



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:43 am BST

PDB ID : 4E5O  
Title : Crystal structure of mouse thymidylate synthase in complex with dUMP  
Authors : Dowiercial, A.; Jarmula, A.; Rypniewski, W.; Sokolowska, M.; Fraczyk, T.; Ciesla, J.; Rode, W.  
Deposited on : 2012-03-14  
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

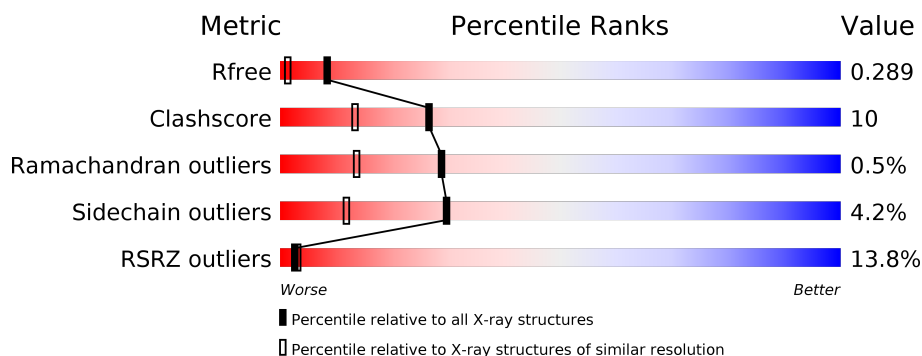
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	307	
1	B	307	
1	C	307	
1	D	307	
1	E	307	
1	F	307	

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
2	UMP	F	502	-	-	X	-
3	BU1	C	503	-	-	X	-

## 2 Entry composition [i](#)

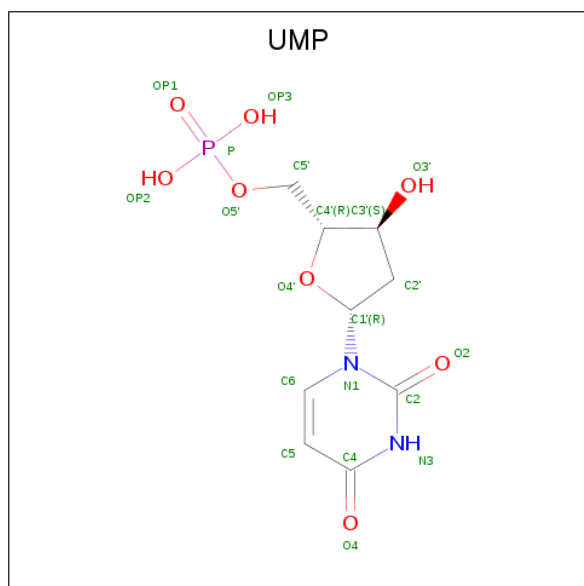
There are 4 unique types of molecules in this entry. The entry contains 15512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

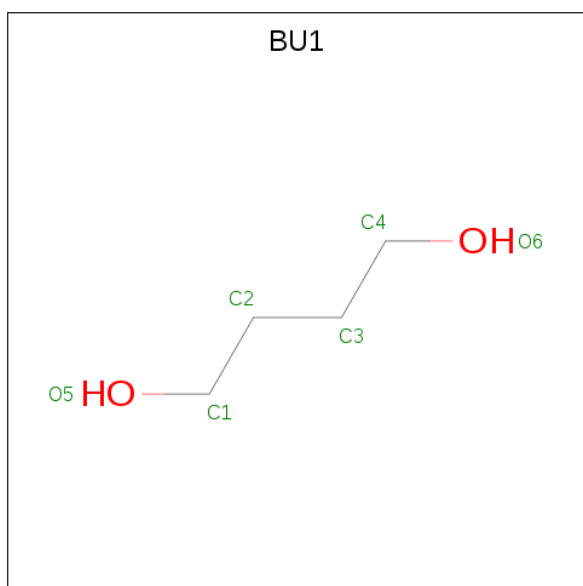
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	3	0
			2346	1501	405	427	13			
1	B	288	Total	C	N	O	S	0	3	0
			2354	1505	409	427	13			
1	C	280	Total	C	N	O	S	0	2	0
			2275	1456	395	413	11			
1	D	283	Total	C	N	O	S	0	1	0
			2298	1472	399	415	12			
1	E	281	Total	C	N	O	S	0	6	0
			2332	1493	407	421	11			
1	F	279	Total	C	N	O	S	0	2	0
			2277	1457	397	412	11			

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



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		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			6	4	2		

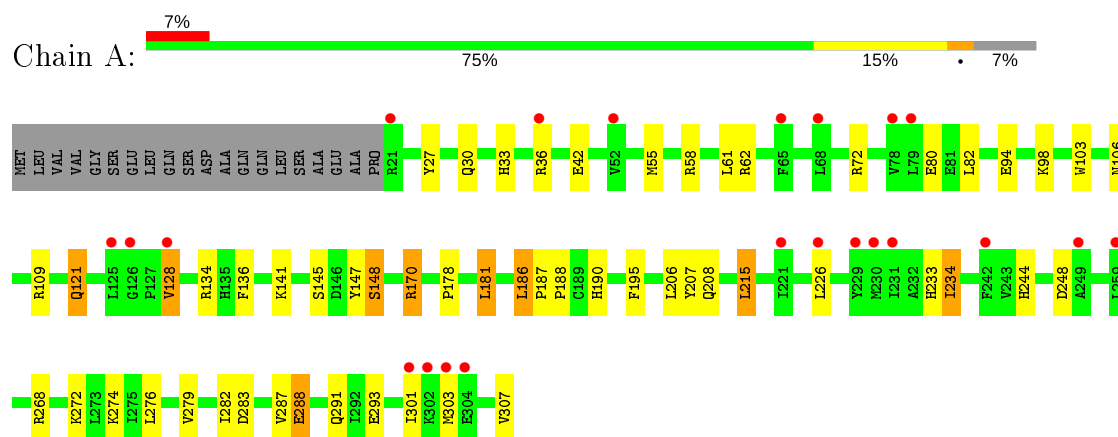
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	344	Total 344	O 344	0	0
4	B	315	Total 315	O 315	0	0
4	C	279	Total 279	O 279	0	0
4	D	242	Total 242	O 242	0	0
4	E	116	Total 116	O 116	0	0
4	F	176	Total 176	O 176	0	0

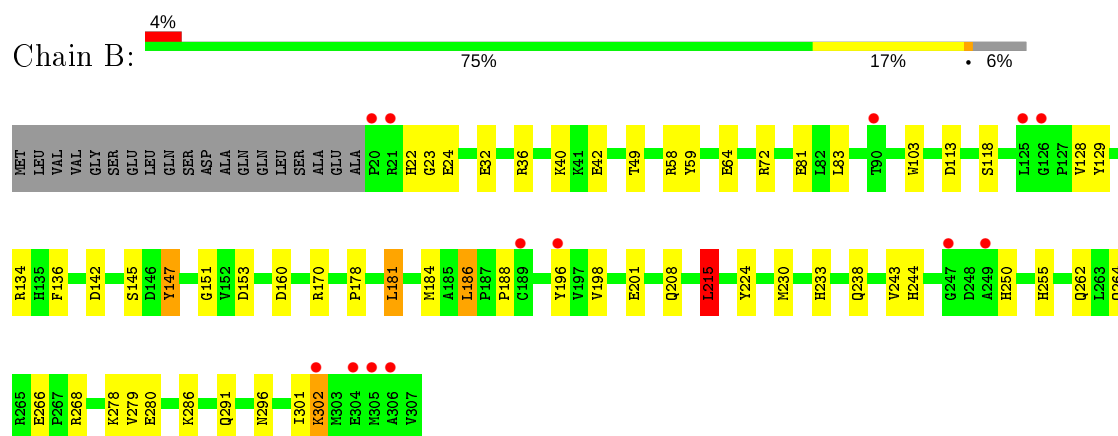
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

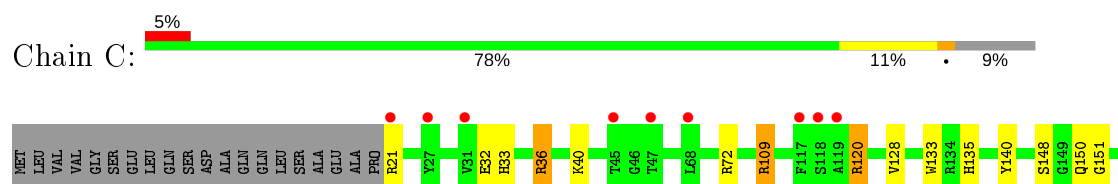
#### • Molecule 1: Thymidylate synthase

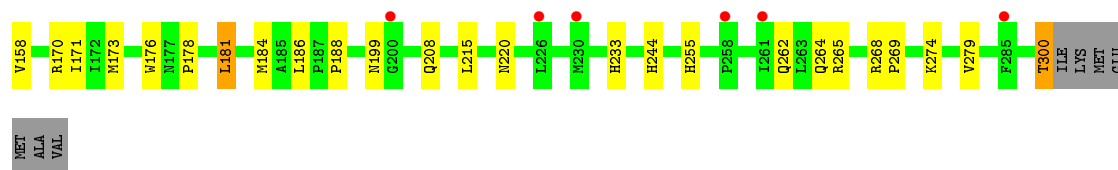


#### • Molecule 1: Thymidylate synthase

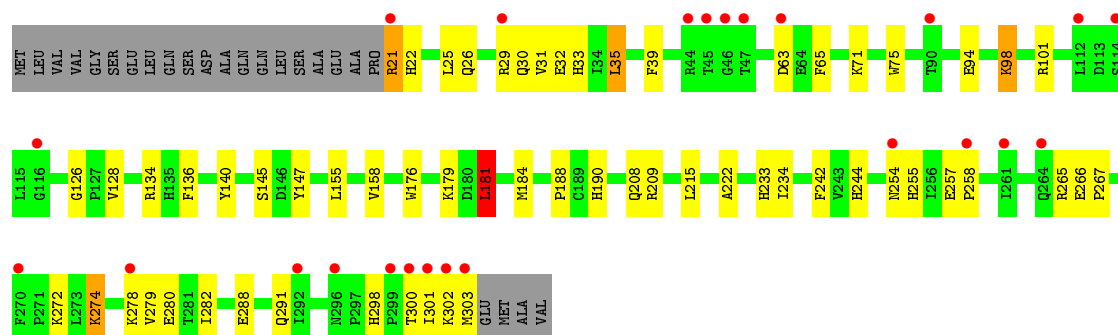
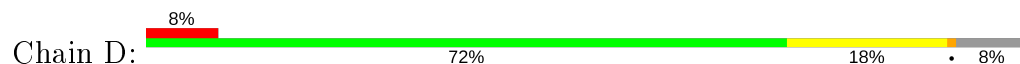


#### • Molecule 1: Thymidylate synthase

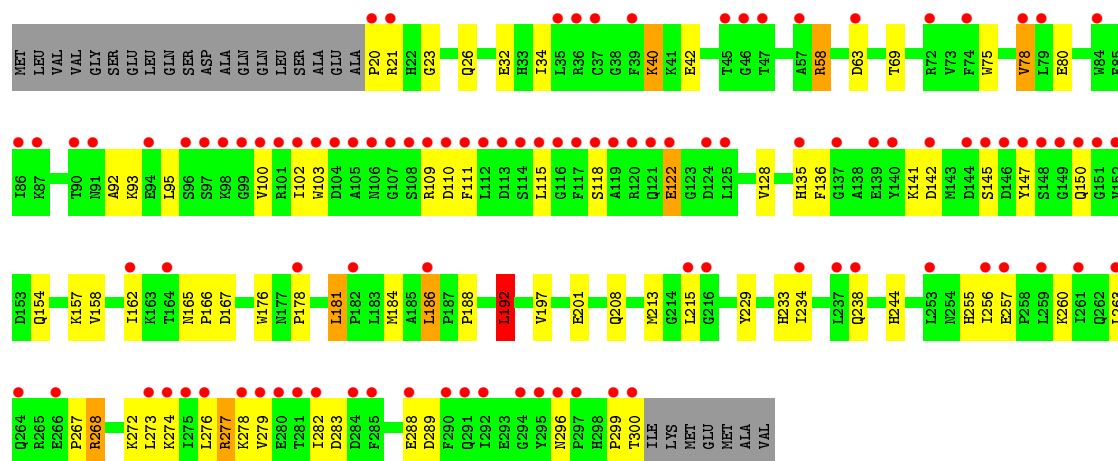




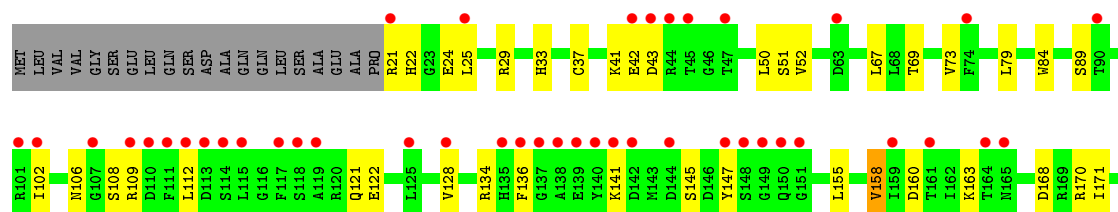
• Molecule 1: Thymidylate synthase



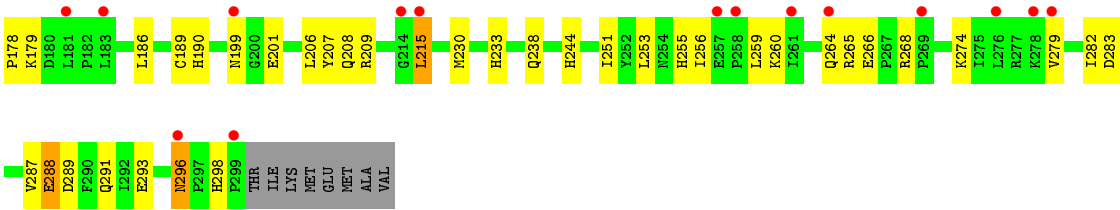
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.35Å 88.54Å 136.76Å 90.00° 95.99° 90.00°	Depositor
Resolution (Å)	19.95 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.95-1.70) 98.6 (19.95-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.235 , 0.292 0.233 , 0.289	Depositor DCC
$R_{free}$ test set	4109 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 40.64 % 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 2.6537e-04.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BU1, UMP

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	1.22	6/2405 (0.2%)	1.20	15/3248 (0.5%)
1	B	1.22	9/2414 (0.4%)	1.12	12/3261 (0.4%)
1	C	1.07	0/2337	1.01	3/3161 (0.1%)
1	D	0.99	1/2357 (0.0%)	0.94	2/3186 (0.1%)
1	E	0.78	0/2394	0.84	2/3237 (0.1%)
1	F	0.91	0/2336	0.92	4/3158 (0.1%)
All	All	1.05	16/14243 (0.1%)	1.01	38/19251 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CB-CG	-6.85	1.39	1.52
1	A	207	TYR	CE1-CZ	6.16	1.46	1.38
1	B	129	TYR	CE2-CZ	6.09	1.46	1.38
1	A	27	TYR	CE1-CZ	6.01	1.46	1.38
1	D	242	PHE	CE1-CZ	5.99	1.48	1.37
1	A	136	PHE	CD1-CE1	5.61	1.50	1.39
1	B	243	VAL	CB-CG2	5.48	1.64	1.52
1	B	59	TYR	CG-CD2	5.45	1.46	1.39
1	B	224	TYR	CG-CD1	5.43	1.46	1.39
1	B	81	GLU	CD-OE1	-5.38	1.19	1.25
1	A	272	LYS	CE-NZ	5.27	1.62	1.49
1	B	198	VAL	CB-CG2	5.27	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	TYR	CD1-CE1	5.22	1.47	1.39
1	A	195	PHE	CE1-CZ	5.09	1.47	1.37
1	A	128	VAL	CA-CB	5.06	1.65	1.54
1	B	196	TYR	CE1-CZ	5.06	1.45	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	109	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	72	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	170	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	268	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	283	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	A	181	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	170	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	215	LEU	CB-CG-CD1	6.51	122.07	111.00
1	A	62	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	58	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	72	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	134	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	109	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	72	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	120	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	268	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	153	ASP	CB-CG-OD1	5.74	123.47	118.30
1	F	230	MET	CG-SD-CE	5.74	109.39	100.20
1	A	195	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	A	248	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	170	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	181	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	234	ILE	CB-CA-C	-5.45	100.71	111.60
1	B	160	ASP	CB-CG-OD1	5.42	123.18	118.30
1	E	192	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	134	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	83	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	E	58	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	72	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	61	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	F	160	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	230	MET	CG-SD-CE	5.12	108.38	100.20
1	B	134	ARG	NE-CZ-NH1	5.11	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	F	209	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	58	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	F	289	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	300	THR	Peptide

## 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	2346	0	2312	42	0
1	B	2354	0	2320	35	1
1	C	2275	0	2238	50	0
1	D	2298	0	2268	57	0
1	E	2332	0	2288	57	0
1	F	2277	0	2238	55	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
2	E	20	0	11	0	0
2	F	40	0	22	8	0
3	C	18	0	30	9	0
4	A	344	0	0	11	1
4	B	315	0	0	7	0
4	C	279	0	0	18	0
4	D	242	0	0	16	0
4	E	116	0	0	10	0
4	F	176	0	0	13	0
All	All	15512	0	13771	287	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 10.

All (287) 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)
2:F:502:UMP:C5	4:F:776:HOH:O	1.72	1.32
1:D:65:PHE:CE2	4:D:654:HOH:O	1.93	1.20
1:F:136:PHE:HE2	4:F:620:HOH:O	1.28	1.16
2:F:502:UMP:O4	4:F:774:HOH:O	1.64	1.16
1:D:188:PRO:HB2	4:D:642:HOH:O	1.47	1.11
1:D:65:PHE:CZ	4:D:654:HOH:O	1.98	1.08
1:C:135:HIS:CE1	3:C:503:BU1:H11	1.93	1.04
1:C:109:ARG:HH11	1:C:109:ARG:CG	1.72	1.03
1:C:199[A]:ASN:OD1	1:D:39:PHE:CD2	2.11	1.03
1:C:109:ARG:HH11	1:C:109:ARG:HG3	0.90	1.02
2:F:502:UMP:H5	4:F:776:HOH:O	1.21	1.01
1:B:264[B]:GLN:NE2	1:B:264[B]:GLN:HA	1.76	1.00
1:C:233:HIS:HE1	1:C:279:VAL:H	1.01	1.00
1:B:42:GLU:OE1	4:B:729:HOH:O	1.79	0.99
1:C:109:ARG:NH1	1:C:109:ARG:HG3	1.75	0.96
1:E:20:PRO:HG3	1:E:58:ARG:O	1.66	0.95
1:A:94[B]:GLU:OE2	4:A:672:HOH:O	1.84	0.95
1:B:233:HIS:HE1	1:B:279:VAL:H	1.02	0.95
1:A:274:LYS:HD2	4:A:863:HOH:O	1.68	0.94
1:F:22:HIS:HD2	1:F:24:GLU:H	1.11	0.93
1:F:233:HIS:HE1	1:F:279:VAL:H	1.16	0.92
1:C:233:HIS:CE1	1:C:279:VAL:H	1.88	0.92
1:A:233:HIS:HE1	1:A:279:VAL:H	1.11	0.91
1:C:135:HIS:HE1	3:C:503:BU1:H11	1.26	0.90
2:F:502:UMP:O2	2:F:502:UMP:H2'	1.72	0.88
1:A:274:LYS:HE2	1:A:293[B]:GLU:OE1	1.77	0.84
1:C:215:LEU:HG	4:C:798:HOH:O	1.79	0.83
1:D:233:HIS:HE1	1:D:279:VAL:H	1.23	0.83
1:A:274:LYS:CD	4:A:863:HOH:O	2.24	0.82
2:F:502:UMP:C4	4:F:776:HOH:O	2.13	0.81
1:B:233:HIS:CE1	1:B:279:VAL:H	1.94	0.81
1:D:272:LYS:HE3	1:D:274:LYS:HZ3	1.46	0.80
1:C:199[A]:ASN:OD1	1:D:39:PHE:HD2	1.62	0.79
1:C:140:TYR:CE2	4:C:684:HOH:O	2.35	0.79
1:B:264[B]:GLN:HE21	1:B:264[B]:GLN:HA	1.45	0.79
1:C:135:HIS:HE1	3:C:503:BU1:C1	1.96	0.76
1:F:141:LYS:HE2	1:F:145:SER:HB3	1.68	0.76
1:D:272:LYS:HE3	1:D:274:LYS:NZ	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:NH2	4:C:684:HOH:O	2.20	0.74
1:D:176:TRP:CZ2	1:D:181:LEU:HD21	2.24	0.73
1:D:257:GLU:HB2	1:D:258:PRO:HD3	1.70	0.73
1:E:192:LEU:HD21	1:F:207:TYR:CD2	2.23	0.73
1:E:109:ARG:HB2	1:E:122:GLU:OE1	1.89	0.71
1:A:106:ASN:OD1	4:A:869:HOH:O	2.07	0.71
1:A:233:HIS:CE1	1:A:279:VAL:H	2.03	0.71
1:E:162:ILE:HA	4:E:648:HOH:O	1.91	0.71
1:C:178:PRO:HA	1:C:181:LEU:HD22	1.72	0.70
1:A:33:HIS:HD2	4:A:868:HOH:O	1.74	0.69
1:D:258:PRO:HG2	1:D:303:MET:HA	1.71	0.69
1:F:288:GLU:H	1:F:288:GLU:CD	1.96	0.69
1:F:163:LYS:NZ	4:F:734:HOH:O	2.25	0.68
1:D:254:ASN:HB2	4:D:732:HOH:O	1.94	0.68
1:D:233:HIS:CE1	1:D:279:VAL:H	2.11	0.68
1:C:135:HIS:CE1	3:C:503:BU1:H32	2.29	0.68
1:D:188:PRO:CB	4:D:642:HOH:O	2.20	0.68
1:C:140:TYR:HE2	4:C:684:HOH:O	1.76	0.67
1:A:274:LYS:CG	1:A:293[A]:GLU:OE2	2.43	0.67
1:A:274:LYS:HG2	1:A:293[A]:GLU:CD	2.15	0.66
1:A:215:LEU:HD12	4:A:718:HOH:O	1.96	0.66
1:E:109:ARG:NH2	1:E:118:SER:O	2.29	0.66
1:D:75:TRP:HZ3	4:D:654:HOH:O	1.80	0.65
1:E:278[B]:LYS:N	1:E:278[B]:LYS:HD2	2.13	0.64
1:C:199[A]:ASN:OD1	1:D:39:PHE:CE2	2.51	0.64
1:F:136:PHE:CE2	4:F:620:HOH:O	2.17	0.64
1:B:103:TRP:CZ3	1:B:186:LEU:HD21	2.33	0.64
1:B:264[B]:GLN:HE21	1:B:264[B]:GLN:CA	2.10	0.64
1:F:134:ARG:NH2	1:F:283:ASP:OD1	2.31	0.63
2:F:502:UMP:O2	2:F:502:UMP:C2'	2.44	0.63
1:E:178:PRO:HD2	1:F:136:PHE:CZ	2.34	0.63
1:D:71:LYS:HE2	1:D:303:MET:SD	2.39	0.62
1:B:208:GLN:OE1	1:B:244:HIS:HE1	1.83	0.62
1:C:32:GLU:HG2	1:C:36:ARG:NH2	2.15	0.61
1:A:190:HIS:HB3	1:A:206:LEU:HD11	1.82	0.61
1:F:233:HIS:CE1	1:F:279:VAL:H	2.07	0.61
1:A:234:ILE:HD11	1:A:282:ILE:HB	1.81	0.61
1:F:208:GLN:OE1	1:F:244:HIS:HE1	1.83	0.61
1:C:151:GLY:O	3:C:504:BU1:H22	2.01	0.61
1:C:233:HIS:HE1	1:C:279:VAL:N	1.85	0.61
1:E:208:GLN:OE1	1:E:244:HIS:HE1	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:CYS:SG	2:F:501:UMP:C6	2.94	0.61
1:A:141[A]:LYS:HE3	1:A:145:SER:HB3	1.82	0.60
1:F:22:HIS:CD2	1:F:24:GLU:H	2.04	0.60
1:F:274:LYS:HE3	1:F:293:GLU:OE1	2.01	0.60
1:E:167:ASP:OD2	1:F:42:GLU:HG2	2.01	0.59
1:B:278:LYS:NZ	1:B:280:GLU:OE2	2.28	0.59
1:F:190:HIS:HB3	1:F:206:LEU:HD11	1.84	0.59
1:A:30:GLN:HB3	1:A:55:MET:HE1	1.84	0.59
1:E:95:LEU:HD12	4:E:695:HOH:O	2.02	0.58
1:F:108:SER:O	1:F:112:LEU:HD13	2.03	0.58
1:A:42:GLU:OE2	4:A:858:HOH:O	2.17	0.58
1:D:65:PHE:HE2	4:D:654:HOH:O	1.51	0.58
1:D:65:PHE:HZ	4:D:654:HOH:O	1.61	0.58
1:E:277:ARG:HD3	1:E:289:ASP:OD1	2.03	0.58
1:B:22:HIS:CD2	4:B:897:HOH:O	2.57	0.57
1:D:222:ALA:HB1	4:D:654:HOH:O	2.04	0.57
1:A:274:LYS:HG2	1:A:293[A]:GLU:OE2	2.03	0.57
1:E:20:PRO:HB2	1:E:26[B]:GLN:NE2	2.19	0.57
1:A:274:LYS:HG3	1:A:293[A]:GLU:OE2	2.05	0.57
1:E:244:HIS:HD2	4:E:633:HOH:O	1.86	0.57
1:E:197:VAL:HG21	4:E:648:HOH:O	2.04	0.57
1:B:233:HIS:HE1	1:B:279:VAL:N	1.87	0.56
1:E:166:PRO:HA	4:E:648:HOH:O	2.05	0.56
1:C:215:LEU:HD13	1:C:255:HIS:CE1	2.41	0.56
1:B:291:GLN:HG3	1:E:21:ARG:HE	1.69	0.56
1:C:300:THR:OG1	1:C:300:THR:O	2.23	0.55
1:D:155:LEU:HD21	1:D:282:ILE:HG12	1.89	0.55
1:B:22:HIS:HB2	4:B:897:HOH:O	2.06	0.55
1:E:256:ILE:CG2	1:E:260:LYS:HE3	2.37	0.55
1:F:233:HIS:HE1	1:F:279:VAL:N	1.96	0.55
1:E:154:GLN:O	1:E:158:VAL:HG13	2.07	0.55
1:E:165:ASN:HB2	4:E:620:HOH:O	2.06	0.55
1:F:141:LYS:HE2	1:F:145:SER:CB	2.35	0.54
1:A:301:ILE:O	1:A:301:ILE:HD12	2.07	0.54
1:F:141:LYS:CE	1:F:145:SER:HB3	2.35	0.54
1:A:30:GLN:CD	1:A:55:MET:HE3	2.27	0.54
1:F:51:SER:HB3	4:F:684:HOH:O	2.07	0.54
1:A:288:GLU:H	1:A:288:GLU:CD	2.11	0.54
1:B:22:HIS:HD2	4:B:897:HOH:O	1.89	0.54
1:C:135:HIS:HE1	3:C:503:BU1:H32	1.70	0.54
1:E:63:ASP:O	1:E:272:LYS:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:HIS:HB3	1:E:150:GLN:O	2.09	0.53
1:E:80:GLU:HB3	4:E:695:HOH:O	2.07	0.53
1:A:233:HIS:HD2	4:A:922:HOH:O	1.91	0.53
1:A:208:GLN:OE1	1:A:244:HIS:HE1	1.91	0.53
1:C:274:LYS:HG3	4:C:745:HOH:O	2.08	0.53
1:E:278[B]:LYS:N	1:E:278[B]:LYS:CD	2.73	0.52
1:E:296:ASN:ND2	4:E:704:HOH:O	2.37	0.52
1:E:93:LYS:NZ	1:E:122:GLU:HG2	2.24	0.52
1:C:148[A]:SER:HB3	4:C:879:HOH:O	2.08	0.52
1:E:257:GLU:HA	1:E:257:GLU:OE1	2.09	0.52
1:E:234:ILE:HD11	1:E:282:ILE:HA	1.92	0.52
1:D:208:GLN:OE1	1:D:244:HIS:HE1	1.92	0.52
1:C:135:HIS:HE1	3:C:503:BU1:C2	2.22	0.52
1:C:140:TYR:CD2	4:C:684:HOH:O	2.60	0.52
1:D:155:LEU:O	1:D:158:VAL:HG22	2.10	0.52
1:B:244:HIS:HD2	4:B:613:HOH:O	1.92	0.52
1:E:40:LYS:NZ	1:E:42:GLU:OE2	2.43	0.52
1:C:208:GLN:OE1	1:C:244:HIS:HE1	1.92	0.52
1:D:188:PRO:C	4:D:642:HOH:O	2.47	0.52
1:A:291:GLN:NE2	1:A:293[A]:GLU:OE2	2.43	0.51
1:C:220:ASN:ND2	4:C:682:HOH:O	2.43	0.51
1:E:178:PRO:HA	1:E:181:LEU:HD22	1.91	0.51
1:B:215:LEU:HD13	1:B:255:HIS:CE1	2.46	0.51
1:C:170:ARG:HG3	1:D:209:ARG:NH1	2.25	0.51
1:C:176:TRP:CZ2	1:C:181:LEU:HD21	2.45	0.51
1:D:190:HIS:N	4:D:642:HOH:O	2.44	0.51
1:D:98:LYS:HD2	1:D:98:LYS:N	2.25	0.51
1:A:244:HIS:HD2	4:A:606:HOH:O	1.95	0.50
1:C:244:HIS:HD2	4:C:614:HOH:O	1.93	0.50
1:F:244:HIS:HD2	4:F:612:HOH:O	1.94	0.50
1:C:148[B]:SER:HB2	4:C:879:HOH:O	2.11	0.50
1:D:265:ARG:NH1	1:D:298:HIS:HB3	2.26	0.50
1:F:41:LYS:HG3	4:F:684:HOH:O	2.11	0.50
1:F:215:LEU:HD22	1:F:255:HIS:CE1	2.47	0.50
1:D:244:HIS:HD2	4:D:603:HOH:O	1.94	0.49
1:D:234:ILE:HD11	1:D:282:ILE:HA	1.95	0.49
1:A:186:LEU:N	1:A:186:LEU:HD23	2.27	0.49
1:B:22:HIS:NE2	1:B:268:ARG:O	2.45	0.49
1:E:192:LEU:HD21	1:F:207:TYR:CE2	2.48	0.49
1:B:178:PRO:HA	1:B:181:LEU:HD22	1.95	0.49
1:D:21:ARG:NH2	4:D:686:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:HIS:HE1	1:F:268:ARG:O	1.96	0.49
1:A:121:GLN:HG3	4:A:745:HOH:O	2.13	0.49
1:A:186:LEU:N	1:A:186:LEU:CD2	2.76	0.49
1:A:80:GLU:OE2	1:A:287:VAL:HG21	2.13	0.48
1:B:296:ASN:HB3	1:F:37:CYS:HB2	1.94	0.48
1:F:158:VAL:HB	1:F:171:ILE:CG2	2.43	0.48
1:B:40:LYS:NZ	1:B:42:GLU:OE2	2.40	0.48
1:C:178:PRO:HD2	1:D:136:PHE:CZ	2.48	0.48
1:C:32:GLU:HG2	1:C:36:ARG:HH21	1.77	0.48
1:F:145:SER:HB2	1:F:147:TYR:CZ	2.49	0.48
1:E:176:TRP:CZ2	1:E:181:LEU:HD21	2.49	0.48
1:E:215:LEU:HG	1:E:255:HIS:CE1	2.48	0.48
1:D:302:LYS:HG3	1:D:303:MET:N	2.29	0.48
1:F:268:ARG:HD3	1:F:296:ASN:O	2.14	0.48
1:E:20:PRO:HB3	1:E:58:ARG:HB3	1.95	0.48
1:D:265:ARG:HD3	1:D:298:HIS:CG	2.49	0.47
1:D:215:LEU:HG	1:D:255:HIS:CE1	2.50	0.47
1:E:111:PHE:HZ	1:E:186:LEU:HD13	1.79	0.47
1:C:135:HIS:HD2	1:C:150:GLN:O	1.97	0.47
1:C:33:HIS:HE1	4:C:806:HOH:O	1.96	0.47
1:F:51:SER:CB	4:F:684:HOH:O	2.62	0.47
1:D:126:GLY:HA2	1:D:140:TYR:CE2	2.49	0.47
1:A:145:SER:HB2	1:A:147:TYR:CZ	2.50	0.47
1:E:63:ASP:O	1:E:272:LYS:CD	2.63	0.47
1:A:301:ILE:C	1:A:301:ILE:HD12	2.35	0.46
1:B:184:MET:SD	1:B:188:PRO:HD3	2.56	0.46
1:D:288:GLU:CD	1:D:288:GLU:H	2.17	0.46
1:E:136:PHE:CZ	1:F:178:PRO:HD2	2.50	0.46
1:E:256:ILE:HG22	1:E:260:LYS:HE3	1.97	0.46
1:F:121:GLN:HG2	1:F:122:GLU:N	2.29	0.46
1:D:179:LYS:HD3	4:D:671:HOH:O	2.15	0.46
1:E:92:ALA:HB1	1:E:103[B]:TRP:O	2.15	0.46
1:D:21:ARG:HD2	1:D:29:ARG:HH22	1.79	0.46
1:F:84:TRP:CD1	1:F:89:SER:HB3	2.51	0.46
1:A:274:LYS:CG	1:A:293[A]:GLU:CD	2.82	0.46
1:F:102:ILE:HB	2:F:502:UMP:H3'	1.97	0.46
1:C:148[A]:SER:CB	4:C:879:HOH:O	2.64	0.46
1:D:258:PRO:CG	1:D:303:MET:HA	2.42	0.46
1:E:145:SER:HB2	1:E:147:TYR:CZ	2.51	0.46
1:B:151:GLY:HA2	4:B:712:HOH:O	2.14	0.46
1:D:26[A]:GLN:O	1:D:30:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:GLU:O	1:D:98:LYS:HD3	2.16	0.46
1:E:20:PRO:HB2	1:E:26[B]:GLN:HE22	1.80	0.46
1:E:201:GLU:HA	1:E:238:GLN:O	2.15	0.46
1:E:75:TRP:HA	1:E:78:VAL:HG13	1.98	0.46
1:D:21:ARG:HH22	1:D:26[A]:GLN:HG3	1.82	0.45
1:F:67:LEU:HD11	1:F:73:VAL:HB	1.97	0.45
1:F:168:ASP:OD1	1:F:170:ARG:HB2	2.16	0.45
1:B:145:SER:HB2	1:B:147:TYR:CZ	2.52	0.45
1:A:234:ILE:HD13	1:A:234:ILE:HG21	1.39	0.45
1:A:276:LEU:HD11	1:A:291:GLN:HB2	1.98	0.45
1:C:120:ARG:CZ	4:C:684:HOH:O	2.63	0.45
1:C:148[B]:SER:CB	4:C:879:HOH:O	2.65	0.45
1:E:34:ILE:HD12	1:E:213:MET:HG3	1.96	0.45
1:C:40:LYS:HD3	4:C:733:HOH:O	2.16	0.45
1:A:178:PRO:HD2	1:B:136:PHE:CZ	2.52	0.45
1:F:33:HIS:HE1	4:F:634:HOH:O	1.99	0.45
1:C:135:HIS:HE1	3:C:503:BU1:C3	2.29	0.44
1:E:229:TYR:CD2	1:E:273:LEU:HD23	2.52	0.44
1:D:22:HIS:CD2	1:D:267:PRO:HB2	2.51	0.44
1:E:274:LYS:HG3	1:E:276:LEU:HD22	1.99	0.44
1:C:133:TRP:CE2	1:C:173:MET:HE3	2.52	0.44
1:B:262:GLN:HB2	1:B:301:ILE:CD1	2.48	0.44
1:D:31:VAL:HG12	1:D:35:LEU:HD22	2.00	0.44
1:D:33:HIS:HE1	4:D:753:HOH:O	2.00	0.44
1:D:266:GLU:OE1	1:D:266:GLU:HA	2.18	0.44
1:D:234:ILE:HD11	1:D:282:ILE:CA	2.47	0.44
1:A:147:TYR:O	1:A:148:SER:C	2.56	0.43
1:F:121:GLN:HG2	1:F:122:GLU:H	1.83	0.43
1:B:208:GLN:OE1	1:B:244:HIS:CE1	2.68	0.43
1:C:264:GLN:NE2	4:C:665:HOH:O	2.50	0.43
1:D:145:SER:HB2	1:D:147:TYR:CZ	2.53	0.43
3:C:504:BU1:H32	4:C:675:HOH:O	2.18	0.43
1:E:267:PRO:HD2	4:E:604:HOH:O	2.18	0.43
1:E:32:GLU:HG2	1:E:263:LEU:CD2	2.49	0.43
1:F:251:ILE:HG23	1:F:259:LEU:HD12	2.01	0.43
1:F:260:LYS:O	1:F:264:GLN:HG3	2.19	0.43
1:F:69:THR:HG21	1:F:268:ARG:O	2.19	0.42
1:B:22:HIS:CE1	1:B:24:GLU:HB2	2.54	0.42
1:B:233:HIS:HD2	4:B:777:HOH:O	2.01	0.42
1:F:158:VAL:HB	1:F:171:ILE:HG22	2.01	0.42
1:B:302:LYS:HD3	1:B:302:LYS:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:THR:HB	1:B:250:HIS:HB2	2.02	0.42
1:A:187:PRO:HA	1:A:188:PRO:HD3	1.91	0.42
1:C:178:PRO:HD2	1:D:136:PHE:CE1	2.54	0.42
1:F:288:GLU:N	1:F:288:GLU:CD	2.70	0.42
1:B:22:HIS:ND1	1:B:23:GLY:N	2.68	0.42
1:B:103:TRP:HZ3	1:B:186:LEU:HD21	1.84	0.42
1:D:184:MET:SD	1:D:188:PRO:HD3	2.59	0.42
1:D:32:GLU:HG3	4:D:646:HOH:O	2.19	0.42
1:F:155:LEU:HD21	1:F:282:ILE:HG12	2.02	0.42
1:F:79:LEU:HD23	1:F:287:VAL:HG23	2.02	0.42
1:B:186:LEU:N	1:B:186:LEU:HD23	2.35	0.41
1:F:106:ASN:ND2	1:F:186:LEU:HG	2.35	0.41
1:A:170:ARG:NH2	4:A:769:HOH:O	2.34	0.41
1:A:82:LEU:HD23	1:A:226:LEU:HG	2.03	0.41
1:E:257:GLU:OE1	1:E:260:LYS:HD2	2.21	0.41
1:A:103:TRP:CZ3	1:A:186:LEU:HD21	2.55	0.41
1:D:265:ARG:HH11	1:D:298:HIS:HB3	1.83	0.41
1:F:22:HIS:CE1	1:F:268:ARG:O	2.74	0.41
1:A:186:LEU:H	1:A:186:LEU:HD23	1.84	0.41
1:C:170:ARG:HG3	1:D:209:ARG:CZ	2.50	0.41
1:B:201:GLU:HA	1:B:238:GLN:O	2.21	0.41
1:D:302:LYS:HG3	1:D:303:MET:H	1.84	0.41
1:E:69:THR:HB	1:E:268:ARG:HG2	2.02	0.41
1:E:299:PRO:O	1:E:300:THR:HB	2.21	0.41
1:F:25:LEU:HD13	1:F:29:ARG:NH2	2.35	0.41
1:F:253:LEU:HD23	1:F:256:ILE:HD11	2.02	0.41
1:C:40:LYS:CD	4:C:733:HOH:O	2.69	0.41
1:F:179:LYS:HE2	4:F:762:HOH:O	2.20	0.41
1:B:113:ASP:OD1	1:B:118:SER:HA	2.21	0.41
1:D:21:ARG:NH1	1:D:29:ARG:NH1	2.69	0.41
1:E:93:LYS:HZ1	1:E:122:GLU:HG2	1.86	0.41
1:F:265:ARG:HG2	1:F:298:HIS:ND1	2.35	0.41
1:E:167:ASP:OD2	1:F:42:GLU:CG	2.69	0.41
1:F:201:GLU:HA	1:F:238:GLN:O	2.21	0.41
1:C:262:GLN:HA	1:C:265:ARG:HD2	2.03	0.40
1:E:184:MET:SD	1:E:188:PRO:HD3	2.61	0.40
1:E:95:LEU:CD1	4:E:695:HOH:O	2.65	0.40
1:C:184:MET:SD	1:C:188:PRO:HD3	2.62	0.40
1:A:121:GLN:HA	1:A:121:GLN:HE21	1.87	0.40
1:C:158:VAL:HG13	1:C:171:ILE:CG2	2.51	0.40
1:D:21:ARG:HG2	1:D:25:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:VAL:HG12	1:E:102:ILE:HG12	2.04	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:B:36[B]:ARG:NH1	4:A:858:HOH:O[4_545]	2.00	0.20

## 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	288/307 (94%)	279 (97%)	7 (2%)	2 (1%)	22	8
1	B	289/307 (94%)	283 (98%)	5 (2%)	1 (0%)	41	24
1	C	280/307 (91%)	273 (98%)	6 (2%)	1 (0%)	34	18
1	D	282/307 (92%)	272 (96%)	9 (3%)	1 (0%)	34	18
1	E	285/307 (93%)	268 (94%)	15 (5%)	2 (1%)	22	8
1	F	279/307 (91%)	271 (97%)	7 (2%)	1 (0%)	34	18
All	All	1703/1842 (92%)	1646 (97%)	49 (3%)	8 (0%)	29	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	23	GLY
1	A	148	SER
1	E	128	VAL
1	F	128	VAL
1	A	128	VAL
1	B	128	VAL
1	D	128	VAL

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Mol	Chain	Res	Type
1	C	128	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	253/266 (95%)	244 (96%)	9 (4%)	35	16
1	B	254/266 (96%)	247 (97%)	7 (3%)	43	25
1	C	246/266 (92%)	239 (97%)	7 (3%)	43	25
1	D	248/266 (93%)	237 (96%)	11 (4%)	28	11
1	E	251/266 (94%)	234 (93%)	17 (7%)	16	4
1	F	245/266 (92%)	233 (95%)	12 (5%)	25	9
All	All	1497/1596 (94%)	1434 (96%)	63 (4%)	30	12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	98	LYS
1	A	121	GLN
1	A	181	LEU
1	A	186	LEU
1	A	215	LEU
1	A	288	GLU
1	A	303	MET
1	A	307	VAL
1	B	32	GLU
1	B	181	LEU
1	B	186	LEU
1	B	215	LEU
1	B	266	GLU
1	B	286	LYS
1	B	302	LYS
1	C	21	ARG

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Mol	Chain	Res	Type
1	C	36	ARG
1	C	109	ARG
1	C	181	LEU
1	C	186	LEU
1	C	269	PRO
1	C	300	THR
1	D	21	ARG
1	D	35	LEU
1	D	63	ASP
1	D	98	LYS
1	D	101	ARG
1	D	181	LEU
1	D	274	LYS
1	D	278	LYS
1	D	280	GLU
1	D	291	GLN
1	D	301	ILE
1	E	40	LYS
1	E	78	VAL
1	E	110	ASP
1	E	115	LEU
1	E	122	GLU
1	E	141	LYS
1	E	142	ASP
1	E	157	LYS
1	E	181	LEU
1	E	186	LEU
1	E	192	LEU
1	E	268	ARG
1	E	277	ARG
1	E	279	VAL
1	E	283	ASP
1	E	288[A]	GLU
1	E	288[B]	GLU
1	F	21	ARG
1	F	43	ASP
1	F	50	LEU
1	F	52	VAL
1	F	109	ARG
1	F	158	VAL
1	F	199	ASN
1	F	215	LEU

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Mol	Chain	Res	Type
1	F	266	GLU
1	F	288	GLU
1	F	291	GLN
1	F	296	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	56	GLN
1	A	121	GLN
1	A	205	GLN
1	A	233	HIS
1	A	244	HIS
1	A	262	GLN
1	A	291	GLN
1	B	33	HIS
1	B	205	GLN
1	B	233	HIS
1	B	244	HIS
1	C	33	HIS
1	C	135	HIS
1	C	233	HIS
1	C	244	HIS
1	C	264	GLN
1	D	33	HIS
1	D	205	GLN
1	D	233	HIS
1	D	244	HIS
1	E	22	HIS
1	E	33	HIS
1	E	205	GLN
1	E	233	HIS
1	E	244	HIS
1	E	255	HIS
1	F	22	HIS
1	F	33	HIS
1	F	106	ASN
1	F	233	HIS
1	F	244	HIS
1	F	255	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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$
3	BU1	C	503	-	5,5,5	0.35	0	4,4,4	0.50	0
2	UMP	F	501	-	18,21,21	1.30	2 (11%)	21,31,31	0.93	0
2	UMP	A	501	-	18,21,21	1.03	1 (5%)	21,31,31	0.92	1 (4%)
2	UMP	D	501	-	18,21,21	1.19	2 (11%)	21,31,31	0.99	1 (4%)
2	UMP	B	501	-	18,21,21	1.34	1 (5%)	21,31,31	0.89	1 (4%)
2	UMP	F	502	-	18,21,21	1.07	1 (5%)	21,31,31	1.31	2 (9%)
3	BU1	C	504	-	5,5,5	0.31	0	4,4,4	0.49	0
2	UMP	C	501	-	18,21,21	1.39	2 (11%)	21,31,31	1.31	3 (14%)
2	UMP	E	501	-	18,21,21	0.98	1 (5%)	21,31,31	0.98	2 (9%)
3	BU1	C	502	-	5,5,5	0.29	0	4,4,4	0.52	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
3	BU1	C	503	-	-	0/3/3/3	-
2	UMP	F	501	-	-	2/7/22/22	0/2/2/2
2	UMP	A	501	-	-	2/7/22/22	0/2/2/2
2	UMP	D	501	-	-	1/7/22/22	0/2/2/2
2	UMP	B	501	-	-	1/7/22/22	0/2/2/2
2	UMP	F	502	-	-	3/7/22/22	0/2/2/2
3	BU1	C	504	-	-	0/3/3/3	-
2	UMP	C	501	-	-	1/7/22/22	0/2/2/2
2	UMP	E	501	-	-	2/7/22/22	0/2/2/2
3	BU1	C	502	-	-	2/3/3/3	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	UMP	C6-N1	3.29	1.39	1.35
2	D	501	UMP	C4-N3	3.08	1.38	1.33
2	B	501	UMP	C4-N3	3.02	1.38	1.33
2	F	501	UMP	C6-N1	3.02	1.39	1.35
2	F	502	UMP	C4-N3	3.00	1.38	1.33
2	F	501	UMP	C4-N3	2.90	1.38	1.33
2	E	501	UMP	C4-N3	2.54	1.37	1.33
2	C	501	UMP	C4-N3	2.37	1.37	1.33
2	A	501	UMP	C6-N1	2.37	1.38	1.35
2	D	501	UMP	C6-N1	2.15	1.38	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UMP	OP3-P-O5'	2.71	113.96	106.73
2	D	501	UMP	P-O5'-C5'	2.71	125.76	118.30
2	F	502	UMP	O4'-C1'-C2'	-2.51	101.50	106.25
2	F	502	UMP	O5'-P-OP1	2.50	113.50	106.47
2	C	501	UMP	P-O5'-C5'	2.38	124.85	118.30
2	C	501	UMP	C5-C4-N3	-2.37	118.09	123.31
2	E	501	UMP	O3'-C3'-C2'	-2.37	102.42	110.90
2	B	501	UMP	P-O5'-C5'	2.15	124.22	118.30
2	E	501	UMP	C5-C4-N3	-2.03	118.84	123.31
2	C	501	UMP	C6-N1-C2	-2.02	117.99	121.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

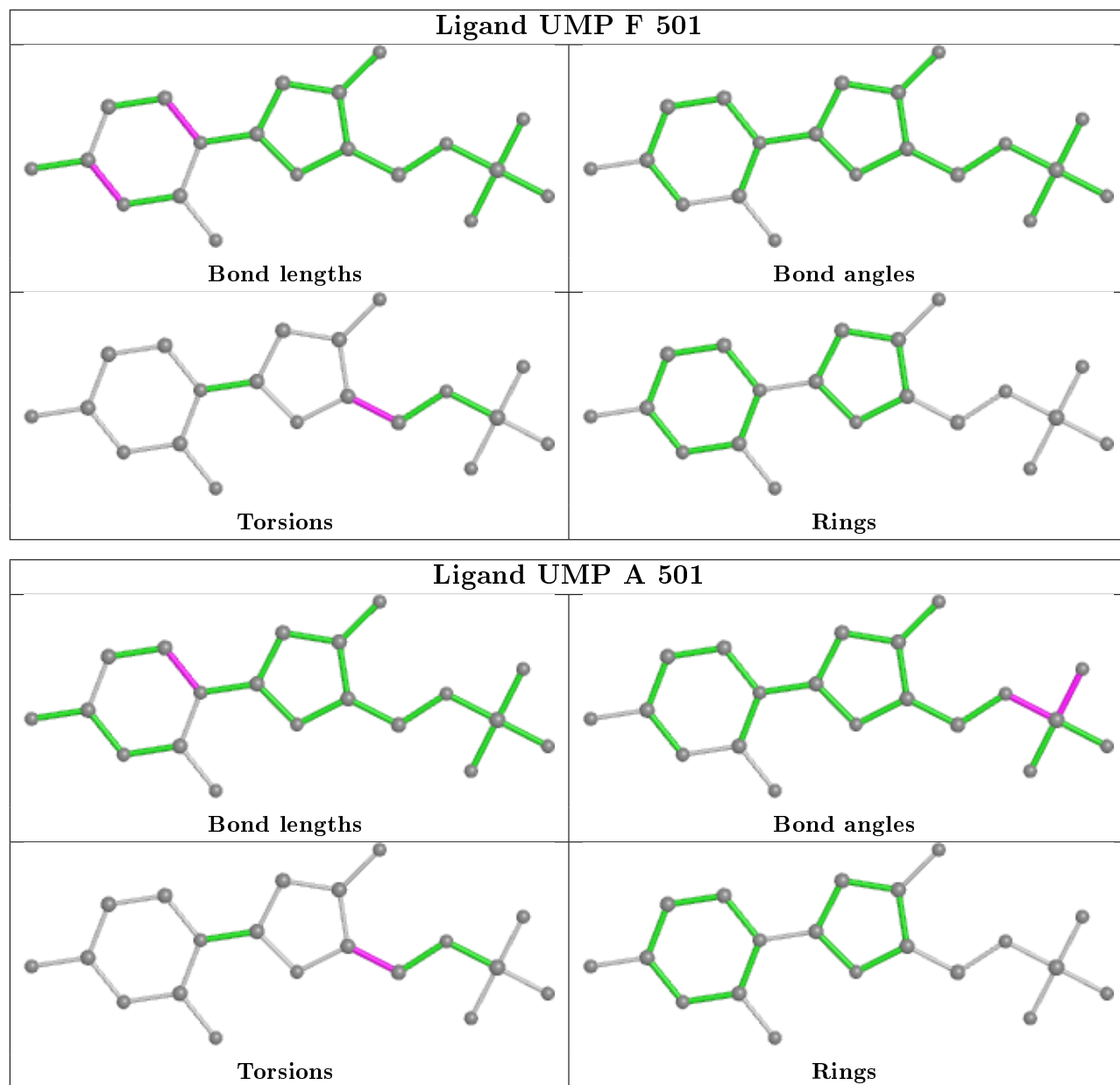
Mol	Chain	Res	Type	Atoms
2	F	502	UMP	O4'-C1'-N1-C6
2	F	502	UMP	C3'-C4'-C5'-O5'
2	F	502	UMP	O4'-C4'-C5'-O5'
3	C	502	BU1	C2-C3-C4-O6
3	C	502	BU1	O5-C1-C2-C3
2	A	501	UMP	O4'-C4'-C5'-O5'
2	E	501	UMP	O4'-C4'-C5'-O5'
2	F	501	UMP	O4'-C4'-C5'-O5'
2	B	501	UMP	O4'-C4'-C5'-O5'
2	C	501	UMP	O4'-C4'-C5'-O5'
2	E	501	UMP	C3'-C4'-C5'-O5'
2	F	501	UMP	C3'-C4'-C5'-O5'
2	A	501	UMP	C3'-C4'-C5'-O5'
2	D	501	UMP	O4'-C4'-C5'-O5'

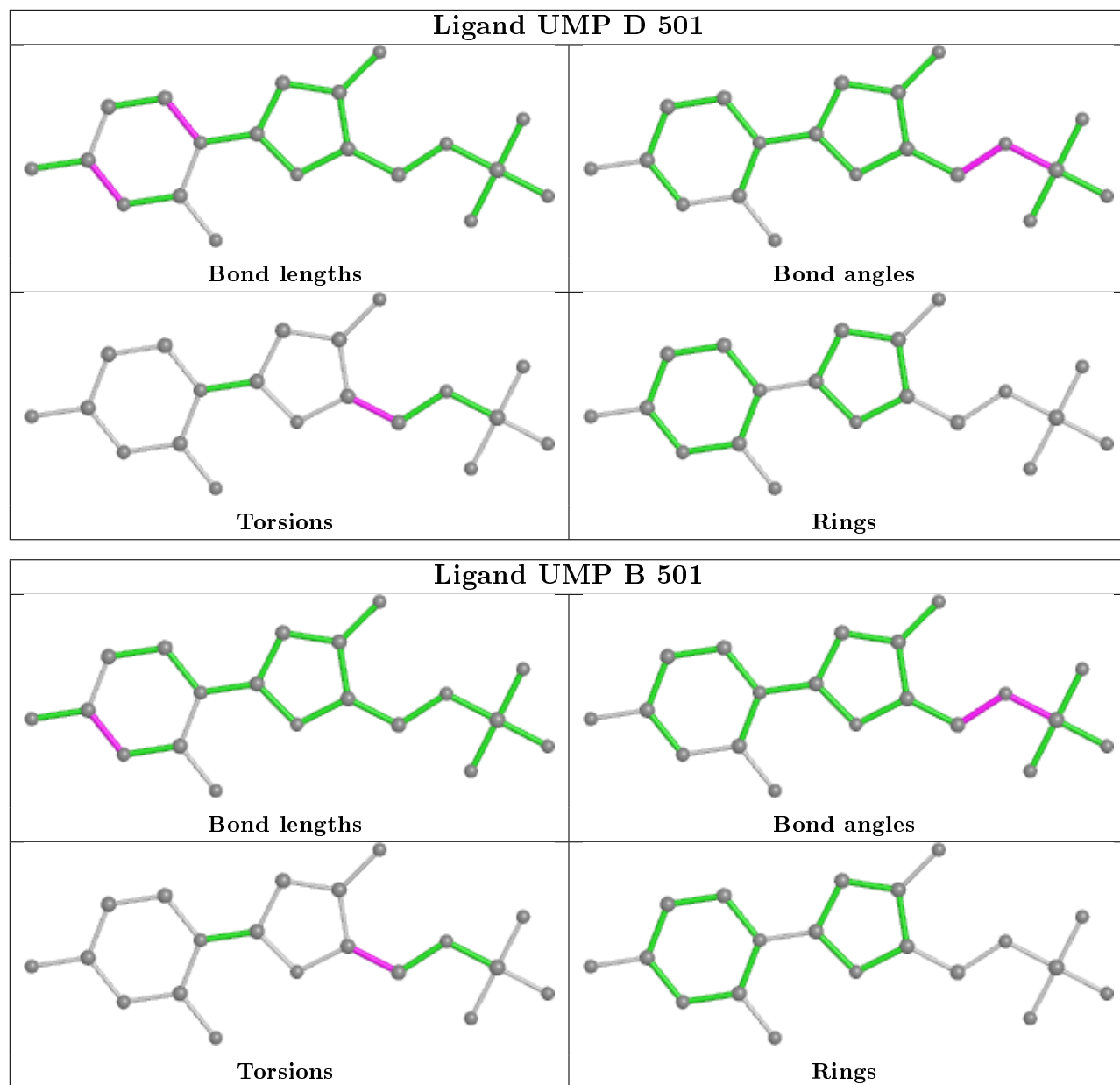
There are no ring outliers.

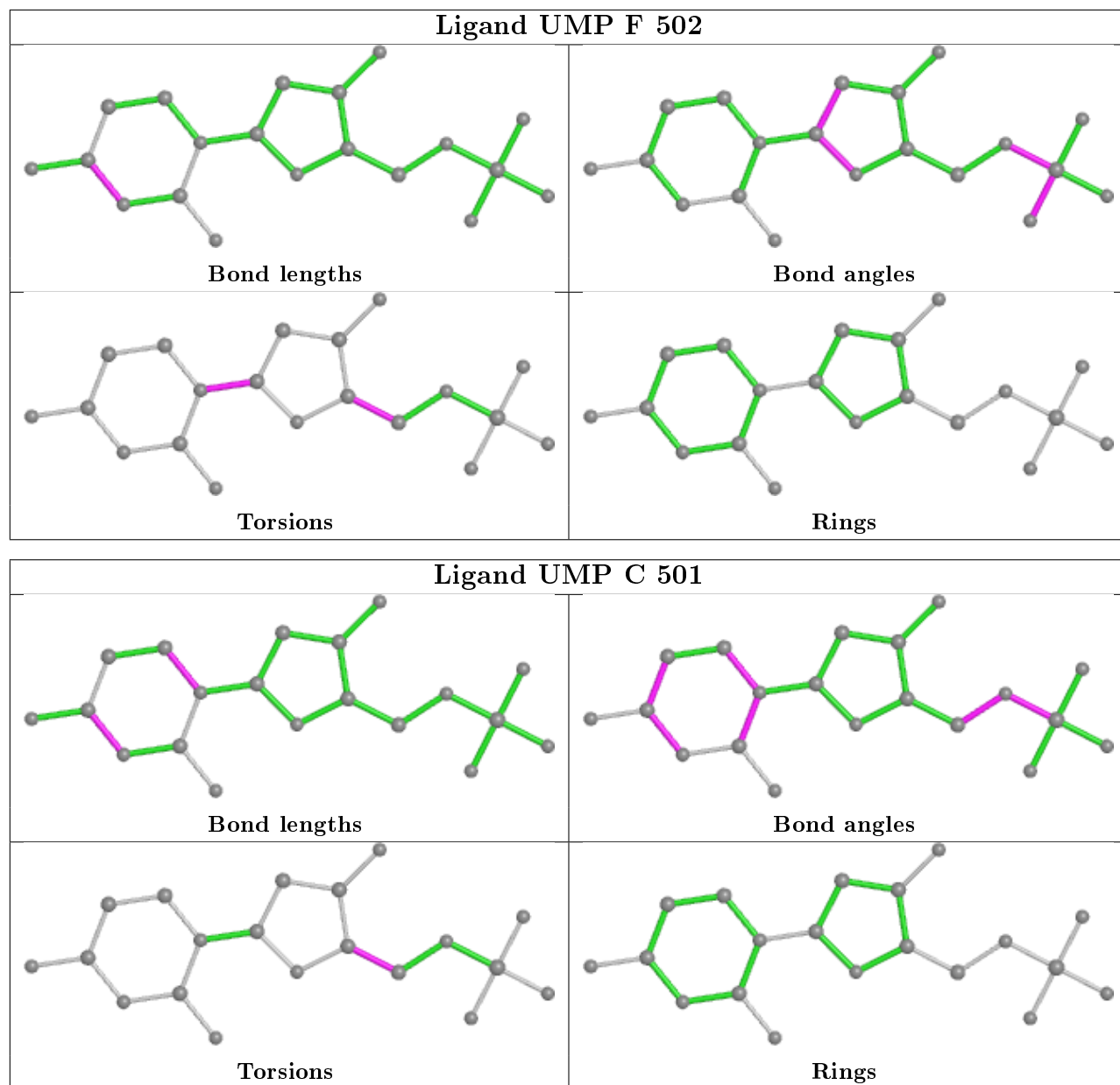
4 monomers are involved in 17 short contacts:

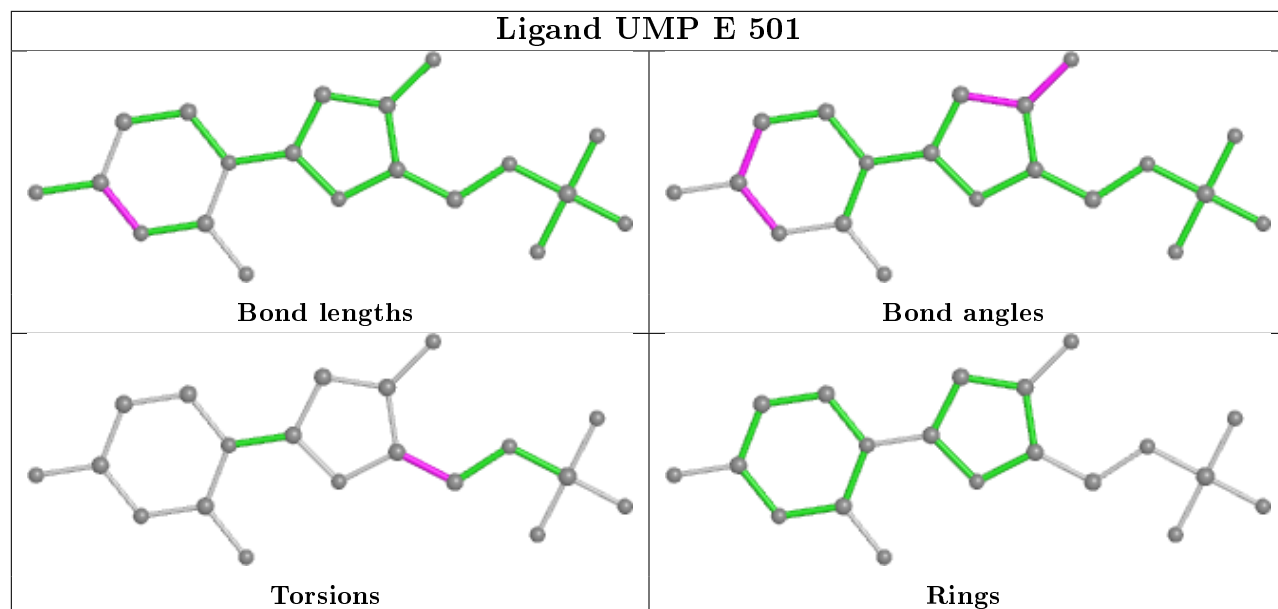
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	BU1	7	0
2	F	501	UMP	1	0
2	F	502	UMP	7	0
3	C	504	BU1	2	0

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, 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	287/307 (93%)	0.55	22 (7%)	13 15	12, 20, 33, 43	0
1	B	288/307 (93%)	0.48	13 (4%)	33 37	13, 21, 31, 54	0
1	C	280/307 (91%)	0.56	15 (5%)	25 28	16, 24, 36, 43	0
1	D	283/307 (92%)	0.81	24 (8%)	10 12	18, 27, 44, 69	0
1	E	281/307 (91%)	1.99	103 (36%)	0 0	23, 39, 69, 86	0
1	F	279/307 (90%)	1.24	58 (20%)	1 0	20, 31, 50, 55	0
All	All	1698/1842 (92%)	0.94	235 (13%)	2 3	12, 26, 49, 86	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	117	PHE	12.5
1	E	112	LEU	12.4
1	E	119	ALA	10.4
1	E	100	VAL	10.1
1	E	115	LEU	9.9
1	E	116	GLY	9.9
1	E	45	THR	8.1
1	D	45	THR	7.8
1	E	111	PHE	7.6
1	B	20	PRO	7.5
1	D	300	THR	7.3
1	E	300	THR	7.3
1	E	103[A]	TRP	6.9
1	F	44[A]	ARG	6.7
1	E	110	ASP	6.5
1	E	118	SER	6.5
1	F	118	SER	6.1
1	E	113	ASP	5.9
1	E	39	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	148	SER	5.8
1	D	47	THR	5.8
1	F	45	THR	5.7
1	F	276	LEU	5.7
1	F	119	ALA	5.5
1	E	46	GLY	5.5
1	E	149	GLY	5.5
1	F	111	PHE	5.4
1	E	47	THR	5.3
1	E	137	GLY	5.3
1	E	101	ARG	5.3
1	E	102	ILE	5.3
1	F	110	ASP	5.2
1	C	45	THR	5.1
1	F	117	PHE	5.0
1	F	215	LEU	4.9
1	E	151	GLY	4.9
1	E	108	SER	4.8
1	E	114	SER	4.8
1	E	97	SER	4.7
1	E	299	PRO	4.7
1	F	142	ASP	4.7
1	E	215	LEU	4.7
1	E	261	ILE	4.7
1	F	47	THR	4.6
1	D	302	LYS	4.5
1	F	144	ASP	4.5
1	F	299	PRO	4.3
1	F	149	GLY	4.3
1	F	261	ILE	4.3
1	D	46	GLY	4.3
1	E	150	GLN	4.2
1	F	21	ARG	4.2
1	D	261	ILE	4.2
1	E	98	LYS	4.1
1	F	125	LEU	4.1
1	F	42	GLU	4.0
1	E	280	GLU	3.9
1	E	125	LEU	3.9
1	E	257	GLU	3.9
1	E	146	ASP	3.8
1	E	263	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	261	ILE	3.8
1	A	301	ILE	3.8
1	E	79	LEU	3.7
1	F	296	ASN	3.7
1	E	37	CYS	3.6
1	F	63	ASP	3.6
1	E	36	ARG	3.6
1	E	20	PRO	3.6
1	E	186	LEU	3.6
1	E	281	THR	3.6
1	D	116	GLY	3.6
1	E	294	GLY	3.6
1	C	68	LEU	3.5
1	F	114	SER	3.5
1	E	152	VAL	3.5
1	E	264	GLN	3.5
1	E	99	GLY	3.4
1	E	120	ARG	3.4
1	F	43	ASP	3.4
1	A	302	LYS	3.4
1	F	137	GLY	3.4
1	E	276	LEU	3.4
1	A	21	ARG	3.3
1	C	226	LEU	3.3
1	E	87	LYS	3.3
1	E	147	TYR	3.3
1	F	109	ARG	3.3
1	F	113	ASP	3.3
1	B	304	GLU	3.3
1	E	144	ASP	3.2
1	E	96	SER	3.2
1	E	124	ASP	3.2
1	B	306	ALA	3.2
1	F	165	ASN	3.2
1	F	151	GLY	3.2
1	E	145	SER	3.2
1	E	74	PHE	3.2
1	D	21	ARG	3.1
1	D	301	ILE	3.1
1	E	121[A]	GLN	3.1
1	E	274	LYS	3.1
1	E	140	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	164	THR	3.1
1	F	181	LEU	3.0
1	A	226	LEU	3.0
1	E	178	PRO	3.0
1	E	238	GLN	3.0
1	B	21	ARG	3.0
1	E	275	ILE	3.0
1	C	258	PRO	3.0
1	E	288[A]	GLU	3.0
1	F	164	THR	2.9
1	E	291	GLN	2.9
1	F	140	TYR	2.9
1	F	136	PHE	2.9
1	E	279	VAL	2.9
1	E	91	ASN	2.9
1	D	264	GLN	2.9
1	A	303	MET	2.9
1	E	273	LEU	2.8
1	E	109	ARG	2.8
1	F	102	ILE	2.8
1	D	299	PRO	2.8
1	D	303	MET	2.8
1	C	119	ALA	2.8
1	E	57	ALA	2.8
1	F	279	VAL	2.7
1	D	254	ASN	2.7
1	E	266	GLU	2.7
1	E	105	ALA	2.7
1	F	183	LEU	2.7
1	C	117	PHE	2.7
1	F	74	PHE	2.7
1	C	27	TYR	2.7
1	B	125	LEU	2.7
1	A	68	LEU	2.7
1	A	128	VAL	2.7
1	E	63	ASP	2.7
1	E	278[A]	LYS	2.7
1	F	269	PRO	2.7
1	F	138	ALA	2.6
1	F	199	ASN	2.6
1	E	107	GLY	2.6
1	F	107	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	256	ILE	2.6
1	B	126	GLY	2.6
1	D	44	ARG	2.5
1	F	141	LYS	2.5
1	F	148	SER	2.5
1	B	90	THR	2.5
1	B	189	CYS	2.5
1	D	29	ARG	2.5
1	F	128	VAL	2.5
1	C	21	ARG	2.5
1	E	297	PRO	2.5
1	A	231	ILE	2.5
1	E	292	ILE	2.5
1	F	147	TYR	2.5
1	B	302	LYS	2.5
1	D	90	THR	2.5
1	E	259	LEU	2.5
1	C	200	GLY	2.5
1	F	264	GLN	2.5
1	F	101	ARG	2.4
1	D	296	ASN	2.4
1	F	159	ILE	2.4
1	E	253	LEU	2.4
1	E	296	ASN	2.4
1	D	278	LYS	2.4
1	E	106	ASN	2.4
1	E	216	GLY	2.4
1	E	290	PHE	2.4
1	E	182	PRO	2.4
1	F	258	PRO	2.4
1	B	305	MET	2.4
1	A	249	ALA	2.4
1	C	31	VAL	2.3
1	E	86	ILE	2.3
1	A	125	LEU	2.3
1	E	78	VAL	2.3
1	E	282	ILE	2.3
1	D	63	ASP	2.3
1	E	284	ASP	2.3
1	F	161	THR	2.3
1	A	229	TYR	2.3
1	E	72[A]	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	2.2
1	E	142	ASP	2.2
1	A	36	ARG	2.2
1	E	21	ARG	2.2
1	D	270	PHE	2.2
1	E	122	GLU	2.2
1	E	237	LEU	2.2
1	E	162	ILE	2.2
1	F	278	LYS	2.2
1	B	196	TYR	2.2
1	E	139	GLU	2.2
1	C	230	MET	2.2
1	A	52	VAL	2.2
1	A	78	VAL	2.2
1	A	79	LEU	2.2
1	E	135	HIS	2.2
1	F	112	LEU	2.2
1	F	257	GLU	2.2
1	B	247	GLY	2.2
1	A	230	MET	2.1
1	E	285	PHE	2.1
1	F	90	THR	2.1
1	F	135	HIS	2.1
1	F	139[A]	GLU	2.1
1	A	126	GLY	2.1
1	A	221	ILE	2.1
1	E	234	ILE	2.1
1	A	304	GLU	2.1
1	C	47	THR	2.1
1	E	90	THR	2.1
1	E	295	TYR	2.1
1	A	242	PHE	2.1
1	C	285	PHE	2.1
1	B	249	ALA	2.1
1	A	259	LEU	2.1
1	E	35	LEU	2.1
1	F	25	LEU	2.1
1	F	214	GLY	2.1
1	C	118	SER	2.1
1	E	94	GLU	2.0
1	D	114	SER	2.0
1	F	115	LEU	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	150	GLN	2.0
1	D	292	ILE	2.0
1	D	258	PRO	2.0
1	E	104	ASP	2.0
1	A	65	PHE	2.0
1	E	84	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

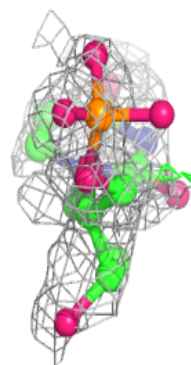
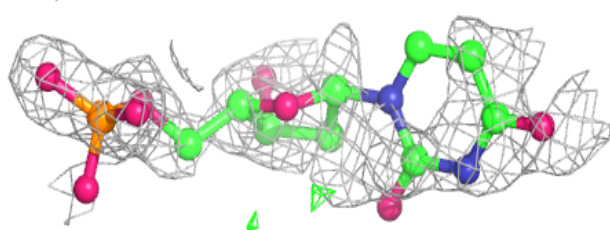
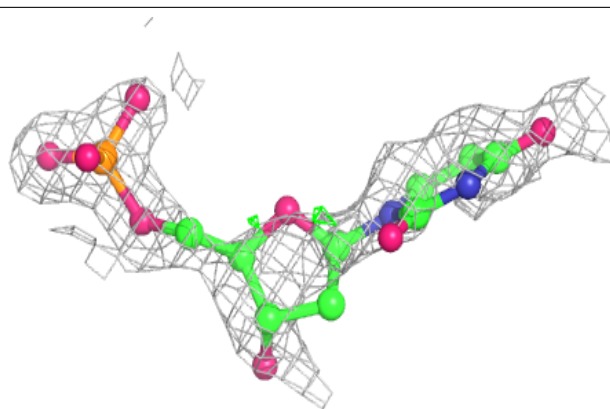
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UMP	F	502	20/20	0.70	0.30	23,41,46,46	20
3	BU1	C	504	6/6	0.75	0.26	40,47,51,54	0
3	BU1	C	502	6/6	0.83	0.26	56,57,57,58	0
3	BU1	C	503	6/6	0.85	0.15	37,45,47,48	0
2	UMP	F	501	20/20	0.86	0.16	24,31,32,34	0
2	UMP	D	501	20/20	0.92	0.10	21,24,29,29	0
2	UMP	E	501	20/20	0.93	0.19	23,29,35,36	0
2	UMP	C	501	20/20	0.95	0.07	19,22,29,30	0
2	UMP	B	501	20/20	0.98	0.09	13,17,21,23	0
2	UMP	A	501	20/20	0.98	0.07	13,16,24,24	0

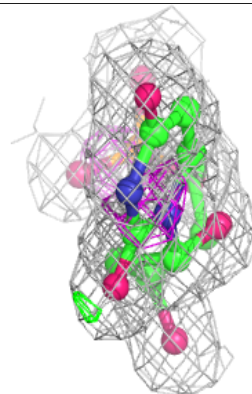
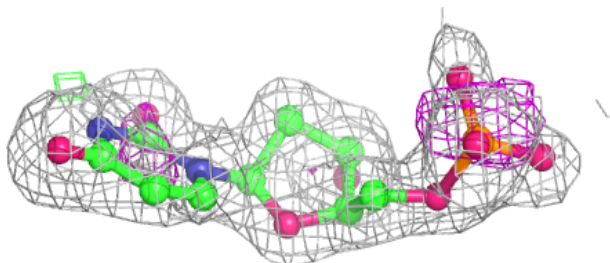
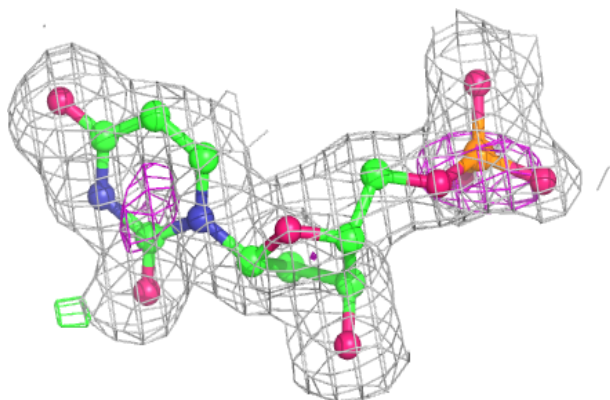
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UMP F 502:**

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

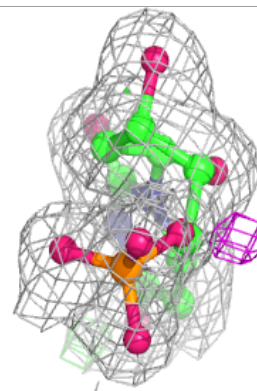
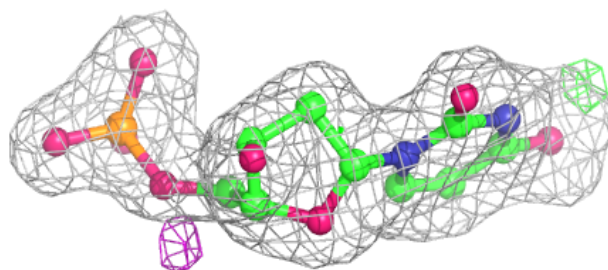
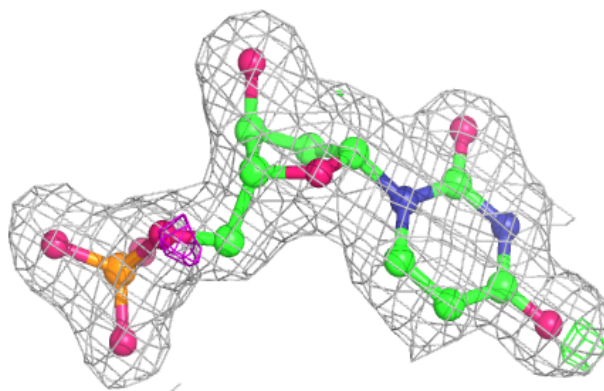
**Electron density around UMP F 501:**

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

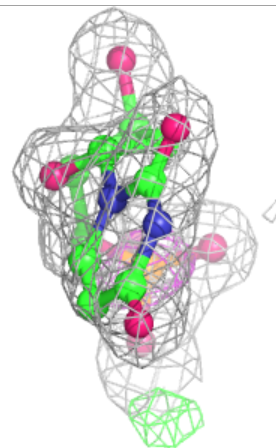
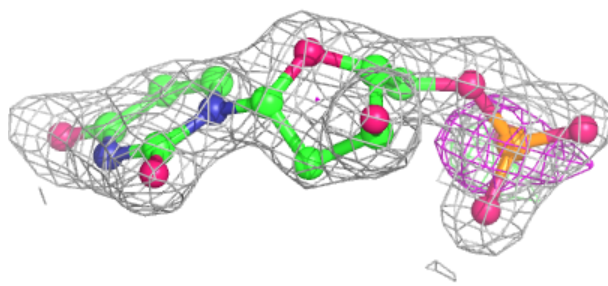
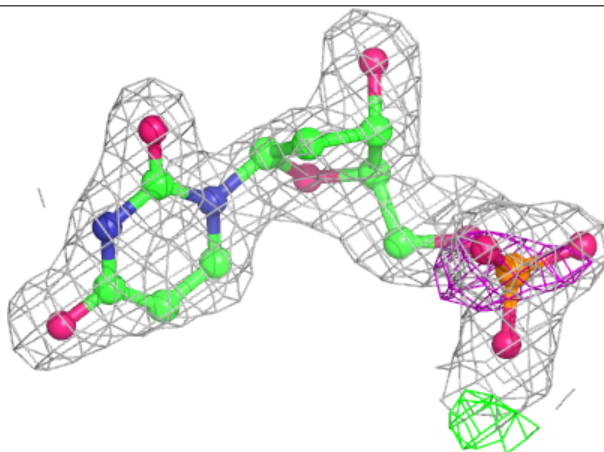


**Electron density around UMP D 501:**

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

**Electron density around UMP E 501:**

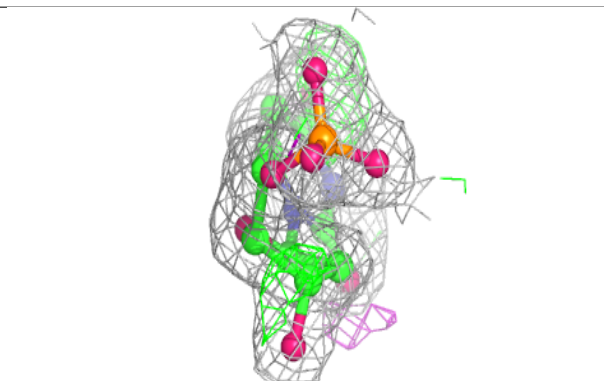
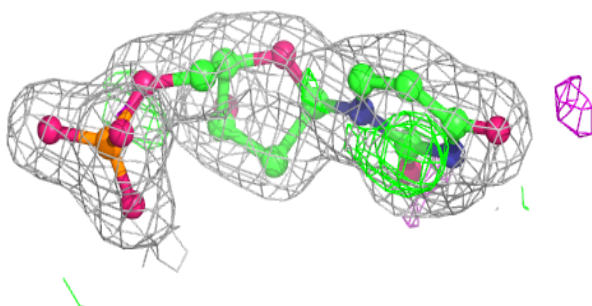
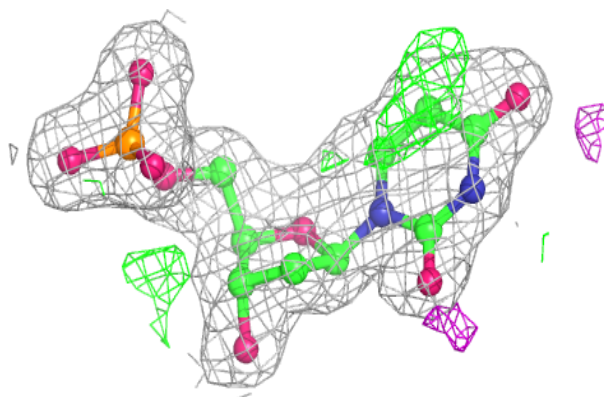
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



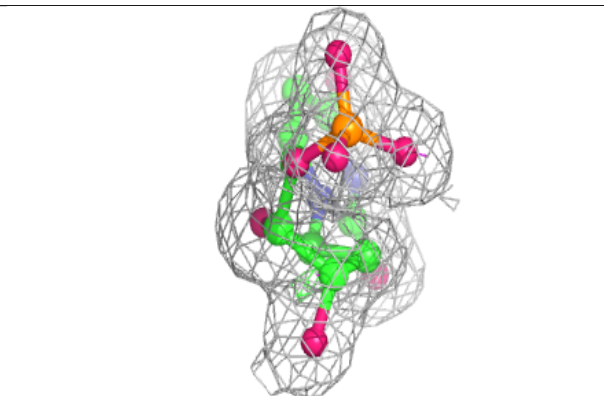
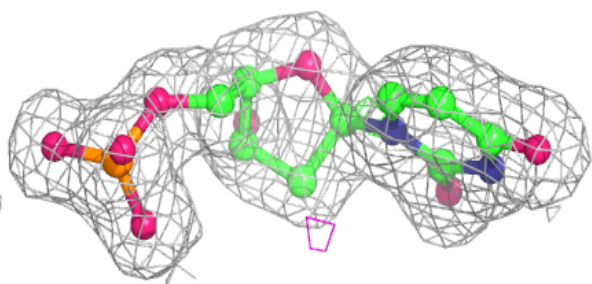
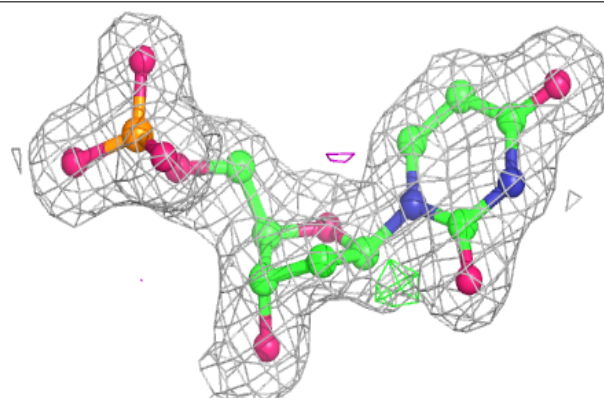


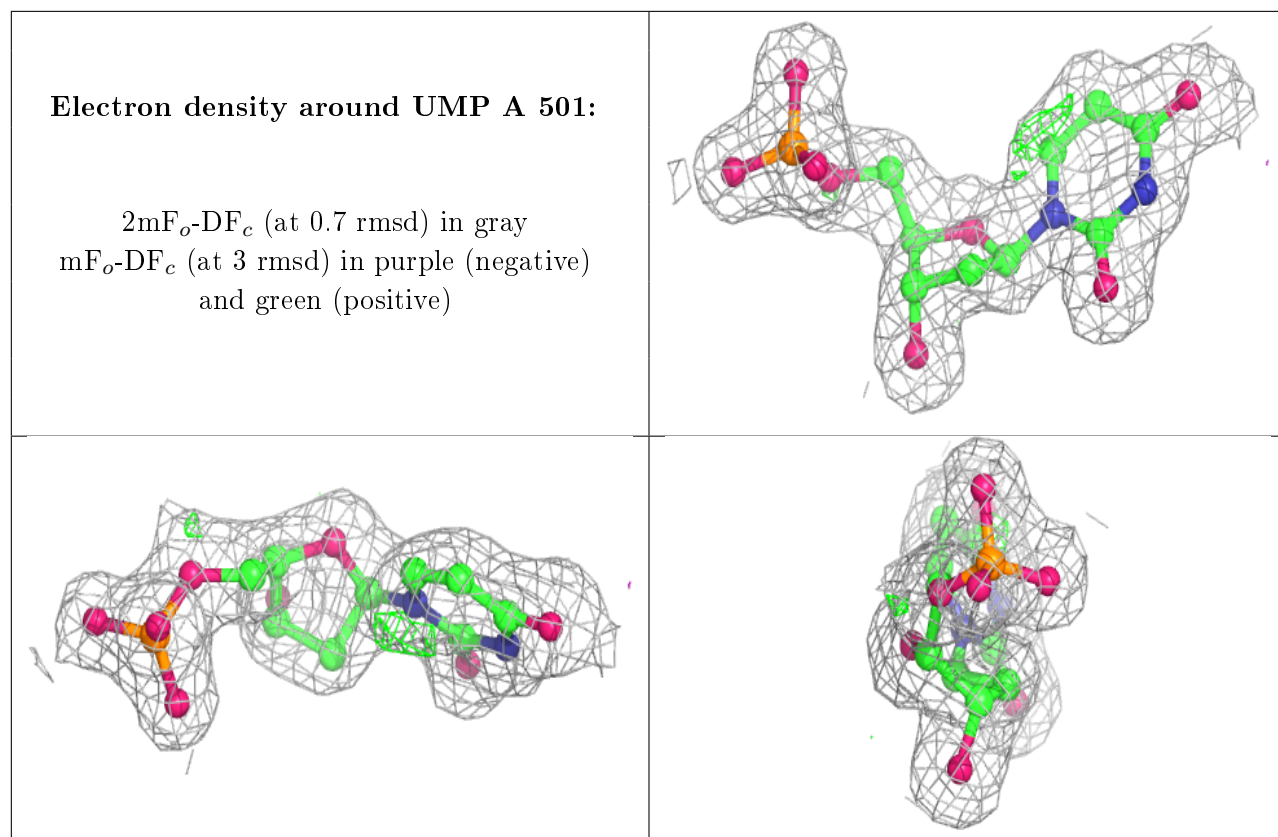
**Electron density around UMP C 501:**

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

**Electron density around UMP B 501:**

$2mF_o-DF_c$  (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.