



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 7XYJ / pdb_00007xyj
Title : Structure of WSSV thymidylate synthase in complex with dUMP
Authors : Ma, Q.; Liu, C.; Zang, K.
Deposited on : 2022-06-01
Resolution : 2.27 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

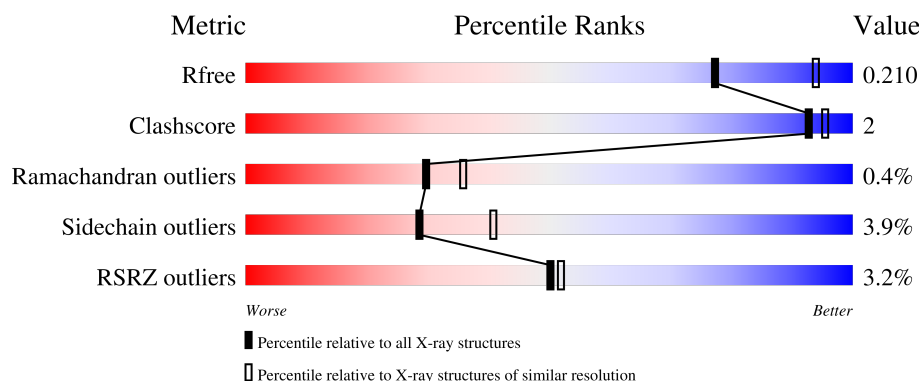
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	292	3% 87% 9% ..
1	B	292	3% 88% 8% .
1	C	292	2% 88% 8% .
1	D	292	4% 84% 10% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9433 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.

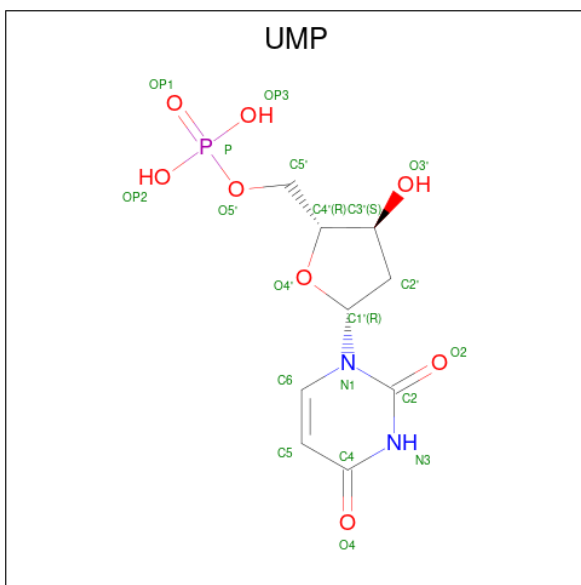
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2277	1454	395	413	15			
1	B	279	Total	C	N	O	S	0	0	0
			2250	1439	390	407	14			
1	C	280	Total	C	N	O	S	0	0	0
			2258	1444	391	408	15			
1	D	278	Total	C	N	O	S	0	0	0
			2241	1434	389	404	14			

There are 12 discrepancies between the modelled and reference sequences:

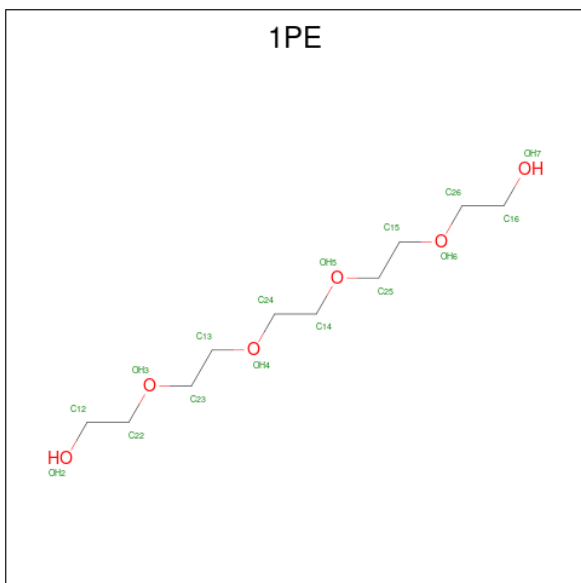
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q77J90
A	-1	ASN	-	expression tag	UNP Q77J90
A	0	ALA	-	expression tag	UNP Q77J90
B	-2	SER	-	expression tag	UNP Q77J90
B	-1	ASN	-	expression tag	UNP Q77J90
B	0	ALA	-	expression tag	UNP Q77J90
C	-2	SER	-	expression tag	UNP Q77J90
C	-1	ASN	-	expression tag	UNP Q77J90
C	0	ALA	-	expression tag	UNP Q77J90
D	-2	SER	-	expression tag	UNP Q77J90
D	-1	ASN	-	expression tag	UNP Q77J90
D	0	ALA	-	expression tag	UNP Q77J90

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



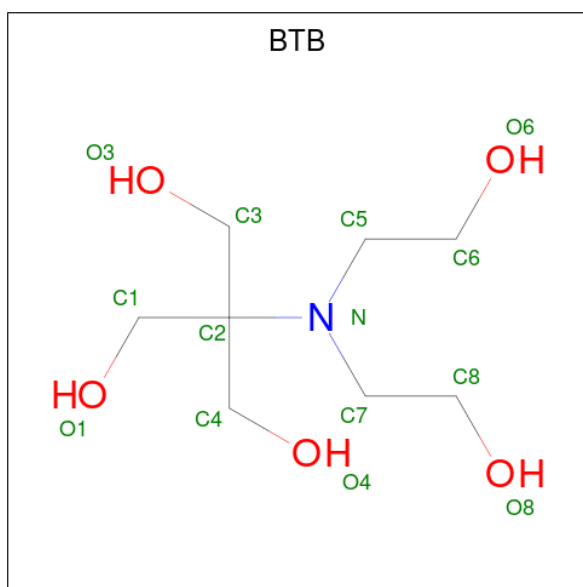
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	1
			32	20	12		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0

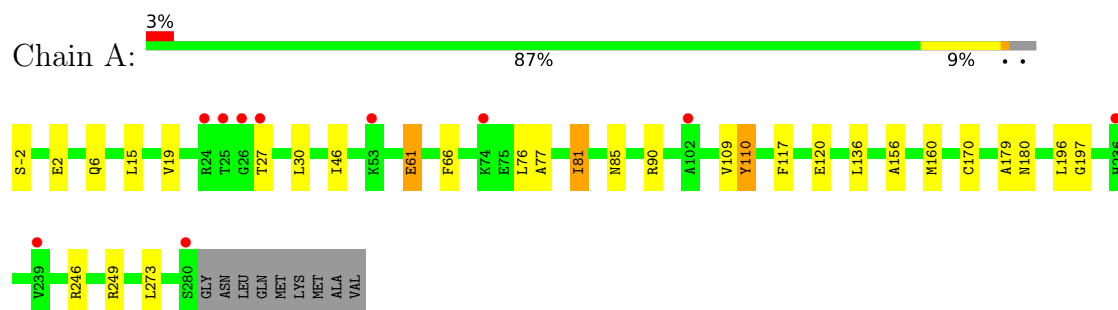
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	B	57	Total O 57 57	0	0
6	C	40	Total O 40 40	0	0
6	D	62	Total O 62 62	0	0

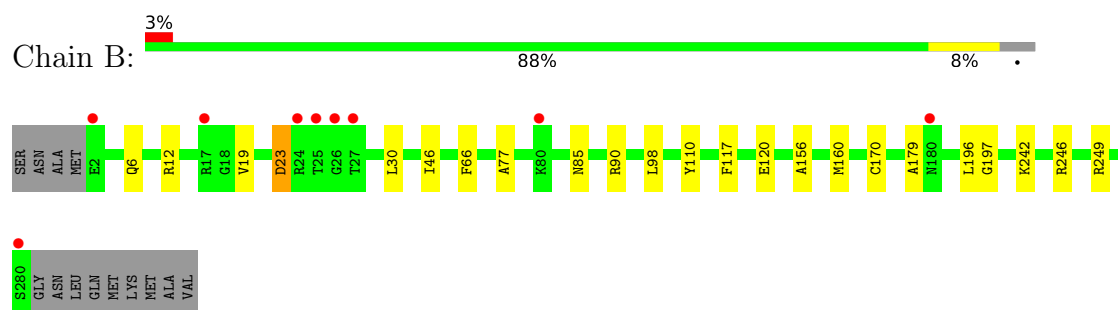
3 Residue-property plots [i](#)

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.

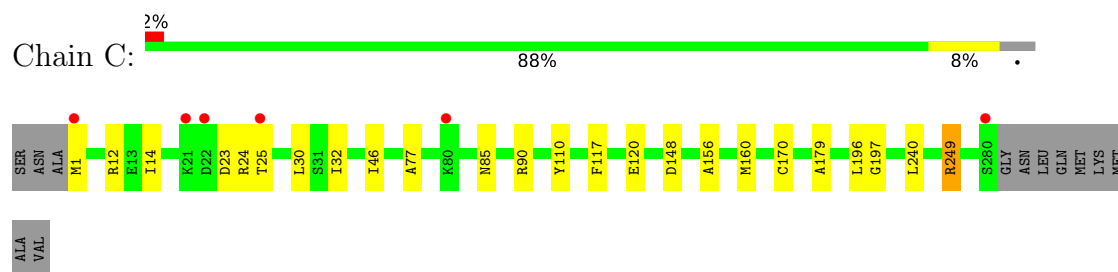
• Molecule 1: Thymidylate synthase



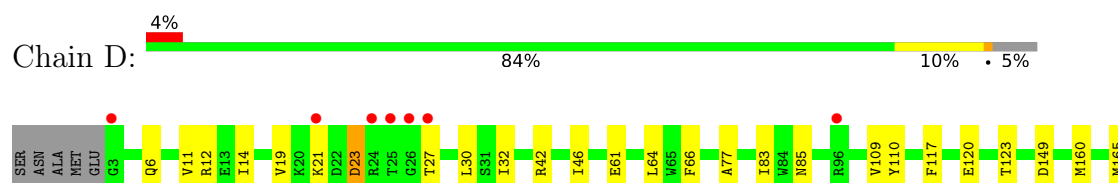
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.91Å 132.35Å 234.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.05 – 2.27 117.05 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.3 (117.05-2.27) 99.9 (117.05-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.188 , 0.208 0.190 , 0.210	Depositor DCC
R_{free} test set	3955 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9433	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6160e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1PE, BTB, UMP, SO4

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	0.81	0/2333	1.28	13/3154 (0.4%)
1	B	0.85	0/2306	1.26	9/3118 (0.3%)
1	C	0.82	0/2314	1.28	7/3128 (0.2%)
1	D	0.87	1/2297 (0.0%)	1.28	14/3106 (0.5%)
All	All	0.84	1/9250 (0.0%)	1.27	43/12506 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	196	LEU	CA-C	5.33	1.57	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	GLY	CA-C-N	7.58	126.39	120.33
1	C	197	GLY	C-N-CA	7.58	126.39	120.33
1	A	197	GLY	CA-C-N	6.14	125.25	120.33
1	A	197	GLY	C-N-CA	6.14	125.25	120.33
1	C	30	LEU	N-CA-C	-6.07	99.30	109.07
1	D	6	GLN	N-CA-C	-6.06	104.36	110.97
1	D	23	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	46	ILE	CB-CA-C	6.03	116.25	110.16
1	B	30	LEU	N-CA-C	-6.00	99.41	109.07
1	D	30	LEU	N-CA-C	-5.95	99.49	109.07
1	B	197	GLY	CA-C-N	5.91	125.06	120.33
1	B	197	GLY	C-N-CA	5.91	125.06	120.33
1	D	197	GLY	CA-C-N	5.86	125.02	120.33
1	D	197	GLY	C-N-CA	5.86	125.02	120.33
1	D	249	ARG	N-CA-C	-5.86	102.72	110.40
1	B	23	ASP	CA-CB-CG	5.73	118.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	30	LEU	N-CA-C	-5.62	100.03	109.07
1	D	66	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	23	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	46	ILE	CB-CA-C	5.54	115.75	110.16
1	B	249	ARG	N-CA-C	-5.46	103.24	110.40
1	A	180	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	66	PHE	CA-CB-CG	5.38	119.18	113.80
1	C	46	ILE	CB-CA-C	5.33	115.55	110.16
1	A	249	ARG	N-CA-C	-5.32	103.43	110.40
1	B	46	ILE	CB-CA-C	5.27	115.48	110.16
1	D	171	HIS	N-CA-C	-5.25	99.21	108.23
1	B	156	ALA	N-CA-C	-5.18	106.98	113.72
1	C	249	ARG	N-CA-C	-5.16	103.64	110.40
1	D	11	VAL	CA-C-N	5.16	127.50	120.54
1	D	11	VAL	C-N-CA	5.16	127.50	120.54
1	A	61	GLU	CB-CG-CD	5.13	121.32	112.60
1	D	109	VAL	CA-C-N	5.11	131.31	121.54
1	D	109	VAL	C-N-CA	5.11	131.31	121.54
1	A	109	VAL	CA-C-N	5.11	131.29	121.54
1	A	109	VAL	C-N-CA	5.11	131.29	121.54
1	B	6	GLN	CB-CG-CD	-5.10	103.92	112.60
1	C	156	ALA	N-CA-C	-5.08	107.11	113.72
1	D	61	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	110	TYR	CA-C-N	5.08	125.72	120.03
1	A	110	TYR	C-N-CA	5.08	125.72	120.03
1	A	156	ALA	N-CA-C	-5.00	107.21	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2277	0	2257	11	0
1	B	2250	0	2229	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2258	0	2241	11	0
1	D	2241	0	2223	13	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
3	A	16	0	22	0	0
3	B	32	0	44	0	0
3	C	16	0	22	0	0
3	D	16	0	22	1	0
4	A	5	0	0	0	0
4	C	20	0	0	0	0
5	C	14	0	19	0	0
5	D	14	0	19	2	0
6	A	35	0	0	0	0
6	B	57	0	0	0	0
6	C	40	0	0	0	0
6	D	62	0	0	0	0
All	All	9433	0	9142	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (28) 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:D:83:ILE:HD12	3:D:302:1PE:H142	1.69	0.73
1:A:160:MET:HE1	1:B:160:MET:HE1	1.73	0.69
1:C:160:MET:HE1	1:D:160:MET:HE1	1.79	0.65
1:A:117:PHE:HE1	1:B:160:MET:HE2	1.65	0.62
1:A:179:ALA:HB1	1:B:19:VAL:HG21	1.83	0.61
1:C:117:PHE:HE1	1:D:160:MET:HE2	1.66	0.60
1:A:19:VAL:HG21	1:B:179:ALA:HB1	1.83	0.60
1:A:160:MET:HE2	1:B:117:PHE:HE1	1.67	0.58
1:A:2:GLU:HB3	1:A:6:GLN:HG3	1.89	0.55
1:A:-2:SER:O	1:C:24:ARG:HD3	2.08	0.54
1:C:160:MET:HE2	1:D:117:PHE:HE1	1.72	0.54
1:C:148:ASP:HA	1:D:21:LYS:HZ1	1.73	0.53
1:A:77:ALA:HB2	1:A:85:ASN:HD21	1.73	0.52
1:C:117:PHE:CE1	1:D:160:MET:HE2	2.45	0.51
1:B:77:ALA:HB2	1:B:85:ASN:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ALA:HB2	1:D:85:ASN:HD21	1.77	0.49
1:C:148:ASP:HA	1:D:21:LYS:NZ	2.28	0.48
1:D:149:ASP:OD1	5:D:303:BTB:H31	2.15	0.47
1:C:179:ALA:HB1	1:D:19:VAL:HG21	1.96	0.47
1:A:117:PHE:CE1	1:B:160:MET:HE2	2.47	0.47
5:D:303:BTB:H71	5:D:303:BTB:H32	1.61	0.46
1:C:160:MET:HE2	1:D:117:PHE:CE1	2.52	0.45
1:A:61:GLU:HB2	1:A:81:ILE:HD13	2.00	0.43
1:A:160:MET:HE2	1:B:117:PHE:CE1	2.49	0.43
1:C:77:ALA:HB2	1:C:85:ASN:HD21	1.84	0.42
1:D:165:MET:SD	1:D:169:PRO:HD3	2.60	0.42
1:C:14:ILE:HG12	1:C:32:ILE:HG12	2.03	0.41
1:D:14:ILE:HG12	1:D:32:ILE:HG12	2.02	0.41

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	281/292 (96%)	272 (97%)	8 (3%)	1 (0%)	30	36
1	B	277/292 (95%)	268 (97%)	8 (3%)	1 (0%)	30	36
1	C	278/292 (95%)	271 (98%)	6 (2%)	1 (0%)	30	36
1	D	276/292 (94%)	267 (97%)	8 (3%)	1 (0%)	30	36
All	All	1112/1168 (95%)	1078 (97%)	30 (3%)	4 (0%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	B	110	TYR

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Mol	Chain	Res	Type
1	C	110	TYR
1	D	110	TYR

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	245/252 (97%)	234 (96%)	11 (4%)	24	35
1	B	242/252 (96%)	233 (96%)	9 (4%)	30	43
1	C	243/252 (96%)	234 (96%)	9 (4%)	30	43
1	D	241/252 (96%)	232 (96%)	9 (4%)	30	43
All	All	971/1008 (96%)	933 (96%)	38 (4%)	28	41

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	27	THR
1	A	76	LEU
1	A	81	ILE
1	A	90	ARG
1	A	120	GLU
1	A	136	LEU
1	A	170	CYS
1	A	196	LEU
1	A	246	ARG
1	A	273	LEU
1	B	12	ARG
1	B	23	ASP
1	B	90	ARG
1	B	98	LEU
1	B	120	GLU
1	B	170	CYS
1	B	196	LEU
1	B	242	LYS

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Mol	Chain	Res	Type
1	B	246	ARG
1	C	1	MET
1	C	12	ARG
1	C	25	THR
1	C	90	ARG
1	C	120	GLU
1	C	170	CYS
1	C	196	LEU
1	C	240	LEU
1	C	249	ARG
1	D	12	ARG
1	D	23	ASP
1	D	27	THR
1	D	42	ARG
1	D	64	LEU
1	D	120	GLU
1	D	123	THR
1	D	170	CYS
1	D	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	36	GLN
1	A	85	ASN
1	A	87	ASN
1	A	186	GLN
1	B	85	ASN
1	B	180	ASN
1	C	85	ASN
1	C	146	ASN
1	D	85	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	1PE	A	302	-	15,15,15	0.26	0	14,14,14	0.15	0
3	1PE	B	302[A]	-	15,15,15	0.21	0	14,14,14	0.13	0
4	SO4	C	306	-	4,4,4	0.33	0	6,6,6	0.04	0
4	SO4	C	305	-	4,4,4	0.28	0	6,6,6	0.06	0
3	1PE	B	302[B]	-	15,15,15	0.24	0	14,14,14	0.12	0
4	SO4	C	304	-	4,4,4	0.29	0	6,6,6	0.20	0
2	UMP	B	301	-	21,21,21	0.30	0	30,31,31	0.30	0
3	1PE	C	302	-	15,15,15	0.36	0	14,14,14	0.31	0
2	UMP	A	301	-	21,21,21	0.46	0	30,31,31	0.33	0
4	SO4	C	307	-	4,4,4	0.28	0	6,6,6	0.14	0
3	1PE	D	302	-	15,15,15	0.23	0	14,14,14	0.16	0
4	SO4	A	303	-	4,4,4	0.26	0	6,6,6	0.10	0
2	UMP	D	301	-	21,21,21	0.31	0	30,31,31	0.34	0
5	BTB	D	303	-	13,13,13	1.08	1 (7%)	7,16,16	1.20	0
2	UMP	C	301	-	21,21,21	0.37	0	30,31,31	0.41	0
5	BTB	C	303	-	13,13,13	1.19	1 (7%)	7,16,16	1.25	1 (14%)

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	1PE	A	302	-	-	8/13/13/13	-
3	1PE	B	302[A]	-	-	8/13/13/13	-
3	1PE	B	302[B]	-	-	7/13/13/13	-
2	UMP	B	301	-	-	0/10/22/22	0/2/2/2
3	1PE	C	302	-	-	9/13/13/13	-
2	UMP	A	301	-	-	0/10/22/22	0/2/2/2
5	BTB	D	303	-	-	11/21/21/21	-
3	1PE	D	302	-	-	4/13/13/13	-
2	UMP	D	301	-	-	0/10/22/22	0/2/2/2
2	UMP	C	301	-	-	0/10/22/22	0/2/2/2
5	BTB	C	303	-	-	9/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	303	BTB	C2-N	4.05	1.56	1.48
5	D	303	BTB	C2-N	3.63	1.55	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	BTB	O1-C1-C2	2.31	116.84	111.40

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	303	BTB	C4-C2-C3-O3
5	C	303	BTB	N-C2-C3-O3
5	C	303	BTB	C1-C2-N-C5
5	C	303	BTB	C3-C2-N-C5
5	C	303	BTB	C4-C2-N-C5
5	C	303	BTB	C4-C2-N-C7
5	D	303	BTB	O1-C1-C2-C3
5	D	303	BTB	O1-C1-C2-C4
5	D	303	BTB	O1-C1-C2-N
5	D	303	BTB	C1-C2-C3-O3
5	D	303	BTB	C4-C2-C3-O3
5	D	303	BTB	N-C2-C3-O3
5	D	303	BTB	C6-C5-N-C7
3	B	302[A]	1PE	OH5-C14-C24-OH4

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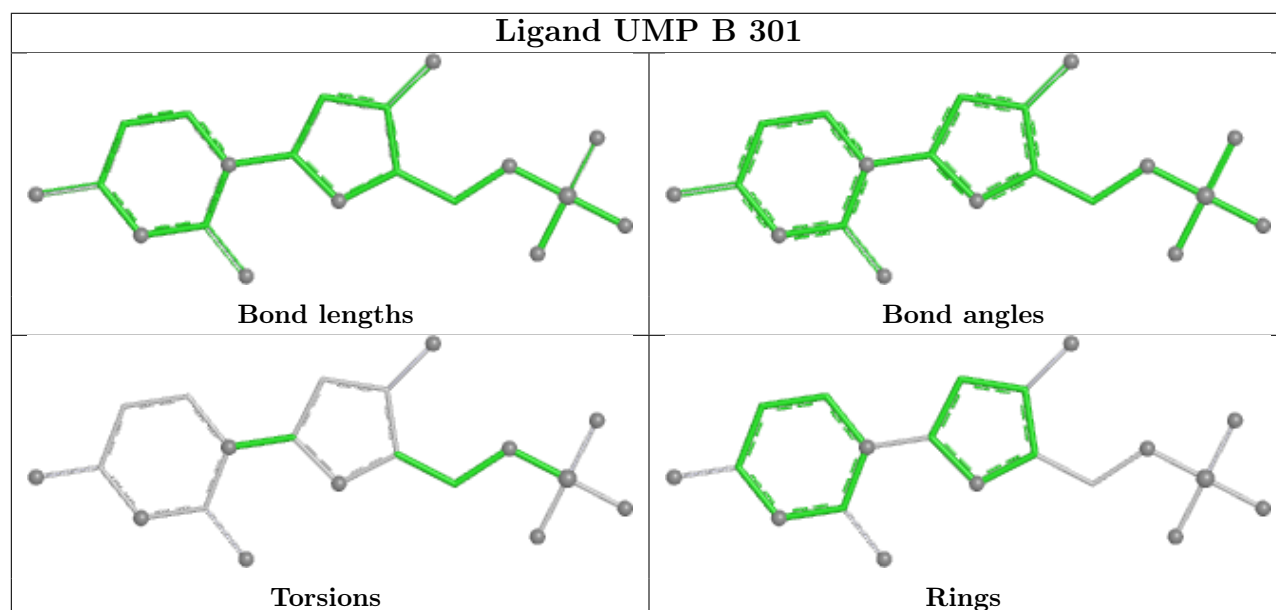
Mol	Chain	Res	Type	Atoms
3	C	302	1PE	OH6-C15-C25-OH5
3	D	302	1PE	OH2-C12-C22-OH3
3	A	302	1PE	OH6-C15-C25-OH5
3	B	302[B]	1PE	OH4-C13-C23-OH3
3	C	302	1PE	OH5-C14-C24-OH4
3	B	302[B]	1PE	OH5-C14-C24-OH4
3	D	302	1PE	OH6-C15-C25-OH5
3	A	302	1PE	C15-C25-OH5-C14
5	D	303	BTB	N-C7-C8-O8
3	A	302	1PE	C13-C23-OH3-C22
3	B	302[A]	1PE	C16-C26-OH6-C15
3	B	302[A]	1PE	C23-C13-OH4-C24
3	A	302	1PE	C12-C22-OH3-C23
3	A	302	1PE	C24-C14-OH5-C25
3	A	302	1PE	C23-C13-OH4-C24
3	B	302[B]	1PE	C12-C22-OH3-C23
3	C	302	1PE	OH7-C16-C26-OH6
3	B	302[B]	1PE	C15-C25-OH5-C14
3	C	302	1PE	C14-C24-OH4-C13
3	D	302	1PE	C12-C22-OH3-C23
3	B	302[A]	1PE	C13-C23-OH3-C22
5	C	303	BTB	C3-C2-N-C7
5	D	303	BTB	C1-C2-N-C7
5	D	303	BTB	C3-C2-N-C7
5	D	303	BTB	C4-C2-N-C7
3	C	302	1PE	C13-C23-OH3-C22
3	B	302[B]	1PE	C14-C24-OH4-C13
3	B	302[B]	1PE	C23-C13-OH4-C24
3	B	302[A]	1PE	OH4-C13-C23-OH3
3	C	302	1PE	C15-C25-OH5-C14
3	D	302	1PE	C25-C15-OH6-C26
3	A	302	1PE	C16-C26-OH6-C15
3	B	302[A]	1PE	C24-C14-OH5-C25
3	B	302[A]	1PE	C15-C25-OH5-C14
3	B	302[A]	1PE	C12-C22-OH3-C23
3	B	302[B]	1PE	C16-C26-OH6-C15
3	C	302	1PE	C16-C26-OH6-C15
3	C	302	1PE	C25-C15-OH6-C26
5	C	303	BTB	N-C5-C6-O6
3	A	302	1PE	OH4-C13-C23-OH3
5	C	303	BTB	C1-C2-N-C7
3	C	302	1PE	OH4-C13-C23-OH3

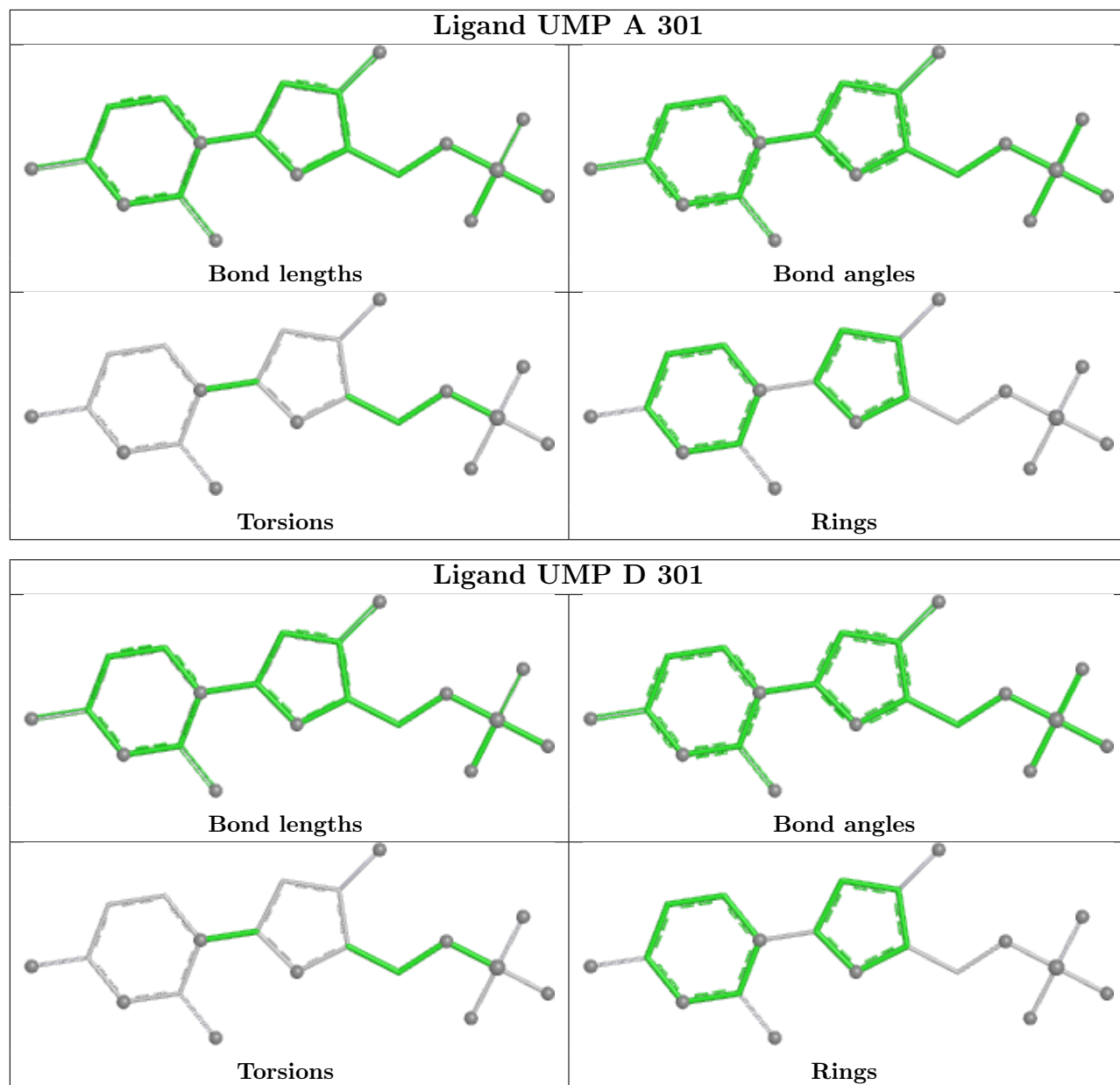
There are no ring outliers.

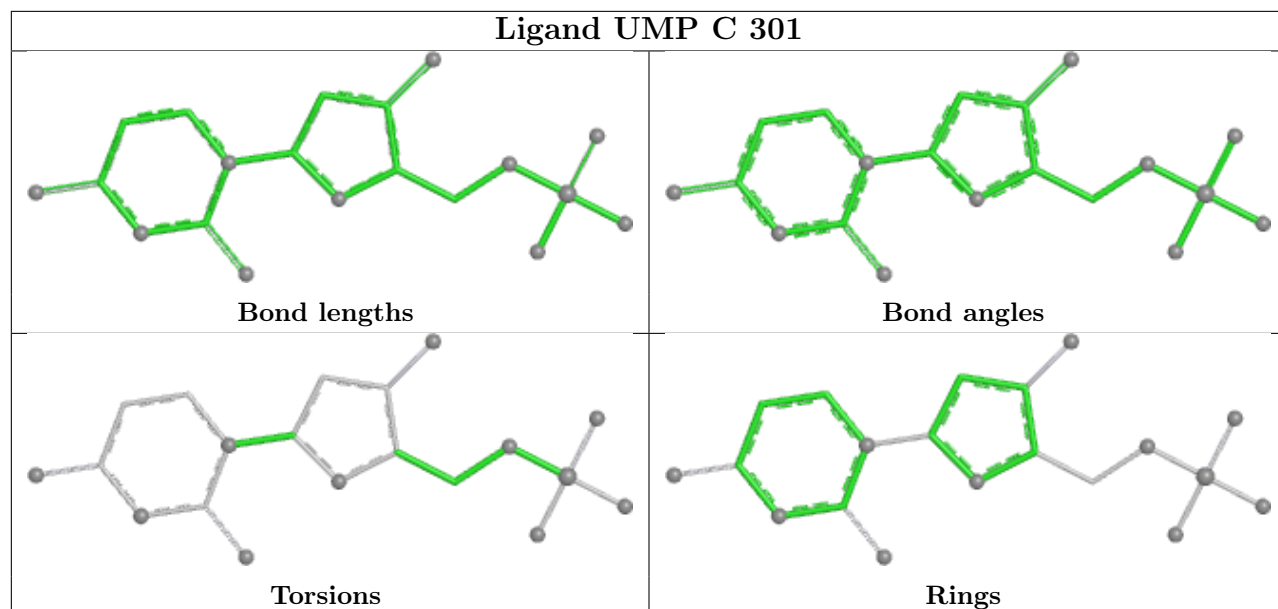
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	1PE	1	0
5	D	303	BTB	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/292 (96%)	0.23	10 (3%) 47 49	41, 61, 102, 120	0
1	B	279/292 (95%)	0.05	9 (3%) 50 52	39, 53, 90, 107	0
1	C	280/292 (95%)	0.11	6 (2%) 63 65	41, 57, 85, 108	0
1	D	278/292 (95%)	0.06	11 (3%) 42 44	38, 53, 90, 114	0
All	All	1120/1168 (95%)	0.11	36 (3%) 50 52	38, 56, 91, 120	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	SER	4.8
1	A	27	THR	4.6
1	D	280	SER	4.3
1	D	26	GLY	4.1
1	C	1	MET	4.1
1	C	280	SER	4.1
1	B	280	SER	3.9
1	C	25	THR	3.7
1	D	25	THR	3.6
1	B	27	THR	3.0
1	A	236	HIS	3.0
1	B	80	LYS	2.9
1	B	25	THR	2.8
1	A	26	GLY	2.8
1	D	24	ARG	2.8
1	D	235	THR	2.8
1	C	80	LYS	2.7
1	D	3	GLY	2.7
1	D	236	HIS	2.6
1	A	25	THR	2.6
1	A	24	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	27	THR	2.5
1	B	26	GLY	2.5
1	A	239	VAL	2.4
1	C	22	ASP	2.3
1	B	17	ARG	2.3
1	C	21	LYS	2.3
1	A	102	ALA	2.3
1	D	21	LYS	2.2
1	D	96	ARG	2.2
1	A	53	LYS	2.1
1	A	74	LYS	2.1
1	B	180	ASN	2.1
1	B	2	GLU	2.1
1	D	239	VAL	2.0
1	B	24	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

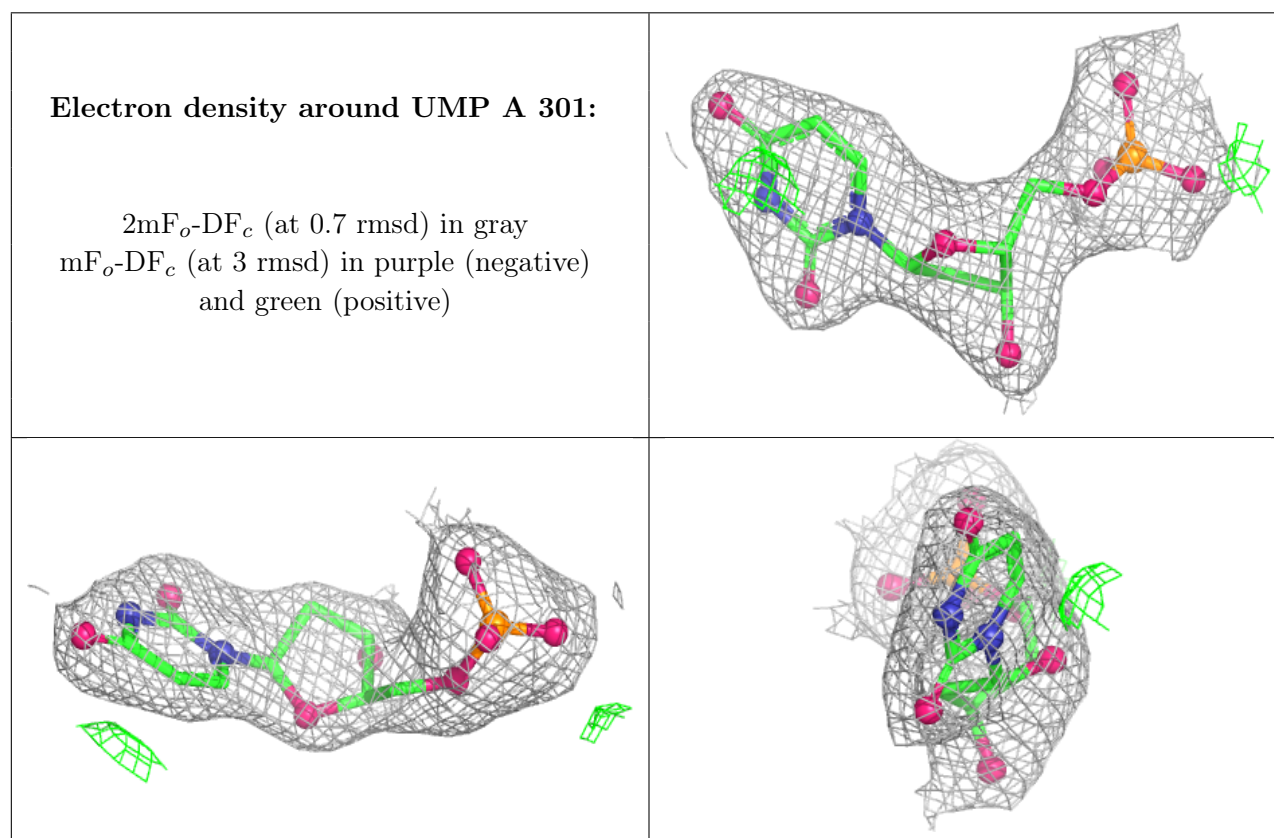
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	307	5/5	0.45	0.16	146,148,148,149	0
4	SO4	C	305	5/5	0.67	0.12	133,133,134,137	0
4	SO4	C	306	5/5	0.71	0.13	131,132,132,135	0
4	SO4	C	304	5/5	0.71	0.10	110,111,112,112	0
3	1PE	C	302	16/16	0.78	0.23	76,84,93,94	0
5	BTB	C	303	14/14	0.81	0.23	85,91,100,102	0
3	1PE	A	302	16/16	0.82	0.23	86,93,98,99	0
3	1PE	B	302[A]	16/16	0.83	0.24	55,72,76,76	16

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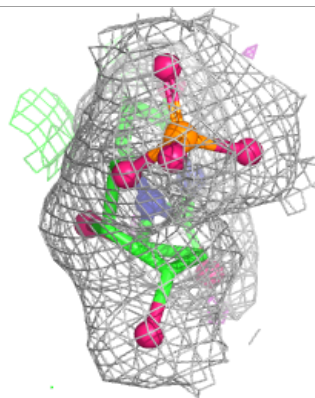
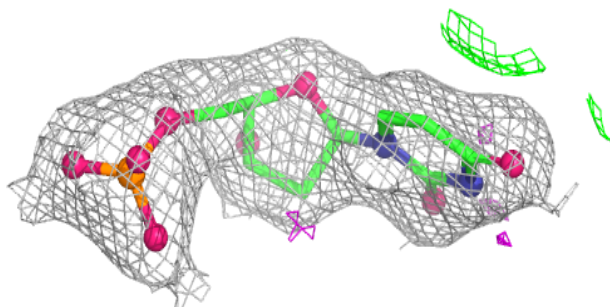
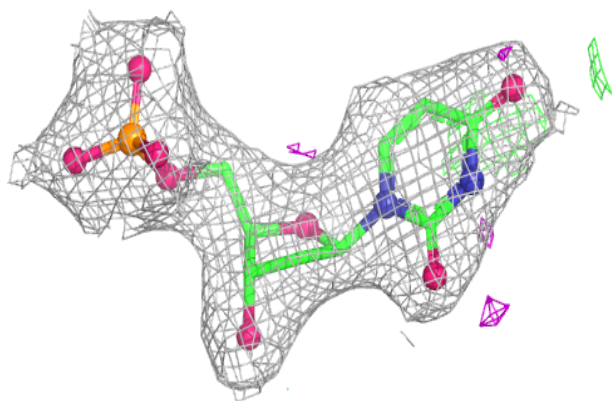
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1PE	B	302[B]	16/16	0.83	0.24	66,88,93,93	16
4	SO4	A	303	5/5	0.86	0.08	132,133,134,136	0
5	BTB	D	303	14/14	0.86	0.17	58,74,79,80	0
3	1PE	D	302	16/16	0.88	0.17	73,76,90,93	0
2	UMP	A	301	20/20	0.98	0.06	48,57,62,63	0
2	UMP	B	301	20/20	0.98	0.05	43,47,50,51	0
2	UMP	C	301	20/20	0.98	0.05	43,47,51,51	0
2	UMP	D	301	20/20	0.98	0.05	49,54,58,58	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.

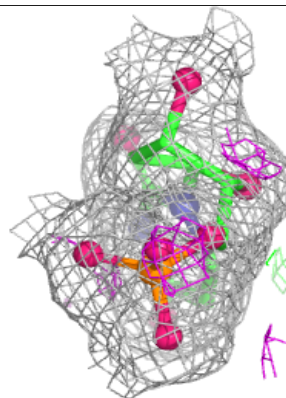
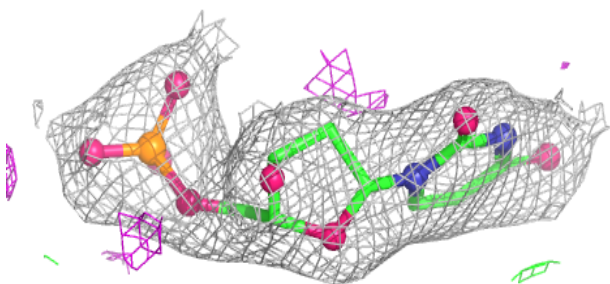
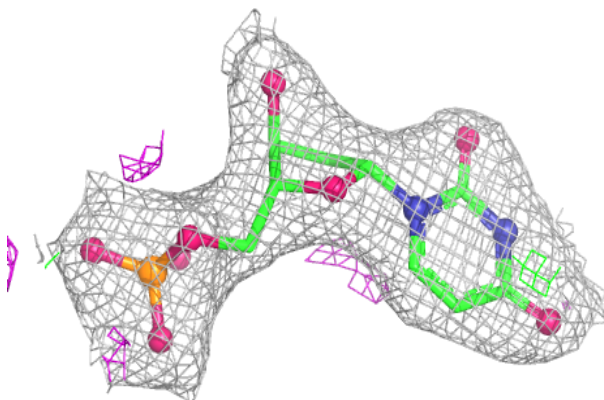


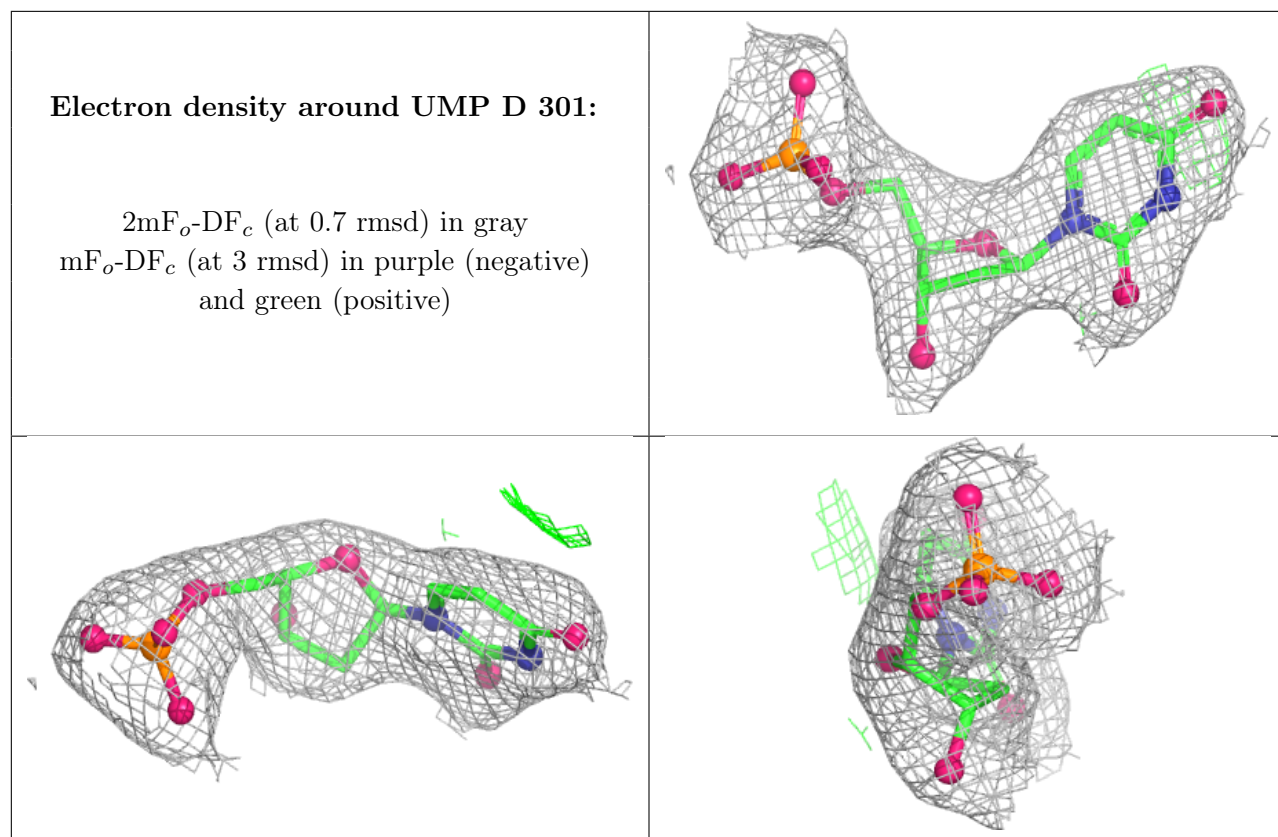
Electron density around UMP B 301:

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

**Electron density around UMP C 301:**

$2mF_o-DF_c$ (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.