-C5B	2.74	1.39	1.34
2	C	211	T5A	C4B-C5B	2.72	1.49	1.44
2	B	211	T5A	C6B-C5B	2.70	1.39	1.34
2	C	211	T5A	PA-O3A	2.66	1.62	1.59
2	C	211	T5A	C2B-N1B	2.59	1.42	1.38
2	C	211	T5A	C4B-N3B	-2.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	T5A	C2B-N3B	-2.38	1.33	1.38
2	A	211	T5A	C6B-C5B	2.31	1.38	1.34
2	B	211	T5A	C2B-N1B	2.30	1.42	1.38
2	C	211	T5A	C6B-N1B	-2.27	1.34	1.38
2	A	211	T5A	C4B-N3B	-2.19	1.34	1.38
2	A	211	T5A	C6B-N1B	-2.14	1.34	1.38
2	C	211	T5A	C2A-N3A	2.10	1.35	1.32
2	A	211	T5A	C4B-C5B	2.03	1.48	1.44
2	B	211	T5A	PD-O3D	2.01	1.61	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	211	T5A	N3A-C2A-N1A	-6.77	119.48	128.67
2	B	211	T5A	C5B-C4B-N3B	6.30	120.80	115.32
2	A	211	T5A	C4B-N3B-C2B	-6.02	119.45	127.34
2	A	211	T5A	N3B-C2B-N1B	5.91	122.58	114.89
2	B	211	T5A	N3B-C2B-N1B	5.87	122.53	114.89
2	C	211	T5A	C4B-N3B-C2B	-5.84	119.68	127.34
2	B	211	T5A	C4B-N3B-C2B	-5.84	119.69	127.34
2	A	211	T5A	O2B-C2B-N1B	-5.79	115.25	122.80
2	C	211	T5A	N3A-C2A-N1A	-5.36	121.39	128.67
2	C	211	T5A	N3B-C2B-N1B	5.28	121.77	114.89
2	B	211	T5A	N3A-C2A-N1A	-5.19	121.63	128.67
2	B	211	T5A	O4B-C4B-C5B	-5.12	119.06	124.92
2	C	211	T5A	C5B-C4B-N3B	4.82	119.52	115.32
2	A	211	T5A	O4B-C4B-C5B	-4.74	119.49	124.92
2	A	211	T5A	C5B-C4B-N3B	4.70	119.41	115.32
2	C	211	T5A	C7B-C5B-C4B	4.00	123.06	118.78
2	C	211	T5A	O1D-PD-O3C	3.92	117.88	107.27
2	C	211	T5A	O2B-C2B-N1B	-3.68	118.01	122.80
2	C	211	T5A	C5B-C6B-N1B	-3.62	119.39	123.31
2	C	211	T5A	O4B-C4B-C5B	-3.58	120.82	124.92
2	B	211	T5A	O4E-C1E-C2E	-3.57	99.58	106.25
2	A	211	T5A	O3B-PB-O1B	-3.51	100.13	110.70
2	C	211	T5A	C7B-C5B-C6B	-3.50	118.12	122.85
2	A	211	T5A	O2X-PB-O3A	3.28	116.14	107.27
2	C	211	T5A	O4F-C1F-N9A	-3.21	104.48	108.75
2	B	211	T5A	C5B-C6B-N1B	-3.11	119.93	123.31
2	C	211	T5A	C4F-O4F-C1F	3.04	112.71	109.92
2	C	211	T5A	O2X-PB-O3A	2.99	115.35	107.27
2	A	211	T5A	O1E-PE-O3D	2.88	115.05	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	211	T5A	C5B-C6B-N1B	-2.87	120.19	123.31
2	C	211	T5A	O2C-PC-O3C	2.81	114.88	107.27
2	B	211	T5A	C1E-N1B-C2B	2.53	122.61	117.66
2	A	211	T5A	O1D-PD-O3C	2.46	113.92	107.27
2	B	211	T5A	C4F-O4F-C1F	2.45	112.17	109.92
2	C	211	T5A	O1A-PA-O2A	2.34	123.33	112.44
2	B	211	T5A	O2B-C2B-N3B	-2.31	117.22	121.49
2	C	211	T5A	O1A-PA-O3A	-2.31	101.03	107.27
2	A	211	T5A	C1F-N9A-C4A	-2.28	122.64	126.64
2	B	211	T5A	C7B-C5B-C4B	2.22	121.15	118.78
2	A	211	T5A	C2E-C3E-C4E	2.18	107.22	102.80
2	B	211	T5A	O3B-PB-O1B	-2.17	104.18	110.70
2	A	211	T5A	C7B-C5B-C4B	2.10	121.02	118.78
2	A	211	T5A	O4E-C1E-N1B	-2.07	104.19	107.86
2	A	211	T5A	O3D-PE-O2E	-2.07	104.48	110.70
2	A	211	T5A	O2C-PC-O3C	2.05	112.81	107.27
2	B	211	T5A	C6B-N1B-C2B	-2.05	119.27	121.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	211	T5A	C5E-O5E-PA-O1A
2	C	211	T5A	C5E-O5E-PA-O3A
2	C	211	T5A	C5F-O5F-PE-O1E
2	A	211	T5A	O4E-C4E-C5E-O5E
2	A	211	T5A	C3E-C4E-C5E-O5E
2	A	211	T5A	PB-O3A-PA-O5E
2	A	211	T5A	PB-O3B-PC-O2C
2	B	211	T5A	PE-O3D-PD-O2D
2	C	211	T5A	PB-O3A-PA-O2A
2	A	211	T5A	C5E-O5E-PA-O2A
2	C	211	T5A	C5F-O5F-PE-O3D
2	C	211	T5A	C5F-O5F-PE-O2E
2	A	211	T5A	PD-O3C-PC-O1C
2	C	211	T5A	PB-O3A-PA-O1A
2	A	211	T5A	PD-O3C-PC-O2C
2	C	211	T5A	PD-O3C-PC-O1C
2	A	211	T5A	PB-O3B-PC-O1C
2	B	211	T5A	PC-O3B-PB-O1B
2	B	211	T5A	PC-O3C-PD-O1D
2	B	211	T5A	PE-O3D-PD-O1D

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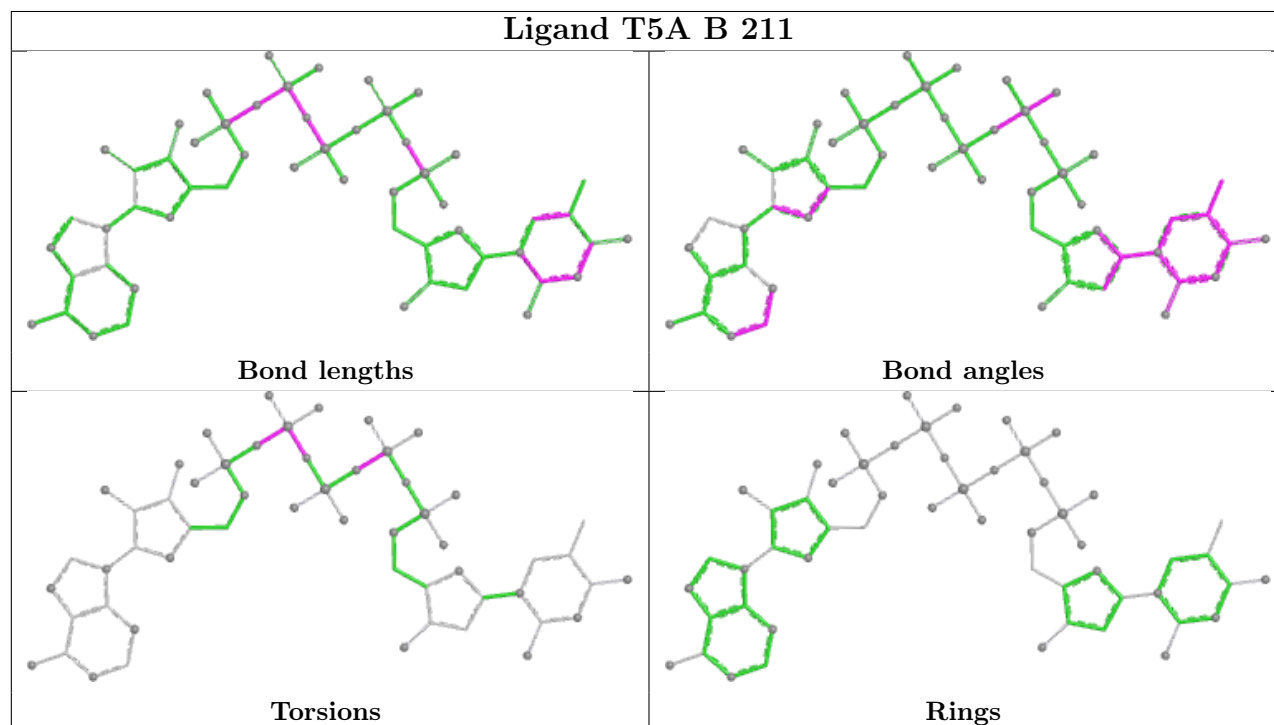
Mol	Chain	Res	Type	Atoms
2	C	211	T5A	PB-O3B-PC-O2C

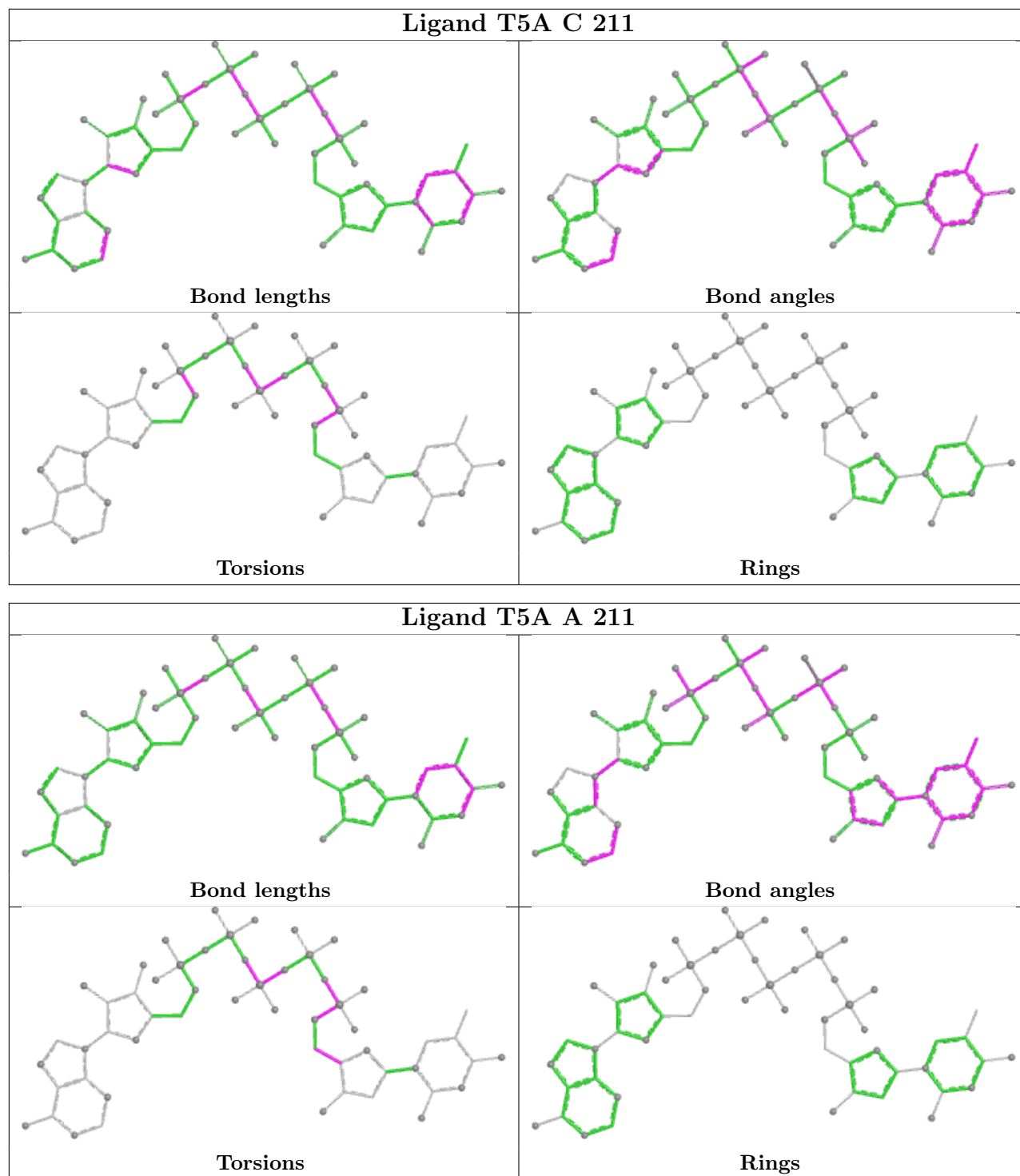
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	211	T5A	4	0
2	C	211	T5A	2	0
2	A	211	T5A	5	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	-1:HIS	C	1:MET	N	2.45

## 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	211/212 (99%)	-0.41	2 (0%) 84 85	12, 27, 48, 87	11 (5%)
1	B	210/212 (99%)	-0.23	4 (1%) 66 69	25, 40, 62, 71	15 (7%)
1	C	210/212 (99%)	-0.09	8 (3%) 40 39	28, 43, 63, 68	23 (10%)
All	All	631/636 (99%)	-0.24	14 (2%) 62 63	12, 38, 61, 87	49 (7%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	TYR	3.3
1	B	2	THR	3.0
1	C	198	ILE	3.0
1	B	145	ARG	2.9
1	C	189	ASN	2.6
1	C	196	THR	2.5
1	C	195	VAL	2.3
1	C	30	GLU	2.1
1	C	27	LEU	2.1
1	A	2	THR	2.1
1	B	4	ASP	2.1
1	C	35	ASN	2.0
1	A	196	THR	2.0
1	B	183	LYS	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](#)

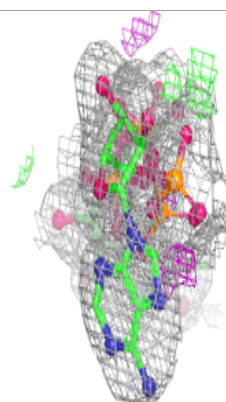
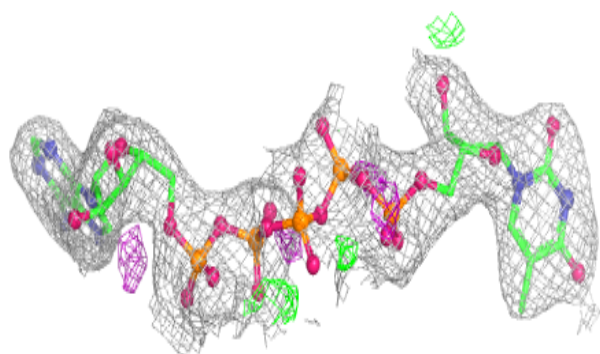
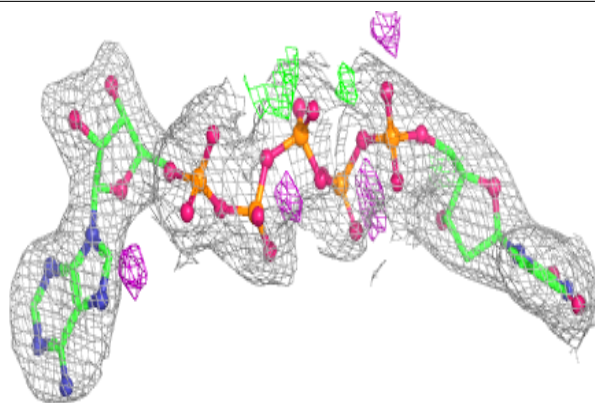
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	NA	B	212	1/1	0.71	0.20	51,51,51,51	0
3	NA	C	212	1/1	0.92	0.08	38,38,38,38	0
3	NA	A	212	1/1	0.93	0.12	43,43,43,43	0
3	NA	C	213	1/1	0.94	0.06	49,49,49,49	0
2	T5A	C	211	55/55	0.95	0.12	31,40,50,50	0
3	NA	A	213	1/1	0.96	0.10	23,23,23,23	0
2	T5A	B	211	55/55	0.97	0.12	24,40,48,49	0
2	T5A	A	211	55/55	0.98	0.12	17,28,34,37	0

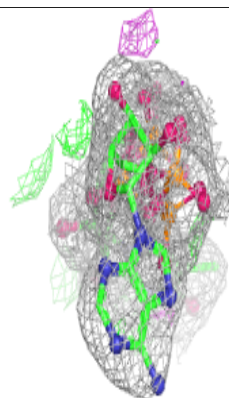
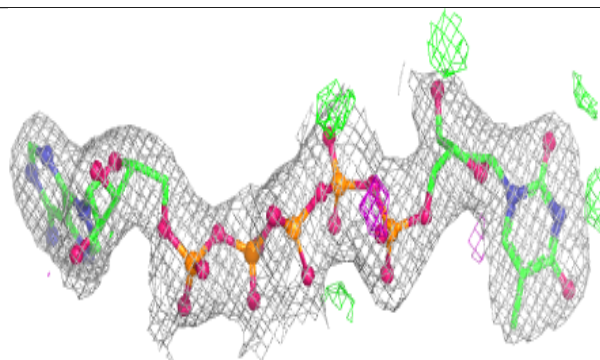
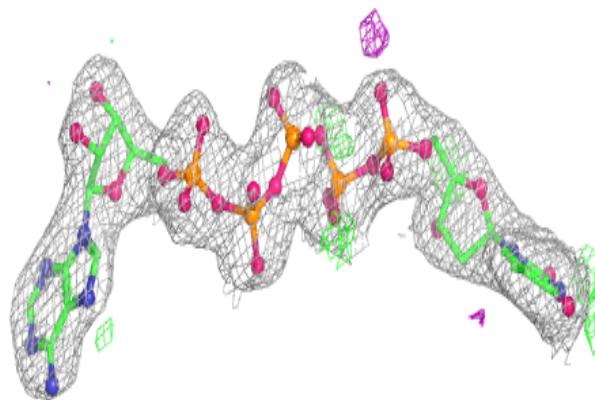
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

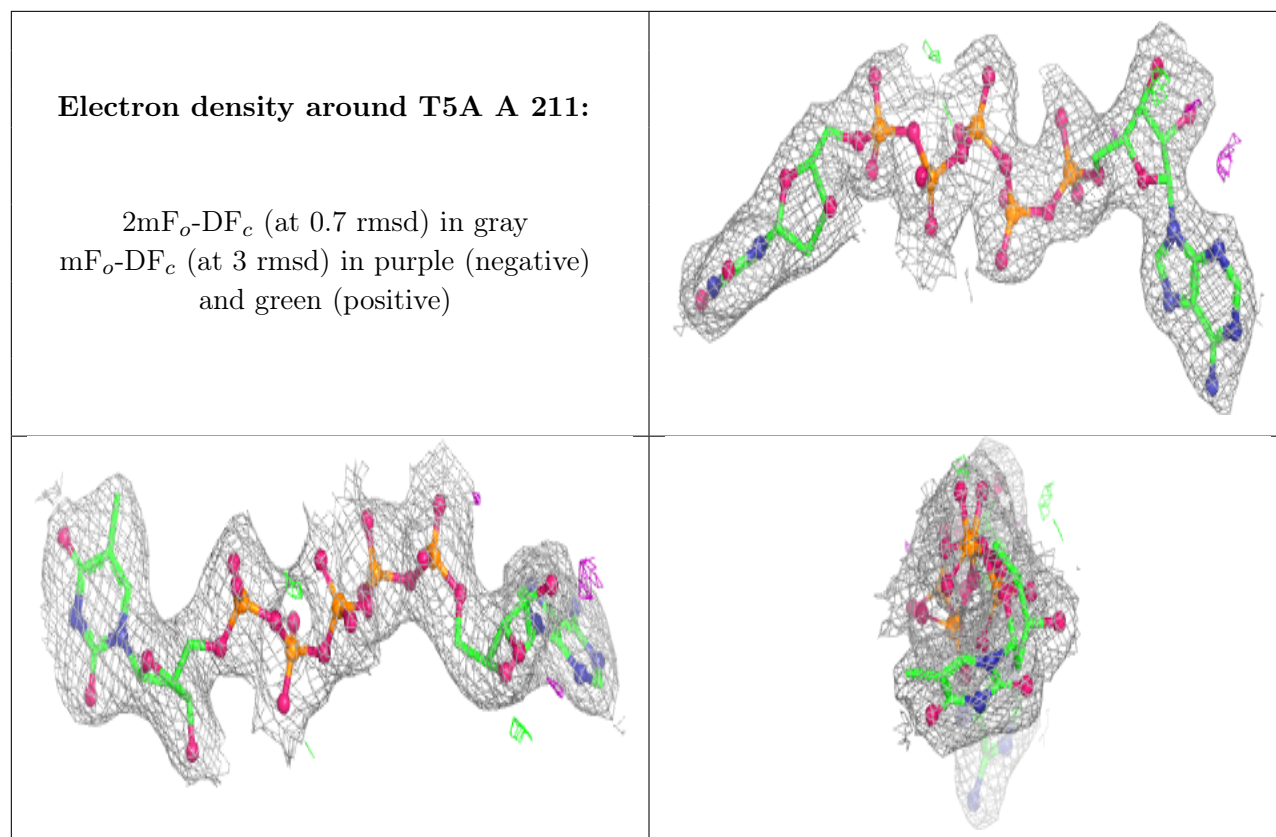
**Electron density around T5A C 211:**

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

**Electron density around T5A B 211:**

$2mF_o-DF_c$  (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.