Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:04 pm BST

PDB ID	:	5T7O
Title	:	Crystal structure of Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase in complex with (6S)-5,6,7,8-TETRAHYDROFOLATE
Authors	:	Di Pisa, F.; Dello Iacono, L.; Bonucci, A.; Mangani, S.
Deposited on	:	2016-09-05
Resolution	:	1.80 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:

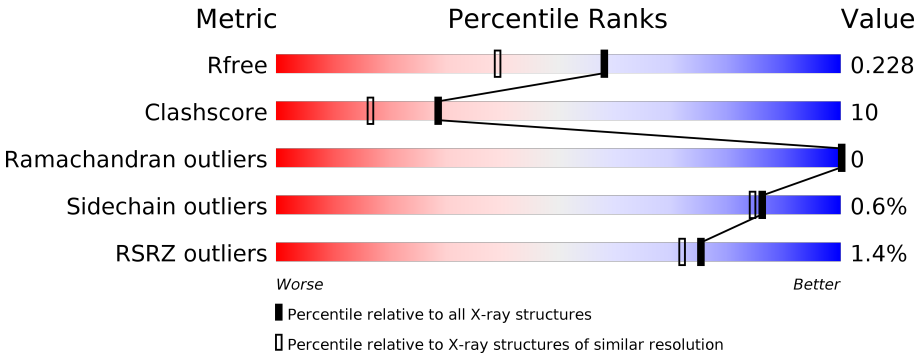
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	521	84% 11% 5%
1	B	521	80% 15% 5%
1	C	521	82% 11% 7%
1	D	521	80% 13% 6%

2 Entry composition

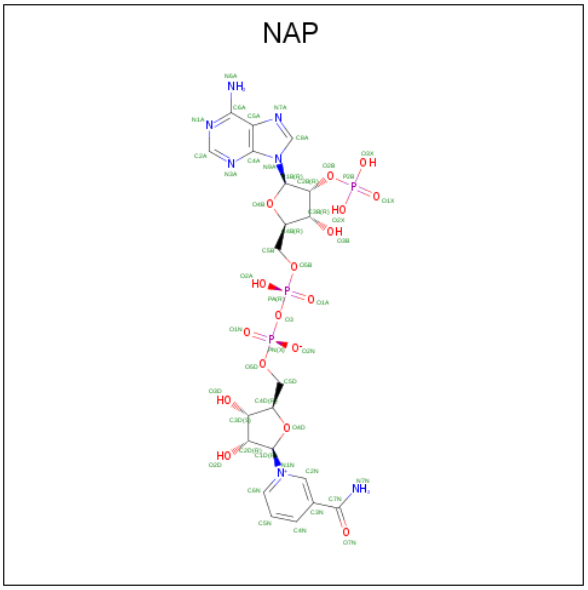
There are 6 unique types of molecules in this entry. The entry contains 18488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	25	0
			4003	2563	698	720	22			
1	B	495	Total	C	N	O	S	0	21	0
			4017	2572	701	722	22			
1	C	487	Total	C	N	O	S	0	23	0
			3947	2531	689	707	20			
1	D	489	Total	C	N	O	S	0	13	0
			3909	2501	684	707	17			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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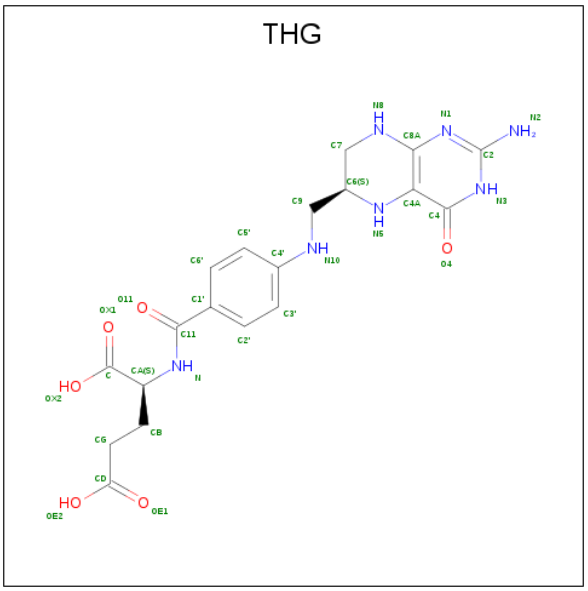
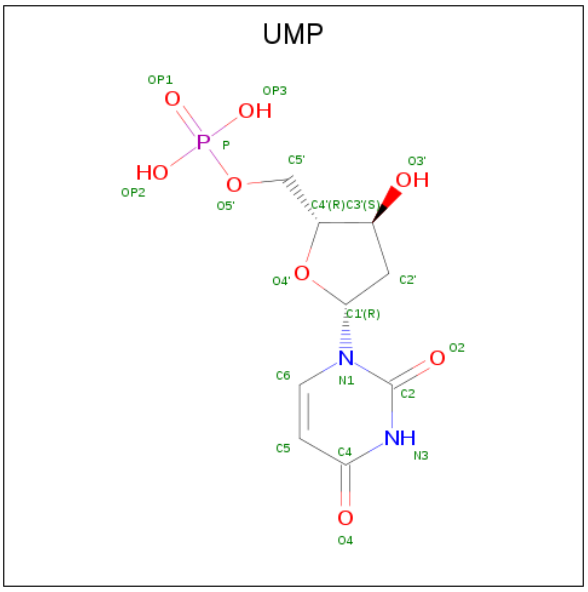
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).



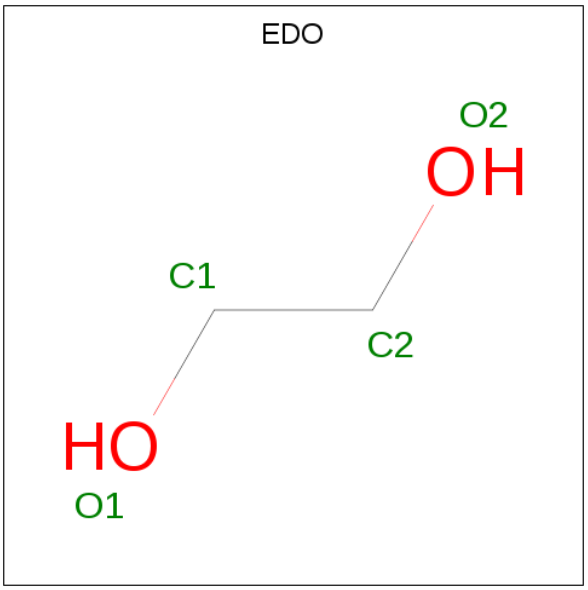
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	7	6		
3	B	1	Total	C	N	O	0	0
			32	19	7	6		
3	C	1	Total	C	N	O	0	0
			32	19	7	6		
3	D	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

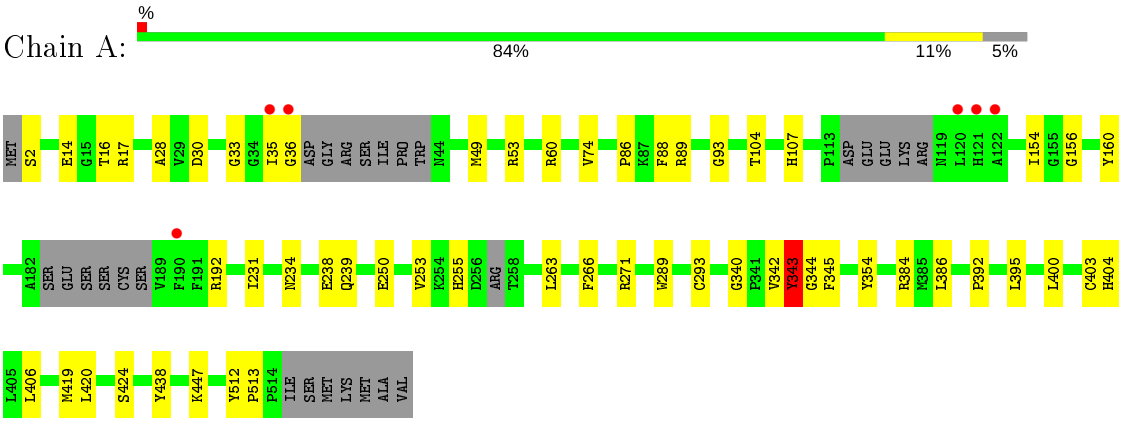
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	527	Total O 527 527	0	0
6	B	514	Total O 514 514	0	4
6	C	518	Total O 518 518	0	1
6	D	465	Total O 465 465	0	0

3 Residue-property plots (i)

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

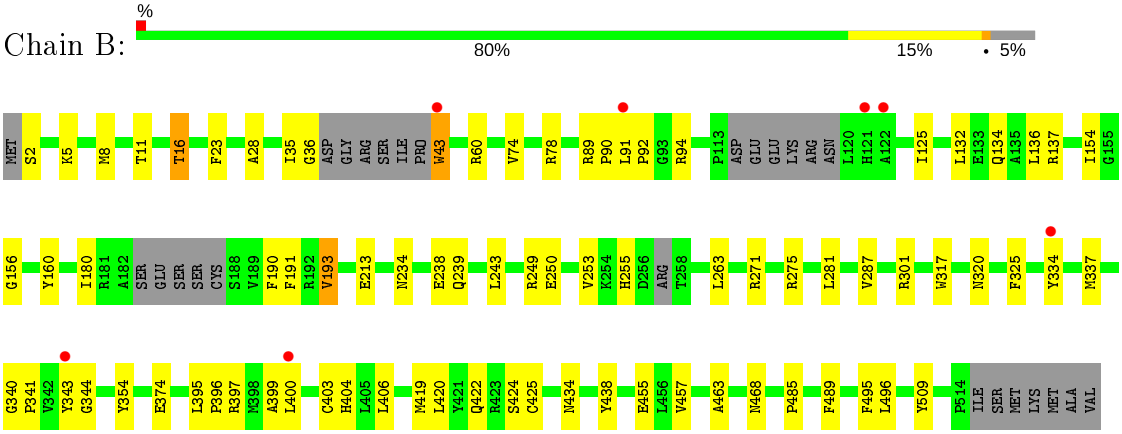
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:



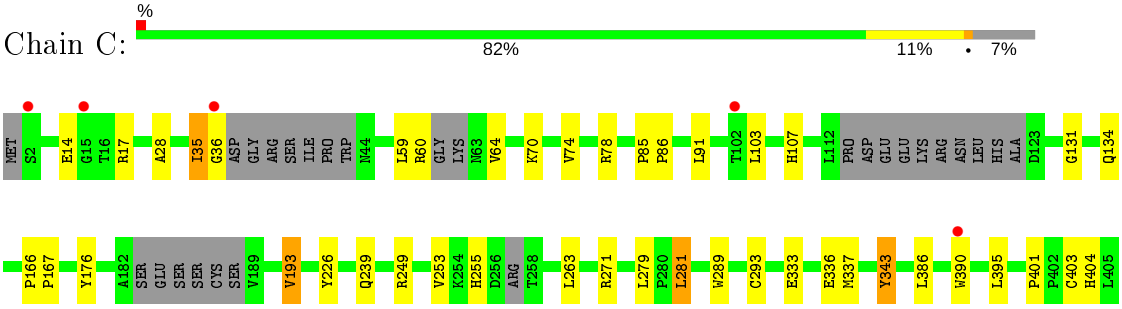
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

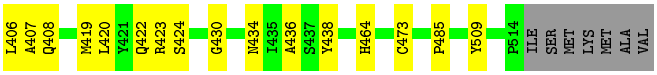
Chain B:



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

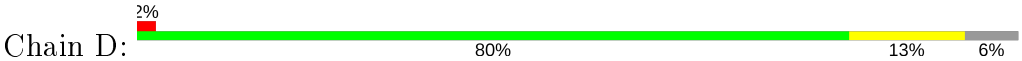
Chain C:

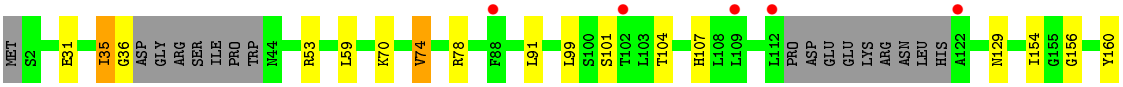


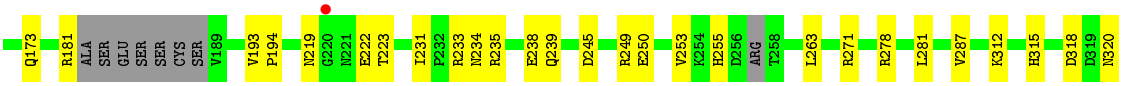


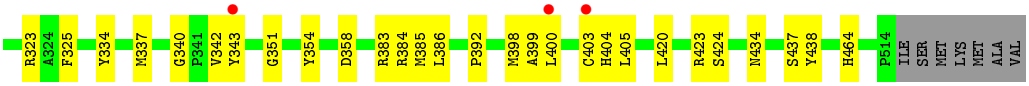
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.55Å 173.54Å 174.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.77 – 1.80 69.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.77-1.80) 99.2 (69.51-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.220 0.188 , 0.228	Depositor DCC
R_{free} test set	10547 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0996e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: THG, NAP, UMP, EDO

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	1.24	2/4161 (0.0%)	1.08	4/5648 (0.1%)
1	B	1.23	0/4169	1.07	0/5659
1	C	1.25	1/4092 (0.0%)	1.12	3/5550 (0.1%)
1	D	1.23	1/4027 (0.0%)	1.08	2/5467 (0.0%)
All	All	1.24	4/16449 (0.0%)	1.09	9/22324 (0.0%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	343	TYR	CB-CG	19.02	1.80	1.51
1	D	385	MET	C-N	-8.31	1.15	1.34
1	A	344	GLY	N-CA	6.48	1.55	1.46
1	A	344	GLY	CA-C	-5.03	1.43	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	343	TYR	CA-CB-CG	-6.66	100.75	113.40
1	C	343	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	343	TYR	CB-CG-CD1	6.38	124.83	121.00
1	A	400	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	74[A]	VAL	CB-CA-C	5.39	121.65	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	74[B]	VAL	CB-CA-C	5.39	121.65	111.40
1	A	386	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	386	LEU	CB-CA-C	-5.22	100.29	110.20
1	A	343	TYR	N-CA-CB	5.14	119.85	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	TYR	Mainchain

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	4003	0	3985	65	0
1	B	4017	0	3996	99	0
1	C	3947	0	3957	72	0
1	D	3909	0	3857	82	0
2	A	48	0	25	5	0
2	B	48	0	25	11	0
2	C	48	0	25	3	0
2	D	48	0	25	8	0
3	A	32	0	21	3	0
3	B	32	0	21	2	0
3	C	32	0	21	1	0
3	D	32	0	21	3	0
4	A	20	0	11	4	0
4	B	20	0	11	3	0
4	C	20	0	11	5	0
4	D	20	0	11	2	0
5	A	56	0	84	5	0
5	B	48	0	72	8	0
5	C	44	0	66	9	0
5	D	40	0	60	3	0
6	A	527	0	0	12	0
6	B	514	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	518	0	0	9	0
6	D	465	0	0	15	0
All	All	18488	0	16305	319	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 10.

All (319) 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:343:TYR:CB	1:C:343:TYR:CG	1.80	1.64
1:B:337:MET:HG3	6:B:1142:HOH:O	1.42	1.19
1:B:8[B]:MET:CE	1:B:496:LEU:N	2.07	1.15
1:D:337:MET:HG3	6:D:1228:HOH:O	1.47	1.15
6:C:1040:HOH:O	1:D:400:LEU:HD23	1.50	1.11
1:B:8[B]:MET:HE3	1:B:496:LEU:N	1.63	1.06
1:A:253[B]:VAL:HG22	6:A:968:HOH:O	1.53	1.05
1:D:238:GLU:OE1	6:D:801:HOH:O	1.78	1.01
1:A:238:GLU:OE1	6:A:801:HOH:O	1.81	0.98
1:A:403[C]:CYS:SG	4:A:703:UMP:C5	2.57	0.97
1:C:35[A]:ILE:HG13	1:C:36[A]:GLY:N	1.78	0.96
1:B:8[B]:MET:HE3	1:B:495:PHE:C	1.86	0.95
1:B:8[B]:MET:HE1	1:B:496:LEU:N	1.79	0.95
1:B:334:TYR:OH	1:B:397[B]:ARG:NH2	1.99	0.95
1:A:403[C]:CYS:SG	4:A:703:UMP:C4	2.60	0.94
1:A:253[B]:VAL:HG21	6:D:919:HOH:O	1.70	0.92
1:B:320:ASN:CG	1:B:400:LEU:HD11	1.91	0.91
1:C:390:TRP:CE2	1:D:386:LEU:HD22	2.05	0.90
1:C:289:TRP:CZ2	1:C:293[B]:CYS:SG	2.64	0.90
1:D:343:TYR:OH	6:D:802:HOH:O	1.90	0.89
1:D:222:GLU:HG3	6:D:1014:HOH:O	1.73	0.88
1:B:403[C]:CYS:SG	4:B:602:UMP:C4	2.68	0.86
1:C:343:TYR:CA	1:C:343:TYR:CG	2.60	0.85
1:C:289:TRP:CE2	1:C:293[B]:CYS:SG	2.69	0.85
1:B:35[A]:ILE:HD12	2:B:603:NAP:C5N	2.07	0.84
1:C:166:PRO:HB2	5:C:610:EDO:H22	1.58	0.84
1:B:8[B]:MET:HE1	1:B:496:LEU:H	1.39	0.83
1:B:43:TRP:HZ3	2:B:603:NAP:H71N	1.26	0.83
1:B:320:ASN:ND2	1:B:400:LEU:HD11	1.95	0.82
1:D:239:GLN:HE22	1:D:271:ARG:H	1.28	0.82
5:A:714:EDO:H11	6:A:811:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:CYS:SG	1:D:424:SER:O	2.40	0.79
1:A:104:THR:H	1:A:107[B]:HIS:HD2	1.26	0.78
1:B:334:TYR:OH	1:B:397[B]:ARG:CZ	2.31	0.78
1:C:434[A]:ASN:HD21	4:C:603:UMP:HN3	1.32	0.78
1:A:35[A]:ILE:HG13	1:A:36[A]:GLY:N	1.98	0.77
1:A:35[A]:ILE:CG1	1:A:36[A]:GLY:N	2.47	0.77
1:C:28:ALA:O	2:C:602:NAP:N7N	2.17	0.77
1:B:400:LEU:HD23	6:B:1063:HOH:O	1.84	0.77
1:C:78:ARG:HD3	2:C:602:NAP:O2X	1.85	0.77
1:D:253:VAL:HG22	1:D:263[A]:LEU:CD2	2.15	0.76
1:A:384:ARG:HD2	6:A:1025:HOH:O	1.86	0.75
1:B:43:TRP:HZ3	2:B:603:NAP:N7N	1.84	0.74
1:C:390:TRP:NE1	1:D:386:LEU:HD22	2.02	0.74
1:B:74:VAL:HG21	1:B:91:LEU:HD12	1.70	0.74
1:D:400:LEU:O	6:D:803:HOH:O	2.05	0.73
1:D:315:HIS:HE1	6:D:1135:HOH:O	1.72	0.72
1:B:400:LEU:O	6:B:701:HOH:O	2.06	0.72
1:A:156:GLY:HA2	2:A:701:NAP:H5N	1.72	0.72
1:C:253:VAL:HG22	1:C:263[A]:LEU:CD2	2.20	0.72
1:A:234:ASN:O	1:A:238:GLU:HG3	1.90	0.71
1:B:255:HIS:HD2	6:C:1068:HOH:O	1.73	0.71
1:A:192:ARG:H	5:A:713:EDO:H22	1.54	0.71
1:A:404:HIS:HD2	1:A:438:TYR:OH	1.74	0.70
1:C:166:PRO:CB	5:C:610:EDO:H22	2.22	0.70
1:D:323:ARG:NH2	1:D:334:TYR:O	2.16	0.70
1:D:253:VAL:HG22	1:D:263[A]:LEU:HD21	1.73	0.70
1:A:406:LEU:HD21	1:B:406:LEU:CD2	2.23	0.69
1:B:403[C]:CYS:SG	4:B:602:UMP:C5	2.86	0.69
1:D:233:ARG:NH2	1:D:235:ARG:NH1	2.41	0.68
1:D:233:ARG:HH21	1:D:235:ARG:NH1	1.92	0.68
1:B:8[B]:MET:HE3	1:B:496:LEU:CA	2.23	0.68
1:B:374:GLU:HG3	6:B:1076:HOH:O	1.94	0.67
1:B:78:ARG:HD3	2:B:603:NAP:O2X	1.94	0.67
1:A:104:THR:H	1:A:107[B]:HIS:CD2	2.11	0.67
2:B:603:NAP:H52N	2:B:603:NAP:H6N	1.77	0.67
1:C:14:GLU:OE1	1:C:17:ARG:NH1	2.26	0.67
1:D:233:ARG:NE	1:D:235:ARG:CZ	2.58	0.67
1:A:404:HIS:HB2	1:A:420[A]:LEU:HD11	1.76	0.67
1:C:343:TYR:CB	1:C:343:TYR:CD2	2.72	0.66
1:C:386[B]:LEU:CD2	1:C:408:GLN:HB2	2.25	0.66
1:D:249:ARG:O	1:D:250:GLU:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:HE2	2:A:701:NAP:H4N	1.61	0.66
1:A:93:GLY:HA2	5:A:717:EDO:H22	1.77	0.66
1:B:8[B]:MET:CE	1:B:496:LEU:CA	2.74	0.66
1:C:239:GLN:HE22	1:C:271:ARG:H	1.42	0.66
1:C:509:TYR:HD2	5:C:614:EDO:H21	1.61	0.66
1:B:320:ASN:CG	1:B:400:LEU:CD1	2.64	0.65
1:A:255:HIS:HD2	6:A:1197:HOH:O	1.80	0.65
1:A:406:LEU:HD21	1:B:406:LEU:HD21	1.78	0.65
1:B:253:VAL:HG22	1:B:263[B]:LEU:CD2	2.26	0.65
1:D:320:ASN:ND2	1:D:400:LEU:HD11	2.12	0.65
1:B:43:TRP:CZ3	2:B:603:NAP:N7N	2.65	0.64
1:D:384:ARG:HD2	6:D:966:HOH:O	1.96	0.64
1:C:509:TYR:CD2	5:C:614:EDO:H21	2.32	0.64
1:C:253:VAL:HG22	1:C:263[A]:LEU:HD21	1.79	0.64
1:A:53:ARG:NH2	3:A:702:THG:OE2	2.30	0.64
1:D:281[A]:LEU:HD22	1:D:287:VAL:HB	1.78	0.64
6:A:1136:HOH:O	1:D:255:HIS:HD2	1.80	0.63
1:D:78:ARG:HD3	2:D:701:NAP:O2X	1.98	0.63
1:B:419[B]:MET:HG2	1:B:457:VAL:HB	1.80	0.63
1:A:239:GLN:HE22	1:A:271:ARG:H	1.47	0.63
1:B:404:HIS:HB2	1:B:420:LEU:HD11	1.81	0.63
1:B:134[B]:GLN:NE2	1:B:137:ARG:HH11	1.98	0.62
1:B:92:PRO:HD2	1:B:94:ARG:NH2	2.14	0.62
1:B:403[A]:CYS:SG	1:B:424:SER:O	2.57	0.62
1:A:16[B]:THR:HG21	1:A:447:LYS:HZ3	1.63	0.62
1:C:404:HIS:HD2	1:C:438:TYR:OH	1.82	0.62
1:D:234:ASN:O	1:D:238:GLU:HG3	1.99	0.62
1:A:49[B]:MET:HE2	1:A:49[B]:MET:HA	1.81	0.62
1:B:404:HIS:HD2	1:B:438:TYR:OH	1.81	0.62
1:C:35[A]:ILE:HG13	1:C:36[A]:GLY:H	1.62	0.61
1:B:134[B]:GLN:NE2	1:B:137:ARG:NH1	2.49	0.61
1:D:405:LEU:HD23	1:D:423:ARG:HG2	1.83	0.61
1:B:239:GLN:HE22	1:B:271:ARG:H	1.47	0.61
1:D:343:TYR:CE1	1:D:404:HIS:CE1	2.88	0.61
1:C:390:TRP:NE1	1:D:386:LEU:CD2	2.62	0.61
1:D:74[A]:VAL:HG11	1:D:91:LEU:HD12	1.81	0.61
1:B:422[B]:GLN:HE22	1:B:434[B]:ASN:CG	2.04	0.61
1:A:403[B]:CYS:SG	4:A:703:UMP:C6	2.94	0.60
1:A:403[A]:CYS:SG	1:A:424:SER:O	2.59	0.60
1:D:59[B]:LEU:HD21	1:D:70:LYS:HG3	1.84	0.60
1:B:35[A]:ILE:HG13	1:B:36[A]:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8[B]:MET:CE	1:B:495:PHE:C	2.56	0.60
1:D:404:HIS:HD2	1:D:438:TYR:OH	1.85	0.60
1:D:59[B]:LEU:CD2	1:D:70:LYS:HG3	2.31	0.60
1:B:92:PRO:HD2	1:B:94:ARG:HH21	1.66	0.59
1:C:249:ARG:NH1	5:C:607:EDO:H12	2.17	0.59
4:B:602:UMP:O4	5:B:611:EDO:H11	2.02	0.59
1:C:279:LEU:HG	1:C:281[C]:LEU:HD13	1.84	0.59
1:C:403[A]:CYS:SG	1:C:424:SER:O	2.61	0.58
1:B:253:VAL:HG22	1:B:263[B]:LEU:HD21	1.84	0.58
1:A:156:GLY:CA	2:A:701:NAP:H5N	2.34	0.57
1:A:16[B]:THR:HG21	1:A:447:LYS:NZ	2.19	0.57
1:D:358:ASP:H	5:D:708:EDO:C1	2.17	0.57
1:D:35[A]:ILE:CG1	1:D:36[A]:GLY:N	2.68	0.57
1:A:35[A]:ILE:CG1	1:A:36[A]:GLY:H	2.16	0.56
1:B:160:TYR:HE2	2:B:603:NAP:H4N	1.69	0.56
1:A:35[A]:ILE:HG12	1:A:36[A]:GLY:H	1.71	0.56
1:D:104:THR:H	1:D:107[B]:HIS:HD2	1.53	0.56
1:A:406:LEU:CD2	1:B:406:LEU:CD2	2.84	0.56
1:D:315:HIS:HD2	1:D:318:ASP:OD2	1.89	0.56
1:B:16[A]:THR:HG22	6:B:756:HOH:O	2.05	0.56
1:B:154:ILE:O	3:B:601:THG:HC72	2.05	0.55
1:C:176:TYR:HE2	5:C:611:EDO:H21	1.71	0.55
1:A:406:LEU:CD2	1:B:406:LEU:HD23	2.36	0.55
2:A:701:NAP:H6N	2:A:701:NAP:H52N	1.89	0.55
1:A:271:ARG:HD2	6:A:980:HOH:O	2.06	0.55
1:C:386[B]:LEU:HD11	1:D:423:ARG:HD3	1.89	0.55
1:C:386[B]:LEU:HD21	1:C:408:GLN:HB2	1.88	0.55
2:D:701:NAP:C7N	6:D:813:HOH:O	2.54	0.55
1:C:253:VAL:HG22	1:C:263[A]:LEU:HD23	1.88	0.55
6:B:898:HOH:O	1:C:193[B]:VAL:HG22	2.07	0.55
1:D:233:ARG:NH2	1:D:235:ARG:HH12	2.04	0.55
1:D:358:ASP:H	5:D:708:EDO:H12	1.73	0.54
1:C:473:CYS:SG	6:C:1116:HOH:O	2.58	0.54
1:B:374:GLU:CG	6:B:1076:HOH:O	2.52	0.54
1:C:422:GLN:HE22	1:C:434[A]:ASN:ND2	2.04	0.54
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.90	0.54
1:B:325:PHE:HZ	1:B:400:LEU:HD21	1.72	0.54
1:C:404:HIS:HB2	1:C:420[A]:LEU:HD11	1.88	0.54
1:B:249:ARG:NH1	5:B:606:EDO:H11	2.23	0.54
1:D:156:GLY:HA2	2:D:701:NAP:H5N	1.90	0.54
1:D:245:ASP:O	1:D:249:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:VAL:HG22	1:D:263[A]:LEU:HD23	1.91	0.54
1:A:266:PHE:CZ	1:B:419[B]:MET:HB2	2.43	0.53
1:A:60[A]:ARG:NH1	6:A:810:HOH:O	2.42	0.53
1:D:343:TYR:CE1	1:D:404:HIS:NE2	2.75	0.53
1:A:404:HIS:CD2	1:A:438:TYR:OH	2.58	0.53
1:A:343:TYR:CE1	1:A:404:HIS:CE1	2.97	0.53
1:D:315:HIS:CD2	1:D:318:ASP:OD2	2.61	0.53
1:A:342:VAL:O	1:A:343:TYR:C	2.45	0.53
1:C:404:HIS:CD2	1:C:438:TYR:OH	2.61	0.53
1:A:406:LEU:HD21	1:B:406:LEU:HD23	1.91	0.53
1:D:74[B]:VAL:HG11	1:D:154:ILE:HD13	1.91	0.53
1:D:231:ILE:HG13	6:D:858:HOH:O	2.09	0.52
1:D:253:VAL:HG22	1:D:263[B]:LEU:HD22	1.91	0.52
1:B:340:GLY:HA2	1:B:354:TYR:CE2	2.44	0.52
1:C:386[B]:LEU:HD23	1:C:408:GLN:CB	2.39	0.52
6:B:898:HOH:O	1:C:193[B]:VAL:CG2	2.57	0.52
1:B:35[A]:ILE:HD12	2:B:603:NAP:H5N	1.87	0.52
1:A:16[B]:THR:HG21	1:A:447:LYS:HG2	1.92	0.52
1:B:281[A]:LEU:HD22	1:B:287:VAL:HB	1.92	0.52
1:B:404:HIS:CD2	1:B:438:TYR:OH	2.62	0.52
1:D:399:ALA:O	1:D:400:LEU:HG	2.10	0.52
1:A:253[B]:VAL:CG2	6:D:919:HOH:O	2.43	0.52
5:A:714:EDO:C1	6:A:811:HOH:O	2.51	0.52
1:D:383:ARG:NH2	6:D:804:HOH:O	2.26	0.51
1:D:101:SER:HA	1:D:129:ASN:ND2	2.26	0.51
1:C:464:HIS:CE1	4:C:603:UMP:HO3'	2.24	0.51
1:B:253:VAL:HG22	1:B:263[B]:LEU:HD23	1.91	0.51
1:B:250:GLU:HA	5:B:612:EDO:H21	1.93	0.51
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.45	0.51
1:C:35[A]:ILE:HD12	2:C:602:NAP:H2N	1.92	0.51
1:C:131:GLY:H	1:C:134:GLN:HE21	1.59	0.51
1:D:312:LYS:HE2	6:D:843:HOH:O	2.11	0.51
1:D:173:GLN:HE22	1:D:278:ARG:HH12	1.59	0.50
6:B:1070:HOH:O	1:C:255:HIS:HD2	1.93	0.50
1:B:156:GLY:HA2	2:B:603:NAP:H5N	1.93	0.50
5:C:604:EDO:H22	5:C:611:EDO:O1	2.11	0.50
1:B:2:SER:CB	6:B:1096:HOH:O	2.60	0.50
1:D:160:TYR:HE2	2:D:701:NAP:H4N	1.76	0.50
1:B:43:TRP:CD1	1:B:180:ILE:HG21	2.47	0.50
1:D:35[A]:ILE:HG12	1:D:36[A]:GLY:N	2.27	0.49
1:D:320:ASN:CG	1:D:400:LEU:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LEU:HD22	1:C:401:PRO:HB3	1.93	0.49
1:B:213:GLU:HG2	5:B:614:EDO:O2	2.13	0.49
1:C:386[B]:LEU:CD2	1:C:408:GLN:CB	2.91	0.49
1:D:104:THR:O	1:D:107[B]:HIS:HB2	2.11	0.49
1:D:104:THR:H	1:D:107[B]:HIS:CD2	2.30	0.49
1:A:250:GLU:HA	5:A:708:EDO:H11	1.93	0.49
5:B:609:EDO:H11	6:B:871:HOH:O	2.12	0.49
1:C:343:TYR:HA	1:C:343:TYR:CG	2.45	0.49
1:B:90:PRO:HG3	1:B:125:ILE:HD11	1.95	0.49
1:C:386[B]:LEU:HD23	1:C:408:GLN:HB2	1.93	0.49
1:C:60:ARG:HD3	6:C:704:HOH:O	2.13	0.48
1:D:404:HIS:CD2	1:D:438:TYR:OH	2.66	0.48
1:A:49[B]:MET:HE2	1:A:49[B]:MET:CA	2.42	0.48
1:C:59:LEU:HD12	1:C:64:VAL:HB	1.96	0.48
1:D:156:GLY:HA3	2:D:701:NAP:O1N	2.13	0.48
1:C:406:LEU:HD12	1:C:406:LEU:C	2.34	0.48
1:D:219:ASN:HD21	1:D:223:THR:HG23	1.79	0.48
1:B:325:PHE:CZ	1:B:400:LEU:HD21	2.49	0.48
1:B:341:PRO:HD2	1:B:397[B]:ARG:O	2.15	0.47
1:B:406:LEU:C	1:B:406:LEU:HD12	2.34	0.47
1:D:434[B]:ASN:HA	1:D:437[B]:SER:HB2	1.94	0.47
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.95	0.47
1:C:386[B]:LEU:CD1	1:D:423:ARG:HD3	2.45	0.47
1:D:154:ILE:O	3:D:703:THG:HC72	2.14	0.47
1:B:425[A]:CYS:HB2	1:B:463:ALA:HA	1.96	0.47
1:D:323:ARG:O	1:D:323:ARG:HD3	2.14	0.47
1:B:23:PHE:CE1	1:B:136:LEU:HD11	2.50	0.47
1:A:154:ILE:O	3:A:702:THG:HC72	2.15	0.47
1:C:107:HIS:HB2	6:C:1042:HOH:O	2.15	0.46
1:D:342:VAL:HG12	1:D:398:MET:HB3	1.97	0.46
1:C:167:PRO:N	5:C:610:EDO:H21	2.29	0.46
1:A:49[B]:MET:HA	1:A:49[B]:MET:CE	2.46	0.46
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.98	0.46
1:B:317:TRP:CZ2	1:B:343:TYR:HE2	2.34	0.46
1:B:317:TRP:HZ2	1:B:343:TYR:CE2	2.33	0.46
1:B:399:ALA:O	1:B:400:LEU:HG	2.15	0.46
1:D:464:HIS:NE2	4:D:702:UMP:O3'	2.40	0.46
1:B:243[B]:LEU:HG	6:B:791:HOH:O	2.15	0.45
1:C:333:GLU:HB2	6:C:1009:HOH:O	2.16	0.45
2:B:603:NAP:H2N	6:B:714:HOH:O	2.15	0.45
1:C:134:GLN:HG3	6:C:1114:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:O	1:B:238:GLU:HG3	2.16	0.45
1:B:275:ARG:HH22	1:B:455[B]:GLU:HG3	1.81	0.45
1:A:403[C]:CYS:SG	1:A:404:HIS:N	2.90	0.45
1:B:28:ALA:HB3	2:B:603:NAP:H72N	1.82	0.45
1:A:392:PRO:HA	1:A:395:LEU:HG	1.98	0.45
1:D:343:TYR:HE1	1:D:404:HIS:CE1	2.33	0.45
1:D:343:TYR:HE1	1:D:404:HIS:NE2	2.15	0.45
1:B:275:ARG:NH2	1:B:455[B]:GLU:HG3	2.32	0.45
1:B:420:LEU:HD22	1:B:438:TYR:CD1	2.51	0.45
1:B:23:PHE:CZ	1:B:132:LEU:HD21	2.52	0.44
1:C:386[B]:LEU:HD23	1:C:408:GLN:CA	2.47	0.44
1:B:406:LEU:HD12	1:B:406:LEU:O	2.17	0.44
3:B:601:THG:HC5	3:B:601:THG:HC92	1.66	0.44
1:C:464:HIS:NE2	4:C:603:UMP:O3'	2.34	0.44
1:A:74[B]:VAL:HG11	1:A:154:ILE:HD13	2.00	0.44
1:A:345:PHE:CZ	1:A:354:TYR:HD1	2.35	0.44
1:B:11:THR:HA	6:B:1084:HOH:O	2.16	0.44
1:D:351:GLY:HA2	5:D:710:EDO:H12	1.99	0.44
1:C:59:LEU:HD13	1:C:70:LYS:HG3	2.00	0.43
1:D:233:ARG:HE	1:D:235:ARG:CZ	2.30	0.43
1:B:60:ARG:NH2	6:B:702:HOH:O	2.29	0.43
1:C:176:TYR:CE2	5:C:611:EDO:H21	2.52	0.43
1:C:279:LEU:CG	1:C:281[C]:LEU:HD13	2.48	0.43
1:C:281[A]:LEU:HD23	1:C:436:ALA:HB2	1.99	0.43
1:C:74:VAL:HG21	1:C:91:LEU:HD12	1.99	0.43
1:B:253:VAL:HG11	1:C:226:TYR:OH	2.19	0.43
1:A:107[B]:HIS:CD2	6:A:888:HOH:O	2.71	0.43
1:A:30:ASP:OD1	1:A:33:GLY:N	2.51	0.43
1:A:86:PRO:HD3	1:A:89[A]:ARG:HH21	1.83	0.43
1:D:342:VAL:O	1:D:343:TYR:C	2.56	0.43
1:D:53:ARG:NH1	3:D:703:THG:OE1	2.51	0.43
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.53	0.43
1:B:317:TRP:CZ2	1:B:343:TYR:CE2	3.07	0.43
1:B:485:PRO:HB3	1:B:509:TYR:HA	2.00	0.43
1:A:30:ASP:OD1	1:A:30:ASP:C	2.57	0.43
1:B:91:LEU:HB3	1:B:94:ARG:CZ	2.48	0.43
1:D:320:ASN:CG	1:D:400:LEU:HD12	2.39	0.43
1:A:14:GLU:OE1	1:A:17:ARG:NH1	2.51	0.43
1:B:343:TYR:HB3	1:B:344:GLY:H	1.55	0.43
1:C:336:GLU:O	1:C:337[B]:MET:HB2	2.19	0.43
1:B:5:LYS:NZ	6:B:723:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:HA	5:B:613:EDO:H22	2.00	0.43
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.00	0.43
1:A:28:ALA:O	2:A:701:NAP:N7N	2.52	0.42
1:C:406:LEU:HD12	1:C:406:LEU:O	2.19	0.42
1:D:31:GLU:HG3	1:D:181:ARG:HA	2.02	0.42
1:A:289:TRP:CZ2	1:A:293[B]:CYS:SG	3.12	0.42
2:D:701:NAP:O7N	3:D:703:THG:HC71	2.20	0.42
1:A:2:SER:CB	6:A:1233:HOH:O	2.67	0.42
1:A:403[B]:CYS:SG	4:A:703:UMP:C5	3.13	0.42
1:C:134:GLN:NE2	1:C:134:GLN:H	2.18	0.42
1:C:407:ALA:HA	1:C:419:MET:O	2.19	0.42
1:A:88:PHE:CE2	3:A:702:THG:HCG2	2.54	0.42
1:B:89:ARG:HA	1:B:90:PRO:HA	1.91	0.42
1:C:103:LEU:HD22	1:C:107:HIS:CD2	2.55	0.42
1:D:99:LEU:O	2:D:701:NAP:H1B	2.20	0.42
4:D:702:UMP:H5	6:D:802:HOH:O	2.01	0.42
1:C:430:GLY:HA3	4:C:603:UMP:O2	2.20	0.42
1:B:193[B]:VAL:HG22	6:B:1066:HOH:O	2.20	0.42
1:B:16[A]:THR:HG21	1:B:489:PHE:CD1	2.54	0.42
1:B:193[B]:VAL:CG2	6:B:1066:HOH:O	2.68	0.42
1:B:343:TYR:CE1	1:B:404:HIS:CE1	3.08	0.42
1:B:60:ARG:HD3	6:B:1152[A]:HOH:O	2.18	0.42
1:D:325:PHE:HZ	1:D:400:LEU:HD21	1.84	0.42
1:B:301:ARG:NH2	6:B:717:HOH:O	2.51	0.41
6:C:1183:HOH:O	1:D:392:PRO:HB3	2.19	0.41
1:B:190:PHE:O	5:B:613:EDO:H22	2.20	0.41
1:B:399:ALA:C	1:B:400:LEU:HG	2.41	0.41
1:D:193:VAL:HA	1:D:194:PRO:HD3	1.77	0.41
1:D:315:HIS:CE1	6:D:1135:HOH:O	2.57	0.41
1:A:49[B]:MET:CA	1:A:49[B]:MET:CE	2.99	0.41
1:C:434[B]:ASN:ND2	4:C:603:UMP:O4	2.48	0.41
1:C:85:PRO:HA	1:C:86:PRO:HD2	1.77	0.41
1:C:423:ARG:NH1	1:D:383:ARG:O	2.48	0.41
2:D:701:NAP:H6N	2:D:701:NAP:H52N	2.03	0.41
1:A:35[B]:ILE:H	1:A:35[B]:ILE:HG12	1.68	0.41
1:C:386[B]:LEU:HD23	1:C:408:GLN:HA	2.02	0.41
1:B:249:ARG:HH12	5:B:606:EDO:H11	1.86	0.41
1:A:231:ILE:HG13	6:A:869:HOH:O	2.21	0.40
3:C:601:THG:HC5	3:C:601:THG:HC92	1.56	0.40
6:C:1040:HOH:O	1:D:400:LEU:CD2	2.31	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	508/521 (98%)	494 (97%)	14 (3%)	0	100	100
1	B	506/521 (97%)	495 (98%)	11 (2%)	0	100	100
1	C	497/521 (95%)	485 (98%)	12 (2%)	0	100	100
1	D	491/521 (94%)	474 (96%)	17 (4%)	0	100	100
All	All	2002/2084 (96%)	1948 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	429/446 (96%)	428 (100%)	1 (0%)	93	92
1	B	431/446 (97%)	425 (99%)	6 (1%)	67	59
1	C	424/446 (95%)	418 (99%)	6 (1%)	67	59
1	D	413/446 (93%)	411 (100%)	2 (0%)	88	87
All	All	1697/1784 (95%)	1682 (99%)	15 (1%)	86	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	MET
1	B	16[A]	THR

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Mol	Chain	Res	Type
1	B	16[B]	THR
1	B	43	TRP
1	B	193[A]	VAL
1	B	193[B]	VAL
1	B	468	ASN
1	C	35[A]	ILE
1	C	35[B]	ILE
1	C	193[A]	VAL
1	C	193[B]	VAL
1	C	281[A]	LEU
1	C	281[C]	LEU
1	D	35[A]	ILE
1	D	35[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	404	HIS
1	A	476	GLN
1	B	129	ASN
1	B	143	ASN
1	B	239	GLN
1	B	277	ASN
1	B	404	HIS
1	B	469	HIS
1	B	474	ASN
1	C	107	HIS
1	C	129	ASN
1	C	134	GLN
1	C	143	ASN
1	C	239	GLN
1	C	277	ASN
1	C	356	HIS
1	C	379	ASN
1	C	404	HIS
1	C	469	HIS
1	D	129	ASN
1	D	143	ASN
1	D	173	GLN
1	D	239	GLN
1	D	252	ASN

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Mol	Chain	Res	Type
1	D	277	ASN
1	D	315	HIS
1	D	320	ASN
1	D	404	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

59 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	EDO	B	613	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	C	613	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	608	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	609	-	3,3,3	0.46	0	2,2,2	0.34	0
2	NAP	B	603	-	45,52,52	1.16	5 (11%)	56,80,80	1.61	14 (25%)
5	EDO	B	615	-	3,3,3	0.82	0	2,2,2	0.41	0
5	EDO	A	712	-	3,3,3	0.44	0	2,2,2	0.49	0
5	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	C	606	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	C	611	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	708	-	3,3,3	0.41	0	2,2,2	0.37	0
5	EDO	C	604	-	3,3,3	0.70	0	2,2,2	0.39	0
5	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	716	-	3,3,3	0.47	0	2,2,2	1.19	0
5	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.34	0
4	UMP	C	603	-	18,21,21	1.10	1 (5%)	21,31,31	1.09	2 (9%)
5	EDO	A	713	-	3,3,3	0.98	0	2,2,2	0.50	0
5	EDO	B	605	-	3,3,3	0.73	0	2,2,2	0.72	0
5	EDO	C	609	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	709	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	C	607	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	C	608	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	705	-	3,3,3	0.59	0	2,2,2	0.77	0
4	UMP	B	602	-	18,21,21	1.28	4 (22%)	21,31,31	1.30	3 (14%)
5	EDO	D	707	-	3,3,3	0.42	0	2,2,2	0.61	0
4	UMP	A	703	-	18,21,21	1.10	1 (5%)	21,31,31	1.10	2 (9%)
5	EDO	A	706	-	3,3,3	0.68	0	2,2,2	0.79	0
5	EDO	A	714	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	711	-	3,3,3	0.46	0	2,2,2	0.34	0
2	NAP	A	701	-	45,52,52	1.12	4 (8%)	56,80,80	1.61	9 (16%)
5	EDO	C	605	-	3,3,3	0.34	0	2,2,2	0.81	0
5	EDO	D	705	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	D	709	-	3,3,3	0.94	0	2,2,2	0.74	0
5	EDO	D	713	-	3,3,3	0.45	0	2,2,2	0.34	0
3	THG	D	703	-	26,34,34	1.34	2 (7%)	31,47,47	1.60	5 (16%)
5	EDO	D	704	-	3,3,3	0.45	0	2,2,2	0.87	0
5	EDO	D	708	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	D	711	-	3,3,3	0.44	0	2,2,2	0.74	0
5	EDO	C	610	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	B	610	-	3,3,3	0.53	0	2,2,2	0.61	0
5	EDO	C	614	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	614	-	3,3,3	0.34	0	2,2,2	0.98	0
5	EDO	D	712	-	3,3,3	0.40	0	2,2,2	0.17	0
5	EDO	B	607	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	612	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	717	-	3,3,3	0.48	0	2,2,2	0.78	0
5	EDO	C	612	-	3,3,3	0.87	0	2,2,2	0.68	0
4	UMP	D	702	-	18,21,21	1.09	1 (5%)	21,31,31	1.09	2 (9%)
5	EDO	B	611	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	D	710	-	3,3,3	0.46	0	2,2,2	0.34	0
3	THG	A	702	-	26,34,34	1.96	5 (19%)	31,47,47	2.11	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	D	701	-	45,52,52	1.10	4 (8%)	56,80,80	1.49	9 (16%)
2	NAP	C	602	-	45,52,52	1.22	5 (11%)	56,80,80	1.92	16 (28%)
5	EDO	D	706	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	715	-	3,3,3	0.50	0	2,2,2	0.75	0
3	THG	C	601	-	26,34,34	1.79	4 (15%)	31,47,47	2.80	11 (35%)
3	THG	B	601	-	26,34,34	2.29	6 (23%)	31,47,47	2.00	9 (29%)
5	EDO	A	707	-	3,3,3	0.46	0	2,2,2	0.82	0
5	EDO	A	710	-	3,3,3	0.56	0	2,2,2	0.75	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
5	EDO	B	613	-	-	1/1/1/1	-
5	EDO	C	613	-	-	1/1/1/1	-
5	EDO	B	608	-	-	1/1/1/1	-
5	EDO	B	609	-	-	1/1/1/1	-
2	NAP	B	603	-	-	4/31/67/67	0/5/5/5
5	EDO	B	615	-	-	0/1/1/1	-
5	EDO	A	712	-	-	0/1/1/1	-
5	EDO	B	606	-	-	0/1/1/1	-
5	EDO	C	606	-	-	1/1/1/1	-
5	EDO	C	611	-	-	1/1/1/1	-
5	EDO	A	708	-	-	1/1/1/1	-
5	EDO	C	604	-	-	0/1/1/1	-
5	EDO	A	704	-	-	1/1/1/1	-
5	EDO	A	716	-	-	0/1/1/1	-
5	EDO	B	604	-	-	1/1/1/1	-
4	UMP	C	603	-	-	1/7/22/22	0/2/2/2
5	EDO	A	713	-	-	1/1/1/1	-
5	EDO	B	605	-	-	0/1/1/1	-
5	EDO	C	609	-	-	1/1/1/1	-
5	EDO	A	709	-	-	0/1/1/1	-
5	EDO	C	607	-	-	1/1/1/1	-
5	EDO	C	608	-	-	1/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-
4	UMP	B	602	-	-	2/7/22/22	0/2/2/2
5	EDO	D	707	-	-	1/1/1/1	-
4	UMP	A	703	-	-	1/7/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	A	714	-	-	0/1/1/1	-
5	EDO	A	711	-	-	1/1/1/1	-
2	NAP	A	701	-	-	5/31/67/67	0/5/5/5
5	EDO	C	605	-	-	1/1/1/1	-
5	EDO	D	705	-	-	0/1/1/1	-
5	EDO	D	709	-	-	0/1/1/1	-
5	EDO	D	713	-	-	0/1/1/1	-
3	THG	D	703	-	-	4/16/31/31	0/3/3/3
5	EDO	D	704	-	-	0/1/1/1	-
5	EDO	D	708	-	-	1/1/1/1	-
5	EDO	D	711	-	-	0/1/1/1	-
5	EDO	C	610	-	-	1/1/1/1	-
5	EDO	B	610	-	-	0/1/1/1	-
5	EDO	C	614	-	-	0/1/1/1	-
5	EDO	B	614	-	-	1/1/1/1	-
5	EDO	D	712	-	-	1/1/1/1	-
5	EDO	B	607	-	-	1/1/1/1	-
5	EDO	B	612	-	-	0/1/1/1	-
5	EDO	A	717	-	-	0/1/1/1	-
5	EDO	C	612	-	-	0/1/1/1	-
4	UMP	D	702	-	-	1/7/22/22	0/2/2/2
5	EDO	B	611	-	-	1/1/1/1	-
5	EDO	D	710	-	-	1/1/1/1	-
3	THG	A	702	-	-	1/16/31/31	0/3/3/3
2	NAP	D	701	-	-	2/31/67/67	0/5/5/5
2	NAP	C	602	-	-	5/31/67/67	0/5/5/5
5	EDO	D	706	-	-	1/1/1/1	-
5	EDO	A	715	-	-	1/1/1/1	-
3	THG	C	601	-	-	5/16/31/31	0/3/3/3
3	THG	B	601	-	-	1/16/31/31	0/3/3/3
5	EDO	A	707	-	-	1/1/1/1	-
5	EDO	A	710	-	-	0/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	THG	C4-C4A	7.36	1.51	1.41
3	A	702	THG	C4-C4A	5.91	1.49	1.41
3	B	601	THG	C4A-C8A	5.76	1.52	1.41
3	C	601	THG	C4-C4A	5.67	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	THG	C4-C4A	5.09	1.48	1.41
3	A	702	THG	C4A-C8A	4.92	1.50	1.41
3	D	703	THG	C4A-C8A	3.56	1.48	1.41
3	C	601	THG	C4A-C8A	3.49	1.48	1.41
4	C	603	UMP	C4-N3	3.11	1.38	1.33
4	A	703	UMP	C4-N3	3.11	1.38	1.33
4	D	702	UMP	C4-N3	3.08	1.38	1.33
4	B	602	UMP	C4-N3	2.95	1.38	1.33
2	B	603	NAP	P2B-O2B	2.94	1.64	1.59
2	A	701	NAP	P2B-O2B	2.92	1.64	1.59
3	C	601	THG	C4-N3	2.92	1.38	1.33
2	D	701	NAP	O4D-C1D	2.92	1.45	1.41
2	D	701	NAP	C5A-C4A	2.84	1.48	1.40
2	C	602	NAP	C8A-N7A	2.73	1.39	1.34
3	C	601	THG	C2'-C1'	2.73	1.44	1.39
2	C	602	NAP	P2B-O2B	2.63	1.64	1.59
2	C	602	NAP	O4D-C1D	2.57	1.44	1.41
2	A	701	NAP	C4A-N3A	2.47	1.39	1.35
4	B	602	UMP	P-OP2	-2.43	1.45	1.54
2	B	603	NAP	C4A-N3A	2.42	1.39	1.35
2	B	603	NAP	O4D-C1D	2.39	1.44	1.41
3	A	702	THG	C9-N10	2.36	1.50	1.45
2	B	603	NAP	C5A-C4A	2.25	1.46	1.40
2	D	701	NAP	P2B-O2B	2.25	1.63	1.59
3	A	702	THG	C4-N3	2.21	1.36	1.33
3	B	601	THG	O4-C4	2.19	1.30	1.24
2	C	602	NAP	C5A-N7A	-2.17	1.31	1.39
2	A	701	NAP	O4D-C1D	2.17	1.44	1.41
3	A	702	THG	C3'-C4'	2.16	1.42	1.39
3	B	601	THG	CB-CA	2.15	1.56	1.53
4	B	602	UMP	P-OP3	-2.13	1.46	1.54
4	B	602	UMP	C6-C5	-2.09	1.33	1.38
2	D	701	NAP	C8A-N7A	2.08	1.38	1.34
3	B	601	THG	C5'-C4'	2.04	1.42	1.39
2	B	603	NAP	P2B-O3X	-2.03	1.47	1.54
2	A	701	NAP	C5A-C4A	2.02	1.46	1.40
2	C	602	NAP	C2A-N3A	2.01	1.35	1.32
3	B	601	THG	C3'-C4'	2.00	1.42	1.39

All (89) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	THG	C4-C4A-N5	9.15	126.80	119.12
3	A	702	THG	C4-C4A-N5	5.50	123.74	119.12
3	C	601	THG	C9-C6-C7	-5.34	102.63	112.64
3	B	601	THG	C4-N3-C2	5.19	124.17	115.93
2	A	701	NAP	N3A-C2A-N1A	-5.15	120.63	128.68
3	C	601	THG	C4-N3-C2	5.03	123.91	115.93
3	D	703	THG	C4-C4A-N5	4.94	123.27	119.12
2	C	602	NAP	C1B-N9A-C4A	-4.86	118.11	126.64
3	A	702	THG	C4-N3-C2	4.69	123.39	115.93
3	B	601	THG	C4-C4A-C8A	4.64	118.69	114.57
3	A	702	THG	CA-N-C11	4.62	128.30	122.34
2	C	602	NAP	N3A-C2A-N1A	-4.54	121.59	128.68
3	C	601	THG	N3-C2-N1	-4.31	118.66	125.42
3	C	601	THG	C2-N1-C8A	4.13	123.80	114.54
3	A	702	THG	C2-N1-C8A	4.00	123.51	114.54
3	D	703	THG	C4-N3-C2	3.97	122.24	115.93
4	D	702	UMP	C5-C4-N3	-3.96	114.60	123.31
4	A	703	UMP	C5-C4-N3	-3.95	114.61	123.31
4	C	603	UMP	C5-C4-N3	-3.93	114.65	123.31
4	B	602	UMP	C5-C4-N3	-3.90	114.72	123.31
2	D	701	NAP	C3D-C2D-C1D	3.81	106.72	100.98
2	B	603	NAP	N3A-C2A-N1A	-3.69	122.91	128.68
3	B	601	THG	CA-N-C11	3.65	127.05	122.34
2	D	701	NAP	N3A-C2A-N1A	-3.65	122.97	128.68
2	A	701	NAP	C3D-C2D-C1D	3.65	106.47	100.98
2	A	701	NAP	C2A-N1A-C6A	3.57	124.86	118.75
2	C	602	NAP	O7N-C7N-C3N	3.47	123.78	119.63
3	A	702	THG	N3-C2-N1	-3.45	120.00	125.42
2	C	602	NAP	C3N-C2N-N1N	-3.42	117.08	120.43
2	C	602	NAP	C3N-C7N-N7N	-3.38	113.69	117.75
3	B	601	THG	C4-C4A-N5	3.37	121.95	119.12
2	A	701	NAP	C1B-N9A-C4A	-3.26	120.92	126.64
2	C	602	NAP	C2N-C3N-C4N	3.25	121.95	118.26
2	A	701	NAP	O2A-PA-O1A	3.24	128.26	112.24
3	C	601	THG	CB-CA-N	3.22	114.88	110.19
2	D	701	NAP	C2A-N1A-C6A	3.18	124.19	118.75
2	B	603	NAP	O2A-PA-O1A	3.17	127.93	112.24
3	B	601	THG	C2-N1-C8A	3.08	121.45	114.54
4	B	602	UMP	OP3-P-OP2	3.05	119.31	107.64
2	D	701	NAP	C1B-N9A-C4A	-3.02	121.33	126.64
3	B	601	THG	C4A-C4-N3	-3.01	115.44	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	602	NAP	C2N-N1N-C1D	2.98	125.77	119.14
2	D	701	NAP	C4A-C5A-N7A	-2.97	106.30	109.40
3	D	703	THG	C2-N1-C8A	2.97	121.20	114.54
3	C	601	THG	C9-C6-N5	2.97	115.22	108.83
2	C	602	NAP	O5D-C5D-C4D	2.93	119.07	108.99
3	C	601	THG	C9-N10-C4'	-2.89	114.66	122.14
2	B	603	NAP	C2A-N1A-C6A	2.87	123.66	118.75
3	A	702	THG	CB-CA-N	2.87	114.37	110.19
2	C	602	NAP	C5N-C6N-N1N	2.87	124.51	120.40
2	C	602	NAP	C4N-C3N-C7N	-2.85	113.41	121.04
2	B	603	NAP	O3X-P2B-O2X	2.83	118.44	107.64
2	B	603	NAP	O4D-C1D-C2D	-2.82	102.80	106.93
2	B	603	NAP	C4N-C3N-C7N	-2.76	113.66	121.04
3	D	703	THG	C4-C4A-C8A	2.75	117.02	114.57
2	B	603	NAP	C1B-N9A-C4A	-2.75	121.82	126.64
3	A	702	THG	N2-C2-N1	2.74	121.52	117.25
2	D	701	NAP	O2A-PA-O1A	2.69	125.56	112.24
2	D	701	NAP	C5A-C6A-N6A	2.67	124.41	120.35
2	D	701	NAP	O2N-PN-O1N	2.64	125.27	112.24
2	B	603	NAP	C2N-C3N-C7N	2.60	127.01	119.46
2	C	602	NAP	O2B-P2B-O1X	-2.57	99.45	109.39
2	A	701	NAP	O7N-C7N-C3N	2.53	122.66	119.63
2	C	602	NAP	C2A-N1A-C6A	2.53	123.08	118.75
2	B	603	NAP	O2B-P2B-O1X	-2.52	99.67	109.39
3	C	601	THG	O11-C11-C1'	-2.51	116.45	120.94
2	B	603	NAP	C3D-C2D-C1D	2.47	104.70	100.98
2	D	701	NAP	O3X-P2B-O2X	2.45	117.01	107.64
4	B	602	UMP	OP2-P-O5'	-2.43	100.27	106.73
3	C	601	THG	N2-C2-N3	2.41	121.00	117.25
2	B	603	NAP	O2N-PN-O1N	2.41	124.13	112.24
2	B	603	NAP	C2N-N1N-C1D	2.36	124.40	119.14
2	B	603	NAP	O3D-C3D-C4D	-2.36	104.23	111.05
2	A	701	NAP	O2N-PN-O5D	-2.32	96.97	107.75
4	A	703	UMP	OP2-P-OP1	2.29	119.63	110.68
4	D	702	UMP	OP2-P-OP1	2.28	119.60	110.68
4	C	603	UMP	OP2-P-OP1	2.27	119.57	110.68
2	C	602	NAP	C6N-C5N-C4N	-2.26	116.16	119.44
2	C	602	NAP	O3X-P2B-O2X	2.22	116.11	107.64
2	A	701	NAP	O4B-C4B-C5B	-2.15	102.30	109.37
2	C	602	NAP	C5D-C4D-C3D	-2.11	107.27	115.18
3	B	601	THG	N2-C2-N1	2.09	120.51	117.25
2	A	701	NAP	O2N-PN-O1N	2.09	122.56	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	703	THG	C4A-C4-N3	-2.04	118.22	124.01
3	C	601	THG	C4A-C4-N3	-2.04	118.22	124.01
3	B	601	THG	N3-C2-N1	-2.03	122.23	125.42
3	B	601	THG	C9-N10-C4'	-2.01	116.94	122.14
2	C	602	NAP	O2A-PA-O1A	2.01	122.18	112.24
2	B	603	NAP	O5D-PN-O1N	-2.00	101.24	109.07

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	603	NAP	C3D-C4D-C5D-O5D
2	C	602	NAP	C2N-C3N-C7N-O7N
2	C	602	NAP	C2N-C3N-C7N-N7N
2	C	602	NAP	C4N-C3N-C7N-N7N
3	C	601	THG	C7-C6-C9-N10
3	C	601	THG	N5-C6-C9-N10
2	C	602	NAP	C4N-C3N-C7N-O7N
2	B	603	NAP	O4D-C4D-C5D-O5D
2	A	701	NAP	C4N-C3N-C7N-N7N
5	C	608	EDO	O1-C1-C2-O2
5	A	704	EDO	O1-C1-C2-O2
5	C	609	EDO	O1-C1-C2-O2
5	D	708	EDO	O1-C1-C2-O2
5	D	710	EDO	O1-C1-C2-O2
5	B	608	EDO	O1-C1-C2-O2
5	C	605	EDO	O1-C1-C2-O2
5	A	715	EDO	O1-C1-C2-O2
2	A	701	NAP	C4N-C3N-C7N-O7N
3	C	601	THG	CB-CA-N-C11
2	D	701	NAP	C3D-C4D-C5D-O5D
3	C	601	THG	C6-C9-N10-C4'
5	B	613	EDO	O1-C1-C2-O2
5	C	606	EDO	O1-C1-C2-O2
5	B	604	EDO	O1-C1-C2-O2
5	A	713	EDO	O1-C1-C2-O2
5	B	614	EDO	O1-C1-C2-O2
5	D	707	EDO	O1-C1-C2-O2
5	C	610	EDO	O1-C1-C2-O2
5	B	607	EDO	O1-C1-C2-O2
5	B	611	EDO	O1-C1-C2-O2
2	A	701	NAP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
5	C	613	EDO	O1-C1-C2-O2
2	A	701	NAP	C3D-C4D-C5D-O5D
3	D	703	THG	C5'-C4'-N10-C9
5	B	609	EDO	O1-C1-C2-O2
5	A	707	EDO	O1-C1-C2-O2
2	A	701	NAP	C2N-C3N-C7N-O7N
4	B	602	UMP	O4'-C4'-C5'-O5'
5	D	712	EDO	O1-C1-C2-O2
4	C	603	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	O4'-C4'-C5'-O5'
3	D	703	THG	C6-C9-N10-C4'
3	A	702	THG	C6-C9-N10-C4'
3	B	601	THG	C6-C9-N10-C4'
2	B	603	NAP	PA-O3-PN-O1N
5	A	711	EDO	O1-C1-C2-O2
4	D	702	UMP	O4'-C4'-C5'-O5'
3	C	601	THG	C-CA-N-C11
3	D	703	THG	N-CA-CB-CG
3	D	703	THG	C3'-C4'-N10-C9
5	C	611	EDO	O1-C1-C2-O2
5	A	708	EDO	O1-C1-C2-O2
5	D	706	EDO	O1-C1-C2-O2
2	B	603	NAP	C5D-O5D-PN-O3
2	C	602	NAP	C5D-O5D-PN-O3
2	D	701	NAP	PA-O3-PN-O1N
4	B	602	UMP	C3'-C4'-C5'-O5'
5	C	607	EDO	O1-C1-C2-O2

There are no ring outliers.

29 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	613	EDO	2	0
5	B	609	EDO	1	0
2	B	603	NAP	11	0
5	B	606	EDO	2	0
5	C	611	EDO	3	0
5	A	708	EDO	1	0
5	C	604	EDO	1	0
4	C	603	UMP	5	0
5	A	713	EDO	1	0
5	C	607	EDO	1	0

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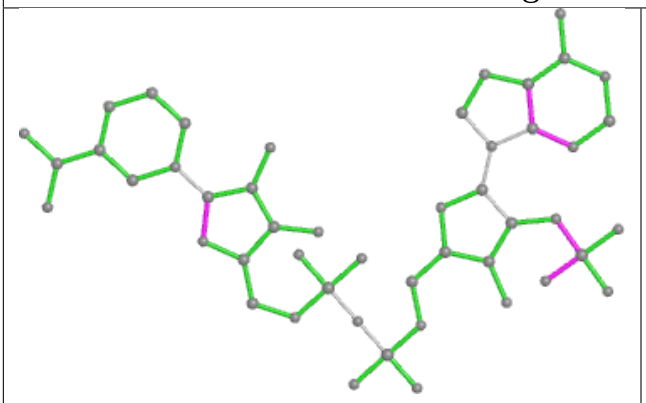
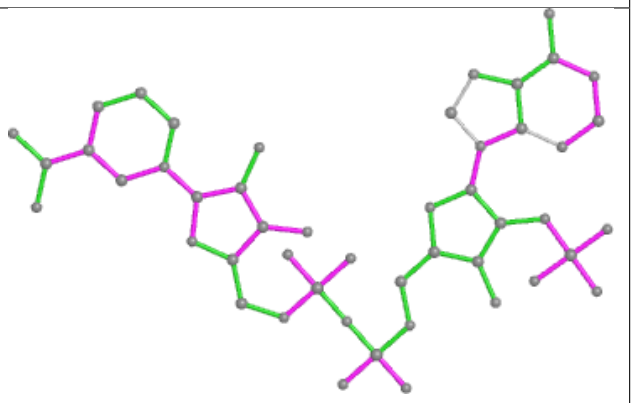
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	UMP	3	0
4	A	703	UMP	4	0
5	A	714	EDO	2	0
2	A	701	NAP	5	0
3	D	703	THG	3	0
5	D	708	EDO	2	0
5	C	610	EDO	3	0
5	C	614	EDO	2	0
5	B	614	EDO	1	0
5	B	612	EDO	1	0
5	A	717	EDO	1	0
4	D	702	UMP	2	0
5	B	611	EDO	1	0
5	D	710	EDO	1	0
3	A	702	THG	3	0
2	D	701	NAP	8	0
2	C	602	NAP	3	0
3	C	601	THG	1	0
3	B	601	THG	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 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.

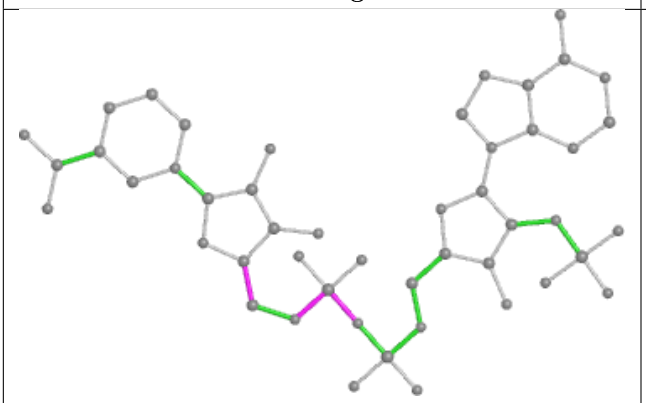
Ligand NAP B 603



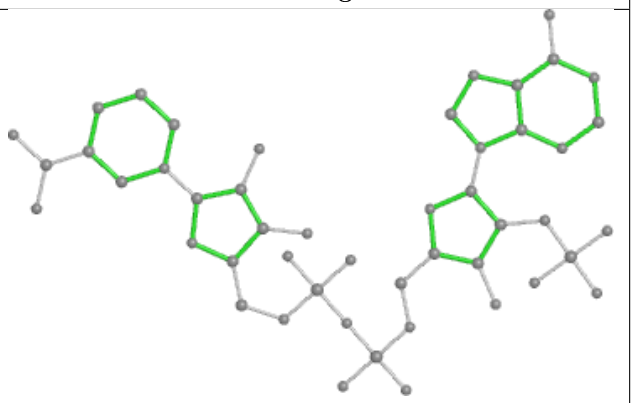
Bond lengths



Bond angles

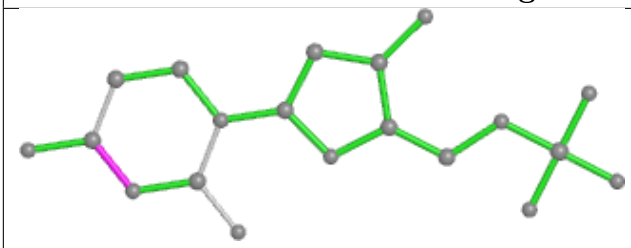


Torsions

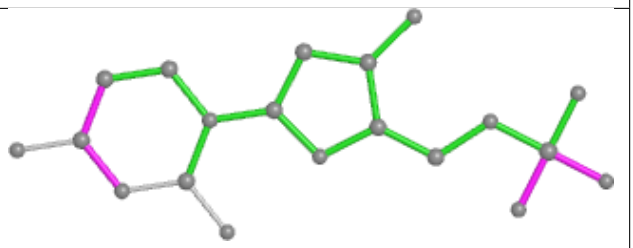


Rings

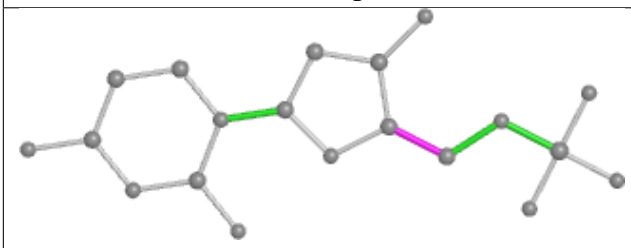
Ligand UMP C 603



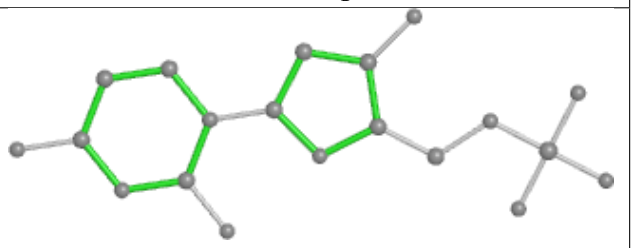
Bond lengths



Bond angles

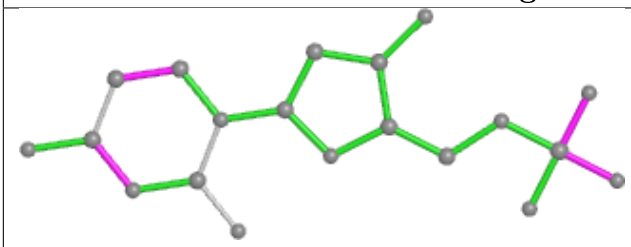


Torsions

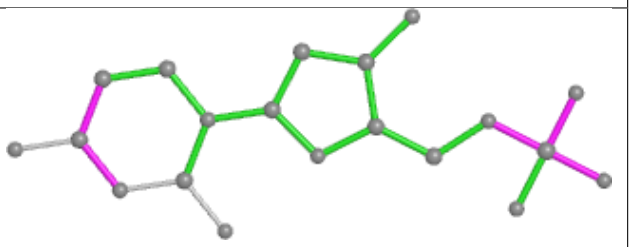


Rings

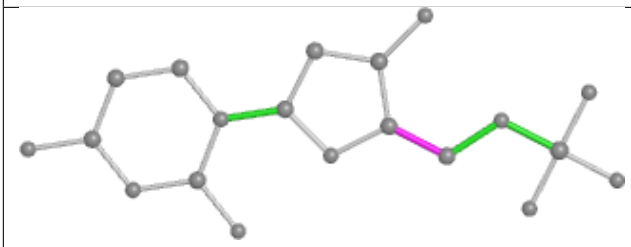
Ligand UMP B 602



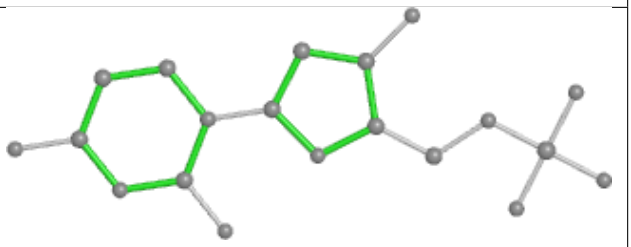
Bond lengths



Bond angles

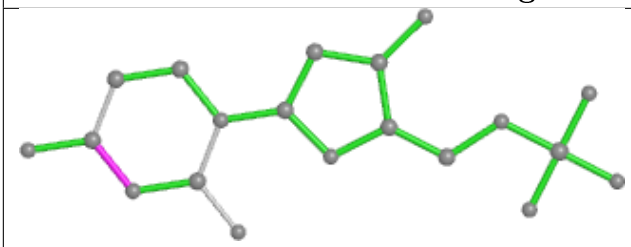


Torsions

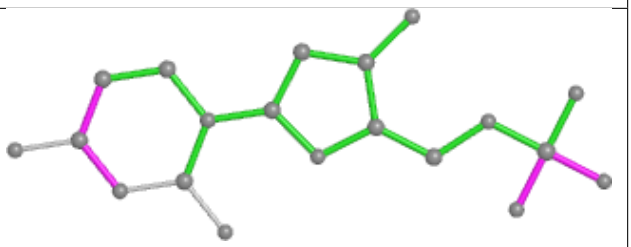


Rings

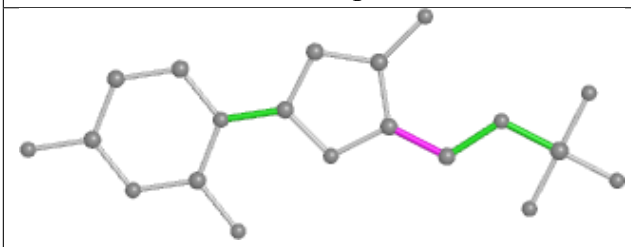
Ligand UMP A 703



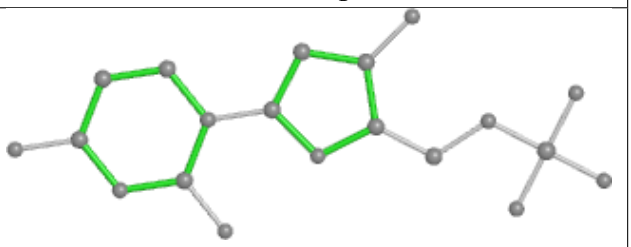
Bond lengths



Bond angles

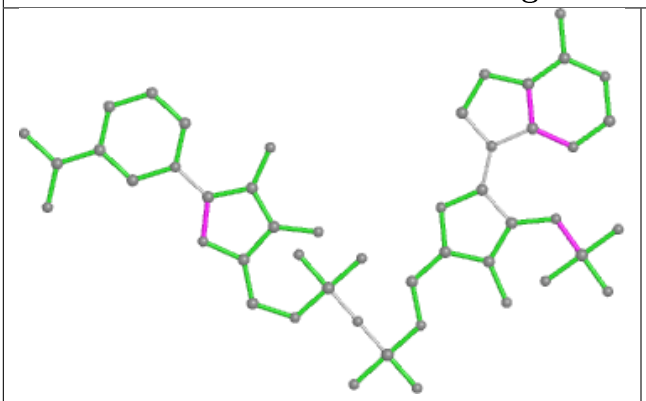


Torsions

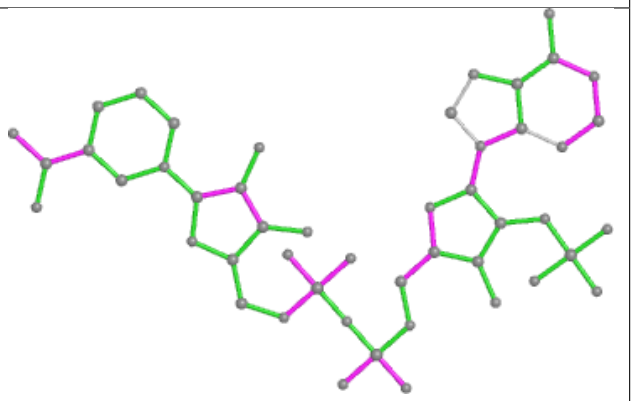


Rings

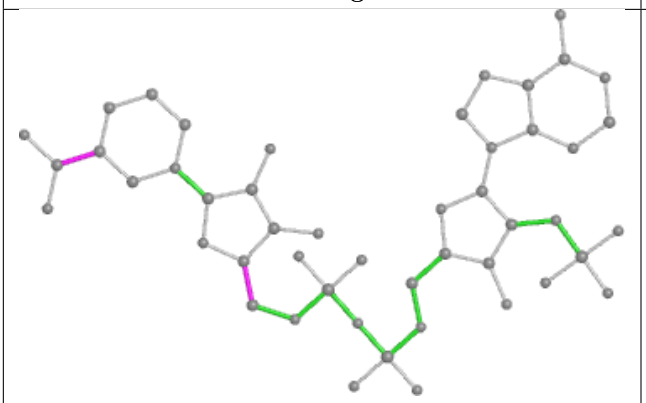
Ligand NAP A 701



Bond lengths



Bond angles



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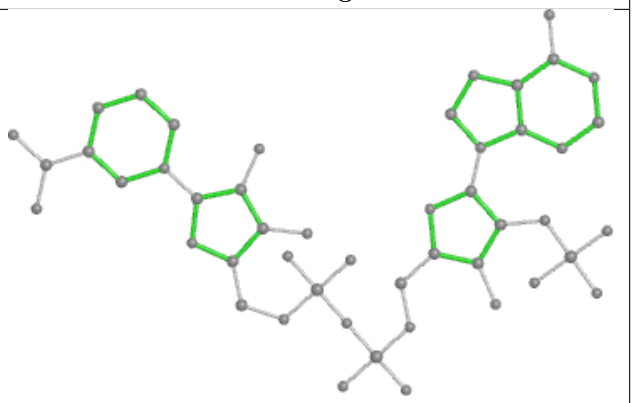
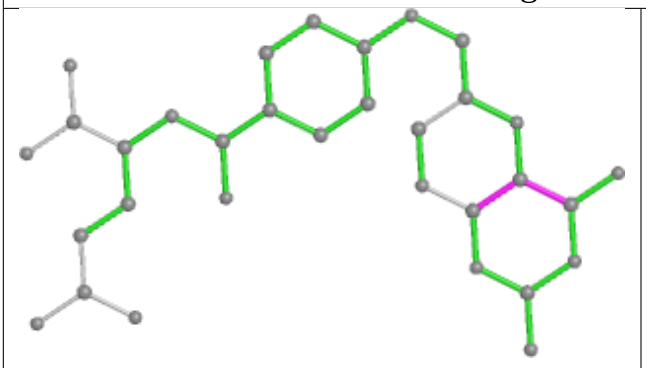


Rings

Ligand THG D 703



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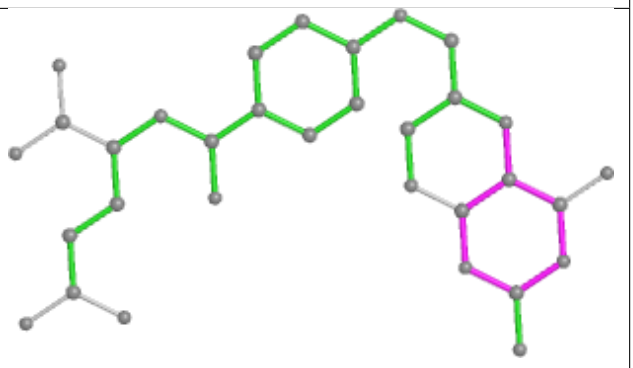
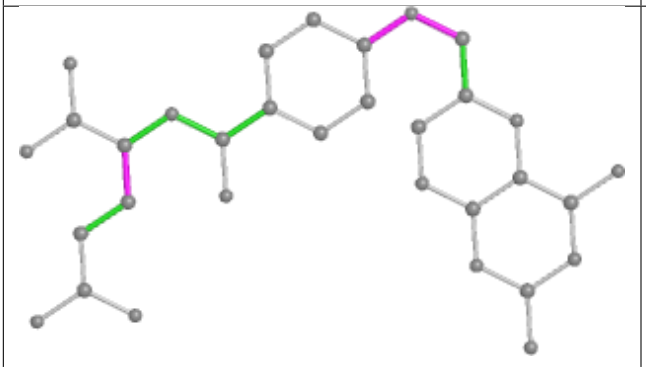
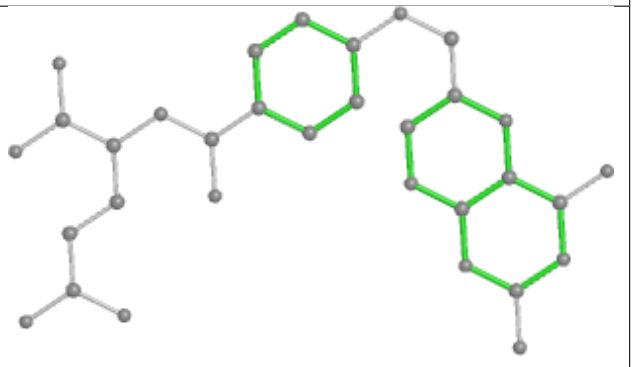


Bond angles

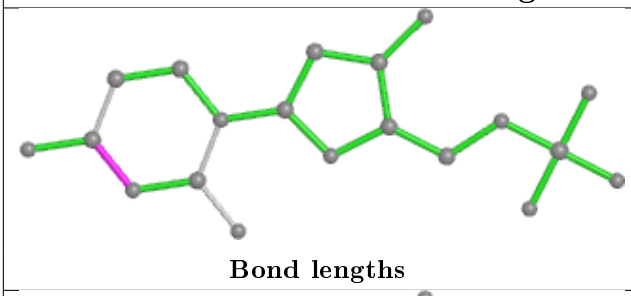


Torsions

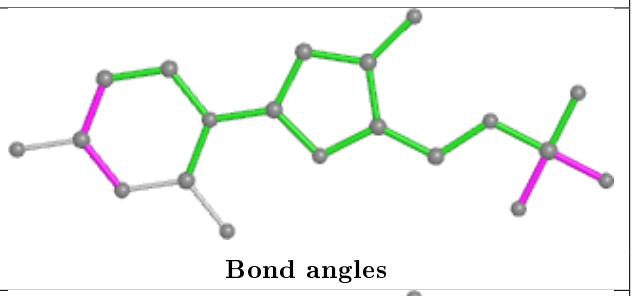


Rings

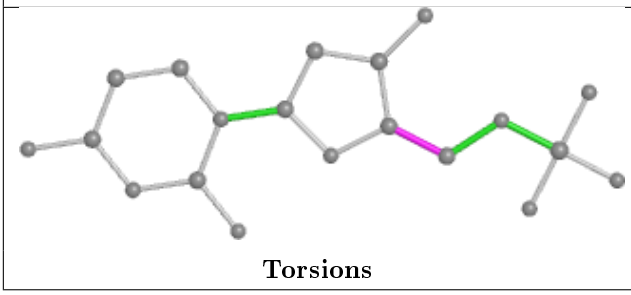
Ligand UMP D 702



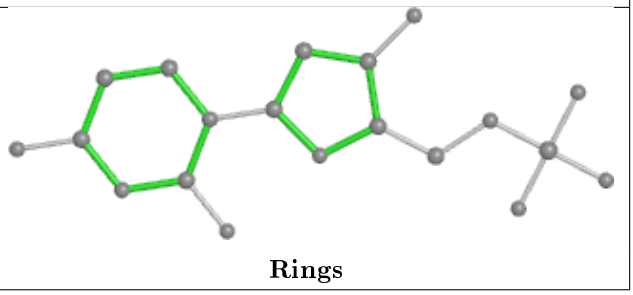
Bond lengths



Bond angles

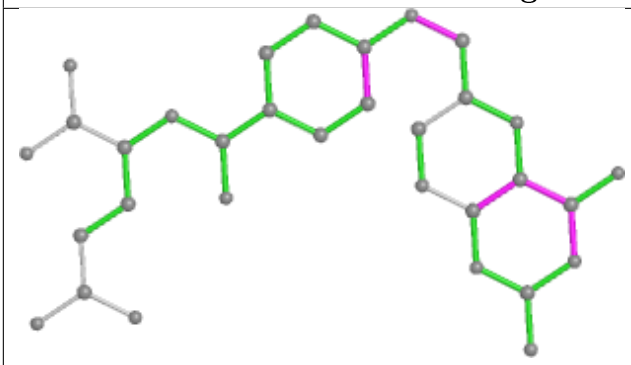


Torsions

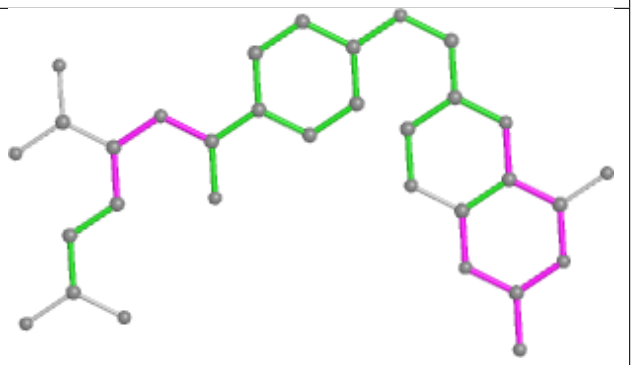


Rings

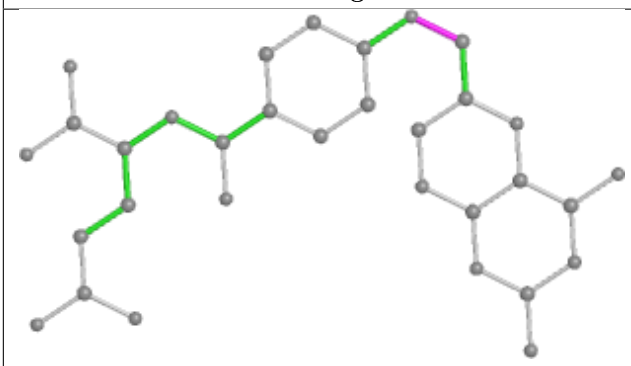
Ligand THG A 702



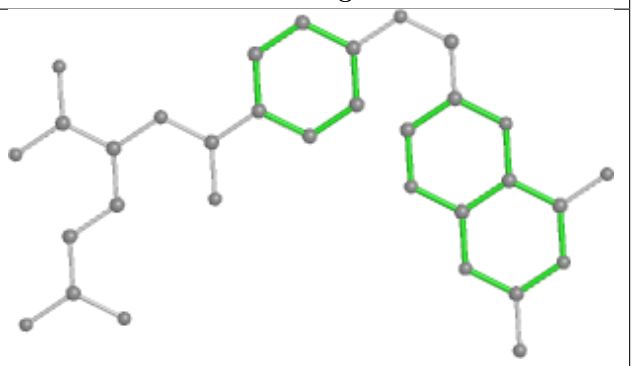
Bond lengths



Bond angles

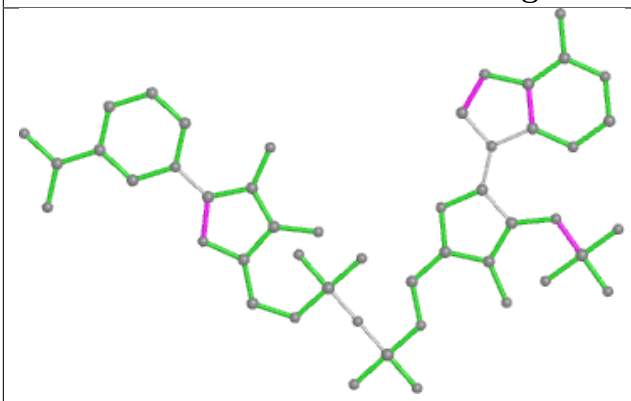


Torsions

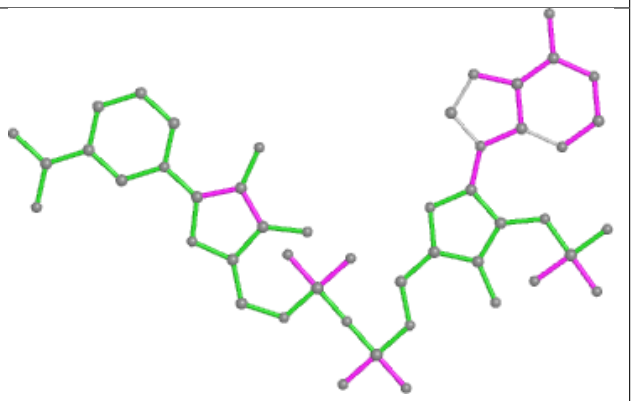


Rings

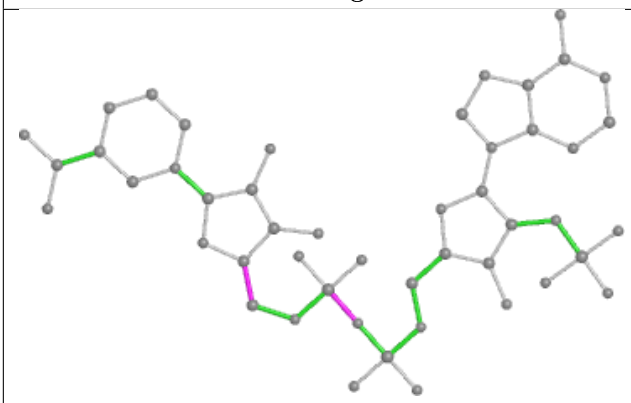
Ligand NAP D 701



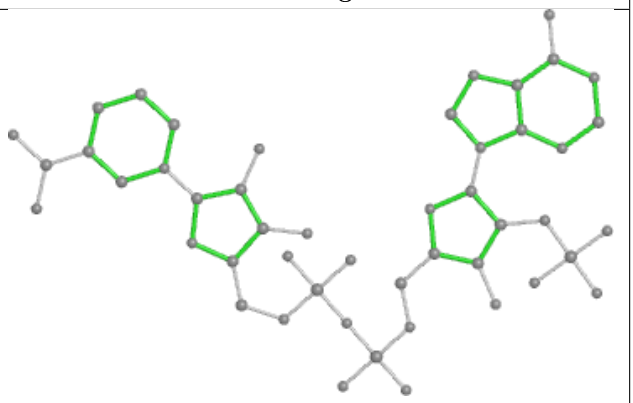
Bond lengths



Bond angles

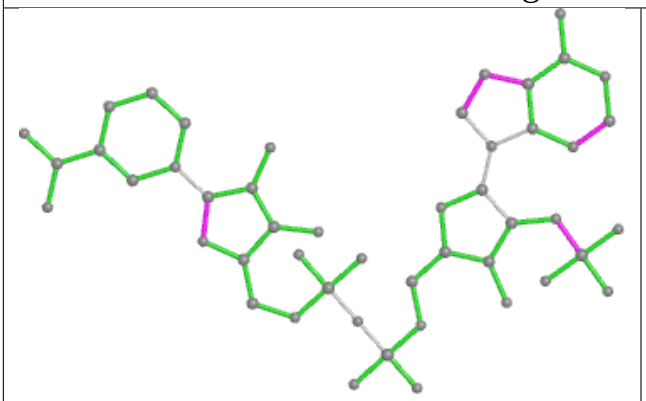


Torsions

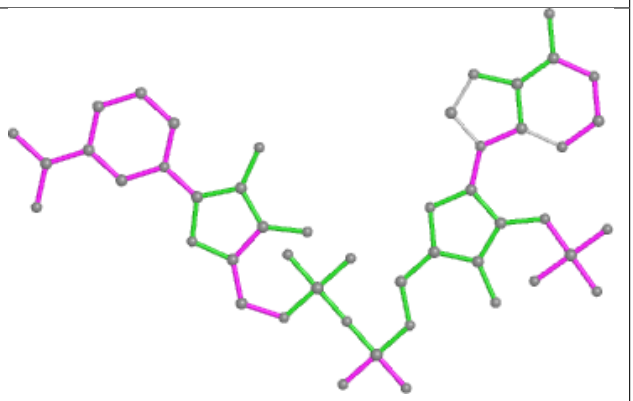


Rings

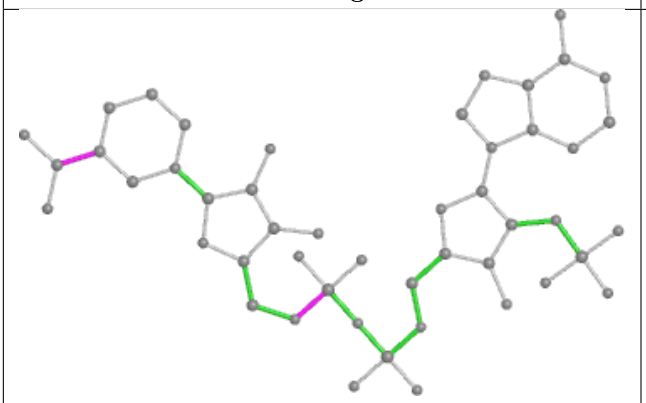
Ligand NAP C 602



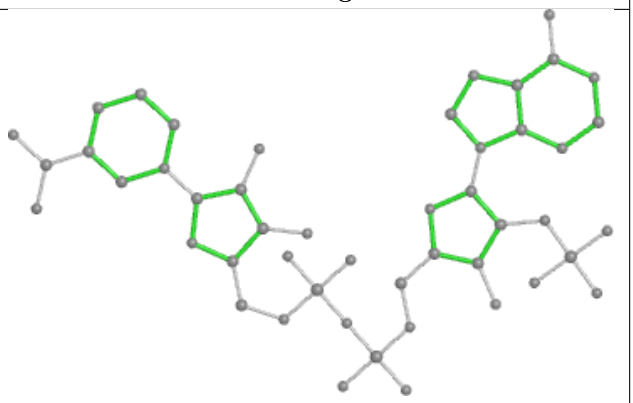
Bond lengths



Bond angles

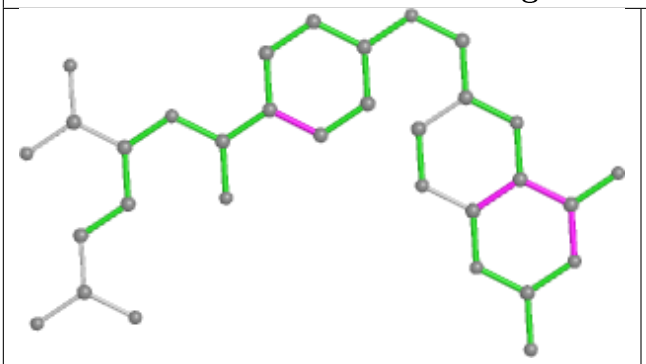


Torsions

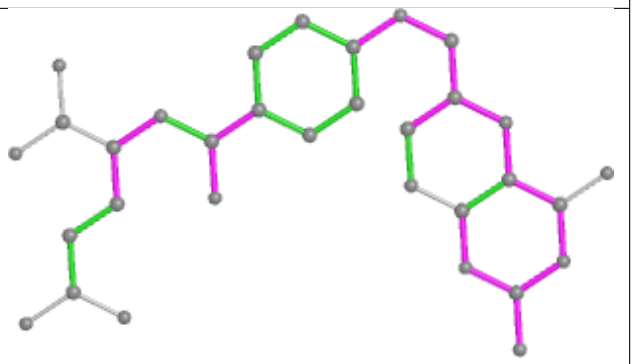


Rings

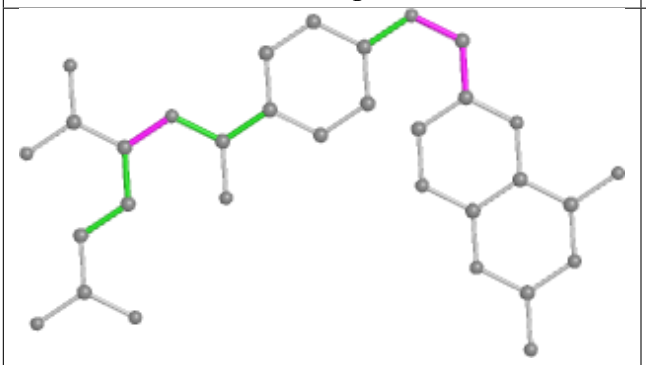
Ligand THG C 601



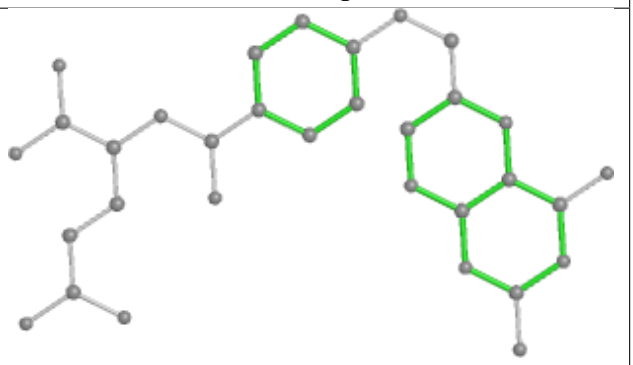
Bond lengths



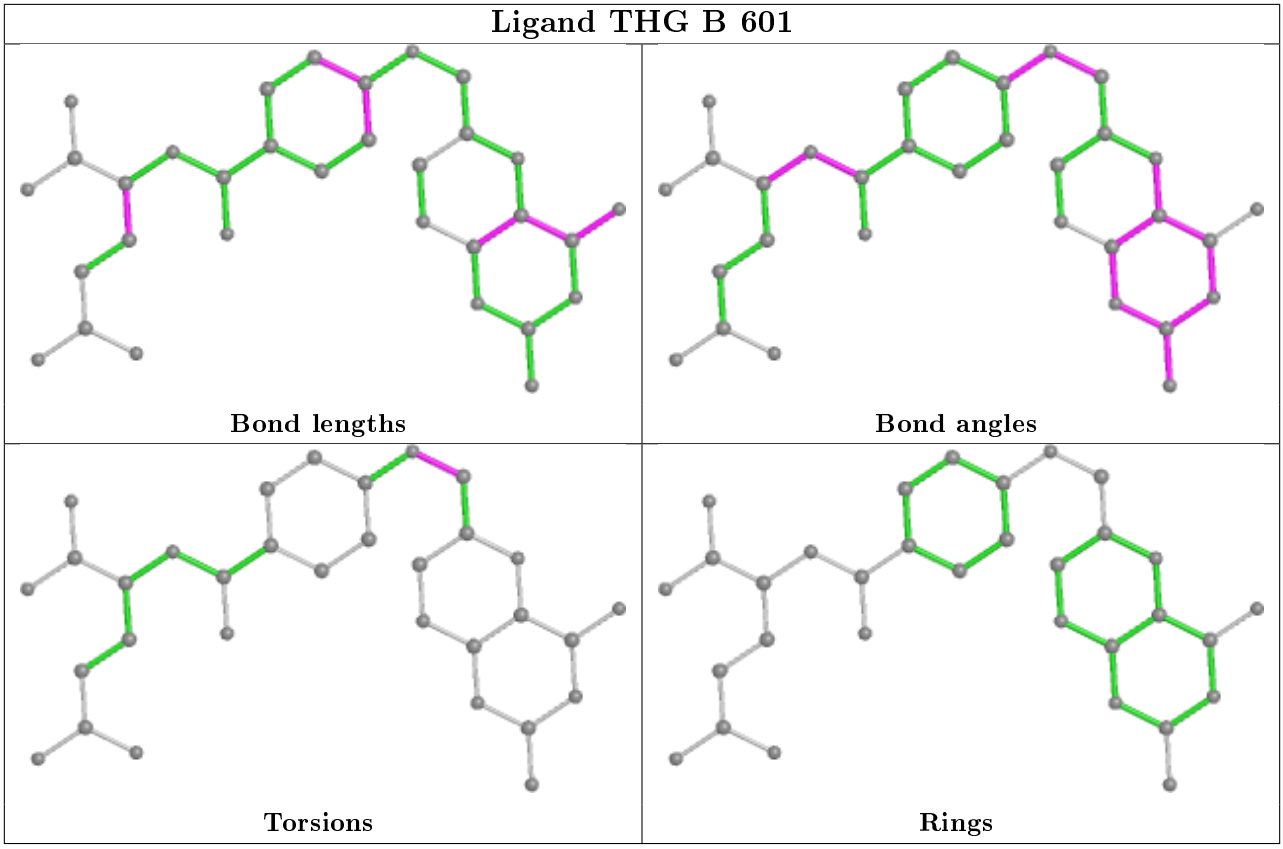
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	385:MET	C	386:LEU	N	1.14

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	494/521 (94%)	-0.32	6 (1%)	79	76	13, 22, 45, 66	0
1	B	495/521 (95%)	-0.31	7 (1%)	75	72	13, 21, 44, 69	1 (0%)
1	C	487/521 (93%)	-0.39	5 (1%)	82	80	13, 22, 42, 65	0
1	D	489/521 (93%)	-0.29	9 (1%)	68	64	13, 23, 48, 69	0
All	All	1965/2084 (94%)	-0.33	27 (1%)	75	72	13, 22, 45, 69	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	LEU	4.8
1	B	400	LEU	4.1
1	D	88	PHE	4.0
1	B	334	TYR	3.9
1	B	343	TYR	3.8
1	B	121	HIS	3.7
1	B	122	ALA	3.7
1	A	120	LEU	3.7
1	B	43	TRP	3.5
1	D	343	TYR	3.4
1	D	403	CYS	3.3
1	D	102	THR	3.2
1	D	109	LEU	3.1
1	A	190	PHE	3.0
1	A	122	ALA	3.0
1	A	121	HIS	2.8
1	A	36[A]	GLY	2.7
1	C	102	THR	2.6
1	C	36[A]	GLY	2.5
1	D	112	LEU	2.3
1	B	91	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	35[A]	ILE	2.3
1	D	122	ALA	2.2
1	C	390	TRP	2.2
1	C	15	GLY	2.1
1	D	220	GLY	2.1
1	C	2	SER	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	EDO	A	714	4/4	0.72	0.19	38,39,49,51	0
5	EDO	C	610	4/4	0.72	0.31	32,37,46,47	0
5	EDO	A	713	4/4	0.76	0.19	42,42,42,57	0
3	THG	D	703	32/32	0.78	0.24	30,46,64,65	0
4	UMP	D	702	20/20	0.79	0.26	32,48,62,62	0
4	UMP	C	603	20/20	0.80	0.24	27,46,54,54	0
5	EDO	C	614	4/4	0.81	0.20	38,39,49,53	0
5	EDO	D	710	4/4	0.81	0.18	40,41,45,47	0
4	UMP	A	703	20/20	0.83	0.23	25,39,48,50	15
5	EDO	B	608	4/4	0.83	0.18	39,39,41,48	0
5	EDO	B	610	4/4	0.84	0.11	47,51,54,56	0
5	EDO	B	607	4/4	0.84	0.20	33,36,48,63	0
5	EDO	C	611	4/4	0.85	0.26	22,24,26,31	4
5	EDO	D	711	4/4	0.85	0.11	49,52,52,62	0
5	EDO	C	607	4/4	0.85	0.16	36,38,40,42	0
5	EDO	B	606	4/4	0.86	0.16	37,38,39,42	0
5	EDO	A	715	4/4	0.86	0.17	52,55,57,58	0

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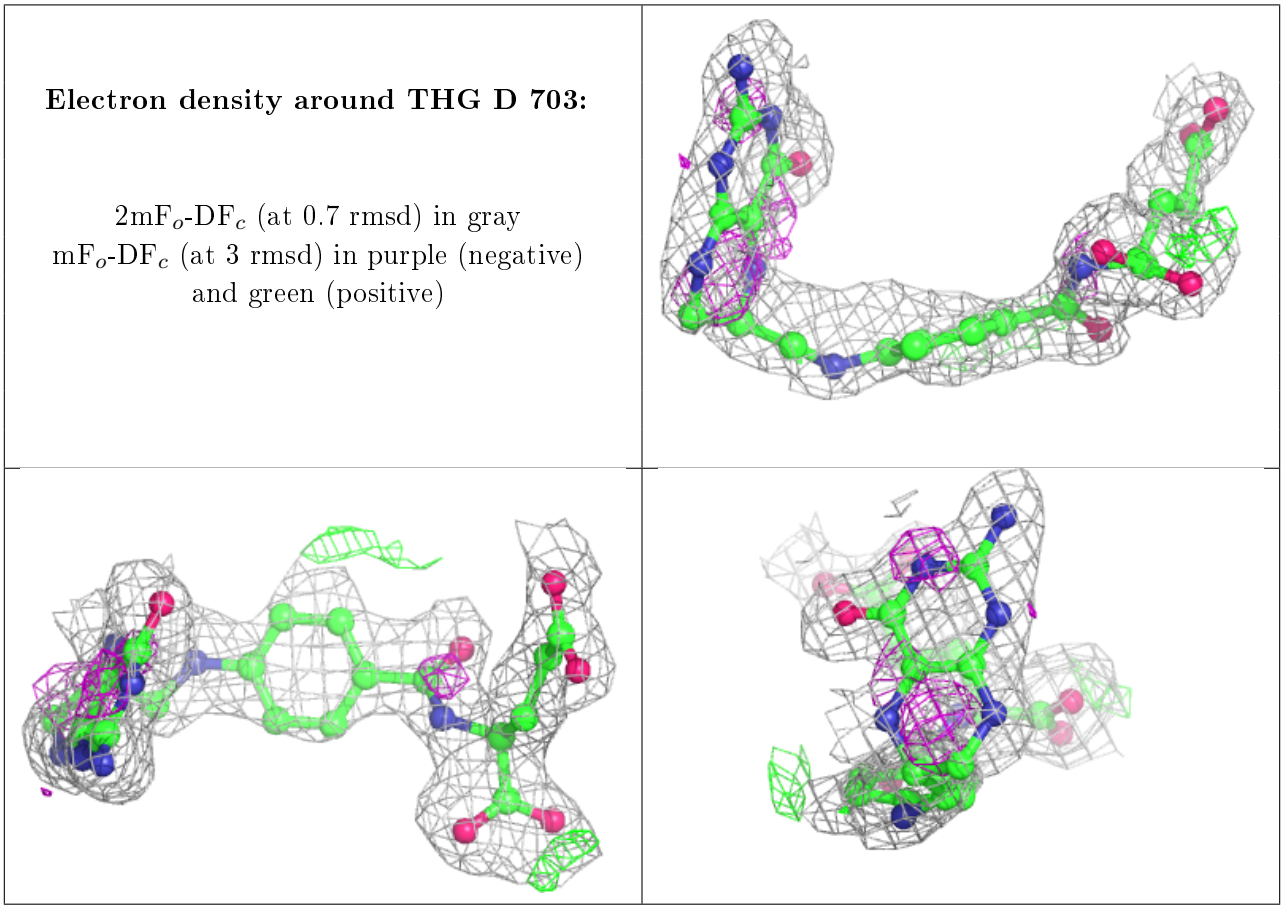
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	608	4/4	0.87	0.17	35,47,49,71	0
5	EDO	B	609	4/4	0.87	0.19	34,47,48,49	0
5	EDO	D	706	4/4	0.87	0.17	39,42,44,45	0
5	EDO	D	707	4/4	0.87	0.16	49,49,52,54	0
5	EDO	C	613	4/4	0.89	0.28	38,39,40,41	0
3	THG	A	702	32/32	0.89	0.16	24,38,50,55	0
5	EDO	C	609	4/4	0.89	0.13	32,34,39,39	0
5	EDO	B	611	4/4	0.89	0.25	30,39,43,47	0
5	EDO	C	606	4/4	0.90	0.21	34,36,38,43	0
5	EDO	A	711	4/4	0.90	0.17	38,39,44,47	0
4	UMP	B	602	20/20	0.90	0.19	27,42,48,49	0
5	EDO	D	708	4/4	0.91	0.20	29,32,35,38	0
3	THG	C	601	32/32	0.91	0.13	27,44,53,55	0
5	EDO	A	709	4/4	0.92	0.12	30,31,43,55	0
5	EDO	B	612	4/4	0.92	0.21	34,39,40,41	0
5	EDO	A	717	4/4	0.92	0.23	46,46,47,54	0
5	EDO	D	705	4/4	0.92	0.14	31,43,43,51	0
5	EDO	B	604	4/4	0.92	0.14	33,36,36,37	0
3	THG	B	601	32/32	0.92	0.14	24,36,44,54	0
5	EDO	A	716	4/4	0.93	0.13	34,40,42,43	0
5	EDO	B	613	4/4	0.93	0.17	38,45,48,52	0
5	EDO	B	614	4/4	0.93	0.09	41,42,45,54	0
5	EDO	A	707	4/4	0.93	0.15	31,32,32,45	0
5	EDO	D	709	4/4	0.94	0.11	24,25,28,29	0
5	EDO	A	704	4/4	0.94	0.11	27,30,30,34	0
5	EDO	D	712	4/4	0.94	0.12	27,32,33,42	0
5	EDO	B	615	4/4	0.95	0.09	26,26,27,29	0
5	EDO	B	605	4/4	0.95	0.10	23,23,24,25	0
5	EDO	C	612	4/4	0.95	0.09	23,24,25,27	0
5	EDO	A	712	4/4	0.95	0.10	35,43,46,54	0
5	EDO	C	605	4/4	0.95	0.10	36,38,43,51	0
5	EDO	A	708	4/4	0.95	0.11	37,41,43,54	0
5	EDO	A	710	4/4	0.95	0.10	28,29,36,44	0
5	EDO	C	604	4/4	0.96	0.10	21,21,22,22	0
2	NAP	D	701	48/48	0.96	0.14	31,37,112,117	0
2	NAP	A	701	48/48	0.97	0.12	25,31,88,97	0
5	EDO	D	713	4/4	0.97	0.13	30,35,36,38	0
2	NAP	B	603	48/48	0.97	0.12	23,30,95,101	0
5	EDO	D	704	4/4	0.97	0.10	21,22,23,25	0
5	EDO	A	706	4/4	0.97	0.08	22,23,23,26	0
2	NAP	C	602	48/48	0.97	0.10	25,32,101,111	0
5	EDO	A	705	4/4	0.98	0.08	20,22,22,23	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.

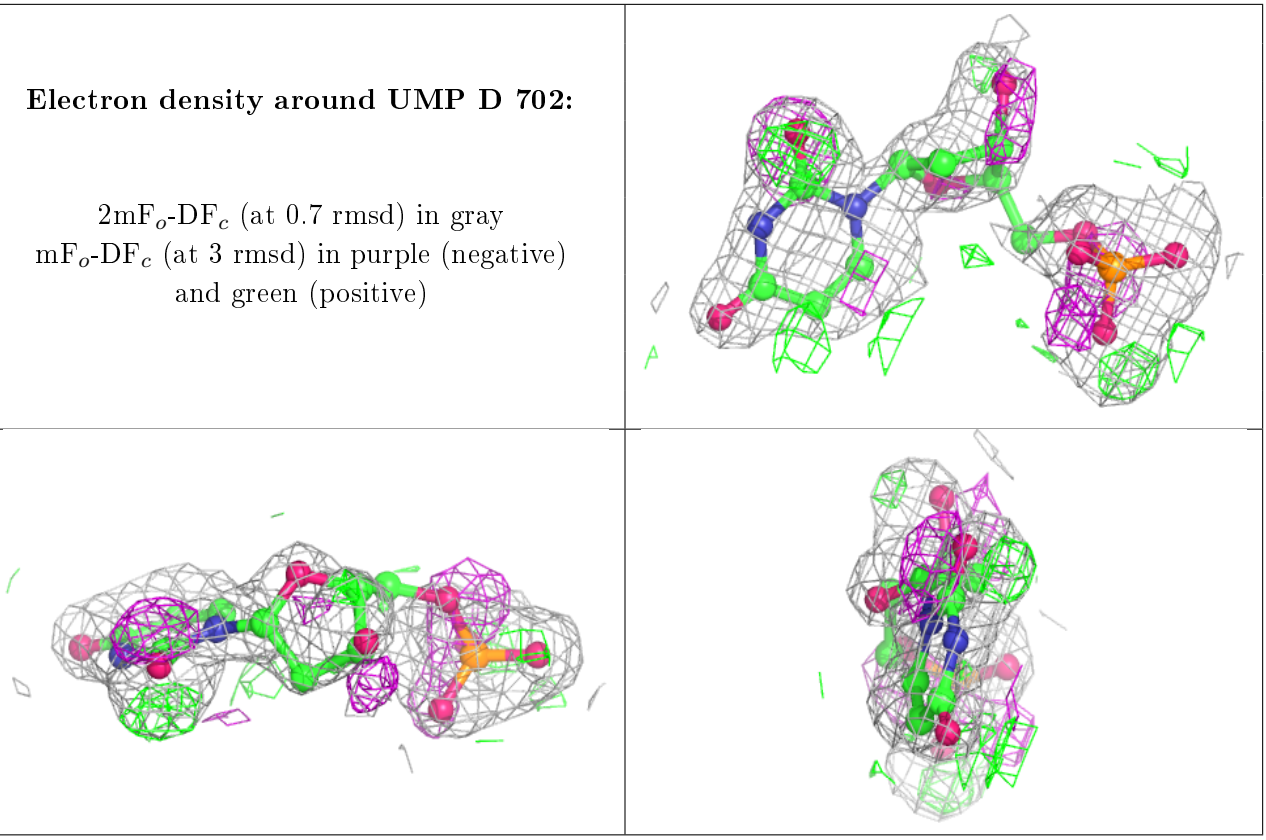
Electron density around THG D 703:

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



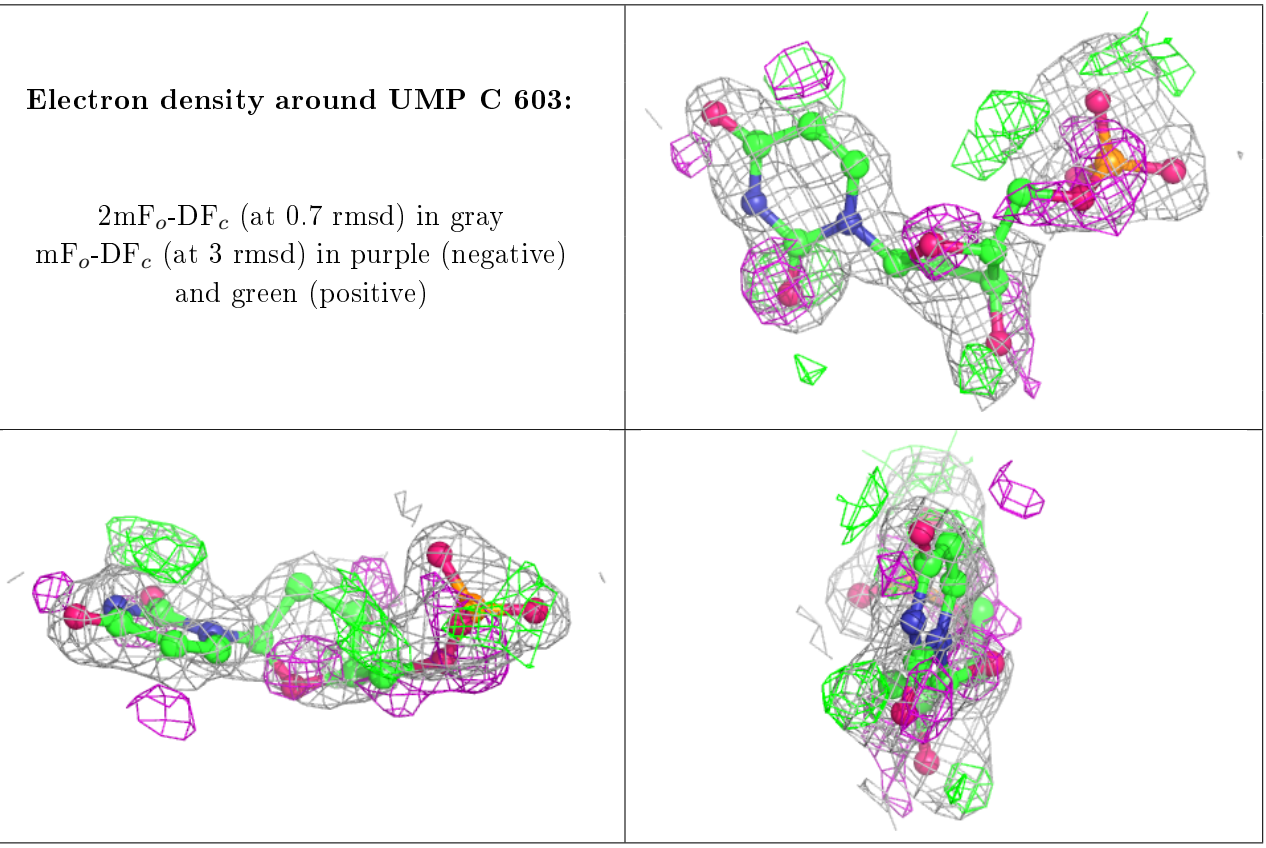
Electron density around UMP D 702:

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



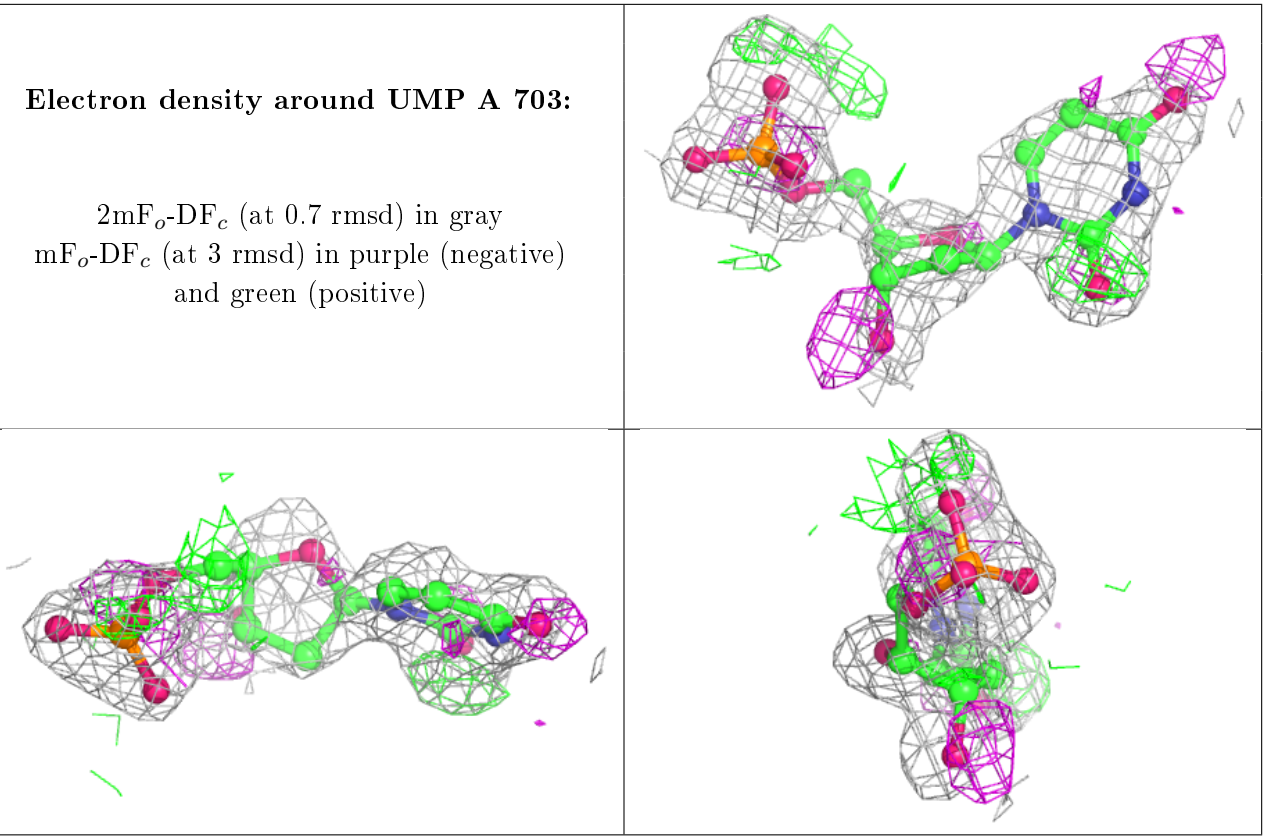
Electron density around UMP C 603:

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



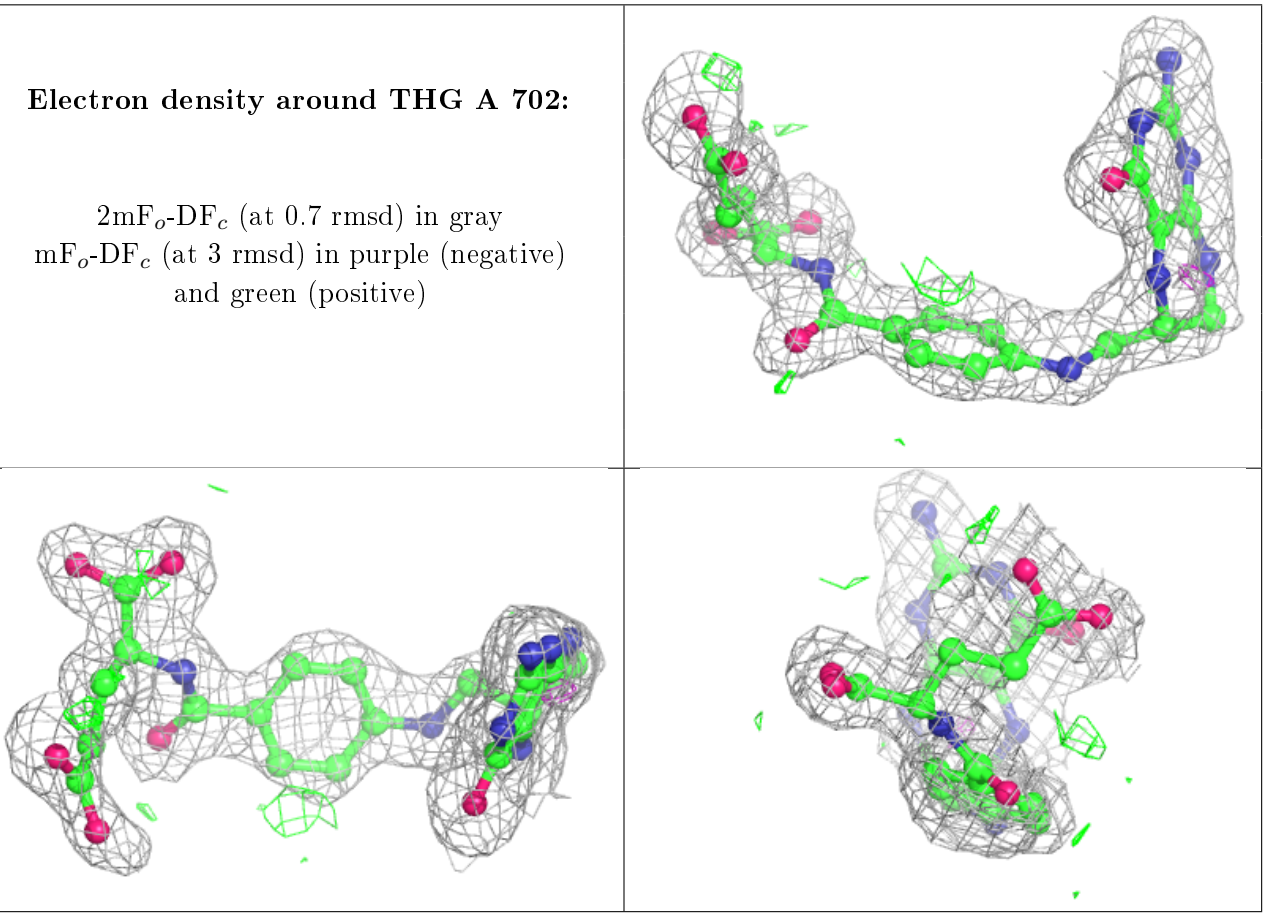
Electron density around UMP A 703:

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



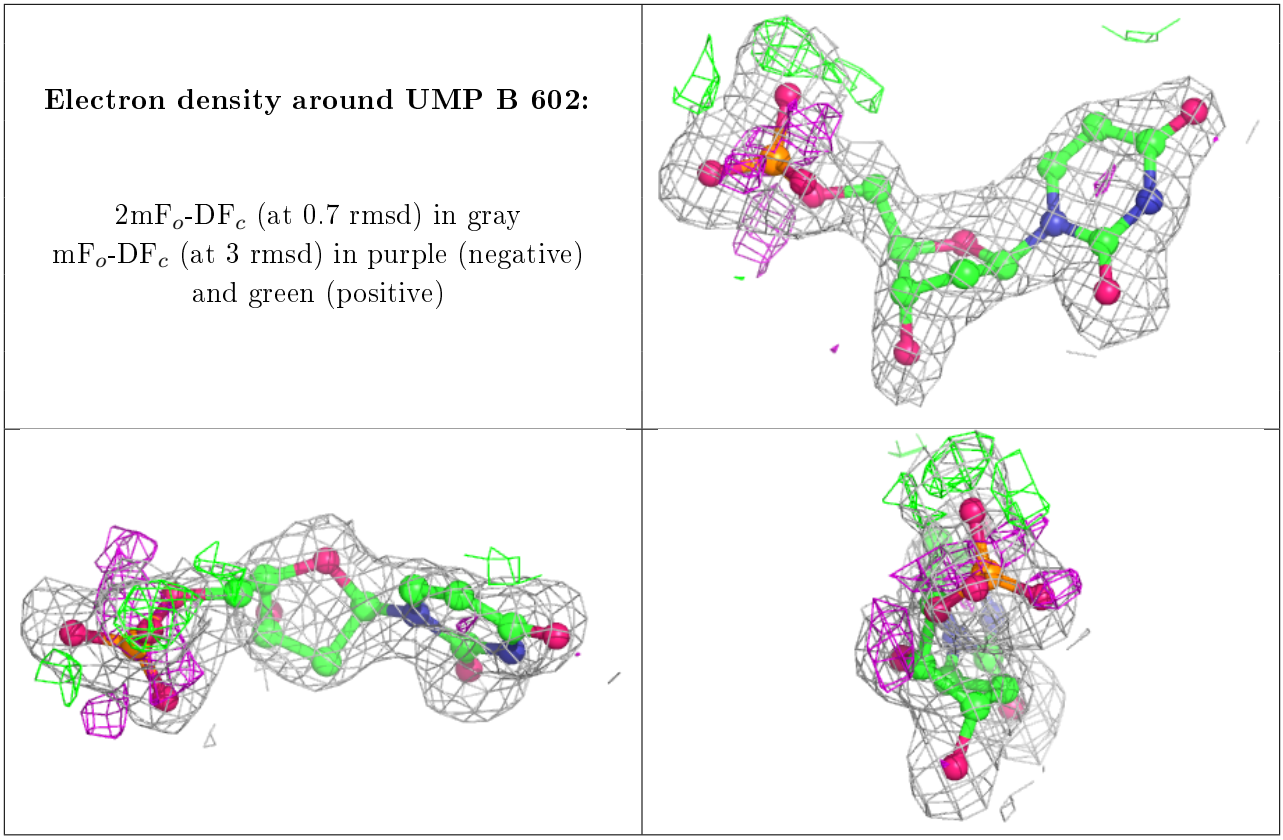
Electron density around THG A 702:

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



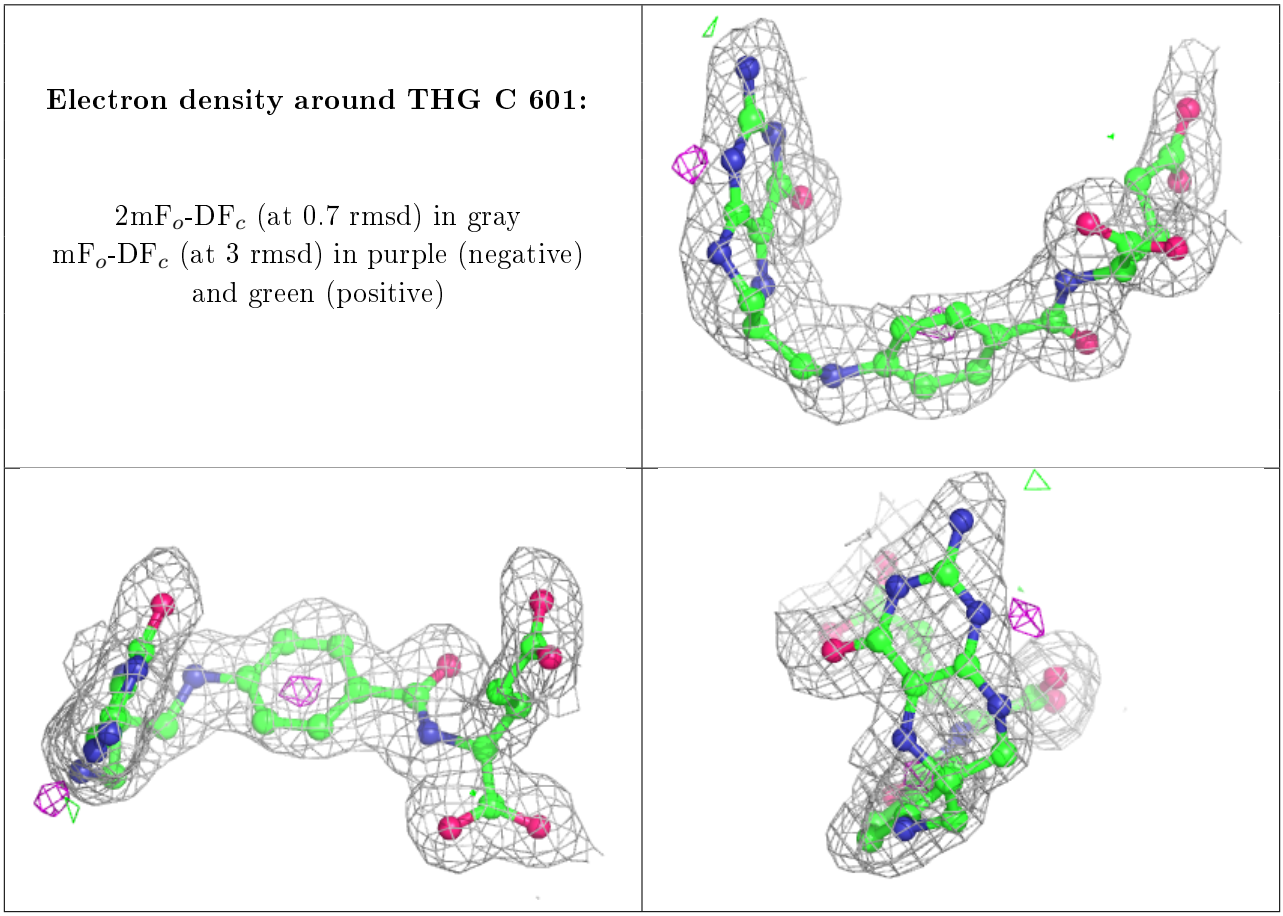
Electron density around UMP B 602:

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



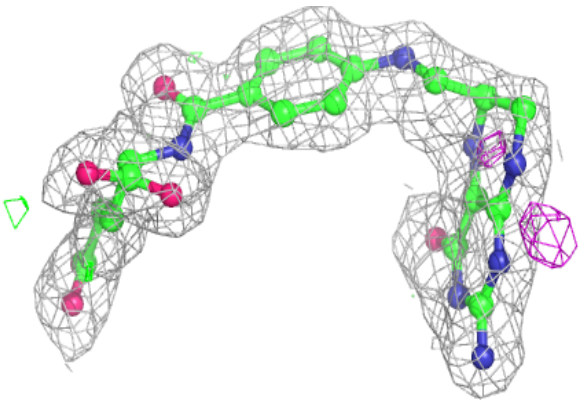
Electron density around THG C 601:

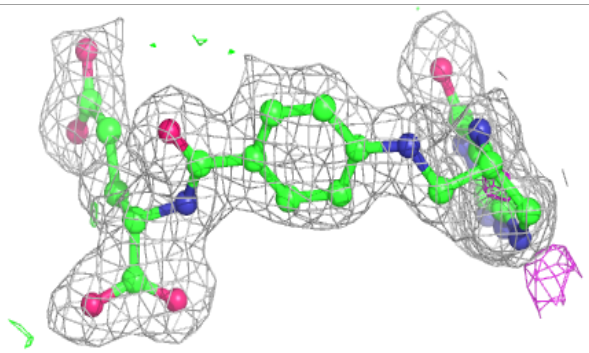
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

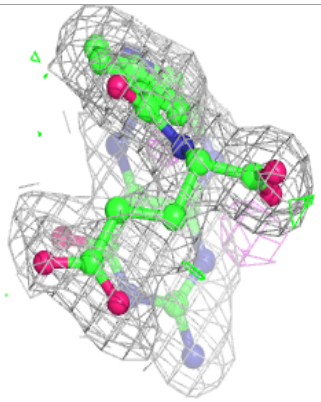


Electron density around THG B 601:

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

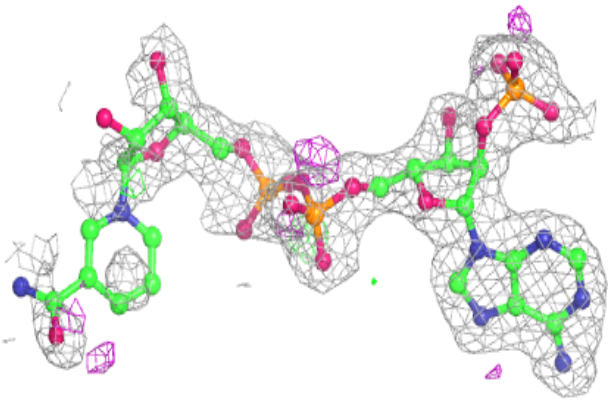


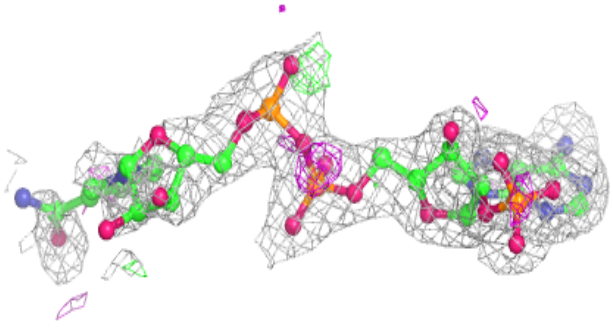


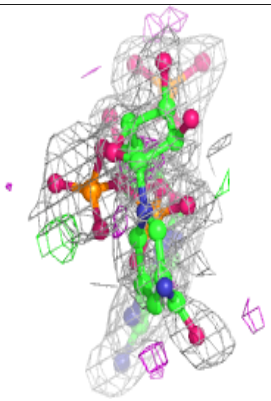


Electron density around NAP D 701:

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

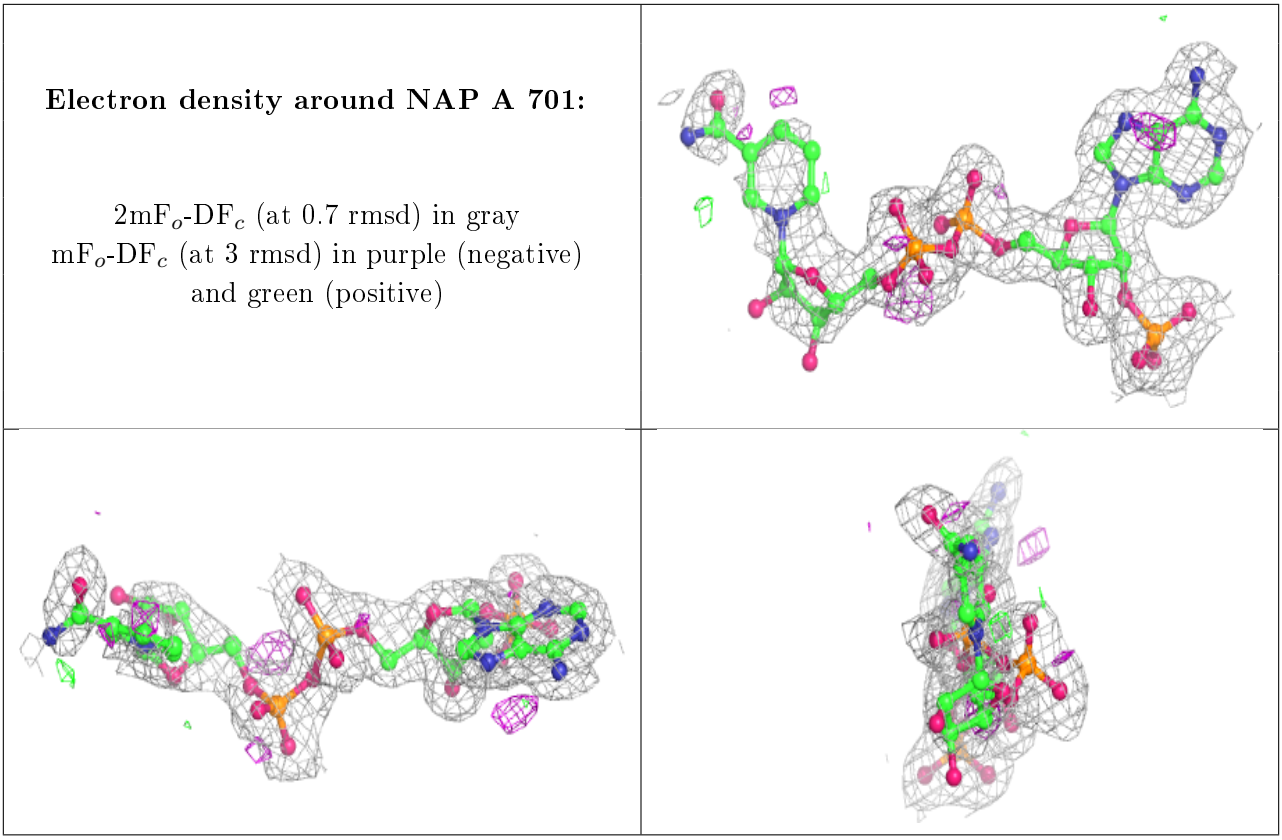






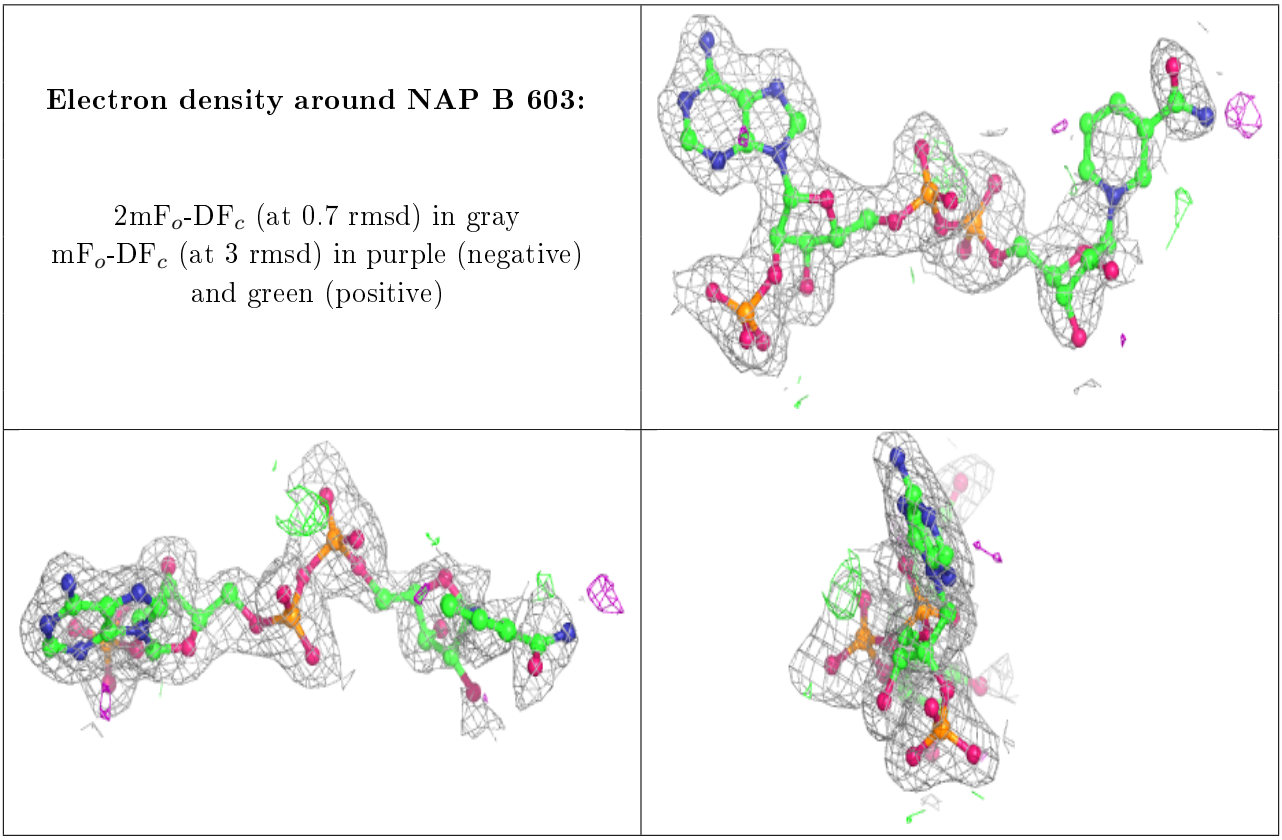
Electron density around NAP A 701:

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



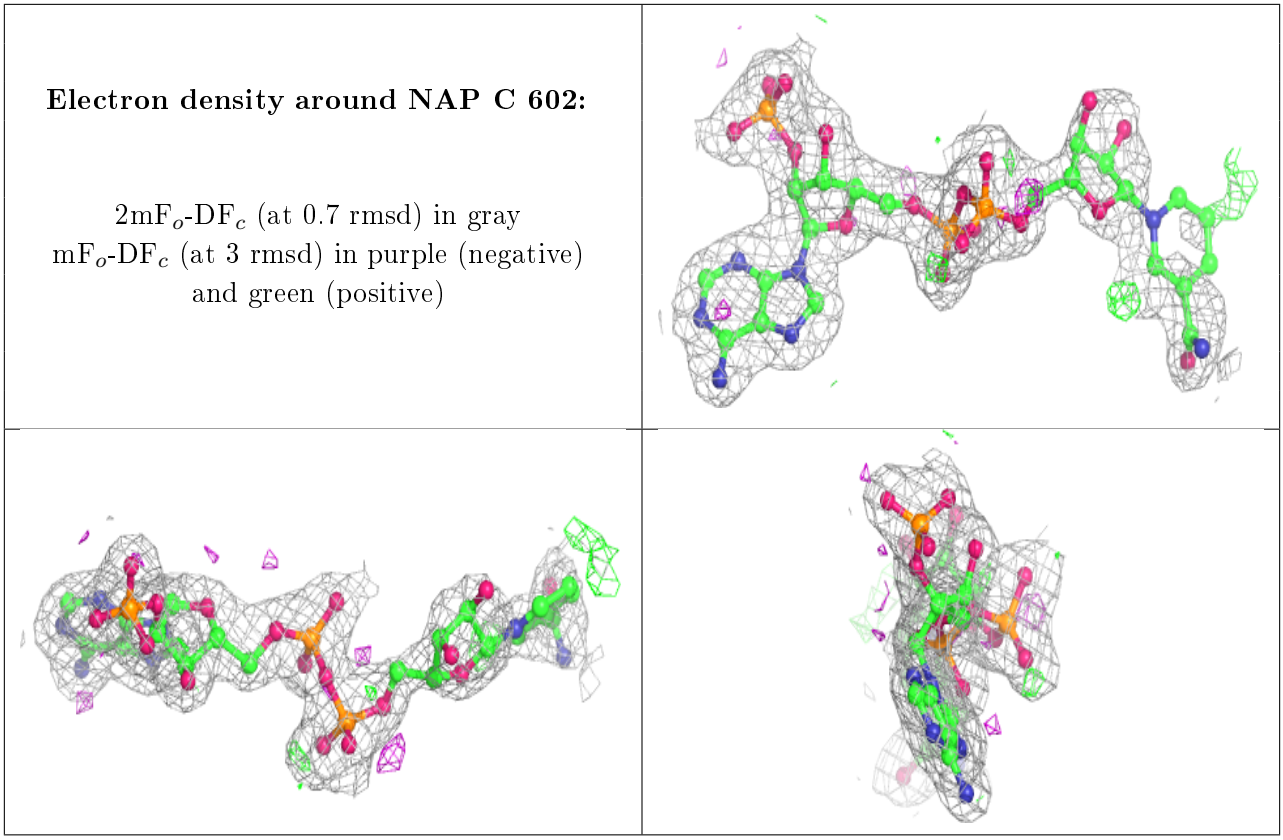
Electron density around NAP B 603:

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



Electron density around NAP C 602:

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



6.5 Other polymers

There are no such residues in this entry.