



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:16 AM UTC

PDB ID : 2TSR / pdb_00002tsr
Title : THYMIDYLATE SYNTHASE FROM RAT IN TERNARY COMPLEX
WITH DUMP AND TOMUDEX
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Hardy, L.W.; Montfort, W.R.
Deposited on : 1998-06-19
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

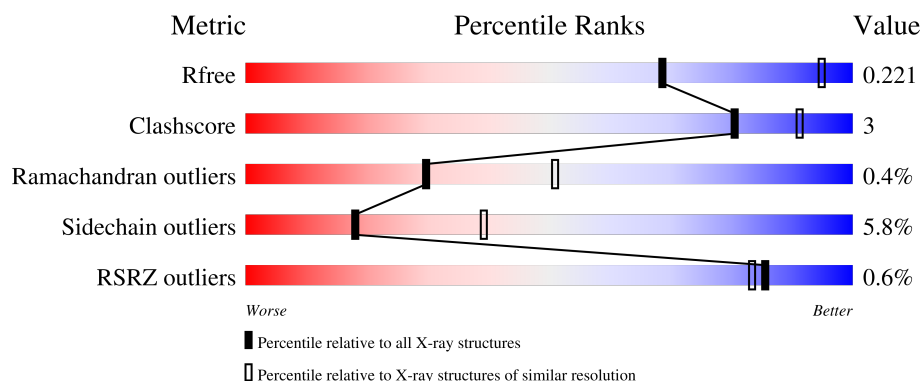
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

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

2 Entry composition [i](#)

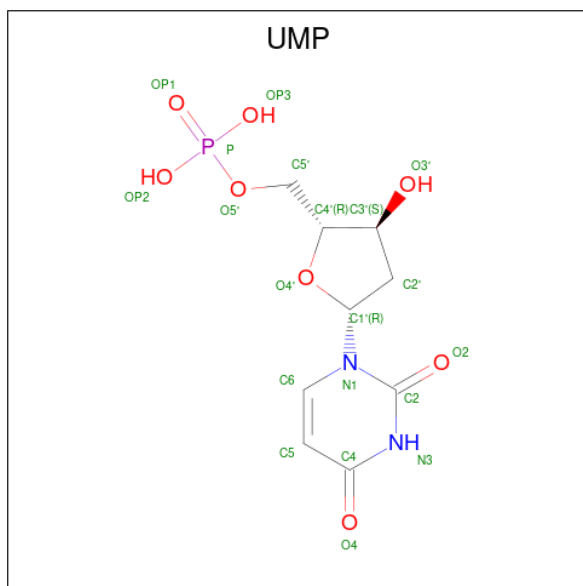
There are 4 unique types of molecules in this entry. The entry contains 9367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	281	Total	C	N	O	S	0	0	0
			2271	1453	394	412	12			
1	B	281	Total	C	N	O	S	0	0	0
			2271	1453	394	412	12			
1	C	281	Total	C	N	O	S	0	0	0
			2271	1453	394	412	12			
1	D	281	Total	C	N	O	S	0	0	0
			2271	1453	394	412	12			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



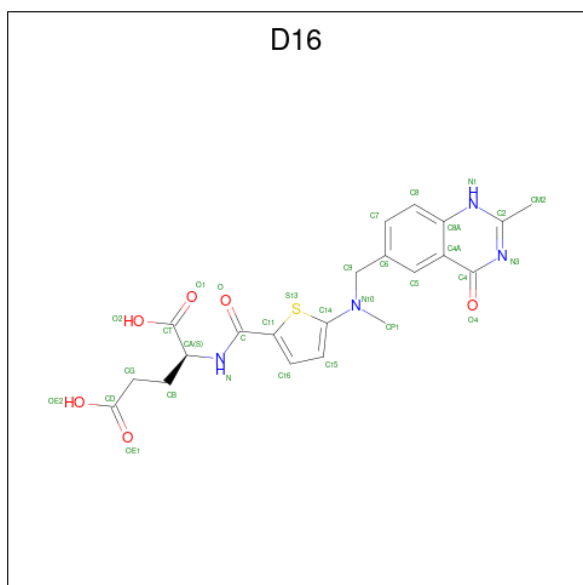
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	26	Total	O	0	0
			26	26		
4	C	9	Total	O	0	0
			9	9		

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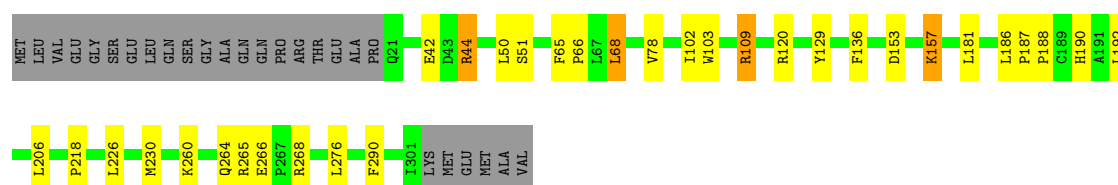
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	16	Total	O	0	0
			16	16		

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.

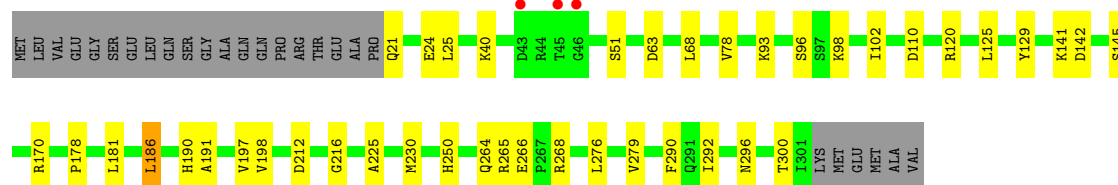
• Molecule 1: THYMIDYLATE SYNTHASE

Chain A: 



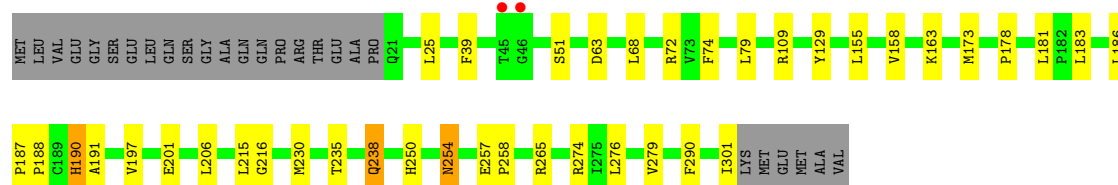
• Molecule 1: THYMIDYLATE SYNTHASE

Chain B: 



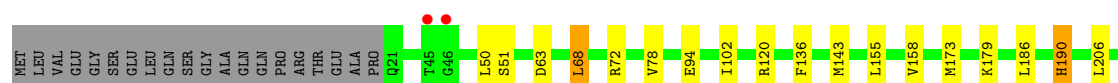
• Molecule 1: THYMIDYLATE SYNTHASE

Chain C: 



• Molecule 1: THYMIDYLATE SYNTHASE

Chain D: 



D212		G216	V217	P218	A225	L226	M230	G247	H250	R265	E266	P267	R268		R274	I275	L276		V279		F290		N296	P297	H298	P299	T300	I301	LYS	MET	GLU	MET	ALA	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 101.60Å 140.80Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.9 (8.00-2.60) 79.9 (8.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.162 , 0.222 0.165 , 0.221	Depositor DCC
R_{free} test set	1760 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9367	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, D16

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/2330	0.89	5/3152 (0.2%)
1	B	0.37	0/2330	0.92	8/3152 (0.3%)
1	C	0.37	0/2330	0.89	6/3152 (0.2%)
1	D	0.38	0/2330	0.91	11/3152 (0.3%)
All	All	0.37	0/9320	0.90	30/12608 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	ALA	N-CA-C	8.73	120.88	111.36
1	C	216	GLY	N-CA-C	7.97	122.29	112.73
1	D	276	LEU	N-CA-C	7.66	119.63	111.28
1	B	216	GLY	N-CA-C	7.54	121.25	112.50
1	D	247	GLY	N-CA-C	-7.15	103.70	110.21
1	B	276	LEU	N-CA-C	6.71	121.06	113.01
1	B	102	ILE	N-CA-C	6.59	120.27	111.17
1	A	276	LEU	N-CA-C	6.40	120.69	113.01
1	D	51	SER	N-CA-C	6.38	119.41	109.52
1	B	51	SER	N-CA-C	6.33	119.50	109.50
1	A	51	SER	N-CA-C	6.01	118.55	109.23
1	D	68	LEU	N-CA-C	5.96	118.70	110.35
1	B	191	ALA	N-CA-C	5.91	118.67	111.82
1	B	197	VAL	N-CA-C	5.81	116.48	108.12
1	C	276	LEU	N-CA-C	5.66	119.45	112.54
1	D	250	HIS	N-CA-C	5.65	117.77	109.24
1	C	250	HIS	N-CA-C	5.64	117.75	109.24
1	D	225	ALA	N-CA-C	-5.55	105.24	112.23
1	D	216	GLY	N-CA-C	5.53	119.85	112.77
1	A	50	LEU	N-CA-C	-5.52	100.19	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	HIS	N-CA-C	-5.45	102.29	110.24
1	C	51	SER	N-CA-C	5.35	118.28	109.72
1	A	68	LEU	N-CA-C	5.35	117.78	110.24
1	D	143	MET	N-CA-C	5.27	117.77	111.71
1	D	102	ILE	N-CA-C	5.23	119.40	112.76
1	B	250	HIS	N-CA-C	5.20	117.10	109.24
1	B	225	ALA	N-CA-C	-5.11	105.79	111.36
1	C	197	VAL	N-CA-C	5.11	115.63	108.17
1	D	50	LEU	N-CA-C	-5.05	100.94	109.07
1	A	44	ARG	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2271	0	2230	13	0
1	B	2271	0	2230	11	0
1	C	2271	0	2230	11	0
1	D	2271	0	2230	12	0
2	A	20	0	11	0	0
2	B	20	0	11	2	0
2	C	20	0	11	2	0
2	D	20	0	11	3	0
3	A	32	0	20	0	0
3	B	32	0	20	1	0
3	C	32	0	20	1	0
3	D	32	0	20	1	0
4	A	24	0	0	0	0
4	B	26	0	0	0	0
4	C	9	0	0	1	0
4	D	16	0	0	0	0
All	All	9367	0	9044	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (48) 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:44:ARG:HH11	1:B:170:ARG:NH2	1.85	0.74
1:A:68:LEU:HD12	1:A:218:PRO:HB3	1.71	0.72
1:D:190:HIS:HB3	1:D:206:LEU:HD11	1.73	0.71
1:D:212:ASP:HB2	2:D:608:UMP:H2''	1.76	0.67
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.77	0.66
1:C:190:HIS:HB2	1:C:206:LEU:HD11	1.77	0.66
2:D:608:UMP:H1'	3:D:609:D16:C4	2.26	0.66
1:A:44:ARG:HH11	1:B:170:ARG:HH21	1.44	0.63
1:B:21:GLN:HG3	1:B:25:LEU:HD12	1.82	0.62
1:A:190:HIS:HB3	1:A:206:LEU:HD11	1.83	0.61
2:B:408:UMP:H1'	3:B:409:D16:C4	2.31	0.61
2:C:508:UMP:H1'	3:C:509:D16:C4	2.34	0.57
1:B:230:MET:HE2	1:B:290:PHE:CZ	2.43	0.54
1:D:68:LEU:HD22	1:D:218:PRO:HB3	1.90	0.53
1:C:254:ASN:ND2	1:C:254:ASN:H	2.06	0.52
1:D:155:LEU:HD13	1:D:173:MET:HE1	1.92	0.51
1:A:102:ILE:HG13	1:A:103:TRP:CD1	2.46	0.51
2:C:508:UMP:O2	2:C:508:UMP:H2'	2.12	0.49
1:D:226:LEU:HG	1:D:230:MET:HE3	1.96	0.47
1:D:268:ARG:HD2	1:D:296:ASN:O	2.15	0.46
1:D:155:LEU:O	1:D:158:VAL:HG22	2.16	0.45
1:B:141:LYS:HG2	1:B:142:ASP:N	2.31	0.45
1:C:257:GLU:HB2	1:C:258:PRO:HD3	1.98	0.45
2:D:608:UMP:O2	2:D:608:UMP:H2'	2.16	0.44
1:C:163:LYS:HG3	1:C:235:THR:HG22	2.00	0.44
1:B:96:SER:C	1:B:98:LYS:H	2.26	0.43
1:A:136:PHE:CE1	1:B:178:PRO:HD2	2.54	0.43
1:C:178:PRO:HD2	1:D:136:PHE:CE1	2.53	0.43
1:A:226:LEU:HG	1:A:230:MET:HE3	2.00	0.43
1:C:230:MET:HE2	1:C:290:PHE:CZ	2.54	0.43
1:C:39:PHE:HD2	4:C:511:HOH:O	2.01	0.42
1:C:155:LEU:O	1:C:158:VAL:HG22	2.19	0.42
1:D:266:GLU:HA	1:D:267:PRO:HD3	1.90	0.42
1:A:153:ASP:O	1:A:157:LYS:HB2	2.19	0.42
1:B:125:LEU:HD13	1:B:186:LEU:HD21	2.01	0.42
1:B:212:ASP:HB2	2:B:408:UMP:H2''	2.02	0.42
1:B:268:ARG:HD2	1:B:296:ASN:O	2.18	0.42
1:D:230:MET:HE2	1:D:290:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASN:N	1:C:254:ASN:HD22	2.18	0.41
1:A:230:MET:HE2	1:A:290:PHE:CZ	2.55	0.41
1:C:201:GLU:HA	1:C:238:GLN:O	2.20	0.41
1:A:109:ARG:NH2	1:A:120:ARG:O	2.54	0.41
1:B:24:GLU:HG3	1:B:68:LEU:HD22	2.03	0.41
1:D:72:ARG:O	1:D:300:THR:HG23	2.21	0.41
1:C:187:PRO:HA	1:C:188:PRO:HD3	1.90	0.40
1:D:265:ARG:NH2	1:D:299:PRO:O	2.54	0.40
1:A:65:PHE:HA	1:A:66:PRO:HD3	1.84	0.40
1:A:187:PRO:HA	1:A:188:PRO:HD3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/307 (91%)	264 (95%)	14 (5%)	1 (0%)	30	51
1	B	279/307 (91%)	267 (96%)	11 (4%)	1 (0%)	30	51
1	C	279/307 (91%)	264 (95%)	13 (5%)	2 (1%)	18	38
1	D	279/307 (91%)	268 (96%)	11 (4%)	0	100	100
All	All	1116/1228 (91%)	1063 (95%)	49 (4%)	4 (0%)	30	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	TYR
1	C	129	TYR
1	B	129	TYR
1	C	74	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/266 (92%)	234 (96%)	11 (4%)	24	50
1	B	245/266 (92%)	228 (93%)	17 (7%)	14	32
1	C	245/266 (92%)	227 (93%)	18 (7%)	13	29
1	D	245/266 (92%)	234 (96%)	11 (4%)	24	50
All	All	980/1064 (92%)	923 (94%)	57 (6%)	18	39

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	78	VAL
1	A	109	ARG
1	A	157	LYS
1	A	181	LEU
1	A	192	LEU
1	A	260	LYS
1	A	264	GLN
1	A	265	ARG
1	A	266	GLU
1	A	268	ARG
1	B	40	LYS
1	B	63	ASP
1	B	78	VAL
1	B	93	LYS
1	B	110	ASP
1	B	120	ARG
1	B	145	SER
1	B	181	LEU
1	B	186	LEU
1	B	190	HIS
1	B	198	VAL
1	B	264	GLN
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	266	GLU
1	B	279	VAL
1	B	292	ILE
1	B	300	THR
1	C	25	LEU
1	C	63	ASP
1	C	68	LEU
1	C	72	ARG
1	C	79	LEU
1	C	109	ARG
1	C	173	MET
1	C	181	LEU
1	C	183	LEU
1	C	186	LEU
1	C	190	HIS
1	C	215	LEU
1	C	238	GLN
1	C	254	ASN
1	C	265	ARG
1	C	274	ARG
1	C	279	VAL
1	C	301	ILE
1	D	63	ASP
1	D	78	VAL
1	D	94	GLU
1	D	120	ARG
1	D	179	LYS
1	D	186	LEU
1	D	190	HIS
1	D	265	ARG
1	D	274	ARG
1	D	279	VAL
1	D	300	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	132	GLN
1	A	135	HIS
1	A	177	ASN
1	A	190	HIS

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Mol	Chain	Res	Type
1	A	233	HIS
1	A	254	ASN
1	B	56	GLN
1	B	156	GLN
1	B	199	ASN
1	B	205	GLN
1	B	298	HIS
1	C	33	HIS
1	C	250	HIS
1	C	254	ASN
1	C	255	HIS
1	D	30	GLN
1	D	33	HIS
1	D	56	GLN
1	D	121	GLN
1	D	165	ASN
1	D	205	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	D	608	-	21,21,21	0.47	0	30,31,31	0.88	1 (3%)
3	D16	A	309	-	33,34,34	2.36	13 (39%)	46,48,48	1.92	12 (26%)
3	D16	C	509	-	33,34,34	2.31	14 (42%)	46,48,48	1.95	14 (30%)
2	UMP	A	308	-	21,21,21	0.44	0	30,31,31	0.41	0
2	UMP	B	408	-	21,21,21	0.47	0	30,31,31	0.75	1 (3%)
3	D16	D	609	-	33,34,34	2.24	14 (42%)	46,48,48	2.04	13 (28%)
3	D16	B	409	-	33,34,34	2.32	15 (45%)	46,48,48	1.92	12 (26%)
2	UMP	C	508	-	21,21,21	0.47	0	30,31,31	0.80	1 (3%)

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	D	608	-	-	2/10/22/22	0/2/2/2
3	D16	A	309	-	-	8/25/25/25	0/3/3/3
3	D16	C	509	-	-	6/25/25/25	0/3/3/3
2	UMP	A	308	-	-	0/10/22/22	0/2/2/2
2	UMP	B	408	-	-	3/10/22/22	0/2/2/2
3	D16	D	609	-	-	4/25/25/25	0/3/3/3
3	D16	B	409	-	-	4/25/25/25	0/3/3/3
2	UMP	C	508	-	-	3/10/22/22	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	409	D16	C2-N3	5.57	1.43	1.31
3	A	309	D16	C2-N3	5.53	1.43	1.31
3	C	509	D16	C2-N3	5.52	1.43	1.31
3	D	609	D16	C2-N3	5.20	1.42	1.31
3	A	309	D16	C9-C6	4.50	1.59	1.51
3	D	609	D16	C9-C6	4.37	1.59	1.51
3	C	509	D16	C9-C6	4.37	1.59	1.51
3	B	409	D16	CG-CD	3.94	1.59	1.50
3	A	309	D16	C9-N10	3.84	1.57	1.46
3	A	309	D16	CG-CD	3.81	1.59	1.50
3	C	509	D16	C9-N10	3.64	1.56	1.46
3	B	409	D16	C9-C6	3.62	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	509	D16	CG-CD	3.57	1.58	1.50
3	B	409	D16	C9-N10	3.54	1.56	1.46
3	D	609	D16	C9-N10	3.50	1.56	1.46
3	B	409	D16	C-C11	3.47	1.55	1.48
3	D	609	D16	CG-CD	3.35	1.58	1.50
3	D	609	D16	C-C11	3.32	1.55	1.48
3	B	409	D16	C8-C7	3.30	1.44	1.38
3	D	609	D16	C5-C6	3.28	1.44	1.39
3	C	509	D16	C5-C6	3.28	1.44	1.39
3	A	309	D16	C7-C6	3.24	1.45	1.38
3	C	509	D16	C-C11	3.22	1.55	1.48
3	A	309	D16	CB-CA	3.16	1.60	1.53
3	B	409	D16	CB-CA	3.06	1.60	1.53
3	A	309	D16	C8-C7	3.06	1.43	1.38
3	C	509	D16	C7-C6	3.05	1.44	1.38
3	C	509	D16	C8-C7	3.04	1.43	1.38
3	A	309	D16	C5-C6	2.99	1.44	1.39
3	A	309	D16	C2-N1	2.98	1.44	1.36
3	D	609	D16	C7-C6	2.97	1.44	1.38
3	B	409	D16	C2-N1	2.94	1.44	1.36
3	B	409	D16	C7-C6	2.94	1.44	1.38
3	A	309	D16	C-C11	2.87	1.54	1.48
3	B	409	D16	C4A-C4	2.85	1.53	1.48
3	C	509	D16	C2-N1	2.84	1.44	1.36
3	C	509	D16	C4A-C4	2.79	1.52	1.48
3	D	609	D16	C8-C7	2.72	1.43	1.38
3	A	309	D16	CB-CG	2.71	1.61	1.52
3	A	309	D16	C4A-C4	2.70	1.52	1.48
3	B	409	D16	CB-CG	2.68	1.60	1.52
3	B	409	D16	C5-C6	2.67	1.43	1.39
3	D	609	D16	C2-N1	2.64	1.43	1.36
3	D	609	D16	CB-CA	2.54	1.59	1.53
3	D	609	D16	C4A-C4	2.53	1.52	1.48
3	C	509	D16	CB-CA	2.48	1.59	1.53
3	D	609	D16	CA-CT	2.46	1.58	1.52
3	A	309	D16	CA-CT	2.46	1.58	1.52
3	C	509	D16	CA-CT	2.37	1.58	1.52
3	D	609	D16	CB-CG	2.36	1.60	1.52
3	B	409	D16	C-N	2.35	1.39	1.34
3	C	509	D16	CB-CG	2.32	1.59	1.52
3	D	609	D16	C-N	2.25	1.38	1.34
3	B	409	D16	CA-CT	2.22	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	409	D16	C4-N3	2.12	1.43	1.38
3	C	509	D16	C-N	2.10	1.38	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	609	D16	S13-C14-N10	6.66	127.24	120.99
3	B	409	D16	S13-C14-N10	5.79	126.42	120.99
3	C	509	D16	S13-C14-N10	5.61	126.25	120.99
3	C	509	D16	CG-CB-CA	5.58	123.44	113.16
3	A	309	D16	S13-C14-N10	5.39	126.04	120.99
3	B	409	D16	CG-CB-CA	5.36	123.03	113.16
3	D	609	D16	CG-CB-CA	5.32	122.96	113.16
3	A	309	D16	CG-CB-CA	4.94	122.27	113.16
3	A	309	D16	C15-C14-S13	-3.59	107.92	111.97
3	B	409	D16	C15-C14-S13	-3.55	107.96	111.97
3	D	609	D16	C15-C14-S13	-3.51	108.00	111.97
3	C	509	D16	C6-C9-N10	3.35	119.33	113.02
3	C	509	D16	C15-C14-S13	-3.28	108.26	111.97
3	A	309	D16	CB-CA-CT	3.17	117.88	110.35
3	A	309	D16	N1-C2-N3	-3.14	118.89	122.96
3	D	609	D16	N1-C2-N3	-3.11	118.93	122.96
3	C	509	D16	N1-C2-N3	-3.11	118.94	122.96
3	D	609	D16	CB-CA-CT	3.09	117.69	110.35
3	D	609	D16	C6-C9-N10	3.07	118.80	113.02
3	C	509	D16	CB-CA-CT	3.03	117.54	110.35
3	D	609	D16	C15-C14-N10	-3.01	124.74	127.84
3	B	409	D16	N1-C2-N3	-3.00	119.07	122.96
3	D	609	D16	C16-C15-C14	2.97	116.36	112.01
3	B	409	D16	CB-CA-CT	2.96	117.39	110.35
3	B	409	D16	C16-C15-C14	2.85	116.18	112.01
2	D	608	UMP	C2'-C1'-N1	2.73	120.64	113.81
3	D	609	D16	C8-C8A-C4A	2.70	122.91	119.37
3	A	309	D16	CA-N-C	-2.66	117.51	122.00
3	C	509	D16	C16-C15-C14	2.59	115.80	112.01
3	A	309	D16	C6-C9-N10	2.58	117.88	113.02
3	A	309	D16	C16-C15-C14	2.57	115.78	112.01
2	C	508	UMP	C2'-C1'-N1	2.56	120.21	113.81
3	C	509	D16	C8-C8A-C4A	2.53	122.68	119.37
3	B	409	D16	C8-C8A-C4A	2.53	122.68	119.37
3	A	309	D16	C8-C8A-C4A	2.52	122.66	119.37
3	A	309	D16	CM2-C2-N1	2.48	121.19	116.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	509	D16	CM2-C2-N1	2.42	121.08	116.41
3	B	409	D16	CA-N-C	-2.41	117.94	122.00
3	D	609	D16	CM2-C2-N1	2.38	121.01	116.41
3	C	509	D16	C5-C4A-C8A	-2.38	116.96	119.09
3	D	609	D16	OE1-CD-CG	-2.37	115.57	123.09
3	B	409	D16	CM2-C2-N1	2.36	120.95	116.41
3	B	409	D16	C5-C4A-C8A	-2.30	117.02	119.09
3	C	509	D16	C15-C14-N10	-2.29	125.48	127.84
3	B	409	D16	C15-C14-N10	-2.27	125.50	127.84
3	D	609	D16	C5-C4A-C8A	-2.26	117.06	119.09
2	B	408	UMP	O4'-C1'-C2'	2.25	110.45	106.25
3	A	309	D16	OE1-CD-CG	-2.25	115.96	123.09
3	C	509	D16	CA-N-C	-2.24	118.22	122.00
3	C	509	D16	OE1-CD-CG	-2.19	116.15	123.09
3	A	309	D16	C5-C4A-C8A	-2.15	117.17	119.09
3	B	409	D16	OE1-CD-CG	-2.07	116.51	123.09
3	D	609	D16	CA-N-C	-2.03	118.58	122.00
3	C	509	D16	O1-CT-CA	-2.00	115.80	122.26

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	309	D16	N-CA-CB-CG
3	C	509	D16	N-CA-CB-CG
2	C	508	UMP	C2'-C1'-N1-C2
3	A	309	D16	CT-CA-CB-CG
3	C	509	D16	CT-CA-CB-CG
2	C	508	UMP	C2'-C1'-N1-C6
2	D	608	UMP	C2'-C1'-N1-C6
2	B	408	UMP	C2'-C1'-N1-C2
2	D	608	UMP	C2'-C1'-N1-C2
2	B	408	UMP	C2'-C1'-N1-C6
3	B	409	D16	CT-CA-CB-CG
3	D	609	D16	N-CA-CT-O2
3	D	609	D16	N-CA-CT-O1
3	C	509	D16	C6-C9-N10-CP1
3	A	309	D16	CB-CA-CT-O2
3	A	309	D16	CB-CA-CT-O1
3	C	509	D16	OE1-CD-CG-CB
3	B	409	D16	OE2-CD-CG-CB
3	B	409	D16	OE1-CD-CG-CB

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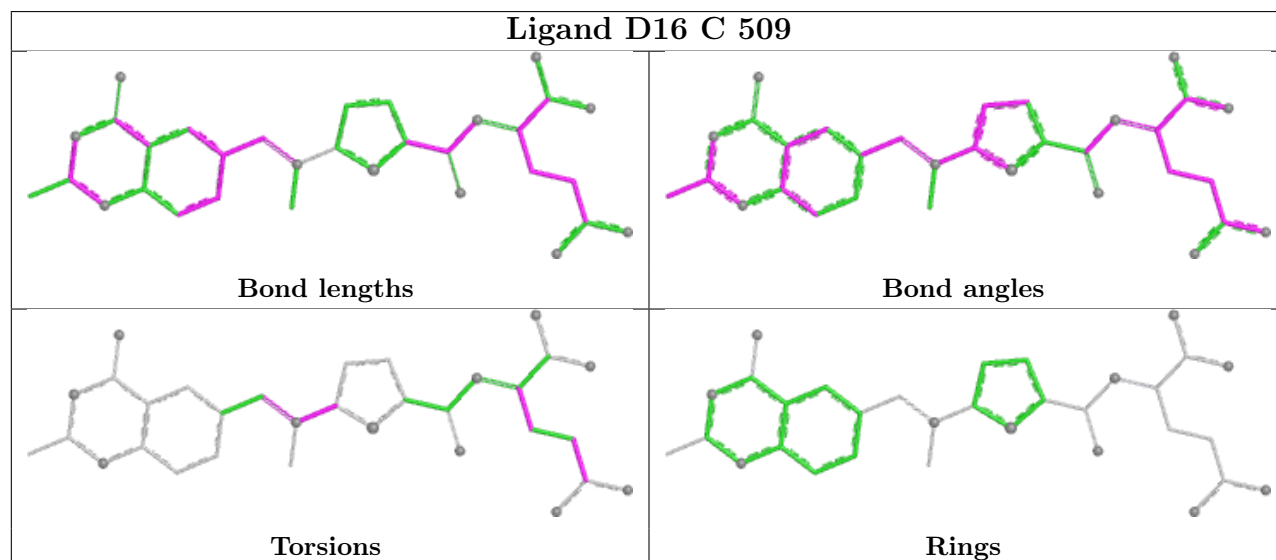
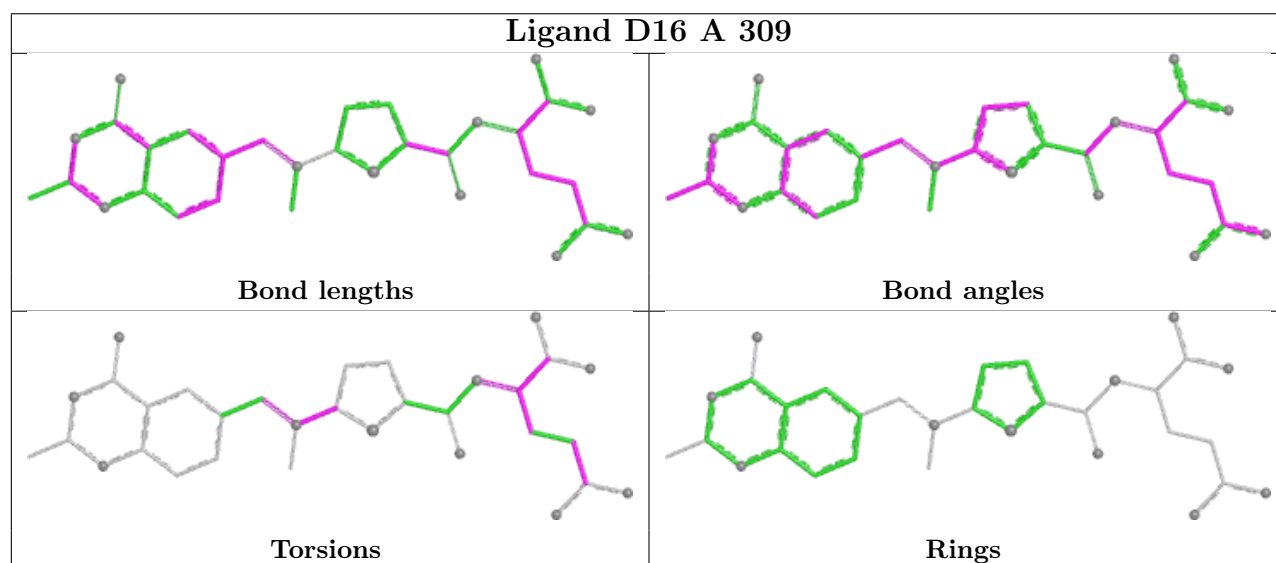
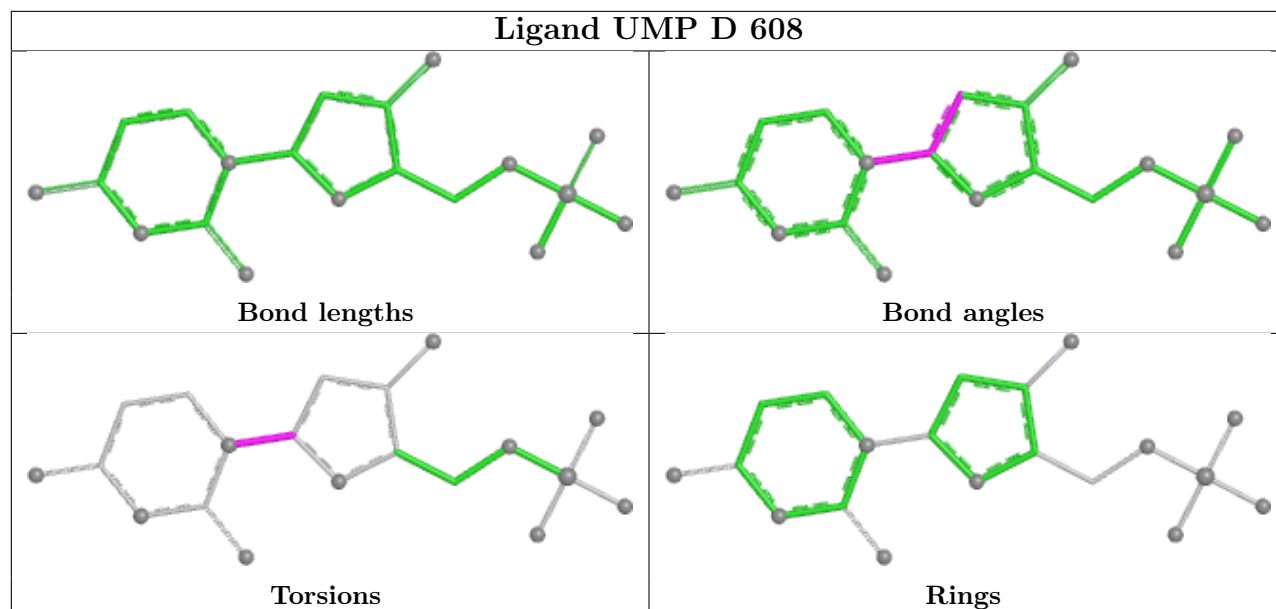
Mol	Chain	Res	Type	Atoms
3	C	509	D16	OE2-CD-CG-CB
3	A	309	D16	C6-C9-N10-CP1
3	A	309	D16	C15-C14-N10-CP1
3	C	509	D16	C15-C14-N10-CP1
2	B	408	UMP	O4'-C4'-C5'-O5'
3	D	609	D16	OE1-CD-CG-CB
3	A	309	D16	CB-CA-N-C
3	D	609	D16	OE2-CD-CG-CB
2	C	508	UMP	O4'-C4'-C5'-O5'
3	A	309	D16	OE2-CD-CG-CB
3	B	409	D16	CA-CB-CG-CD

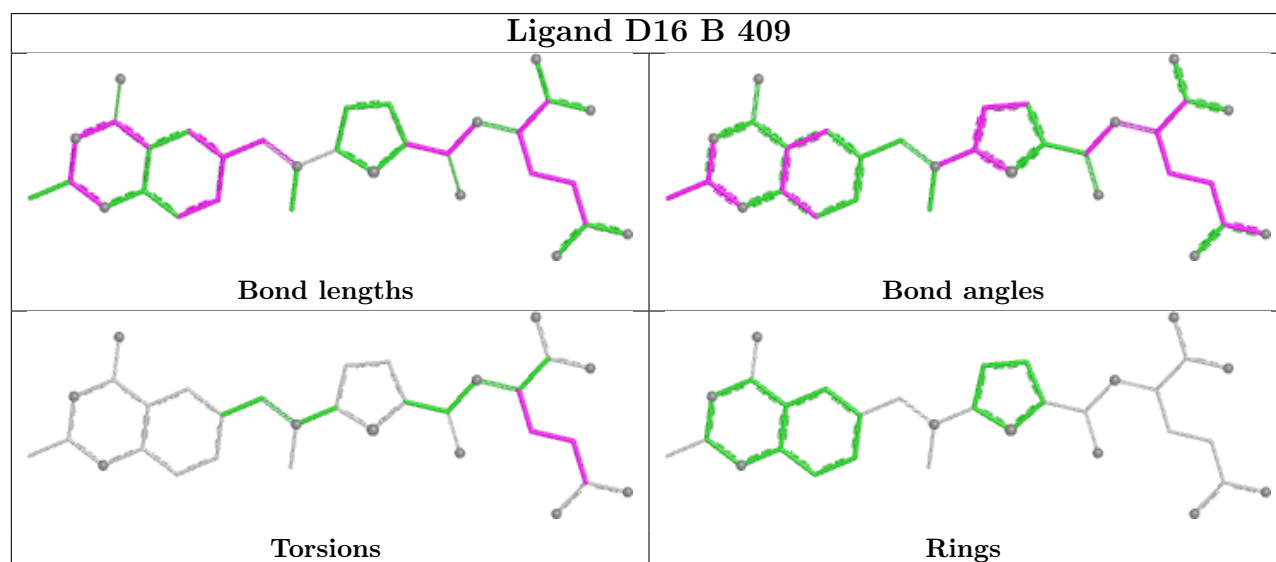
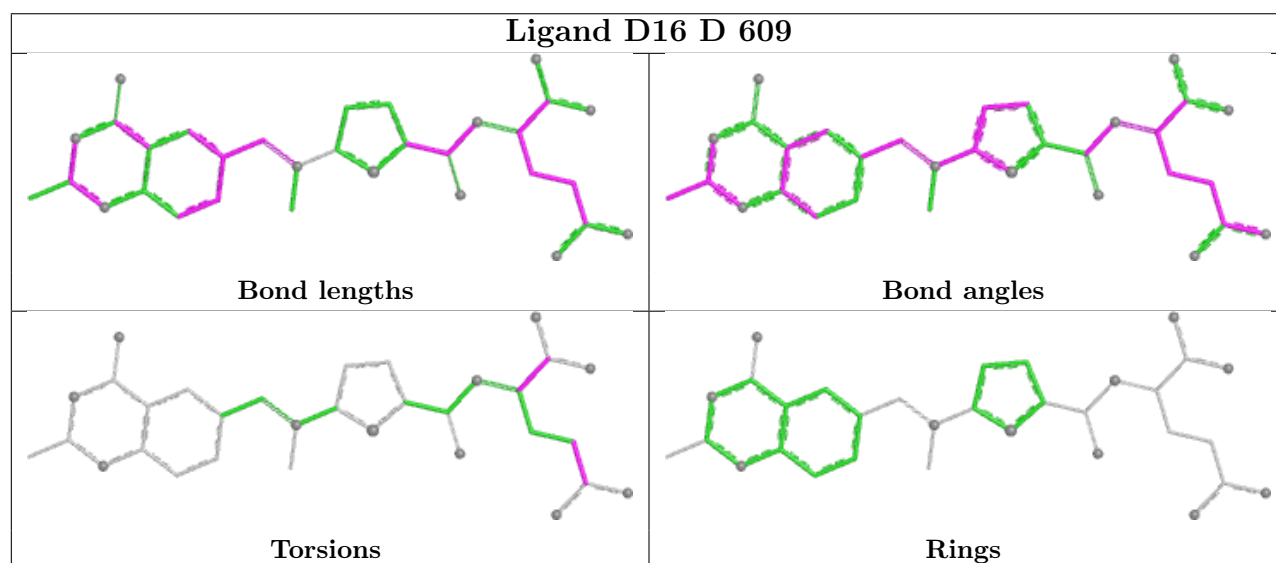
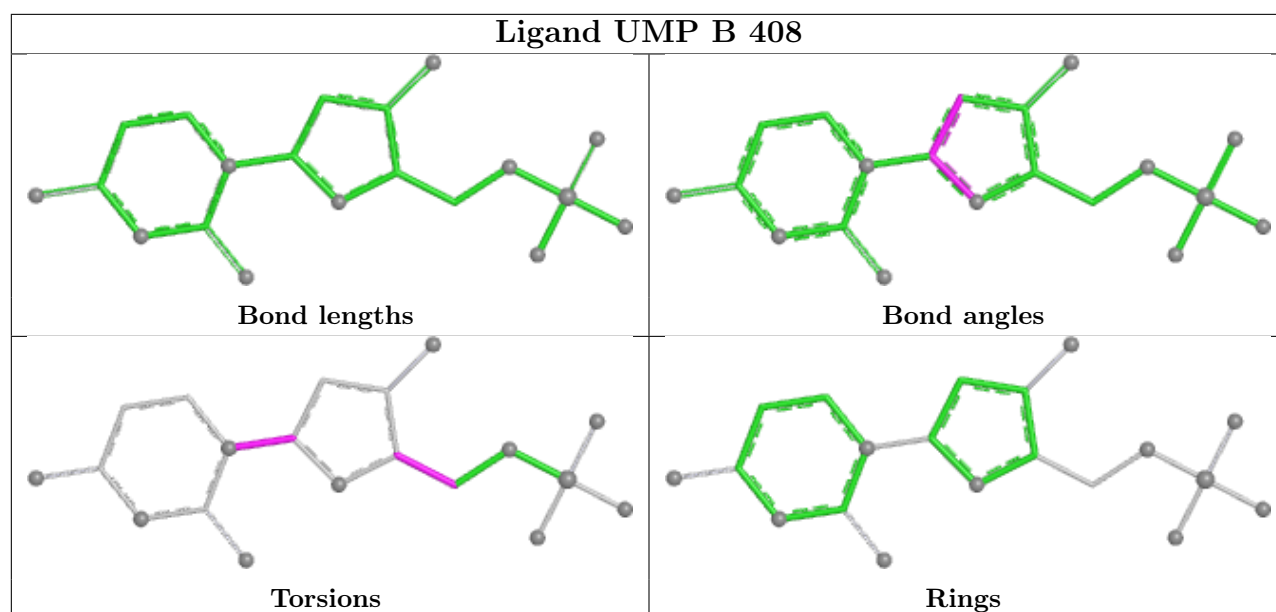
There are no ring outliers.

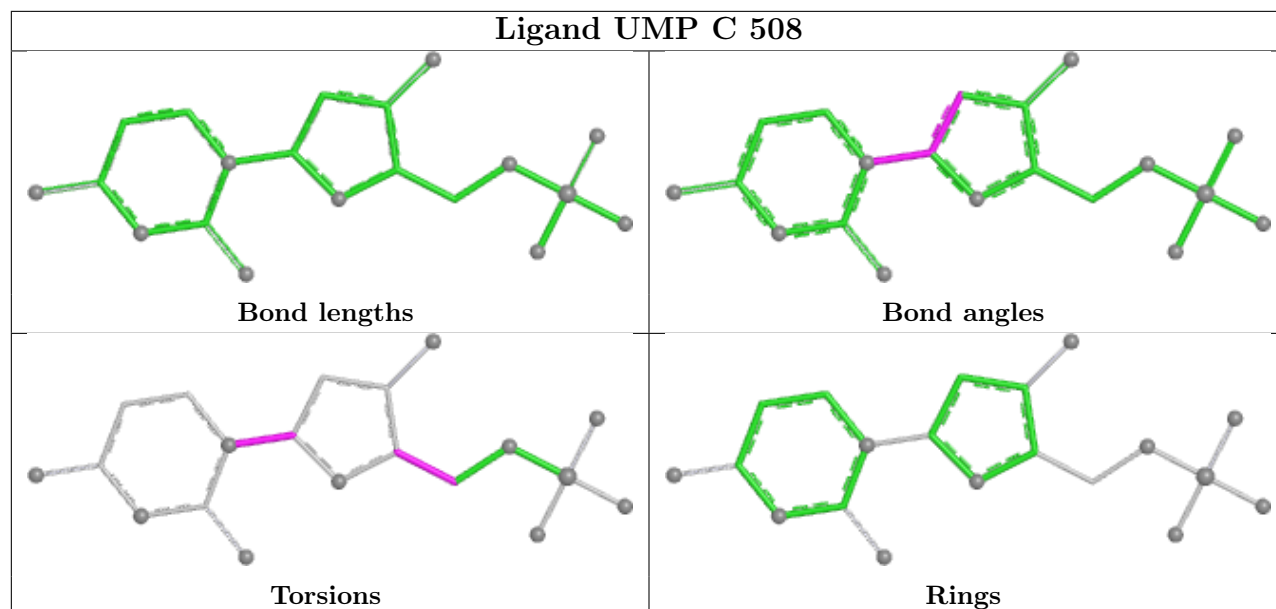
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	608	UMP	3	0
3	C	509	D16	1	0
2	B	408	UMP	2	0
3	D	609	D16	1	0
3	B	409	D16	1	0
2	C	508	UMP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/307 (91%)	-1.01	0 100 100	10, 27, 61, 89	0
1	B	281/307 (91%)	-0.95	3 (1%) 78 74	11, 26, 63, 97	0
1	C	281/307 (91%)	-0.70	2 (0%) 84 82	15, 40, 75, 95	0
1	D	281/307 (91%)	-0.90	2 (0%) 84 82	17, 33, 62, 96	0
All	All	1124/1228 (91%)	-0.89	7 (0%) 85 83	10, 32, 67, 97	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	GLY	3.7
1	D	46	GLY	3.3
1	B	45	THR	2.8
1	C	45	THR	2.8
1	B	46	GLY	2.6
1	D	45	THR	2.3
1	B	43	ASP	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 ⓘ

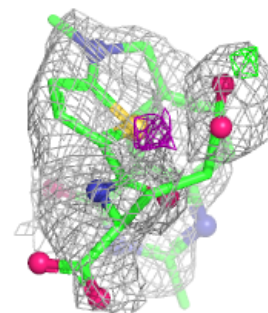
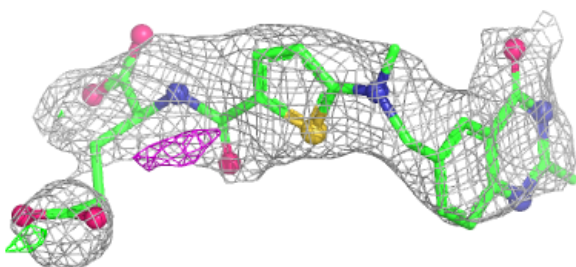
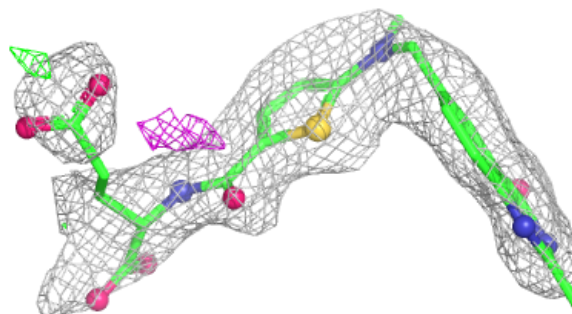
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	D16	B	409	32/32	0.83	0.09	60,71,85,89	0
3	D16	A	309	32/32	0.88	0.10	65,72,96,99	0
2	UMP	B	408	20/20	0.89	0.12	43,67,70,70	0
3	D16	D	609	32/32	0.91	0.07	48,59,72,72	0
2	UMP	D	608	20/20	0.92	0.10	46,53,64,65	0
2	UMP	C	508	20/20	0.92	0.09	40,52,63,64	0
2	UMP	A	308	20/20	0.93	0.09	33,50,63,67	0
3	D16	C	509	32/32	0.94	0.06	47,54,82,86	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.

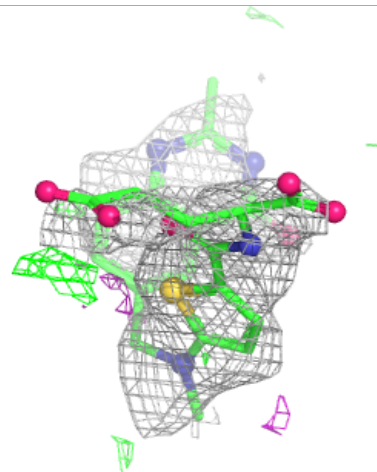
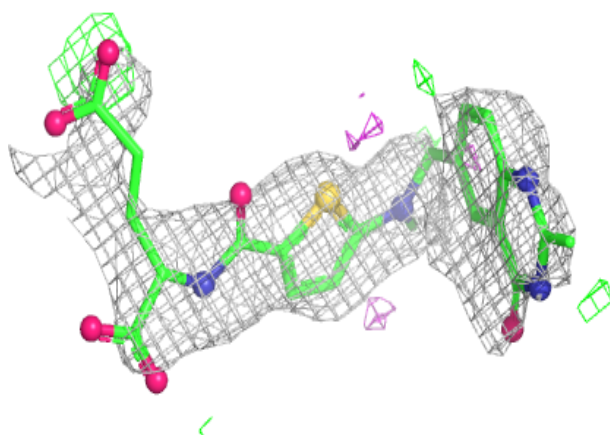
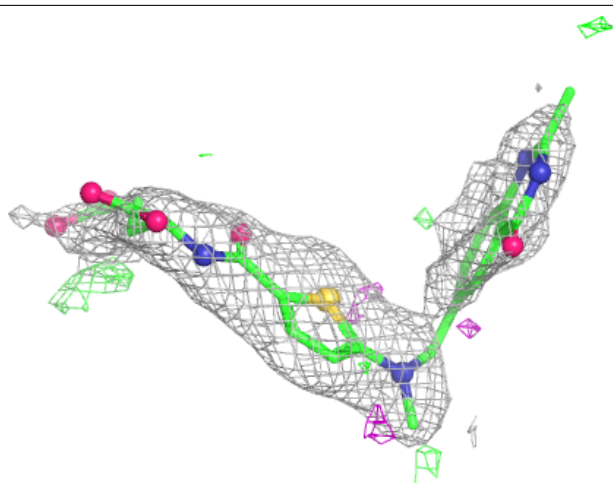
Electron density around D16 B 409:

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



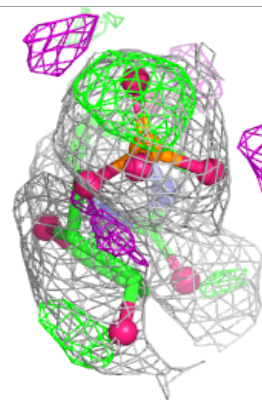
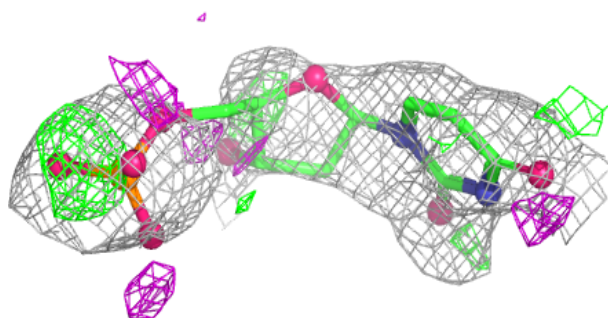
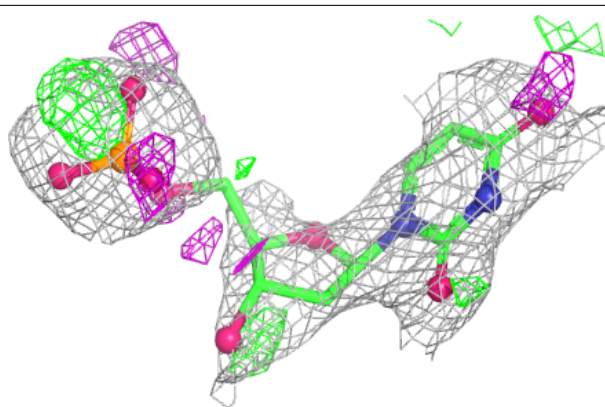
Electron density around D16 A 309:

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

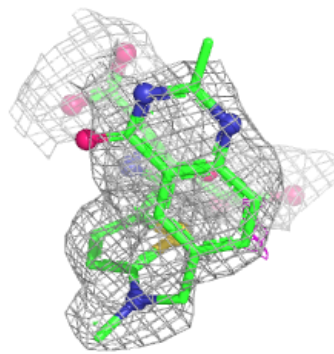
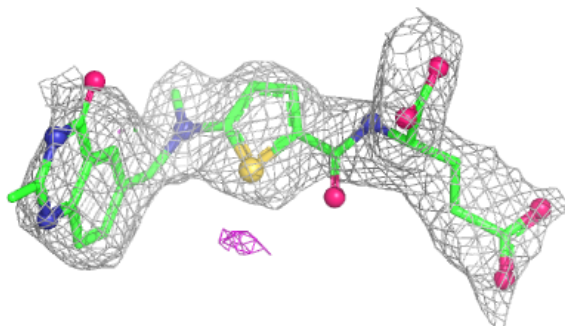
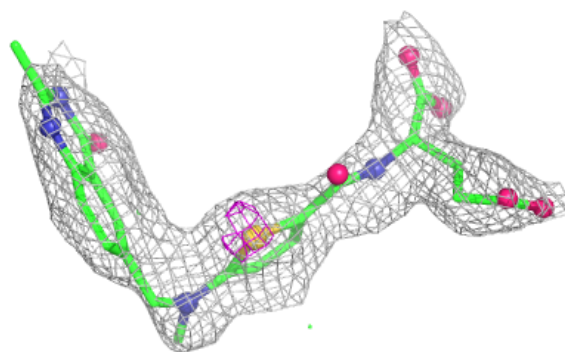


Electron density around UMP B 408:

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

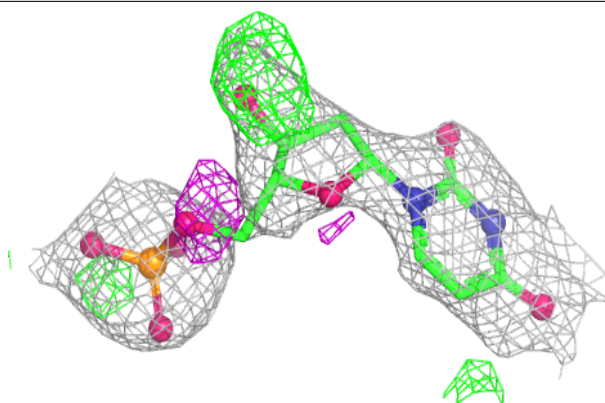
**Electron density around D16 D 609:**

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

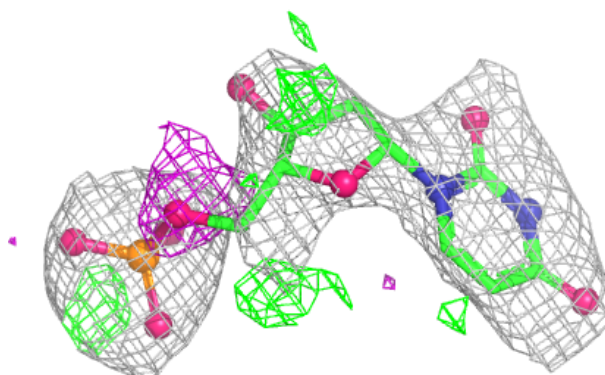


Electron density around UMP D 608:

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

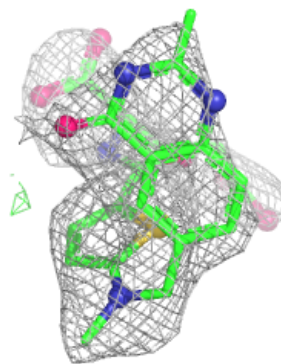
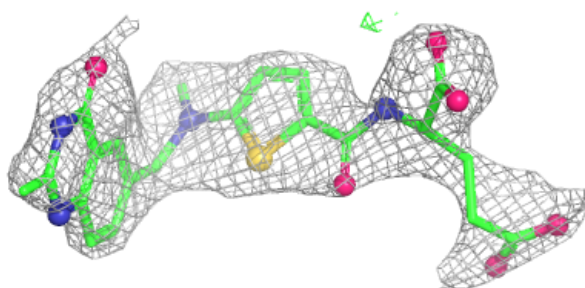
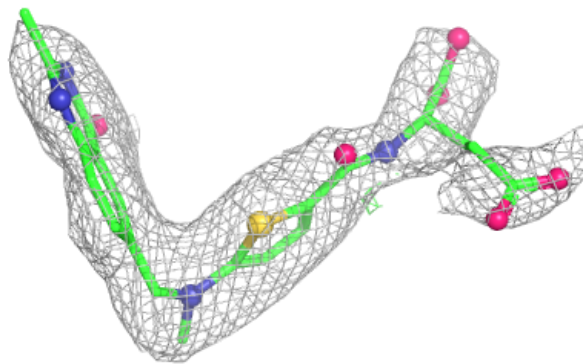
**Electron density around UMP C 508:**

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



Electron density around D16 C 509:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.