



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:38 pm BST

PDB ID : 3UDG  
Title : Structure of Deinococcus radiodurans SSB bound to ssDNA  
Authors : George, N.P.; Ngo, K.V.; Chitteni-Patu, S.; Norais, C.A.; Battista, J.R.; Cox, M.M.; Keck, J.L.  
Deposited on : 2011-10-28  
Resolution : 2.40 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.

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

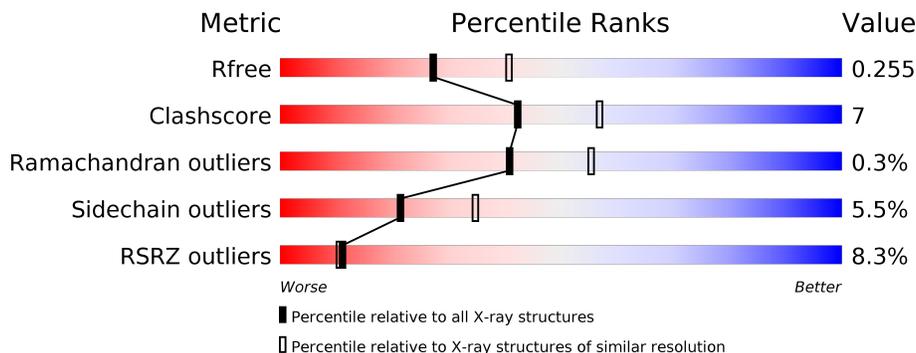
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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.

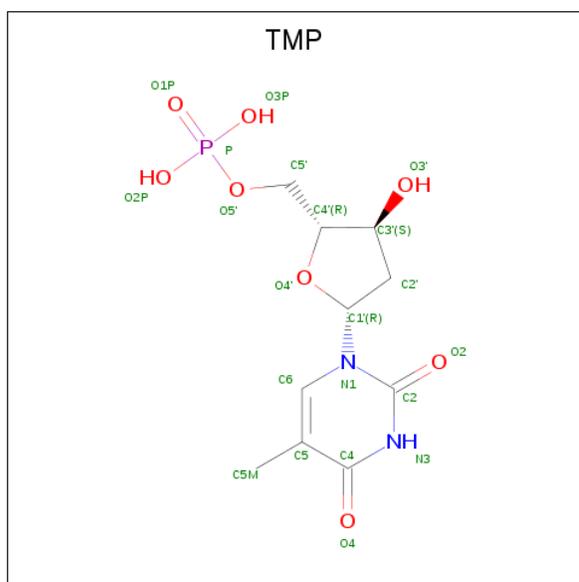
Mol	Chain	Length	Quality of chain
1	A	301	 3% 58% 11% 30%
1	B	301	 4% 58% 12% 29%
1	C	301	 11% 58% 12% 29%
2	D	35	 9% 6% 86%
2	E	35	 9% 6% 86%
2	F	35	 3% 6% 89%

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Mol	Chain	Length	Quality of chain
2	G	35	 11% . 86%
2	H	35	 6% . 91%
2	I	35	 . . . 91%





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

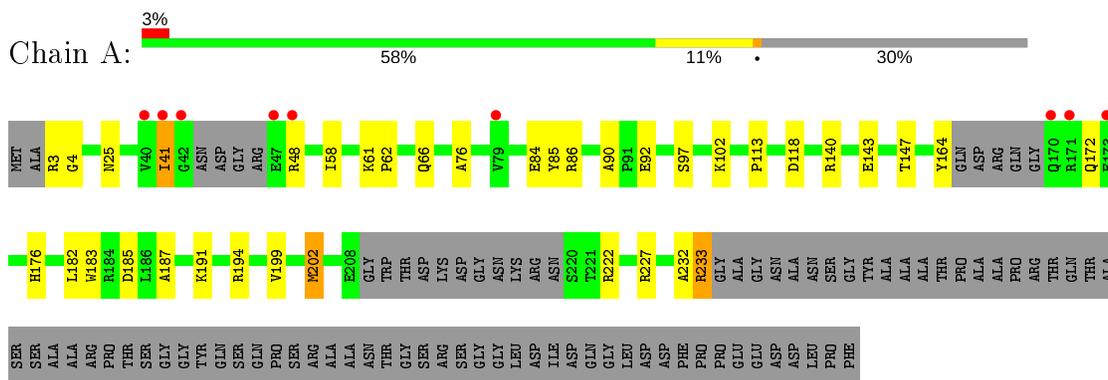
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	37	Total	O	0	0
			37	37		
4	C	23	Total	O	0	0
			23	23		
4	D	1	Total	O	0	0
			1	1		
4	E	5	Total	O	0	0
			5	5		
4	G	1	Total	O	0	0
			1	1		

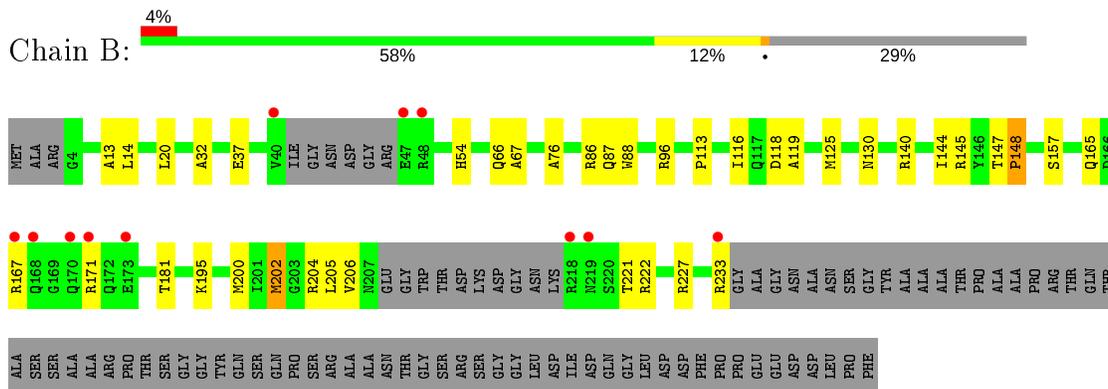
### 3 Residue-property plots i

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

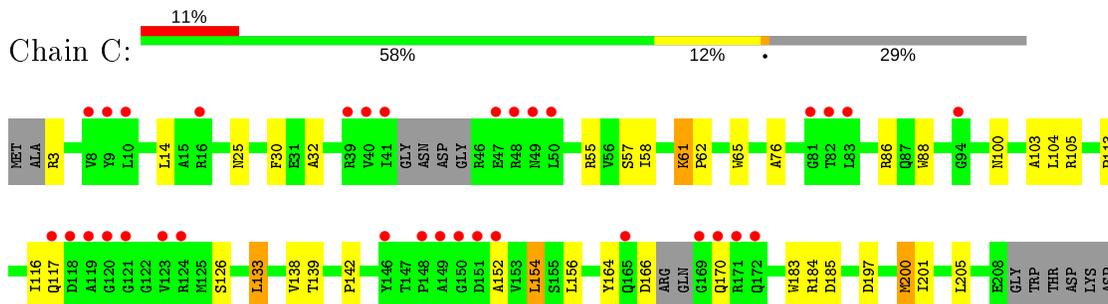
- Molecule 1: Single-stranded DNA-binding protein



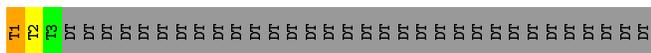
- Molecule 1: Single-stranded DNA-binding protein



- Molecule 1: Single-stranded DNA-binding protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.14Å 95.67Å 65.73Å 90.00° 94.12° 90.00°	Depositor
Resolution (Å)	28.38 – 2.40 28.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (28.38-2.40) 94.1 (28.38-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.201 , 0.261 0.198 , 0.255	Depositor DCC
$R_{free}$ test set	1836 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtrriage
Anisotropy	0.610	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.86	0/1670	0.92	0/2253
1	B	0.80	1/1699 (0.1%)	0.88	0/2293
1	C	0.67	3/1698 (0.2%)	0.77	0/2290
2	D	0.32	0/109	1.14	2/166 (1.2%)
2	E	0.40	0/109	1.09	1/166 (0.6%)
2	F	0.35	0/86	0.89	1/128 (0.8%)
2	G	0.49	0/99	1.14	1/150 (0.7%)
2	H	0.37	0/65	0.64	0/98
2	I	0.38	0/65	0.96	1/98 (1.0%)
All	All	0.75	4/5600 (0.1%)	0.88	6/7642 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TRP	CD2-CE2	6.49	1.49	1.41
1	C	65	TRP	CD2-CE2	5.61	1.48	1.41
1	C	183	TRP	CD2-CE2	5.58	1.48	1.41
1	C	88	TRP	CD2-CE2	5.47	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	1	DT	P-O3'-C3'	8.21	129.56	119.70
2	E	1	DT	P-O3'-C3'	7.58	128.80	119.70
2	G	1	DT	P-O3'-C3'	6.81	127.87	119.70
2	F	1	DT	P-O3'-C3'	6.42	127.41	119.70
2	I	1	DT	P-O3'-C3'	6.37	127.34	119.70
2	D	2	DT	P-O3'-C3'	5.85	126.72	119.70

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	1647	0	1639	18	0
1	B	1675	0	1662	24	0
1	C	1675	0	1664	29	0
2	D	100	0	61	0	0
2	E	100	0	61	1	0
2	F	80	0	50	3	0
2	G	91	0	55	0	0
2	H	60	0	37	2	0
2	I	60	0	37	3	0
3	A	21	0	13	1	0
3	B	42	0	26	6	0
3	C	21	0	13	1	0
4	A	39	0	0	0	0
4	B	37	0	0	2	0
4	C	23	0	0	2	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	G	1	0	0	0	0
All	All	5678	0	5318	75	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 7.

All (75) 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:133:LEU:HD21	1:C:200:MET:HE1	1.55	0.88
1:A:118:ASP:HB2	3:A:302:TMP:H5'2	1.53	0.88
1:B:118:ASP:HB2	3:B:302:TMP:H3'	1.56	0.85
1:C:133:LEU:HD21	1:C:200:MET:CE	2.06	0.84
2:I:1:DT:H4'	2:I:2:DT:OP1	1.81	0.78
1:B:118:ASP:HB2	3:B:302:TMP:C3'	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:HE21	1:B:171:ARG:HG2	1.51	0.74
1:C:142:PRO:HB2	1:C:154:LEU:CD2	2.18	0.73
1:C:138:VAL:HG23	1:C:197:ASP:O	1.90	0.72
1:B:14:LEU:HD22	1:B:32:ALA:HB1	1.74	0.69
1:A:76:ALA:HB2	1:A:113:PRO:HG3	1.77	0.66
1:B:205:LEU:HD11	1:B:221:THR:CG2	2.28	0.64
1:C:142:PRO:HB2	1:C:154:LEU:HD21	1.80	0.63
1:A:140:ARG:HH22	2:H:1:DT:H72	1.66	0.60
1:B:86:ARG:NH2	4:B:326:HOH:O	2.34	0.59
1:B:76:ALA:HB2	1:B:113:PRO:HG3	1.88	0.56
1:C:76:ALA:HB2	1:C:113:PRO:HG3	1.87	0.56
1:A:147:THR:HG21	1:A:183:TRP:HZ3	1.70	0.56
1:A:232:ALA:O	1:A:233:ARG:HB2	2.06	0.55
1:B:54:HIS:ND1	4:B:316:HOH:O	2.34	0.54
1:C:205:LEU:HD11	1:C:221:THR:CG2	2.38	0.54
1:C:133:LEU:HD21	1:C:200:MET:HE2	1.89	0.53
1:A:202:MET:HG2	1:A:227:ARG:HB3	1.90	0.52
1:B:181:THR:OG1	1:B:222:ARG:NH1	2.35	0.52
1:A:86:ARG:O	1:A:97:SER:HA	2.09	0.52
1:C:133:LEU:CD2	1:C:200:MET:CE	2.85	0.52
1:C:133:LEU:CD2	1:C:200:MET:HE2	2.40	0.51
1:A:140:ARG:HH22	2:H:1:DT:C7	2.22	0.51
1:B:37:GLU:OE2	1:B:116:ILE:HD13	2.10	0.51
1:C:156:LEU:HD23	1:C:201:ILE:HD11	1.93	0.50
1:A:90:ALA:HB1	1:A:92:GLU:OE1	2.13	0.49
1:B:86:ARG:NE	2:E:5:DT:C7	2.76	0.49
1:A:85:TYR:HB3	1:A:176:HIS:HA	1.94	0.48
1:A:58:ILE:HD12	1:A:66:GLN:HG2	1.94	0.48
1:B:118:ASP:HB2	3:B:302:TMP:C2'	2.42	0.48
1:C:142:PRO:HB2	1:C:154:LEU:HD22	1.96	0.48
1:B:118:ASP:HB2	3:B:302:TMP:H2'2	1.94	0.48
1:B:144:ILE:O	1:B:145:ARG:HD3	2.12	0.48
1:A:84:GLU:OE1	1:A:102:LYS:NZ	2.35	0.47
2:F:1:DT:H4'	2:F:2:DT:OP1	2.14	0.47
1:B:165:GLN:NE2	1:B:171:ARG:HG2	2.24	0.47
1:A:3:ARG:HG2	1:A:4:GLY:N	2.29	0.46
1:B:20:LEU:HD22	1:B:67:ALA:CB	2.46	0.46
1:C:55:ARG:HH12	3:C:302:TMP:H51	1.79	0.46
1:C:139:THR:O	2:F:2:DT:H5'	2.15	0.46
1:C:166:ASP:OD2	1:C:170:GLN:HB2	2.16	0.46
1:C:61:LYS:N	1:C:62:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HH22	1:C:100:ASN:HB2	1.82	0.45
1:B:195:LYS:HE2	2:I:2:DT:H5'	1.99	0.45
1:C:152:ALA:O	1:C:184:ARG:N	2.50	0.44
1:C:116:ILE:CD1	1:C:126:SER:HB3	2.47	0.44
1:C:3:ARG:HH11	2:F:3:DT:H2''	1.83	0.44
1:C:14:LEU:HD22	1:C:32:ALA:HB1	1.99	0.44
1:B:119:ALA:HB3	3:B:302:TMP:H2'1	1.98	0.44
1:A:164:TYR:CE2	1:A:172:GLN:HB2	2.53	0.44
1:B:145:ARG:HD2	1:B:145:ARG:HA	1.74	0.43
1:C:116:ILE:N	1:C:116:ILE:HD12	2.33	0.43
1:B:13:ALA:HB2	1:B:125:MET:HB2	1.99	0.43
1:C:164:TYR:HB2	4:C:320:HOH:O	2.18	0.43
2:I:1:DT:P	2:I:1:DT:H3'	2.58	0.43
1:A:61:LYS:N	1:A:62:PRO:CD	2.81	0.42
1:A:41:ILE:HG13	1:A:41:ILE:H	1.44	0.42
1:C:58:ILE:HG12	1:C:103:ALA:HB3	2.00	0.42
1:A:194:ARG:HD3	1:A:194:ARG:HA	1.86	0.42
3:B:302:TMP:H6	3:B:302:TMP:H2'2	1.74	0.42
1:C:30:PHE:O	1:C:57:SER:HA	2.19	0.42
1:C:205:LEU:HD11	1:C:221:THR:HG22	2.01	0.42
1:B:147:THR:O	1:B:148:PRO:C	2.57	0.42
1:A:182:LEU:O	1:A:187:ALA:HB2	2.20	0.41
1:B:20:LEU:HD22	1:B:67:ALA:HB2	2.03	0.41
1:C:55:ARG:HB3	1:C:100:ASN:HD22	1.85	0.41
1:C:86:ARG:NH2	4:C:313:HOH:O	2.53	0.41
1:B:130:ASN:O	1:B:204:ARG:HD3	2.21	0.41
1:C:116:ILE:HD13	1:C:126:SER:HB3	2.02	0.41
1:B:202:MET:HG2	1:B:227:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	203/301 (67%)	197 (97%)	5 (2%)	1 (0%)	29	41
1	B	208/301 (69%)	200 (96%)	7 (3%)	1 (0%)	29	41
1	C	206/301 (68%)	200 (97%)	6 (3%)	0	100	100
All	All	617/903 (68%)	597 (97%)	18 (3%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	B	167	ARG

### 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	169/233 (72%)	160 (95%)	9 (5%)	22	37
1	B	172/233 (74%)	162 (94%)	10 (6%)	20	32
1	C	172/233 (74%)	163 (95%)	9 (5%)	23	38
All	All	513/699 (73%)	485 (94%)	28 (6%)	21	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	48	ARG
1	A	143	GLU
1	A	185	ASP
1	A	191	LYS
1	A	199	VAL
1	A	202	MET
1	A	222	ARG
1	A	233	ARG
1	B	66	GLN
1	B	87	GLN

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Mol	Chain	Res	Type
1	B	96	ARG
1	B	140	ARG
1	B	148	PRO
1	B	157	SER
1	B	200	MET
1	B	202	MET
1	B	206	VAL
1	B	233	ARG
1	C	25	ASN
1	C	61	LYS
1	C	104	LEU
1	C	105	ARG
1	C	117	GLN
1	C	133	LEU
1	C	154	LEU
1	C	185	ASP
1	C	200	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	B	165	GLN
1	B	172	GLN
1	B	219	ASN
1	C	87	GLN
1	C	117	GLN
1	C	163	ASN
1	C	165	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	TMP	A	302	-	19,22,22	1.09	1 (5%)	23,33,33	1.82	2 (8%)
3	TMP	B	303	-	19,22,22	1.10	1 (5%)	23,33,33	1.79	1 (4%)
3	TMP	B	302	-	19,22,22	1.05	1 (5%)	23,33,33	2.02	2 (8%)
3	TMP	C	302	-	19,22,22	1.11	1 (5%)	23,33,33	1.85	2 (8%)

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	TMP	A	302	-	-	3/7/22/22	0/2/2/2
3	TMP	B	303	-	-	7/7/22/22	0/2/2/2
3	TMP	B	302	-	-	2/7/22/22	0/2/2/2
3	TMP	C	302	-	-	6/7/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	TMP	C4-C5	4.13	1.50	1.41
3	B	303	TMP	C4-C5	3.96	1.49	1.41
3	B	302	TMP	C4-C5	3.80	1.49	1.41
3	A	302	TMP	C4-C5	3.78	1.49	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	TMP	C4-N3-C2	8.24	122.10	115.14
3	C	302	TMP	C4-N3-C2	7.76	121.69	115.14
3	A	302	TMP	C4-N3-C2	7.42	121.41	115.14
3	B	303	TMP	C4-N3-C2	7.25	121.26	115.14
3	C	302	TMP	P-O5'-C5'	2.26	124.53	118.30
3	B	302	TMP	O5'-P-O1P	-2.16	100.42	106.47
3	A	302	TMP	C2'-C3'-C4'	2.10	107.14	102.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	TMP	C3'-C4'-C5'-O5'
3	B	303	TMP	C5'-O5'-P-O1P
3	B	303	TMP	C5'-O5'-P-O2P
3	B	303	TMP	C5'-O5'-P-O3P
3	B	303	TMP	O4'-C1'-N1-C6
3	B	302	TMP	C3'-C4'-C5'-O5'
3	C	302	TMP	C5'-O5'-P-O1P
3	C	302	TMP	C5'-O5'-P-O2P
3	C	302	TMP	C5'-O5'-P-O3P
3	C	302	TMP	O4'-C4'-C5'-O5'
3	C	302	TMP	C3'-C4'-C5'-O5'
3	A	302	TMP	O4'-C4'-C5'-O5'
3	B	303	TMP	C3'-C4'-C5'-O5'
3	B	302	TMP	O4'-C4'-C5'-O5'
3	B	303	TMP	O4'-C4'-C5'-O5'
3	C	302	TMP	C4'-C5'-O5'-P
3	A	302	TMP	C4'-C5'-O5'-P
3	B	303	TMP	C4'-C5'-O5'-P

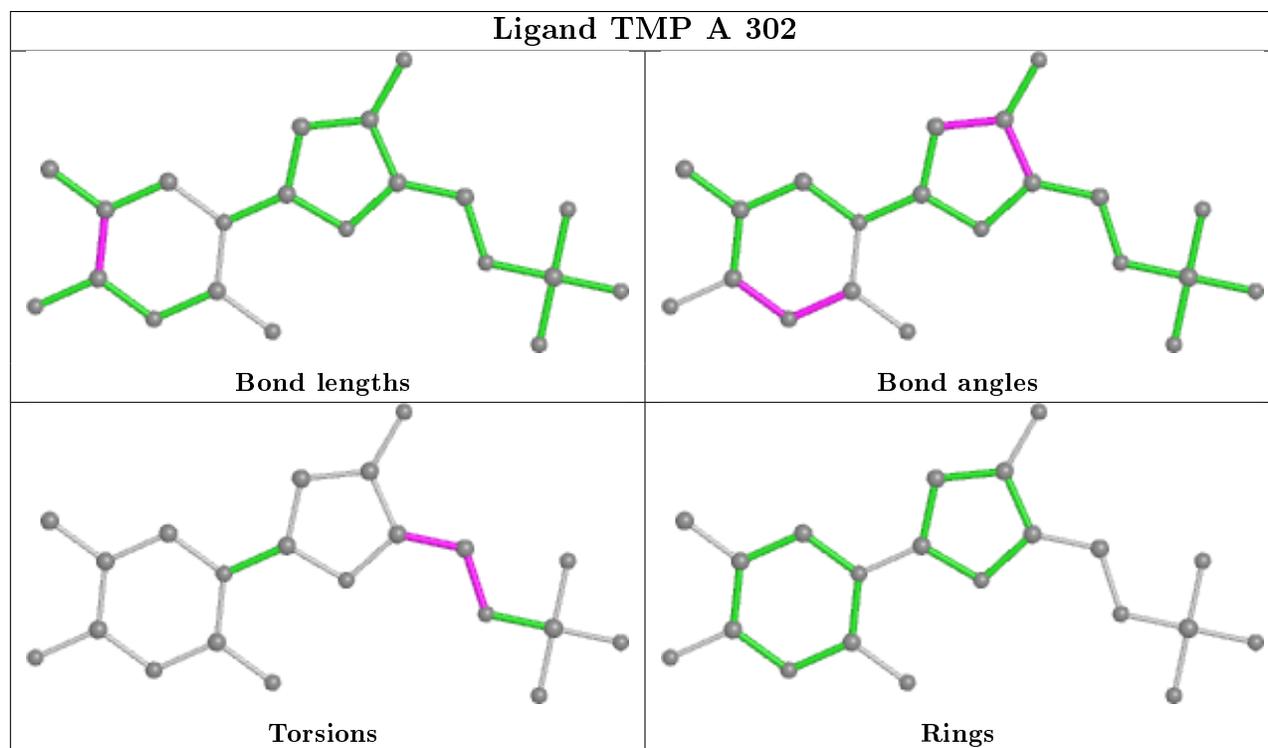
There are no ring outliers.

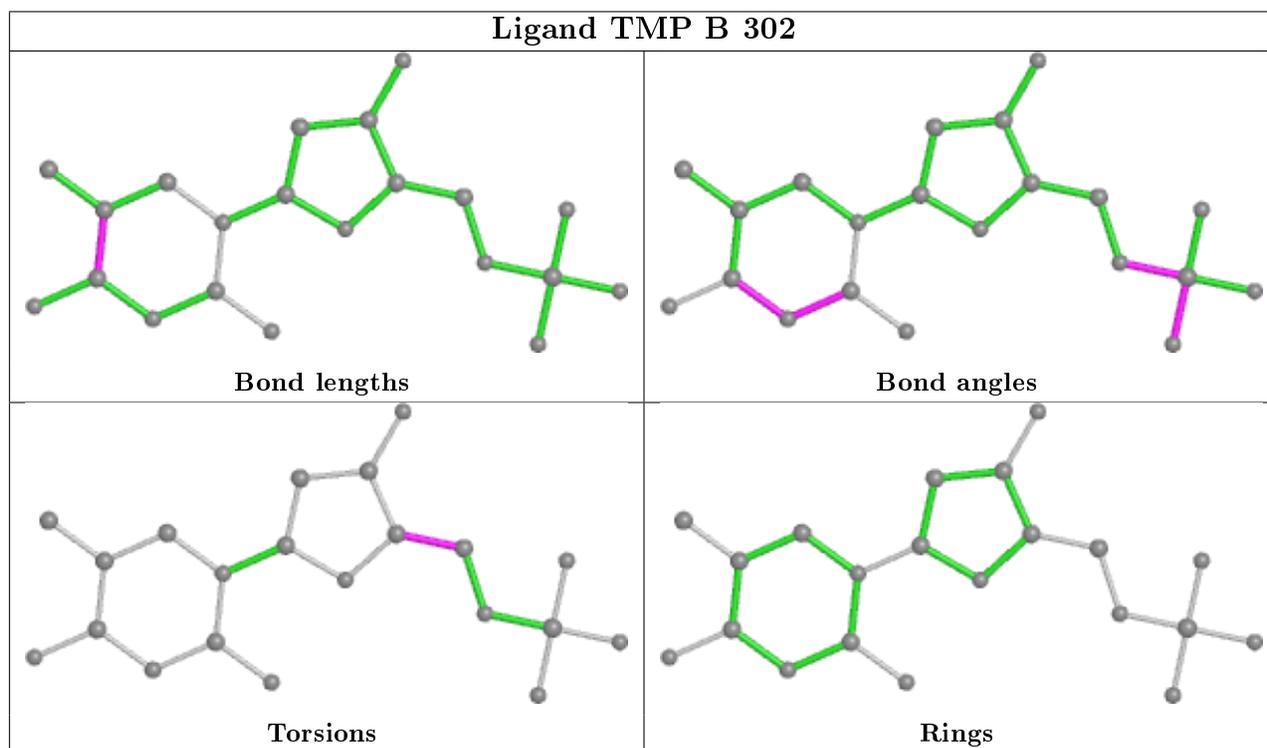
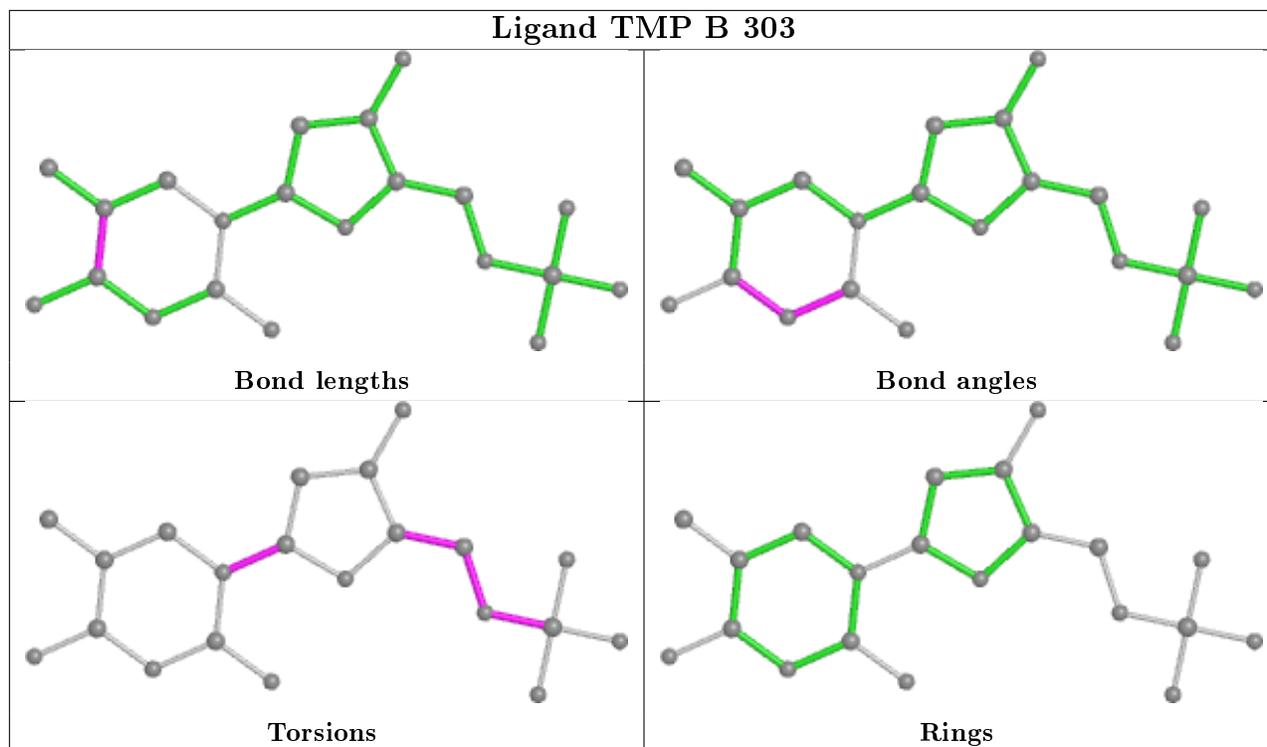
3 monomers are involved in 8 short contacts:

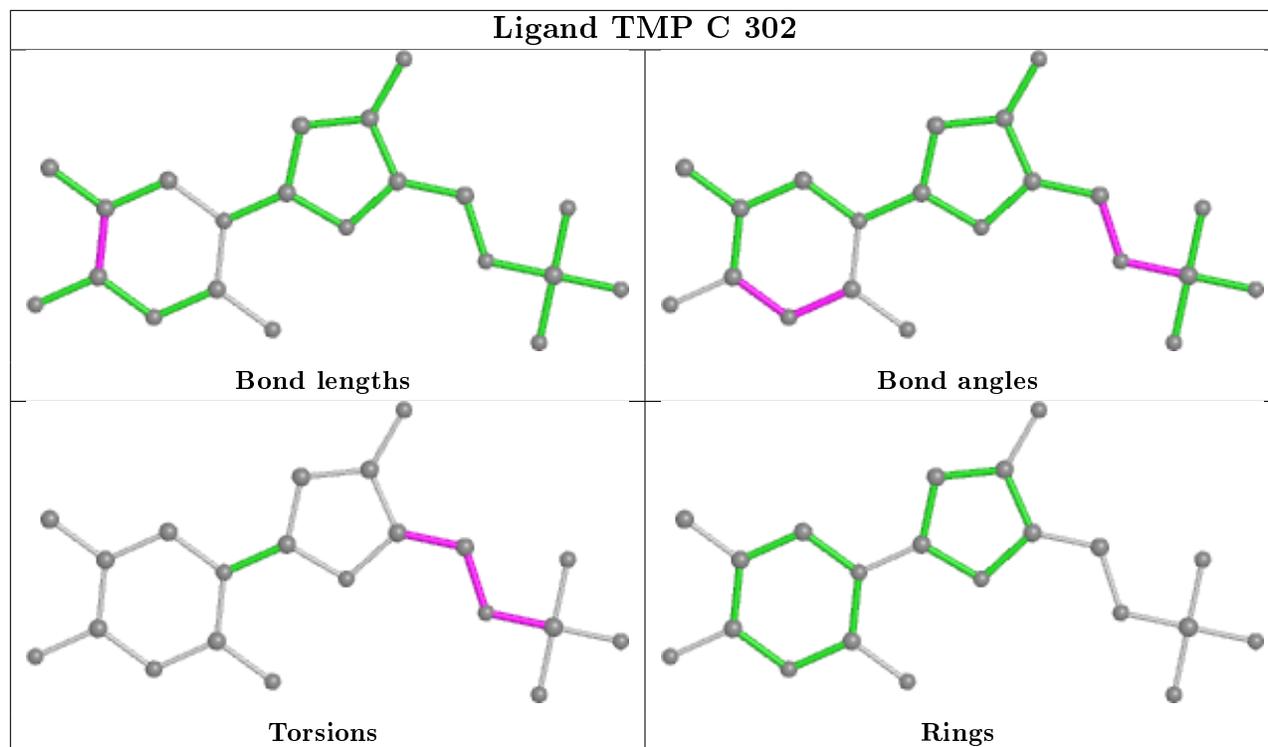
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	TMP	1	0
3	B	302	TMP	6	0
3	C	302	TMP	1	0

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, 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	211/301 (70%)	0.24	9 (4%) 35 33	23, 41, 72, 109	0
1	B	214/301 (71%)	0.30	11 (5%) 28 26	24, 46, 78, 108	0
1	C	214/301 (71%)	0.73	34 (15%) 1 1	33, 59, 100, 121	0
2	D	5/35 (14%)	-0.55	0 100 100	56, 63, 76, 117	0
2	E	5/35 (14%)	-0.32	0 100 100	40, 54, 64, 101	0
2	F	4/35 (11%)	1.60	1 (25%) 0 0	78, 89, 101, 125	1 (25%)
2	G	5/35 (14%)	-0.39	0 100 100	56, 60, 76, 101	0
2	H	3/35 (8%)	0.75	0 100 100	64, 64, 81, 86	0
2	I	3/35 (8%)	0.61	0 100 100	66, 66, 72, 81	1 (33%)
All	All	664/1113 (59%)	0.42	55 (8%) 11 10	23, 49, 92, 125	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLU	6.6
1	A	171	ARG	6.2
1	C	170	GLN	5.5
1	A	41	ILE	5.4
1	B	167	ARG	5.0
1	A	42	GLY	4.7
1	C	119	ALA	4.6
1	C	171	ARG	4.4
1	B	218	ARG	4.3
1	A	48	ARG	4.1
1	C	40	VAL	4.0
1	C	48	ARG	4.0
1	C	146	TYR	3.8
1	C	152	ALA	3.7
1	B	171	ARG	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	170	GLN	3.5
1	C	233	ARG	3.5
1	C	120	GLY	3.5
1	C	117	GLN	3.4
1	C	149	ALA	3.4
1	C	169	GLY	3.3
1	C	150	GLY	3.2
1	C	121	GLY	3.0
1	B	233	ARG	3.0
1	C	94	GLY	2.9
1	B	40	VAL	2.9
1	C	16	ARG	2.8
1	B	48	ARG	2.8
1	B	170	GLN	2.8
1	C	83	LEU	2.8
1	C	49	ASN	2.7
1	B	168	GLN	2.7
1	C	39	ARG	2.6
1	B	47	GLU	2.6
1	C	50	LEU	2.6
1	C	151	ASP	2.6
1	A	79	VAL	2.5
1	C	165	GLN	2.5
1	C	172	GLN	2.5
1	C	148	PRO	2.4
1	A	47	GLU	2.4
1	C	123	VAL	2.4
1	C	82	THR	2.4
1	C	41	ILE	2.3
2	F	5	DT	2.3
1	A	40	VAL	2.2
1	B	219	ASN	2.2
1	C	9	TYR	2.2
1	C	81	GLY	2.2
1	C	118	ASP	2.1
1	B	173	GLU	2.1
1	C	8	VAL	2.1
1	A	173	GLU	2.1
1	C	124	ARG	2.0
1	C	10	LEU	2.0

## 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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

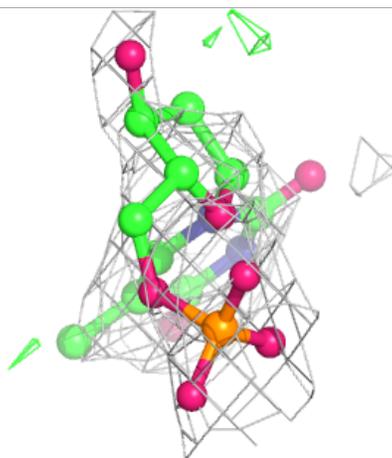
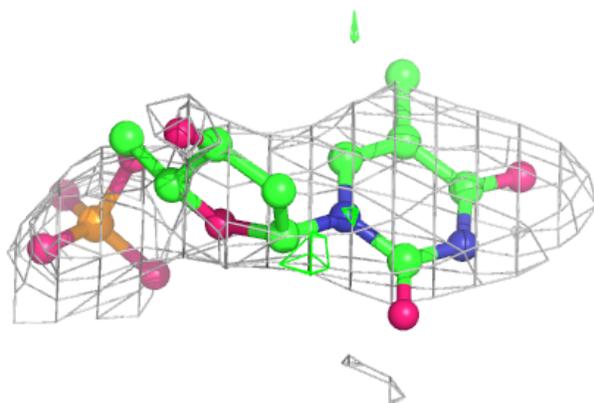
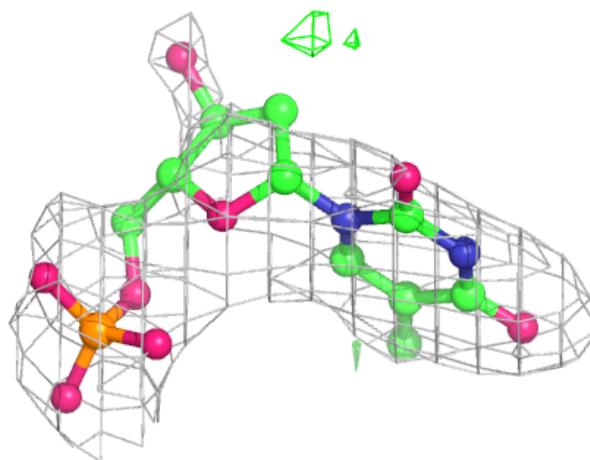
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	TMP	C	302	21/21	0.69	0.23	80,118,141,145	0
3	TMP	B	303	21/21	0.73	0.30	71,103,132,136	0
3	TMP	B	302	21/21	0.73	0.25	82,97,109,115	0
3	TMP	A	302	21/21	0.73	0.29	89,108,119,123	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.

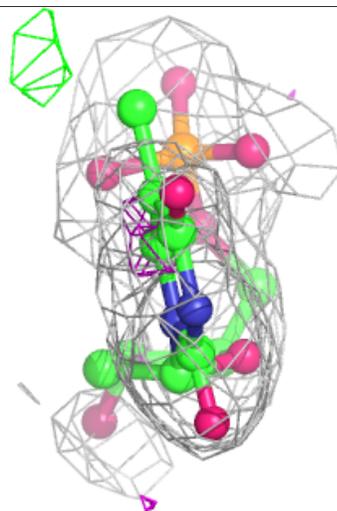
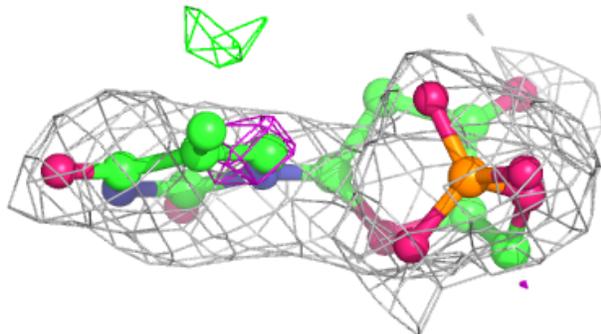
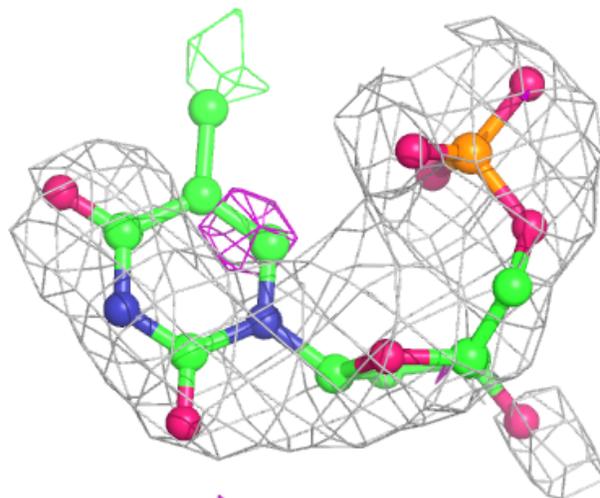
**Electron density around TMP C 302:**

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



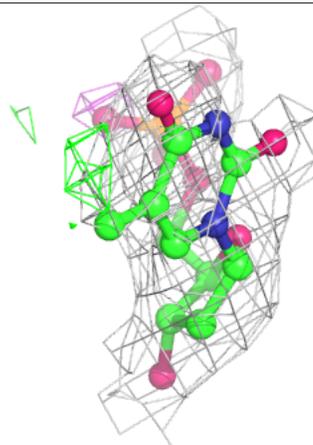
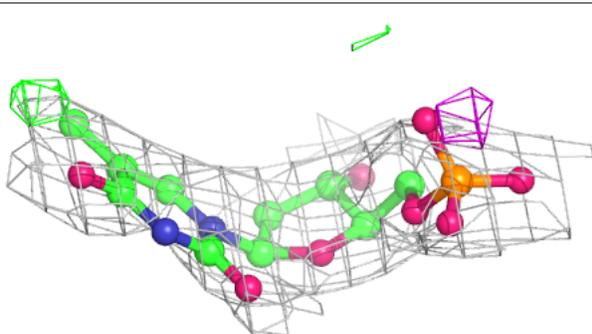
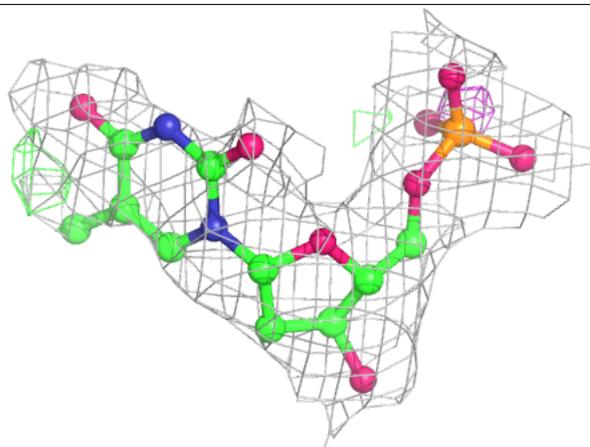
**Electron density around TMP B 303:**

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

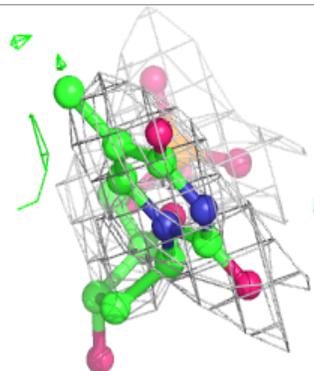
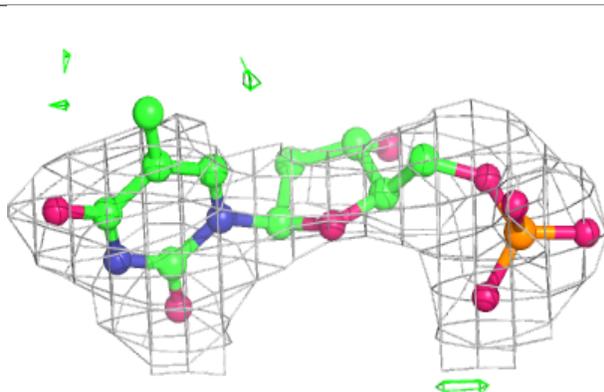
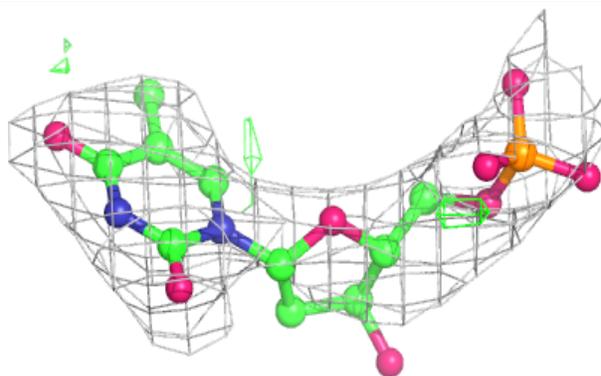


**Electron density around TMP B 302:**

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

**Electron density around TMP A 302:**

$2mF_o-DF_c$  (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.