



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:45 am BST

PDB ID : 1KZI
Title : Crystal Structure of EcTS/dUMP/THF Complex
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Deposited on : 2002-02-06
Resolution : 1.75 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 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

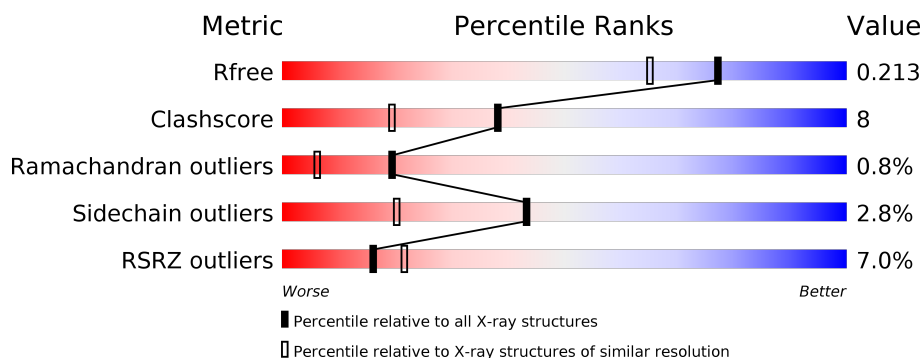
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 ≥ 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	264	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
1	B	264	<div> <div>11%</div> <div>75%</div> <div>23%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DTU	A	800	X	-	-	-
7	DTT	B	802	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4805 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.

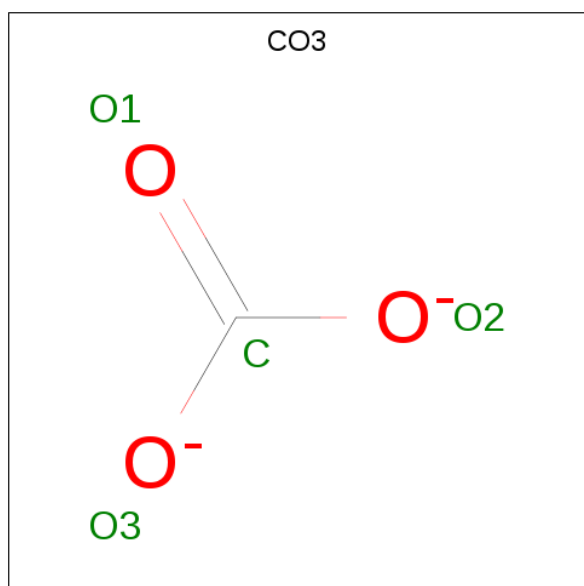
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			
1	B	264	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P0A884
B	1	CXM	MET	MODIFIED RESIDUE	UNP P0A884

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



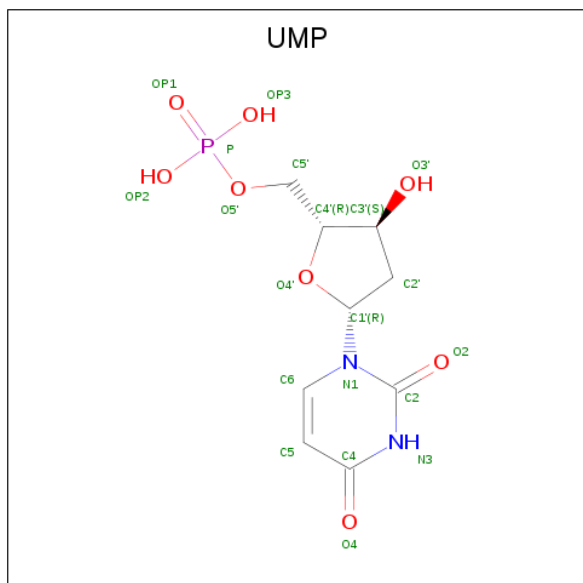
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		

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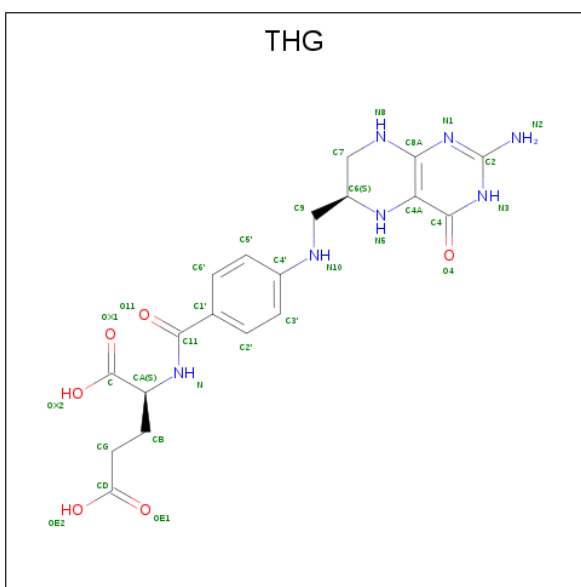
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



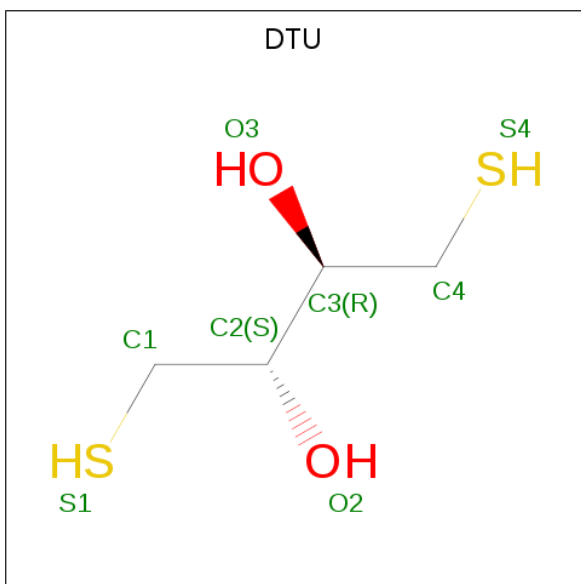
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 32	C 19	N 7	O 6	0	0
4	B	1	Total 32	C 19	N 7	O 6	0	0

- Molecule 5 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: $C_4H_{10}O_2S_2$).



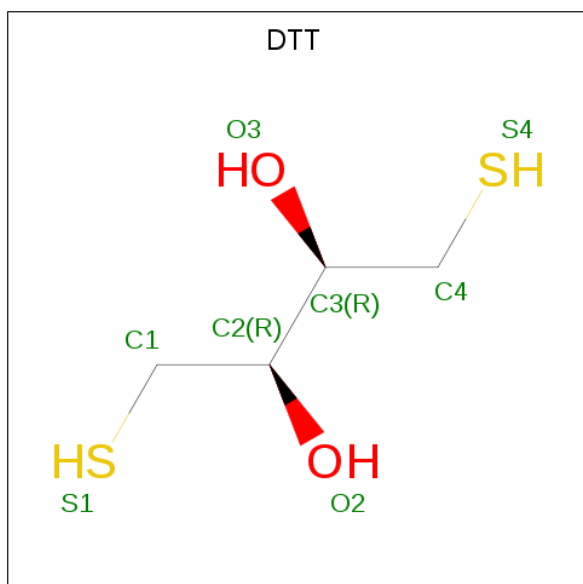
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			8	4	2	2		

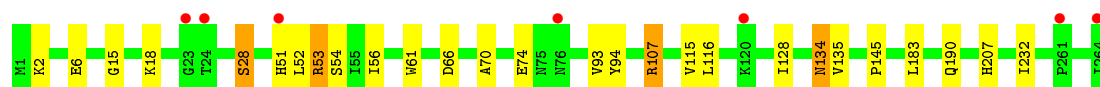
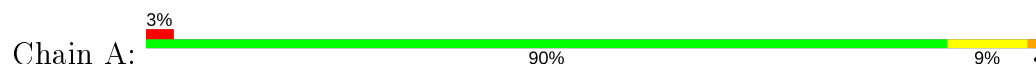
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	224	Total 224	O 224	0	0
8	B	137	Total 137	O 137	0	0

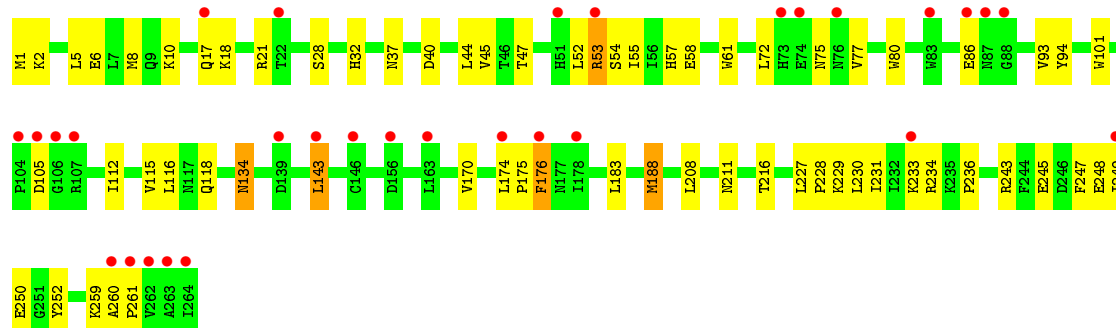
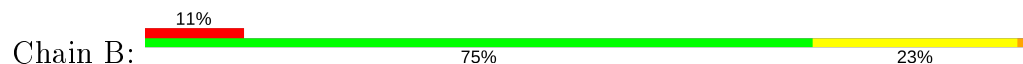
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	125.30 Å 125.30 Å 66.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.46 – 1.75 29.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.46-1.75) 98.7 (29.46-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.75 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.221 0.191 , 0.213	Depositor DCC
R_{free} test set	3007 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4805	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: GOL, CO3, UMP, THG, CXM, DTU, DTT

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	0.33	0/2202	0.67	0/2990
1	B	0.35	0/2202	0.64	0/2990
All	All	0.34	0/4404	0.65	0/5980

There are no bond length outliers.

There are no bond angle outliers.

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	2153	0	2078	18	1
1	B	2153	0	2079	47	0
2	A	12	0	0	0	0
3	A	20	0	10	1	0
3	B	20	0	10	1	0
4	A	32	0	21	1	0
4	B	32	0	21	1	0
5	A	8	0	9	1	0
6	A	6	0	8	0	0
7	B	8	0	8	0	0
8	A	224	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	137	0	0	4	0
All	All	4805	0	4244	66	1

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 8.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TRP:HZ3	1:B:143:LEU:HD21	1.25	1.00
1:A:51:HIS:HD2	1:A:54:SER:H	1.17	0.91
1:B:80:TRP:CZ3	1:B:143:LEU:HD21	2.10	0.86
1:A:190:GLN:HE22	1:A:232:ILE:HG21	1.43	0.81
1:B:116:LEU:HD22	1:B:188:MET:HE1	1.62	0.80
1:A:51:HIS:CD2	1:A:54:SER:H	2.02	0.77
1:A:116:LEU:HD13	5:A:800:DTU:S1	2.27	0.74
1:A:190:GLN:NE2	1:A:232:ILE:HG21	2.03	0.73
1:B:52:LEU:HD11	1:B:249:ILE:HG13	1.72	0.71
1:B:86:GLU:CD	1:B:86:GLU:H	1.94	0.70
1:A:190:GLN:HE22	1:A:232:ILE:CG2	2.07	0.68
1:B:116:LEU:CD2	1:B:188:MET:HE1	2.23	0.68
1:A:2:LYS:O	1:A:6:GLU:HG3	1.96	0.65
1:B:72:LEU:HB3	1:B:77:VAL:HB	1.81	0.63
1:A:51:HIS:NE2	1:A:53:ARG:HB3	2.13	0.63
1:B:229:LYS:HG3	8:B:698:HOH:O	2.00	0.62
1:B:1:CXM:ON2	1:B:45:VAL:HG13	2.02	0.59
1:B:234:ARG:O	1:B:236:PRO:HD3	2.04	0.58
1:A:28:SER:HB2	1:A:207:HIS:HB3	1.87	0.57
1:A:56:ILE:HG12	1:A:183:LEU:HD21	1.88	0.56
1:B:115:VAL:HA	1:B:118:GLN:HE21	1.71	0.56
3:A:302:UMP:C5	4:A:303:THG:N5	2.74	0.55
1:B:211:ASN:ND2	1:B:261:PRO:HG2	2.22	0.55
3:B:304:UMP:C5	4:B:305:THG:N5	2.74	0.55
1:B:18:LYS:HG3	1:B:28:SER:HB3	1.90	0.54
1:B:2:LYS:O	1:B:6:GLU:HG3	2.07	0.54
1:A:70:ALA:O	1:A:74:GLU:HG3	2.08	0.53
1:B:259:LYS:HD3	1:B:260:ALA:N	2.24	0.53
1:B:53:ARG:HG3	1:B:54:SER:N	2.24	0.52
1:B:170:VAL:HB	1:B:208:LEU:HD23	1.91	0.52
1:B:52:LEU:CD1	1:B:249:ILE:HG13	2.40	0.51
1:B:52:LEU:HD23	1:B:55:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:CE1	1:B:75:ASN:ND2	2.80	0.49
1:B:134:ASN:C	1:B:134:ASN:HD22	2.16	0.49
1:A:134:ASN:C	1:A:134:ASN:HD22	2.15	0.49
1:A:145:PRO:HG3	8:A:506:HOH:O	2.13	0.49
1:A:51:HIS:CD2	1:A:53:ARG:HB3	2.47	0.49
1:B:44:LEU:HD13	1:B:52:LEU:HD21	1.95	0.48
1:B:10:LYS:NZ	1:B:32:HIS:HD2	2.11	0.48
1:A:61:TRP:CD1	1:A:66:ASP:HB3	2.49	0.48
1:B:18:LYS:CE	8:B:722:HOH:O	2.62	0.48
1:B:233:LYS:HD2	1:B:248:GLU:HG3	1.97	0.47
1:B:243:ARG:HH21	1:B:243:ARG:HG2	1.78	0.47
1:B:1:CXM:HG3	1:B:227:LEU:HD21	1.97	0.47
1:B:231:ILE:HD13	1:B:250:GLU:HB2	1.96	0.47
1:B:5:LEU:HD11	1:B:47:THR:HG21	1.97	0.46
1:B:116:LEU:CD2	1:B:188:MET:CE	2.93	0.46
1:B:17:GLN:HG3	8:B:628:HOH:O	2.17	0.45
1:B:37:ASN:HB3	1:B:40:ASP:OD2	2.16	0.45
1:B:18:LYS:HE3	8:B:722:HOH:O	2.16	0.45
1:A:53:ARG:HB2	1:A:53:ARG:HE	1.51	0.45
1:B:228:PRO:HB2	1:B:249:ILE:HG23	1.98	0.44
1:B:249:ILE:CG2	1:B:252:TYR:HB2	2.48	0.43
1:B:230:LEU:HA	1:B:249:ILE:HD13	2.00	0.43
1:B:233:LYS:HD2	1:B:248:GLU:CG	2.49	0.43
1:B:58:GLU:O	1:B:61:TRP:HB3	2.19	0.43
1:B:183:LEU:HD11	1:B:247:PHE:CE1	2.54	0.43
1:B:55:ILE:HG12	1:B:176:PHE:CD2	2.55	0.42
1:A:135:VAL:HB	1:B:101:TRP:CE2	2.54	0.42
1:B:188:MET:HB3	1:B:188:MET:HE2	1.79	0.42
1:A:115:VAL:HG13	1:A:128:ILE:CG2	2.49	0.42
1:B:112:ILE:O	1:B:116:LEU:HD23	2.20	0.41
1:B:174:LEU:HB3	1:B:175:PRO:HD3	2.01	0.41
1:B:245:GLU:CD	1:B:245:GLU:H	2.24	0.41
1:B:8:MET:CG	1:B:216:THR:HG23	2.51	0.40
1:B:231:ILE:HD12	1:B:231:ILE:N	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLY:O	1:A:107:ARG:NH2[6_545]	2.03	0.17

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	262/264 (99%)	258 (98%)	2 (1%)	2 (1%)	19	6
1	B	262/264 (99%)	254 (97%)	6 (2%)	2 (1%)	19	6
All	All	524/528 (99%)	512 (98%)	8 (2%)	4 (1%)	19	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	B	94	TYR
1	A	93	VAL
1	B	93	VAL

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	232/232 (100%)	226 (97%)	6 (3%)	46	23
1	B	232/232 (100%)	225 (97%)	7 (3%)	41	18
All	All	464/464 (100%)	451 (97%)	13 (3%)	43	20

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	28	SER

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Mol	Chain	Res	Type
1	A	52	LEU
1	A	53	ARG
1	A	107	ARG
1	A	134	ASN
1	B	21	ARG
1	B	53	ARG
1	B	105	ASP
1	B	134	ASN
1	B	143	LEU
1	B	176	PHE
1	B	188	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	51	HIS
1	A	87	ASN
1	A	121	ASN
1	A	134	ASN
1	A	151	GLN
1	A	190	GLN
1	A	217	HIS
1	B	32	HIS
1	B	39	GLN
1	B	75	ASN
1	B	117	ASN
1	B	118	GLN
1	B	134	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CXM	A	1	1	6,10,11	1.09	1 (16%)	5,11,13	0.75	0
1	CXM	B	1	1	6,10,11	0.96	1 (16%)	5,11,13	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	A	1	1	-	0/7/10/12	-
1	CXM	B	1	1	-	1/7/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CXM	CA-N	2.43	1.49	1.46
1	B	1	CXM	CA-N	2.14	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1	CXM	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	CXM	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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
2	CO3	A	805	-	0,3,3	0.00	-	0,3,3	0.00	-
4	THG	A	303	-	26,34,34	1.69	5 (19%)	31,47,47	2.06	5 (16%)
2	CO3	A	804	-	0,3,3	0.00	-	0,3,3	0.00	-
7	DTT	B	802	-	7,7,7	0.71	0	4,8,8	1.19	0
6	GOL	A	801	-	5,5,5	0.38	0	5,5,5	0.15	0
4	THG	B	305	-	26,34,34	1.69	5 (19%)	31,47,47	2.09	7 (22%)
2	CO3	A	803	-	0,3,3	0.00	-	0,3,3	0.00	-
3	UMP	A	302	1	18,21,21	4.48	4 (22%)	21,31,31	1.34	2 (9%)
3	UMP	B	304	1	18,21,21	4.85	4 (22%)	21,31,31	1.75	2 (9%)
5	DTU	A	800	1	7,7,7	1.83	1 (14%)	4,8,8	1.38	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	THG	A	303	-	-	3/16/31/31	0/3/3/3
7	DTT	B	802	-	1/1/2/2	0/8/8/8	-
6	GOL	A	801	-	-	0/4/4/4	-
4	THG	B	305	-	-	1/16/31/31	0/3/3/3
3	UMP	A	302	1	-	1/7/22/22	0/2/2/2
3	UMP	B	304	1	-	1/7/22/22	0/2/2/2
5	DTU	A	800	1	2/2/2/2	6/8/8/8	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	304	UMP	C6-N1	15.04	1.54	1.35
3	A	302	UMP	C6-N1	14.55	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	304	UMP	C6-C5	10.88	1.62	1.38
3	A	302	UMP	C6-C5	9.11	1.58	1.38
3	B	304	UMP	O4-C4	7.22	1.42	1.24
3	A	302	UMP	O4-C4	6.84	1.41	1.24
4	B	305	THG	C4-N3	4.42	1.40	1.33
4	A	303	THG	C4-N3	4.11	1.40	1.33
5	A	800	DTU	C4-S4	3.64	1.89	1.81
3	B	304	UMP	C4-N3	3.60	1.39	1.33
4	A	303	THG	C2-N3	3.21	1.41	1.35
3	A	302	UMP	C4-N3	3.11	1.38	1.33
4	B	305	THG	C2-N2	2.98	1.39	1.33
4	A	303	THG	C2-N2	2.84	1.39	1.33
4	B	305	THG	C2-N3	2.69	1.40	1.35
4	B	305	THG	C7-N8	2.62	1.49	1.44
4	A	303	THG	C7-N8	2.44	1.48	1.44
4	B	305	THG	C4A-N5	2.38	1.42	1.38
4	A	303	THG	C4A-N5	2.14	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	THG	C4-C4A-C8A	7.76	121.47	114.57
4	B	305	THG	C4-C4A-C8A	6.99	120.78	114.57
3	B	304	UMP	C5-C6-N1	-6.70	105.72	120.68
3	A	302	UMP	C5-C6-N1	-5.09	109.32	120.68
4	B	305	THG	N2-C2-N1	3.88	123.29	117.25
4	B	305	THG	C4-N3-C2	3.54	121.55	115.93
4	A	303	THG	C4A-C4-N3	-3.35	114.48	124.01
4	A	303	THG	C4-N3-C2	3.33	121.22	115.93
4	B	305	THG	C4A-C4-N3	-3.14	115.08	124.01
4	A	303	THG	N2-C2-N1	2.99	121.90	117.25
4	B	305	THG	N3-C2-N1	-2.60	121.35	125.42
3	B	304	UMP	C6-N1-C2	2.49	125.16	121.20
4	B	305	THG	C9-C6-N5	-2.41	103.64	108.83
5	A	800	DTU	C3-C4-S4	-2.39	107.52	114.47
3	A	302	UMP	P-O5'-C5'	2.12	124.12	118.30
4	B	305	THG	C2-N1-C8A	2.06	119.15	114.54
4	A	303	THG	C4-C4A-N5	-2.06	117.40	119.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	802	DTT	C3
5	A	800	DTU	C2
5	A	800	DTU	C3

All (12) torsion outliers are listed below:

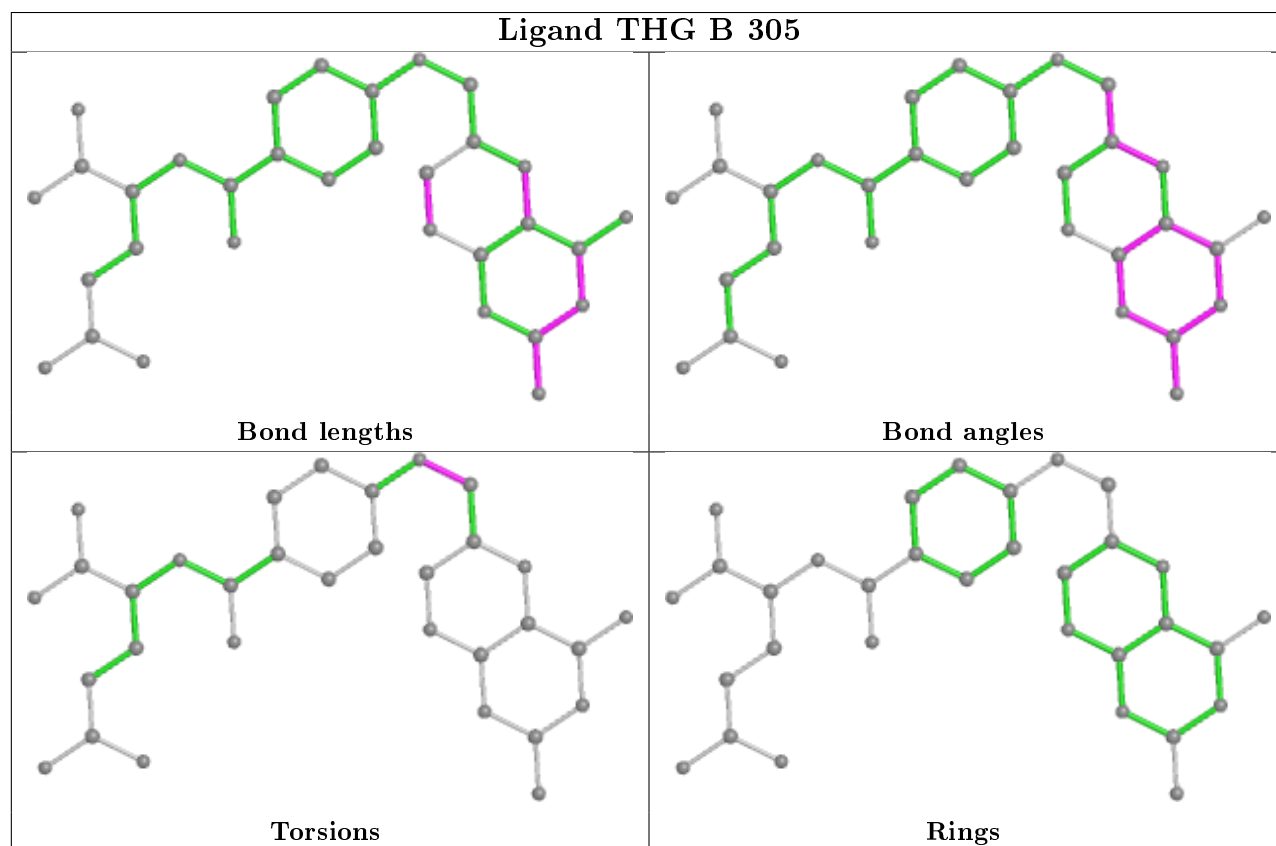
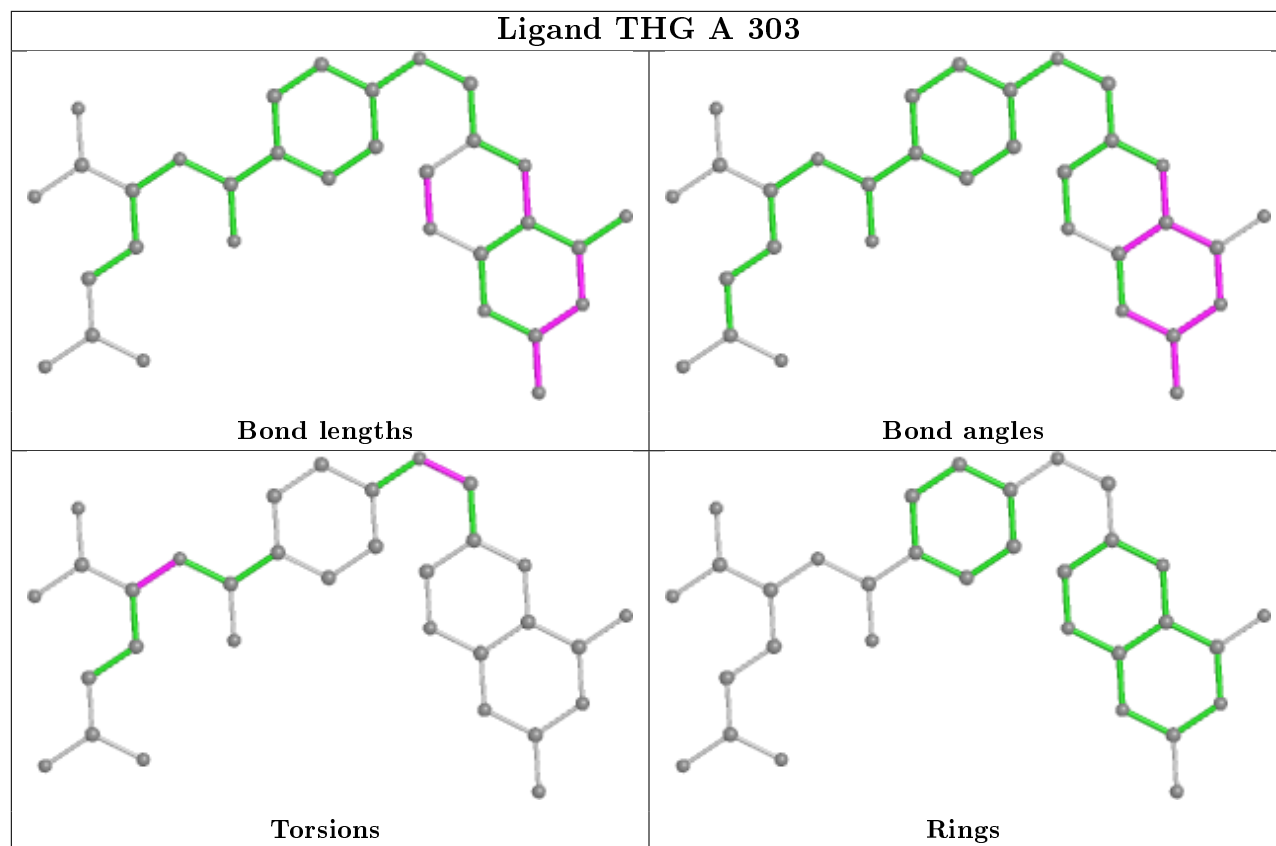
Mol	Chain	Res	Type	Atoms
5	A	800	DTU	S1-C1-C2-C3
5	A	800	DTU	C1-C2-C3-O3
5	A	800	DTU	C1-C2-C3-C4
5	A	800	DTU	O2-C2-C3-O3
5	A	800	DTU	O2-C2-C3-C4
4	A	303	THG	C-CA-N-C11
5	A	800	DTU	S1-C1-C2-O2
4	A	303	THG	C6-C9-N10-C4'
4	B	305	THG	C6-C9-N10-C4'
4	A	303	THG	CB-CA-N-C11
3	A	302	UMP	O4'-C4'-C5'-O5'
3	B	304	UMP	O4'-C4'-C5'-O5'

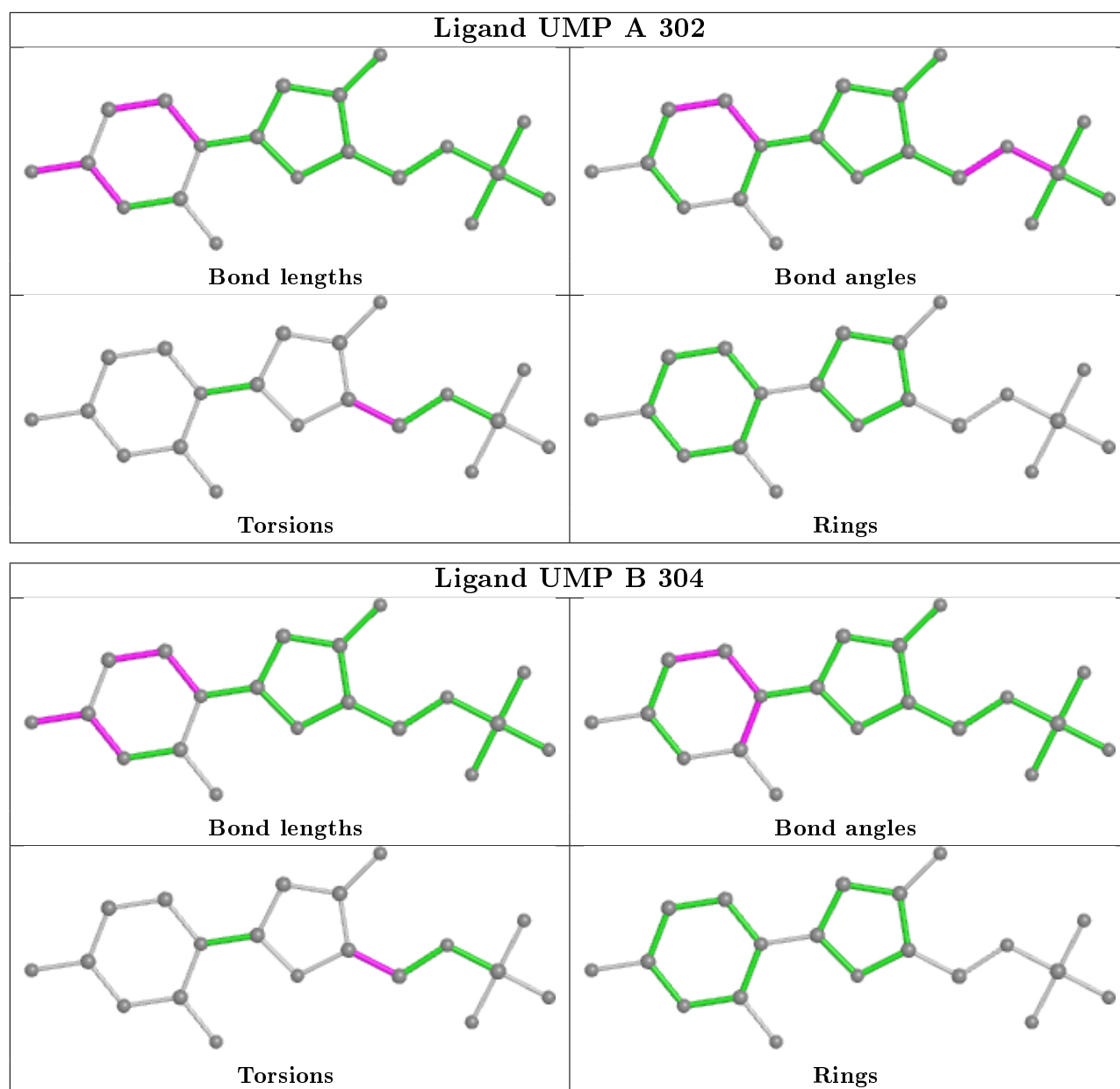
There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	THG	1	0
4	B	305	THG	1	0
3	A	302	UMP	1	0
3	B	304	UMP	1	0
5	A	800	DTU	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/264 (99%)	0.21	7 (2%) 54 60	15, 21, 34, 43	0
1	B	263/264 (99%)	0.71	30 (11%) 5 7	16, 27, 48, 60	0
All	All	526/528 (99%)	0.46	37 (7%) 16 21	15, 24, 43, 60	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ILE	8.7
1	B	262	VAL	5.0
1	B	176	PHE	4.6
1	B	104	PRO	4.1
1	B	105	ASP	4.1
1	B	156	ASP	4.0
1	B	86	GLU	3.9
1	B	106	GLY	3.7
1	B	76	ASN	3.6
1	B	143	LEU	3.6
1	B	22	THR	3.6
1	B	260	ALA	3.5
1	B	178	ILE	3.4
1	B	263	ALA	3.1
1	B	74	GLU	3.1
1	B	88	GLY	3.0
1	B	53	ARG	2.9
1	B	83	TRP	2.8
1	A	76	ASN	2.8
1	B	261	PRO	2.8
1	B	174	LEU	2.7
1	B	51	HIS	2.7
1	A	264	ILE	2.6
1	B	17	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	2.5
1	B	249	ILE	2.5
1	B	163	LEU	2.5
1	B	146	CYS	2.4
1	A	51	HIS	2.3
1	A	261	PRO	2.3
1	B	73	HIS	2.3
1	B	107	ARG	2.2
1	A	120	LYS	2.2
1	A	24	THR	2.1
1	B	233	LYS	2.0
1	B	139	ASP	2.0
1	B	87	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CXM	B	1	11/12	0.95	0.09	21,22,23,25	0
1	CXM	A	1	11/12	0.97	0.07	16,18,20,21	0

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, 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.

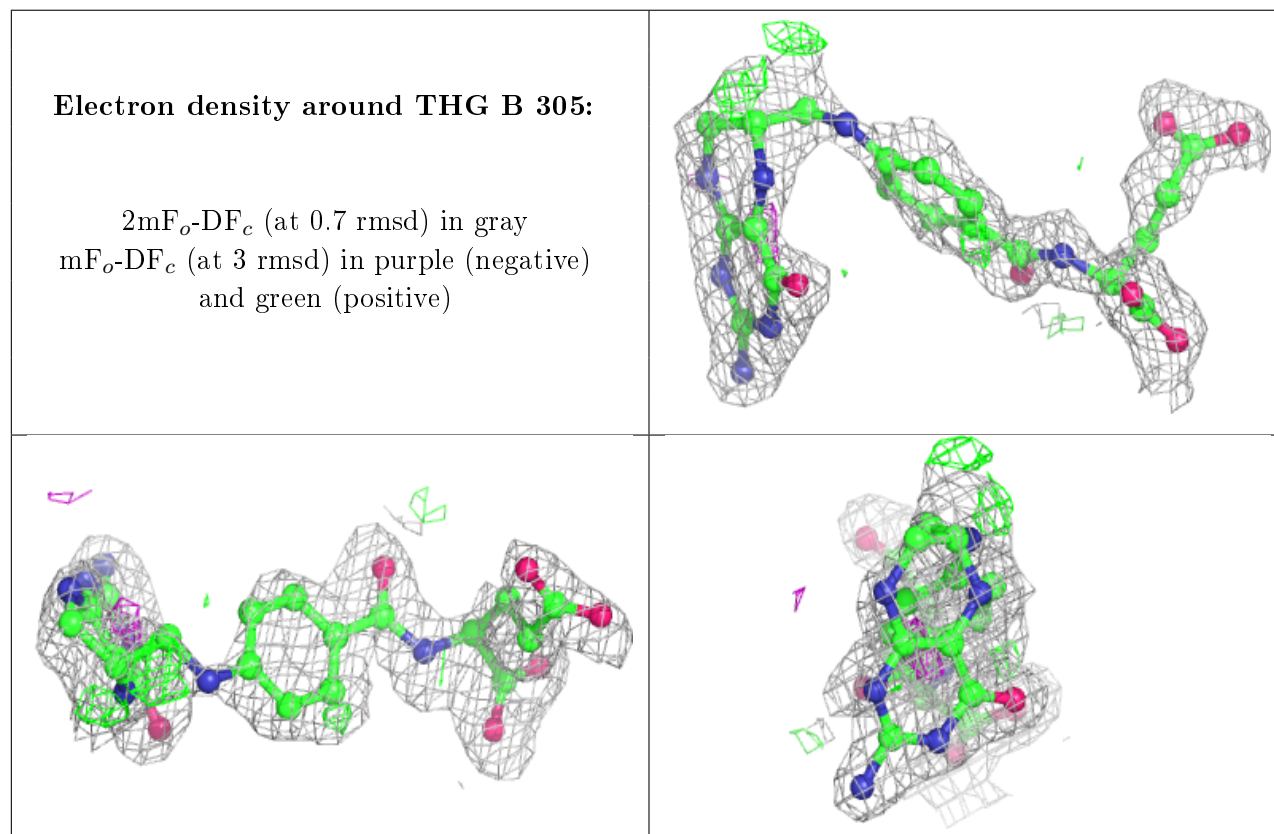
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	THG	B	305	32/32	0.54	0.23	54,56,58,58	0
7	DTT	B	802	8/8	0.76	0.21	59,60,60,61	0
6	GOL	A	801	6/6	0.82	0.23	53,54,55,56	0

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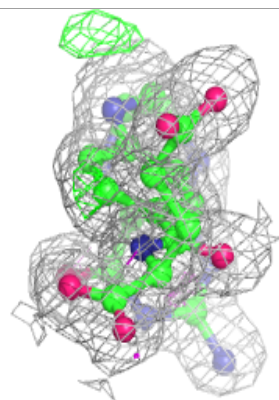
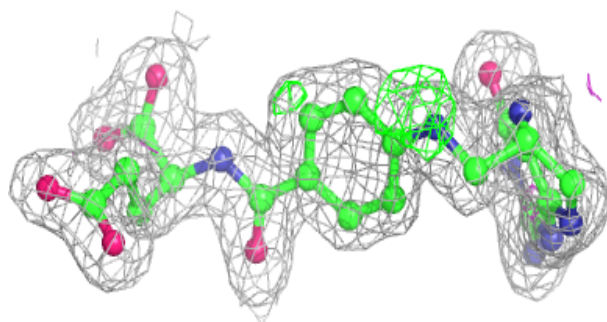
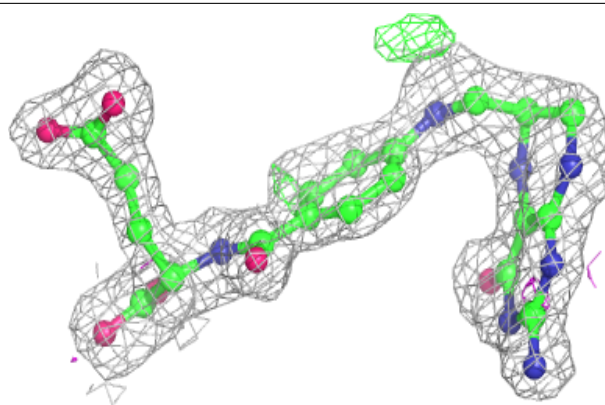
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	THG	A	303	32/32	0.82	0.15	27,30,32,35	0
2	CO3	A	803	4/4	0.85	0.20	39,39,40,43	0
3	UMP	B	304	20/20	0.85	0.22	34,41,43,43	0
5	DTU	A	800	8/8	0.85	0.16	36,48,55,60	0
2	CO3	A	804	4/4	0.86	0.13	42,43,43,44	0
2	CO3	A	805	4/4	0.90	0.12	38,39,41,42	0
3	UMP	A	302	20/20	0.92	0.13	21,26,28,30	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.

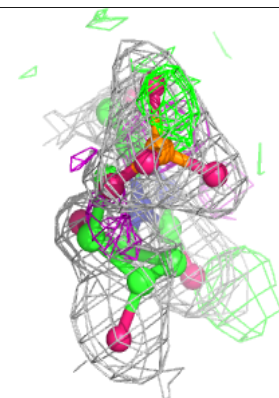
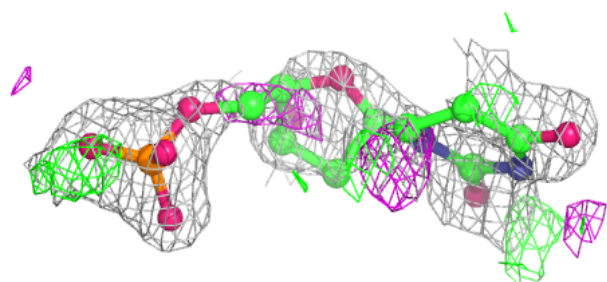
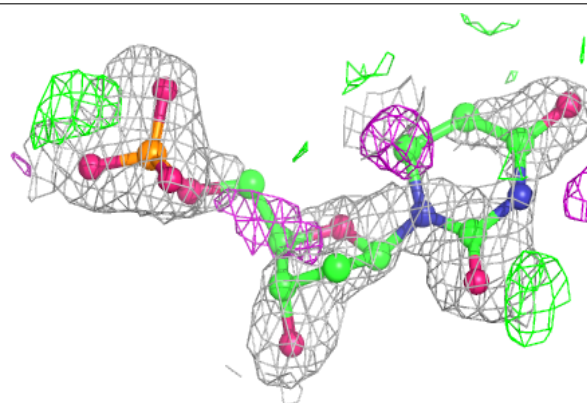


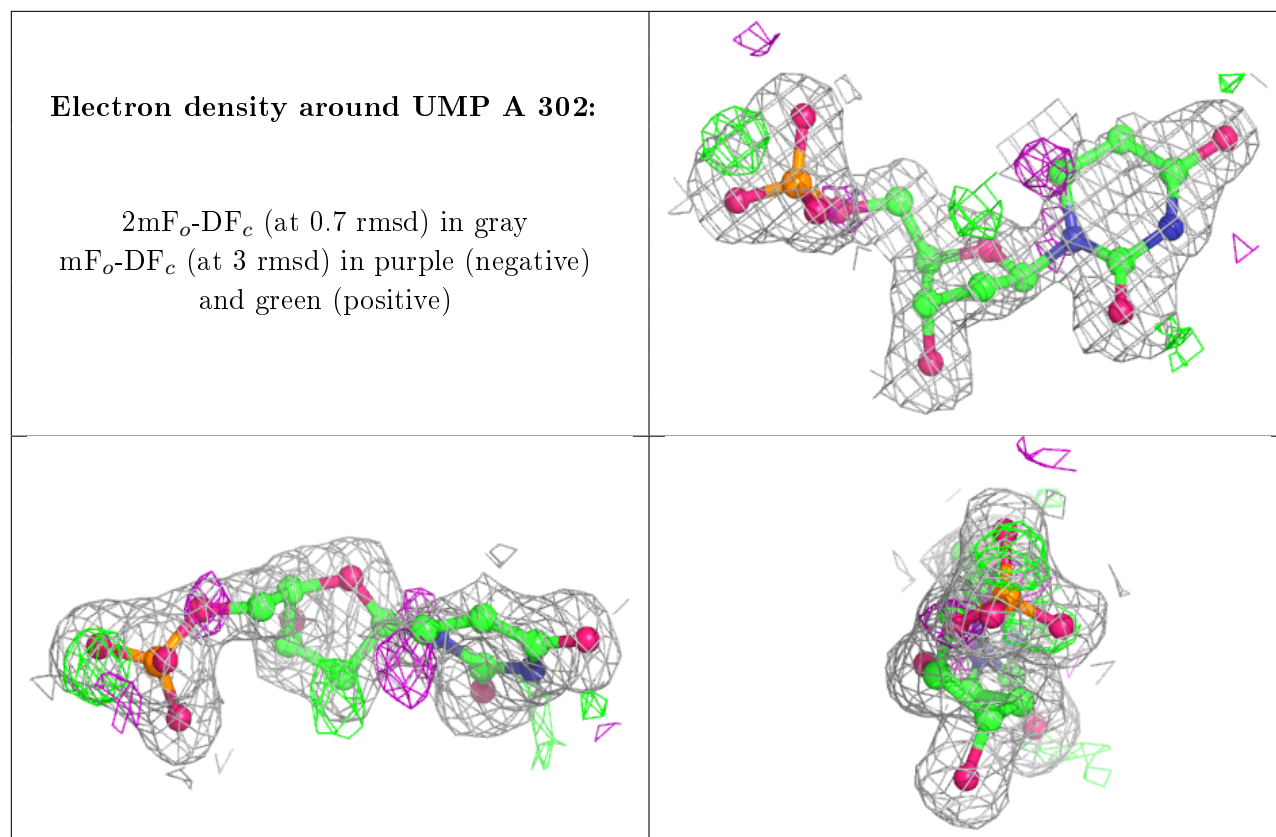
Electron density around THG A 303:

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

**Electron density around UMP B 304:**

$2mF_o-DF_c$ (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.