Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:28 pm BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

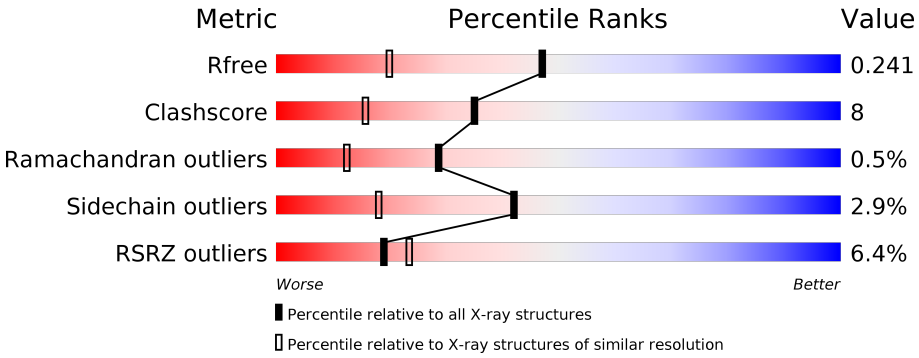
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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

Mol	Chain	Length	Quality of chain
1	A	307	2% 83% 13%
1	B	307	88% 9%
1	C	307	12% 79% 15%
1	D	307	9% 84% 12%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	A	403	-	X	-	-
5	GOL	A	407[B]	-	-	X	-

2 Entry composition

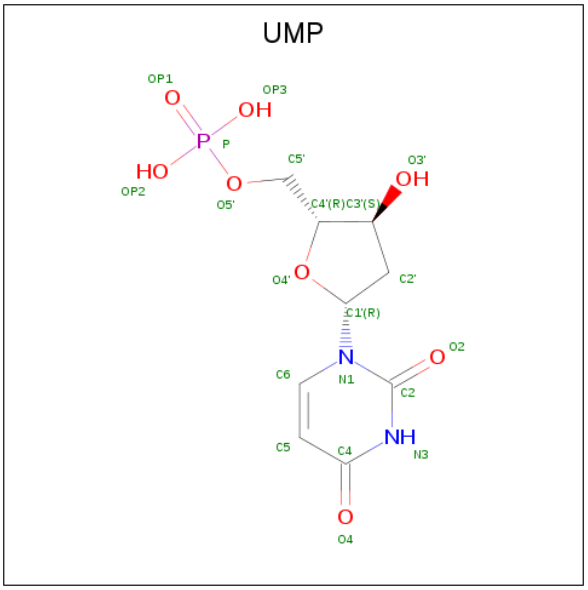
There are 8 unique types of molecules in this entry. The entry contains 11513 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thymidylate synthase.

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

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (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		

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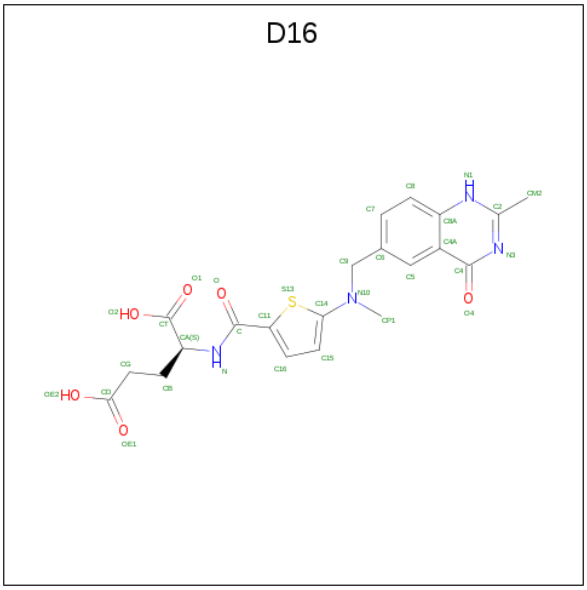
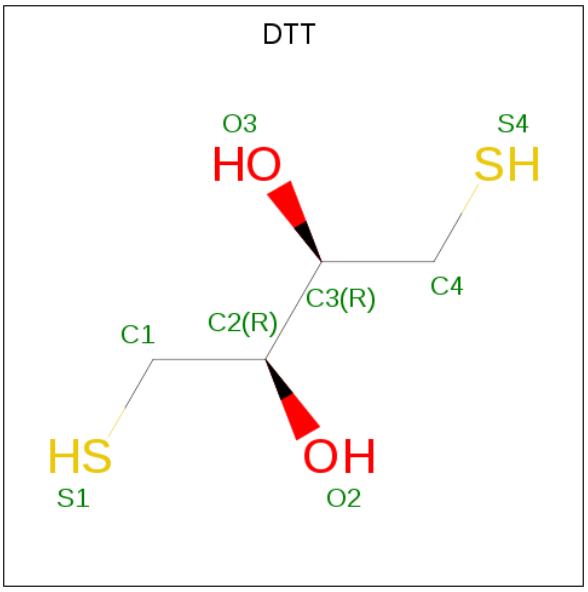
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is TOMUDEX (three-letter code: D16) (formula: $C_{21}H_{22}N_4O_6S$).



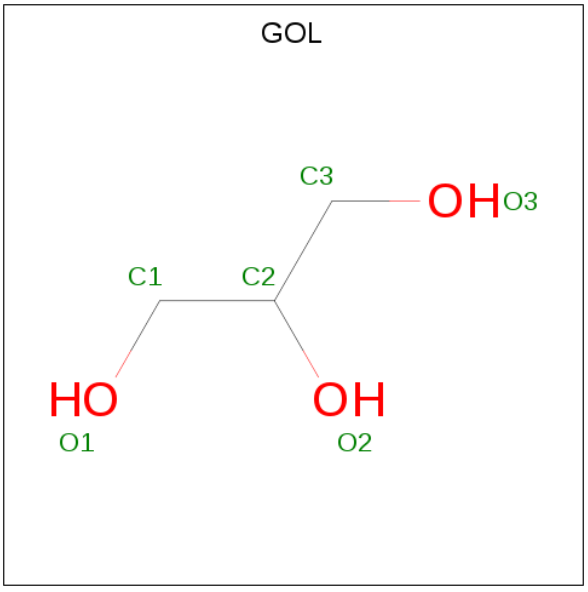
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
3	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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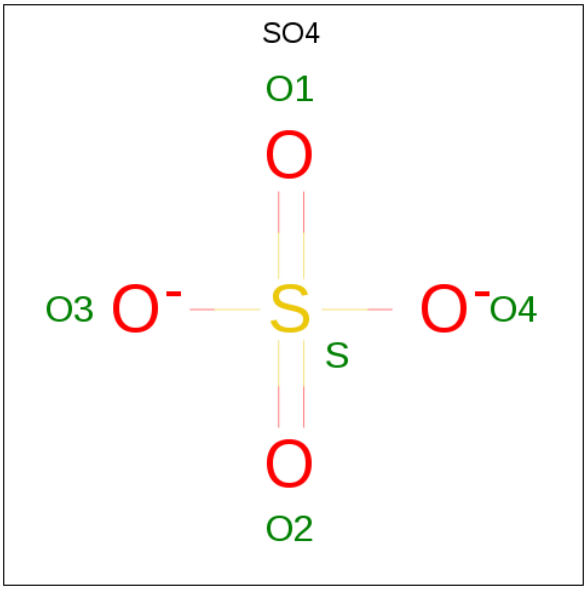
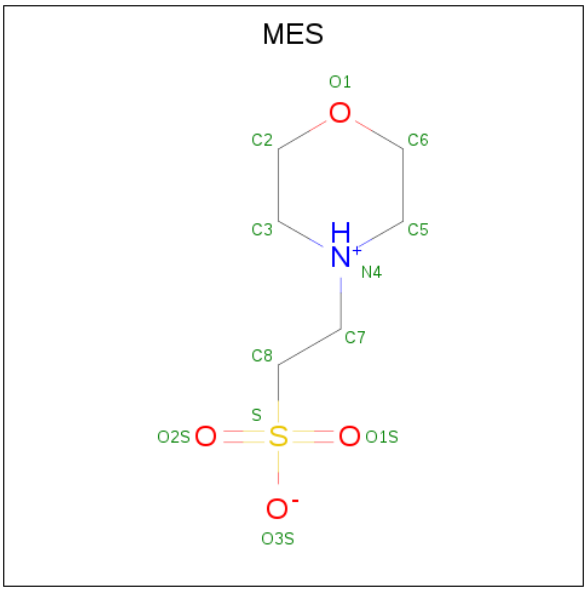
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 6 6	0	1
5	B	1	Total C O 12 6 6	0	1
5	B	1	Total C O 12 6 6	0	1
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 8 is water.

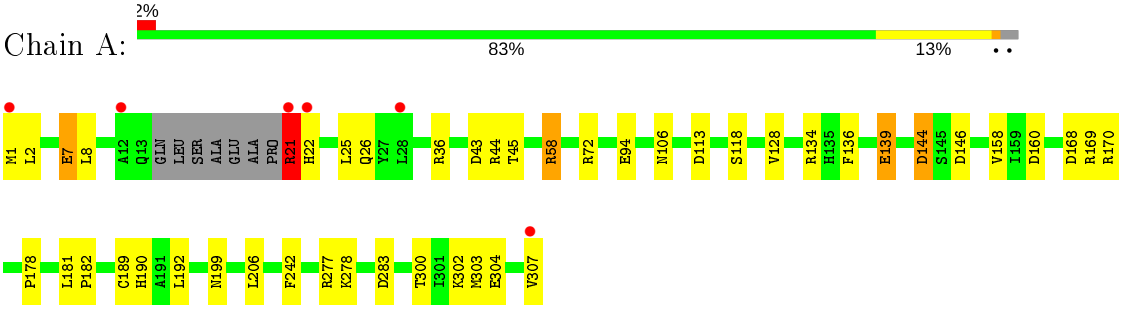
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	394	Total	O	0	0
			394	394		
8	B	362	Total	O	0	0
			362	362		
8	C	264	Total	O	0	0
			264	264		
8	D	202	Total	O	0	0
			202	202		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

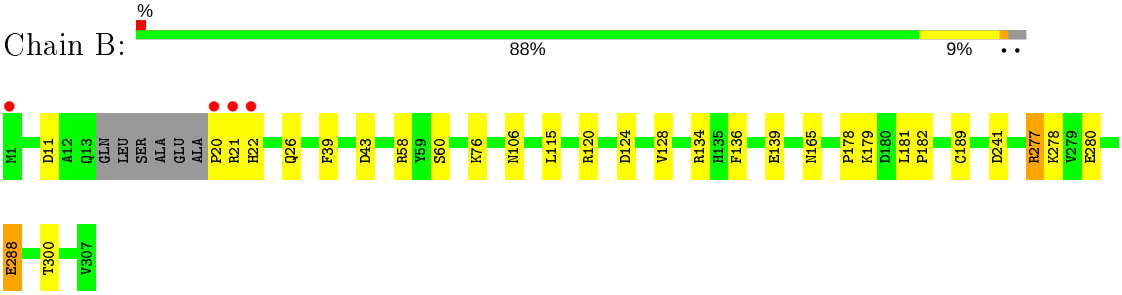
- Molecule 1: Thymidylate synthase

Chain A:



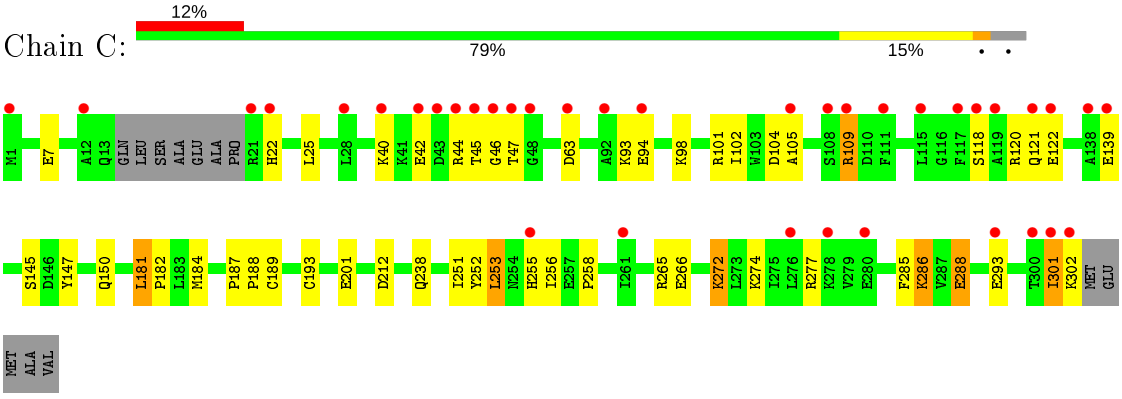
- Molecule 1: Thymidylate synthase

Chain B:



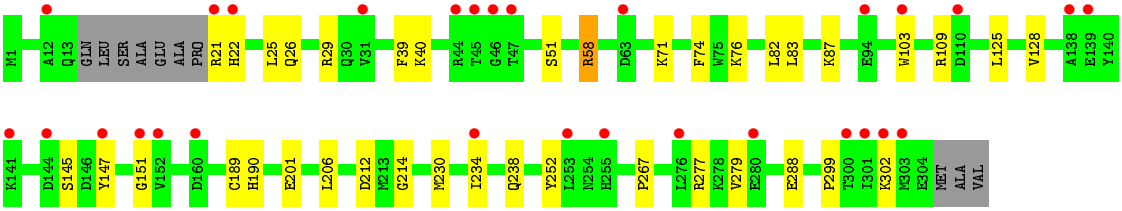
- Molecule 1: Thymidylate synthase

Chain C:



- Molecule 1: Thymidylate synthase

Chain D:


M1
A12
Q13
GLN
LEU
SER
ALA
GLU
ALA
PRO
R21
H22
L25
Q26
R29
Q30
V31
F39
K40
R44
T45
G46
T47
S51
R58
D63
K71
F74
W75
K76
L82
L83
K87
E94
W103
R109
D110
L125
V128
A138
E139
Y140
K141
D144
S145
D146
Y147
G151
V152
D160
C189
H190
E201
L206
D212
M213
G214
M230
I234
Q238
Y252
L253
M254
H255
P267
L276
R277
K278
V279
E280
E288
P299
T300
I301
K302
N303
E304
MET
ALA
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.80Å 114.22Å 123.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.74 20.04 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.74) 99.6 (20.04-1.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.238 0.194 , 0.241	Depositor DCC
R_{free} test set	7435 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, D16, UMP, SO4, MES, DTT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.12	1/2564 (0.0%)	1.07	12/3459 (0.3%)
1	B	1.07	1/2521 (0.0%)	1.02	7/3406 (0.2%)
1	C	1.03	1/2568 (0.0%)	0.95	1/3466 (0.0%)
1	D	0.98	1/2570 (0.0%)	0.92	3/3471 (0.1%)
All	All	1.05	4/10223 (0.0%)	0.99	23/13802 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	GLU	CG-CD	5.54	1.60	1.51
1	D	51	SER	CB-OG	-5.29	1.35	1.42
1	C	193	CYS	CB-SG	5.12	1.91	1.82
1	A	139	GLU	CB-CG	5.05	1.61	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	ARG	NE-CZ-NH2	9.39	125.00	120.30
1	A	144[A]	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	144[B]	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	169	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	134	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	58	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	B	58	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	212	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	B	134	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	D	58	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	277	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	D	212	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	160	ASP	CB-CG-OD1	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	277	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	B	277	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	21	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	277	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	11	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	120	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	242	PHE	CB-CG-CD2	5.61	124.73	120.80
1	B	241	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	36	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2501	0	2462	41	0
1	B	2462	0	2434	22	0
1	C	2503	0	2445	70	0
1	D	2508	0	2444	31	0
2	A	20	0	11	2	0
2	B	20	0	11	3	0
2	C	20	0	11	2	0
2	D	20	0	11	2	0
3	A	32	0	20	1	0
3	B	32	0	20	0	0
3	C	32	0	20	3	0
3	D	32	0	20	1	0
4	A	8	0	10	1	0
5	A	36	0	48	11	0
5	B	30	0	40	4	0
5	C	6	0	8	0	0
5	D	12	0	16	2	0
6	A	5	0	0	0	0
7	B	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	394	0	0	7	2
8	B	362	0	0	11	0
8	C	264	0	0	17	2
8	D	202	0	0	4	0
All	All	11513	0	10043	168	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (168) 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:C:63[A]:ASP:HB3	8:C:572:HOH:O	1.36	1.25
1:A:307:VAL:HG21	8:A:871:HOH:O	1.30	1.24
1:C:63[A]:ASP:OD1	8:C:748:HOH:O	1.66	1.11
1:B:189:CYS:SG	2:B:401:UMP:C6	2.43	1.11
1:C:181:LEU:HA	1:C:184[B]:MET:CE	1.81	1.10
1:C:181:LEU:HA	1:C:184[B]:MET:HE2	1.11	1.09
1:C:266[B]:GLU:CD	8:C:687:HOH:O	1.93	1.07
1:A:189:CYS:SG	2:A:401:UMP:C6	2.48	1.07
1:A:278[B]:LYS:H	5:A:407[B]:GOL:H31	1.11	1.07
1:A:94[A]:GLU:OE2	8:A:886:HOH:O	1.77	1.01
1:A:144[A]:ASP:OD1	8:A:886:HOH:O	1.83	0.96
1:A:106[A]:ASN:OD1	8:A:850:HOH:O	1.86	0.94
1:B:106[A]:ASN:ND2	8:B:502:HOH:O	2.01	0.94
1:A:7:GLU:OE2	1:A:8:LEU:HD12	1.69	0.92
1:C:181:LEU:HD22	1:C:184[B]:MET:HE1	1.51	0.91
1:A:307:VAL:HG23	8:A:837:HOH:O	1.70	0.90
1:A:278[B]:LYS:HG3	5:A:407[B]:GOL:H12	1.56	0.85
1:D:151:GLY:O	8:D:586:HOH:O	1.94	0.85
1:C:139[C]:GLU:CD	1:C:139[C]:GLU:H	1.74	0.85
1:A:44:ARG:HH22	1:A:307:VAL:HG11	1.42	0.84
1:C:255[A]:HIS:CE1	8:C:751:HOH:O	2.31	0.83
5:B:403[A]:GOL:O1	8:B:532:HOH:O	1.91	0.81
1:A:278[B]:LYS:H	5:A:407[B]:GOL:C3	1.91	0.81
1:D:288[B]:GLU:CD	1:D:288[B]:GLU:H	1.83	0.81
1:C:288:GLU:OE2	8:C:703:HOH:O	1.99	0.81
1:C:266[B]:GLU:OE2	8:C:687:HOH:O	1.91	0.80
1:D:189:CYS:SG	2:D:401:UMP:C6	2.76	0.79
1:C:181:LEU:HD22	1:C:184[B]:MET:CE	2.14	0.78
1:C:181:LEU:CA	1:C:184[B]:MET:HE2	2.05	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ARG:HG3	1:D:25:LEU:HD12	1.65	0.78
1:C:189:CYS:SG	2:C:401:UMP:C6	2.78	0.77
1:C:181:LEU:CD2	1:C:184[B]:MET:CE	2.62	0.76
1:C:122:GLU:N	8:C:690:HOH:O	2.17	0.76
1:A:278[B]:LYS:N	5:A:407[B]:GOL:H31	1.95	0.76
1:D:288[B]:GLU:OE1	1:D:288[B]:GLU:N	2.19	0.76
1:D:21:ARG:HE	1:D:29:ARG:HH12	1.36	0.72
1:C:181:LEU:CD2	1:C:184[B]:MET:HE1	2.19	0.72
1:C:7[B]:GLU:H	1:C:7[B]:GLU:CD	1.93	0.71
1:C:101:ARG:O	8:C:554:HOH:O	2.09	0.71
5:A:404[A]:GOL:H11	8:A:767:HOH:O	1.90	0.70
1:C:181:LEU:HD23	1:C:184[B]:MET:HE2	1.74	0.69
1:D:189:CYS:SG	2:D:401:UMP:C5	2.85	0.69
1:D:21:ARG:O	1:D:22[B]:HIS:ND1	2.25	0.68
1:C:181:LEU:CD2	1:C:184[B]:MET:HE2	2.24	0.68
5:B:403[A]:GOL:O2	8:B:512:HOH:O	2.07	0.67
1:C:22[B]:HIS:O	8:C:754:HOH:O	2.14	0.66
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.60	0.66
1:C:22[A]:HIS:O	8:C:754:HOH:O	2.14	0.66
1:C:139[C]:GLU:HG2	8:C:565:HOH:O	1.95	0.65
1:A:7:GLU:H	1:A:7:GLU:CD	2.01	0.64
1:B:22:HIS:HA	5:B:405:GOL:H31	1.78	0.64
1:B:165:ASN:OD1	8:B:614:HOH:O	2.15	0.63
1:C:94[B]:GLU:O	1:C:98[B]:LYS:HD3	1.99	0.63
1:C:98[B]:LYS:HD2	1:C:98[B]:LYS:N	2.14	0.63
1:C:22[A]:HIS:HB2	1:C:25:LEU:HG	1.81	0.62
1:D:190[B]:HIS:H	1:D:190[B]:HIS:CD2	2.17	0.62
1:C:109:ARG:CD	1:C:122:GLU:HG3	2.29	0.62
1:C:109:ARG:HD2	1:C:122:GLU:HG3	1.80	0.62
1:A:44:ARG:NH2	1:A:307:VAL:HG11	2.14	0.62
1:D:71:LYS:NZ	1:D:214:GLY:O	2.32	0.62
1:B:300:THR:HG23	8:B:624:HOH:O	1.99	0.61
1:D:190[B]:HIS:CB	1:D:206:LEU:HD11	2.31	0.61
1:A:45:THR:HG22	1:A:307:VAL:HB	1.82	0.60
1:C:189:CYS:SG	2:C:401:UMP:C5	2.94	0.60
1:C:63[A]:ASP:CB	8:C:572:HOH:O	2.15	0.60
1:A:278[B]:LYS:HE3	5:A:407[B]:GOL:H2	1.83	0.60
1:B:300:THR:CG2	8:B:570:HOH:O	2.49	0.59
1:C:181:LEU:HD23	1:C:184[B]:MET:CE	2.31	0.59
1:C:7[B]:GLU:HG2	1:C:25:LEU:HD21	1.84	0.59
1:A:158:VAL:HG23	4:A:403:DTT:S1	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:HIS:HB2	1:A:25:LEU:HG	1.85	0.58
1:C:139[C]:GLU:CD	1:C:139[C]:GLU:N	2.54	0.58
1:A:190:HIS:HB3	1:A:206:LEU:HD11	1.86	0.57
1:C:252:TYR:CE1	3:C:402:D16:HM21	2.40	0.57
1:C:139[B]:GLU:OE1	1:C:150:GLN:NE2	2.37	0.57
1:B:39:PHE:CE2	7:B:406:MES:H31	2.40	0.57
1:C:272:LYS:HB2	1:C:293[B]:GLU:HG3	1.85	0.57
1:A:72:ARG:HB3	1:A:300:THR:HG22	1.87	0.56
1:B:20:PRO:HG2	1:B:60:SER:HB2	1.87	0.56
1:D:22[A]:HIS:HB3	1:D:25:LEU:HG	1.86	0.55
1:D:190[B]:HIS:HB3	1:D:206:LEU:HD11	1.87	0.55
1:A:189:CYS:SG	2:A:401:UMP:C5	3.00	0.55
1:D:40:LYS:HG3	5:D:404:GOL:H31	1.89	0.55
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.21	0.54
1:D:190[A]:HIS:HB3	1:D:206:LEU:HD11	1.90	0.54
1:D:26[A]:GLN:NE2	8:D:627:HOH:O	2.40	0.54
1:A:7:GLU:OE2	1:A:8:LEU:CD1	2.51	0.54
1:B:189:CYS:SG	2:B:401:UMP:H6	2.26	0.54
1:C:45:THR:HG1	1:C:47:THR:HG1	1.53	0.54
1:D:26[B]:GLN:NE2	1:D:58:ARG:O	2.41	0.54
1:D:103[B]:TRP:CE3	1:D:125:LEU:HD13	2.44	0.53
1:C:121:GLN:HB3	8:C:690:HOH:O	2.08	0.53
1:D:201:GLU:HA	1:D:238:GLN:O	2.09	0.53
1:C:181:LEU:HA	1:C:184[B]:MET:HE3	1.86	0.52
1:A:136:PHE:CZ	1:B:178:PRO:HD2	2.44	0.52
1:D:22[B]:HIS:HB2	1:D:25:LEU:HG	1.91	0.51
1:B:120:ARG:HD3	1:B:124:ASP:HB3	1.91	0.51
1:C:181:LEU:HB2	1:C:182:PRO:HD3	1.93	0.51
1:B:189:CYS:SG	2:B:401:UMP:C5	3.01	0.50
1:D:22[B]:HIS:CD2	8:D:688:HOH:O	2.64	0.50
3:C:402:D16:O2	8:C:564:HOH:O	2.20	0.50
1:D:22[B]:HIS:HD2	8:D:688:HOH:O	1.95	0.50
1:A:168:ASP:OD2	1:A:170:ARG:HB2	2.11	0.49
1:A:1:MET:HG2	1:A:2:LEU:H	1.76	0.49
1:D:234:ILE:HD11	1:D:279:VAL:HG12	1.94	0.49
1:D:39:PHE:HD2	5:D:404:GOL:H2	1.77	0.49
1:B:288:GLU:CD	1:B:288:GLU:H	2.15	0.49
1:C:212:ASP:OD1	1:C:255[B]:HIS:NE2	2.46	0.48
1:C:184[B]:MET:HE1	1:C:188:PRO:HD3	1.94	0.48
1:C:201:GLU:HA	1:C:238:GLN:O	2.14	0.48
1:C:288:GLU:H	1:C:288:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286[A]:LYS:HB2	1:C:286[A]:LYS:NZ	2.29	0.48
1:D:145:SER:HB2	1:D:147:TYR:CZ	2.48	0.48
1:D:252:TYR:CE2	3:D:402:D16:HM21	2.49	0.48
1:A:146[A]:ASP:OD1	1:A:146[A]:ASP:C	2.52	0.47
1:C:46:GLY:O	8:C:704:HOH:O	2.20	0.47
1:B:278:LYS:HD3	1:B:280:GLU:OE2	2.13	0.47
1:A:192:LEU:HD12	1:A:192:LEU:C	2.34	0.47
1:C:255[A]:HIS:NE2	8:C:751:HOH:O	2.35	0.47
1:C:94[B]:GLU:O	1:C:98[B]:LYS:CD	2.62	0.47
1:C:258:PRO:CB	1:C:301:ILE:HD11	2.45	0.46
1:C:258:PRO:HB2	1:C:301:ILE:HD11	1.96	0.46
1:C:145:SER:HB2	1:C:147:TYR:CZ	2.50	0.46
1:C:286[B]:LYS:HA	1:C:286[B]:LYS:HD2	1.61	0.46
1:C:286[B]:LYS:HB3	1:C:286[B]:LYS:NZ	2.31	0.46
5:A:405:GOL:H32	1:B:179:LYS:HD3	1.98	0.46
1:B:26:GLN:HG2	8:B:853:HOH:O	2.16	0.46
1:C:286[B]:LYS:HB3	1:C:286[B]:LYS:HZ2	1.80	0.45
1:C:293[B]:GLU:OE2	1:C:293[B]:GLU:O	2.35	0.45
1:A:7:GLU:N	1:A:7:GLU:CD	2.70	0.45
1:C:265:ARG:NH2	1:C:301:ILE:HG22	2.32	0.45
1:A:303:MET:O	3:A:402:D16:OE2	2.35	0.45
1:C:251:ILE:HG23	1:C:255[B]:HIS:CE1	2.51	0.45
1:C:181:LEU:CA	1:C:184[B]:MET:CE	2.74	0.44
3:C:402:D16:HP11	3:C:402:D16:H15	1.53	0.44
1:C:272:LYS:HB2	1:C:293[B]:GLU:CG	2.48	0.44
1:A:22:HIS:CE1	8:A:880:HOH:O	2.71	0.43
1:C:63[A]:ASP:CA	8:C:572:HOH:O	2.59	0.43
1:B:277:ARG:HB2	8:B:820:HOH:O	2.18	0.43
1:C:104:ASP:O	1:C:105:ALA:C	2.57	0.43
1:B:278:LYS:CD	1:B:280:GLU:OE2	2.67	0.43
1:D:83:LEU:O	1:D:87:LYS:HG3	2.19	0.43
1:A:113:ASP:OD1	1:A:118:SER:HA	2.20	0.42
1:A:278[B]:LYS:HE3	5:A:407[B]:GOL:C2	2.48	0.42
1:C:181:LEU:CB	1:C:182:PRO:HD3	2.49	0.42
1:A:1:MET:HG2	1:A:2:LEU:N	2.34	0.42
1:A:199:ASN:N	5:A:404[A]:GOL:O3	2.40	0.42
1:A:278[B]:LYS:CE	5:A:407[B]:GOL:H12	2.49	0.42
1:B:76:LYS:NZ	8:B:830:HOH:O	2.45	0.42
1:B:181[A]:LEU:HB2	1:B:182:PRO:HD3	2.01	0.42
1:D:82:LEU:HD23	1:D:230:MET:HE1	2.00	0.42
1:D:190[B]:HIS:N	1:D:190[B]:HIS:CD2	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26[A]:GLN:NE2	1:A:58:ARG:O	2.28	0.42
1:B:300:THR:HA	8:B:624:HOH:O	2.19	0.42
1:C:285:PHE:O	1:C:286[B]:LYS:HD2	2.21	0.41
1:A:199:ASN:H	5:A:404[B]:GOL:H32	1.85	0.41
1:C:187:PRO:HA	1:C:188:PRO:HD3	1.92	0.41
1:A:181:LEU:N	1:A:182:PRO:CD	2.84	0.41
1:C:22[B]:HIS:HB3	1:C:25:LEU:HG	2.02	0.40
1:C:98[B]:LYS:CD	1:C:98[B]:LYS:N	2.83	0.40
1:D:22[A]:HIS:HD2	1:D:267:PRO:HB2	1.86	0.40
1:A:178:PRO:HD2	1:B:136:PHE:CZ	2.56	0.40
1:C:45:THR:OG1	1:C:47:THR:OG1	2.28	0.40
1:D:74:PHE:CE1	1:D:76:LYS:HB3	2.56	0.40
1:C:286[A]:LYS:HZ2	1:C:286[A]:LYS:HB2	1.86	0.40
5:B:403[B]:GOL:H31	8:B:738:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:860:HOH:O	8:C:506:HOH:O[3_545]	1.96	0.24
8:A:557:HOH:O	8:C:506:HOH:O[3_545]	2.01	0.19

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/307 (100%)	296 (97%)	9 (3%)	1 (0%)	41 23
1	B	302/307 (98%)	288 (95%)	13 (4%)	1 (0%)	41 23
1	C	305/307 (99%)	289 (95%)	14 (5%)	2 (1%)	22 8
1	D	305/307 (99%)	287 (94%)	16 (5%)	2 (1%)	22 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1218/1228 (99%)	1160 (95%)	52 (4%)	6 (0%)	29 12

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/266 (102%)	263 (97%)	9 (3%)	38 14
1	B	267/266 (100%)	263 (98%)	4 (2%)	65 47
1	C	272/266 (102%)	255 (94%)	17 (6%)	18 3
1	D	271/266 (102%)	268 (99%)	3 (1%)	73 59
All	All	1082/1064 (102%)	1049 (97%)	33 (3%)	42 17

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	21	ARG
1	A	43	ASP
1	A	139	GLU
1	A	283[A]	ASP
1	A	283[B]	ASP
1	A	302[A]	LYS
1	A	302[B]	LYS
1	A	304	GLU

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Mol	Chain	Res	Type
1	B	21	ARG
1	B	43	ASP
1	B	115	LEU
1	B	288	GLU
1	C	40	LYS
1	C	42	GLU
1	C	93	LYS
1	C	102	ILE
1	C	109	ARG
1	C	118	SER
1	C	181	LEU
1	C	253	LEU
1	C	256	ILE
1	C	272	LYS
1	C	274	LYS
1	C	277	ARG
1	C	286[A]	LYS
1	C	286[B]	LYS
1	C	288	GLU
1	C	301	ILE
1	C	302	LYS
1	D	109	ARG
1	D	277	ARG
1	D	302	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	B	165	ASN
1	C	150	GLN
1	C	165	ASN
1	C	296	ASN
1	D	291	GLN
1	D	296	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	404[B]	-	5,5,5	0.48	0	5,5,5	0.87	0
5	GOL	A	404[A]	-	5,5,5	0.68	0	5,5,5	1.03	0
3	D16	C	402	-	23,34,34	1.35	2 (8%)	25,48,48	3.30	11 (44%)
2	UMP	B	401	-	18,21,21	1.26	4 (22%)	21,31,31	1.35	3 (14%)
3	D16	B	402	-	23,34,34	1.04	1 (4%)	25,48,48	3.54	11 (44%)
2	UMP	A	401	-	18,21,21	1.43	2 (11%)	21,31,31	1.26	2 (9%)
5	GOL	B	405	-	5,5,5	0.42	0	5,5,5	0.57	0
5	GOL	B	403[B]	-	5,5,5	0.27	0	5,5,5	0.62	0
5	GOL	D	404	-	5,5,5	0.41	0	5,5,5	0.38	0
5	GOL	A	406	-	5,5,5	0.26	0	5,5,5	0.63	0
2	UMP	D	401	-	18,21,21	1.09	2 (11%)	21,31,31	1.47	6 (28%)
3	D16	A	402	-	23,34,34	1.19	2 (8%)	25,48,48	3.14	11 (44%)
2	UMP	C	401	-	18,21,21	1.63	3 (16%)	21,31,31	1.57	4 (19%)
5	GOL	A	407[A]	-	5,5,5	0.29	0	5,5,5	0.33	0
5	GOL	D	403	-	5,5,5	0.43	0	5,5,5	0.34	0
5	GOL	B	403[A]	-	5,5,5	0.65	0	5,5,5	0.71	0
4	DTT	A	403	-	7,7,7	1.94	5 (71%)	4,8,8	2.15	2 (50%)
5	GOL	A	407[B]	-	5,5,5	0.32	0	5,5,5	0.56	0
5	GOL	A	405	-	5,5,5	0.64	0	5,5,5	0.57	0
3	D16	D	402	-	23,34,34	1.26	2 (8%)	25,48,48	2.87	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	A	408	-	4,4,4	0.21	0	6,6,6	0.25	0
5	GOL	B	404[A]	-	5,5,5	0.41	0	5,5,5	0.80	0
5	GOL	C	403	-	5,5,5	0.45	0	5,5,5	0.19	0
5	GOL	B	404[B]	-	5,5,5	0.39	0	5,5,5	0.42	0
7	MES	B	406	-	12,12,12	1.94	1 (8%)	14,16,16	2.57	7 (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
5	GOL	A	404[B]	-	-	2/4/4/4	-
5	GOL	A	404[A]	-	-	2/4/4/4	-
3	D16	C	402	-	-	1/13/25/25	0/3/3/3
2	UMP	B	401	-	-	1/7/22/22	0/2/2/2
3	D16	B	402	-	-	1/13/25/25	0/3/3/3
2	UMP	A	401	-	-	1/7/22/22	0/2/2/2
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	B	403[B]	-	-	4/4/4/4	-
5	GOL	D	404	-	-	4/4/4/4	-
5	GOL	A	406	-	-	2/4/4/4	-
2	UMP	D	401	-	-	1/7/22/22	0/2/2/2
3	D16	A	402	-	-	1/13/25/25	0/3/3/3
2	UMP	C	401	-	-	1/7/22/22	0/2/2/2
5	GOL	A	407[A]	-	-	4/4/4/4	-
5	GOL	D	403	-	-	0/4/4/4	-
5	GOL	B	403[A]	-	-	4/4/4/4	-
4	DTT	A	403	-	-	7/8/8/8	-
5	GOL	A	407[B]	-	-	2/4/4/4	-
5	GOL	A	405	-	-	2/4/4/4	-
3	D16	D	402	-	-	1/13/25/25	0/3/3/3
5	GOL	B	404[A]	-	-	2/4/4/4	-
5	GOL	C	403	-	-	2/4/4/4	-
5	GOL	B	404[B]	-	-	4/4/4/4	-
7	MES	B	406	-	-	1/6/14/14	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	406	MES	C8-S	-6.26	1.68	1.77
2	C	401	UMP	C4-N3	4.61	1.41	1.33
3	C	402	D16	C4A-C8A	4.13	1.49	1.41
3	D	402	D16	C4A-C8A	3.98	1.49	1.41
2	A	401	UMP	C4-N3	3.83	1.39	1.33
2	C	401	UMP	C6-N1	3.63	1.40	1.35
2	A	401	UMP	C6-N1	3.16	1.39	1.35
4	A	403	DTT	C4-S4	2.51	1.86	1.81
2	B	401	UMP	C4-N3	2.44	1.37	1.33
2	D	401	UMP	P-OP3	-2.43	1.45	1.54
4	A	403	DTT	C3-C2	2.43	1.59	1.52
3	B	402	D16	C4A-C8A	2.34	1.45	1.41
2	B	401	UMP	P-OP3	-2.31	1.45	1.54
2	B	401	UMP	C6-C5	2.26	1.43	1.38
2	B	401	UMP	C6-N1	2.23	1.38	1.35
3	A	402	D16	C4A-C8A	2.18	1.45	1.41
3	D	402	D16	C8-C8A	-2.15	1.38	1.41
2	D	401	UMP	C4-N3	2.14	1.36	1.33
4	A	403	DTT	C1-C2	2.09	1.57	1.51
4	A	403	DTT	C1-S1	2.07	1.85	1.81
2	C	401	UMP	O4'-C4'	-2.06	1.40	1.45
3	C	402	D16	C8A-N1	-2.02	1.34	1.37
3	A	402	D16	C2-N3	2.02	1.37	1.34
4	A	403	DTT	C4-C3	2.01	1.57	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	D16	C4A-C4-N3	-10.05	117.39	124.40
3	B	402	D16	C4A-C4-N3	-8.82	118.25	124.40
3	B	402	D16	C2-N1-C8A	8.04	121.99	116.54
3	B	402	D16	C4A-C8A-N1	-7.63	119.46	123.60
3	A	402	D16	C4A-C8A-N1	-7.61	119.47	123.60
3	A	402	D16	C4A-C4-N3	-7.55	119.14	124.40
3	D	402	D16	C4A-C4-N3	-7.39	119.25	124.40
3	A	402	D16	C2-N1-C8A	6.65	121.05	116.54
3	C	402	D16	C4A-C8A-N1	-6.47	120.09	123.60
3	D	402	D16	C2-N1-C8A	6.37	120.86	116.54
3	D	402	D16	C4A-C8A-N1	-6.21	120.23	123.60
3	C	402	D16	C2-N1-C8A	5.74	120.43	116.54
3	B	402	D16	C8-C8A-N1	4.74	125.92	118.69
3	B	402	D16	CM2-C2-N1	4.33	123.90	117.16
7	B	406	MES	C5-N4-C3	4.31	118.52	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	D16	C6-C5-C4A	-4.19	116.38	122.65
2	C	401	UMP	C2'-C1'-N1	4.16	123.87	114.27
3	B	402	D16	C8-C8A-C4A	-3.95	114.61	120.05
7	B	406	MES	C7-N4-C3	3.93	121.27	111.23
3	B	402	D16	C4-C4A-C8A	-3.91	115.18	118.59
3	C	402	D16	CG-CB-CA	-3.84	105.29	113.04
3	C	402	D16	C8-C8A-N1	3.79	124.47	118.69
3	D	402	D16	C4-C4A-C8A	-3.57	115.48	118.59
7	B	406	MES	O3S-S-C8	3.56	111.53	105.77
2	B	401	UMP	O5'-P-OP1	-3.50	96.66	106.47
3	C	402	D16	CA-N-C	-3.49	117.85	122.34
7	B	406	MES	C7-N4-C5	3.48	120.15	111.23
4	A	403	DTT	O3-C3-C2	3.38	116.68	109.72
3	C	402	D16	C8-C8A-C4A	-3.36	115.43	120.05
3	C	402	D16	C6-C9-N10	3.33	117.95	113.81
7	B	406	MES	C2-C3-N4	-3.31	105.09	110.10
7	B	406	MES	O1S-S-C8	3.25	110.83	106.92
3	D	402	D16	C8-C8A-N1	3.21	123.58	118.69
2	B	401	UMP	C2'-C1'-N1	3.12	121.47	114.27
2	D	401	UMP	C2'-C1'-N1	2.91	120.98	114.27
2	A	401	UMP	C2'-C1'-N1	2.81	120.76	114.27
3	D	402	D16	C8-C8A-C4A	-2.81	116.19	120.05
2	C	401	UMP	C5-C4-N3	-2.81	117.13	123.31
3	A	402	D16	C7-C8-C8A	-2.74	117.39	120.84
3	A	402	D16	CA-N-C	2.73	125.86	122.34
2	D	401	UMP	C5-C4-N3	-2.68	117.40	123.31
3	A	402	D16	C6-C9-N10	2.68	117.14	113.81
3	C	402	D16	C11-C-N	2.68	120.17	115.21
3	D	402	D16	C11-C-N	2.67	120.16	115.21
3	B	402	D16	N1-C2-N3	-2.62	120.91	125.72
2	A	401	UMP	O4'-C1'-C2'	2.60	111.16	106.25
2	C	401	UMP	O5'-P-OP1	2.58	113.71	106.47
3	D	402	D16	CM2-C2-N1	2.57	121.16	117.16
3	B	402	D16	CA-N-C	2.55	125.62	122.34
2	D	401	UMP	OP3-P-O5'	2.54	113.50	106.73
2	D	401	UMP	P-O5'-C5'	2.51	125.22	118.30
3	A	402	D16	C4-C4A-C8A	-2.44	116.47	118.59
3	B	402	D16	C11-C-N	2.42	119.70	115.21
3	A	402	D16	N1-C2-N3	-2.38	121.34	125.72
3	A	402	D16	CP1-N10-C14	-2.37	115.60	119.96
2	D	401	UMP	C6-N1-C2	-2.35	117.47	121.20
3	D	402	D16	C6-C5-C4A	-2.31	119.19	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	D16	N1-C2-N3	-2.28	121.53	125.72
3	B	402	D16	CG-CB-CA	-2.27	108.45	113.04
3	A	402	D16	C8-C8A-N1	2.26	122.14	118.69
3	C	402	D16	C4-C4A-C8A	-2.20	116.68	118.59
2	C	401	UMP	P-O5'-C5'	2.19	124.32	118.30
7	B	406	MES	O2S-S-O1S	-2.18	106.42	113.95
3	C	402	D16	C6-C5-C4A	-2.13	119.46	122.65
2	B	401	UMP	OP3-P-OP2	2.07	115.56	107.64
4	A	403	DTT	C2-C1-S1	2.05	120.44	114.47
2	D	401	UMP	OP3-P-OP1	2.01	118.53	110.68

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404[B]	GOL	C1-C2-C3-O3
5	A	404[A]	GOL	C1-C2-C3-O3
5	A	404[A]	GOL	O2-C2-C3-O3
5	B	405	GOL	C1-C2-C3-O3
5	B	403[B]	GOL	O1-C1-C2-O2
5	B	403[B]	GOL	O1-C1-C2-C3
5	B	403[B]	GOL	C1-C2-C3-O3
5	D	404	GOL	O1-C1-C2-O2
5	D	404	GOL	O1-C1-C2-C3
5	D	404	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-C3
5	A	407[B]	GOL	C1-C2-C3-O3
5	A	407[A]	GOL	C1-C2-C3-O3
5	B	403[A]	GOL	O1-C1-C2-C3
5	B	403[A]	GOL	C1-C2-C3-O3
5	B	403[A]	GOL	O2-C2-C3-O3
4	A	403	DTT	S1-C1-C2-O2
4	A	403	DTT	S1-C1-C2-C3
4	A	403	DTT	C1-C2-C3-O3
4	A	403	DTT	C1-C2-C3-C4
4	A	403	DTT	O2-C2-C3-O3
4	A	403	DTT	O2-C2-C3-C4
4	A	403	DTT	C2-C3-C4-S4
5	A	405	GOL	C1-C2-C3-O3
5	B	404[A]	GOL	C1-C2-C3-O3
5	B	404[A]	GOL	O2-C2-C3-O3
5	C	403	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	404[B]	GOL	C1-C2-C3-O3
7	B	406	MES	C8-C7-N4-C5
5	A	404[B]	GOL	O2-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
5	B	403[A]	GOL	O1-C1-C2-O2
5	A	405	GOL	O2-C2-C3-O3
5	A	407[A]	GOL	O1-C1-C2-C3
5	D	404	GOL	O2-C2-C3-O3
5	A	407[B]	GOL	O2-C2-C3-O3
5	C	403	GOL	O1-C1-C2-O2
5	B	404[B]	GOL	O2-C2-C3-O3
5	B	403[B]	GOL	O2-C2-C3-O3
5	A	407[A]	GOL	O2-C2-C3-O3
3	C	402	D16	C6-C9-N10-CP1
3	B	402	D16	C6-C9-N10-CP1
3	A	402	D16	C6-C9-N10-CP1
3	D	402	D16	C6-C9-N10-CP1
5	B	405	GOL	O2-C2-C3-O3
5	B	404[B]	GOL	O1-C1-C2-C3
5	A	407[A]	GOL	O1-C1-C2-O2
5	B	404[B]	GOL	O1-C1-C2-O2
2	B	401	UMP	O4'-C4'-C5'-O5'
2	C	401	UMP	O4'-C4'-C5'-O5'
2	A	401	UMP	O4'-C4'-C5'-O5'
2	D	401	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404[B]	GOL	1	0
5	A	404[A]	GOL	2	0
3	C	402	D16	3	0
2	B	401	UMP	3	0
2	A	401	UMP	2	0
5	B	405	GOL	1	0
5	B	403[B]	GOL	1	0
5	D	404	GOL	2	0
2	D	401	UMP	2	0
3	A	402	D16	1	0
2	C	401	UMP	2	0
5	B	403[A]	GOL	2	0

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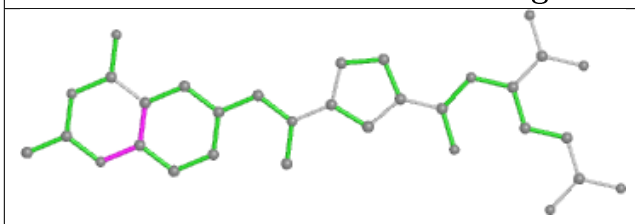
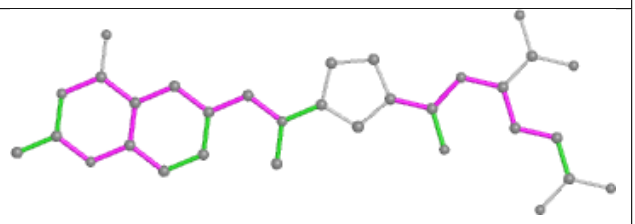
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	DTT	1	0
5	A	407[B]	GOL	7	0
5	A	405	GOL	1	0
3	D	402	D16	1	0
7	B	406	MES	1	0

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

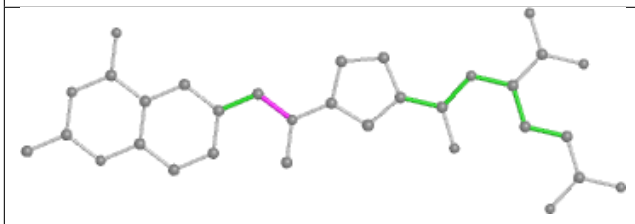
Ligand D16 C 402



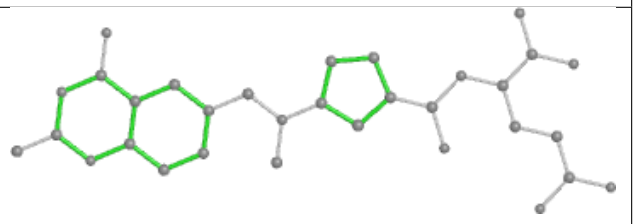
Bond lengths



Bond angles

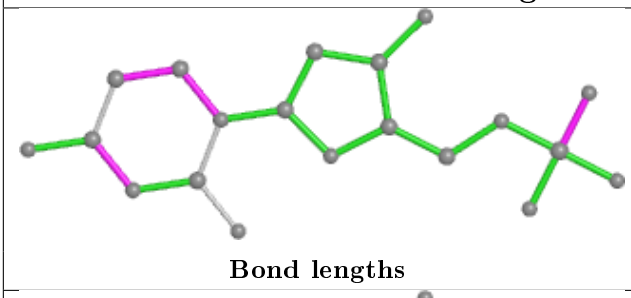


Torsions

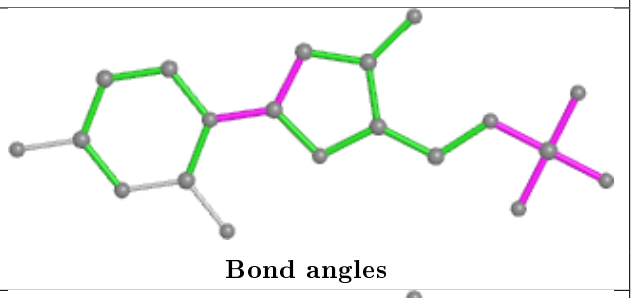


Rings

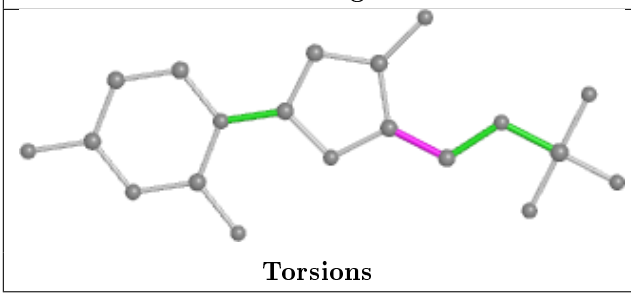
Ligand UMP B 401



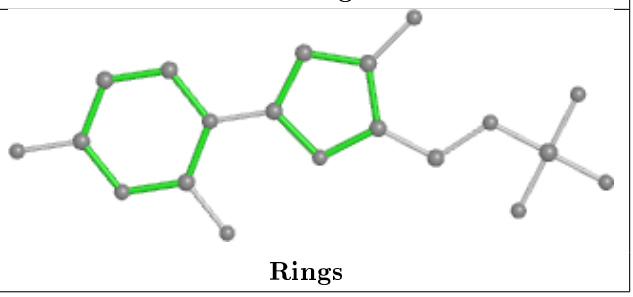
Bond lengths



Bond angles

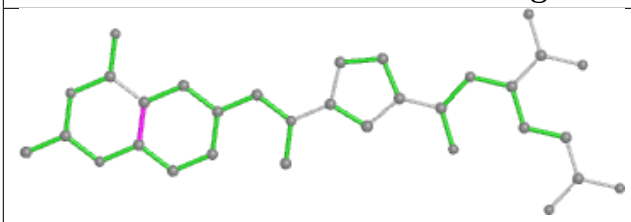


Torsions

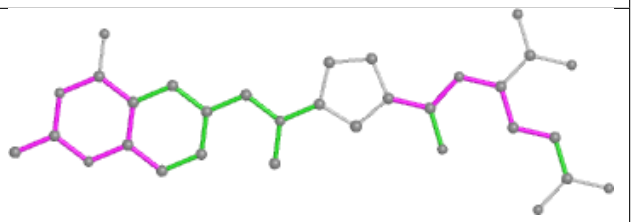


Rings

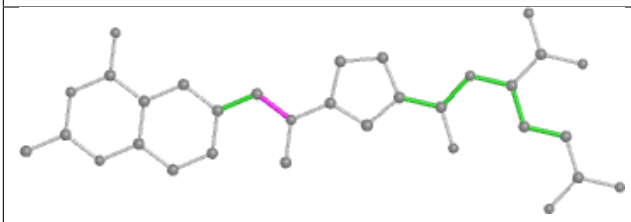
Ligand D16 B 402



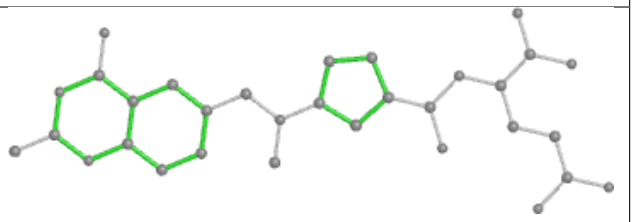
Bond lengths



Bond angles

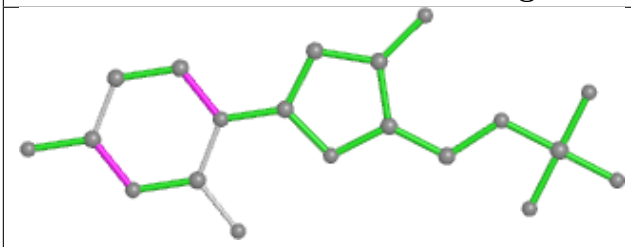


Torsions

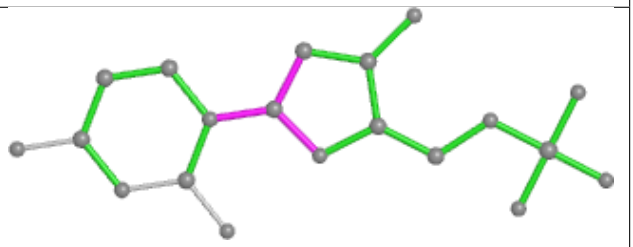


Rings

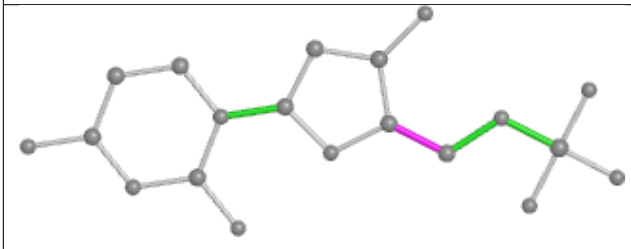
Ligand UMP A 401



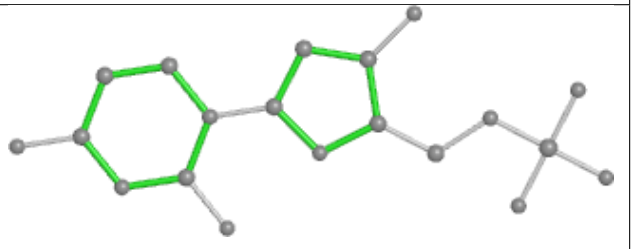
Bond lengths



Bond angles

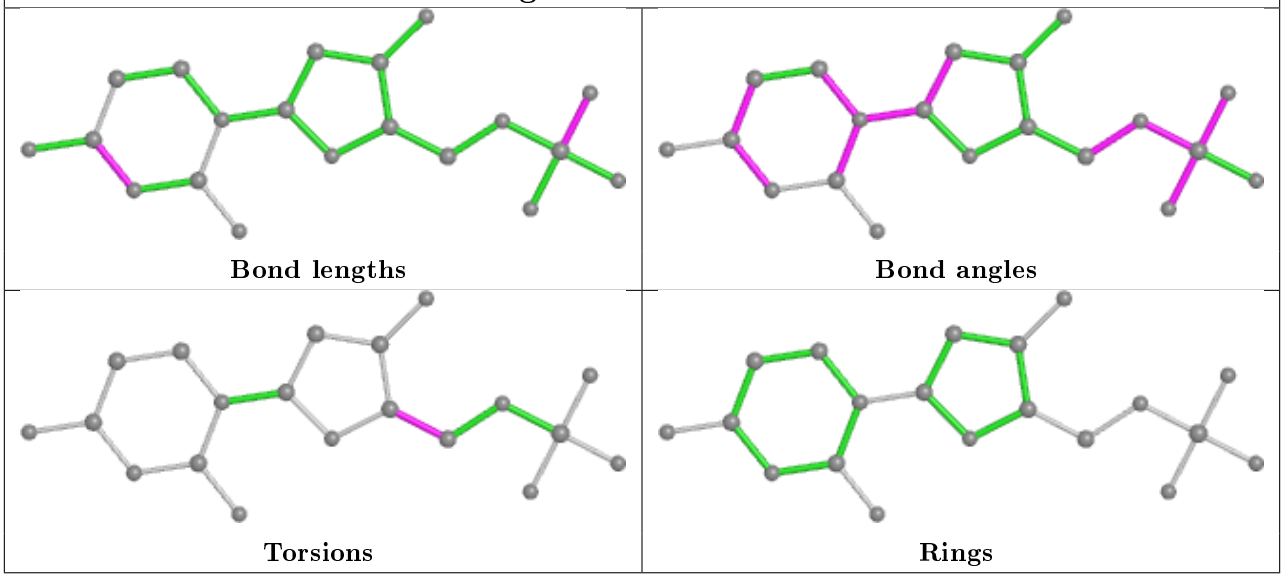


Torsions

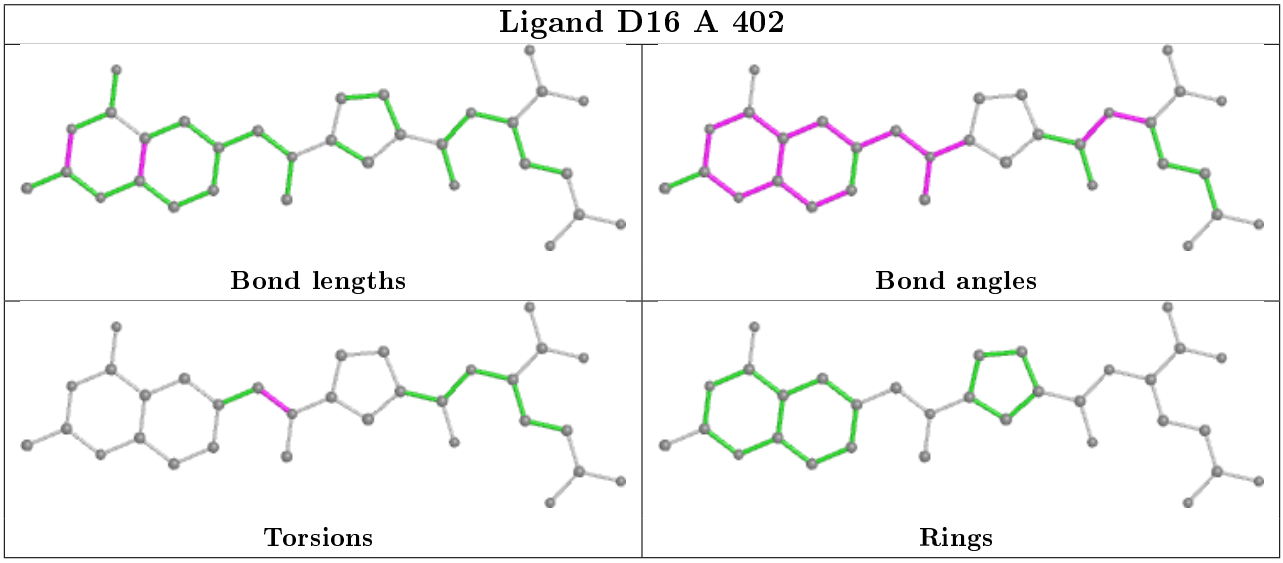


Rings

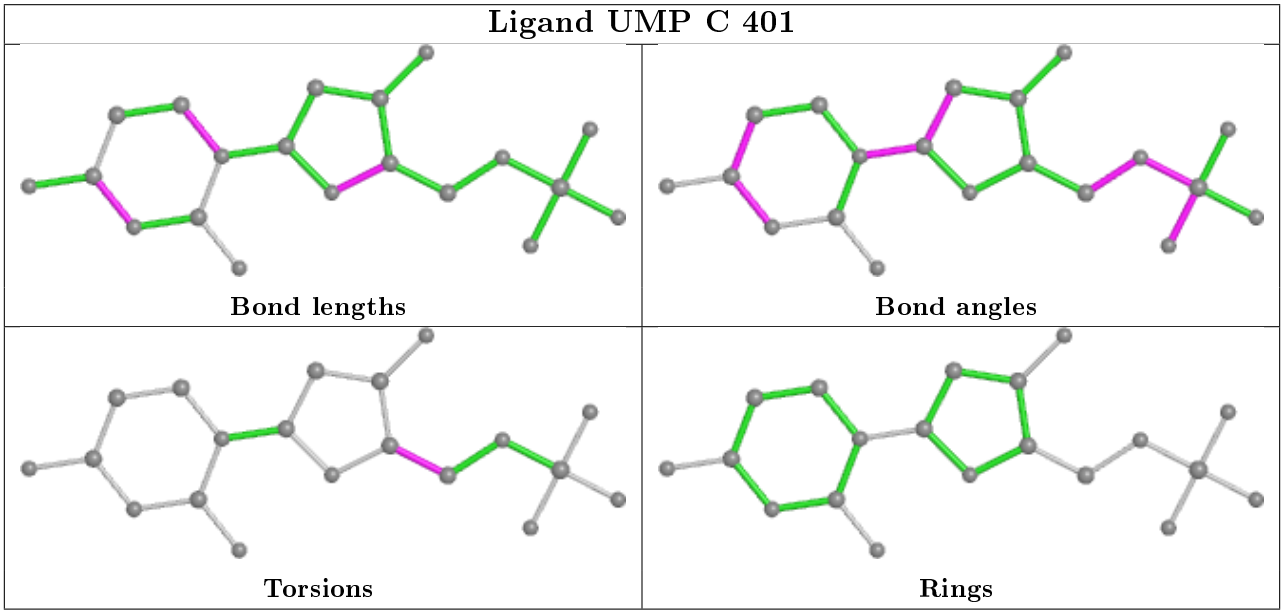
Ligand UMP D 401



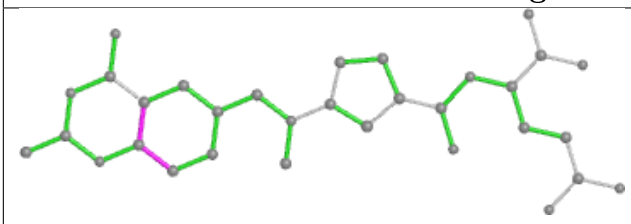
Ligand D16 A 402



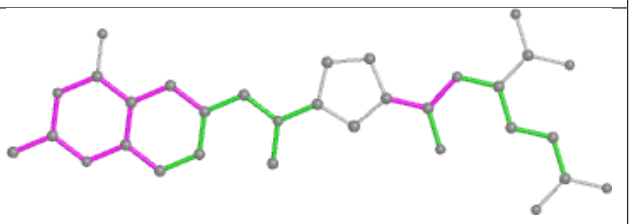
Ligand UMP C 401



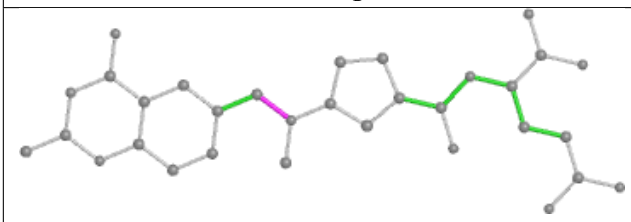
Ligand D16 D 402



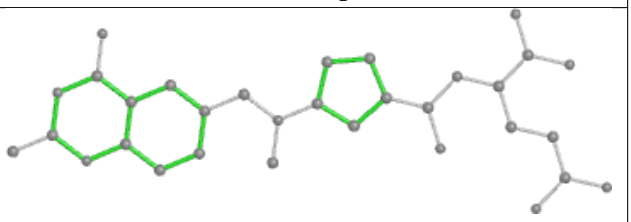
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	300/307 (97%)	0.04	6 (2%) 65 71	15, 22, 36, 60	0
1	B	301/307 (98%)	-0.03	4 (1%) 77 82	15, 22, 35, 60	0
1	C	295/307 (96%)	0.81	37 (12%) 3 4	19, 32, 60, 68	0
1	D	297/307 (96%)	0.65	29 (9%) 7 9	21, 34, 50, 68	0
All	All	1193/1228 (97%)	0.36	76 (6%) 19 23	15, 28, 49, 68	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	LEU	8.7
1	C	45	THR	8.4
1	D	301	ILE	7.6
1	D	45	THR	7.5
1	C	302	LYS	7.5
1	D	300	THR	6.6
1	C	21	ARG	6.4
1	B	20	PRO	6.0
1	B	21	ARG	5.7
1	D	22[A]	HIS	5.6
1	C	301	ILE	5.5
1	A	12	ALA	5.1
1	A	1	MET	5.0
1	D	44	ARG	4.7
1	A	21	ARG	4.7
1	C	111	PHE	4.4
1	B	1	MET	4.3
1	C	22[A]	HIS	4.3
1	C	44	ARG	4.2
1	D	303	MET	4.0
1	D	302	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	46	GLY	3.9
1	C	46	GLY	3.9
1	A	22	HIS	3.9
1	C	47	THR	3.8
1	C	109	ARG	3.7
1	C	139[A]	GLU	3.7
1	C	276	LEU	3.6
1	C	118	SER	3.4
1	D	21	ARG	3.4
1	D	47	THR	3.4
1	C	1	MET	3.3
1	D	110	ASP	3.3
1	C	122	GLU	3.3
1	C	121	GLN	3.3
1	A	307	VAL	3.3
1	C	12	ALA	3.1
1	D	255	HIS	3.0
1	C	300	THR	3.0
1	B	22	HIS	2.9
1	C	280	GLU	2.8
1	D	160[A]	ASP	2.7
1	C	105	ALA	2.7
1	D	276	LEU	2.7
1	C	43	ASP	2.7
1	C	119	ALA	2.6
1	D	141	LYS	2.6
1	C	28	LEU	2.6
1	C	94[A]	GLU	2.6
1	C	63[A]	ASP	2.5
1	C	293[A]	GLU	2.5
1	D	103[A]	TRP	2.5
1	C	255[A]	HIS	2.5
1	C	138	ALA	2.5
1	C	278	LYS	2.4
1	D	152	VAL	2.3
1	C	42	GLU	2.3
1	D	151	GLY	2.3
1	D	12	ALA	2.3
1	D	94	GLU	2.3
1	D	138	ALA	2.3
1	C	108	SER	2.3
1	C	48	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	144	ASP	2.3
1	D	139[A]	GLU	2.2
1	D	147	TYR	2.2
1	D	234	ILE	2.2
1	C	117	PHE	2.1
1	D	63	ASP	2.1
1	D	253	LEU	2.1
1	D	280[A]	GLU	2.1
1	C	40	LYS	2.1
1	C	92	ALA	2.1
1	A	28	LEU	2.1
1	C	261	ILE	2.1
1	D	31	VAL	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^{th} 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
5	GOL	D	404	6/6	0.67	0.16	43,44,45,45	6
5	GOL	C	403	6/6	0.79	0.21	60,61,63,64	0
4	DTT	A	403	8/8	0.80	0.18	32,39,48,50	0
5	GOL	D	403	6/6	0.82	0.21	66,66,67,67	0
5	GOL	A	405	6/6	0.83	0.17	39,40,44,47	0
3	D16	C	402	32/32	0.83	0.14	32,40,54,56	0
7	MES	B	406	12/12	0.83	0.15	44,46,50,51	12
5	GOL	B	405	6/6	0.85	0.12	67,68,69,69	0
5	GOL	A	407[A]	6/6	0.86	0.21	44,49,50,52	6
5	GOL	A	406	6/6	0.86	0.12	53,56,56,57	0

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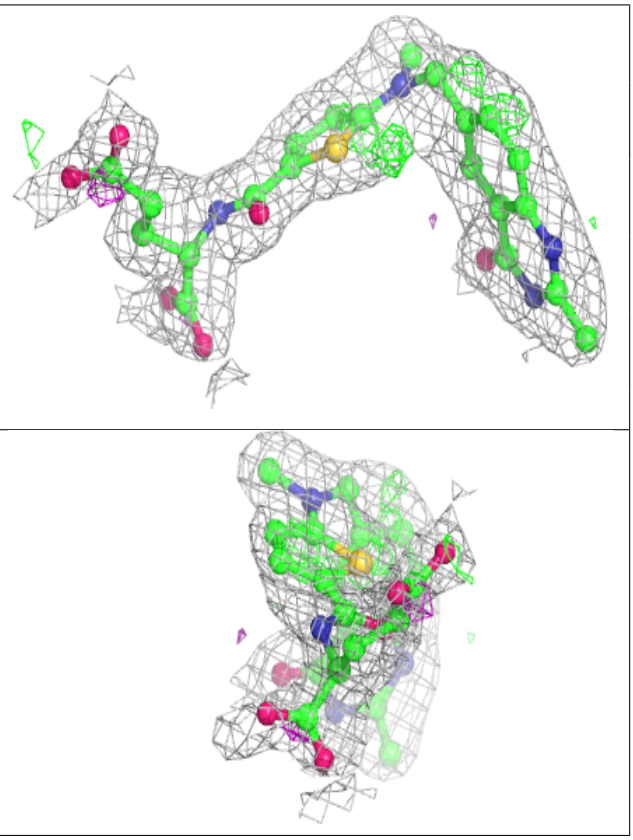
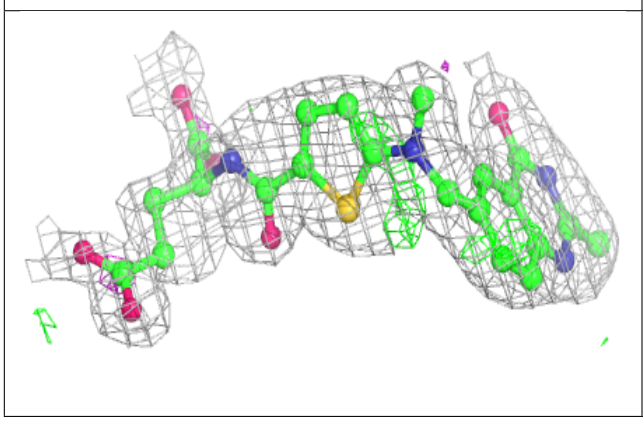
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	407[B]	6/6	0.86	0.21	41,43,45,45	6
5	GOL	B	403[B]	6/6	0.87	0.24	37,39,39,40	6
5	GOL	B	403[A]	6/6	0.87	0.24	36,39,41,42	6
3	D16	D	402	32/32	0.88	0.12	39,44,55,59	0
6	SO4	A	408	5/5	0.89	0.16	41,41,43,44	5
5	GOL	B	404[B]	6/6	0.90	0.22	13,18,19,19	6
5	GOL	B	404[A]	6/6	0.90	0.22	30,33,37,37	6
3	D16	A	402	32/32	0.93	0.09	18,23,31,38	0
3	D16	B	402	32/32	0.93	0.10	13,24,34,41	0
5	GOL	A	404[A]	6/6	0.93	0.19	23,31,31,31	6
5	GOL	A	404[B]	6/6	0.93	0.19	25,30,31,31	6
2	UMP	C	401	20/20	0.94	0.08	29,33,37,40	0
2	UMP	D	401	20/20	0.95	0.08	25,32,36,37	0
2	UMP	A	401	20/20	0.98	0.07	16,17,20,24	0
2	UMP	B	401	20/20	0.99	0.07	14,16,20,21	0

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

Electron density around D16 C 402:

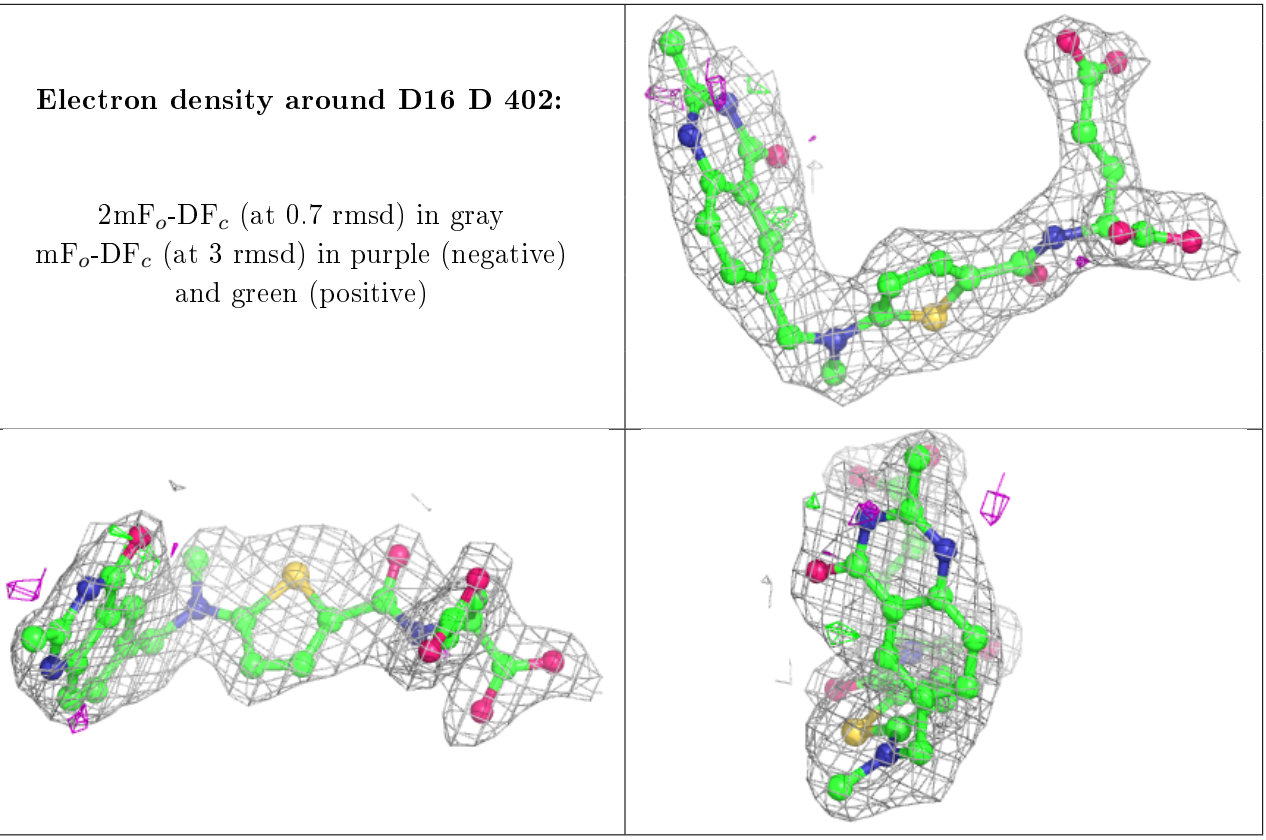
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





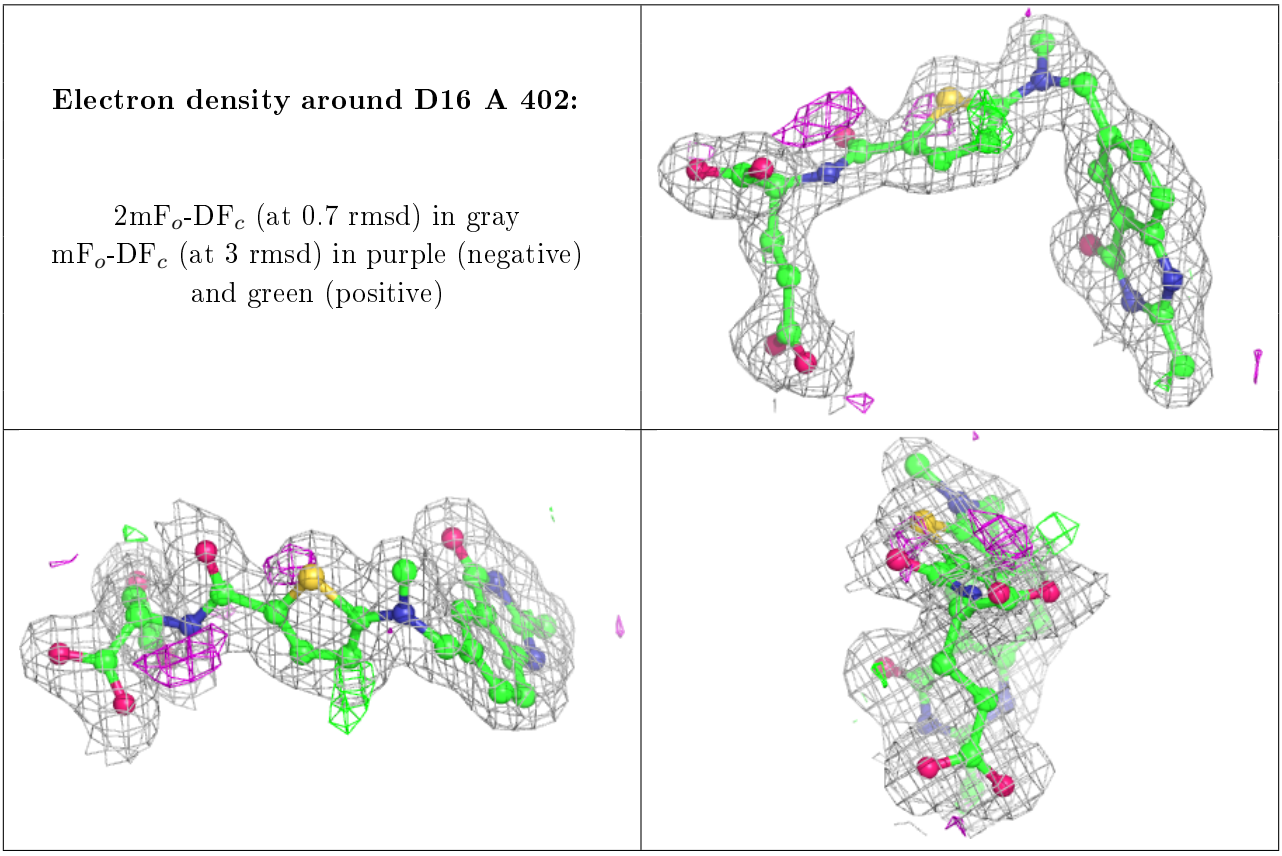
Electron density around D16 D 402:

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



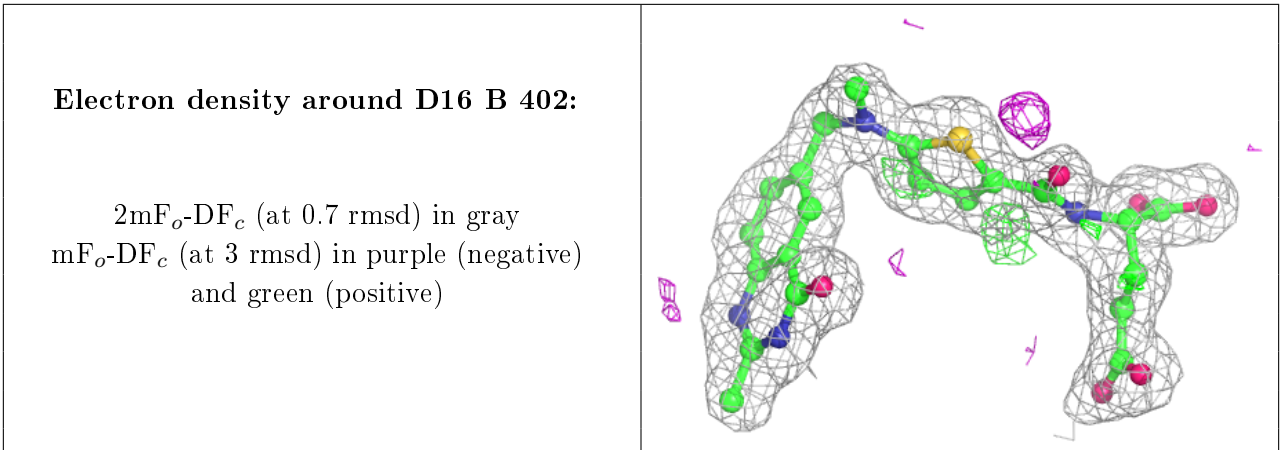
Electron density around D16 A 402:

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



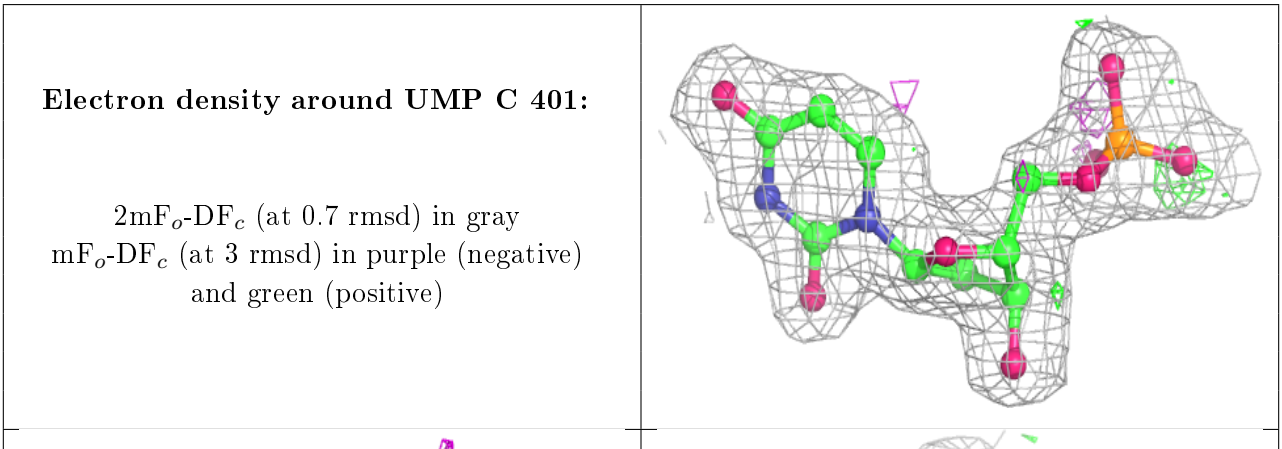
Electron density around D16 B 402:

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



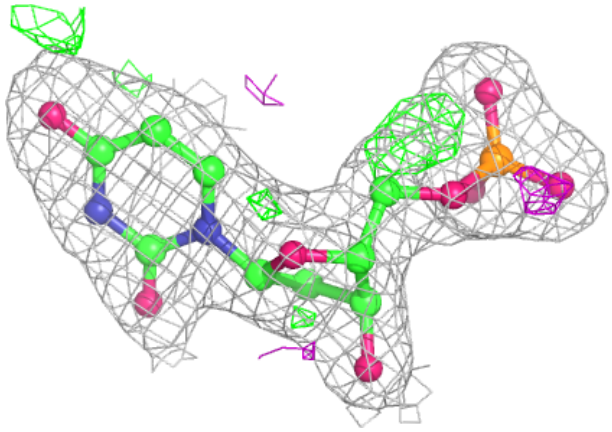
Electron density around UMP C 401:

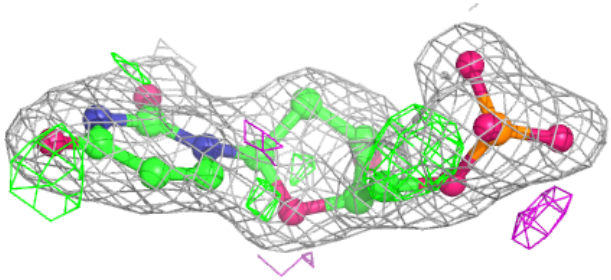
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

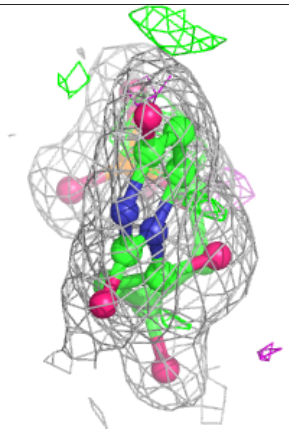


Electron density around UMP D 401:

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

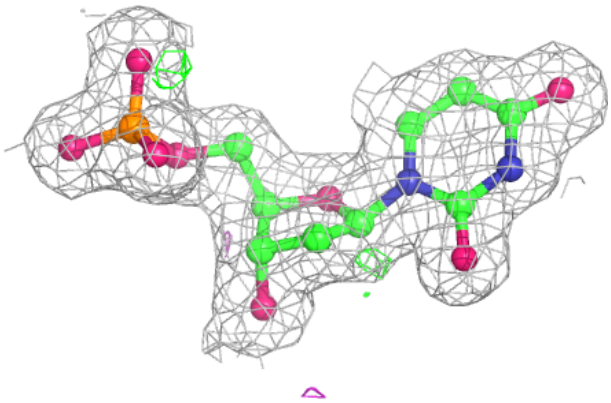


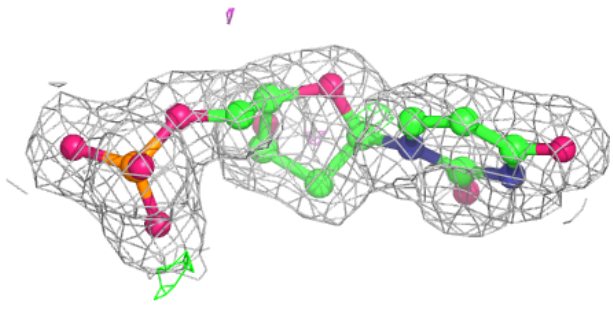


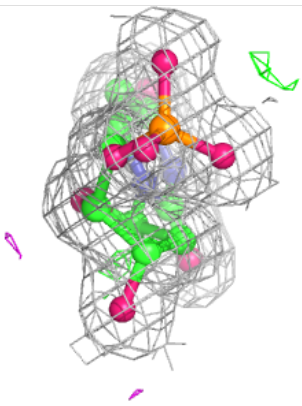


Electron density around UMP A 401:

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

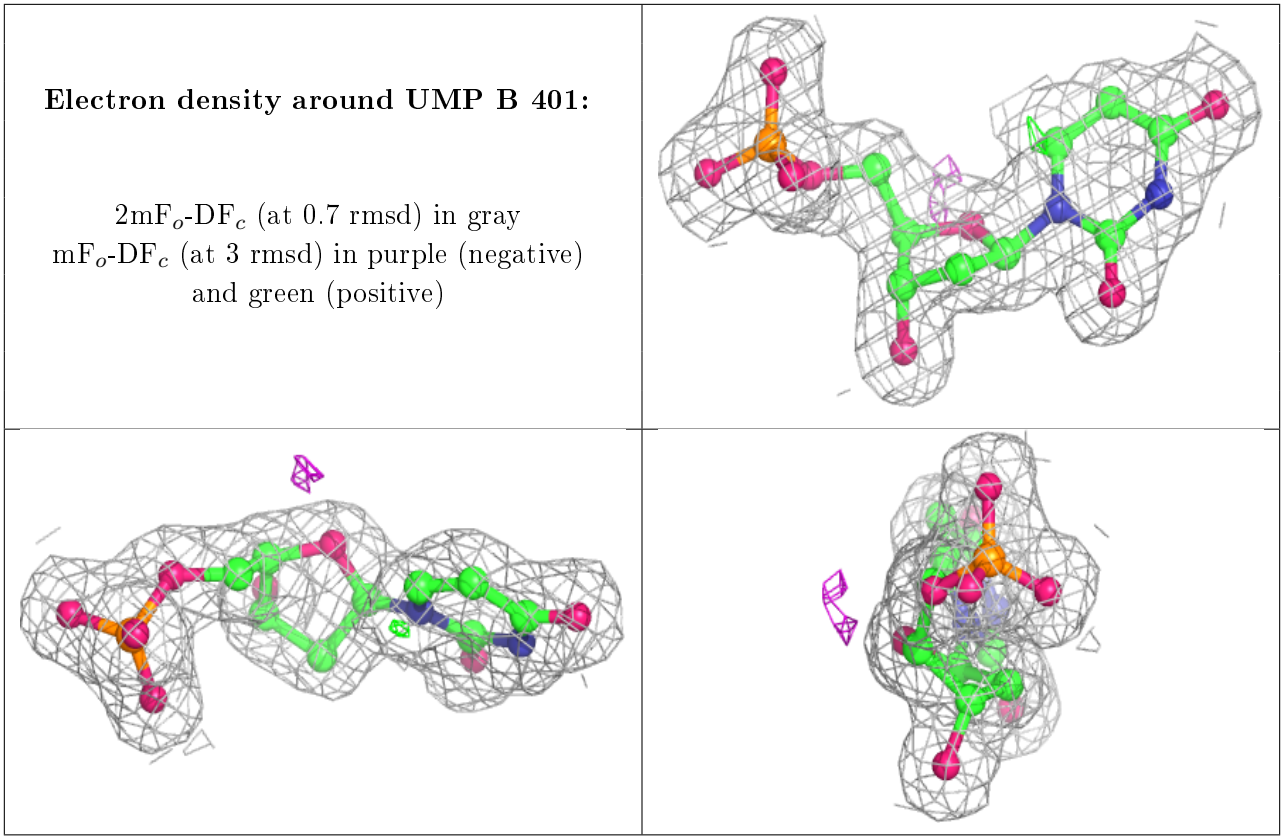






Electron density around UMP B 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.