



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:22 AM UTC

PDB ID : 1HVV / pdb_00001hvv
Title : Human thymidylate synthase complexed with dUMP and Raltitrexed, an antifolate drug, is in the closed conformation
Authors : Phan, J.; Koli, S.; Minor, W.; Dunlap, R.B.; Berger, S.H.; Lebioda, L.
Deposited on : 2001-01-08
Resolution : 1.90 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

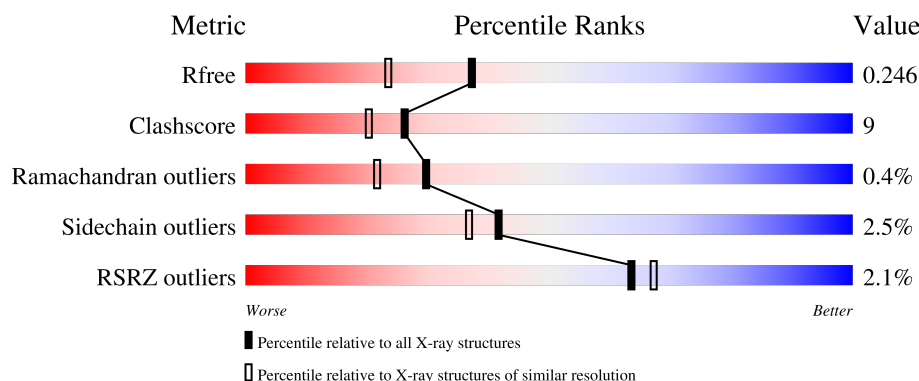
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	288	2% 77% 22% .
1	B	288	3% 81% 19% .
1	C	288	2% 75% 23% .
1	D	288	% 78% 19% .

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	BME	A	1514	-	X	-	-
4	BME	B	1515	-	X	-	-
4	BME	C	1516	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10136 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.

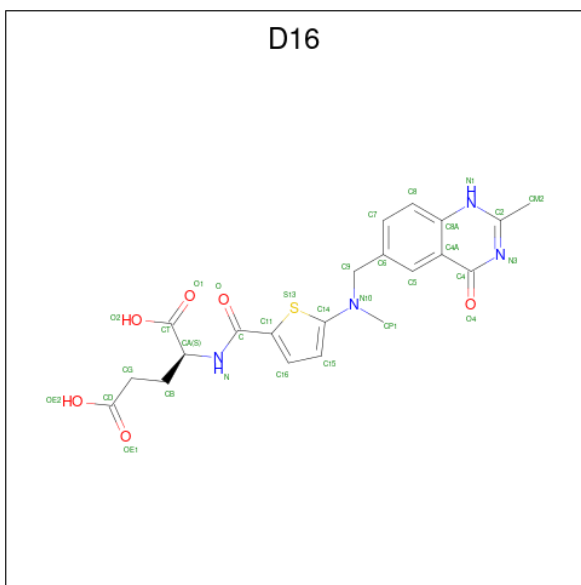
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	B	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	C	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	D	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			

There are 4 discrepancies between the modelled and reference sequences:

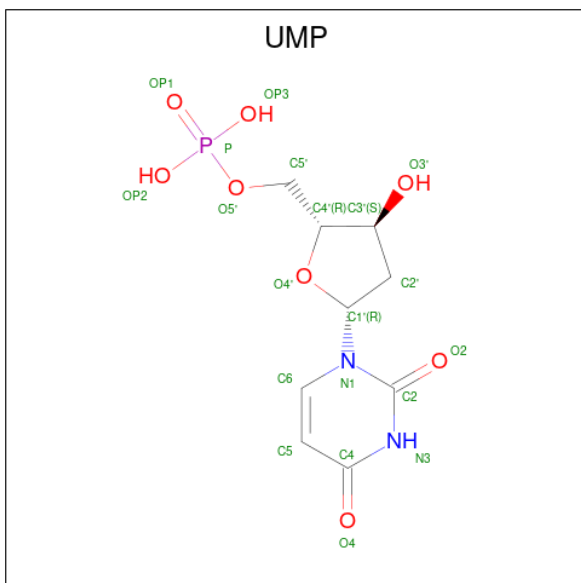
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	CME	CYS	modified residue	UNP P04818
B	43	CME	CYS	modified residue	UNP P04818
C	43	CME	CYS	modified residue	UNP P04818
D	43	CME	CYS	modified residue	UNP P04818

- Molecule 2 is TOMUDEX (CCD ID: D16) (formula: C₂₁H₂₂N₄O₆S).



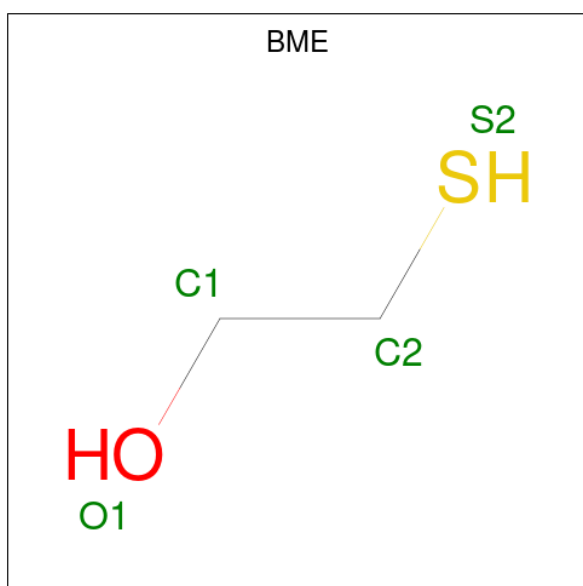
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

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



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

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	119	Total	O	0	0
			119	119		

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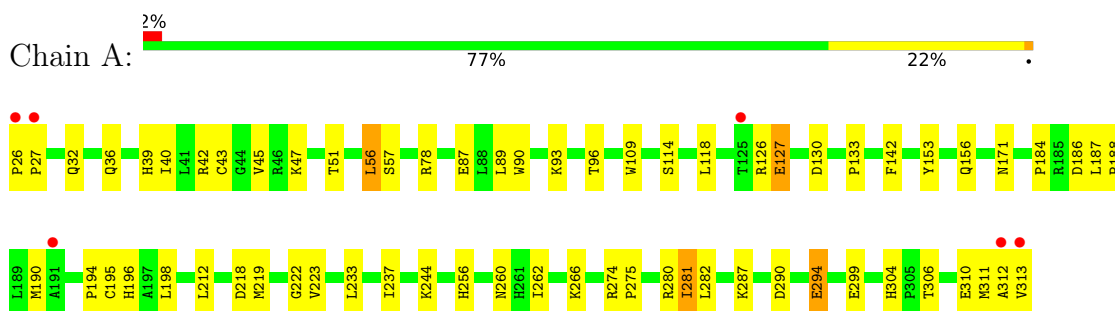
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	151	Total 151	O 151	0	0
5	D	170	Total 170	O 170	0	0

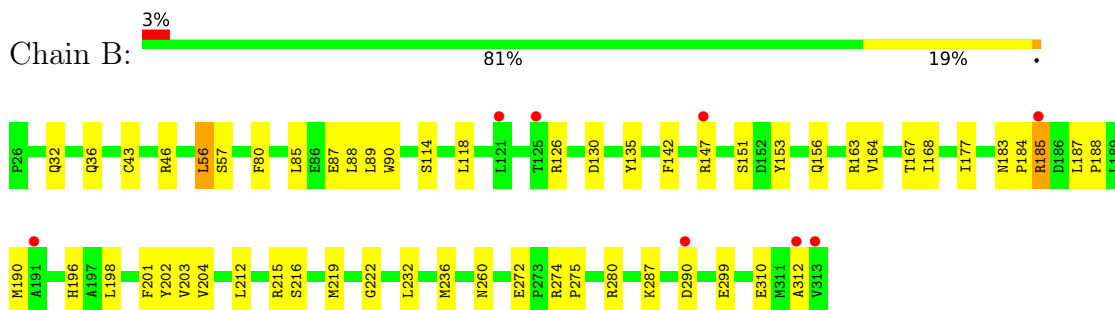
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

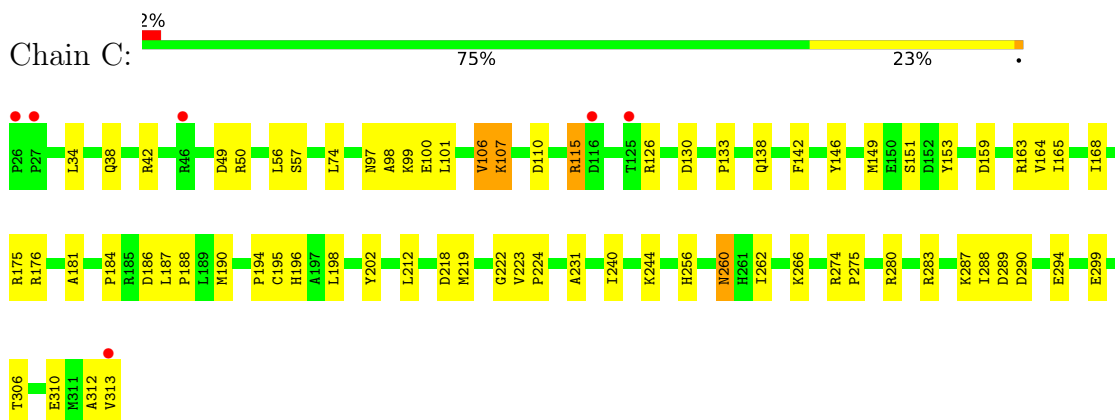
• Molecule 1: THYMIDYLATE SYNTHASE



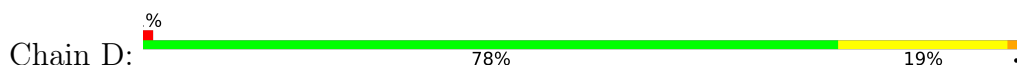
• Molecule 1: THYMIDYLATE SYNTHASE

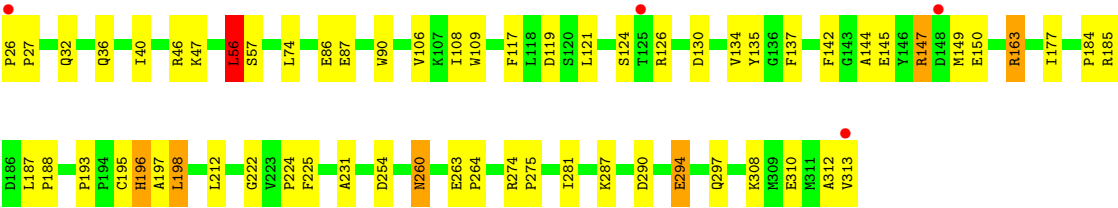


• Molecule 1: THYMIDYLATE SYNTHASE



• Molecule 1: THYMIDYLATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.85Å 70.50Å 74.53Å 70.23° 83.29° 73.28°	Depositor
Resolution (Å)	20.09 – 1.90 20.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	79.2 (20.09-1.90) 94.3 (20.09-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.244 0.209 , 0.246	Depositor DCC
R_{free} test set	6603 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: BME, UMP, CME, 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	0.40	0/2378	0.90	9/3213 (0.3%)
1	B	0.38	0/2378	0.89	4/3213 (0.1%)
1	C	0.39	0/2378	0.89	7/3213 (0.2%)
1	D	0.40	0/2378	0.91	7/3213 (0.2%)
All	All	0.39	0/9512	0.90	27/12852 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	N-CA-C	-8.30	95.70	109.07
1	D	56	LEU	N-CA-C	-8.00	95.49	108.52
1	C	56	LEU	N-CA-C	-7.57	96.18	108.52
1	B	56	LEU	N-CA-C	-7.30	96.63	108.52
1	A	222	GLY	N-CA-C	6.63	120.19	112.50
1	D	281	ILE	N-CA-C	-6.55	98.42	107.99
1	D	222	GLY	N-CA-C	6.53	120.56	112.73
1	A	195	CYS	N-CA-C	-6.23	104.94	112.54
1	D	195	CYS	N-CA-C	-6.07	104.22	111.69
1	D	197	ALA	N-CA-C	5.94	117.43	111.07
1	C	222	GLY	N-CA-C	5.83	119.26	112.50
1	A	282	LEU	N-CA-C	5.83	121.41	113.37
1	C	231	ALA	N-CA-C	-5.77	104.99	111.28
1	B	219	MET	N-CA-C	5.67	117.46	111.28
1	D	231	ALA	N-CA-C	-5.59	105.26	111.36
1	C	195	CYS	N-CA-C	-5.52	106.05	112.89
1	C	218	ASP	N-CA-C	-5.49	98.79	108.23
1	B	222	GLY	N-CA-C	5.41	118.78	112.50
1	C	57	SER	N-CA-C	5.41	118.05	109.50
1	A	57	SER	N-CA-C	5.38	118.01	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	THR	N-CA-C	-5.28	105.12	112.30
1	A	218	ASP	N-CA-C	-5.20	99.28	108.23
1	C	256	HIS	N-CA-C	5.12	117.17	109.23
1	A	256	HIS	N-CA-C	5.09	117.54	109.50
1	A	304	HIS	N-CA-C	-5.07	101.65	109.87
1	D	57	SER	N-CA-C	5.02	117.30	109.52
1	B	57	SER	N-CA-C	5.01	117.41	109.50

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	2329	0	2299	46	0
1	B	2329	0	2299	45	0
1	C	2329	0	2299	50	0
1	D	2329	0	2299	49	0
2	A	32	0	20	1	0
2	B	32	0	20	0	0
2	C	32	0	20	0	0
2	D	32	0	20	1	0
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	4	0	5	0	0
4	B	4	0	5	2	0
4	C	4	0	5	1	0
4	D	4	0	5	1	0
5	A	156	0	0	2	0
5	B	119	0	0	4	0
5	C	151	0	0	3	0
5	D	170	0	0	4	0
All	All	10136	0	9336	178	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 9.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:HH11	1:D:163:ARG:HB3	1.18	1.06
1:D:147:ARG:HB3	1:D:147:ARG:HH11	1.26	0.96
1:C:101:LEU:HG	1:C:106:VAL:HG13	1.63	0.81
1:D:163:ARG:HB3	1:D:163:ARG:NH1	1.98	0.79
1:A:78:ARG:HB3	1:A:306:THR:HG22	1.64	0.79
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.67	0.76
1:D:147:ARG:HB3	1:D:147:ARG:NH1	2.01	0.75
1:D:297:GLN:HG3	5:D:968:HOH:O	1.85	0.74
1:C:107:LYS:HB3	1:C:110:ASP:OD2	1.87	0.74
1:D:260:ASN:HD22	1:D:260:ASN:N	1.87	0.71
1:D:46:ARG:HD3	1:D:46:ARG:C	2.16	0.70
1:C:260:ASN:HD22	1:C:260:ASN:H	1.40	0.70
1:C:260:ASN:HD22	1:C:260:ASN:N	1.89	0.70
1:D:260:ASN:HD22	1:D:260:ASN:H	1.39	0.69
1:B:187:LEU:HA	1:B:190:MET:HE3	1.77	0.66
1:A:294:GLU:H	1:A:294:GLU:CD	2.06	0.64
1:D:193:PRO:HG3	5:D:716:HOH:O	1.96	0.64
1:B:196:HIS:HB3	1:B:212:LEU:HD11	1.80	0.64
1:B:198:LEU:HD12	1:B:198:LEU:C	2.22	0.63
1:C:126:ARG:HG2	1:C:130:ASP:HB3	1.80	0.63
1:A:43:CME:HZ2	1:A:43:CME:HA	1.80	0.63
1:B:43:CME:HZ3	1:B:43:CME:HB2	1.79	0.63
1:D:32:GLN:O	1:D:36:GLN:HG3	1.98	0.63
1:C:97:ASN:ND2	1:C:99:LYS:H	1.96	0.63
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.14	0.62
1:C:159:ASP:O	1:C:163:ARG:HG2	2.00	0.61
1:D:198:LEU:C	1:D:198:LEU:HD12	2.26	0.61
1:D:313:VAL:HA	5:D:908:HOH:O	1.99	0.61
1:A:281:ILE:HD12	1:A:281:ILE:N	2.15	0.61
1:A:51:THR:HB	1:A:313:VAL:HA	1.83	0.60
1:C:163:ARG:HB3	4:C:1516:BME:H21	1.83	0.60
1:C:115:ARG:HG3	1:C:115:ARG:HH11	1.67	0.60
1:A:190:MET:SD	1:A:194:PRO:HD3	2.43	0.59
1:A:312:ALA:O	1:A:313:VAL:HB	2.01	0.59
1:C:262:ILE:O	1:C:266:LYS:HG3	2.04	0.58
1:B:232:LEU:HG	1:B:236:MET:HE3	1.86	0.58
1:D:260:ASN:H	1:D:260:ASN:ND2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:NH1	1:B:151:SER:HB3	2.20	0.57
1:A:89:LEU:O	1:A:93:LYS:HG3	2.04	0.57
1:C:288:ILE:HG23	1:C:289:ASP:OD2	2.05	0.56
1:C:133:PRO:HG3	1:C:146:TYR:CG	2.40	0.56
1:C:190:MET:SD	1:C:194:PRO:HD3	2.46	0.56
1:D:74:LEU:HD22	1:D:224:PRO:HB3	1.87	0.56
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.35	0.56
1:A:233:LEU:O	1:A:237:ILE:HD13	2.05	0.56
1:A:198:LEU:HD12	1:A:198:LEU:C	2.31	0.55
1:B:32:GLN:O	1:B:36:GLN:HG3	2.07	0.55
1:B:290:ASP:HB3	5:B:659:HOH:O	2.06	0.55
1:A:32:GLN:O	1:A:36:GLN:HG3	2.06	0.54
1:C:198:LEU:C	1:C:198:LEU:HD12	2.33	0.54
1:C:260:ASN:H	1:C:260:ASN:ND2	2.04	0.54
1:A:42:ARG:NH1	1:A:43:CME:SG	2.81	0.54
1:A:45:VAL:HG21	1:B:204:VAL:HG21	1.89	0.54
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.89	0.54
1:D:187:LEU:N	1:D:188:PRO:HD2	2.23	0.54
1:B:147:ARG:HB2	1:B:151:SER:OG	2.07	0.54
1:A:313:VAL:HG13	1:A:313:VAL:O	2.08	0.53
1:A:90:TRP:HA	1:A:93:LYS:HD3	1.91	0.53
1:A:127:GLU:HG2	5:A:673:HOH:O	2.07	0.53
1:C:34:LEU:O	1:C:38:GLN:HG3	2.09	0.53
1:D:312:ALA:HB2	5:D:621:HOH:O	2.09	0.53
1:D:196:HIS:CB	1:D:212:LEU:HD11	2.38	0.53
1:D:260:ASN:N	1:D:260:ASN:ND2	2.57	0.53
1:A:187:LEU:N	1:A:188:PRO:HD2	2.24	0.53
1:C:97:ASN:C	1:C:97:ASN:HD22	2.17	0.53
1:C:142:PHE:CE2	1:D:184:PRO:HD2	2.44	0.52
1:C:165:ILE:HD13	1:C:240:ILE:HD11	1.90	0.52
1:C:187:LEU:N	1:C:188:PRO:HD2	2.24	0.52
1:D:294:GLU:CD	1:D:294:GLU:H	2.16	0.52
1:B:280:ARG:HE	1:B:299:GLU:CD	2.18	0.52
1:C:223:VAL:HB	1:C:224:PRO:HD3	1.92	0.51
1:A:280:ARG:HE	1:A:299:GLU:CD	2.18	0.51
1:A:196:HIS:HB3	1:A:212:LEU:HD11	1.93	0.51
1:C:42:ARG:HD3	5:C:704:HOH:O	2.11	0.51
1:D:87:GLU:OE1	1:D:225:PHE:HE2	1.94	0.51
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.45	0.50
1:B:126:ARG:HD3	1:B:130:ASP:O	2.11	0.50
1:D:119:ASP:OD1	1:D:124:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LYS:HE3	1:D:310:GLU:OE2	2.11	0.50
1:A:36:GLN:O	1:A:40:ILE:HG13	2.12	0.50
1:C:38:GLN:O	1:C:42:ARG:HG2	2.12	0.50
1:B:215:ARG:HG3	1:B:216:SER:N	2.27	0.50
1:A:313:VAL:O	1:A:313:VAL:HG22	2.11	0.50
1:B:114:SER:O	1:B:118:LEU:HG	2.12	0.50
1:B:312:ALA:HB2	5:B:669:HOH:O	2.11	0.49
1:C:280:ARG:HE	1:C:299:GLU:CD	2.20	0.49
1:A:153:TYR:HA	1:A:156:GLN:OE1	2.13	0.49
1:C:175:ARG:HG2	1:D:254:ASP:OD2	2.12	0.49
1:D:163:ARG:HH11	1:D:163:ARG:CB	2.06	0.49
1:B:147:ARG:HH11	1:B:151:SER:HB3	1.78	0.48
1:B:43:CME:HZ3	1:B:43:CME:CB	2.44	0.48
1:A:109:TRP:CZ2	2:A:414:D16:H91	2.49	0.47
1:B:183:ASN:HD21	1:B:185:ARG:NH1	2.12	0.47
1:B:183:ASN:OD1	1:B:185:ARG:HG3	2.14	0.47
1:C:312:ALA:HA	5:C:646:HOH:O	2.13	0.47
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.96	0.47
1:C:202:TYR:CE1	1:D:47:LYS:HE2	2.50	0.47
1:C:219:MET:SD	1:C:223:VAL:HG21	2.55	0.47
1:D:87:GLU:O	1:D:90:TRP:HB3	2.14	0.47
1:C:287:LYS:HB2	1:C:290:ASP:OD1	2.15	0.47
1:A:184:PRO:HD2	1:B:142:PHE:CE2	2.50	0.47
1:B:85:LEU:O	1:B:89:LEU:HG	2.15	0.46
1:D:106:VAL:HG12	1:D:108:ILE:HG12	1.97	0.46
1:A:186:ASP:C	1:A:188:PRO:HD2	2.41	0.46
1:A:47:LYS:HE3	1:B:202:TYR:CE1	2.49	0.46
1:D:274:ARG:O	1:D:275:PRO:C	2.58	0.46
1:A:133:PRO:O	1:A:190:MET:HE2	2.16	0.46
1:C:176:ARG:HD3	1:D:193:PRO:HG2	1.98	0.46
1:A:312:ALA:O	1:A:313:VAL:CB	2.64	0.46
1:B:151:SER:HB2	1:B:153:TYR:CZ	2.51	0.46
1:A:262:ILE:O	1:A:266:LYS:HG3	2.16	0.45
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.81	0.45
1:D:126:ARG:HD3	1:D:130:ASP:O	2.15	0.45
1:D:149:MET:HG3	1:D:150:GLU:HG3	1.98	0.45
1:A:287:LYS:O	1:A:290:ASP:HB2	2.17	0.45
1:C:151:SER:HB2	1:C:153:TYR:CZ	2.51	0.45
1:B:88:LEU:HD23	1:B:232:LEU:HG	1.98	0.45
1:B:287:LYS:HE2	5:B:711:HOH:O	2.17	0.45
1:C:142:PHE:CZ	1:D:184:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:O	1:A:43:CME:N	2.49	0.45
1:C:107:LYS:N	1:C:107:LYS:HD2	2.32	0.45
1:C:186:ASP:C	1:C:188:PRO:HD2	2.42	0.45
1:D:117:PHE:CE1	1:D:121:LEU:HD11	2.52	0.45
1:D:46:ARG:HD3	1:D:47:LYS:N	2.33	0.44
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.98	0.44
1:B:187:LEU:N	1:B:188:PRO:CD	2.80	0.44
1:B:87:GLU:O	1:B:90:TRP:HB3	2.18	0.44
1:A:237:ILE:HD12	1:A:237:ILE:N	2.33	0.44
1:B:88:LEU:HD23	1:B:236:MET:HE3	1.99	0.44
1:B:287:LYS:HB2	1:B:290:ASP:OD1	2.18	0.43
1:C:97:ASN:HD22	1:C:98:ALA:N	2.17	0.43
1:C:184:PRO:HD2	1:D:142:PHE:CE2	2.52	0.43
1:B:177:ILE:CG2	1:B:201:PHE:HB2	2.48	0.43
1:D:86:GLU:HB2	1:D:106:VAL:HG21	2.00	0.43
1:A:260:ASN:ND2	1:A:310:GLU:HB3	2.34	0.43
1:B:198:LEU:C	1:B:198:LEU:CD1	2.91	0.43
1:D:145:GLU:OE1	1:D:185:ARG:NH2	2.51	0.43
1:A:26:PRO:N	1:A:27:PRO:HD3	2.34	0.43
1:C:164:VAL:O	1:C:168:ILE:HG13	2.19	0.43
1:A:87:GLU:O	1:A:90:TRP:HB3	2.19	0.43
1:C:50:ARG:HH11	1:C:50:ARG:HG2	1.84	0.43
1:C:313:VAL:OXT	1:C:313:VAL:HG22	2.19	0.43
1:D:26:PRO:HA	1:D:27:PRO:HD3	1.96	0.42
1:B:274:ARG:O	1:B:275:PRO:C	2.62	0.42
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.84	0.42
1:C:283:ARG:HD2	5:C:713:HOH:O	2.18	0.42
1:B:167:THR:HG21	4:B:1515:BME:H11	2.00	0.42
1:A:45:VAL:HG23	1:B:204:VAL:HG21	2.02	0.42
1:C:274:ARG:O	1:C:275:PRO:C	2.61	0.42
1:B:164:VAL:O	1:B:168:ILE:HG13	2.20	0.42
1:D:177:ILE:HA	4:D:1517:BME:H12	2.02	0.42
1:A:274:ARG:O	1:A:275:PRO:C	2.63	0.41
1:B:287:LYS:HB3	5:B:711:HOH:O	2.20	0.41
1:D:109:TRP:CZ2	2:D:417:D16:H91	2.55	0.41
1:C:138:GLN:HG3	1:C:181:ALA:O	2.20	0.41
1:B:164:VAL:HG13	1:B:177:ILE:CG2	2.51	0.41
1:B:183:ASN:HD21	1:B:185:ARG:HH12	1.68	0.41
1:C:294:GLU:H	1:C:294:GLU:CD	2.28	0.41
1:D:287:LYS:HB2	1:D:290:ASP:OD1	2.20	0.41
1:D:145:GLU:OE1	1:D:145:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:ND2	5:A:688:HOH:O	2.52	0.41
1:B:163:ARG:HG3	4:B:1515:BME:H22	2.02	0.41
1:C:126:ARG:CG	1:C:130:ASP:HB3	2.48	0.41
1:D:196:HIS:HB2	1:D:212:LEU:HD11	2.02	0.41
1:C:244:LYS:HE2	1:C:244:LYS:HB2	1.94	0.41
1:C:97:ASN:CG	1:C:149:MET:SD	3.04	0.41
1:A:219:MET:SD	1:A:223:VAL:HG21	2.61	0.41
1:B:168:ILE:HG23	1:B:203:VAL:HG21	2.02	0.41
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.85	0.41
1:C:97:ASN:ND2	1:C:97:ASN:C	2.78	0.41
1:D:137:PHE:CZ	1:D:144:ALA:HB3	2.56	0.41
1:A:114:SER:O	1:A:118:LEU:HG	2.20	0.41
1:B:187:LEU:HD23	1:B:190:MET:CE	2.51	0.41
1:D:36:GLN:O	1:D:40:ILE:HG13	2.21	0.41
1:D:198:LEU:C	1:D:198:LEU:CD1	2.91	0.41
1:A:281:ILE:N	1:A:281:ILE:CD1	2.82	0.40
1:A:126:ARG:CG	1:A:130:ASP:HB3	2.52	0.40
1:C:97:ASN:HB3	1:C:100:GLU:HG3	2.03	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	285/288 (99%)	271 (95%)	14 (5%)	0	100	100
1	B	285/288 (99%)	272 (95%)	11 (4%)	2 (1%)	18	10
1	C	285/288 (99%)	272 (95%)	13 (5%)	0	100	100
1	D	285/288 (99%)	266 (93%)	17 (6%)	2 (1%)	18	10
All	All	1140/1152 (99%)	1081 (95%)	55 (5%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	TYR
1	D	135	TYR
1	B	80	PHE
1	D	134	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	250/250 (100%)	245 (98%)	5 (2%)	48	46
1	B	250/250 (100%)	244 (98%)	6 (2%)	43	38
1	C	250/250 (100%)	243 (97%)	7 (3%)	38	32
1	D	250/250 (100%)	243 (97%)	7 (3%)	38	32
All	All	1000/1000 (100%)	975 (98%)	25 (2%)	42	37

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	127	GLU
1	A	281	ILE
1	A	294	GLU
1	A	311	MET
1	B	46	ARG
1	B	56	LEU
1	B	185	ARG
1	B	260	ASN
1	B	272	GLU
1	B	310	GLU
1	C	49	ASP
1	C	106	VAL
1	C	107	LYS
1	C	115	ARG
1	C	260	ASN
1	C	306	THR
1	C	310	GLU

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Mol	Chain	Res	Type
1	D	56	LEU
1	D	147	ARG
1	D	163	ARG
1	D	196	HIS
1	D	198	LEU
1	D	260	ASN
1	D	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	196	HIS
1	A	200	GLN
1	A	270	GLN
1	B	156	GLN
1	B	196	HIS
1	B	200	GLN
1	B	211	GLN
1	B	260	ASN
1	B	302	ASN
1	C	32	GLN
1	C	39	HIS
1	C	97	ASN
1	C	171	ASN
1	C	196	HIS
1	C	200	GLN
1	C	260	ASN
1	C	270	GLN
1	C	302	ASN
1	D	36	GLN
1	D	38	GLN
1	D	112	ASN
1	D	156	GLN
1	D	171	ASN
1	D	200	GLN
1	D	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	D	43	1	8,9,10	0.49	0	6,9,11	0.53	0
1	CME	C	43	1	8,9,10	0.51	0	6,9,11	0.45	0
1	CME	A	43	1	8,9,10	0.55	0	6,9,11	0.60	0
1	CME	B	43	1	8,9,10	0.49	0	6,9,11	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	D	43	1	-	0/5/8/10	-
1	CME	C	43	1	-	2/5/8/10	-
1	CME	A	43	1	-	2/5/8/10	-
1	CME	B	43	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	43	CME	CZ-CE-SD-SG
1	C	43	CME	CE-SD-SG-CB
1	A	43	CME	CE-SD-SG-CB
1	C	43	CME	SD-CE-CZ-OH
1	A	43	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	43	CME	3	0
1	B	43	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
4	BME	D	1517	-	3,3,3	2.03	1 (33%)	2,2,2	1.95	1 (50%)
3	UMP	B	315	1	21,21,21	2.03	5 (23%)	30,31,31	1.78	7 (23%)
3	UMP	C	316	1	21,21,21	2.01	5 (23%)	30,31,31	1.83	6 (20%)
3	UMP	D	317	1	21,21,21	2.06	6 (28%)	30,31,31	1.79	7 (23%)
2	D16	C	416	-	33,34,34	2.13	12 (36%)	46,48,48	1.79	11 (23%)
2	D16	A	414	-	33,34,34	2.21	10 (30%)	46,48,48	1.67	9 (19%)
2	D16	B	415	-	33,34,34	2.27	11 (33%)	46,48,48	1.76	10 (21%)
4	BME	C	1516	-	3,3,3	2.06	1 (33%)	2,2,2	1.88	1 (50%)
4	BME	A	1514	-	3,3,3	2.04	1 (33%)	2,2,2	1.97	1 (50%)
2	D16	D	417	-	33,34,34	2.21	11 (33%)	46,48,48	1.81	11 (23%)
3	UMP	A	314	1	21,21,21	2.03	5 (23%)	30,31,31	1.83	6 (20%)
4	BME	B	1515	-	3,3,3	2.01	1 (33%)	2,2,2	1.95	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	D	1517	-	-	0/1/1/1	-
3	UMP	B	315	1	-	0/10/22/22	0/2/2/2
3	UMP	C	316	1	-	0/10/22/22	0/2/2/2
3	UMP	D	317	1	-	0/10/22/22	0/2/2/2
2	D16	C	416	-	-	7/25/25/25	0/3/3/3
2	D16	A	414	-	-	6/25/25/25	0/3/3/3
2	D16	B	415	-	-	7/25/25/25	0/3/3/3
4	BME	C	1516	-	-	1/1/1/1	-
4	BME	A	1514	-	-	1/1/1/1	-
2	D16	D	417	-	-	5/25/25/25	0/3/3/3
3	UMP	A	314	1	-	0/10/22/22	0/2/2/2
4	BME	B	1515	-	-	1/1/1/1	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	D16	O4-C4	8.66	1.38	1.23
2	D	417	D16	O4-C4	8.25	1.37	1.23
2	A	414	D16	O4-C4	8.23	1.37	1.23
2	C	416	D16	O4-C4	7.71	1.36	1.23
3	A	314	UMP	C6-N1	5.81	1.51	1.38
3	B	315	UMP	C6-N1	5.60	1.51	1.38
3	D	317	UMP	C6-N1	5.48	1.51	1.38
3	C	316	UMP	C6-N1	5.46	1.51	1.38
3	C	316	UMP	C3'-C4'	-4.60	1.40	1.53
3	D	317	UMP	C3'-C4'	-4.55	1.41	1.53
3	B	315	UMP	C3'-C4'	-4.37	1.41	1.53
3	A	314	UMP	C3'-C4'	-4.31	1.41	1.53
3	D	317	UMP	C6-C5	4.09	1.44	1.35
3	B	315	UMP	C6-C5	3.99	1.44	1.35
3	A	314	UMP	C6-C5	3.77	1.43	1.35
2	C	416	D16	C5-C6	3.74	1.45	1.39
3	C	316	UMP	C6-C5	3.72	1.43	1.35
2	A	414	D16	C4A-C4	-3.70	1.41	1.48
2	D	417	D16	C4A-C4	-3.64	1.41	1.48
2	B	415	D16	C4A-C4	-3.60	1.42	1.48
4	C	1516	BME	O1-C1	-3.55	1.24	1.42
2	D	417	D16	C16-C15	3.53	1.51	1.39
4	A	1514	BME	O1-C1	-3.50	1.24	1.42
2	A	414	D16	C16-C15	3.50	1.51	1.39
4	D	1517	BME	O1-C1	-3.48	1.24	1.42
4	B	1515	BME	O1-C1	-3.44	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	416	D16	C4A-C4	-3.43	1.42	1.48
2	C	416	D16	C16-C15	3.39	1.50	1.39
2	B	415	D16	C16-C15	3.37	1.50	1.39
2	A	414	D16	C5-C6	3.26	1.44	1.39
2	D	417	D16	C5-C6	3.15	1.44	1.39
2	B	415	D16	C5-C6	2.95	1.44	1.39
2	D	417	D16	C8-C7	2.78	1.43	1.38
2	B	415	D16	C4A-C8A	2.65	1.45	1.41
2	B	415	D16	C2-N3	2.57	1.36	1.31
2	D	417	D16	C8-C8A	2.56	1.43	1.39
2	A	414	D16	C8-C7	2.55	1.42	1.38
3	D	317	UMP	O4'-C1'	-2.50	1.36	1.42
2	A	414	D16	C8-C8A	2.48	1.43	1.39
2	B	415	D16	C7-C6	2.40	1.43	1.38
3	A	314	UMP	P-OP3	-2.39	1.45	1.54
3	D	317	UMP	P-OP3	-2.39	1.45	1.54
2	B	415	D16	C8-C7	2.39	1.42	1.38
2	A	414	D16	C2-N3	2.35	1.36	1.31
2	A	414	D16	O2-CT	-2.34	1.23	1.30
3	B	315	UMP	O4'-C1'	-2.33	1.37	1.42
3	C	316	UMP	P-OP3	-2.32	1.46	1.54
2	C	416	D16	C8-C7	2.32	1.42	1.38
2	C	416	D16	C8-C8A	2.32	1.43	1.39
2	B	415	D16	C8-C8A	2.27	1.43	1.39
3	A	314	UMP	P-OP2	-2.27	1.46	1.54
3	C	316	UMP	P-OP2	-2.27	1.46	1.54
2	B	415	D16	O2-CT	-2.26	1.23	1.30
2	D	417	D16	C7-C6	2.26	1.43	1.38
3	B	315	UMP	P-OP3	-2.25	1.46	1.54
2	C	416	D16	C4A-C8A	2.22	1.44	1.41
2	D	417	D16	O2-CT	-2.21	1.23	1.30
2	C	416	D16	OE2-CD	-2.20	1.23	1.30
2	B	415	D16	OE2-CD	-2.20	1.23	1.30
2	A	414	D16	C4A-C8A	2.19	1.44	1.41
3	D	317	UMP	P-OP2	-2.16	1.46	1.54
2	C	416	D16	C2-N3	2.16	1.36	1.31
2	C	416	D16	O2-CT	-2.15	1.23	1.30
2	D	417	D16	C4A-C8A	2.10	1.44	1.41
2	D	417	D16	C2-N3	2.09	1.36	1.31
2	D	417	D16	OE2-CD	-2.05	1.24	1.30
2	C	416	D16	C7-C6	2.05	1.43	1.38
2	C	416	D16	C5-C4A	2.01	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	414	D16	OE2-CD	-2.00	1.24	1.30

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	314	UMP	C5-C6-N1	-6.14	111.86	121.84
3	C	316	UMP	C5-C6-N1	-6.12	111.89	121.84
3	B	315	UMP	C5-C6-N1	-5.84	112.35	121.84
3	D	317	UMP	C5-C6-N1	-5.71	112.56	121.84
2	D	417	D16	CG-CB-CA	5.63	123.55	113.16
2	C	416	D16	CG-CB-CA	5.12	122.60	113.16
2	A	414	D16	CG-CB-CA	4.94	122.27	113.16
2	B	415	D16	CG-CB-CA	4.84	122.08	113.16
3	A	314	UMP	O4'-C1'-N1	4.60	116.02	107.86
3	C	316	UMP	O4'-C1'-N1	4.51	115.86	107.86
2	D	417	D16	S13-C14-N10	4.11	124.84	120.99
2	B	415	D16	S13-C14-N10	3.95	124.69	120.99
3	B	315	UMP	O4'-C1'-N1	3.92	114.82	107.86
3	D	317	UMP	O4'-C1'-N1	3.87	114.72	107.86
2	D	417	D16	C11-S13-C14	3.87	95.30	91.43
2	C	416	D16	C8A-C4A-C4	-3.76	116.05	120.11
2	C	416	D16	S13-C14-N10	3.69	124.45	120.99
2	B	415	D16	C11-S13-C14	3.64	95.08	91.43
2	B	415	D16	C8A-C4A-C4	-3.35	116.50	120.11
2	D	417	D16	C8A-C4A-C4	-3.32	116.53	120.11
2	A	414	D16	S13-C14-N10	3.30	124.09	120.99
2	A	414	D16	C11-S13-C14	3.28	94.72	91.43
2	A	414	D16	C8A-C4A-C4	-3.25	116.60	120.11
2	C	416	D16	C11-S13-C14	3.12	94.55	91.43
2	C	416	D16	C-C11-S13	2.88	124.73	117.18
4	A	1514	BME	O1-C1-C2	2.74	121.51	110.82
2	B	415	D16	C6-C9-N10	2.70	118.11	113.02
4	B	1515	BME	O1-C1-C2	2.70	121.37	110.82
2	B	415	D16	C-C11-S13	2.70	124.24	117.18
4	D	1517	BME	O1-C1-C2	2.70	121.35	110.82
3	A	314	UMP	C5-C4-N3	2.69	118.56	114.80
2	D	417	D16	C-C11-S13	2.67	124.16	117.18
4	C	1516	BME	O1-C1-C2	2.62	121.03	110.82
3	C	316	UMP	C5-C4-N3	2.61	118.45	114.80
2	D	417	D16	CM2-C2-N1	2.61	121.44	116.41
3	C	316	UMP	O4-C4-C5	-2.58	120.72	125.16
3	B	315	UMP	C5-C4-N3	2.57	118.40	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	416	D16	CM2-C2-N1	2.54	121.31	116.41
3	D	317	UMP	C5-C4-N3	2.53	118.34	114.80
3	D	317	UMP	O4'-C1'-C2'	-2.52	101.53	106.25
3	B	315	UMP	O4-C4-C5	-2.51	120.84	125.16
3	A	314	UMP	O4-C4-C5	-2.50	120.85	125.16
3	D	317	UMP	C1'-N1-C6	-2.50	116.61	121.53
2	A	414	D16	C-C11-S13	2.49	123.70	117.18
2	C	416	D16	C6-C9-N10	2.48	117.70	113.02
2	B	415	D16	CM2-C2-N1	2.48	121.19	116.41
2	C	416	D16	CA-N-C	2.45	126.11	122.00
2	D	417	D16	CB-CA-N	2.43	115.72	110.91
3	D	317	UMP	O4-C4-C5	-2.41	121.01	125.16
3	B	315	UMP	O4'-C1'-C2'	-2.37	101.82	106.25
2	A	414	D16	CM2-C2-N1	2.36	120.97	116.41
3	B	315	UMP	C1'-N1-C6	-2.36	116.89	121.53
3	A	314	UMP	C1'-N1-C6	-2.28	117.04	121.53
2	B	415	D16	C15-C14-N10	-2.24	125.53	127.84
3	C	316	UMP	C1'-N1-C6	-2.23	117.14	121.53
2	A	414	D16	C6-C9-N10	2.23	117.22	113.02
2	C	416	D16	N1-C2-N3	-2.21	120.10	122.96
2	B	415	D16	N1-C2-N3	-2.21	120.10	122.96
2	B	415	D16	CB-CA-N	2.18	115.22	110.91
2	C	416	D16	C15-C14-N10	-2.18	125.59	127.84
2	D	417	D16	N1-C2-N3	-2.17	120.15	122.96
2	D	417	D16	C15-C14-S13	-2.17	109.52	111.97
3	D	317	UMP	C4'-O4'-C1'	2.16	114.63	109.51
2	A	414	D16	N1-C2-N3	-2.14	120.19	122.96
2	D	417	D16	C15-C14-N10	-2.14	125.63	127.84
3	C	316	UMP	O4'-C1'-C2'	-2.08	102.36	106.25
2	A	414	D16	CB-CA-N	2.07	115.01	110.91
2	D	417	D16	C6-C9-N10	2.04	116.86	113.02
3	A	314	UMP	C6-N1-C2	2.02	123.46	121.00
2	C	416	D16	C9-C6-C7	-2.02	117.03	120.75
3	B	315	UMP	C4'-O4'-C1'	2.01	114.29	109.51

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	416	D16	N-CA-CB-CG
4	A	1514	BME	O1-C1-C2-S2
2	A	414	D16	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	B	415	D16	N-CA-CB-CG
2	B	415	D16	CT-CA-CB-CG
2	C	416	D16	CT-CA-CB-CG
2	D	417	D16	N-CA-CB-CG
2	A	414	D16	CT-CA-CB-CG
4	C	1516	BME	O1-C1-C2-S2
2	C	416	D16	CA-CB-CG-CD
2	D	417	D16	CT-CA-CB-CG
4	B	1515	BME	O1-C1-C2-S2
2	B	415	D16	OE2-CD-CG-CB
2	B	415	D16	OE1-CD-CG-CB
2	C	416	D16	OE1-CD-CG-CB
2	A	414	D16	OE1-CD-CG-CB
2	A	414	D16	OE2-CD-CG-CB
2	C	416	D16	OE2-CD-CG-CB
2	B	415	D16	C5-C6-C9-N10
2	D	417	D16	C5-C6-C9-N10
2	A	414	D16	C5-C6-C9-N10
2	C	416	D16	C5-C6-C9-N10
2	B	415	D16	C7-C6-C9-N10
2	D	417	D16	C7-C6-C9-N10
2	A	414	D16	C7-C6-C9-N10
2	B	415	D16	C6-C9-N10-CP1
2	D	417	D16	C6-C9-N10-CP1
2	C	416	D16	C7-C6-C9-N10

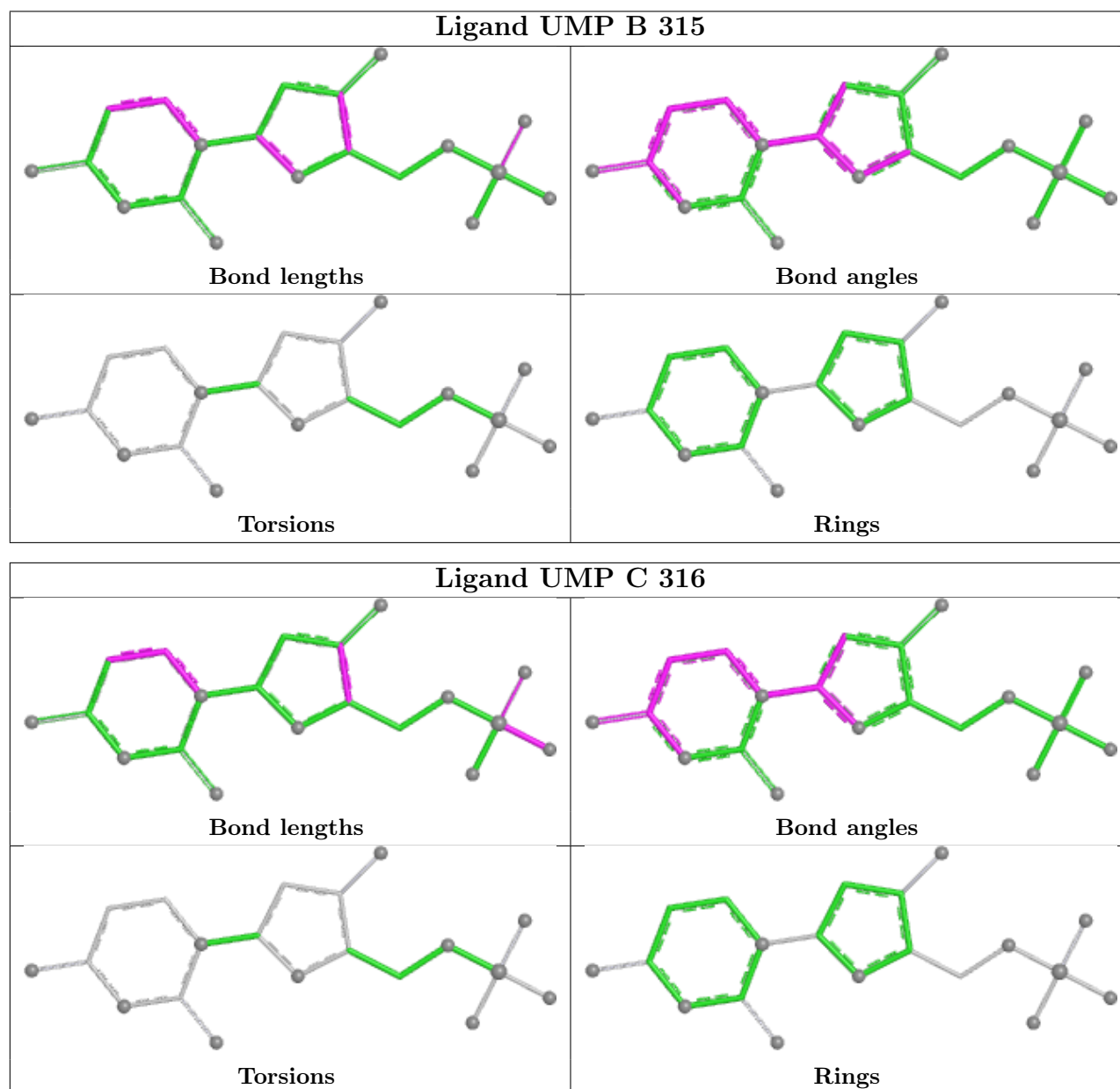
There are no ring outliers.

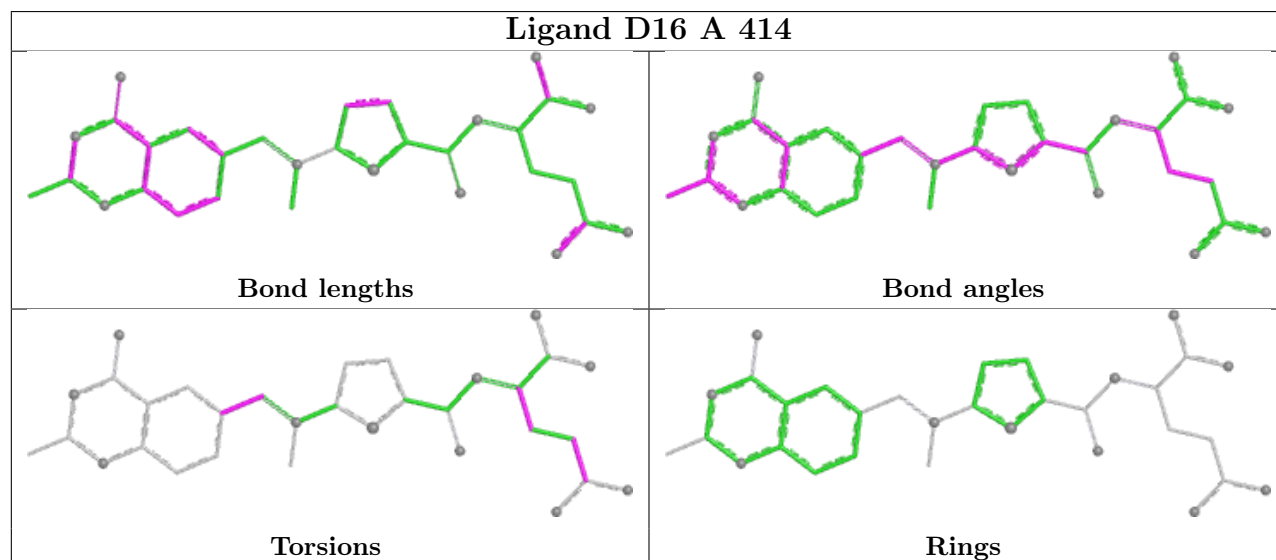
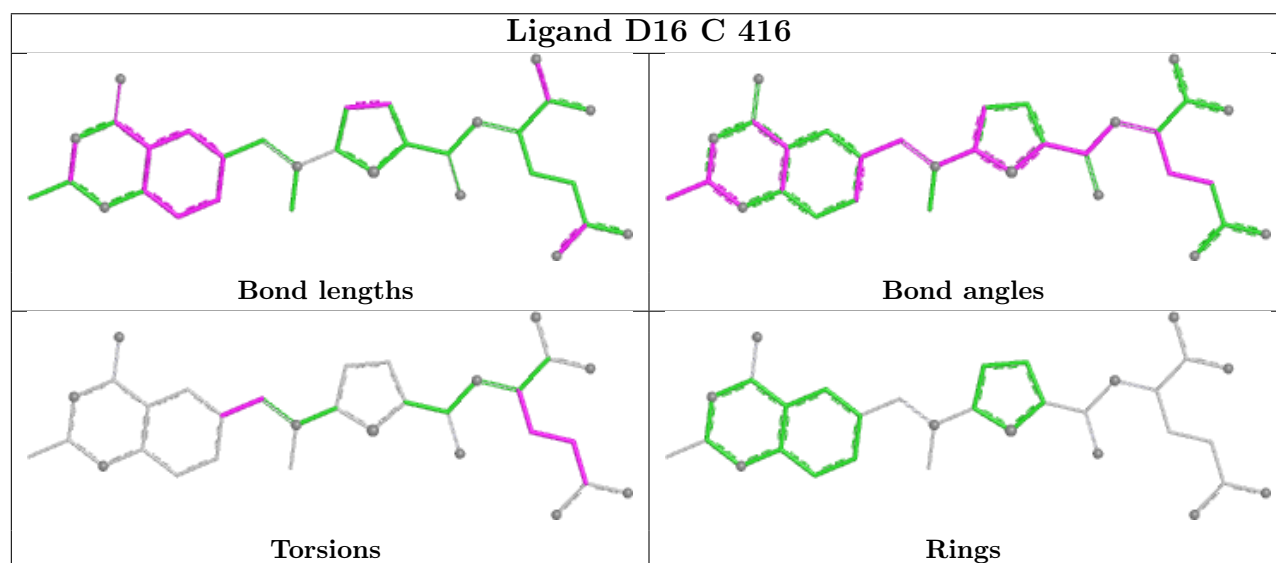
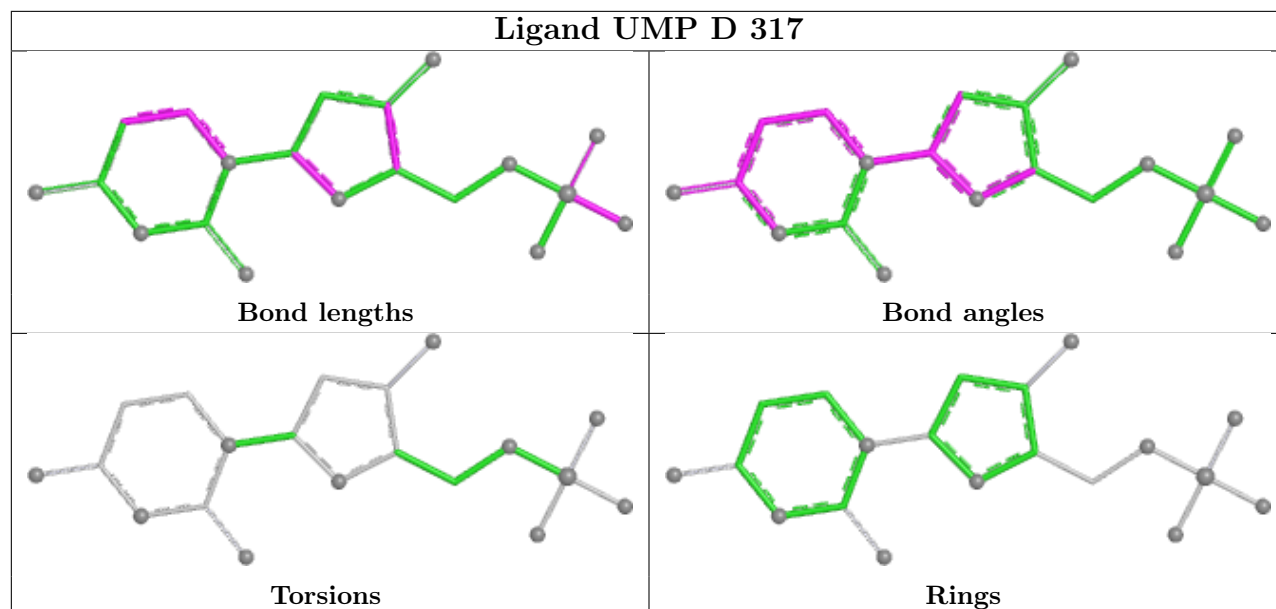
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1517	BME	1	0
2	A	414	D16	1	0
4	C	1516	BME	1	0
2	D	417	D16	1	0
4	B	1515	BME	2	0

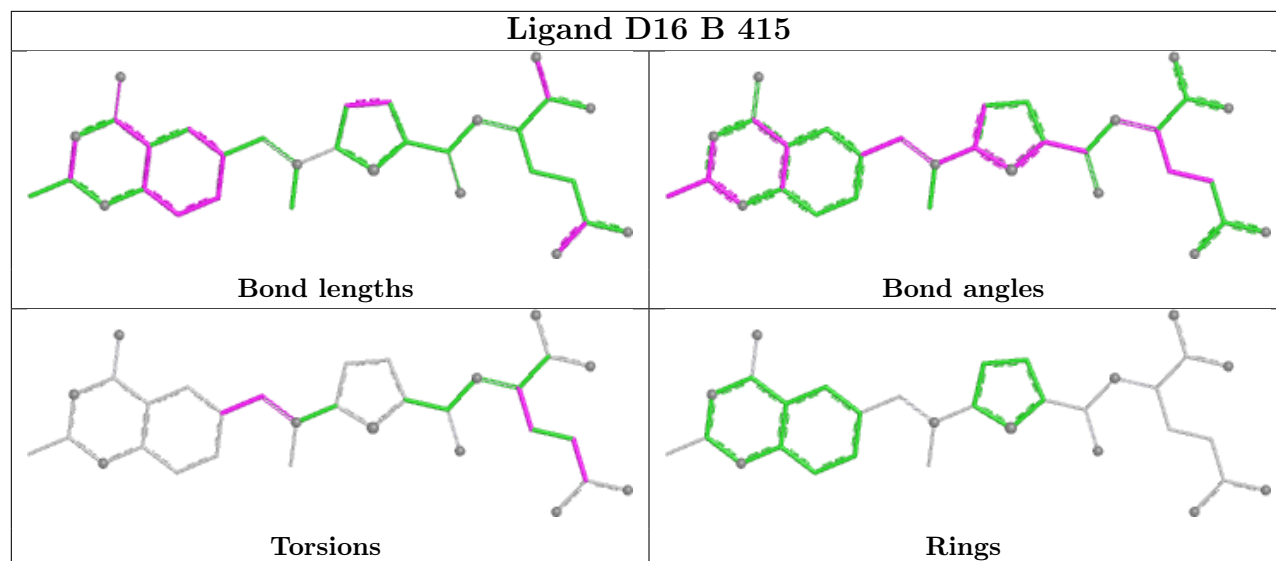
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

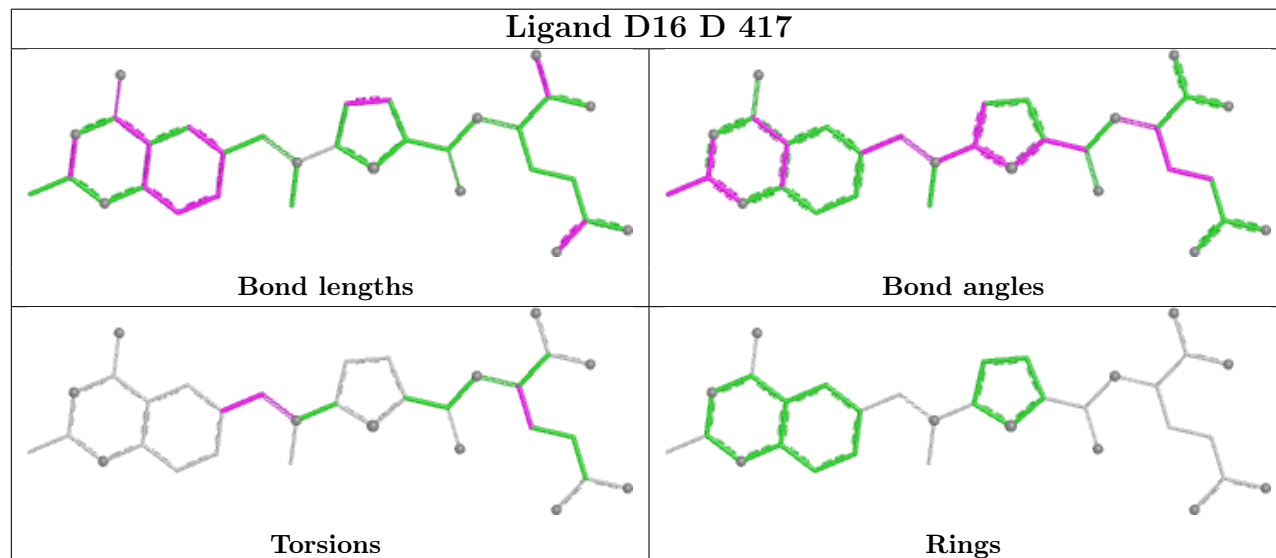




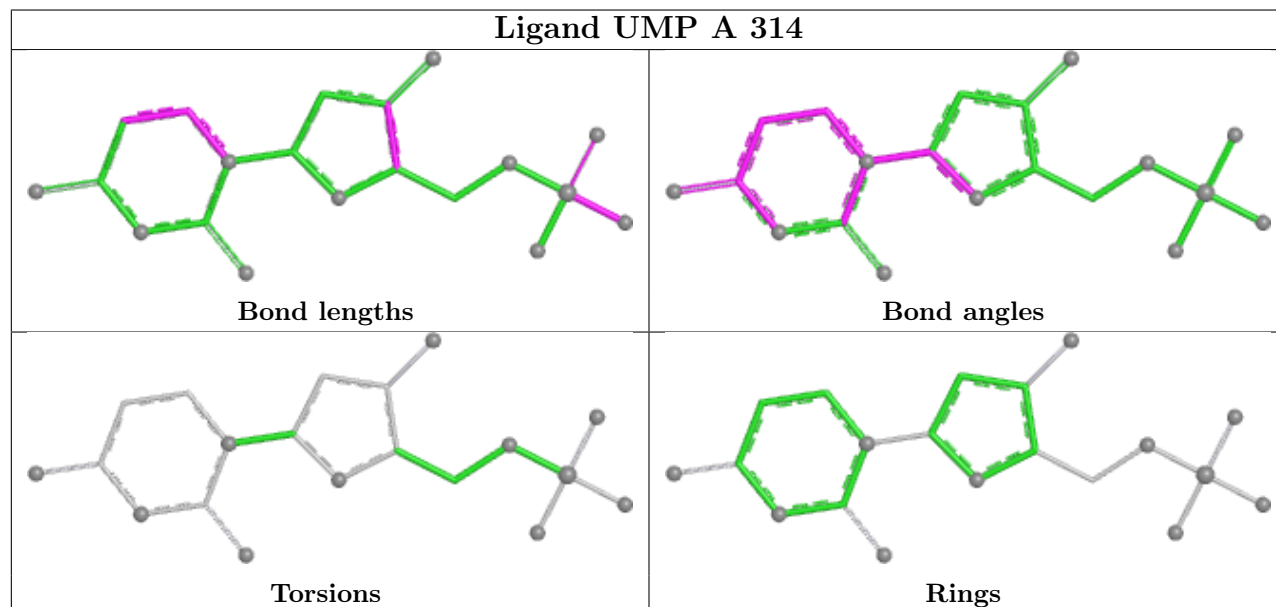
Ligand D16 B 415



Ligand D16 D 417



Ligand UMP A 314



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	287/288 (99%)	0.08	6 (2%) 63 67	9, 19, 35, 41	0
1	B	287/288 (99%)	0.23	8 (2%) 55 59	10, 22, 38, 50	0
1	C	287/288 (99%)	0.05	6 (2%) 63 67	8, 19, 36, 49	0
1	D	287/288 (99%)	0.06	4 (1%) 73 76	9, 20, 35, 50	0
All	All	1148/1152 (99%)	0.10	24 (2%) 63 67	8, 20, 36, 50	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	VAL	7.1
1	A	313	VAL	7.0
1	C	26	PRO	6.0
1	C	313	VAL	4.6
1	A	26	PRO	3.9
1	D	313	VAL	3.6
1	B	191	ALA	3.1
1	C	27	PRO	3.0
1	D	125	THR	2.9
1	C	125	THR	2.9
1	B	185	ARG	2.8
1	B	290	ASP	2.8
1	D	26	PRO	2.7
1	A	191	ALA	2.6
1	A	312	ALA	2.6
1	C	116	ASP	2.5
1	B	312	ALA	2.3
1	D	148	ASP	2.3
1	C	46	ARG	2.3
1	A	125	THR	2.2
1	B	125	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	147	ARG	2.1
1	A	27	PRO	2.0
1	B	121	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	C	43	10/11	0.91	0.11	28,32,44,45	0
1	CME	A	43	10/11	0.92	0.12	28,29,42,44	0
1	CME	B	43	10/11	0.96	0.07	21,24,36,38	0
1	CME	D	43	10/11	0.97	0.06	19,21,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BME	B	1515	4/4	0.75	0.18	40,41,42,42	0
4	BME	D	1517	4/4	0.77	0.18	47,48,49,50	0
4	BME	C	1516	4/4	0.79	0.20	50,52,52,53	0
4	BME	A	1514	4/4	0.80	0.14	34,36,36,37	0
2	D16	B	415	32/32	0.88	0.11	16,26,43,44	0
2	D16	A	414	32/32	0.91	0.10	14,22,39,41	0
2	D16	D	417	32/32	0.91	0.09	15,19,35,36	0
2	D16	C	416	32/32	0.92	0.10	12,26,47,49	0
3	UMP	B	315	20/20	0.95	0.07	11,16,19,21	0
3	UMP	C	316	20/20	0.95	0.07	8,13,16,21	0
3	UMP	A	314	20/20	0.95	0.07	13,15,18,21	0

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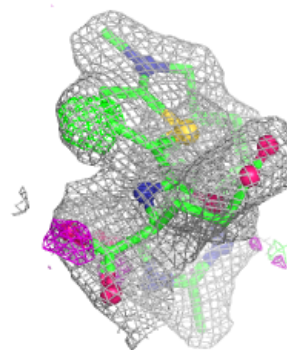
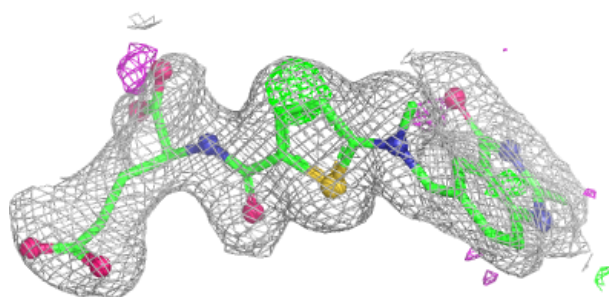
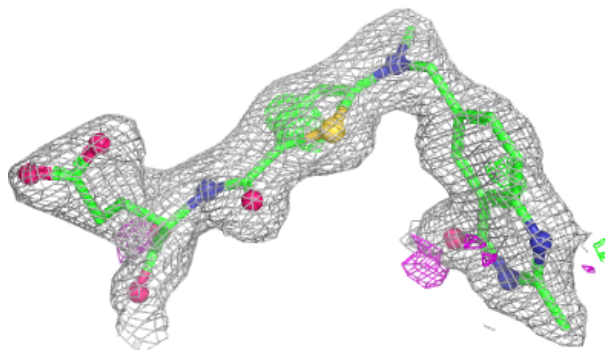
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UMP	D	317	20/20	0.98	0.05	8,14,16,21	0

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.

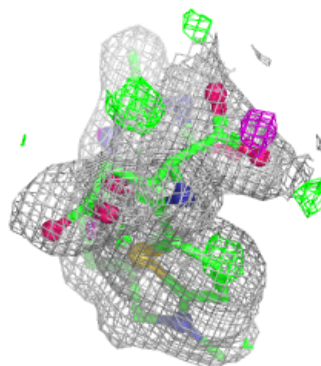
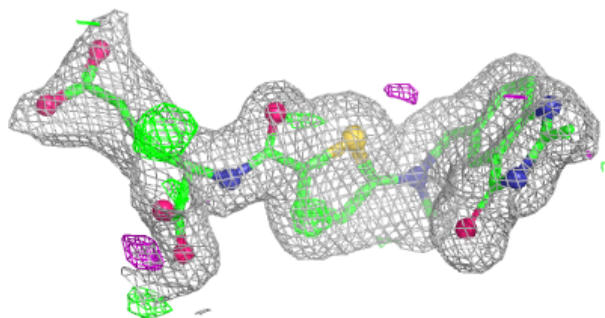
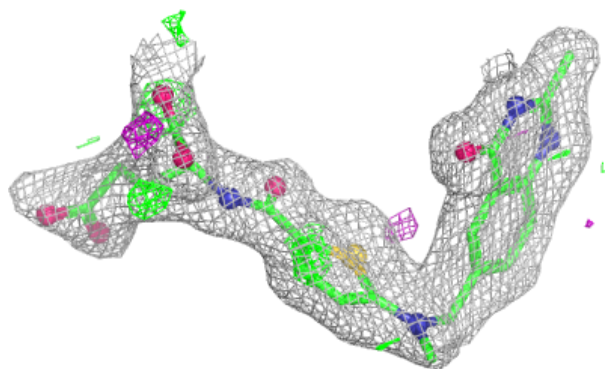
Electron density around D16 B 415:

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

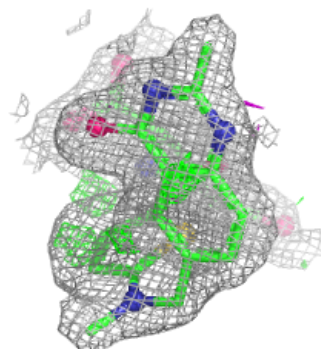
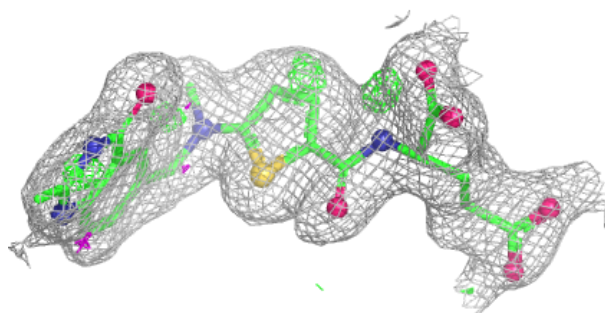
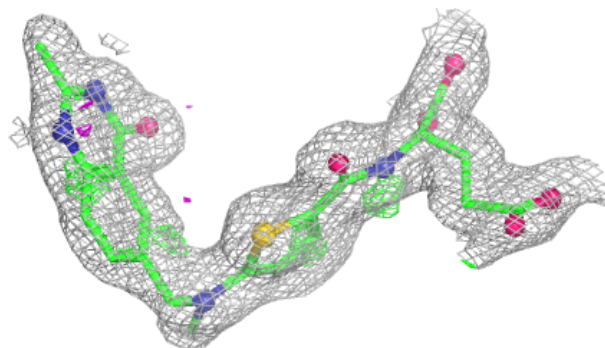


Electron density around D16 A 414:

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

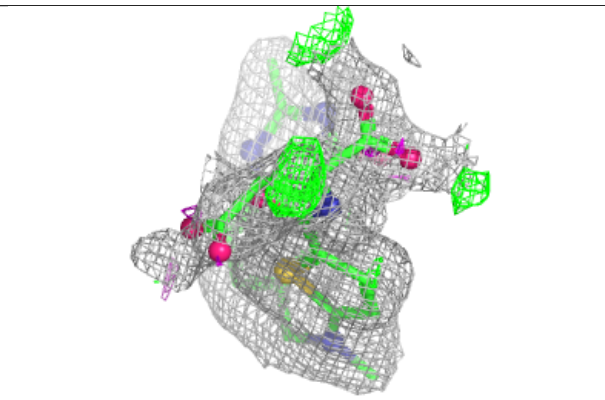
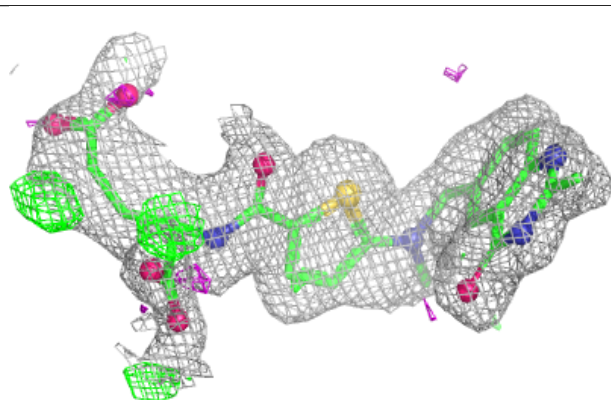
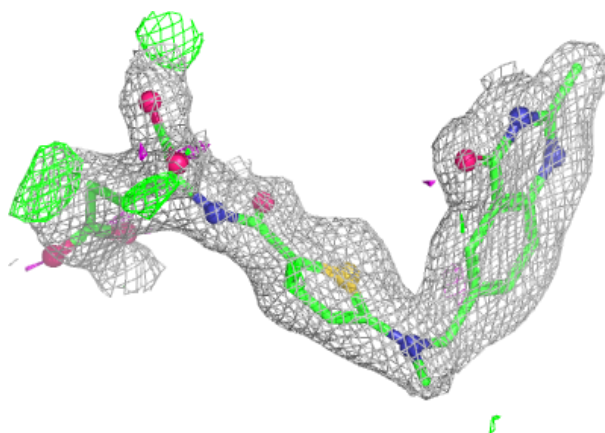
**Electron density around D16 D 417:**

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

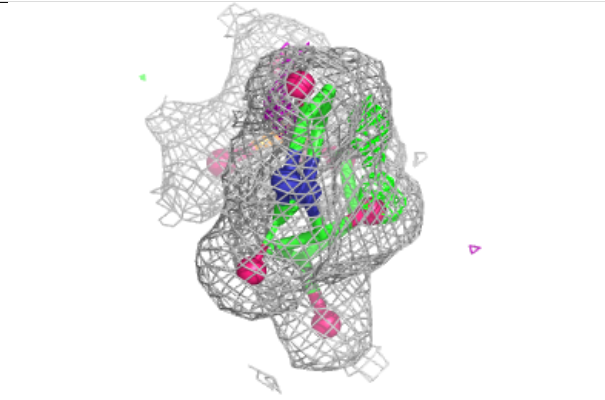
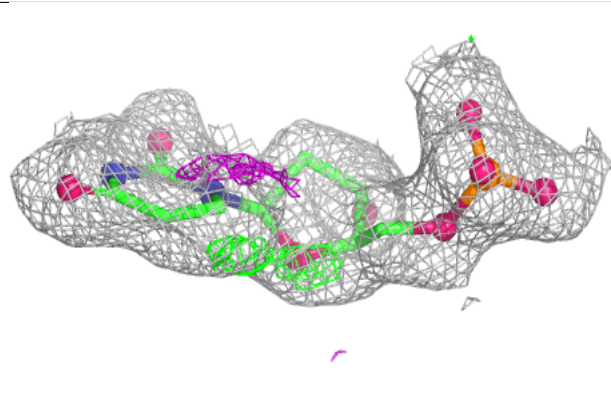
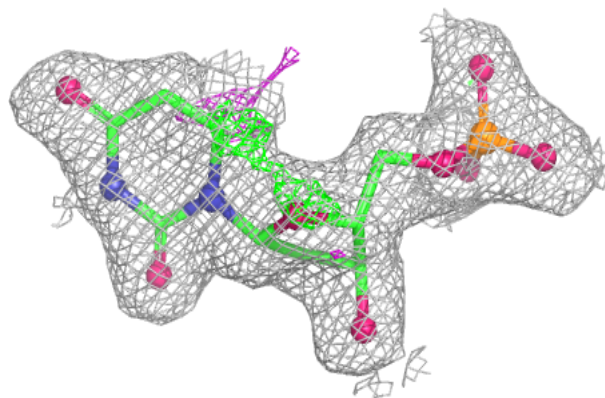


Electron density around D16 C 416:

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

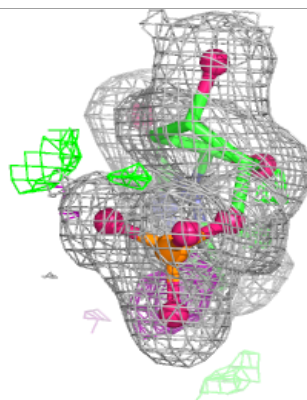
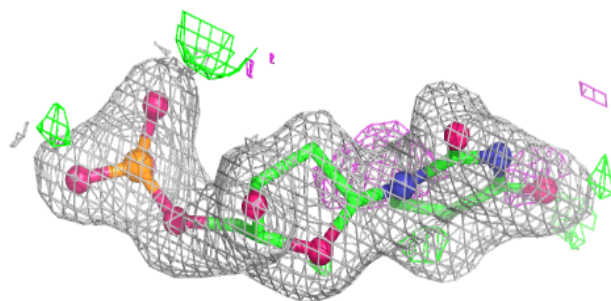
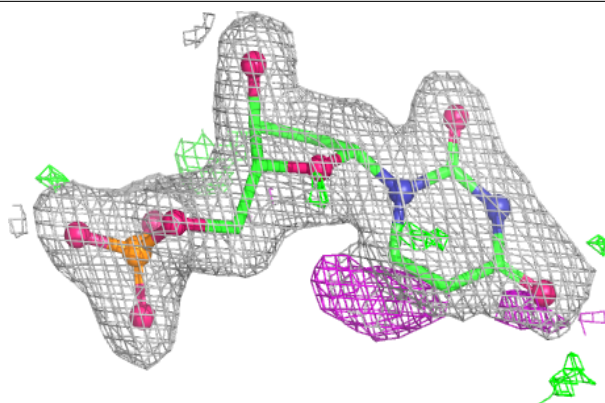
**Electron density around UMP B 315:**

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

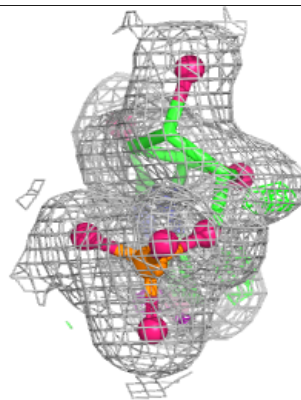
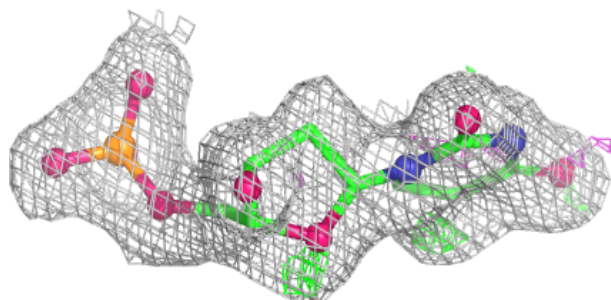
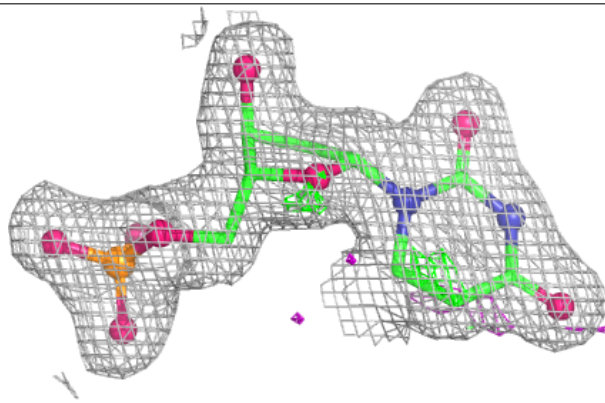


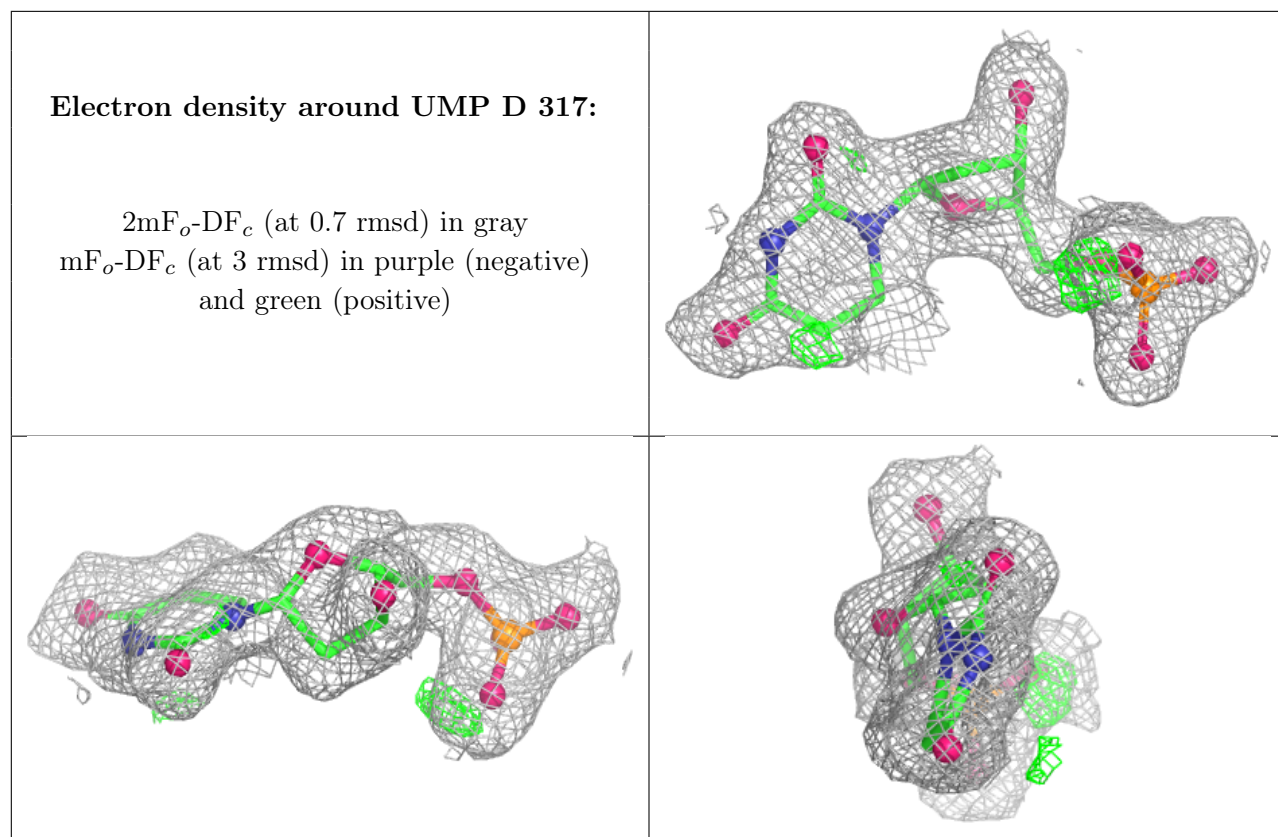
Electron density around UMP C 316:

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

**Electron density around UMP A 314:**

$2mF_o-DF_c$ (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.