



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:31 PM UTC

PDB ID : 4EB4 / pdb\_00004eb4  
Title : Crystal structure of mouse thymidylate synthase in ternary complex with dUMP and Tomudex  
Authors : Dowiercial, A.; Jarmula, A.; Rypniewski, W.R.; Wilk, P.; Rode, W.  
Deposited on : 2012-03-23  
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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)  
Xtrriage (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

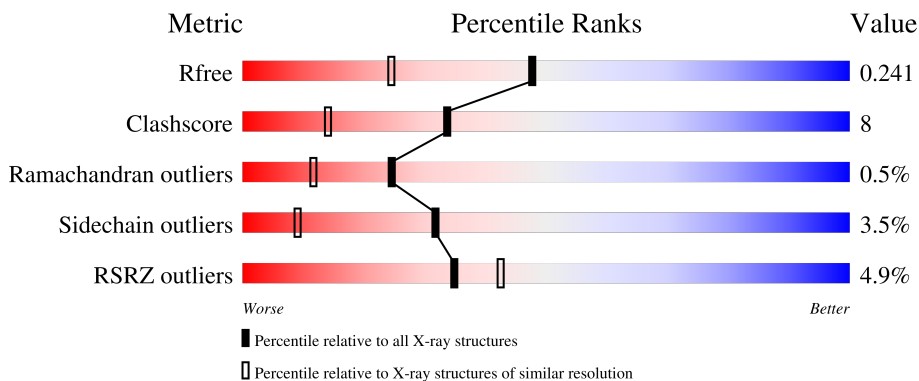
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	 2% 83% 12% ..
1	B	307	 % 88% 9% ..
1	C	307	 11% 75% 19% ..
1	D	307	 6% 81% 15% ..

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
4	DTT	A	403	-	X	-	-
5	GOL	A	407[B]	-	-	X	-

## 2 Entry composition [i](#)

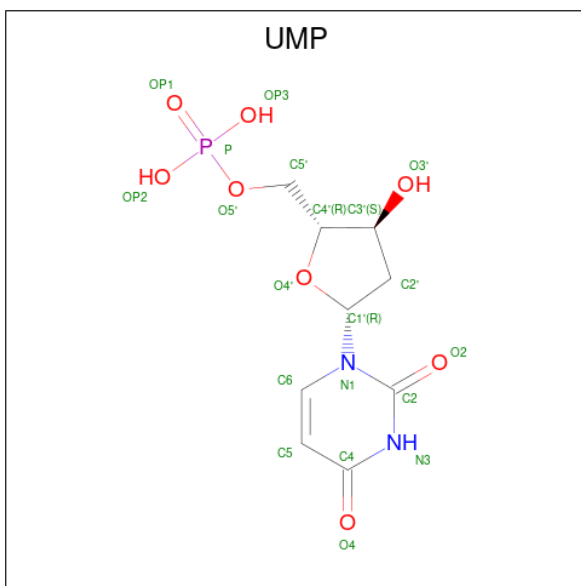
There are 8 unique types of molecules in this entry. The entry contains 11513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	300	Total	C	N	O	S	0	11	0
			2501	1594	431	462	14			
1	B	301	Total	C	N	O	S	0	5	0
			2462	1572	426	450	14			
1	C	295	Total	C	N	O	S	0	14	0
			2503	1594	432	464	13			
1	D	297	Total	C	N	O	S	0	12	0
			2508	1598	436	461	13			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).



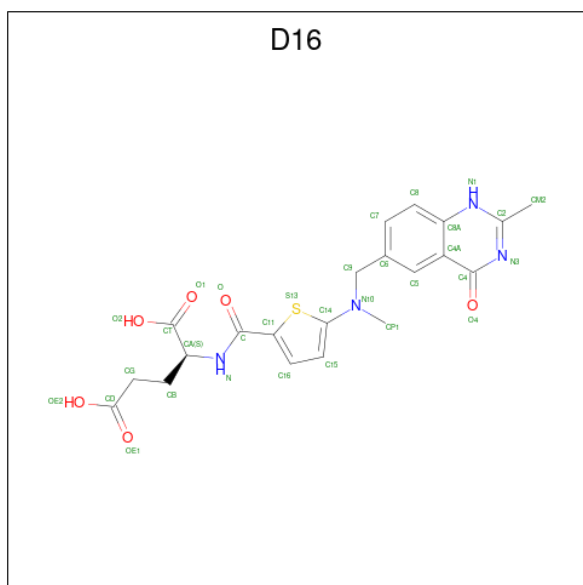
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

*Continued on next page...*

Continued from previous page...

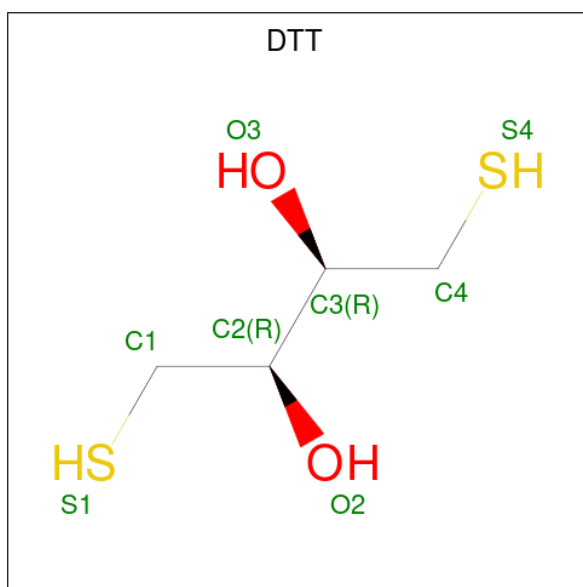
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is TOMUDEX (CCD ID: D16) (formula:  $C_{21}H_{22}N_4O_6S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	12	6	6	0	1
5	A	1	6	3	3	0	0
5	A	1	6	3	3	0	0

*Continued on next page...*

Continued from previous page...

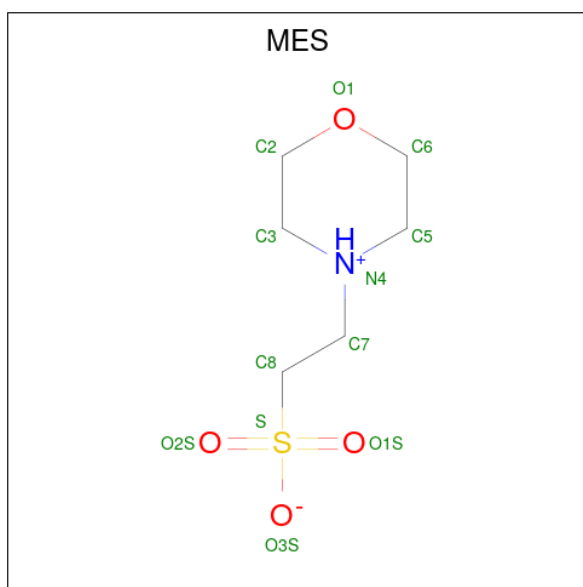
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 6 6	0	1
5	B	1	Total C O 12 6 6	0	1
5	B	1	Total C O 12 6 6	0	1
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	B	1	12	6	1	4	1	0	0

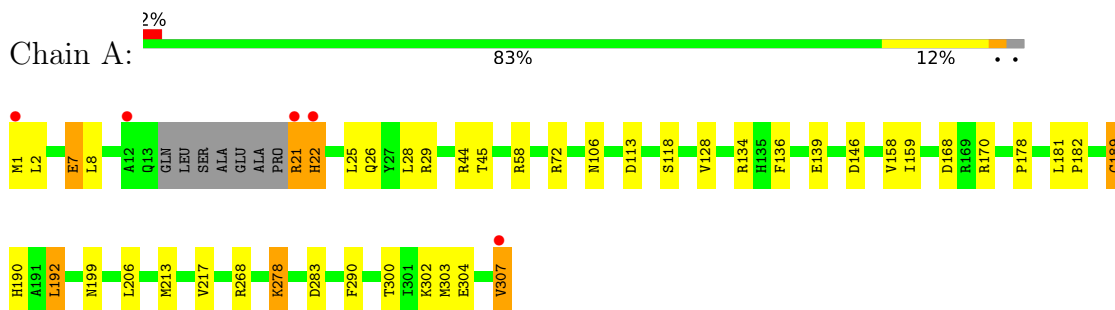
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	394	Total	O	0	0
			394	394		
8	B	362	Total	O	0	0
			362	362		
8	C	264	Total	O	0	0
			264	264		
8	D	202	Total	O	0	0
			202	202		

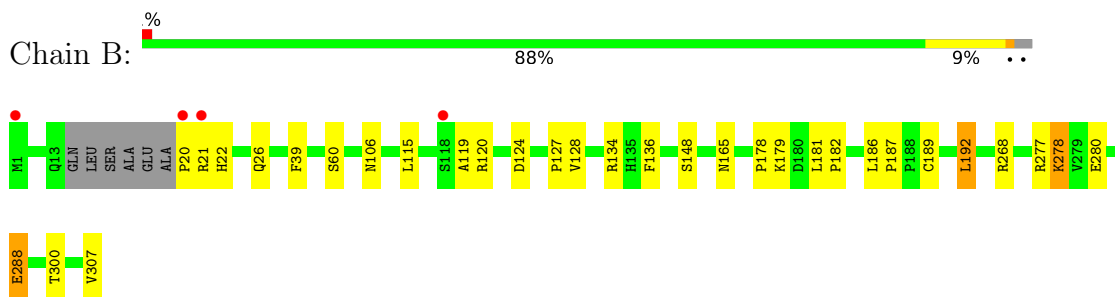
### 3 Residue-property plots [i](#)

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.

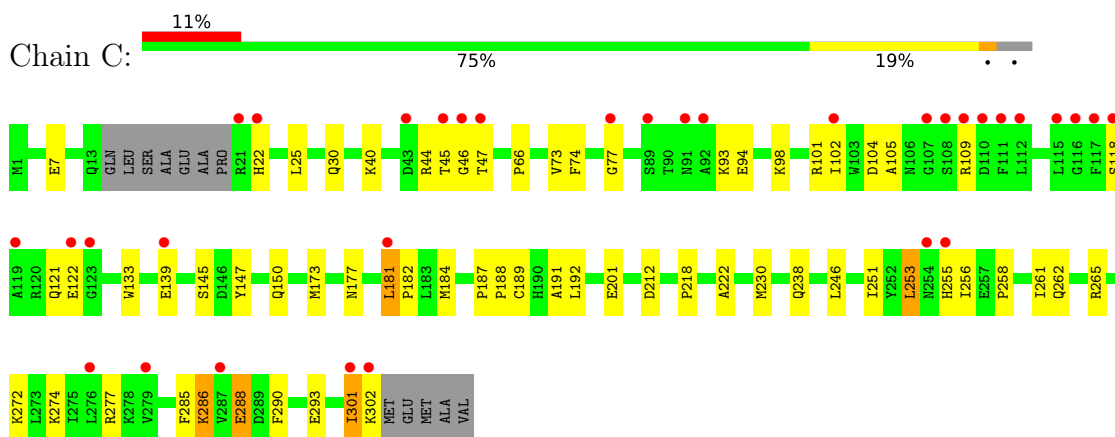
- Molecule 1: Thymidylate synthase



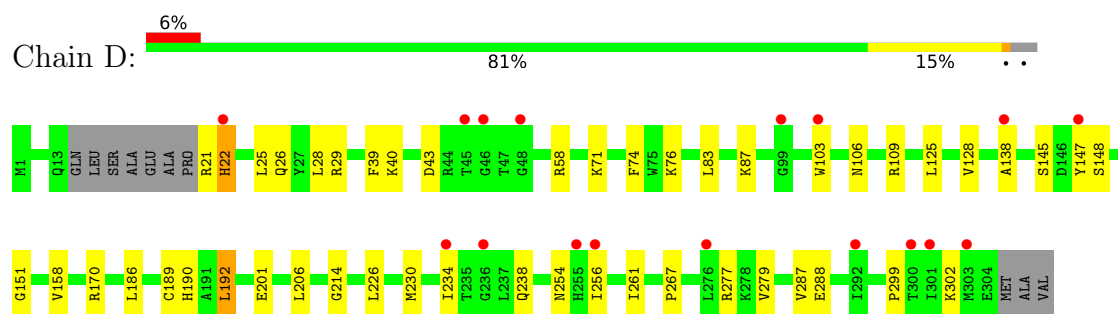
- Molecule 1: Thymidylate synthase



- 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, $\alpha$ , $\beta$ , $\gamma$	101.80Å 114.22Å 123.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.74 20.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.74) 99.8 (20.00-1.74)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.73Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.238 0.194 , 0.241	Depositor DCC
$R_{free}$ test set	7435 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SO4, MES, D16, GOL, UMP, 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	1.35	6/2564 (0.2%)	1.15	5/3459 (0.1%)
1	B	1.29	2/2521 (0.1%)	1.16	8/3406 (0.2%)
1	C	1.26	9/2568 (0.4%)	1.10	5/3466 (0.1%)
1	D	1.17	3/2570 (0.1%)	1.06	3/3471 (0.1%)
All	All	1.27	20/10223 (0.2%)	1.12	21/13802 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	VAL	CA-CB	11.18	1.61	1.53
1	D	261	ILE	CA-CB	6.70	1.62	1.54
1	A	159	ILE	CA-CB	-6.59	1.46	1.54
1	A	213	MET	N-CA	-6.23	1.38	1.46
1	C	66	PRO	CA-C	-5.79	1.48	1.53
1	C	191	ALA	CA-CB	-5.69	1.44	1.53
1	C	73	VAL	CA-C	5.45	1.59	1.52
1	B	127	PRO	CA-C	5.40	1.57	1.52
1	A	290	PHE	C-O	-5.36	1.17	1.24
1	C	218	PRO	N-CA	-5.35	1.40	1.47
1	D	138	ALA	N-CA	5.24	1.52	1.45
1	D	28	LEU	C-O	-5.22	1.17	1.24
1	C	177	ASN	CA-C	-5.21	1.47	1.52
1	C	262	GLN	N-CA	-5.20	1.40	1.46
1	A	29	ARG	C-O	-5.14	1.18	1.24
1	C	77	GLY	CA-C	5.08	1.57	1.52
1	C	222	ALA	CA-CB	5.06	1.61	1.53
1	A	28	LEU	C-O	-5.05	1.18	1.24
1	B	119	ALA	CA-CB	-5.05	1.44	1.53
1	C	73	VAL	N-CA	-5.05	1.40	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ARG	CA-C-N	-7.16	112.40	119.78
1	A	268	ARG	C-N-CA	-7.16	112.40	119.78
1	C	246	LEU	N-CA-C	6.88	120.66	109.59
1	B	187	PRO	CA-C-N	-6.61	113.15	119.76
1	B	187	PRO	C-N-CA	-6.61	113.15	119.76
1	A	134	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	C	74	PHE	CA-C-N	5.68	127.82	120.44
1	C	74	PHE	C-N-CA	5.68	127.82	120.44
1	B	134	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	B	148	SER	N-CA-C	5.52	118.81	110.64
1	B	186	LEU	CA-C-N	-5.44	115.69	119.66
1	B	186	LEU	C-N-CA	-5.44	115.69	119.66
1	B	268	ARG	CA-C-N	-5.40	114.22	119.78
1	B	268	ARG	C-N-CA	-5.40	114.22	119.78
1	D	43	ASP	N-CA-C	5.32	116.08	108.74
1	A	189	CYS	N-CA-C	-5.32	105.65	111.82
1	D	254	ASN	N-CA-C	5.29	117.95	111.82
1	C	261	ILE	CB-CA-C	-5.26	105.23	111.97
1	A	22	HIS	N-CA-C	5.08	116.78	108.55
1	C	30	GLN	N-CA-C	5.06	116.48	111.07
1	D	287	VAL	CB-CA-C	-5.04	105.33	112.14

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	2501	0	2462	39	0
1	B	2462	0	2434	22	0
1	C	2503	0	2445	59	0
1	D	2508	0	2444	32	0
2	A	20	0	11	2	0
2	B	20	0	11	3	0
2	C	20	0	11	2	0
2	D	20	0	11	2	0
3	A	32	0	20	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	20	0	0
3	C	32	0	20	2	0
3	D	32	0	20	0	0
4	A	8	0	10	1	0
5	A	36	0	48	11	0
5	B	30	0	40	4	0
5	C	6	0	8	0	0
5	D	12	0	16	2	0
6	A	5	0	0	0	0
7	B	12	0	12	1	0
8	A	394	0	0	5	2
8	B	362	0	0	10	0
8	C	264	0	0	7	2
8	D	202	0	0	2	0
All	All	11513	0	10043	156	2

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 (156) 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:307:VAL:HG21	8:A:871:HOH:O	1.30	1.24
1:B:189:CYS:SG	2:B:401:UMP:C6	2.43	1.11
1:C:181:LEU:HA	1:C:184[B]:MET:CE	1.81	1.10
1:C:181:LEU:CD2	1:C:184[B]:MET:HE1	1.80	1.09
1:A:189:CYS:SG	2:A:401:UMP:C6	2.48	1.07
1:A:278[B]:LYS:H	5:A:407[B]:GOL:H31	1.11	1.07
1:C:181:LEU:CA	1:C:184[B]:MET:HE2	1.85	1.06
1:C:181:LEU:HD22	1:C:184[B]:MET:HE1	1.40	1.01
1:A:106[A]:ASN:OD1	8:A:850:HOH:O	1.86	0.94
1:B:106[A]:ASN:ND2	8:B:502:HOH:O	2.01	0.94
1:A:7:GLU:OE2	1:A:8:LEU:HD12	1.69	0.92
1:C:139[C]:GLU:H	1:C:139[C]:GLU:CD	1.74	0.90
1:A:307:VAL:HG23	8:A:837:HOH:O	1.70	0.90
1:C:181:LEU:HD23	1:C:184[B]:MET:HE1	1.55	0.87
1:A:278[B]:LYS:HG3	5:A:407[B]:GOL:H12	1.56	0.85
1:D:288[B]:GLU:H	1:D:288[B]:GLU:CD	1.83	0.85
1:D:151:GLY:O	8:D:586:HOH:O	1.94	0.85
1:A:44:ARG:HH22	1:A:307:VAL:HG11	1.42	0.84
1:C:181:LEU:HA	1:C:184[B]:MET:HE2	0.91	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:403[A]:GOL:O1	8:B:532:HOH:O	1.91	0.81
1:A:278[B]:LYS:H	5:A:407[B]:GOL:C3	1.91	0.81
1:C:288:GLU:OE2	8:C:703:HOH:O	1.99	0.81
1:D:189:CYS:SG	2:D:401:UMP:C6	2.76	0.79
1:C:181:LEU:HD22	1:C:184[B]:MET:CE	2.14	0.78
1:D:21:ARG:HG3	1:D:25:LEU:HD12	1.65	0.78
1:C:189:CYS:SG	2:C:401:UMP:C6	2.78	0.77
1:C:7[B]:GLU:H	1:C:7[B]:GLU:CD	1.93	0.76
1:C:122:GLU:N	8:C:690:HOH:O	2.17	0.76
1:A:278[B]:LYS:N	5:A:407[B]:GOL:H31	1.95	0.76
1:C:181:LEU:CD2	1:C:184[B]:MET:CE	2.62	0.76
1:D:288[B]:GLU:N	1:D:288[B]:GLU:OE1	2.19	0.76
1:D:21:ARG:HE	1:D:29:ARG:HH12	1.36	0.72
1:C:101:ARG:O	8:C:554:HOH:O	2.09	0.71
5:A:404[A]:GOL:H11	8:A:767:HOH:O	1.90	0.70
1:D:189:CYS:SG	2:D:401:UMP:C5	2.85	0.69
1:A:7:GLU:H	1:A:7:GLU:CD	2.01	0.69
1:D:21:ARG:O	1:D:22[B]:HIS:ND1	2.25	0.68
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.60	0.66
1:C:139[C]:GLU:HG2	8:C:565:HOH:O	1.95	0.65
1:B:22:HIS:HA	5:B:405:GOL:H31	1.78	0.64
1:B:165:ASN:OD1	8:B:614:HOH:O	2.15	0.63
1:C:94[B]:GLU:O	1:C:98[B]:LYS:HD3	1.99	0.63
1:C:98[B]:LYS:N	1:C:98[B]:LYS:HD2	2.14	0.63
1:C:139[C]:GLU:CD	1:C:139[C]:GLU:N	2.54	0.63
1:C:22[A]:HIS:HB2	1:C:25:LEU:HG	1.81	0.62
1:D:190[B]:HIS:CD2	1:D:190[B]:HIS:H	2.17	0.62
1:C:109:ARG:CD	1:C:122:GLU:HG3	2.29	0.62
1:C:109:ARG:HD2	1:C:122:GLU:HG3	1.80	0.62
1:A:44:ARG:NH2	1:A:307:VAL:HG11	2.14	0.62
1:D:71:LYS:NZ	1:D:214:GLY:O	2.32	0.62
1:B:300:THR:HG23	8:B:624:HOH:O	1.99	0.61
1:D:190[B]:HIS:CB	1:D:206:LEU:HD11	2.31	0.61
1:A:45:THR:HG22	1:A:307:VAL:HB	1.82	0.60
1:C:189:CYS:SG	2:C:401:UMP:C5	2.94	0.60
1:A:278[B]:LYS:HE3	5:A:407[B]:GOL:H2	1.83	0.60
1:B:300:THR:CG2	8:B:570:HOH:O	2.49	0.59
1:C:7[B]:GLU:HG2	1:C:25:LEU:HD21	1.84	0.59
1:A:158:VAL:HG23	4:A:403:DTT:S1	2.42	0.59
1:D:288[B]:GLU:CD	1:D:288[B]:GLU:N	2.60	0.58
1:A:22:HIS:HB2	1:A:25:LEU:HG	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:HIS:HB3	1:A:206:LEU:HD11	1.86	0.57
1:C:139[B]:GLU:OE1	1:C:150:GLN:NE2	2.37	0.57
1:B:39:PHE:CE2	7:B:406:MES:H31	2.40	0.57
1:C:272:LYS:HB2	1:C:293[B]:GLU:HG3	1.85	0.57
1:A:72:ARG:HB3	1:A:300:THR:HG22	1.87	0.56
1:B:20:PRO:HG2	1:B:60:SER:HB2	1.87	0.56
1:D:22[A]:HIS:HB3	1:D:25:LEU:HG	1.86	0.55
1:D:190[B]:HIS:HB3	1:D:206:LEU:HD11	1.87	0.55
1:A:189:CYS:SG	2:A:401:UMP:C5	3.00	0.55
1:D:40:LYS:HG3	5:D:404:GOL:H31	1.89	0.55
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.21	0.54
1:D:26[A]:GLN:NE2	8:D:627:HOH:O	2.40	0.54
1:D:190[A]:HIS:HB3	1:D:206:LEU:HD11	1.90	0.54
1:A:7:GLU:OE2	1:A:8:LEU:CD1	2.51	0.54
1:B:189:CYS:SG	2:B:401:UMP:H6	2.26	0.54
1:D:26[B]:GLN:NE2	1:D:58:ARG:O	2.41	0.54
1:C:45:THR:HG1	1:C:47:THR:HG1	1.53	0.53
1:B:288:GLU:H	1:B:288:GLU:CD	2.15	0.53
1:D:103[B]:TRP:CE3	1:D:125:LEU:HD13	2.44	0.53
1:C:121:GLN:HB3	8:C:690:HOH:O	2.08	0.53
1:C:181:LEU:HD23	1:C:184[B]:MET:CE	2.31	0.53
1:D:201:GLU:HA	1:D:238:GLN:O	2.09	0.53
1:A:136:PHE:CZ	1:B:178:PRO:HD2	2.44	0.52
1:A:146[A]:ASP:OD1	1:A:146[A]:ASP:C	2.52	0.52
1:A:192:LEU:C	1:A:192:LEU:HD12	2.34	0.52
1:C:288:GLU:H	1:C:288:GLU:CD	2.17	0.52
1:D:22[B]:HIS:HB2	1:D:25:LEU:HG	1.91	0.51
1:B:120:ARG:HD3	1:B:124:ASP:HB3	1.91	0.51
1:C:181:LEU:HB2	1:C:182:PRO:HD3	1.93	0.51
1:B:189:CYS:SG	2:B:401:UMP:C5	3.01	0.50
3:C:402:D16:O2	8:C:564:HOH:O	2.20	0.50
1:A:7:GLU:CD	1:A:7:GLU:N	2.70	0.49
1:A:1:MET:HG2	1:A:2:LEU:H	1.76	0.49
1:A:168:ASP:OD2	1:A:170:ARG:HB2	2.11	0.49
1:D:234:ILE:HD11	1:D:279:VAL:HG12	1.94	0.49
1:D:39:PHE:HD2	5:D:404:GOL:H2	1.77	0.49
1:C:212:ASP:OD1	1:C:255[B]:HIS:NE2	2.46	0.48
1:C:104:ASP:O	1:C:105:ALA:C	2.57	0.48
1:C:201:GLU:HA	1:C:238:GLN:O	2.14	0.48
1:C:286[A]:LYS:NZ	1:C:286[A]:LYS:HB2	2.29	0.48
1:D:145:SER:HB2	1:D:147:TYR:CZ	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLY:O	8:C:704:HOH:O	2.20	0.47
1:B:278:LYS:HD3	1:B:280:GLU:OE2	2.13	0.47
1:C:94[B]:GLU:O	1:C:98[B]:LYS:CD	2.62	0.47
1:C:258:PRO:CB	1:C:301:ILE:HD11	2.45	0.46
1:C:258:PRO:HB2	1:C:301:ILE:HD11	1.96	0.46
1:C:145:SER:HB2	1:C:147:TYR:CZ	2.50	0.46
1:C:286[B]:LYS:NZ	1:C:286[B]:LYS:HB3	2.31	0.46
1:C:286[B]:LYS:HD2	1:C:286[B]:LYS:HA	1.61	0.46
5:A:405:GOL:H32	1:B:179:LYS:HD3	1.98	0.46
1:B:26:GLN:HG2	8:B:853:HOH:O	2.16	0.46
1:C:286[B]:LYS:HB3	1:C:286[B]:LYS:HZ2	1.80	0.45
1:C:293[B]:GLU:O	1:C:293[B]:GLU:OE2	2.35	0.45
1:C:265:ARG:NH2	1:C:301:ILE:HG22	2.32	0.45
1:A:303:MET:O	3:A:402:D16:OE2	2.35	0.45
1:C:251:ILE:HG23	1:C:255[B]:HIS:CE1	2.51	0.45
1:D:226:LEU:HG	1:D:230:MET:HE3	1.98	0.45
1:C:192:LEU:C	1:C:192:LEU:HD12	2.42	0.44
5:B:403[A]:GOL:O2	8:B:512:HOH:O	2.07	0.44
3:C:402:D16:HP11	3:C:402:D16:H15	1.53	0.44
1:B:192:LEU:HD12	1:B:192:LEU:C	2.43	0.44
1:C:272:LYS:HB2	1:C:293[B]:GLU:CG	2.48	0.44
1:D:192:LEU:C	1:D:192:LEU:HD12	2.43	0.44
1:C:139[B]:GLU:CD	1:C:139[B]:GLU:H	2.26	0.44
1:A:22:HIS:CE1	8:A:880:HOH:O	2.71	0.43
1:B:277:ARG:HB2	8:B:820:HOH:O	2.18	0.43
1:B:278:LYS:CD	1:B:280:GLU:OE2	2.67	0.43
1:C:7[B]:GLU:CD	1:C:7[B]:GLU:N	2.65	0.43
1:D:106:ASN:CG	1:D:186:LEU:HD11	2.44	0.43
1:D:83:LEU:O	1:D:87:LYS:HG3	2.19	0.43
1:C:230:MET:HE2	1:C:290:PHE:CZ	2.54	0.42
1:A:113:ASP:OD1	1:A:118:SER:HA	2.20	0.42
1:A:278[B]:LYS:HE3	5:A:407[B]:GOL:C2	2.48	0.42
1:C:181:LEU:CB	1:C:182:PRO:HD3	2.49	0.42
1:A:1:MET:HG2	1:A:2:LEU:N	2.34	0.42
1:A:199:ASN:N	5:A:404[A]:GOL:O3	2.40	0.42
1:A:278[B]:LYS:CE	5:A:407[B]:GOL:H12	2.49	0.42
1:B:181[A]:LEU:HB2	1:B:182:PRO:HD3	2.01	0.42
1:D:190[B]:HIS:CD2	1:D:190[B]:HIS:N	2.85	0.42
1:A:26[A]:GLN:NE2	1:A:58:ARG:O	2.28	0.42
1:B:300:THR:HA	8:B:624:HOH:O	2.19	0.42
1:C:285:PHE:O	1:C:286[B]:LYS:HD2	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:H	5:A:404[B]:GOL:H32	1.85	0.41
1:C:187:PRO:HA	1:C:188:PRO:HD3	1.92	0.41
1:D:147:TYR:O	1:D:148:SER:C	2.63	0.41
1:A:181:LEU:N	1:A:182:PRO:CD	2.84	0.41
1:C:22[B]:HIS:HB3	1:C:25:LEU:HG	2.02	0.40
1:C:98[B]:LYS:N	1:C:98[B]:LYS:CD	2.83	0.40
1:D:22[A]:HIS:HD2	1:D:267:PRO:HB2	1.86	0.40
1:A:178:PRO:HD2	1:B:136:PHE:CZ	2.56	0.40
1:C:45:THR:OG1	1:C:47:THR:OG1	2.28	0.40
1:C:133:TRP:CE2	1:C:173:MET:HE3	2.56	0.40
1:D:74:PHE:CE1	1:D:76:LYS:HB3	2.56	0.40
5:B:403[B]:GOL:H31	8:B:738:HOH:O	2.21	0.40

All (2) 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)
8:A:860:HOH:O	8:C:506:HOH:O[3_545]	1.96	0.24
8:A:557:HOH:O	8:C:506:HOH:O[3_545]	2.01	0.19

## 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	306/307 (100%)	296 (97%)	9 (3%)	1 (0%)	36 23
1	B	302/307 (98%)	288 (95%)	13 (4%)	1 (0%)	36 23
1	C	305/307 (99%)	289 (95%)	14 (5%)	2 (1%)	18 6
1	D	305/307 (99%)	287 (94%)	16 (5%)	2 (1%)	18 6
All	All	1218/1228 (99%)	1160 (95%)	52 (4%)	6 (0%)	24 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	ARG
1	C	253	LEU
1	D	299	PRO
1	D	128	VAL
1	A	128	VAL
1	B	128	VAL

### 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	272/266 (102%)	260 (96%)	12 (4%)	25 5
1	B	267/266 (100%)	261 (98%)	6 (2%)	45 22
1	C	272/266 (102%)	258 (95%)	14 (5%)	21 4
1	D	271/266 (102%)	262 (97%)	9 (3%)	33 10
All	All	1082/1064 (102%)	1041 (96%)	41 (4%)	32 8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	21	ARG
1	A	139	GLU
1	A	192	LEU
1	A	278[A]	LYS
1	A	278[B]	LYS
1	A	283[A]	ASP
1	A	283[B]	ASP
1	A	302[A]	LYS
1	A	302[B]	LYS
1	A	304	GLU
1	A	307	VAL
1	B	21	ARG
1	B	115	LEU
1	B	192	LEU
1	B	278	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	288	GLU
1	B	307	VAL
1	C	40	LYS
1	C	93	LYS
1	C	102	ILE
1	C	118	SER
1	C	181	LEU
1	C	253	LEU
1	C	256	ILE
1	C	274	LYS
1	C	277	ARG
1	C	286[A]	LYS
1	C	286[B]	LYS
1	C	288	GLU
1	C	301	ILE
1	C	302	LYS
1	D	22[A]	HIS
1	D	22[B]	HIS
1	D	109	ARG
1	D	158	VAL
1	D	170	ARG
1	D	192	LEU
1	D	256	ILE
1	D	277	ARG
1	D	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	132	GLN
1	A	177	ASN
1	A	291	GLN
1	B	165	ASN
1	B	199	ASN
1	C	150	GLN
1	C	165	ASN
1	C	264	GLN
1	C	296	ASN
1	D	254	ASN
1	D	291	GLN
1	D	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

25 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	UMP	B	401	-	21,21,21	1.11	2 (9%)	30,31,31	1.71	5 (16%)
2	UMP	A	401	-	21,21,21	1.41	3 (14%)	30,31,31	1.63	6 (20%)
2	UMP	C	401	-	21,21,21	1.21	3 (14%)	30,31,31	1.96	6 (20%)
3	D16	B	402	-	33,34,34	1.30	3 (9%)	46,48,48	1.92	11 (23%)
5	GOL	B	404[B]	-	5,5,5	0.39	0	5,5,5	0.44	0
5	GOL	B	404[A]	-	5,5,5	0.43	0	5,5,5	0.83	0
5	GOL	A	404[B]	-	5,5,5	0.49	0	5,5,5	0.94	0
5	GOL	D	404	-	5,5,5	0.42	0	5,5,5	0.40	0
5	GOL	C	403	-	5,5,5	0.46	0	5,5,5	0.18	0
5	GOL	A	404[A]	-	5,5,5	0.70	0	5,5,5	1.12	0
5	GOL	B	403[B]	-	5,5,5	0.27	0	5,5,5	0.66	0
3	D16	A	402	-	33,34,34	1.49	6 (18%)	46,48,48	1.61	10 (21%)
3	D16	C	402	-	33,34,34	1.42	3 (9%)	46,48,48	2.62	14 (30%)
2	UMP	D	401	-	21,21,21	1.09	2 (9%)	30,31,31	1.81	7 (23%)
5	GOL	A	407[B]	-	5,5,5	0.33	0	5,5,5	0.61	0
7	MES	B	406	-	12,12,12	1.99	1 (8%)	15,16,16	2.38	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	403[A]	-	5,5,5	0.66	0	5,5,5	0.75	0
4	DTT	A	403	-	7,7,7	1.99	5 (71%)	4,8,8	2.19	2 (50%)
5	GOL	A	405	-	5,5,5	0.66	0	5,5,5	0.59	0
5	GOL	D	403	-	5,5,5	0.44	0	5,5,5	0.38	0
5	GOL	A	407[A]	-	5,5,5	0.29	0	5,5,5	0.37	0
3	D16	D	402	-	33,34,34	1.44	5 (15%)	46,48,48	1.78	12 (26%)
5	GOL	A	406	-	5,5,5	0.27	0	5,5,5	0.69	0
5	GOL	B	405	-	5,5,5	0.42	0	5,5,5	0.60	0
6	SO4	A	408	-	4,4,4	0.28	0	6,6,6	0.24	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
2	UMP	B	401	-	-	0/10/22/22	0/2/2/2
2	UMP	A	401	-	-	0/10/22/22	0/2/2/2
2	UMP	C	401	-	-	0/10/22/22	0/2/2/2
3	D16	B	402	-	-	0/25/25/25	0/3/3/3
5	GOL	B	404[B]	-	-	4/4/4/4	-
5	GOL	B	404[A]	-	-	2/4/4/4	-
5	GOL	A	404[B]	-	-	2/4/4/4	-
5	GOL	D	404	-	-	4/4/4/4	-
5	GOL	C	403	-	-	2/4/4/4	-
5	GOL	A	404[A]	-	-	2/4/4/4	-
5	GOL	B	403[B]	-	-	4/4/4/4	-
3	D16	A	402	-	-	0/25/25/25	0/3/3/3
3	D16	C	402	-	-	3/25/25/25	0/3/3/3
2	UMP	D	401	-	-	0/10/22/22	0/2/2/2
5	GOL	A	407[B]	-	-	2/4/4/4	-
7	MES	B	406	-	-	1/6/14/14	0/1/1/1
5	GOL	B	403[A]	-	-	4/4/4/4	-
4	DTT	A	403	-	-	7/8/8/8	-
5	GOL	A	405	-	-	2/4/4/4	-
5	GOL	D	403	-	-	0/4/4/4	-
5	GOL	A	407[A]	-	-	4/4/4/4	-
3	D16	D	402	-	-	2/25/25/25	0/3/3/3
5	GOL	A	406	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	405	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	406	MES	C8-S	-6.41	1.68	1.77
3	C	402	D16	C4A-C8A	5.30	1.49	1.41
3	D	402	D16	C4A-C8A	5.12	1.49	1.41
2	A	401	UMP	O2-C2	3.83	1.29	1.23
3	A	402	D16	C4-N3	-3.79	1.31	1.38
2	B	401	UMP	C6-C5	3.44	1.43	1.35
3	C	402	D16	C8A-N1	-3.29	1.34	1.39
3	B	402	D16	C4-N3	-3.21	1.32	1.38
3	B	402	D16	C4A-C8A	3.09	1.45	1.41
3	A	402	D16	C8A-N1	-2.97	1.34	1.39
3	D	402	D16	C8A-N1	-2.93	1.34	1.39
3	A	402	D16	C2-N3	2.90	1.37	1.31
3	A	402	D16	C4A-C8A	2.89	1.45	1.41
2	A	401	UMP	C5-C4	-2.77	1.37	1.43
3	A	402	D16	C-C11	2.75	1.54	1.48
3	C	402	D16	C2-N3	2.74	1.37	1.31
3	B	402	D16	C8A-N1	-2.72	1.35	1.39
4	A	403	DTT	C4-S4	2.59	1.86	1.81
2	C	401	UMP	C6-C5	2.57	1.41	1.35
4	A	403	DTT	C3-C2	2.55	1.59	1.53
2	D	401	UMP	P-OP3	-2.51	1.45	1.54
3	D	402	D16	C2-N3	2.49	1.36	1.31
2	A	401	UMP	C6-C5	2.44	1.40	1.35
2	B	401	UMP	P-OP3	-2.39	1.45	1.54
2	D	401	UMP	C6-C5	2.32	1.40	1.35
2	C	401	UMP	C5-C4	-2.26	1.38	1.43
3	D	402	D16	C4A-C4	-2.20	1.44	1.48
3	A	402	D16	C14-S13	-2.17	1.70	1.73
4	A	403	DTT	C1-S1	2.14	1.85	1.81
4	A	403	DTT	C1-C2	2.09	1.57	1.51
2	C	401	UMP	O4'-C4'	-2.07	1.40	1.45
3	D	402	D16	C4-N3	-2.05	1.34	1.38
4	A	403	DTT	C4-C3	2.01	1.57	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	D16	C15-C14-N10	-10.18	117.34	127.84
3	C	402	D16	S13-C14-N10	7.54	128.06	120.99
2	C	401	UMP	N3-C2-N1	5.54	122.10	114.89
2	B	401	UMP	C6-C5-C4	-5.51	112.49	119.53
3	A	402	D16	C5-C4A-C8A	4.77	123.38	119.09
2	C	401	UMP	C4-N3-C2	-4.74	120.73	126.61
2	D	401	UMP	N3-C2-N1	4.71	121.03	114.89
3	C	402	D16	C11-S13-C14	-4.66	86.76	91.43
3	B	402	D16	C8A-C4A-C4	-4.56	115.18	120.11
7	B	406	MES	C5-N4-C3	4.49	118.52	108.84
3	B	402	D16	S13-C14-N10	4.34	125.06	120.99
3	B	402	D16	C15-C14-N10	-4.33	123.37	127.84
3	D	402	D16	C8A-C4A-C4	-4.28	115.48	120.11
3	C	402	D16	CG-CB-CA	-4.27	105.29	113.16
3	D	402	D16	C11-S13-C14	-4.02	87.39	91.43
2	C	401	UMP	C2'-C1'-N1	4.02	123.87	113.81
3	B	402	D16	CM2-C2-N1	3.88	123.90	116.41
3	D	402	D16	C15-C14-N10	-3.82	123.90	127.84
7	B	406	MES	C7-N4-C3	3.77	121.27	111.24
2	A	401	UMP	C4-N3-C2	-3.73	121.98	126.61
2	B	401	UMP	C5-C4-N3	3.69	119.96	114.80
2	D	401	UMP	C4-N3-C2	-3.68	122.05	126.61
3	B	402	D16	C8-C8A-C4A	-3.64	114.61	119.37
2	B	401	UMP	O5'-P-OP1	-3.62	96.66	106.44
3	B	402	D16	C8-C8A-N1	3.57	125.92	119.91
2	A	401	UMP	O4-C4-N3	-3.53	114.15	119.27
2	A	401	UMP	C5-C4-N3	3.47	119.66	114.80
2	C	401	UMP	O2-C2-N1	-3.45	118.31	122.80
3	C	402	D16	C5-C4A-C8A	3.43	122.18	119.09
4	A	403	DTT	O3-C3-C2	3.38	116.68	109.57
3	A	402	D16	C8A-C4A-C4	-3.37	116.47	120.11
2	D	401	UMP	O2-C2-N1	-3.36	118.42	122.80
7	B	406	MES	C7-N4-C5	3.34	120.15	111.24
3	D	402	D16	C15-C14-S13	3.33	115.72	111.97
7	B	406	MES	C2-C3-N4	-3.31	105.09	110.12
3	A	402	D16	C4A-C5-C6	-3.22	116.38	121.38
3	D	402	D16	C5-C4A-C8A	3.20	121.97	119.09
3	C	402	D16	C8A-C4A-C4	-3.18	116.68	120.11
2	B	401	UMP	C2'-C1'-N1	3.06	121.47	113.81
3	B	402	D16	C5-C4A-C8A	3.02	121.81	119.09
3	C	402	D16	C8-C8A-C4A	-3.02	115.43	119.37
2	D	401	UMP	C6-N1-C2	-2.90	117.47	121.00
2	D	401	UMP	C2'-C1'-N1	2.87	120.98	113.81

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	D16	C16-C11-S13	2.86	114.66	110.49
7	B	406	MES	O3S-S-C8	2.82	111.53	106.00
2	A	401	UMP	C2'-C1'-N1	2.78	120.76	113.81
3	B	402	D16	C8-C7-C6	2.73	124.58	121.00
3	A	402	D16	C8-C7-C6	2.73	124.58	121.00
3	C	402	D16	OE1-CD-CG	-2.72	114.47	123.09
7	B	406	MES	O1S-S-C8	2.71	110.83	106.73
3	C	402	D16	C8-C8A-N1	2.71	124.47	119.91
2	C	401	UMP	O5'-P-OP1	2.69	113.71	106.44
2	A	401	UMP	O4'-C1'-C2'	2.63	111.16	106.25
2	D	401	UMP	OP3-P-O5'	2.62	113.50	106.67
3	C	402	D16	C6-C9-N10	2.62	117.95	113.02
3	A	402	D16	C15-C14-N10	-2.56	125.20	127.84
3	B	402	D16	CG-CB-CA	-2.55	108.45	113.16
2	D	401	UMP	O4-C4-C5	-2.49	120.87	125.16
3	C	402	D16	CA-N-C	-2.47	117.85	122.00
3	D	402	D16	CM2-C2-N1	2.46	121.16	116.41
3	D	402	D16	C8-C8A-C4A	-2.44	116.19	119.37
2	A	401	UMP	N3-C2-N1	2.42	118.04	114.89
3	D	402	D16	OE1-CD-CG	-2.38	115.54	123.09
3	C	402	D16	O4-C4-N3	2.38	123.84	120.23
3	A	402	D16	CP1-N10-C14	-2.34	115.60	120.41
3	C	402	D16	OE2-CD-CG	2.30	121.28	114.00
3	A	402	D16	CA-N-C	2.30	125.86	122.00
7	B	406	MES	O2S-S-O1S	-2.28	106.42	113.82
2	C	401	UMP	C6-N1-C2	-2.22	118.30	121.00
3	A	402	D16	C6-C9-N10	2.19	117.14	113.02
3	D	402	D16	C8-C8A-N1	2.18	123.58	119.91
3	D	402	D16	C16-C11-S13	2.18	113.66	110.49
3	A	402	D16	O-C-N	-2.17	119.28	123.09
3	B	402	D16	CA-N-C	2.15	125.62	122.00
4	A	403	DTT	C2-C1-S1	2.15	120.44	114.43
3	D	402	D16	O-C-N	-2.12	119.35	123.09
3	B	402	D16	O2-CT-CA	2.12	120.69	113.51
3	A	402	D16	C11-S13-C14	-2.07	89.35	91.43
2	B	401	UMP	OP3-P-OP2	2.07	115.56	107.80
3	D	402	D16	C16-C15-C14	-2.03	109.05	112.01

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	DTT	S1-C1-C2-O2
4	A	403	DTT	S1-C1-C2-C3
4	A	403	DTT	C1-C2-C3-O3
4	A	403	DTT	C1-C2-C3-C4
4	A	403	DTT	O2-C2-C3-O3
4	A	403	DTT	O2-C2-C3-C4
4	A	403	DTT	C2-C3-C4-S4
5	A	404[A]	GOL	C1-C2-C3-O3
5	A	404[A]	GOL	O2-C2-C3-O3
5	A	404[B]	GOL	C1-C2-C3-O3
5	A	405	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-C3
5	A	407[A]	GOL	C1-C2-C3-O3
5	A	407[B]	GOL	C1-C2-C3-O3
5	B	403[A]	GOL	O1-C1-C2-C3
5	B	403[A]	GOL	C1-C2-C3-O3
5	B	403[A]	GOL	O2-C2-C3-O3
5	B	403[B]	GOL	O1-C1-C2-O2
5	B	403[B]	GOL	O1-C1-C2-C3
5	B	403[B]	GOL	C1-C2-C3-O3
5	B	404[A]	GOL	C1-C2-C3-O3
5	B	404[A]	GOL	O2-C2-C3-O3
5	B	404[B]	GOL	C1-C2-C3-O3
5	C	403	GOL	O1-C1-C2-C3
5	D	404	GOL	O1-C1-C2-O2
5	D	404	GOL	O1-C1-C2-C3
5	D	404	GOL	C1-C2-C3-O3
7	B	406	MES	C8-C7-N4-C5
5	A	404[B]	GOL	O2-C2-C3-O3
5	A	405	GOL	O2-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
5	B	403[A]	GOL	O1-C1-C2-O2
5	A	407[A]	GOL	O1-C1-C2-C3
5	B	405	GOL	C1-C2-C3-O3
5	A	407[B]	GOL	O2-C2-C3-O3
5	B	404[B]	GOL	O2-C2-C3-O3
5	C	403	GOL	O1-C1-C2-O2
5	D	404	GOL	O2-C2-C3-O3
5	A	407[A]	GOL	O2-C2-C3-O3
5	B	403[B]	GOL	O2-C2-C3-O3
3	C	402	D16	N-CA-CT-O2
3	C	402	D16	N-CA-CT-O1
5	B	405	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

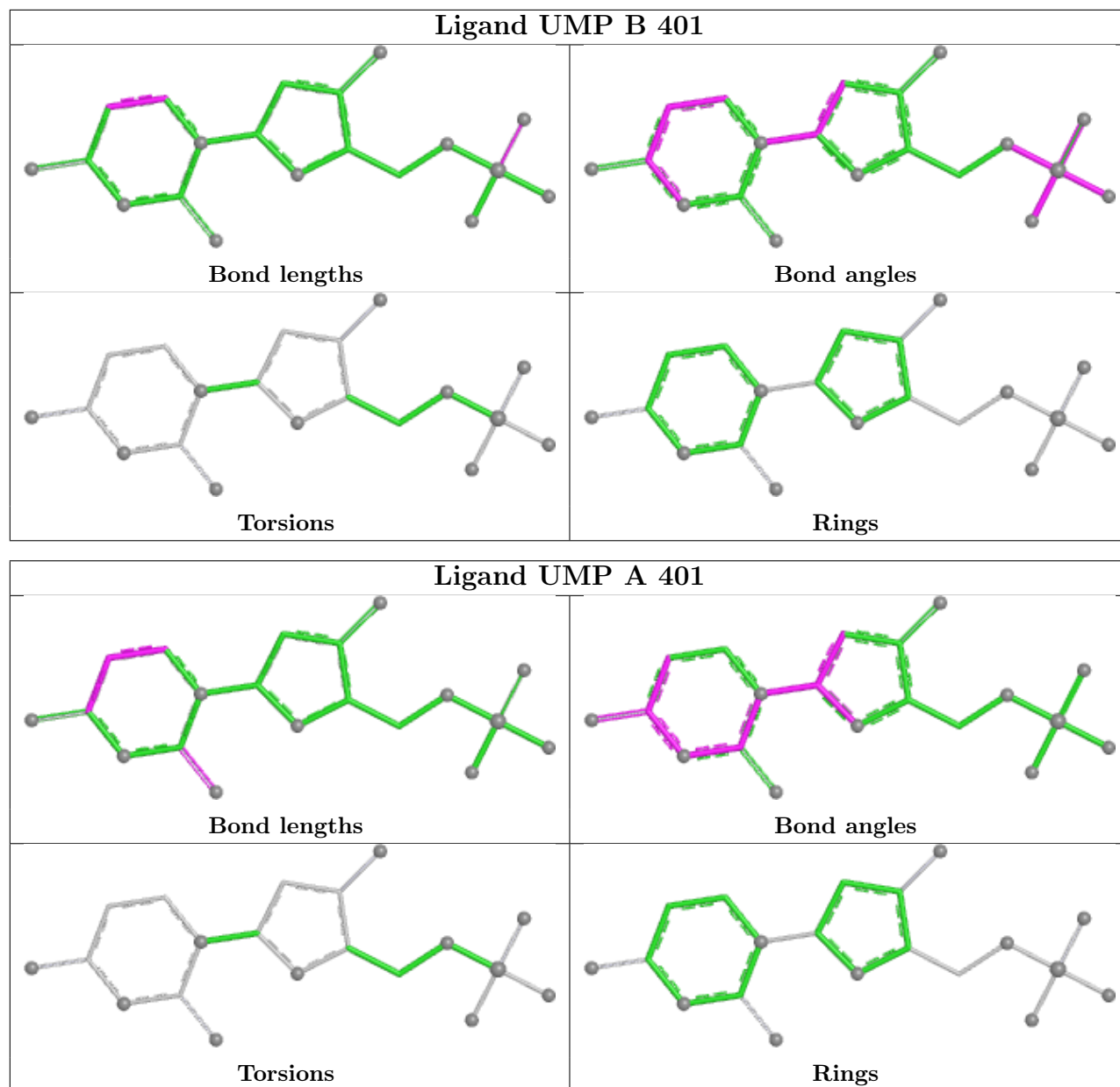
Mol	Chain	Res	Type	Atoms
5	B	404[B]	GOL	O1-C1-C2-C3
5	A	407[A]	GOL	O1-C1-C2-O2
5	B	404[B]	GOL	O1-C1-C2-O2
3	D	402	D16	OE2-CD-CG-CB
3	D	402	D16	OE1-CD-CG-CB
3	C	402	D16	C6-C9-N10-CP1

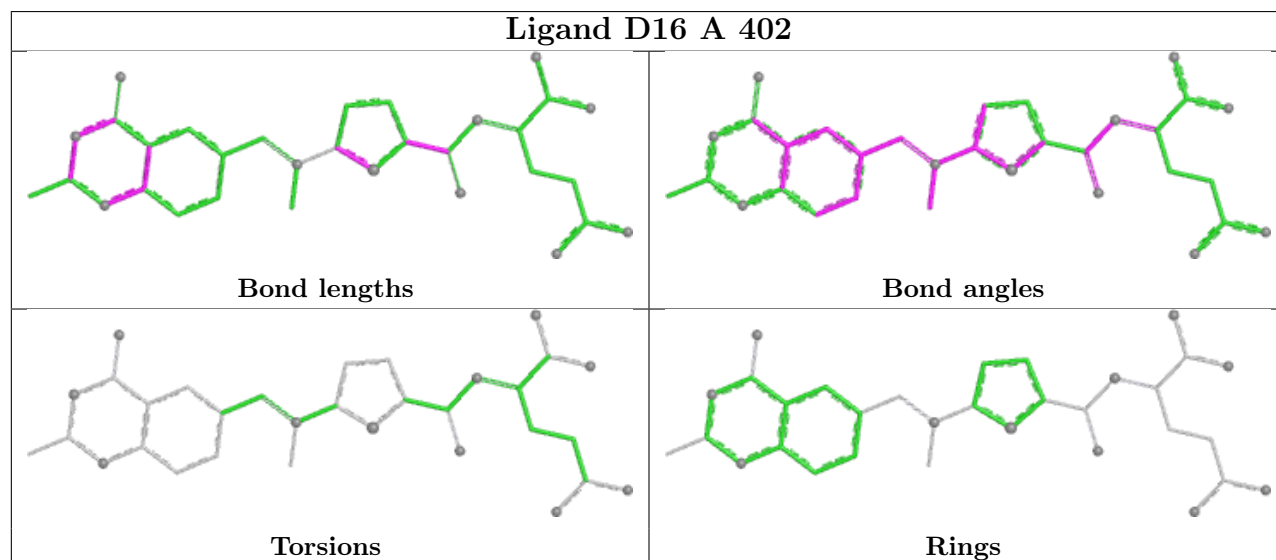
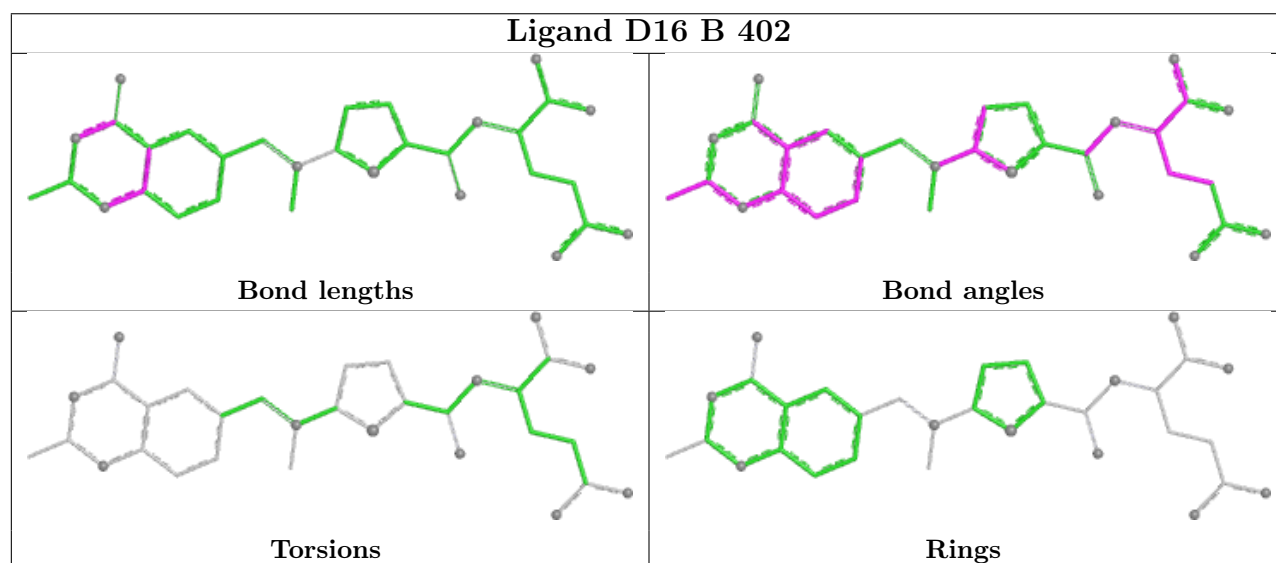
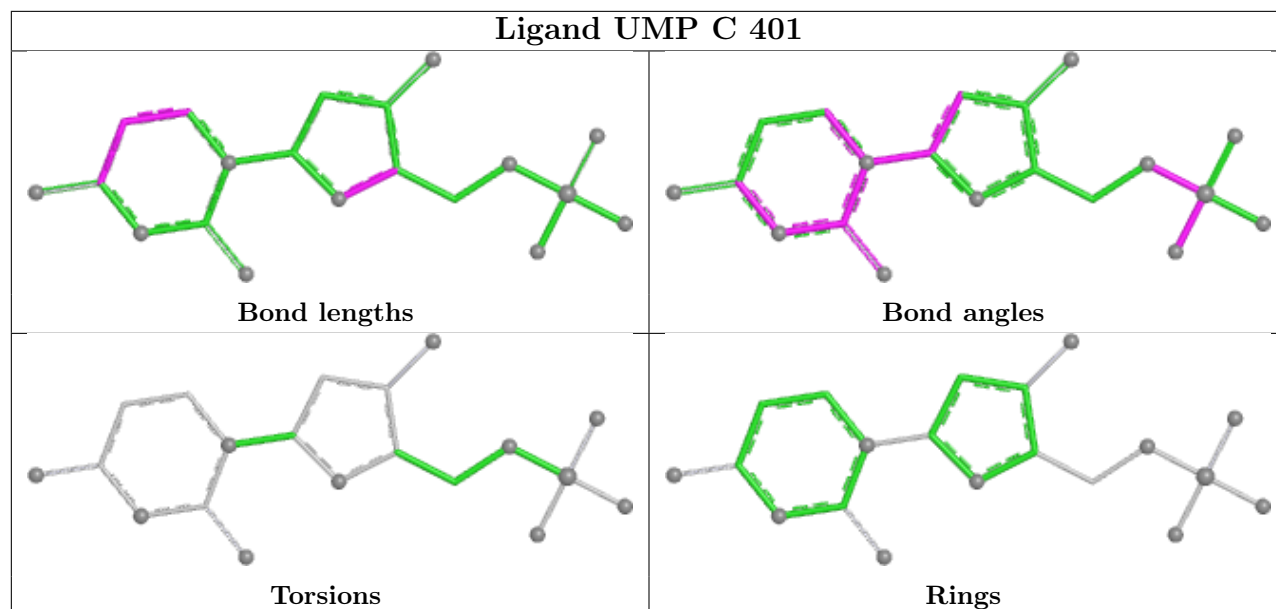
There are no ring outliers.

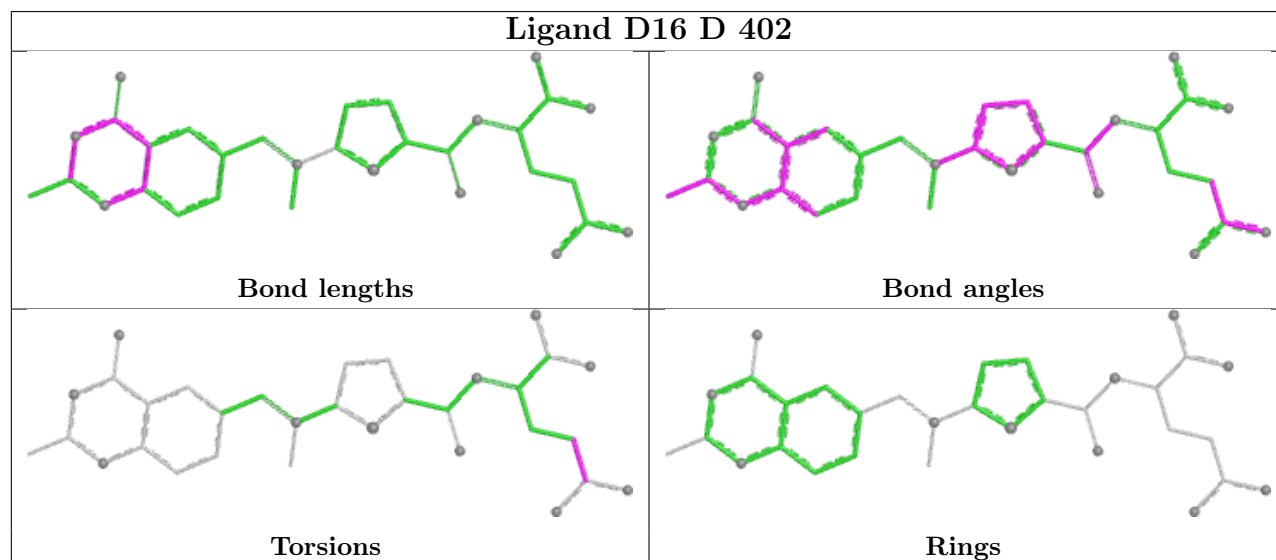
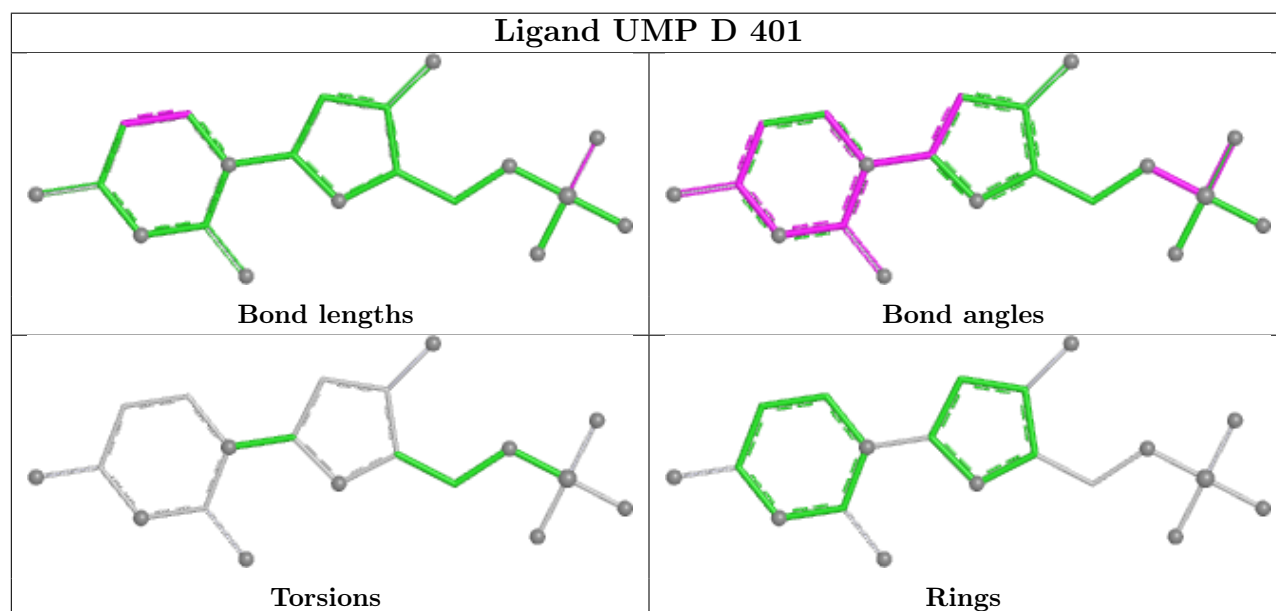
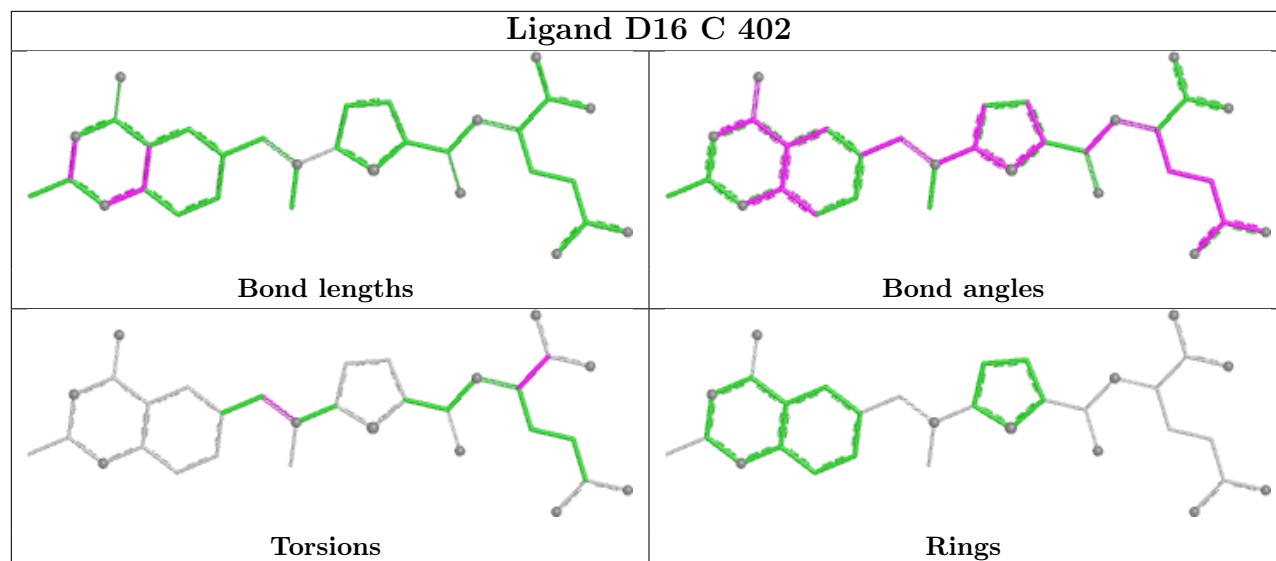
16 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	UMP	3	0
2	A	401	UMP	2	0
2	C	401	UMP	2	0
5	A	404[B]	GOL	1	0
5	D	404	GOL	2	0
5	A	404[A]	GOL	2	0
5	B	403[B]	GOL	1	0
3	A	402	D16	1	0
3	C	402	D16	2	0
2	D	401	UMP	2	0
5	A	407[B]	GOL	7	0
7	B	406	MES	1	0
5	B	403[A]	GOL	2	0
4	A	403	DTT	1	0
5	A	405	GOL	1	0
5	B	405	GOL	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, 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	300/307 (97%)	-0.15	5 (1%) 69 76	10, 22, 35, 60	11 (3%)
1	B	301/307 (98%)	-0.24	4 (1%) 75 82	10, 22, 35, 60	5 (1%)
1	C	295/307 (96%)	0.82	33 (11%) 10 13	11, 31, 60, 68	14 (4%)
1	D	297/307 (96%)	0.72	17 (5%) 29 35	13, 34, 50, 68	12 (4%)
All	All	1193/1228 (97%)	0.28	59 (4%) 35 42	10, 27, 48, 68	42 (3%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139[A]	GLU	4.7
1	B	20	PRO	4.4
1	D	22[A]	HIS	4.3
1	D	301	ILE	3.9
1	C	22[A]	HIS	3.9
1	D	45	THR	3.9
1	A	12	ALA	3.8
1	C	112	LEU	3.6
1	C	301	ILE	3.5
1	D	255	HIS	3.5
1	A	22	HIS	3.4
1	B	1	MET	3.2
1	C	255[A]	HIS	3.2
1	C	107	GLY	3.1
1	A	307	VAL	3.1
1	C	116	GLY	3.0
1	C	77	GLY	3.0
1	C	111	PHE	3.0
1	D	147	TYR	2.9
1	C	115	LEU	2.9
1	D	300	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	108	SER	2.7
1	A	1	MET	2.7
1	B	21	ARG	2.7
1	C	118	SER	2.7
1	C	92	ALA	2.6
1	D	46	GLY	2.6
1	C	119	ALA	2.6
1	D	276	LEU	2.5
1	C	122	GLU	2.5
1	C	276	LEU	2.5
1	C	89	SER	2.4
1	C	279	VAL	2.4
1	C	110	ASP	2.4
1	D	303	MET	2.4
1	C	46	GLY	2.4
1	B	118	SER	2.4
1	C	45	THR	2.4
1	C	254	ASN	2.4
1	C	47	THR	2.3
1	D	138	ALA	2.3
1	A	21	ARG	2.3
1	D	234	ILE	2.3
1	D	99	GLY	2.2
1	C	91	ASN	2.2
1	C	117	PHE	2.2
1	C	102	ILE	2.2
1	D	103[A]	TRP	2.2
1	D	48	GLY	2.2
1	C	109	ARG	2.1
1	D	292	ILE	2.1
1	C	123	GLY	2.1
1	C	287	VAL	2.1
1	C	43	ASP	2.1
1	C	181	LEU	2.1
1	C	302	LYS	2.1
1	D	236	GLY	2.0
1	C	21	ARG	2.0
1	D	256	ILE	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](#)

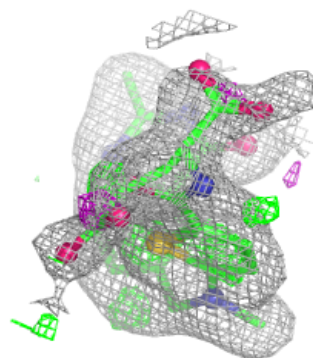
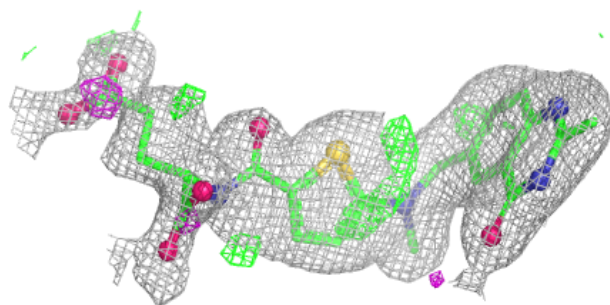
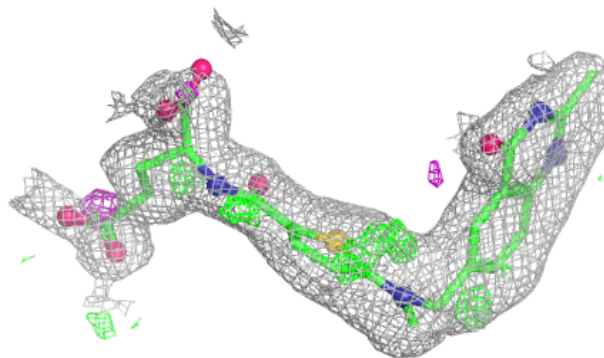
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	GOL	D	404	6/6	0.69	0.16	43,44,45,45	6
5	GOL	C	403	6/6	0.72	0.17	60,61,63,64	0
5	GOL	B	405	6/6	0.75	0.15	67,68,69,69	0
5	GOL	D	403	6/6	0.79	0.12	66,66,67,67	0
5	GOL	A	406	6/6	0.79	0.14	53,56,56,57	0
5	GOL	B	403[A]	6/6	0.82	0.12	36,39,41,42	6
5	GOL	B	403[B]	6/6	0.82	0.12	37,39,39,40	6
7	MES	B	406	12/12	0.82	0.16	44,46,50,51	12
6	SO4	A	408	5/5	0.85	0.20	41,41,43,44	5
3	D16	C	402	32/32	0.85	0.12	32,40,54,56	0
5	GOL	A	405	6/6	0.86	0.13	39,40,44,47	0
4	DTT	A	403	8/8	0.86	0.11	32,39,48,50	0
5	GOL	A	407[A]	6/6	0.86	0.11	44,49,50,52	6
5	GOL	A	407[B]	6/6	0.86	0.11	41,43,45,45	6
3	D16	D	402	32/32	0.87	0.11	39,44,55,59	0
5	GOL	A	404[A]	6/6	0.87	0.11	23,31,31,31	6
5	GOL	A	404[B]	6/6	0.87	0.11	25,30,31,31	6
5	GOL	B	404[A]	6/6	0.90	0.09	30,33,37,37	6
5	GOL	B	404[B]	6/6	0.90	0.09	13,18,19,19	6
2	UMP	C	401	20/20	0.92	0.08	29,33,37,40	0
3	D16	A	402	32/32	0.93	0.07	18,23,31,38	0
2	UMP	D	401	20/20	0.94	0.08	25,32,36,37	0
3	D16	B	402	32/32	0.95	0.08	13,24,34,41	0
2	UMP	A	401	20/20	0.98	0.05	16,17,20,24	0
2	UMP	B	401	20/20	0.99	0.03	14,16,20,21	0

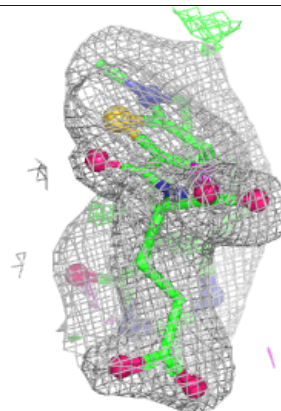
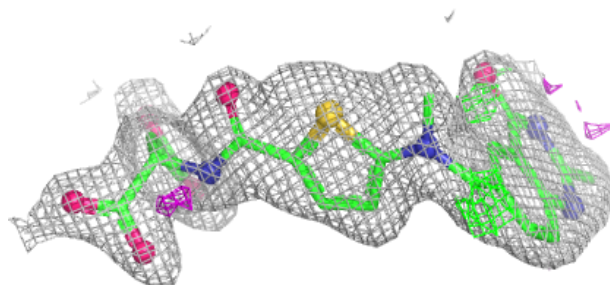
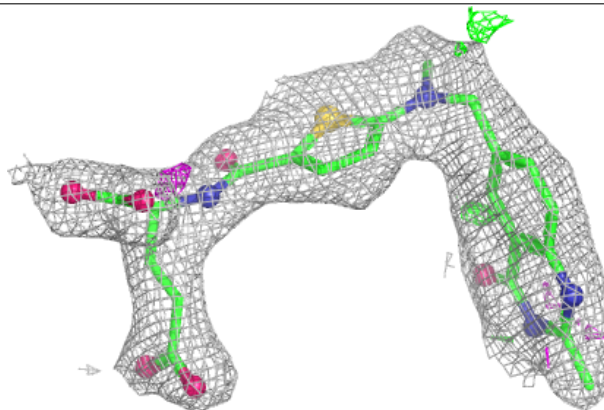
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around D16 C 402:**

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

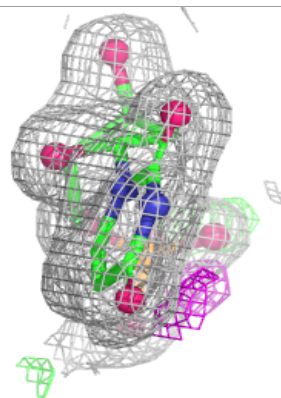
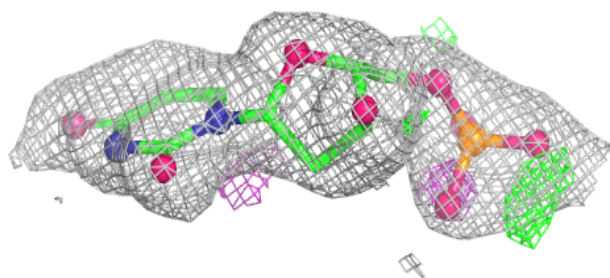
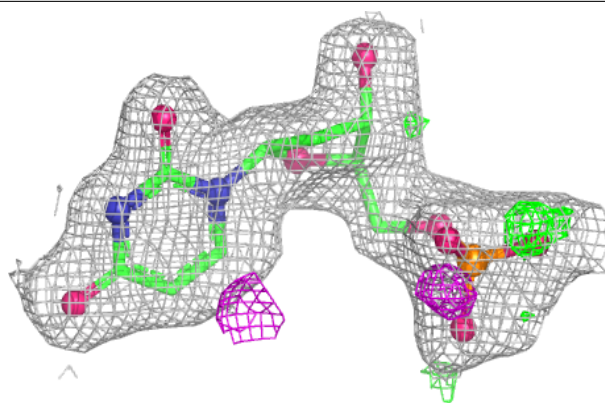
**Electron density around D16 D 402:**

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

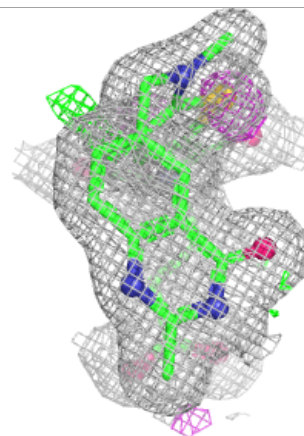
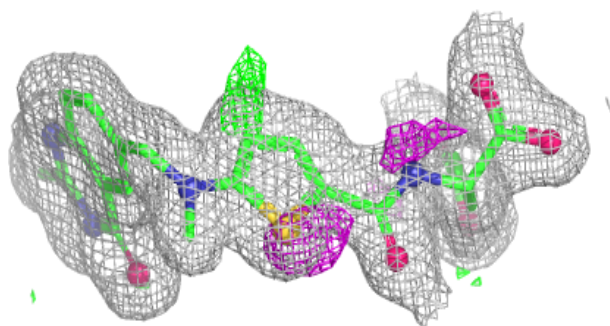
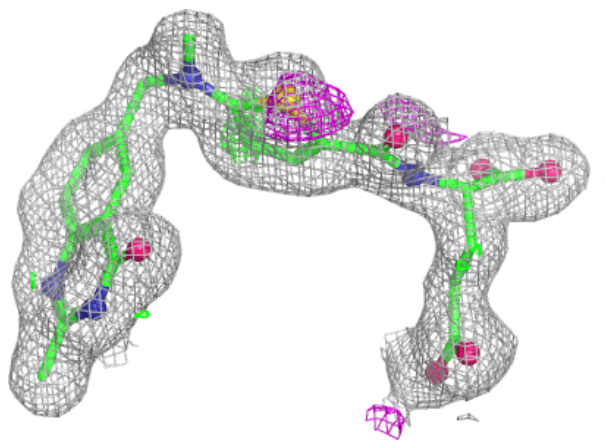


**Electron density around UMP C 401:**

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

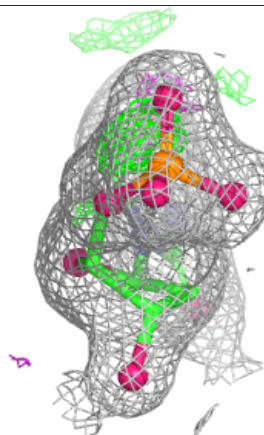
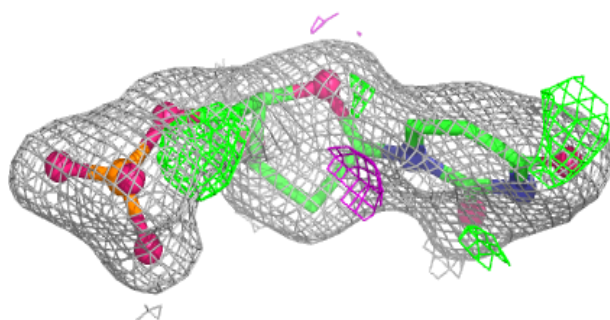
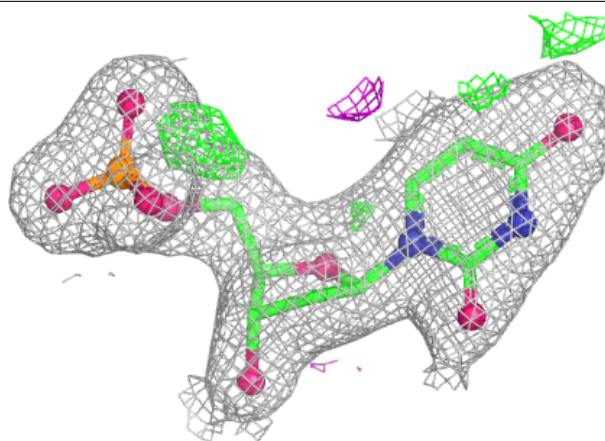
**Electron density around D16 A 402:**

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

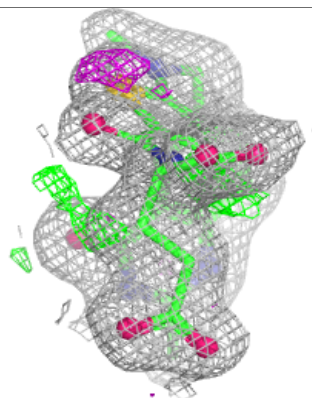
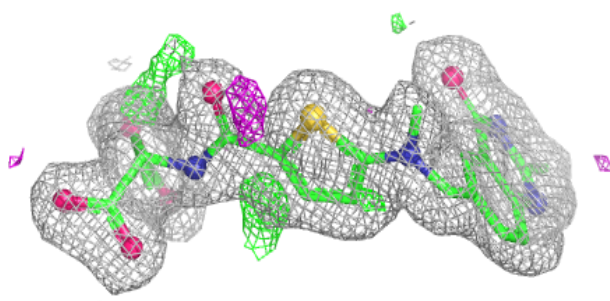
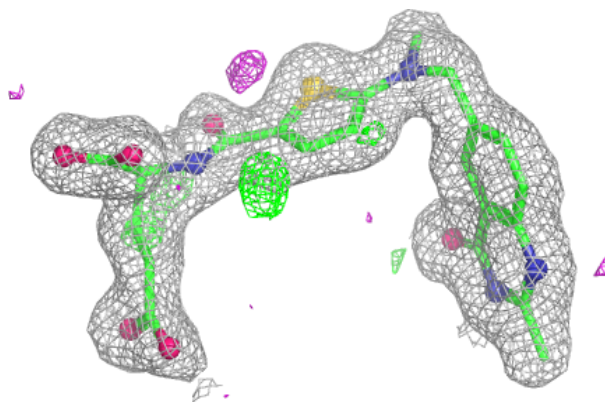


**Electron density around UMP D 401:**

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

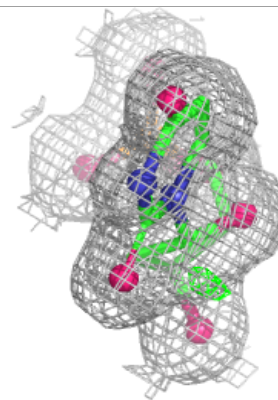
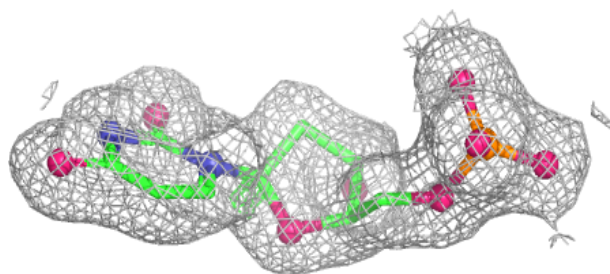
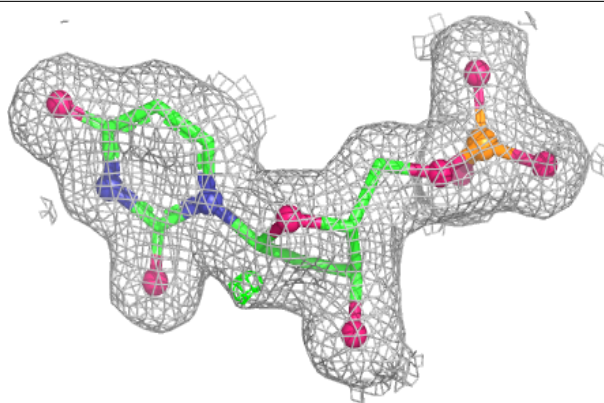
**Electron density around D16 B 402:**

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

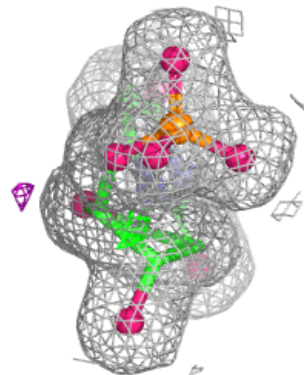
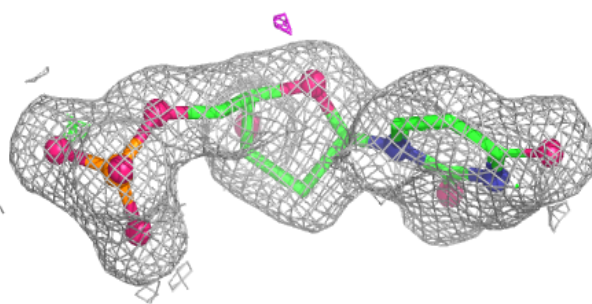
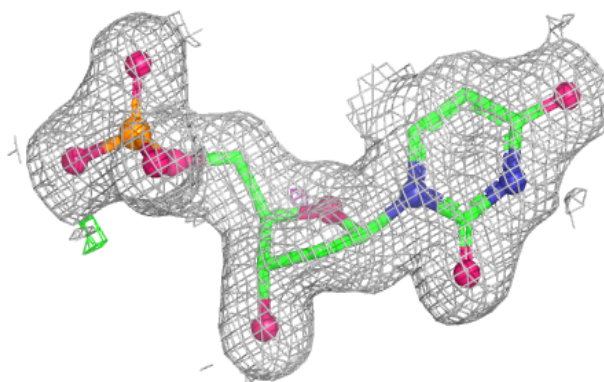


**Electron density around UMP A 401:**

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

**Electron density around UMP B 401:**

$2mF_o-DF_c$  (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.