



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:06 AM UTC

PDB ID : 2WWF / pdb_00002wwf
Title : Plasmodium falciparum thymidylate kinase in complex with TMP and ADP
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 : 1.89 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

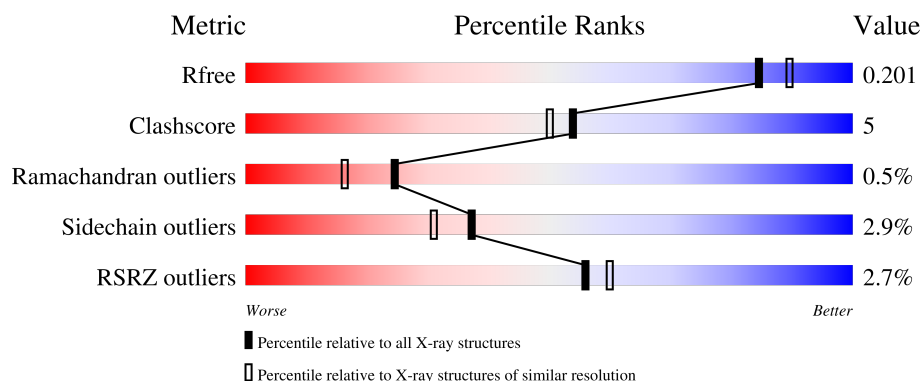
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	212	5% 84% 12% .
1	B	212	5% 83% 13% ..
1	C	212	3% 88% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5987 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.

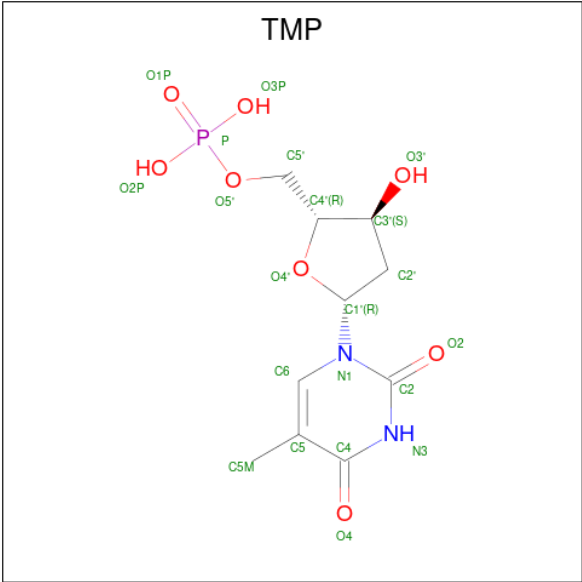
- Molecule 1 is a protein called THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	12	2	0
			1769	1133	295	334	7			
1	B	208	Total	C	N	O	S	27	4	0
			1750	1124	288	332	6			
1	C	212	Total	C	N	O	S	36	2	0
			1774	1135	296	336	7			

There are 6 discrepancies between the modelled and reference sequences:

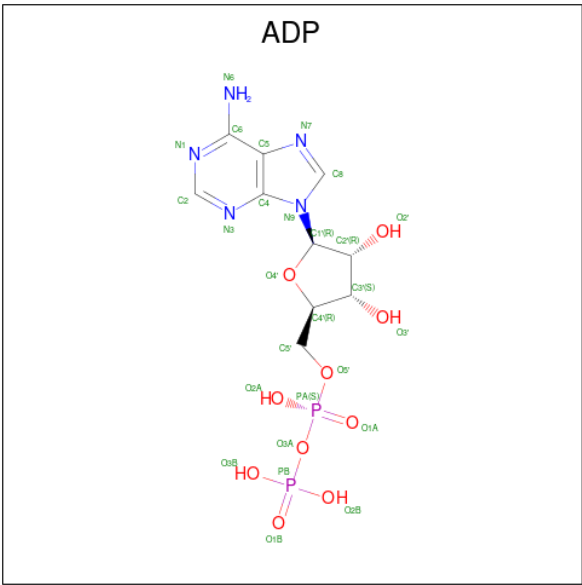
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8I4S1
A	-1	HIS	-	expression tag	UNP Q8I4S1
B	-2	SER	-	expression tag	UNP Q8I4S1
B	-1	HIS	-	expression tag	UNP Q8I4S1
C	-2	SER	-	expression tag	UNP Q8I4S1
C	-1	HIS	-	expression tag	UNP Q8I4S1

- Molecule 2 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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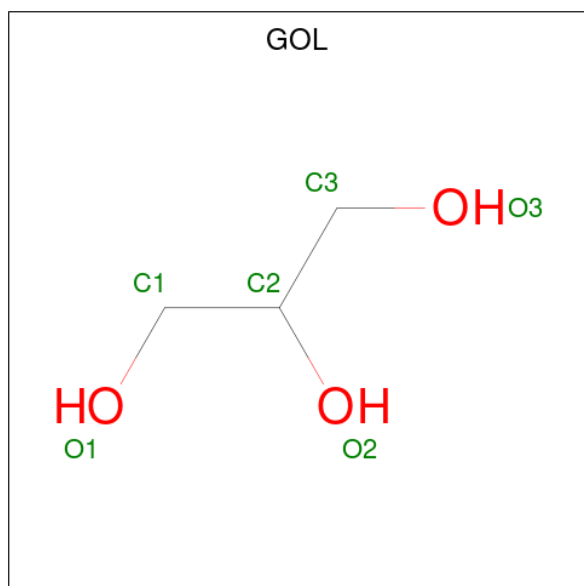
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

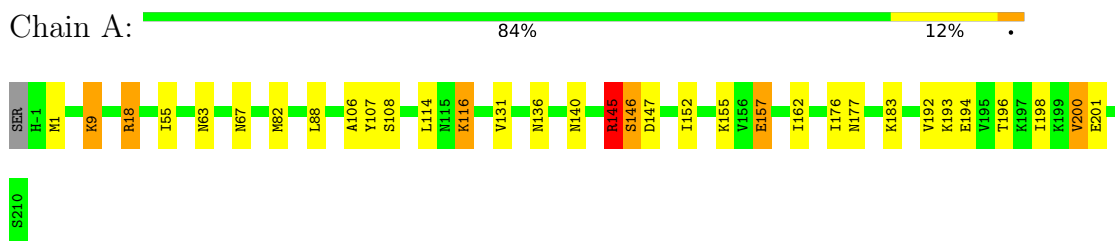
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total	O	0	0
			199	199		
6	B	145	Total	O	0	0
			145	145		
6	C	145	Total	O	0	0
			145	145		

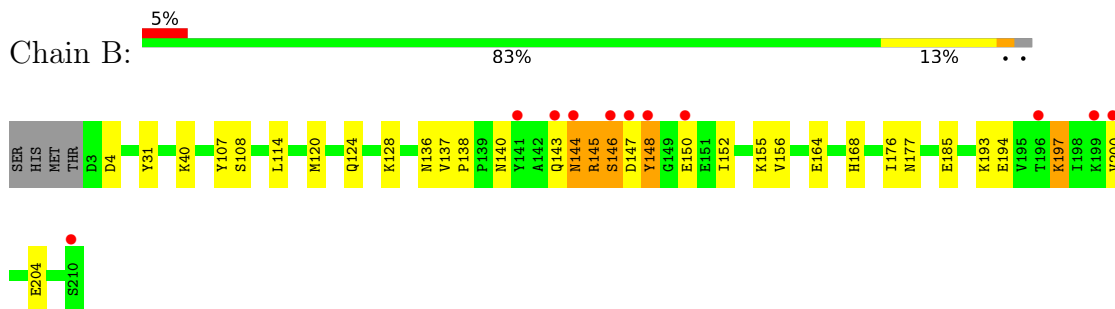
3 Residue-property plots [i](#)

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.

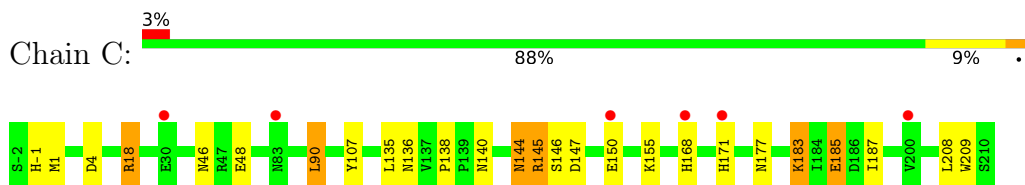
- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.13Å 110.13Å 120.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 1.89 95.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (95.35-1.89) 84.5 (95.35-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.203 0.160 , 0.201	Depositor DCC
R_{free} test set	2902 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5987	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.37	5/1812 (0.3%)	1.16	8/2446 (0.3%)
1	B	1.29	6/1804 (0.3%)	1.15	10/2435 (0.4%)
1	C	1.36	4/1816 (0.2%)	1.22	11/2448 (0.4%)
All	All	1.34	15/5432 (0.3%)	1.18	29/7329 (0.4%)

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	C	1	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	HIS	CB-CG	-10.24	1.35	1.50
1	C	171	HIS	CA-CB	-10.18	1.38	1.54
1	B	138	PRO	CA-C	7.14	1.55	1.51
1	B	197	LYS	CD-CE	-6.95	1.31	1.52
1	A	193	LYS	CB-CG	-6.93	1.31	1.52
1	A	106	ALA	CA-CB	6.79	1.64	1.53
1	A	55	ILE	CA-CB	6.33	1.61	1.54
1	C	155	LYS	CG-CD	-6.31	1.33	1.52
1	A	155	LYS	CG-CD	-6.08	1.34	1.52
1	B	185	GLU	CB-CG	-5.92	1.34	1.52
1	B	128	LYS	CE-NZ	5.86	1.67	1.49
1	A	88	LEU	C-O	5.48	1.30	1.24
1	C	187	ILE	CA-C	5.33	1.59	1.52
1	B	155	LYS	CG-CD	-5.03	1.37	1.52
1	B	193	LYS	CB-CG	-5.01	1.37	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH2	9.70	127.93	119.20
1	C	171	HIS	N-CA-CB	9.54	124.67	110.65
1	A	145	ARG	NE-CZ-NH1	-7.82	113.68	121.50
1	C	145	ARG	NE-CZ-NH2	7.68	126.11	119.20
1	C	18	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	C	18	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	A	146	SER	CA-CB-OG	-7.00	97.11	111.10
1	C	145	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	B	145	ARG	N-CA-C	6.48	119.87	110.28
1	B	150	GLU	N-CA-C	6.41	118.81	111.11
1	C	183	LYS	CB-CG-CD	-6.31	96.79	111.30
1	C	138	PRO	O-C-N	6.22	124.17	121.31
1	C	171	HIS	CB-CA-C	6.15	119.88	109.55
1	B	156	VAL	N-CA-C	6.10	117.57	110.62
1	A	145	ARG	CD-NE-CZ	6.09	132.93	124.40
1	C	18	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	146	SER	CB-CA-C	-5.91	109.77	116.63
1	B	31	TYR	N-CA-C	5.67	117.14	111.07
1	C	-1	HIS	CB-CA-C	-5.62	110.11	116.63
1	A	201	GLU	N-CA-C	5.55	117.75	110.08
1	B	155	LYS	CB-CG-CD	-5.55	98.53	111.30
1	B	144	ASN	N-CA-C	5.47	117.24	111.28
1	A	82	MET	N-CA-C	5.42	117.19	111.28
1	C	18	ARG	CB-CG-CD	5.39	123.69	111.30
1	A	152	ILE	N-CA-C	5.32	116.05	110.62
1	A	200	VAL	N-CA-C	5.30	120.33	113.07
1	B	152	ILE	N-CA-C	5.20	116.55	110.62
1	B	124	GLN	CA-C-N	-5.03	116.29	123.08
1	B	124	GLN	C-N-CA	-5.03	116.29	123.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	171	HIS	CA

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	1769	0	1729	18	0
1	B	1750	0	1717	19	0
1	C	1774	0	1736	15	0
2	A	21	0	13	0	0
2	B	21	0	13	1	0
2	C	21	0	13	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	18	0	24	0	0
5	B	24	0	32	0	0
5	C	12	0	16	0	0
6	A	199	0	0	3	0
6	B	145	0	0	5	0
6	C	145	0	0	2	0
All	All	5987	0	5329	52	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 5.

All (52) 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:176:ILE:HD13	1:A:194:GLU:HG2	1.53	0.91
1:A:116:LYS:NZ	6:A:2095:HOH:O	2.08	0.86
1:A:136:ASN:HD22	1:A:177:ASN:HD21	1.23	0.83
1:C:185:GLU:CD	1:C:185:GLU:H	1.88	0.82
1:B:136:ASN:HD22	1:B:177:ASN:HD21	1.26	0.82
1:C:136:ASN:HD22	1:C:177:ASN:HD21	1.33	0.75
1:B:164:GLU:OE2	6:B:2099:HOH:O	2.12	0.67
1:C:147:ASP:O	1:C:150:GLU:HG2	1.94	0.66
1:C:144:ASN:HD22	1:C:144:ASN:H	1.44	0.64
1:B:147:ASP:O	1:B:148:TYR:C	2.41	0.64
1:B:176:ILE:CD1	1:B:194[A]:GLU:HG2	2.28	0.64
1:B:200:VAL:HG12	1:B:200:VAL:O	1.98	0.63
1:A:176:ILE:HD13	1:A:194:GLU:CG	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB2	6:C:2003:HOH:O	2.02	0.59
1:A:192:VAL:O	1:A:196:THR:HG23	2.04	0.58
1:A:176:ILE:CD1	1:A:194:GLU:HG2	2.32	0.57
1:A:157:GLU:H	1:A:157:GLU:CD	2.12	0.57
1:B:147:ASP:O	1:B:148:TYR:O	2.23	0.57
1:C:46:ASN:HD22	1:C:46:ASN:C	2.13	0.57
1:C:140:ASN:ND2	6:C:2086:HOH:O	2.39	0.54
1:B:40:LYS:HE3	6:B:2060:HOH:O	2.07	0.53
1:B:137:VAL:O	1:B:137:VAL:HG23	2.09	0.53
1:B:147:ASP:C	6:B:2089:HOH:O	2.51	0.53
1:B:176:ILE:HD12	1:B:194[A]:GLU:HG2	1.92	0.50
1:B:143:GLN:HG3	1:B:144:ASN:OD1	2.12	0.50
1:C:4:ASP:HA	1:C:90:LEU:HD21	1.94	0.50
1:C:46:ASN:ND2	1:C:48:GLU:H	2.10	0.49
1:A:9:LYS:HE2	1:A:198:ILE:CG2	2.43	0.49
1:A:131:VAL:HG21	1:A:176:ILE:HD12	1.96	0.48
1:B:194[A]:GLU:OE1	1:B:197:LYS:HE3	2.12	0.48
1:A:9:LYS:HA	1:A:9:LYS:HD2	1.69	0.48
1:A:145:ARG:HD3	6:B:2104:HOH:O	2.14	0.48
1:B:4:ASP:OD1	1:B:4:ASP:N	2.48	0.46
1:A:140:ASN:ND2	6:A:2111:HOH:O	2.46	0.46
1:B:108:SER:HB3	1:B:114:LEU:HD12	1.98	0.45
1:A:67:ASN:ND2	6:A:2054:HOH:O	2.50	0.44
1:B:107:TYR:CE1	2:B:211:TMP:H2'1	2.52	0.43
1:C:107:TYR:CE1	2:C:211:TMP:H2'1	2.53	0.43
1:C:183:LYS:HB3	1:C:185:GLU:OE1	2.18	0.43
1:A:131:VAL:CG2	1:A:176:ILE:HD12	2.49	0.43
1:C:46:ASN:C	1:C:46:ASN:ND2	2.76	0.42
1:B:140:ASN:O	1:B:143:GLN:HG2	2.18	0.42
1:C:208:LEU:HA	1:C:209:TRP:HA	1.83	0.42
1:A:108:SER:HB3	1:A:114:LEU:HD12	2.01	0.42
1:C:185:GLU:CD	1:C:185:GLU:N	2.66	0.42
1:A:63:ASN:OD1	1:A:63:ASN:C	2.62	0.41
1:B:120:MET:SD	1:B:168:HIS:HE1	2.43	0.41
1:A:18:ARG:NH2	1:A:147:ASP:HB2	2.36	0.41
1:B:200:VAL:HG11	6:B:2067:HOH:O	2.20	0.41
1:B:137:VAL:O	1:B:137:VAL:CG2	2.69	0.41
1:C:136:ASN:HD22	1:C:177:ASN:ND2	2.10	0.41
1:A:107:TYR:CE1	1:A:162:ILE:HD13	2.56	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	211/212 (100%)	206 (98%)	4 (2%)	1 (0%)	24	16
1	B	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	16
1	C	211/212 (100%)	206 (98%)	4 (2%)	1 (0%)	24	16
All	All	632/636 (99%)	616 (98%)	13 (2%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	B	148	TYR
1	C	146	SER

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	196/195 (100%)	188 (96%)	8 (4%)	27	19
1	B	195/195 (100%)	192 (98%)	3 (2%)	57	56
1	C	197/195 (101%)	191 (97%)	6 (3%)	36	30
All	All	588/585 (100%)	571 (97%)	17 (3%)	37	31

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	LYS
1	A	18	ARG
1	A	116	LYS
1	A	145	ARG
1	A	157	GLU
1	A	183	LYS
1	A	200	VAL
1	B	145	ARG
1	B	146	SER
1	B	204	GLU
1	C	18	ARG
1	C	90	LEU
1	C	135	LEU
1	C	144	ASN
1	C	145	ARG
1	C	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	34	ASN
1	A	35	ASN
1	A	67	ASN
1	A	144	ASN
1	A	177	ASN
1	A	206	ASN
1	B	34	ASN
1	B	35	ASN
1	B	67	ASN
1	B	168	HIS
1	B	177	ASN
1	C	34	ASN
1	C	35	ASN
1	C	46	ASN
1	C	140	ASN
1	C	143	GLN
1	C	144	ASN
1	C	177	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	TMP	A	211	4	22,22,22	2.37	10 (45%)	32,33,33	3.09	15 (46%)
3	ADP	A	212	4	28,29,29	1.45	4 (14%)	43,45,45	1.86	11 (25%)
3	ADP	C	212	4	28,29,29	1.44	4 (14%)	43,45,45	1.81	9 (20%)
5	GOL	B	218	-	5,5,5	0.46	0	5,5,5	1.23	1 (20%)
5	GOL	A	216	-	5,5,5	0.75	0	5,5,5	0.81	0
5	GOL	A	217	-	5,5,5	0.53	0	5,5,5	1.35	1 (20%)
2	TMP	C	211	-	22,22,22	1.81	6 (27%)	32,33,33	3.23	16 (50%)
5	GOL	B	215	-	5,5,5	0.48	0	5,5,5	1.03	0
2	TMP	B	211	4	22,22,22	1.76	6 (27%)	32,33,33	2.29	8 (25%)
5	GOL	B	217	-	5,5,5	0.60	0	5,5,5	0.37	0
5	GOL	C	215	-	5,5,5	1.10	0	5,5,5	0.82	0
5	GOL	C	216	-	5,5,5	0.38	0	5,5,5	0.50	0
3	ADP	B	212	4	28,29,29	1.76	4 (14%)	43,45,45	1.67	7 (16%)
5	GOL	B	216	-	5,5,5	0.39	0	5,5,5	1.14	1 (20%)
5	GOL	A	215	-	5,5,5	0.54	0	5,5,5	1.80	2 (40%)

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	TMP	A	211	4	-	4/10/22/22	0/2/2/2
3	ADP	A	212	4	-	1/16/32/32	0/3/3/3
3	ADP	C	212	4	-	1/16/32/32	0/3/3/3
5	GOL	B	218	-	-	0/4/4/4	-
5	GOL	A	216	-	-	0/4/4/4	-
5	GOL	A	217	-	-	4/4/4/4	-
2	TMP	C	211	-	-	0/10/22/22	0/2/2/2
5	GOL	B	215	-	-	2/4/4/4	-
2	TMP	B	211	4	-	1/10/22/22	0/2/2/2
5	GOL	B	217	-	-	0/4/4/4	-
5	GOL	C	215	-	-	0/4/4/4	-
5	GOL	C	216	-	-	4/4/4/4	-
3	ADP	B	212	4	-	3/16/32/32	0/3/3/3
5	GOL	B	216	-	-	1/4/4/4	-
5	GOL	A	215	-	-	3/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	212	ADP	PA-O3A	5.58	1.65	1.59
3	B	212	ADP	C5-C4	5.04	1.48	1.39
2	A	211	TMP	P-O3P	-4.50	1.38	1.54
3	A	212	ADP	C5-C4	4.33	1.46	1.39
2	A	211	TMP	C5M-C5	4.30	1.61	1.50
3	C	212	ADP	C5-C4	4.12	1.46	1.39
2	C	211	TMP	C2-N1	4.00	1.44	1.38
2	B	211	TMP	C4-C5	-3.83	1.38	1.44
2	A	211	TMP	P-O1P	-3.70	1.39	1.50
2	A	211	TMP	C6-C5	3.65	1.40	1.34
2	A	211	TMP	P-O5'	3.41	1.71	1.60
2	B	211	TMP	C5M-C5	3.30	1.58	1.50
3	A	212	ADP	C8-N7	3.28	1.38	1.31
3	C	212	ADP	C5-C6	3.20	1.49	1.41
2	A	211	TMP	C4-C5	-3.16	1.39	1.44
2	B	211	TMP	O4'-C4'	2.92	1.51	1.45
2	C	211	TMP	P-O3P	2.92	1.65	1.54
2	B	211	TMP	C2'-C1'	2.86	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	TMP	C6-C5	2.66	1.38	1.34
2	A	211	TMP	P-O2P	-2.58	1.45	1.54
3	B	212	ADP	C5-C6	2.57	1.48	1.41
2	A	211	TMP	C6-N1	2.50	1.42	1.38
2	A	211	TMP	C2-N3	2.49	1.42	1.38
2	C	211	TMP	C6-C5	2.48	1.38	1.34
3	A	212	ADP	PA-O3A	2.43	1.62	1.59
2	C	211	TMP	C5M-C5	2.35	1.56	1.50
3	C	212	ADP	C4-N3	2.35	1.38	1.34
2	C	211	TMP	O3'-C3'	2.20	1.47	1.43
2	B	211	TMP	C5'-C4'	2.19	1.58	1.51
3	C	212	ADP	C8-N7	2.15	1.35	1.31
2	C	211	TMP	C2'-C1'	2.14	1.58	1.52
2	A	211	TMP	O5'-C5'	-2.11	1.36	1.44
3	A	212	ADP	C5-C6	2.04	1.46	1.41
3	B	212	ADP	C8-N7	2.03	1.35	1.31

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	211	TMP	C5-C4-N3	8.90	123.06	115.32
2	C	211	TMP	C4-N3-C2	-8.31	116.45	127.34
2	A	211	TMP	O2P-P-O5'	-8.08	85.59	106.67
2	A	211	TMP	C5-C4-N3	6.68	121.13	115.32
2	A	211	TMP	C4-N3-C2	-6.64	118.64	127.34
2	A	211	TMP	O3P-P-O1P	6.33	135.49	110.83
2	B	211	TMP	C5-C4-N3	5.71	120.29	115.32
2	C	211	TMP	C5-C6-N1	-5.64	117.19	123.31
3	C	212	ADP	C5-C4-N3	-5.56	119.07	126.72
2	B	211	TMP	C4-N3-C2	-5.45	120.20	127.34
3	A	212	ADP	C5-C4-N3	-5.12	119.66	126.72
2	B	211	TMP	C5-C6-N1	-4.86	118.04	123.31
3	C	212	ADP	N3-C4-N9	4.71	135.19	127.17
3	B	212	ADP	C5-C4-N3	-4.65	120.31	126.72
2	A	211	TMP	N3-C2-N1	4.59	120.86	114.89
3	A	212	ADP	N3-C4-N9	4.24	134.38	127.17
3	B	212	ADP	N3-C4-N9	4.21	134.32	127.17
3	B	212	ADP	C2-N1-C6	4.12	125.50	118.73
3	B	212	ADP	N3-C2-N1	-4.09	122.39	128.58
2	C	211	TMP	N3-C2-N1	4.02	120.12	114.89
2	B	211	TMP	N3-C2-N1	4.00	120.09	114.89
3	A	212	ADP	N3-C2-N1	-3.92	122.65	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	TMP	C5M-C5-C6	-3.87	117.62	122.85
3	A	212	ADP	O4'-C1'-N9	-3.86	100.69	108.09
2	C	211	TMP	O3P-P-O2P	-3.79	93.61	107.80
2	C	211	TMP	O5'-P-O1P	3.70	116.43	106.44
2	C	211	TMP	O2P-P-O1P	3.55	124.67	110.83
3	A	212	ADP	C2-N3-C4	3.55	120.50	111.83
2	C	211	TMP	C6-C5-C4	3.41	120.83	118.02
2	A	211	TMP	C5M-C5-C6	-3.40	118.25	122.85
2	C	211	TMP	C5M-C5-C6	-3.37	118.30	122.85
2	B	211	TMP	C6-C5-C4	3.34	120.78	118.02
3	C	212	ADP	C2-N3-C4	3.26	119.79	111.83
3	C	212	ADP	C4-C5-N7	-3.23	106.89	110.58
2	C	211	TMP	O2-C2-N1	-3.14	118.71	122.80
2	C	211	TMP	O4'-C1'-N1	-3.13	102.30	107.86
2	A	211	TMP	C5-C6-N1	-3.13	119.91	123.31
2	C	211	TMP	O3P-P-O5'	-3.11	98.57	106.67
3	C	212	ADP	N3-C2-N1	-3.09	123.90	128.58
3	C	212	ADP	C4-N9-C8	3.09	108.98	105.74
2	C	211	TMP	O3P-P-O1P	-3.09	98.80	110.83
3	B	212	ADP	C2-N3-C4	3.05	119.29	111.83
3	A	212	ADP	N6-C6-N1	3.02	125.10	118.38
2	C	211	TMP	O2P-P-O5'	3.02	114.53	106.67
5	A	215	GOL	O2-C2-C1	2.95	121.39	109.18
3	C	212	ADP	C5-N7-C8	2.88	107.97	103.45
2	C	211	TMP	O4-C4-C5	-2.82	121.69	124.92
3	A	212	ADP	C4-N9-C8	2.81	108.69	105.74
2	B	211	TMP	O2P-P-O1P	2.73	121.46	110.83
2	C	211	TMP	O4-C4-N3	-2.69	115.05	120.11
2	A	211	TMP	C5M-C5-C4	2.65	121.61	118.78
2	B	211	TMP	C5M-C5-C4	2.65	121.61	118.78
2	A	211	TMP	O5'-P-O1P	2.64	113.58	106.44
2	A	211	TMP	O4-C4-N3	-2.63	115.17	120.11
2	A	211	TMP	O4'-C1'-N1	-2.54	103.36	107.86
2	A	211	TMP	C6-C5-C4	2.53	120.11	118.02
2	A	211	TMP	O4'-C4'-C5'	-2.50	101.32	109.33
3	C	212	ADP	N9-C8-N7	-2.50	110.39	113.94
3	A	212	ADP	C5-C6-N6	-2.48	117.14	123.29
2	A	211	TMP	O2-C2-N3	-2.47	116.94	121.49
5	B	216	GOL	C3-C2-C1	-2.45	102.81	111.80
3	B	212	ADP	C4-N9-C8	2.38	108.23	105.74
5	B	218	GOL	C3-C2-C1	-2.33	103.26	111.80
5	A	215	GOL	O2-C2-C3	2.30	118.71	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	212	ADP	C2-N1-C6	2.24	122.42	118.73
2	A	211	TMP	O3P-P-O2P	-2.10	99.93	107.80
3	A	212	ADP	C4-C5-N7	-2.09	108.19	110.58
3	B	212	ADP	C4-C5-N7	-2.07	108.22	110.58
3	C	212	ADP	O3B-PB-O1B	2.06	118.86	110.83
5	A	217	GOL	O1-C1-C2	-2.02	101.26	110.38
3	A	212	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

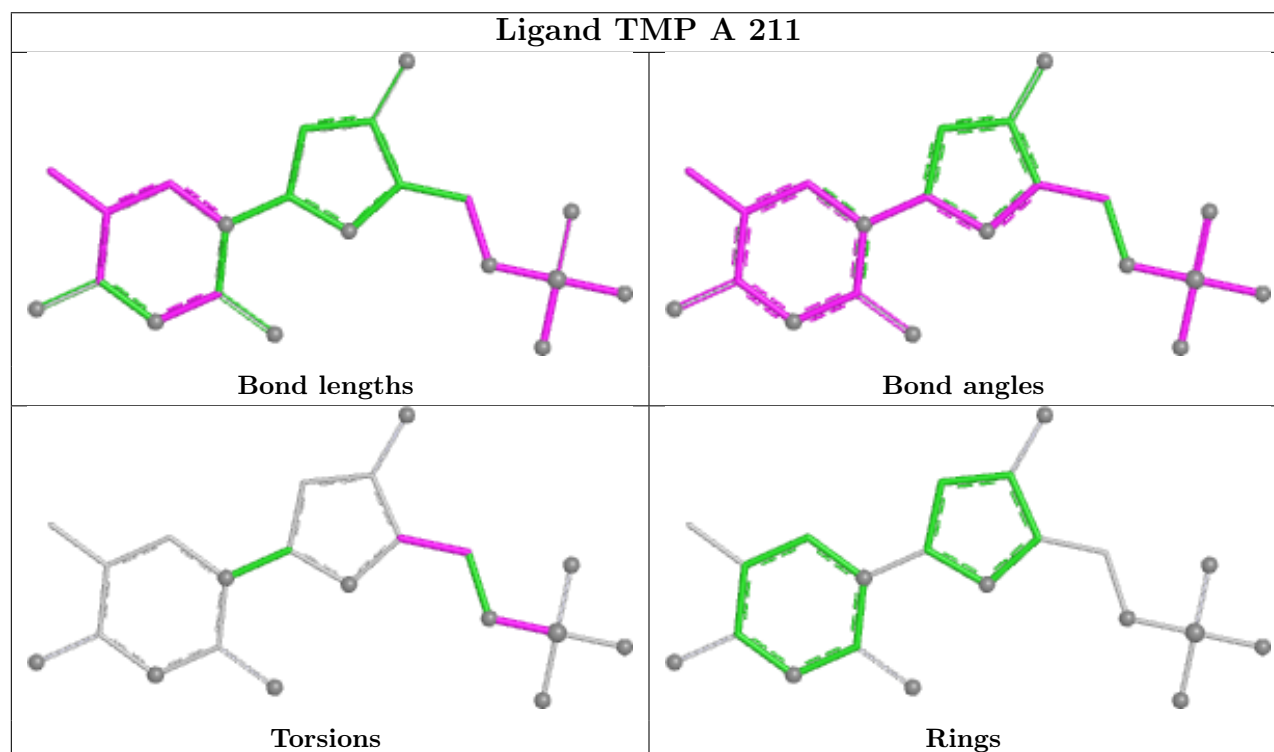
Mol	Chain	Res	Type	Atoms
2	A	211	TMP	C5'-O5'-P-O1P
2	A	211	TMP	C5'-O5'-P-O2P
3	A	212	ADP	PA-O3A-PB-O2B
5	A	217	GOL	O1-C1-C2-C3
5	A	217	GOL	C1-C2-C3-O3
5	B	215	GOL	O1-C1-C2-C3
5	C	216	GOL	O1-C1-C2-C3
5	C	216	GOL	C1-C2-C3-O3
5	A	215	GOL	O1-C1-C2-O2
5	A	215	GOL	O2-C2-C3-O3
5	A	217	GOL	O1-C1-C2-O2
5	A	217	GOL	O2-C2-C3-O3
5	B	215	GOL	O1-C1-C2-O2
5	C	216	GOL	O2-C2-C3-O3
5	B	216	GOL	O1-C1-C2-O2
2	A	211	TMP	C5'-O5'-P-O3P
3	B	212	ADP	PA-O3A-PB-O1B
3	B	212	ADP	PA-O3A-PB-O2B
3	C	212	ADP	PA-O3A-PB-O2B
5	C	216	GOL	O1-C1-C2-O2
3	B	212	ADP	C2'-C1'-N9-C8
5	A	215	GOL	C1-C2-C3-O3
2	A	211	TMP	C3'-C4'-C5'-O5'
2	B	211	TMP	O4'-C4'-C5'-O5'

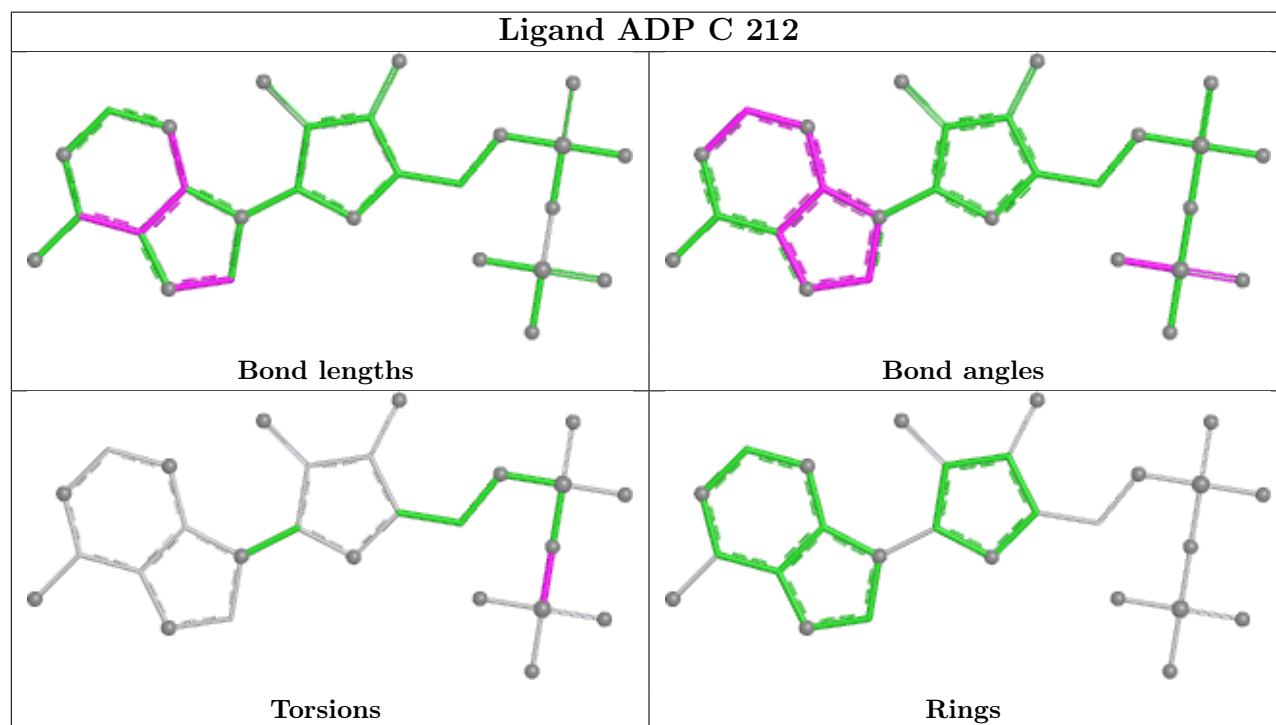
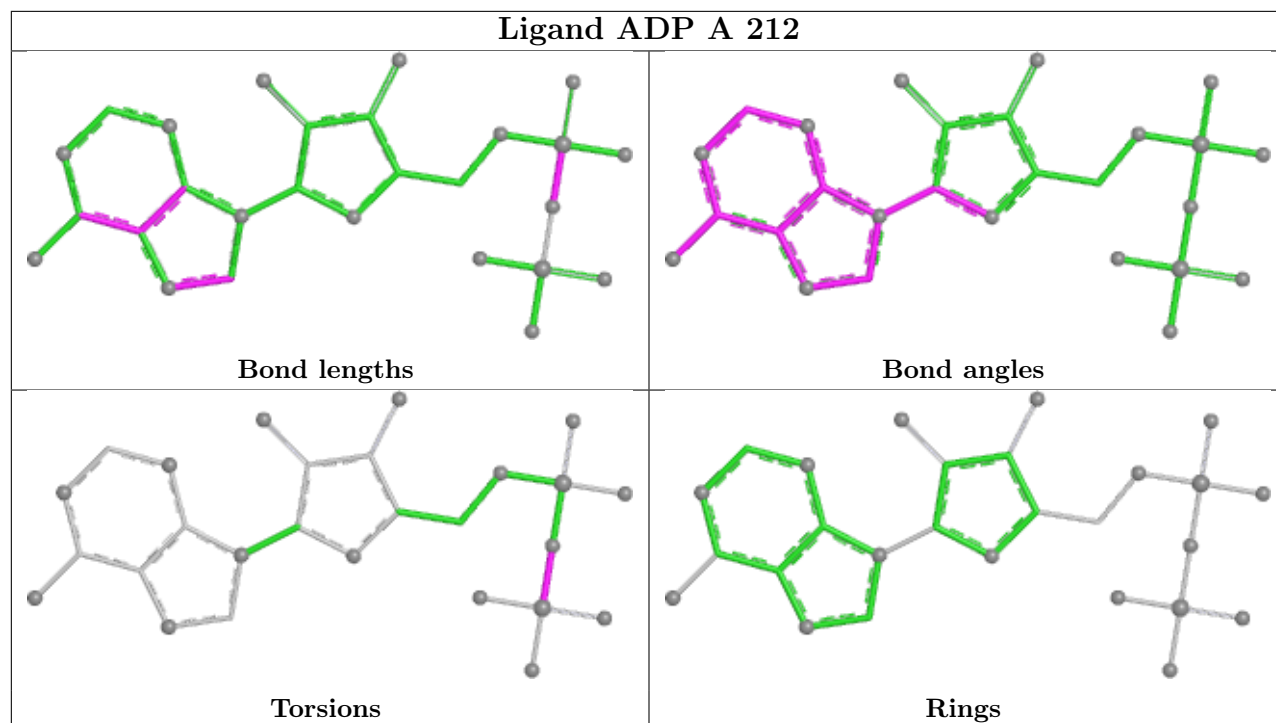
There are no ring outliers.

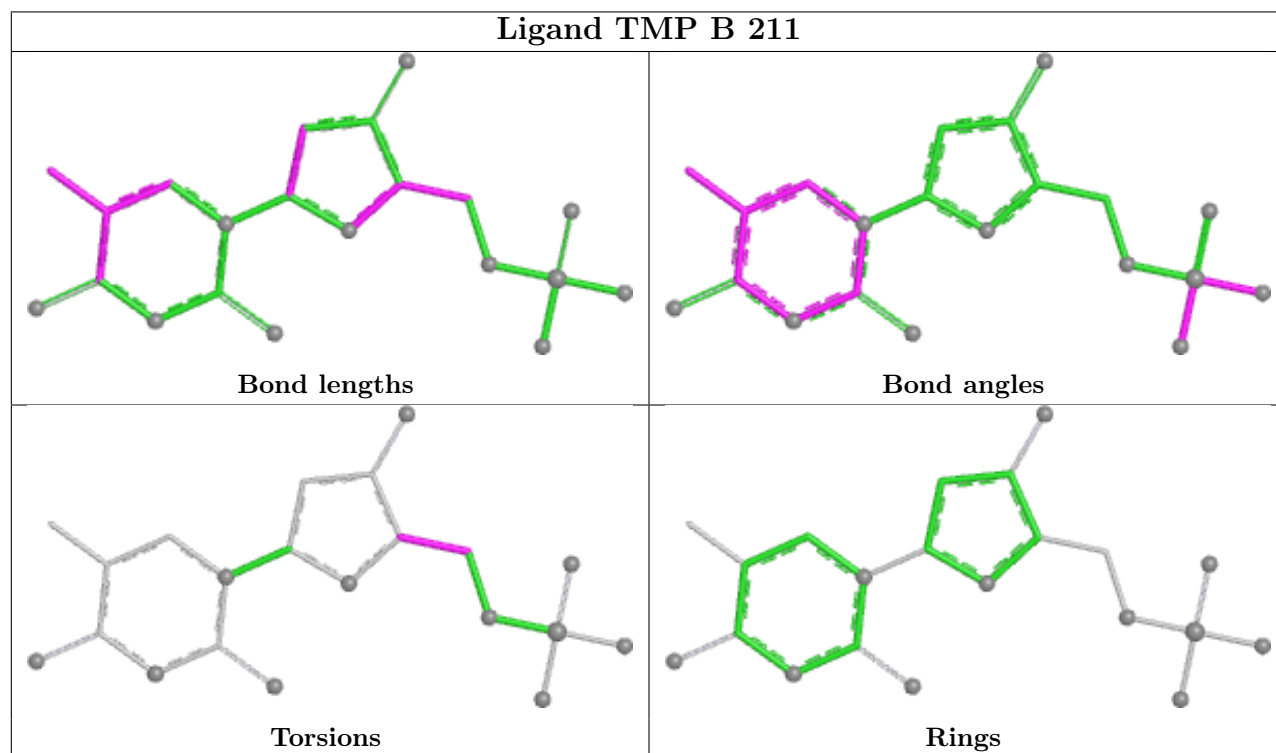
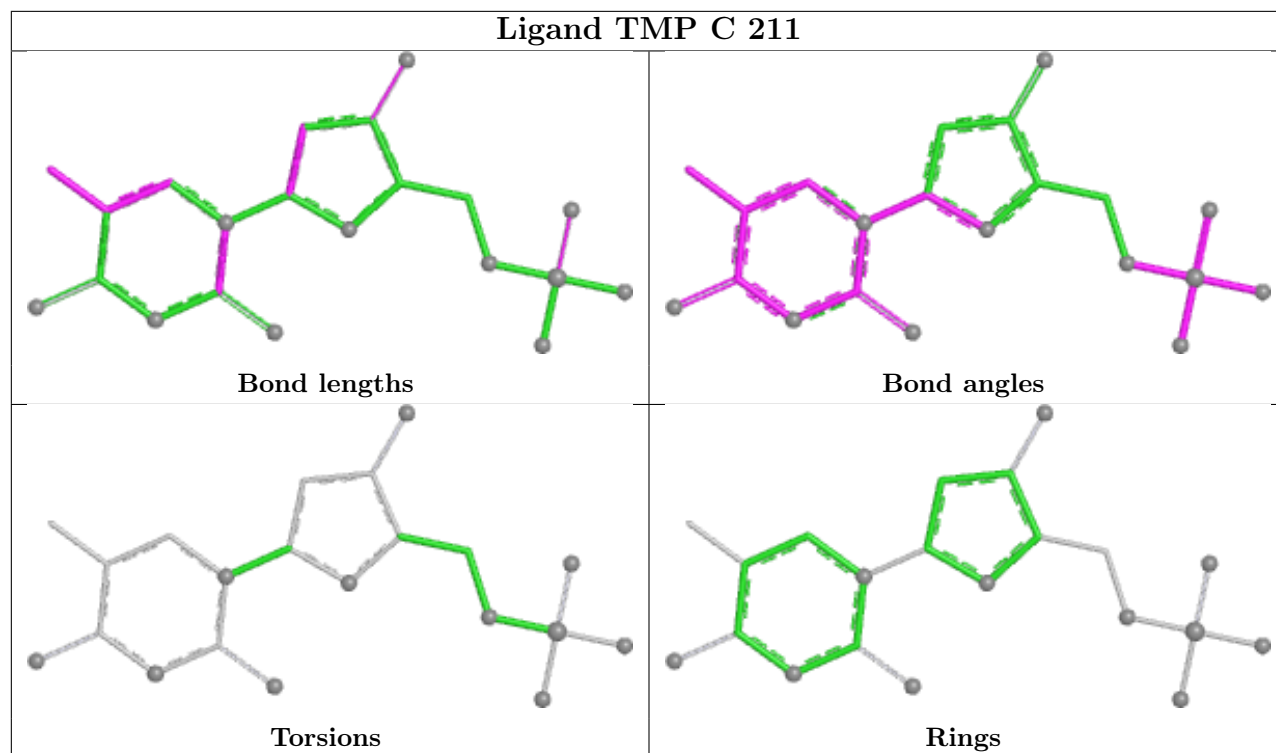
2 monomers are involved in 2 short contacts:

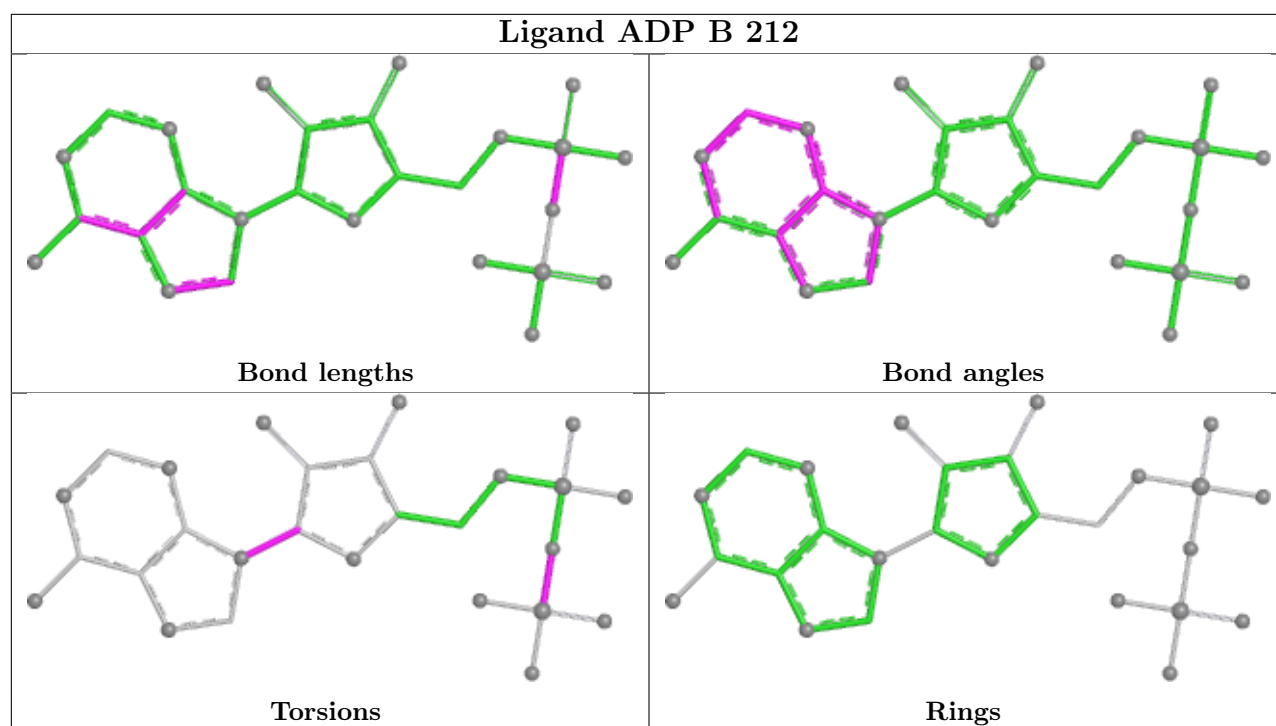
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	211	TMP	1	0
2	B	211	TMP	1	0

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 [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	211/212 (99%)	-0.55	0 100 100	6, 15, 32, 45	6 (2%)
1	B	208/212 (98%)	-0.24	11 (5%) 32 34	11, 18, 36, 47	14 (6%)
1	C	212/212 (100%)	-0.29	6 (2%) 55 59	10, 18, 34, 40	12 (5%)
All	All	631/636 (99%)	-0.36	17 (2%) 56 60	6, 17, 35, 47	32 (5%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ASN	4.6
1	B	143	GLN	4.2
1	B	147	ASP	4.0
1	B	200	VAL	3.6
1	B	141	TYR	3.5
1	B	146	SER	3.4
1	C	200	VAL	2.9
1	B	199	LYS	2.8
1	C	150	GLU	2.6
1	B	150	GLU	2.6
1	C	171	HIS	2.4
1	B	210	SER	2.3
1	C	83	ASN	2.3
1	C	30	GLU	2.2
1	C	168	HIS	2.2
1	B	196	THR	2.2
1	B	148	TYR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

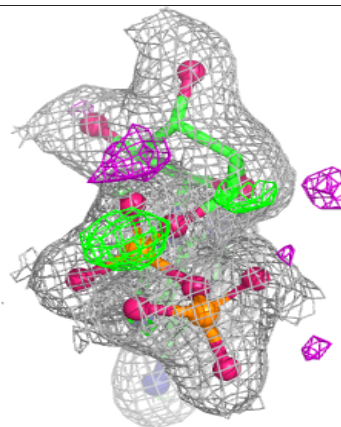
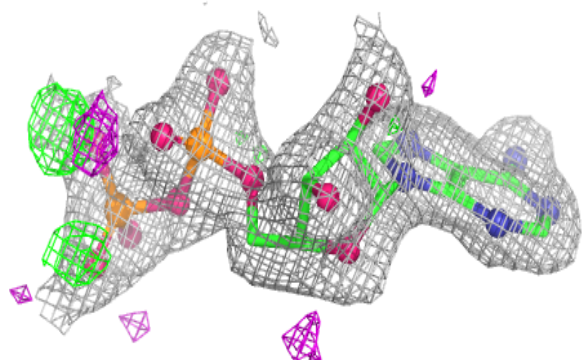
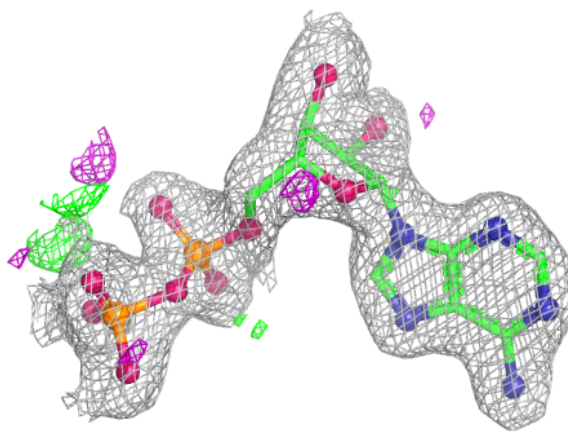
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	217	6/6	0.83	0.13	34,39,43,43	0
5	GOL	B	218	6/6	0.83	0.13	31,34,36,36	0
5	GOL	C	216	6/6	0.87	0.14	37,44,44,49	0
5	GOL	B	215	6/6	0.93	0.09	15,22,28,32	0
4	NA	B	213	1/1	0.94	0.08	37,37,37,37	0
5	GOL	A	215	6/6	0.94	0.08	16,24,28,36	0
5	GOL	C	215	6/6	0.96	0.07	18,20,21,25	0
5	GOL	B	216	6/6	0.96	0.07	15,24,29,34	0
5	GOL	A	216	6/6	0.97	0.05	14,17,19,21	0
4	NA	A	213	1/1	0.97	0.06	25,25,25,25	0
5	GOL	B	217	6/6	0.97	0.04	15,17,19,19	0
3	ADP	C	212	27/27	0.98	0.05	12,23,25,27	0
2	TMP	A	211	21/21	0.98	0.04	5,10,21,27	0
4	NA	A	218	1/1	0.98	0.11	35,35,35,35	0
2	TMP	B	211	21/21	0.98	0.05	10,13,24,27	0
4	NA	C	213	1/1	0.98	0.08	18,18,18,18	0
2	TMP	C	211	21/21	0.98	0.04	9,12,21,31	0
3	ADP	B	212	27/27	0.98	0.06	15,25,29,30	0
4	NA	B	214	1/1	0.99	0.02	22,22,22,22	0
3	ADP	A	212	27/27	0.99	0.04	10,16,19,20	0
4	NA	C	214	1/1	0.99	0.05	15,15,15,15	0
4	NA	A	214	1/1	0.99	0.02	22,22,22,22	0

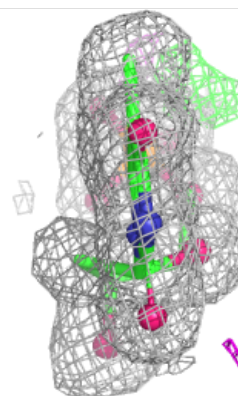
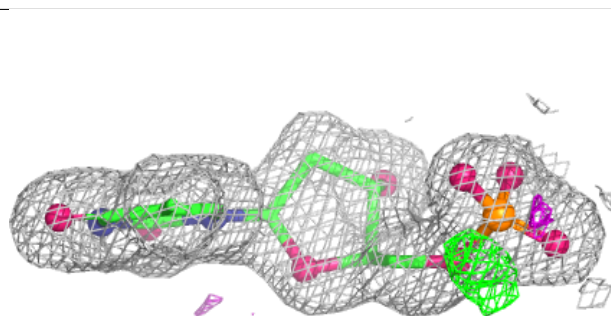
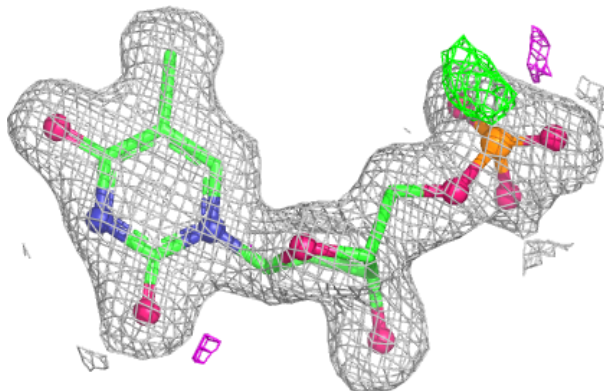
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 212:

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

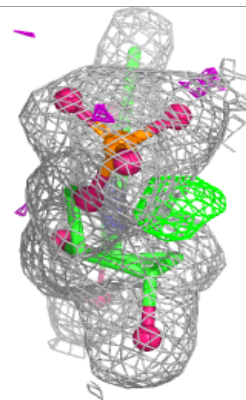
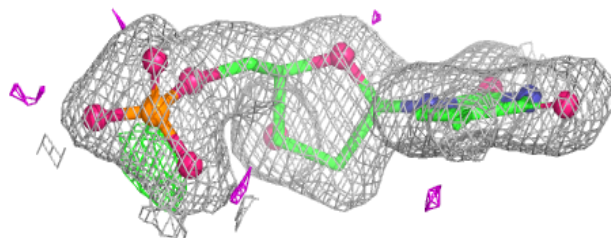
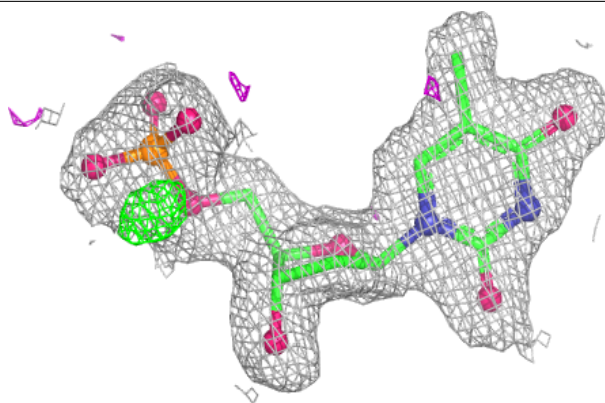
**Electron density around TMP A 211:**

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

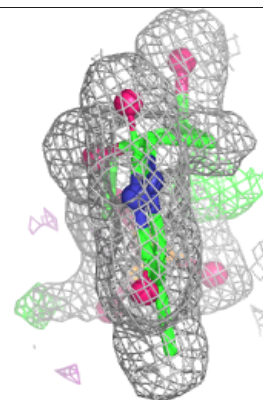
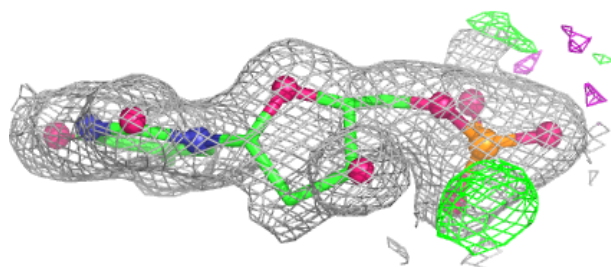
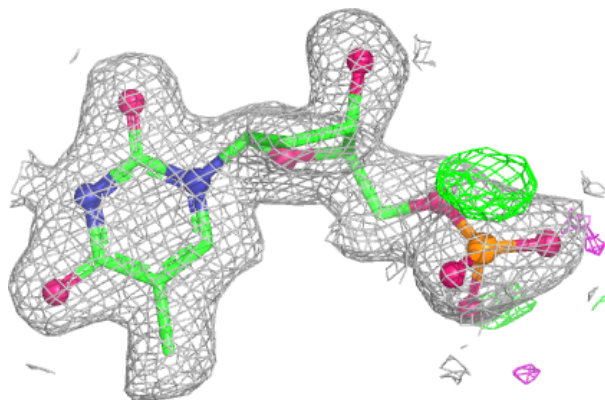


Electron density around TMP B 211:

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

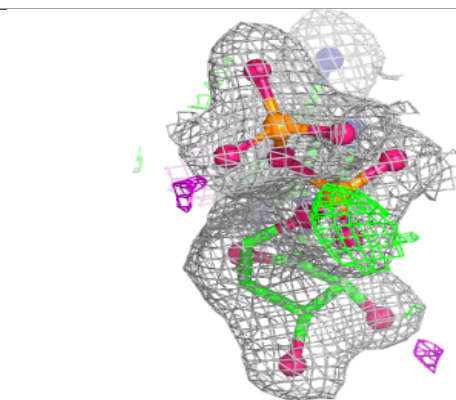
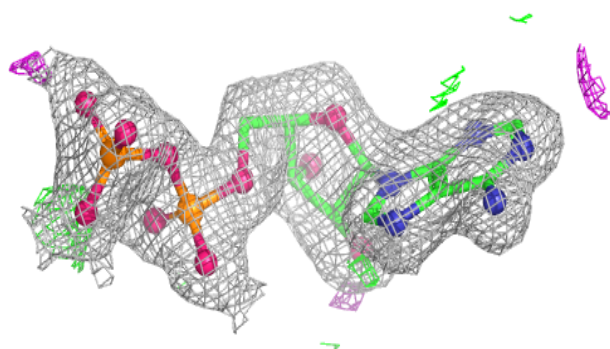
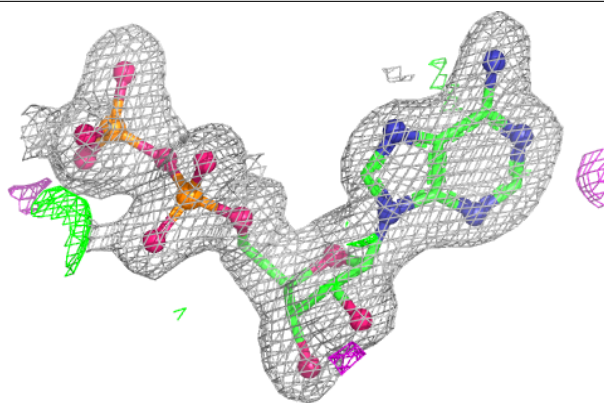
**Electron density around TMP C 211:**

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

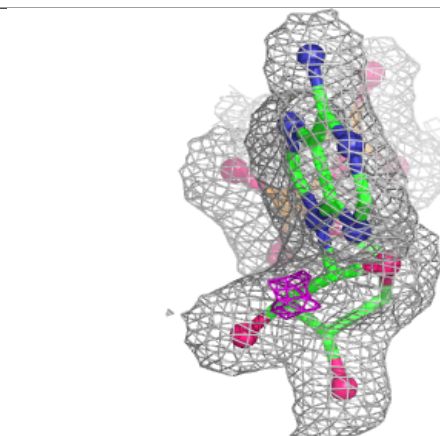
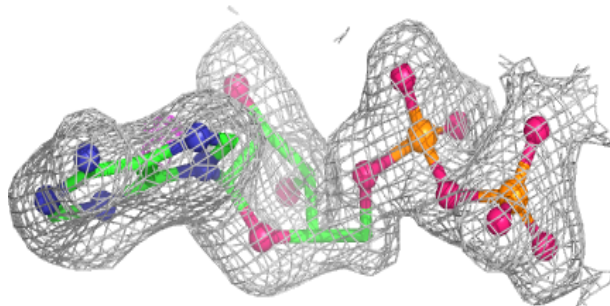
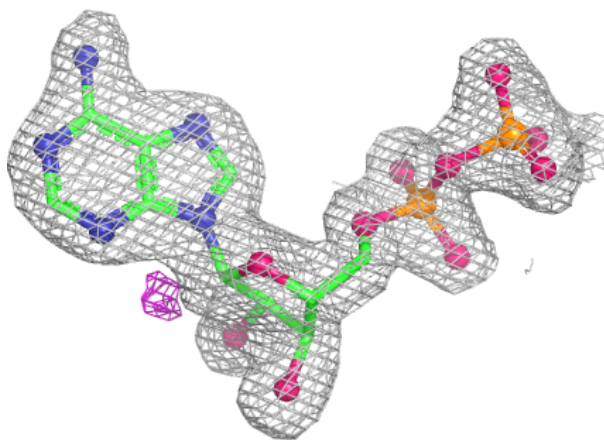


Electron density around ADP B 212:

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

**Electron density around ADP A 212:**

$2mF_o-DF_c$ (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.