Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:47 AM EDT

PDB ID	:	7RSX
Title	:	HIV-1 gp120 complex with CJF-III-049-S
Authors	:	Liang, S.; Hendrickson, W.A.
Deposited on	:	2021-08-12
Resolution	:	2.75 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

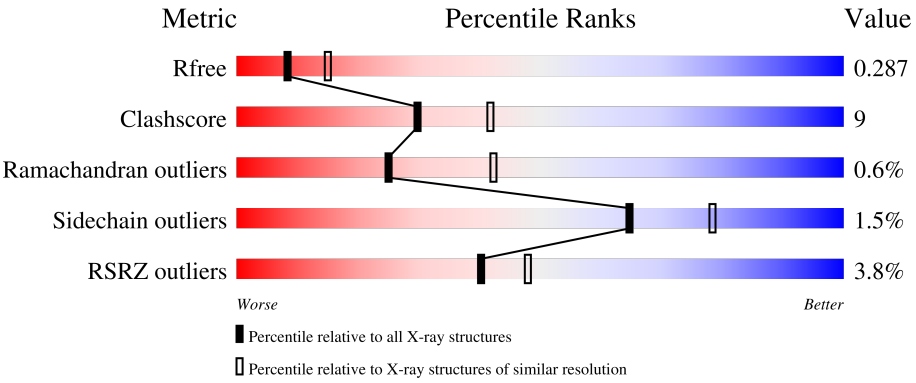
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	362	5% 73% 20% 7%
1	B	362	2% 76% 17% 7%
1	C	362	4% 69% 22% 7%
1	D	362	3% 75% 17% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	506	-	-	-	X
2	NAG	D	501	-	-	-	X
2	NAG	D	504	-	-	-	X
3	7IT	C	506	-	-	-	X

2 Entry composition

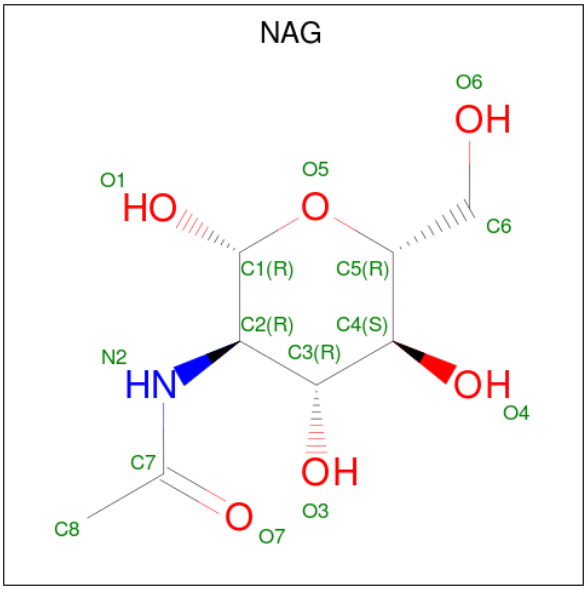
There are 4 unique types of molecules in this entry. The entry contains 11059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	B	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	A	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	D	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

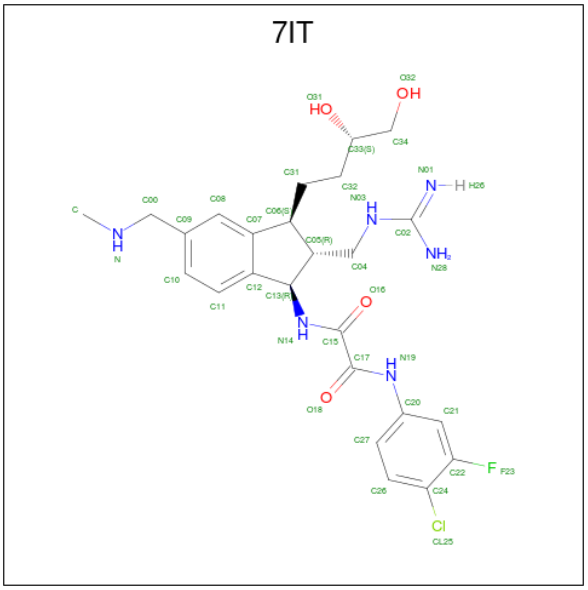
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is N 1 -{(1R,2R,3S)-2-(carbamimidamidomethyl)-3-[(3S)-3,4-dihydroxybutyl]-5-[(methylamino)methyl]-2,3-dihydro-1H-inden-1-yl}-N 2 -(4-chloro-3-fluorophenyl)ethanediamide (three-letter code: 7IT) (formula: $C_{25}H_{32}ClFN_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C Cl F N O 37 25 1 1 6 4	0	0
3	B	1	Total C Cl F N O 37 25 1 1 6 4	0	0
3	A	1	Total C Cl F N O 37 25 1 1 6 4	0	0
3	D	1	Total C Cl F N O 37 25 1 1 6 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	11	Total O 11 11	0	0
4	B	12	Total O 12 12	0	0

Continued on next page...

Continued from previous page...

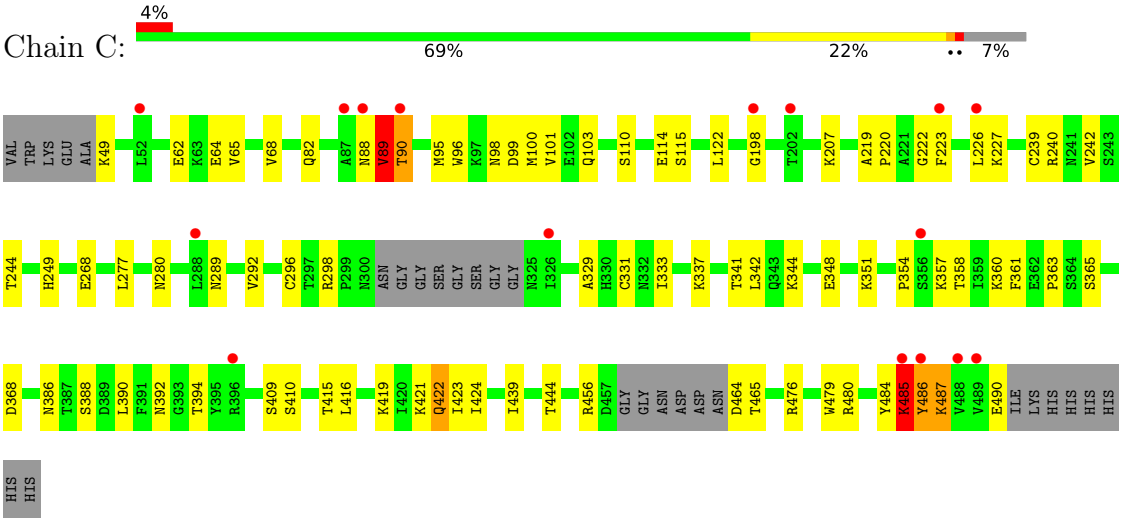
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	D	14	Total O 14 14	0	0

3 Residue-property plots (i)

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

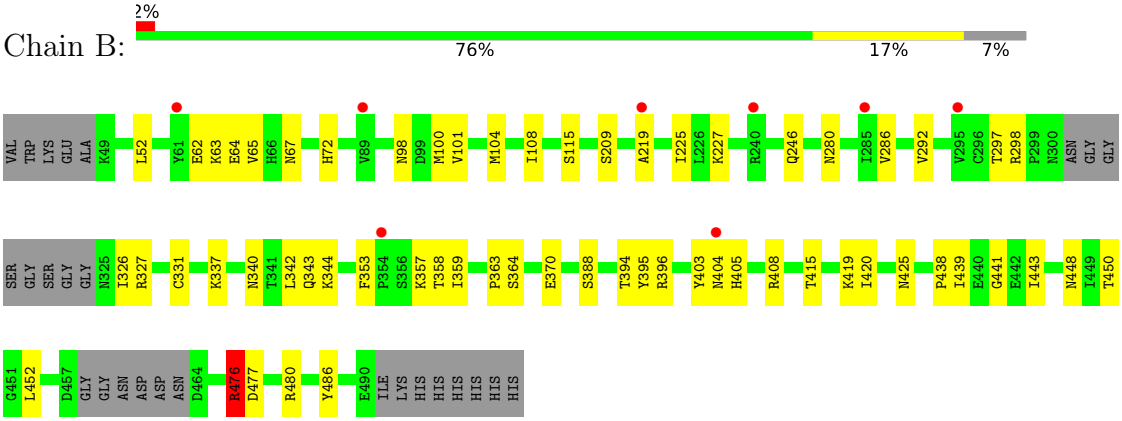
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

Chain C:



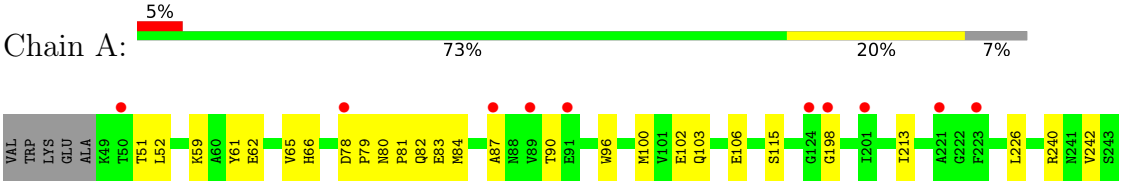
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

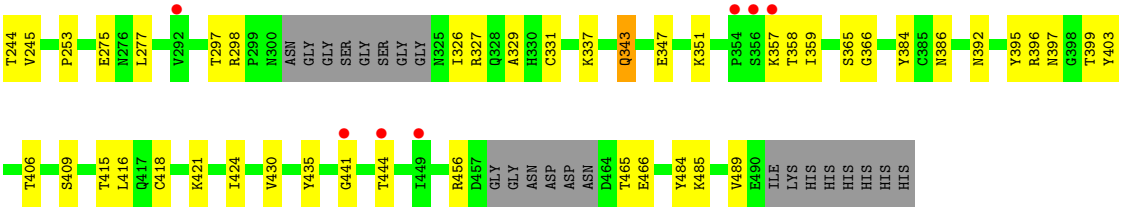
Chain B:



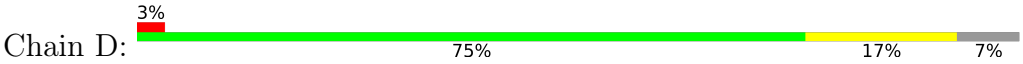
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

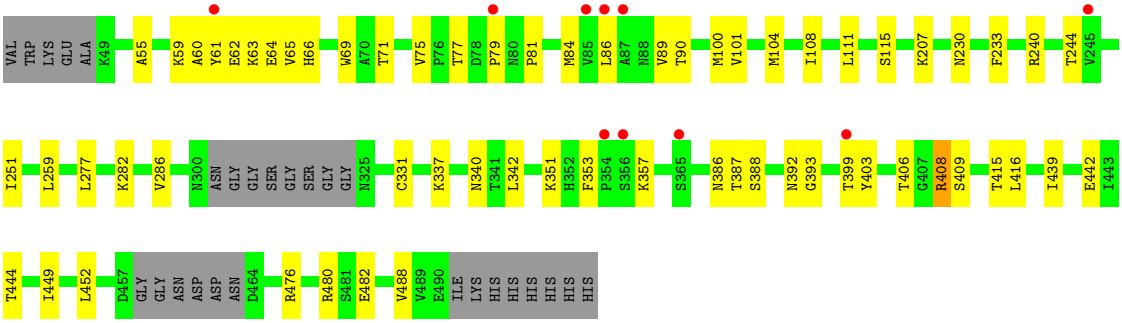
Chain A:





• Molecule 1: ENVELOPE GLYCOPROTEIN GP120





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.81Å 120.66Å 195.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.40 – 2.75 102.64 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.40-2.75) 99.5 (102.64-2.66)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.240 , 0.281 0.246 , 0.287	Depositor DCC
R_{free} test set	2413 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11059	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.58% 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: NAG, 7IT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/2681	0.49	0/3637
1	B	2.67	2/2680 (0.1%)	2.88	3/3634 (0.1%)
1	C	0.28	0/2682	0.51	0/3640
1	D	0.30	0/2680	0.51	2/3634 (0.1%)
All	All	1.36	2/10723 (0.0%)	1.50	5/14545 (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	B	0	1
1	C	0	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	ARG	CZ-NH2	135.57	3.09	1.33
1	B	476	ARG	CZ-NH1	-21.80	1.04	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	476	ARG	NE-CZ-NH2	-133.61	53.50	120.30
1	B	476	ARG	NH1-CZ-NH2	-76.80	34.92	119.40
1	B	476	ARG	NE-CZ-NH1	-74.09	83.25	120.30
1	D	408	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	408	ARG	CA-CB-CG	-5.36	101.61	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	476	ARG	Sidechain
1	C	484	TYR	Peptide
1	C	485	LYS	Peptide
1	C	88	ASN	Peptide
1	C	89	VAL	Peptide

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	2627	0	2539	42	0
1	B	2627	0	2540	55	0
1	C	2627	0	2548	58	0
1	D	2627	0	2538	42	0
2	A	84	0	78	1	0
2	B	70	0	65	2	0
2	C	70	0	65	1	0
2	D	98	0	90	3	0
2	E	28	0	24	2	0
3	A	37	0	0	1	0
3	B	37	0	0	0	0
3	C	37	0	0	0	0
3	D	37	0	0	0	0
4	A	16	0	0	4	0
4	B	12	0	0	6	0
4	C	11	0	0	3	0
4	D	14	0	0	1	0
All	All	11059	0	10487	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (201) 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:B:476:ARG:NH2	1:B:476:ARG:HH11	1.58	1.00
1:B:62:GLU:O	4:B:601:HOH:O	1.85	0.93
1:B:394:THR:O	1:B:404:ASN:HB2	1.76	0.86
1:C:423:ILE:C	1:C:424:ILE:HD12	1.99	0.81
1:A:297:THR:HG23	1:A:444:THR:HG22	1.60	0.81
1:B:364:SER:O	4:B:602:HOH:O	1.98	0.81
1:A:226:LEU:HD12	1:A:489:VAL:HG11	1.64	0.80
1:B:298:ARG:NH2	1:B:439:ILE:O	2.13	0.80
1:C:90:THR:HA	1:C:239:CYS:O	1.83	0.79
1:B:394:THR:O	1:B:404:ASN:CB	2.31	0.78
1:B:476:ARG:NH2	1:B:476:ARG:NH1	2.31	0.77
1:B:476:ARG:NH2	1:B:476:ARG:CD	2.48	0.77
1:D:399:THR:HG1	1:D:403:TYR:N	1.83	0.77
1:B:344:LYS:HD2	2:B:503:NAG:H5	1.71	0.73
1:D:408:ARG:HD3	1:D:409:SER:H	1.53	0.72
1:C:485:LYS:HG2	1:C:486:TYR:HB2	1.70	0.72
1:C:207:LYS:HG2	1:C:439:ILE:HG22	1.73	0.71
1:A:351:LYS:NZ	4:A:602:HOH:O	2.24	0.70
1:A:277:LEU:O	1:A:456:ARG:NH1	2.25	0.70
1:B:298:ARG:NH1	1:B:441:GLY:O	2.25	0.70
1:D:62:GLU:HG3	1:D:64:GLU:H	1.58	0.69
2:D:501:NAG:H83	2:D:501:NAG:H3	1.73	0.69
1:B:326:ILE:O	4:B:603:HOH:O	2.10	0.69
1:C:357:LYS:HB3	1:C:465:THR:HA	1.75	0.68
1:C:344:LYS:HE3	2:C:503:NAG:H5	1.74	0.68
1:A:84:MET:HB3	1:A:244:THR:HG22	1.77	0.67
1:C:358:THR:O	1:C:465:THR:OG1	2.13	0.66
1:A:421:LYS:NZ	4:A:603:HOH:O	2.27	0.66
1:A:253:PRO:O	4:A:601:HOH:O	2.13	0.65
1:C:62:GLU:O	4:C:601:HOH:O	2.15	0.64
1:D:392:ASN:OD1	1:D:406:THR:OG1	2.16	0.63
1:D:230:ASN:ND2	4:D:602:HOH:O	2.24	0.63
1:B:343:GLN:HA	1:B:403:TYR:HB2	1.82	0.62
1:D:408:ARG:NE	1:D:408:ARG:HA	2.08	0.61
1:C:249:HIS:ND1	1:C:486:TYR:OH	2.25	0.61
1:A:52:LEU:HD11	1:A:100:MET:HG2	1.81	0.61
1:A:298:ARG:NH2	1:A:441:GLY:O	2.28	0.61
1:C:99:ASP:OD2	1:C:103:GLN:NE2	2.34	0.60
1:C:98:ASN:HD22	1:C:101:VAL:HG23	1.66	0.60
1:D:331:CYS:O	1:D:415:THR:HA	2.00	0.60
1:C:98:ASN:ND2	1:C:101:VAL:HG23	2.18	0.59
1:B:292:VAL:HG22	1:B:337:LYS:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.85	0.59
1:A:365:SER:OG	1:A:366:GLY:N	2.36	0.58
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.83	0.58
1:C:227:LYS:HB2	1:C:486:TYR:HD1	1.67	0.58
1:A:326:ILE:HD12	1:A:327:ARG:HG3	1.86	0.58
1:A:90:THR:HB	1:A:240:ARG:HA	1.85	0.58
1:A:329:ALA:HB3	1:A:418:CYS:HB2	1.86	0.57
1:D:393:GLY:HA2	1:D:406:THR:HG23	1.86	0.57
1:D:476:ARG:O	1:D:480:ARG:HG3	2.04	0.57
1:D:386:ASN:O	1:D:416:LEU:HD22	2.04	0.57
1:A:79:PRO:C	1:A:81:PRO:HD3	2.26	0.57
1:B:476:ARG:NH2	1:B:476:ARG:NE	2.53	0.56
1:C:101:VAL:HG12	1:C:476:ARG:HG2	1.87	0.56
1:C:65:VAL:HB	1:C:115:SER:HB3	1.87	0.56
1:C:424:ILE:HD12	1:C:424:ILE:N	2.20	0.56
2:D:504:NAG:H83	2:D:504:NAG:H3	1.87	0.56
1:C:486:TYR:O	1:C:487:LYS:HB2	2.06	0.55
1:A:87:ALA:HB1	1:A:240:ARG:HH21	1.72	0.55
1:D:79:PRO:O	1:D:81:PRO:HD3	2.07	0.55
1:A:87:ALA:HB1	1:A:240:ARG:NH2	2.23	0.54
1:C:476:ARG:O	1:C:480:ARG:HG3	2.08	0.54
1:B:476:ARG:NH2	1:B:476:ARG:HD3	2.22	0.54
1:B:298:ARG:NH2	4:B:603:HOH:O	2.40	0.54
1:B:65:VAL:HB	1:B:115:SER:HB3	1.90	0.54
1:C:331:CYS:O	1:C:415:THR:HA	2.08	0.53
1:C:227:LYS:HB2	1:C:486:TYR:CD1	2.44	0.53
1:A:396:ARG:HG2	1:A:397:ASN:HD22	1.73	0.53
1:B:408:ARG:HB2	2:B:505:NAG:O6	2.08	0.53
1:B:52:LEU:HD23	1:B:219:ALA:HA	1.90	0.52
1:B:353:PHE:HB3	1:B:357:LYS:HD3	1.92	0.52
1:A:96:TRP:CG	1:A:275:GLU:HB3	2.45	0.52
1:C:226:LEU:HD22	1:C:244:THR:HG22	1.92	0.52
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.92	0.52
1:C:298:ARG:HB2	1:C:329:ALA:HB2	1.92	0.51
1:A:198:GLY:N	4:A:605:HOH:O	2.36	0.51
1:C:227:LYS:HA	1:C:486:TYR:HA	1.91	0.51
1:B:326:ILE:HB	4:B:603:HOH:O	2.09	0.51
1:C:98:ASN:HD21	1:C:100:MET:HB3	1.76	0.51
1:D:408:ARG:HA	1:D:408:ARG:HE	1.76	0.51
1:B:343:GLN:HA	1:B:403:TYR:CB	2.42	0.50
1:B:227:LYS:HE3	1:B:486:TYR:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TYR:CE2	1:B:405:HIS:HB2	2.46	0.50
1:A:359:ILE:HB	1:A:395:TYR:HB3	1.94	0.49
2:E:2:NAG:H83	2:E:2:NAG:H3	1.92	0.49
1:A:90:THR:CB	1:A:240:ARG:HA	2.41	0.49
1:B:298:ARG:HH21	1:B:438:PRO:HB2	1.77	0.49
1:D:207:LYS:HG3	1:D:439:ILE:HG22	1.94	0.49
1:D:408:ARG:NE	1:D:408:ARG:CA	2.75	0.49
1:B:363:PRO:HG3	1:B:388:SER:HA	1.95	0.49
1:D:84:MET:HB2	1:D:244:THR:CG2	2.43	0.49
1:C:280:ASN:HB2	1:C:456:ARG:O	2.13	0.48
1:C:422:GLN:O	1:C:424:ILE:HD13	2.12	0.48
1:B:370:GLU:CD	1:B:425:ASN:HB2	2.34	0.48
1:A:102:GLU:O	1:A:106:GLU:HG3	2.12	0.48
1:B:104:MET:O	1:B:108:ILE:HG12	2.13	0.48
1:A:357:LYS:N	1:A:357:LYS:HD3	2.29	0.48
1:D:59:LYS:HB3	1:D:61:TYR:CE2	2.49	0.48
1:D:353:PHE:C	1:D:357:LYS:HE3	2.33	0.48
1:C:333:ILE:HD13	1:C:390:LEU:HD13	1.95	0.48
1:A:403:TYR:O	2:A:506:NAG:H81	2.13	0.48
1:B:394:THR:O	1:B:404:ASN:HB3	2.13	0.48
1:D:55:ALA:HB1	1:D:77:THR:HA	1.96	0.47
1:D:65:VAL:HB	1:D:115:SER:HB3	1.96	0.47
1:B:476:ARG:O	1:B:480:ARG:HG3	2.14	0.47
1:D:387:THR:HA	1:D:416:LEU:HD22	1.96	0.47
1:A:392:ASN:OD1	1:A:406:THR:OG1	2.30	0.47
1:B:403:TYR:CG	1:B:404:ASN:N	2.83	0.47
1:B:62:GLU:HG3	1:B:64:GLU:H	1.80	0.47
1:B:340:ASN:O	1:B:343:GLN:HB3	2.15	0.47
1:D:86:LEU:HB2	1:D:89:VAL:CG1	2.44	0.47
1:D:86:LEU:HB2	1:D:89:VAL:HG12	1.97	0.47
1:D:251:ILE:HD12	1:D:482:GLU:HB3	1.95	0.47
1:D:442:GLU:HG2	1:D:444:THR:HG23	1.96	0.47
2:E:1:NAG:H83	2:E:1:NAG:H3	1.96	0.47
1:A:343:GLN:HE21	1:A:399:THR:HA	1.80	0.47
1:D:259:LEU:HD22	1:D:449:ILE:HD13	1.95	0.47
1:B:297:THR:HA	1:B:443:ILE:O	2.15	0.47
1:D:60:ALA:HA	1:D:71:THR:HG21	1.95	0.47
1:D:104:MET:O	1:D:108:ILE:HG12	2.15	0.47
2:D:501:NAG:H3	2:D:501:NAG:C8	2.43	0.47
1:A:331:CYS:O	1:A:415:THR:HA	2.15	0.46
1:A:78:ASP:C	1:A:80:ASN:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HB	1:B:452:LEU:HB2	1.98	0.46
1:A:424:ILE:HD13	1:A:435:TYR:HD1	1.79	0.46
1:D:64:GLU:OE2	1:D:66:HIS:HB2	2.16	0.46
1:C:207:LYS:HG2	1:C:439:ILE:CG2	2.44	0.45
1:C:277:LEU:HD23	1:C:277:LEU:HA	1.83	0.45
1:B:343:GLN:HE22	1:B:403:TYR:N	2.14	0.45
1:D:408:ARG:HD3	1:D:409:SER:N	2.26	0.45
1:A:384:TYR:CE1	1:A:421:LYS:HB2	2.51	0.45
1:A:51:THR:HA	1:A:103:GLN:HE22	1.82	0.45
1:D:69:TRP:CD1	1:D:111:LEU:HA	2.51	0.45
1:C:95:MET:HG3	1:C:96:TRP:CD1	2.52	0.45
1:C:360:LYS:HG2	1:C:394:THR:HG23	1.98	0.45
1:C:422:GLN:O	1:C:424:ILE:CD1	2.64	0.45
1:B:327:ARG:HG2	1:B:420:ILE:O	2.17	0.45
1:B:477:ASP:OD1	1:B:480:ARG:NH1	2.50	0.45
1:C:464:ASP:OD1	1:C:465:THR:N	2.50	0.44
1:C:292:VAL:CG2	1:C:341:THR:HG21	2.47	0.44
1:C:386:ASN:O	1:C:416:LEU:HB3	2.17	0.44
1:C:348:GLU:O	1:C:351:LYS:HG2	2.18	0.44
1:D:100:MET:HE2	1:D:488:VAL:HB	1.99	0.44
1:C:337:LYS:O	1:C:341:THR:HG23	2.17	0.44
1:B:98:ASN:HD21	1:B:100:MET:HE3	1.83	0.44
1:A:357:LYS:HG3	1:A:466:GLU:HG2	2.00	0.44
1:A:347:GLU:HG2	1:A:395:TYR:OH	2.18	0.44
1:A:358:THR:O	1:A:465:THR:OG1	2.36	0.43
1:C:89:VAL:HG23	1:C:90:THR:N	2.34	0.43
1:C:422:GLN:C	1:C:424:ILE:CD1	2.87	0.43
1:A:59:LYS:HB3	1:A:61:TYR:CZ	2.53	0.43
1:C:226:LEU:O	1:C:486:TYR:HA	2.17	0.43
1:C:424:ILE:N	1:C:424:ILE:CD1	2.82	0.43
1:C:409:SER:OG	1:C:410:SER:N	2.51	0.43
1:D:282:LYS:HA	1:D:282:LYS:HD2	1.83	0.43
1:C:227:LYS:O	1:C:242:VAL:HA	2.18	0.43
1:C:296:CYS:O	1:C:444:THR:HA	2.19	0.43
1:A:83:GLU:HA	1:A:245:VAL:HG12	2.01	0.43
1:C:223:PHE:CD1	1:C:490:GLU:HG3	2.54	0.42
1:B:343:GLN:NE2	1:B:403:TYR:N	2.67	0.42
1:A:484:TYR:CZ	1:A:485:LYS:HG2	2.53	0.42
1:A:66:HIS:HB3	1:A:213:ILE:HG12	2.00	0.42
1:D:277:LEU:HD23	1:D:277:LEU:HA	1.91	0.42
1:C:110:SER:O	1:C:114:GLU:HG3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLU:CD	4:C:602:HOH:O	2.57	0.42
1:D:230:ASN:HB3	1:D:233:PHE:HB2	2.01	0.42
1:C:101:VAL:HG21	1:C:480:ARG:HG2	2.01	0.42
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.71	0.42
1:C:421:LYS:NZ	4:C:605:HOH:O	2.42	0.42
1:C:476:ARG:HA	1:C:479:TRP:CD1	2.54	0.42
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.85	0.42
1:D:351:LYS:HB2	1:D:351:LYS:HE3	1.82	0.42
1:D:55:ALA:HA	1:D:75:VAL:O	2.20	0.42
1:A:65:VAL:HB	1:A:115:SER:HB3	2.02	0.42
1:A:226:LEU:HD22	1:A:242:VAL:HG12	2.02	0.42
1:C:361:PHE:O	1:C:392:ASN:HA	2.20	0.41
1:B:219:ALA:HB2	1:B:225:ILE:HD11	2.02	0.41
1:D:337:LYS:HA	1:D:340:ASN:OD1	2.20	0.41
1:B:52:LEU:CD1	1:B:100:MET:HG2	2.50	0.41
1:B:331:CYS:O	1:B:415:THR:HA	2.20	0.41
1:B:403:TYR:HE2	1:B:405:HIS:HB2	1.83	0.41
1:D:251:ILE:CD1	1:D:482:GLU:HB3	2.49	0.41
1:C:219:ALA:HA	1:C:220:PRO:HD3	1.93	0.41
1:A:386:ASN:O	1:A:416:LEU:HB3	2.21	0.41
1:C:363:PRO:HG3	1:C:388:SER:HA	2.01	0.41
1:B:298:ARG:NH2	1:B:438:PRO:HB2	2.36	0.41
1:B:64:GLU:HB3	1:B:67:ASN:HD22	1.86	0.41
1:A:430:VAL:HA	3:A:507:7IT:N28	2.35	0.41
1:B:298:ARG:CZ	4:B:603:HOH:O	2.69	0.41
1:B:476:ARG:HD3	1:B:476:ARG:HH21	1.85	0.41
1:C:64:GLU:O	1:C:68:VAL:HG23	2.21	0.41
1:C:122:LEU:HD21	1:C:198:GLY:CA	2.52	0.40
1:D:90:THR:OG1	1:D:240:ARG:HB2	2.21	0.40
1:C:222:GLY:HA2	1:B:72:HIS:O	2.21	0.40
1:B:359:ILE:HB	1:B:395:TYR:HB3	2.03	0.40
1:B:219:ALA:O	1:B:246:GLN:NE2	2.55	0.40
1:C:122:LEU:HD21	1:C:198:GLY:HA2	2.03	0.40
1:B:358:THR:HG21	1:B:396:ARG:HE	1.86	0.40
1:B:448:ASN:O	1:B:450:THR:HG23	2.21	0.40
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

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	327/362 (90%)	312 (95%)	15 (5%)	0	100 100
1	B	325/362 (90%)	313 (96%)	12 (4%)	0	100 100
1	C	329/362 (91%)	307 (93%)	14 (4%)	8 (2%)	6 9
1	D	325/362 (90%)	312 (96%)	13 (4%)	0	100 100
All	All	1306/1448 (90%)	1244 (95%)	54 (4%)	8 (1%)	25 42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	485	LYS
1	C	486	TYR
1	C	487	LYS
1	C	90	THR
1	C	268	GLU
1	C	354	PRO
1	C	365	SER
1	C	89	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	297/316 (94%)	292 (98%)	5 (2%)	60 76
1	B	297/316 (94%)	293 (99%)	4 (1%)	69 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	297/316 (94%)	290 (98%)	7 (2%)	49 68
1	D	297/316 (94%)	295 (99%)	2 (1%)	84 89
All	All	1188/1264 (94%)	1170 (98%)	18 (2%)	65 78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	LYS
1	C	82	GLN
1	C	240	ARG
1	C	289	ASN
1	C	368	ASP
1	C	419	LYS
1	C	422	GLN
1	B	63	LYS
1	B	209	SER
1	B	280	ASN
1	B	419	LYS
1	A	62	GLU
1	A	82	GLN
1	A	337	LYS
1	A	343	GLN
1	A	409	SER
1	D	63	LYS
1	D	388	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	ASN
1	A	397	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	501	1	14,14,15	0.22	0	17,19,21	0.33	0
3	7IT	D	508	-	37,39,39	3.07	18 (48%)	45,54,54	1.63	9 (20%)
2	NAG	E	2	1	14,14,15	0.26	0	17,19,21	1.36	2 (11%)
2	NAG	D	505	1	14,14,15	0.29	0	17,19,21	0.61	0
3	7IT	A	507	-	37,39,39	3.07	18 (48%)	45,54,54	1.62	9 (20%)
2	NAG	A	504	1	14,14,15	0.31	0	17,19,21	0.49	0
2	NAG	C	502	-	14,14,15	0.64	1 (7%)	17,19,21	0.65	0
2	NAG	B	502	1	14,14,15	0.26	0	17,19,21	0.66	1 (5%)
2	NAG	A	503	1	14,14,15	0.20	0	17,19,21	0.51	0
2	NAG	D	501	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	1 (5%)
2	NAG	D	506	1	14,14,15	0.15	0	17,19,21	0.58	0
2	NAG	A	505	1	14,14,15	0.49	0	17,19,21	0.73	1 (5%)
3	7IT	C	506	-	37,39,39	3.07	18 (48%)	45,54,54	1.62	9 (20%)
2	NAG	C	504	-	14,14,15	0.48	0	17,19,21	0.41	0
2	NAG	D	502	1	14,14,15	0.19	0	17,19,21	0.46	0
3	7IT	B	506	-	37,39,39	3.07	18 (48%)	45,54,54	1.63	9 (20%)
2	NAG	D	507	1	14,14,15	0.45	0	17,19,21	0.64	0
2	NAG	D	503	1	14,14,15	0.22	0	17,19,21	0.86	1 (5%)
2	NAG	B	504	1	14,14,15	0.19	0	17,19,21	0.51	0
2	NAG	C	505	-	14,14,15	0.24	0	17,19,21	0.55	0
2	NAG	A	501	1	14,14,15	0.21	0	17,19,21	0.35	0
2	NAG	C	503	-	14,14,15	0.30	0	17,19,21	0.48	0
2	NAG	A	506	1	14,14,15	0.78	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	B	503	1	14,14,15	0.39	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	1	14,14,15	0.43	0	17,19,21	1.40	2 (11%)
2	NAG	B	505	1	14,14,15	0.41	0	17,19,21	0.61	0
2	NAG	C	501	-	14,14,15	0.31	0	17,19,21	0.37	0
2	NAG	D	504	1	14,14,15	0.37	0	17,19,21	1.34	2 (11%)
2	NAG	A	502	1	14,14,15	0.32	0	17,19,21	0.57	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
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	7IT	D	508	-	-	3/26/43/43	0/3/3/3
2	NAG	E	2	1	-	5/6/23/26	0/1/1/1
2	NAG	D	505	1	-	2/6/23/26	0/1/1/1
3	7IT	A	507	-	-	3/26/43/43	0/3/3/3
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
2	NAG	C	502	-	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	3/6/23/26	0/1/1/1
2	NAG	D	501	1	-	4/6/23/26	0/1/1/1
2	NAG	D	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	4/6/23/26	0/1/1/1
3	7IT	C	506	-	-	3/26/43/43	0/3/3/3
2	NAG	C	504	-	-	2/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
3	7IT	B	506	-	-	3/26/43/43	0/3/3/3
2	NAG	D	507	1	-	4/6/23/26	0/1/1/1
2	NAG	D	503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	C	505	-	-	4/6/23/26	0/1/1/1
2	NAG	A	501	1	-	1/6/23/26	0/1/1/1
2	NAG	C	503	-	-	2/6/23/26	0/1/1/1
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
2	NAG	C	501	-	-	1/6/23/26	0/1/1/1
2	NAG	D	504	1	-	5/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	506	7IT	C02-N03	10.11	1.53	1.33
3	B	506	7IT	C02-N03	10.08	1.53	1.33
3	D	508	7IT	C02-N03	10.08	1.53	1.33
3	A	507	7IT	C02-N03	10.07	1.53	1.33
3	C	506	7IT	C15-N14	6.26	1.46	1.34
3	D	508	7IT	C15-N14	6.25	1.46	1.34
3	A	507	7IT	C15-N14	6.24	1.46	1.34
3	B	506	7IT	C15-N14	6.24	1.46	1.34
3	A	507	7IT	C17-N19	4.86	1.46	1.35
3	B	506	7IT	C17-N19	4.84	1.46	1.35
3	D	508	7IT	C17-N19	4.83	1.46	1.35
3	C	506	7IT	C17-N19	4.80	1.46	1.35
3	D	508	7IT	C20-N19	4.71	1.51	1.41
3	B	506	7IT	C20-N19	4.70	1.51	1.41
3	C	506	7IT	C20-N19	4.69	1.51	1.41
3	A	507	7IT	C20-N19	4.67	1.51	1.41
3	B	506	7IT	C08-C09	4.19	1.46	1.39
3	D	508	7IT	C08-C09	4.19	1.46	1.39
3	A	507	7IT	C08-C09	4.18	1.46	1.39
3	C	506	7IT	C08-C09	4.17	1.46	1.39
3	C	506	7IT	C00-N	4.15	1.52	1.46
3	B	506	7IT	C00-N	4.15	1.52	1.46
3	A	507	7IT	C00-N	4.14	1.52	1.46
3	D	508	7IT	C00-N	4.14	1.52	1.46
3	A	507	7IT	C11-C10	3.53	1.45	1.38
3	D	508	7IT	C11-C10	3.53	1.45	1.38
3	B	506	7IT	C11-C10	3.50	1.45	1.38
3	C	506	7IT	C11-C10	3.49	1.45	1.38
3	D	508	7IT	C12-C07	3.36	1.45	1.40
3	C	506	7IT	O18-C17	-3.35	1.17	1.23
3	B	506	7IT	C12-C07	3.33	1.45	1.40
3	C	506	7IT	C12-C07	3.33	1.45	1.40
3	B	506	7IT	O18-C17	-3.32	1.17	1.23
3	A	507	7IT	O18-C17	-3.32	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	7IT	C12-C07	3.30	1.45	1.40
3	D	508	7IT	O18-C17	-3.30	1.17	1.23
2	D	501	NAG	C1-C2	3.24	1.57	1.52
3	C	506	7IT	C24-CL25	3.20	1.81	1.73
3	A	507	7IT	C24-CL25	3.19	1.81	1.73
3	B	506	7IT	C24-CL25	3.18	1.81	1.73
3	D	508	7IT	C24-CL25	3.18	1.81	1.73
3	C	506	7IT	C11-C12	3.01	1.43	1.39
3	B	506	7IT	C12-C13	2.99	1.54	1.51
3	A	507	7IT	C12-C13	2.99	1.54	1.51
3	B	506	7IT	C11-C12	2.98	1.43	1.39
3	D	508	7IT	C11-C12	2.97	1.43	1.39
3	A	507	7IT	C11-C12	2.95	1.43	1.39
3	C	506	7IT	C17-C15	2.95	1.59	1.53
3	B	506	7IT	C17-C15	2.91	1.58	1.53
3	C	506	7IT	C12-C13	2.91	1.54	1.51
3	A	507	7IT	C17-C15	2.90	1.58	1.53
3	D	508	7IT	C12-C13	2.88	1.54	1.51
3	D	508	7IT	C17-C15	2.87	1.58	1.53
3	C	506	7IT	O16-C15	-2.46	1.18	1.23
3	A	507	7IT	O16-C15	-2.45	1.18	1.23
3	B	506	7IT	O16-C15	-2.44	1.18	1.23
3	D	508	7IT	O16-C15	-2.41	1.19	1.23
3	A	507	7IT	C32-C33	2.35	1.59	1.52
3	D	508	7IT	C32-C33	2.34	1.59	1.52
3	C	506	7IT	C32-C33	2.33	1.59	1.52
3	B	506	7IT	C32-C33	2.33	1.59	1.52
2	C	502	NAG	O5-C1	-2.17	1.40	1.43
3	A	507	7IT	C10-C09	2.14	1.43	1.38
3	D	508	7IT	C10-C09	2.13	1.43	1.38
3	B	506	7IT	C10-C09	2.12	1.43	1.38
3	C	506	7IT	O31-C33	-2.12	1.37	1.43
3	A	507	7IT	C08-C07	2.12	1.43	1.39
3	A	507	7IT	O31-C33	-2.11	1.37	1.43
3	C	506	7IT	C10-C09	2.11	1.43	1.38
3	B	506	7IT	O31-C33	-2.11	1.37	1.43
3	C	506	7IT	C08-C07	2.11	1.43	1.39
3	B	506	7IT	C08-C07	2.10	1.43	1.39
3	D	508	7IT	O31-C33	-2.09	1.37	1.43
3	D	508	7IT	C08-C07	2.08	1.43	1.39
2	A	506	NAG	O5-C1	2.07	1.47	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	506	7IT	C12-C13-N14	-4.71	107.06	114.61
3	D	508	7IT	C12-C13-N14	-4.70	107.07	114.61
3	C	506	7IT	C12-C13-N14	-4.69	107.08	114.61
3	A	507	7IT	C12-C13-N14	-4.68	107.09	114.61
2	E	2	NAG	C2-N2-C7	4.66	129.53	122.90
2	E	1	NAG	C2-N2-C7	4.55	129.38	122.90
2	D	504	NAG	C2-N2-C7	4.44	129.23	122.90
2	D	501	NAG	C2-N2-C7	4.10	128.74	122.90
2	A	506	NAG	C1-O5-C5	3.70	117.20	112.19
3	A	507	7IT	C31-C06-C07	3.35	122.16	113.03
3	B	506	7IT	C31-C06-C07	3.34	122.11	113.03
3	D	508	7IT	C31-C06-C07	3.33	122.09	113.03
3	C	506	7IT	C31-C06-C07	3.32	122.06	113.03
3	A	507	7IT	C26-C24-C22	3.20	121.50	118.94
3	B	506	7IT	C26-C24-C22	3.17	121.48	118.94
3	D	508	7IT	C26-C24-C22	3.17	121.48	118.94
3	C	506	7IT	C26-C24-C22	3.13	121.45	118.94
3	D	508	7IT	C15-C17-N19	3.08	117.18	112.31
3	C	506	7IT	C15-C17-N19	3.05	117.12	112.31
3	A	507	7IT	C15-C17-N19	3.05	117.12	112.31
3	B	506	7IT	O16-C15-N14	-3.04	117.75	123.08
3	B	506	7IT	C15-C17-N19	3.04	117.12	112.31
3	D	508	7IT	O16-C15-N14	-3.03	117.76	123.08
3	A	507	7IT	O16-C15-N14	-3.03	117.77	123.08
3	C	506	7IT	O16-C15-N14	-3.01	117.80	123.08
2	D	503	NAG	C1-O5-C5	2.99	116.24	112.19
3	D	508	7IT	C17-C15-N14	2.83	120.51	113.73
3	B	506	7IT	C17-C15-N14	2.82	120.50	113.73
3	A	507	7IT	C17-C15-N14	2.82	120.49	113.73
3	C	506	7IT	C17-C15-N14	2.81	120.47	113.73
3	B	506	7IT	C20-N19-C17	-2.43	123.31	127.53
3	C	506	7IT	C20-N19-C17	-2.43	123.31	127.53
3	A	507	7IT	C20-N19-C17	-2.42	123.32	127.53
3	D	508	7IT	C20-N19-C17	-2.41	123.35	127.53
2	A	505	NAG	C1-O5-C5	2.34	115.36	112.19
2	E	1	NAG	C1-C2-N2	2.31	114.43	110.49
2	D	504	NAG	C1-C2-N2	2.28	114.38	110.49
2	E	2	NAG	C1-C2-N2	2.27	114.37	110.49
2	B	502	NAG	C1-O5-C5	2.26	115.25	112.19
3	C	506	7IT	C07-C08-C09	-2.15	119.97	121.98
3	D	508	7IT	C07-C08-C09	-2.15	119.97	121.98
3	B	506	7IT	C07-C08-C09	-2.14	119.98	121.98
3	A	507	7IT	C07-C08-C09	-2.12	119.99	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	507	7IT	F23-C22-C24	2.12	120.93	118.98
3	B	506	7IT	F23-C22-C24	2.10	120.92	118.98
3	D	508	7IT	F23-C22-C24	2.10	120.92	118.98
3	C	506	7IT	F23-C22-C24	2.09	120.91	118.98

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	506	7IT	N03-C04-C05-C13
3	C	506	7IT	N03-C04-C05-C06
3	B	506	7IT	N03-C04-C05-C13
3	B	506	7IT	N03-C04-C05-C06
3	A	507	7IT	N03-C04-C05-C13
3	A	507	7IT	N03-C04-C05-C06
3	D	508	7IT	N03-C04-C05-C13
3	D	508	7IT	N03-C04-C05-C06
2	A	504	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	504	NAG	C4-C5-C6-O6
2	C	503	NAG	C8-C7-N2-C2
2	C	503	NAG	O7-C7-N2-C2
2	C	505	NAG	C8-C7-N2-C2
2	C	505	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	B	505	NAG	C8-C7-N2-C2
2	B	505	NAG	O7-C7-N2-C2
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	A	505	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

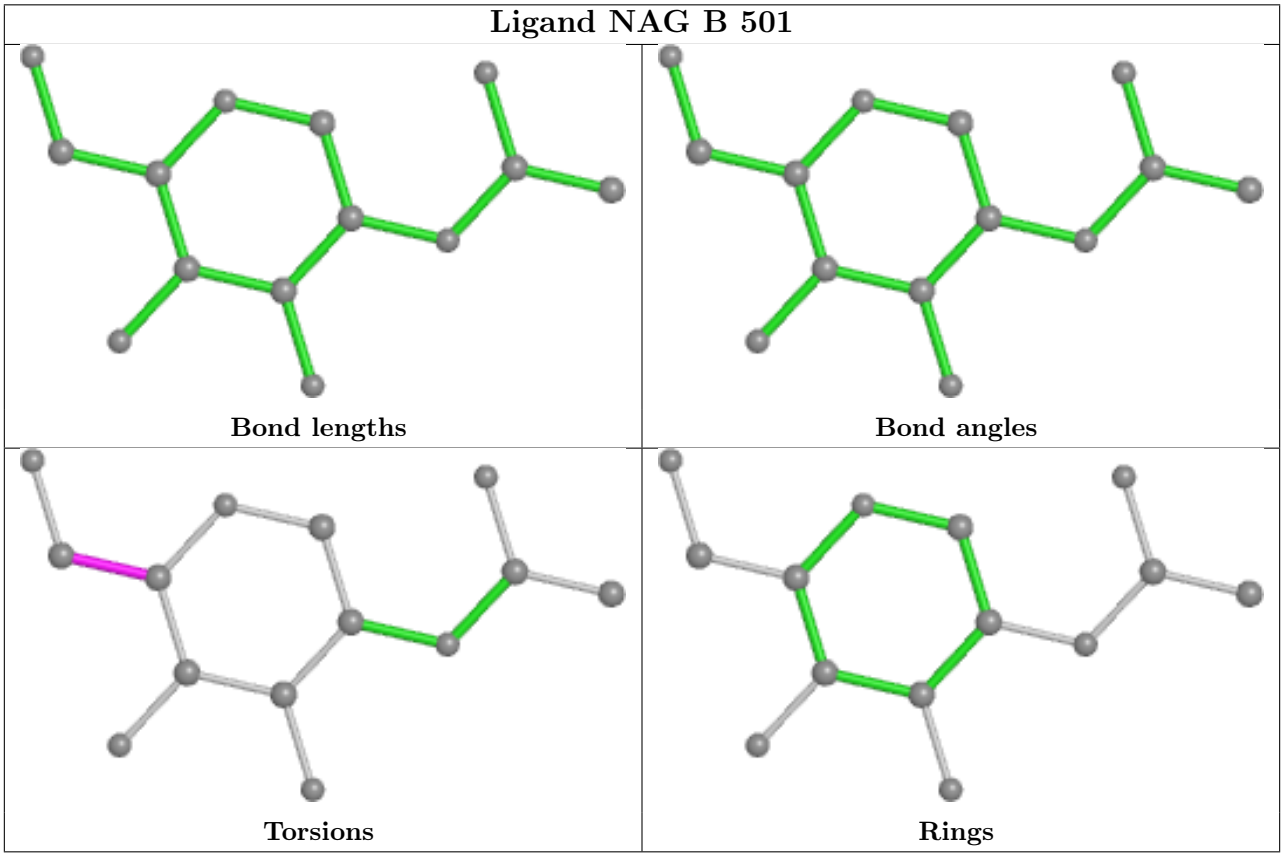
Mol	Chain	Res	Type	Atoms
2	A	505	NAG	O7-C7-N2-C2
2	D	501	NAG	C8-C7-N2-C2
2	D	501	NAG	O7-C7-N2-C2
2	D	504	NAG	C8-C7-N2-C2
2	D	504	NAG	O7-C7-N2-C2
2	D	505	NAG	C8-C7-N2-C2
2	D	505	NAG	O7-C7-N2-C2
2	D	507	NAG	C8-C7-N2-C2
2	D	507	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	C	505	NAG	O5-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	D	507	NAG	O5-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	B	502	NAG	O5-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	B	502	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	D	507	NAG	C4-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
3	C	506	7IT	C07-C06-C31-C32
3	B	506	7IT	C07-C06-C31-C32
3	A	507	7IT	C07-C06-C31-C32
3	D	508	7IT	C07-C06-C31-C32
2	D	503	NAG	O5-C5-C6-O6
2	D	501	NAG	O5-C5-C6-O6
2	C	501	NAG	C3-C2-N2-C7
2	D	501	NAG	C3-C2-N2-C7
2	D	504	NAG	C3-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	A	501	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

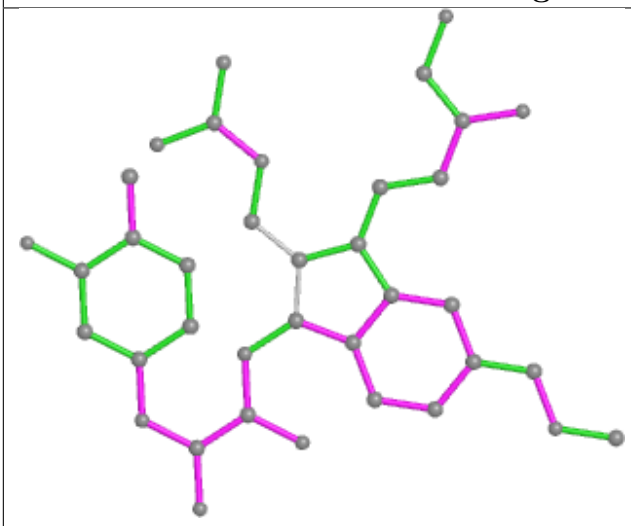
9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	A	507	7IT	1	0
2	D	501	NAG	2	0
2	C	503	NAG	1	0
2	A	506	NAG	1	0
2	B	503	NAG	1	0
2	E	1	NAG	1	0
2	B	505	NAG	1	0
2	D	504	NAG	1	0

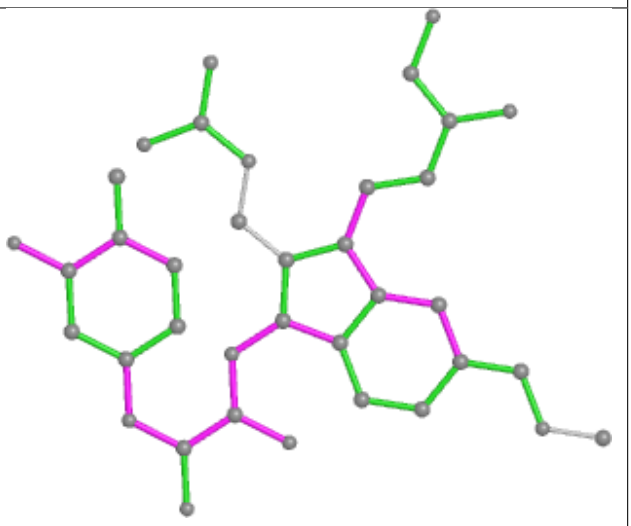
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



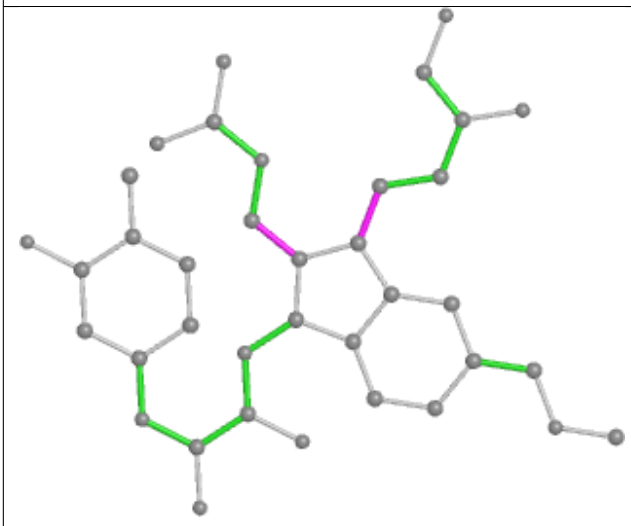
Ligand 7IT D 508



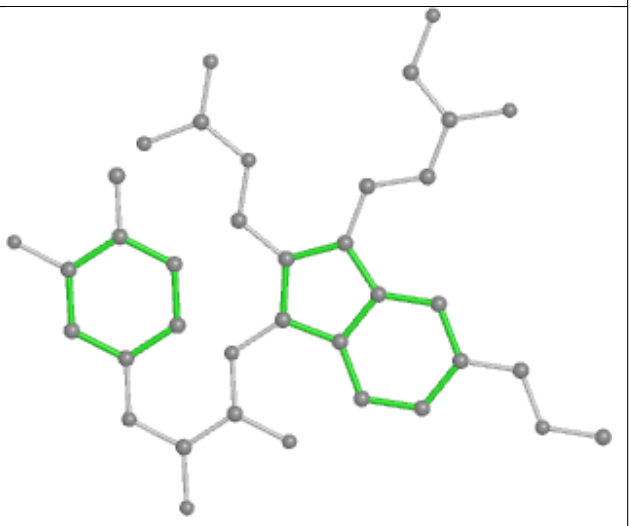
Bond lengths



Bond angles

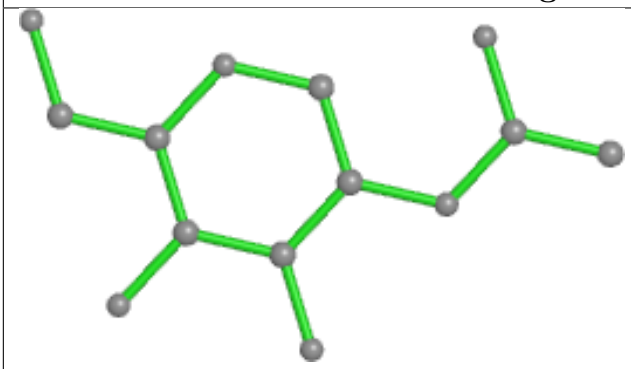


Torsions

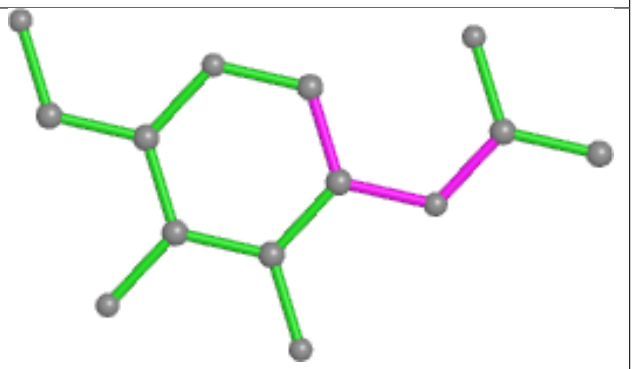


Rings

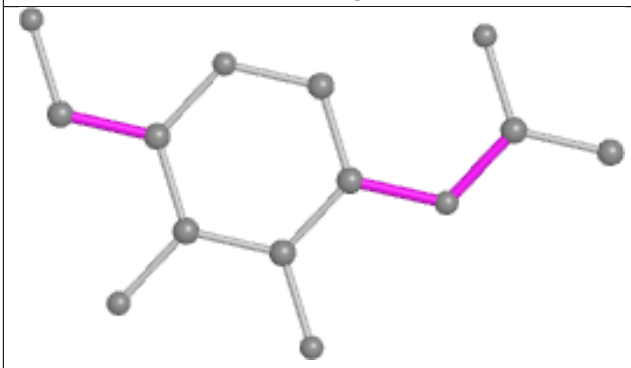
Ligand NAG E 2



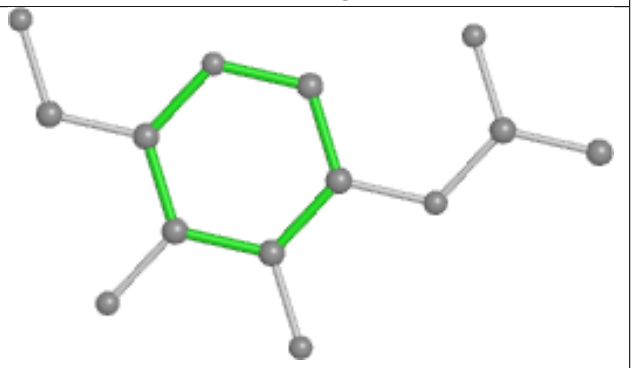
Bond lengths



Bond angles

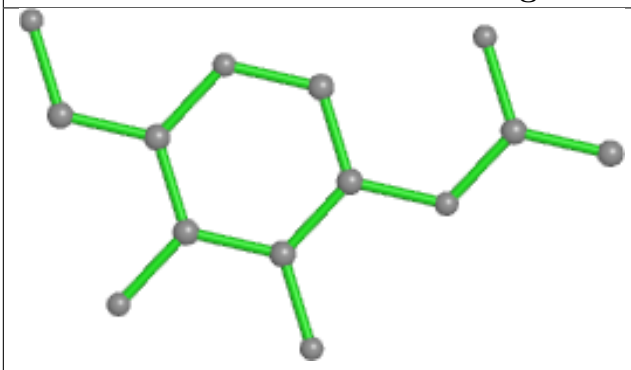


Torsions

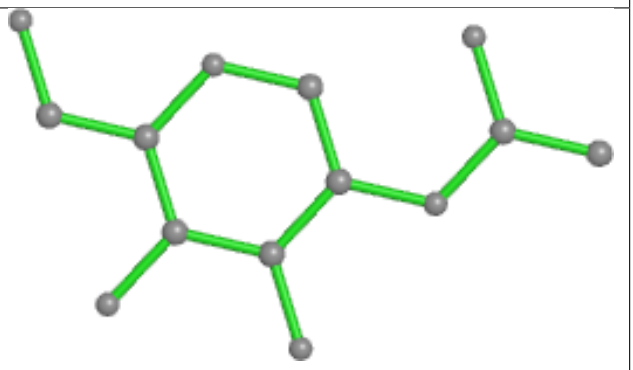


Rings

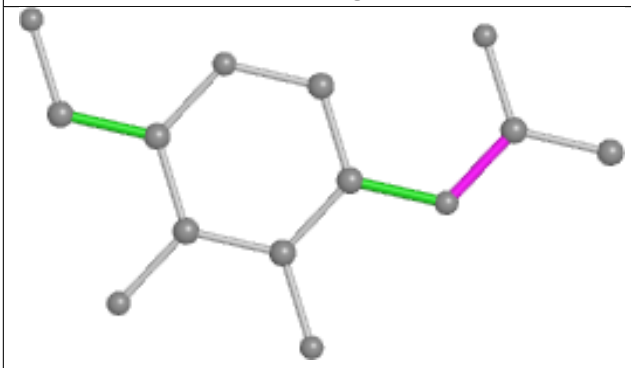
Ligand NAG D 505



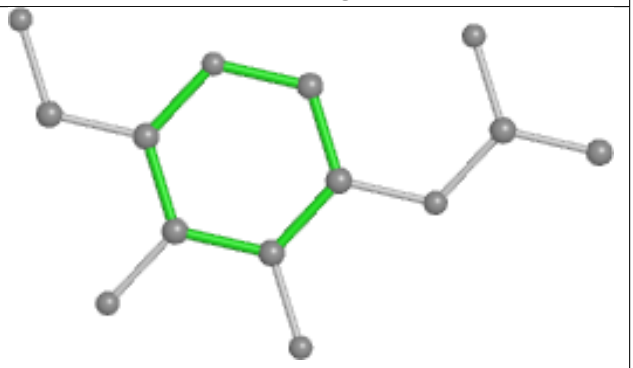
Bond lengths



Bond angles

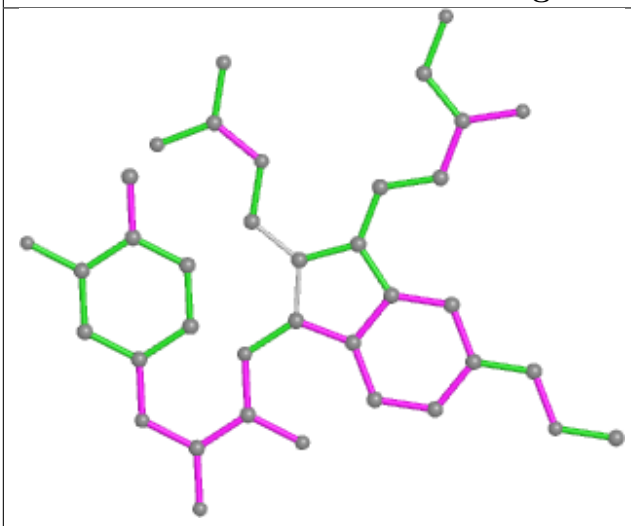


Torsions

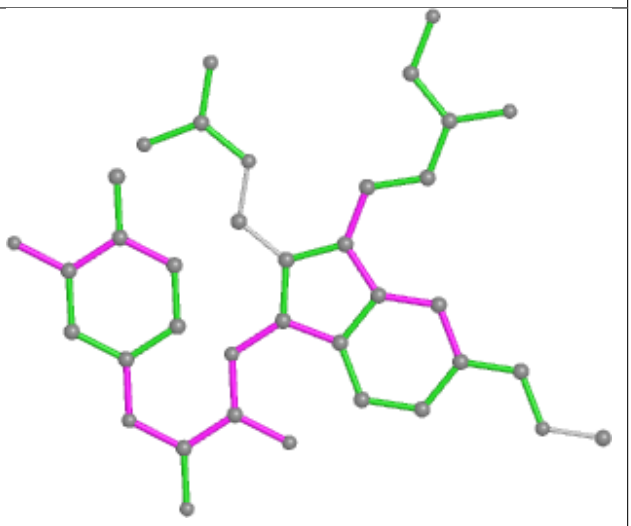


Rings

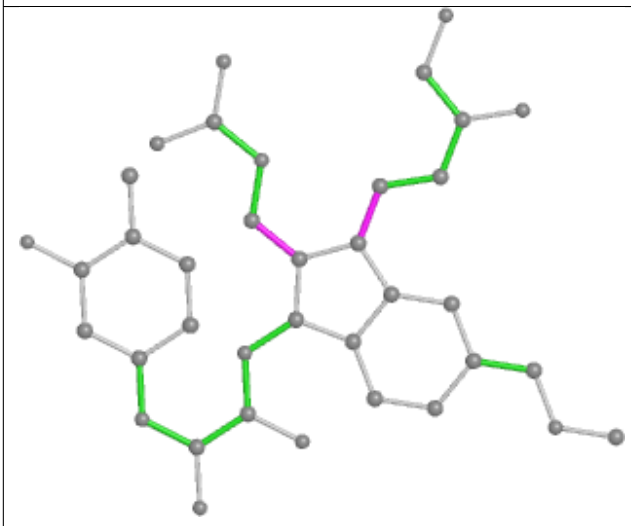
Ligand 7IT A 507



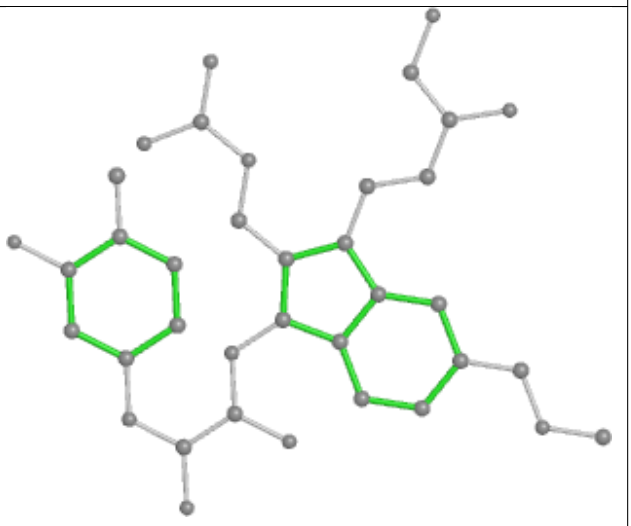
Bond lengths



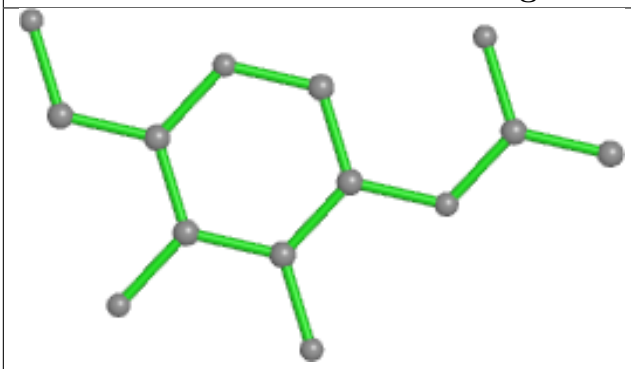
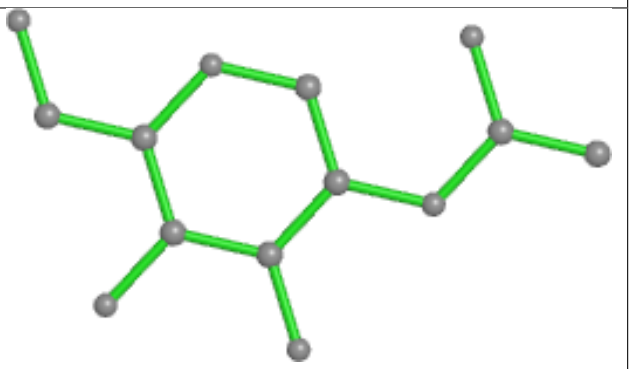
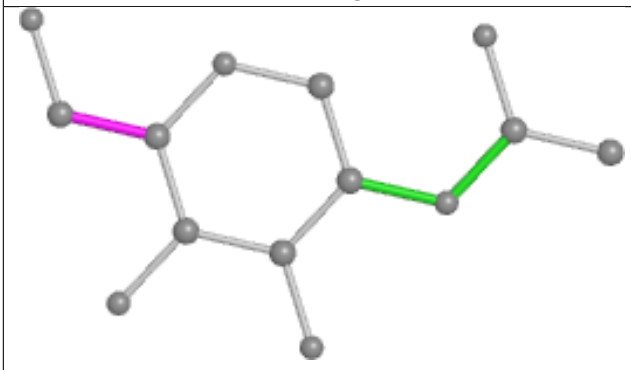
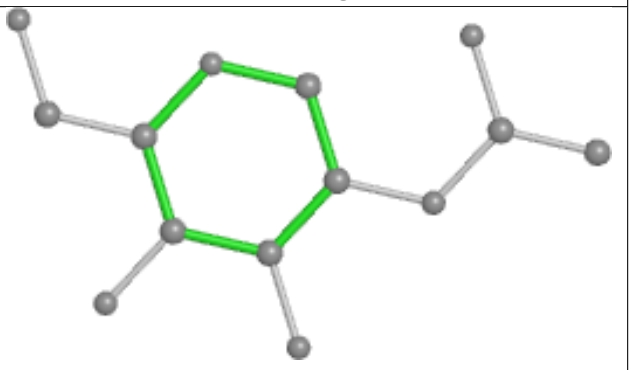
Bond angles

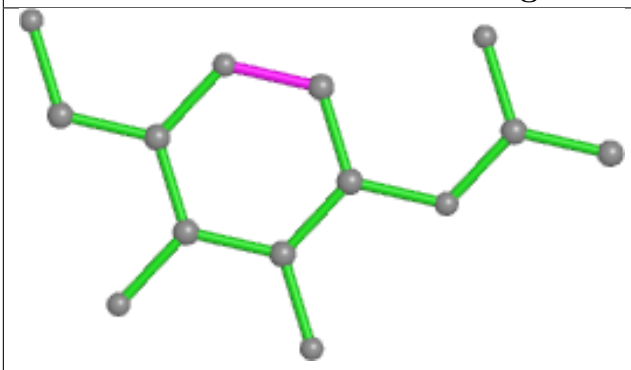
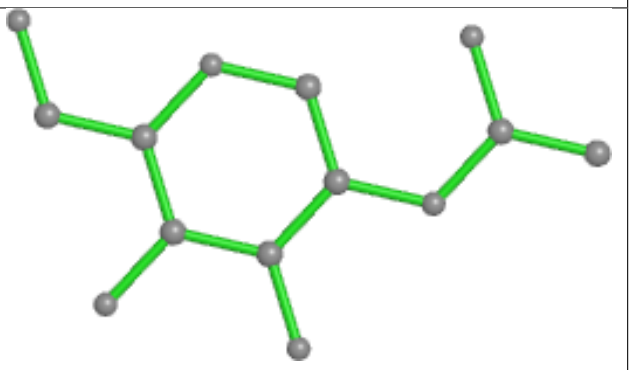
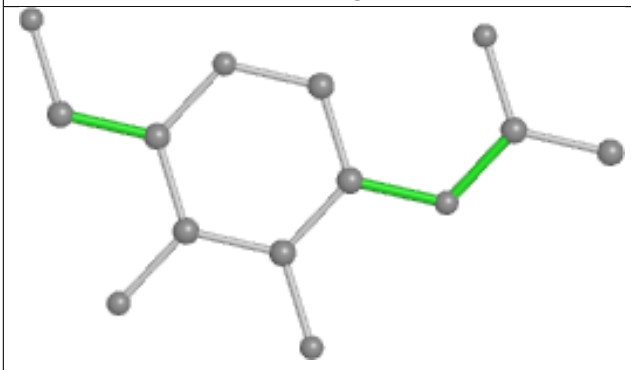
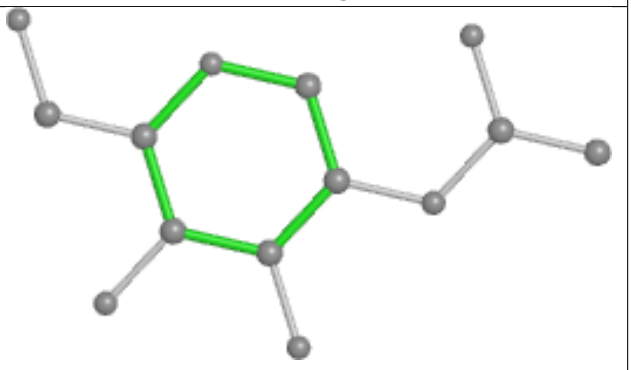


Torsions

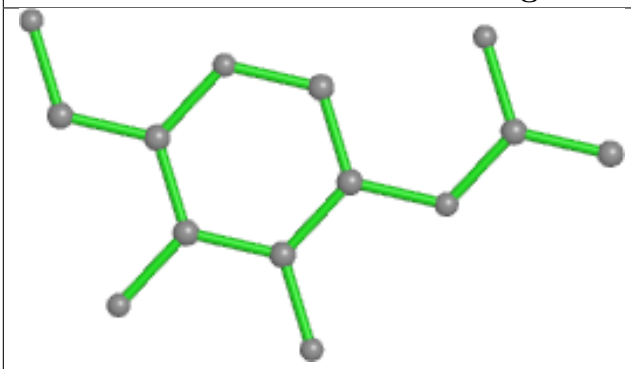


Rings

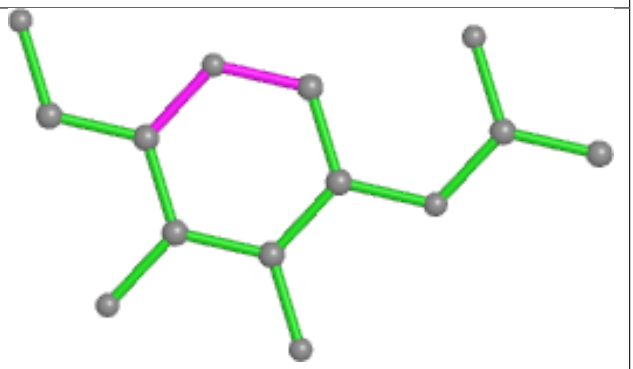
Ligand NAG A 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

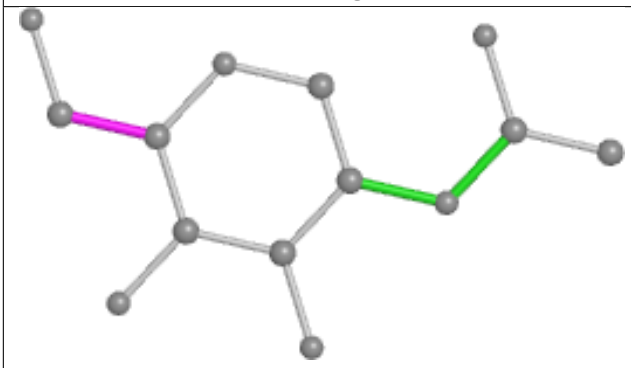
Ligand NAG B 502



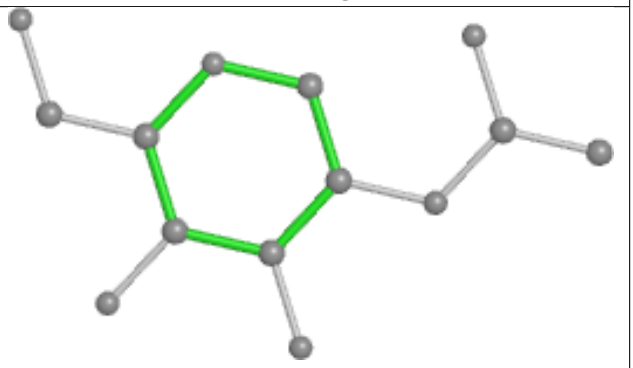
Bond lengths



Bond angles

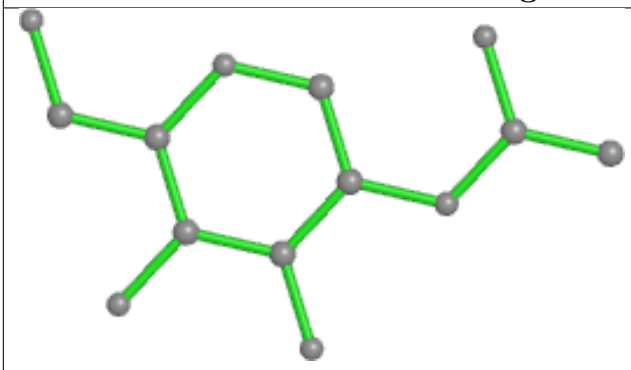


Torsions

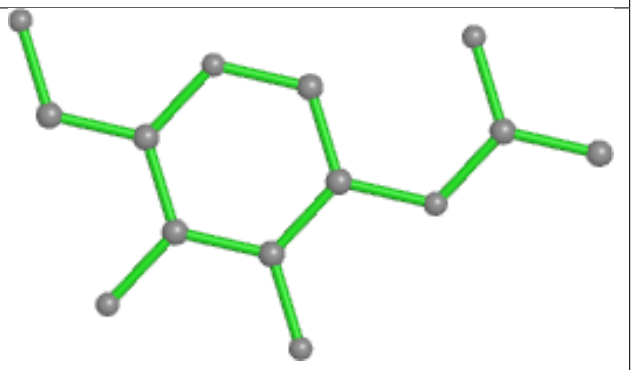


Rings

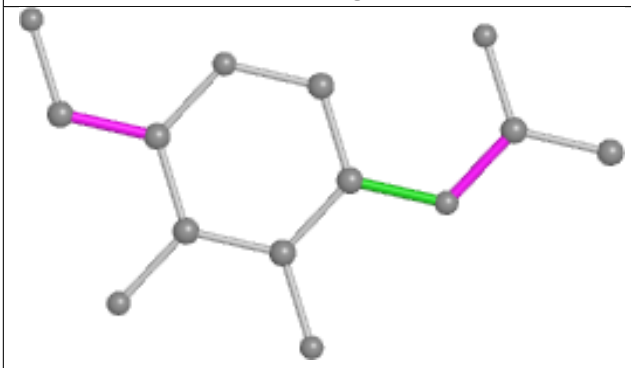
Ligand NAG A 503



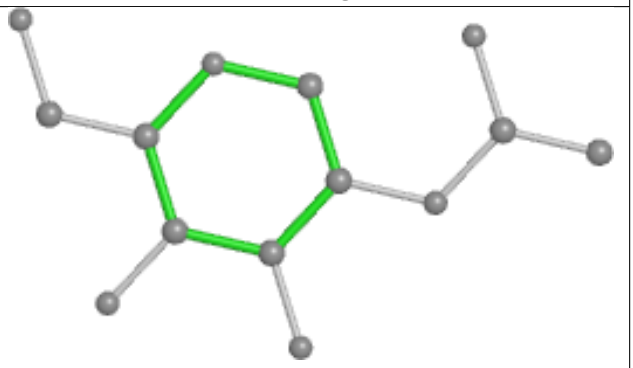
Bond lengths



Bond angles

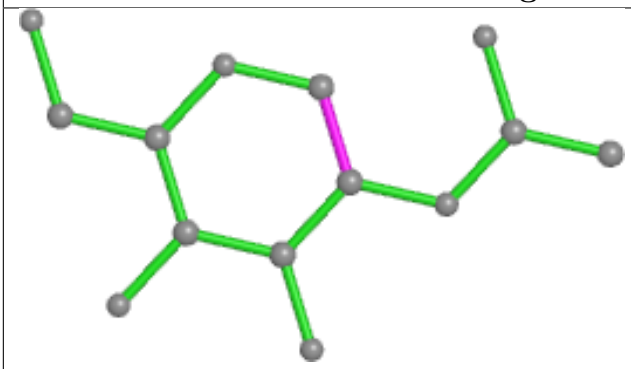


Torsions

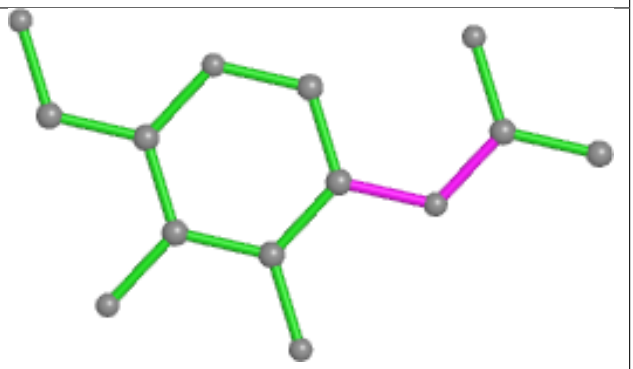


Rings

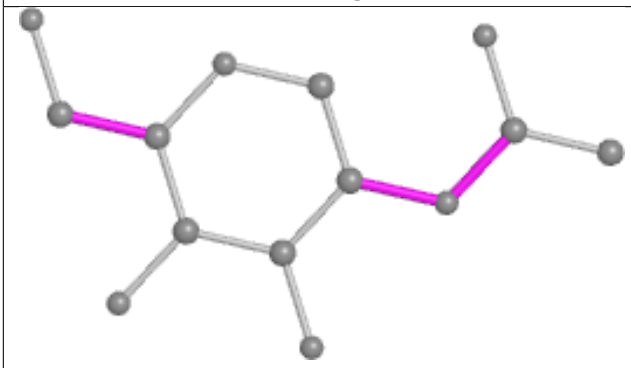
Ligand NAG D 501



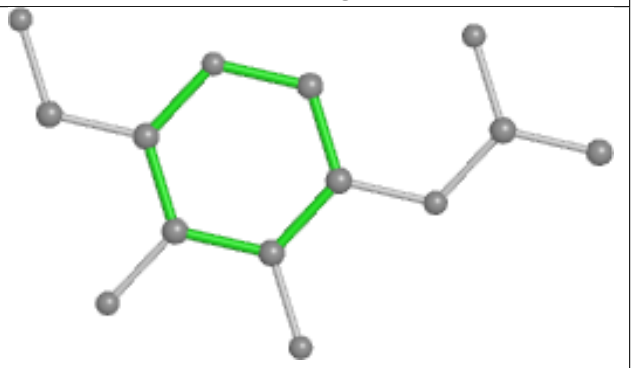
Bond lengths



Bond angles

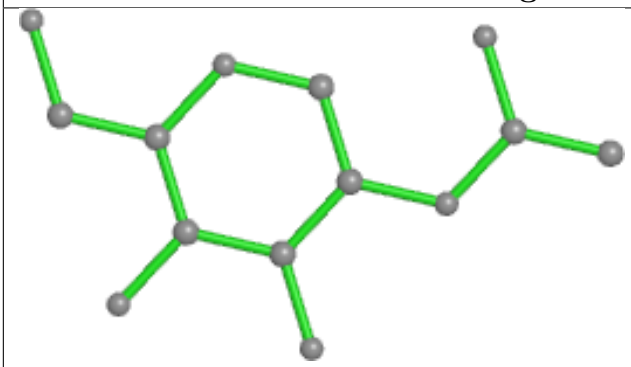


Torsions

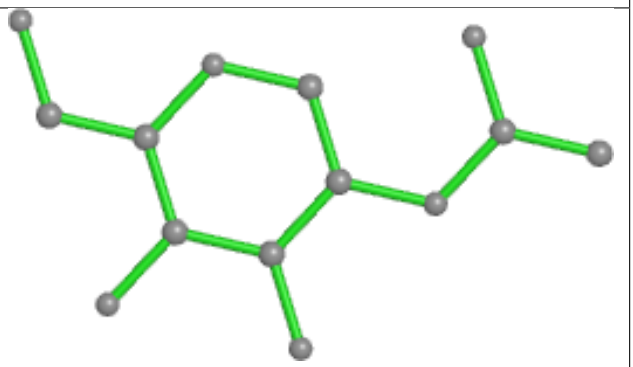


Rings

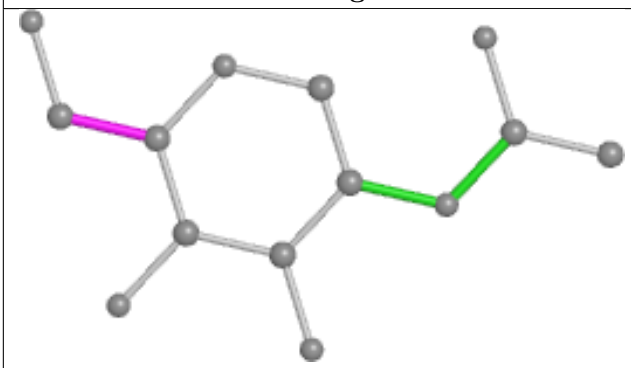
Ligand NAG D 506



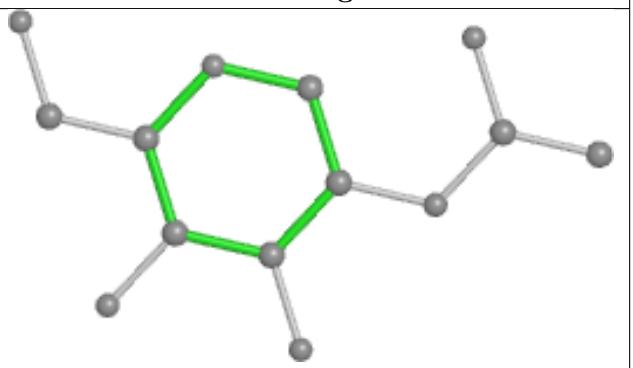
Bond lengths



Bond angles

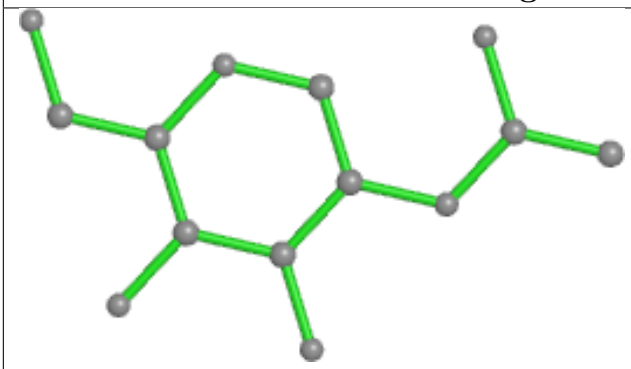


Torsions

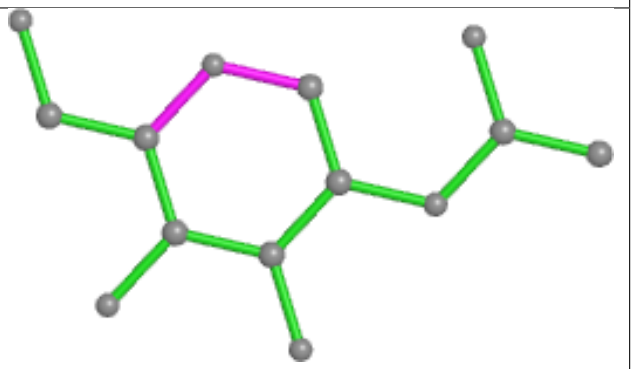


Rings

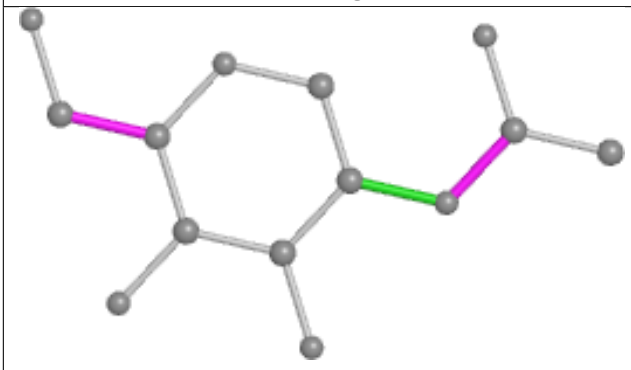
Ligand NAG A 505



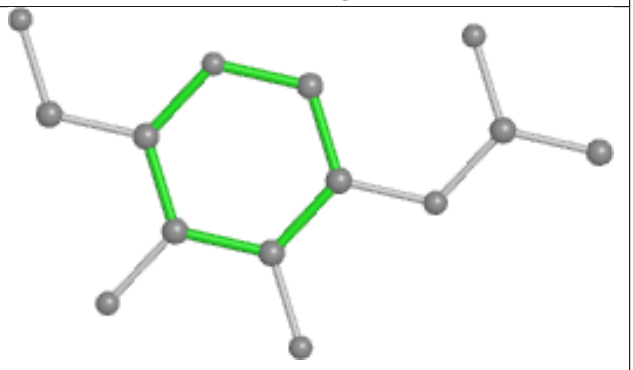
Bond lengths



Bond angles

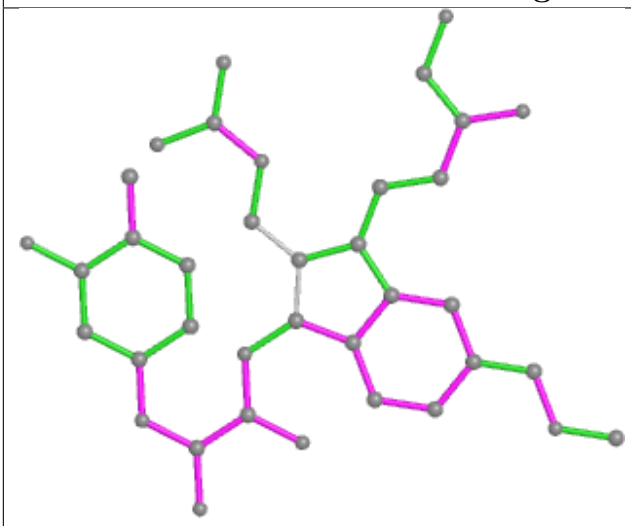


Torsions

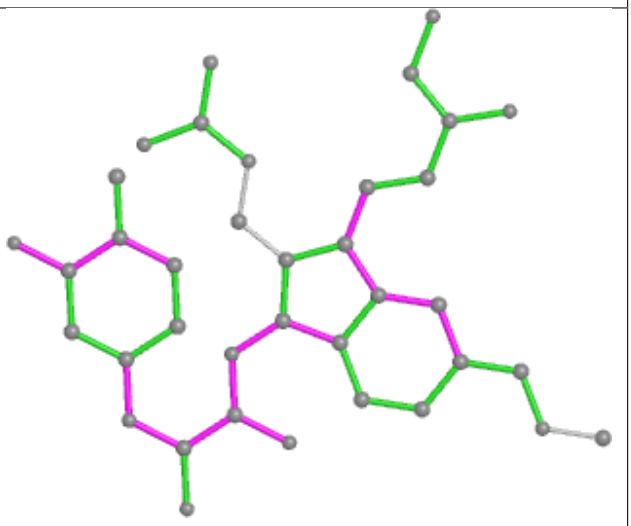


Rings

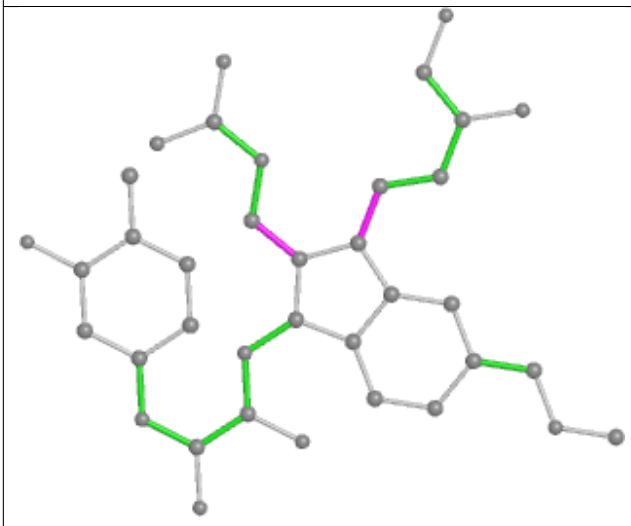
Ligand 7IT C 506



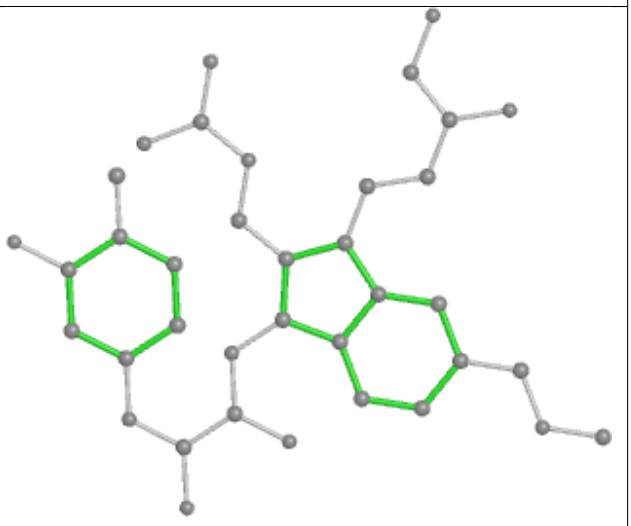
Bond lengths



Bond angles

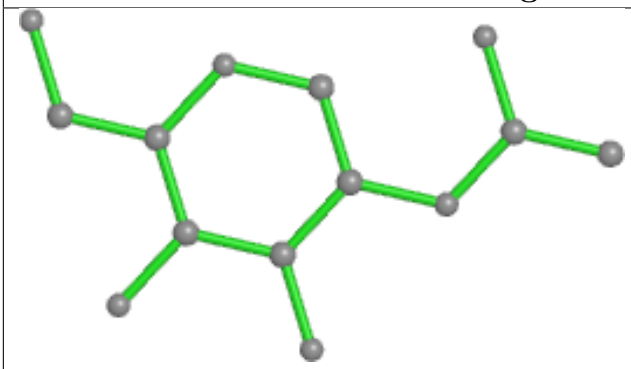


Torsions

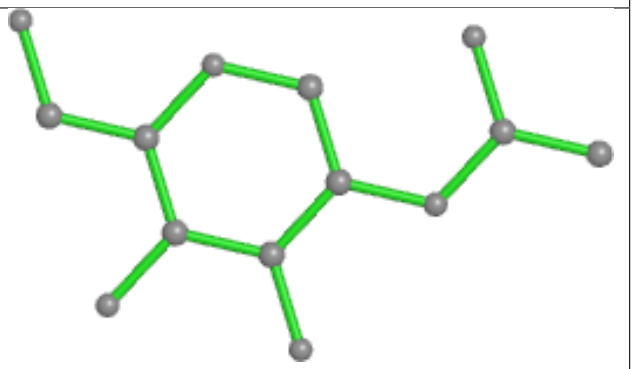


Rings

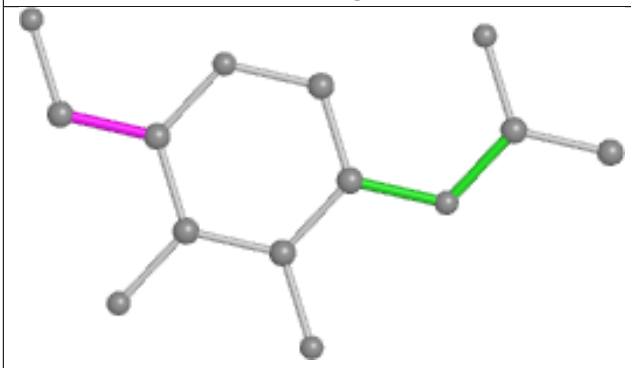
Ligand NAG C 504



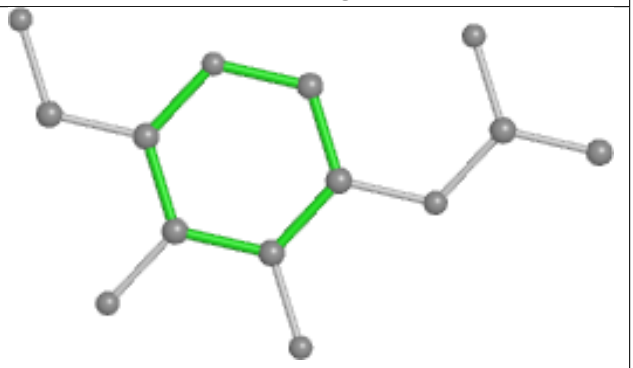
Bond lengths



Bond angles

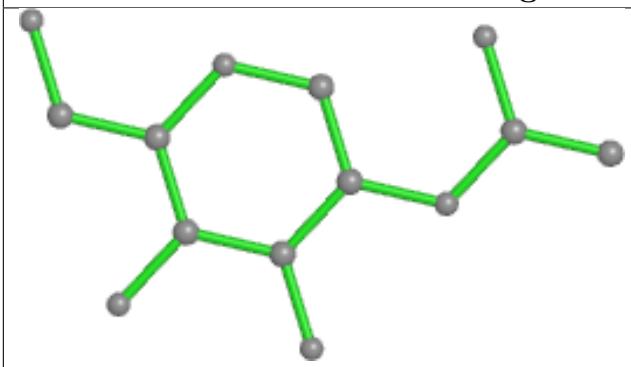


Torsions

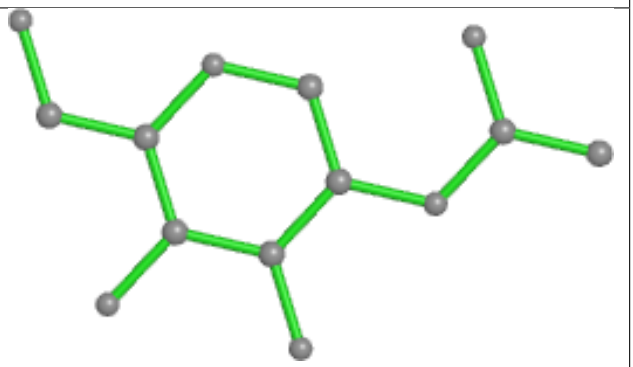


Rings

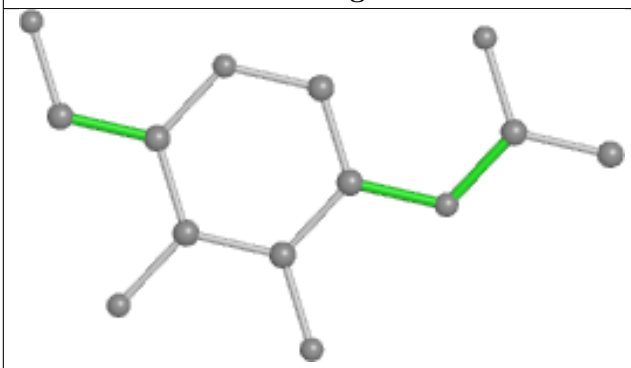
Ligand NAG D 502



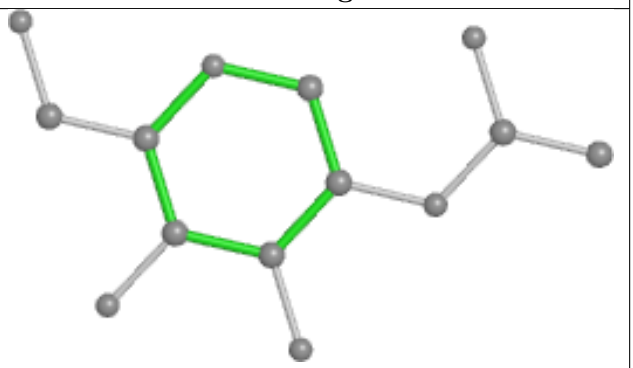
Bond lengths



Bond angles

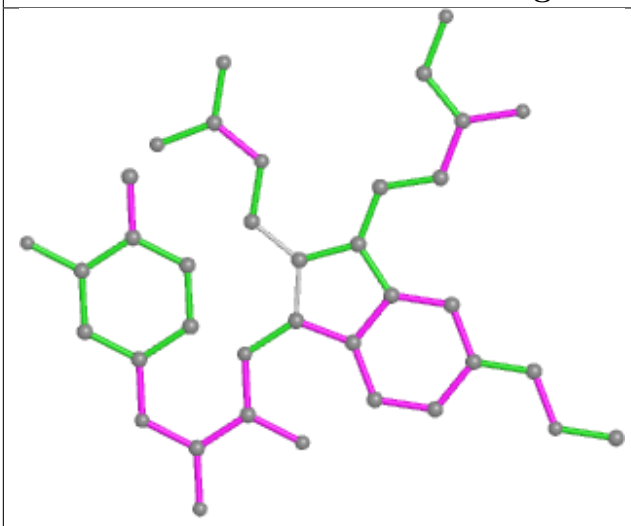


Torsions

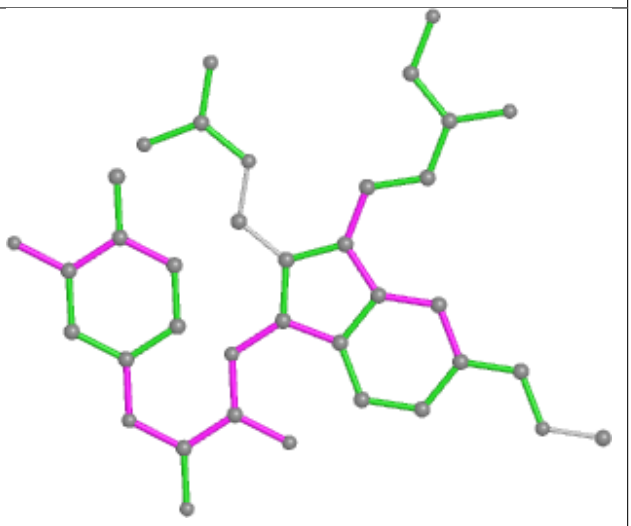


Rings

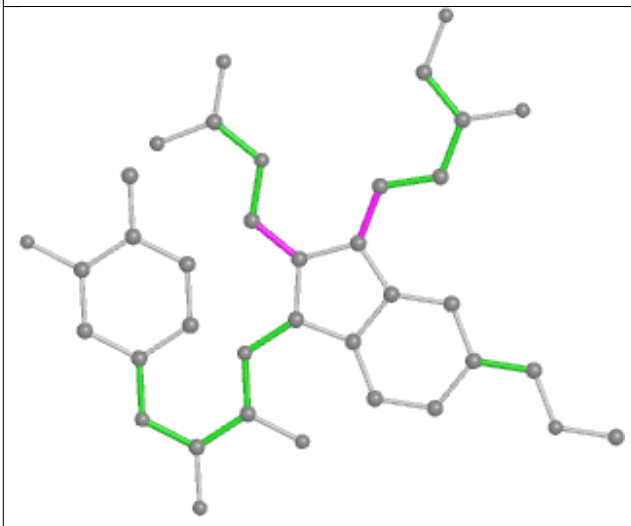
Ligand 7IT B 506



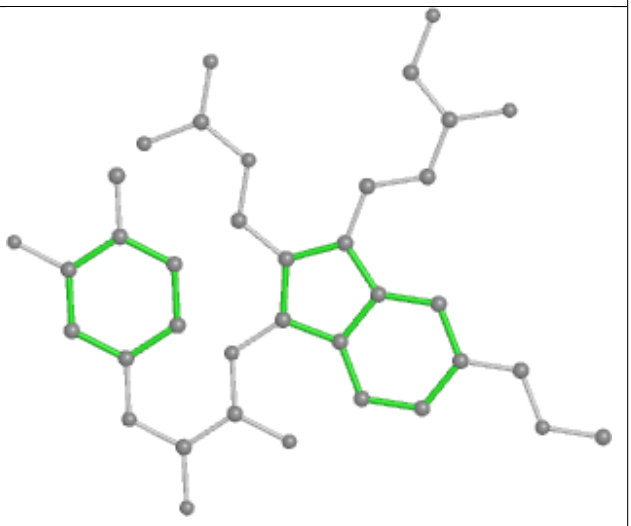
Bond lengths



Bond angles

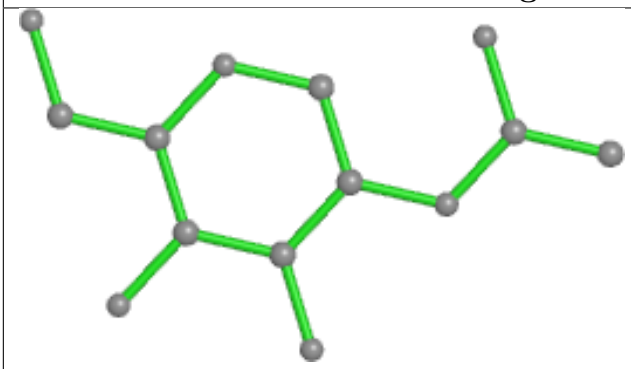


Torsions

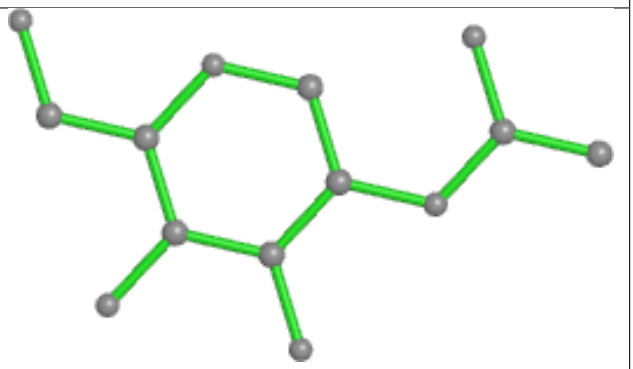


Rings

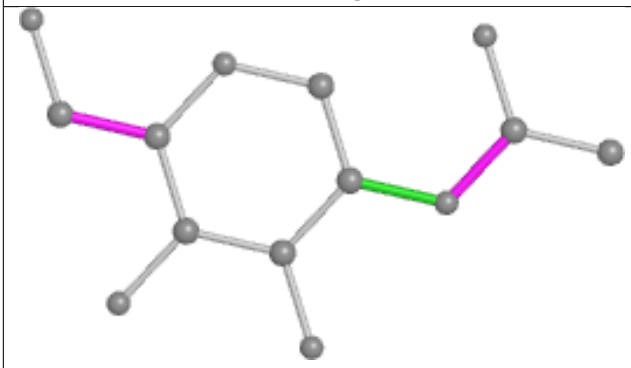
Ligand NAG D 507



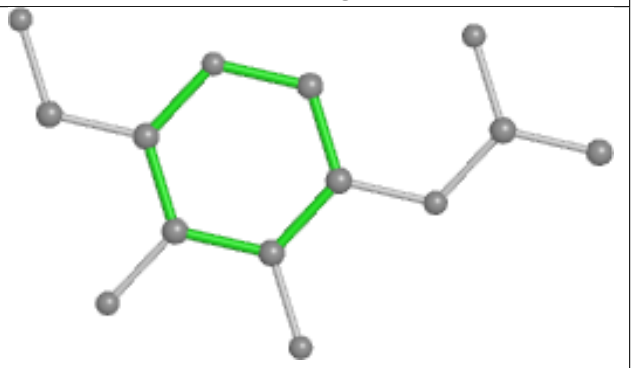
Bond lengths



Bond angles

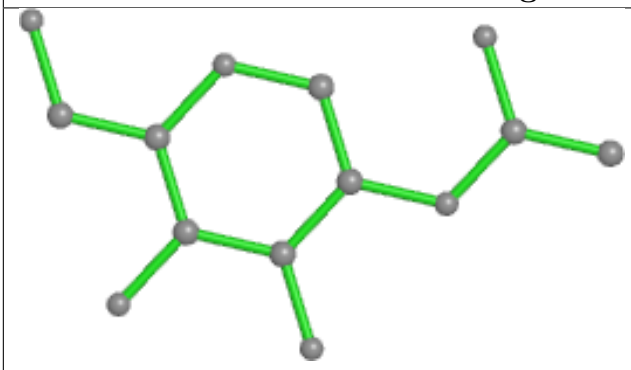


Torsions

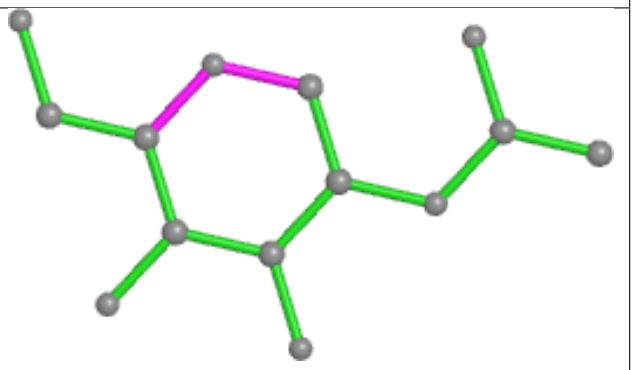


Rings

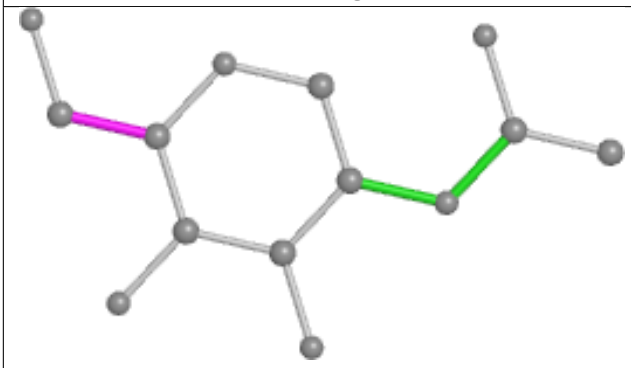
Ligand NAG D 503



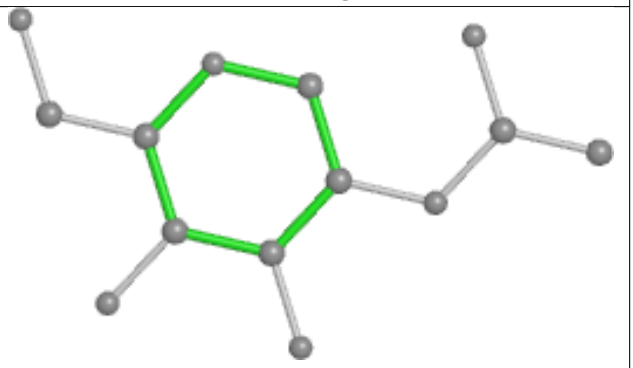
Bond lengths



Bond angles

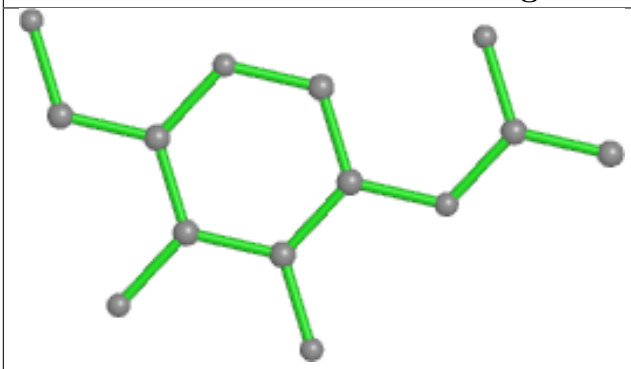


Torsions

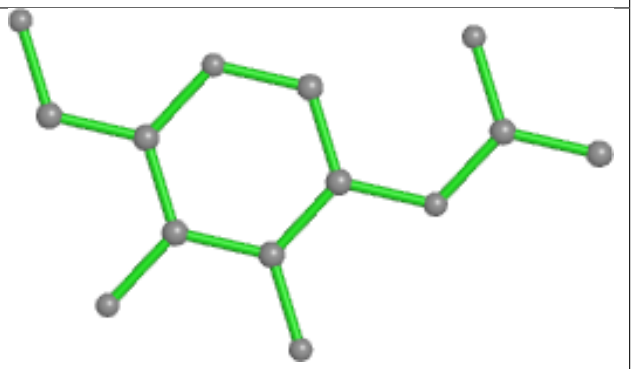


Rings

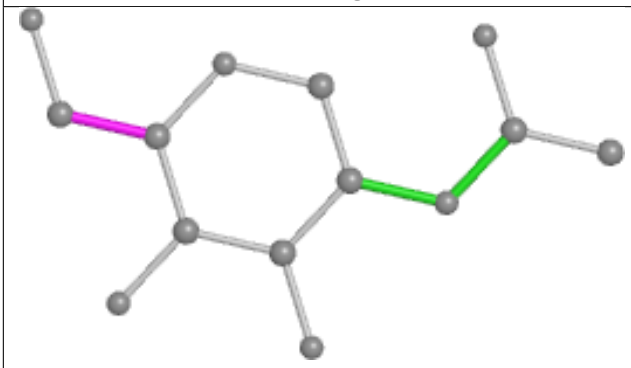
Ligand NAG B 504



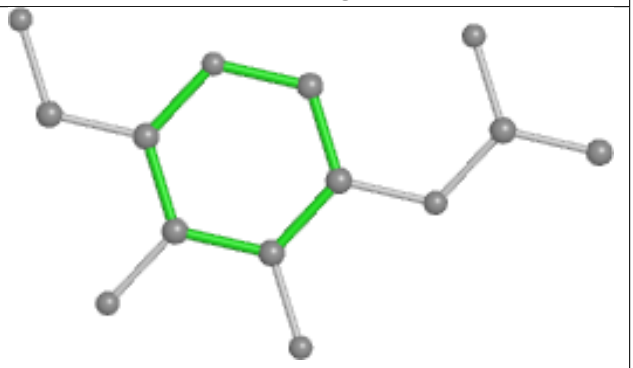
Bond lengths



Bond angles

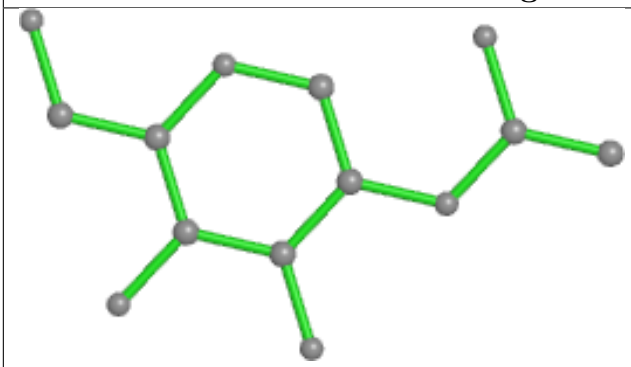


Torsions

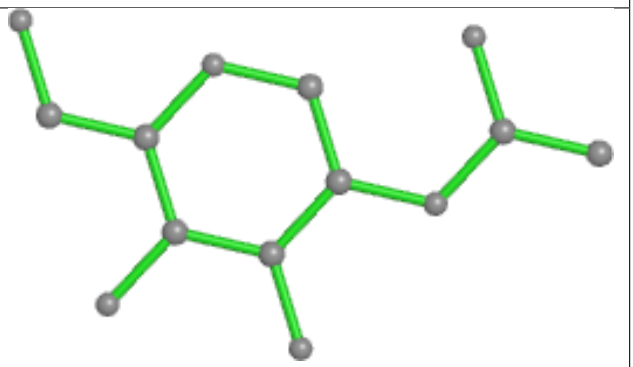


Rings

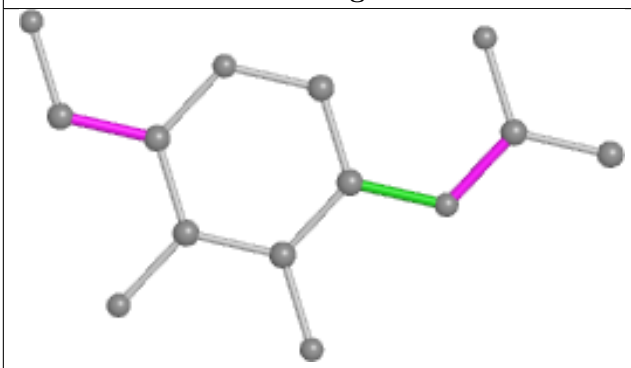
Ligand NAG C 505



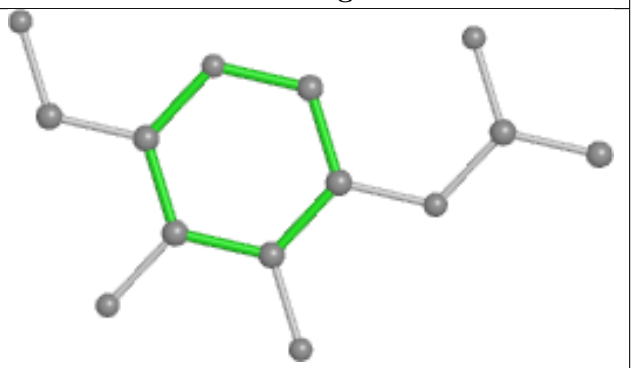
Bond lengths



Bond angles

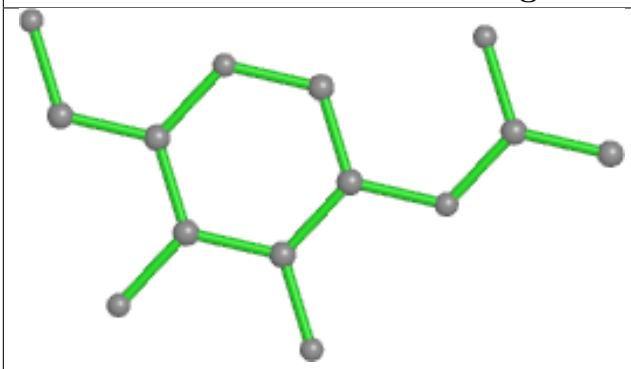


Torsions

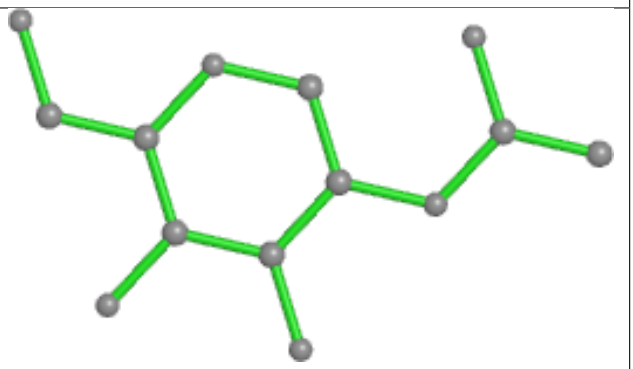


Rings

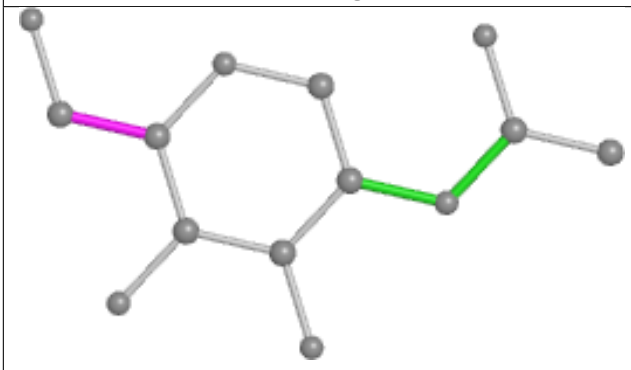
Ligand NAG A 501



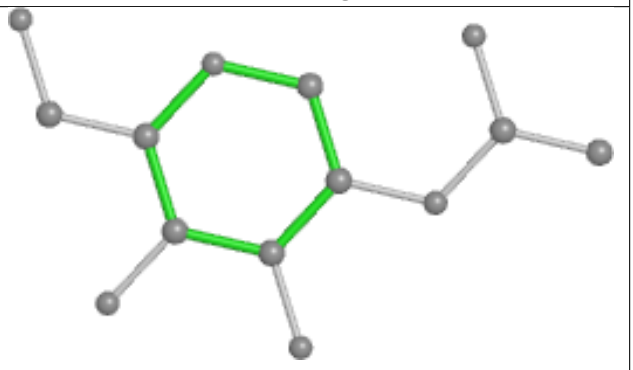
Bond lengths



Bond angles

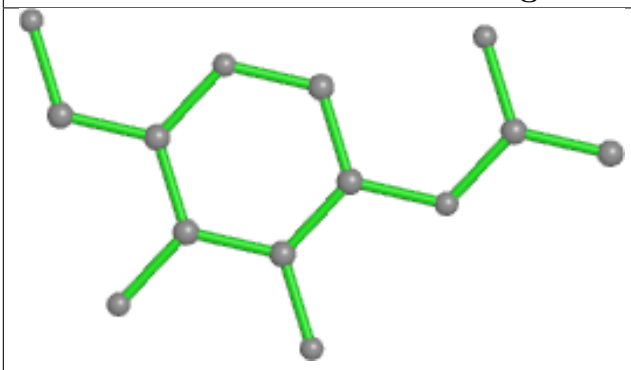


Torsions

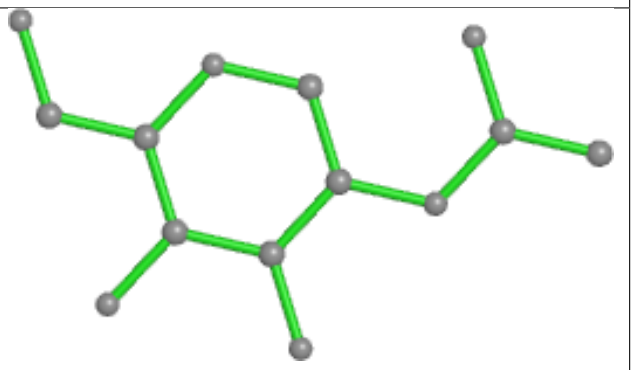


Rings

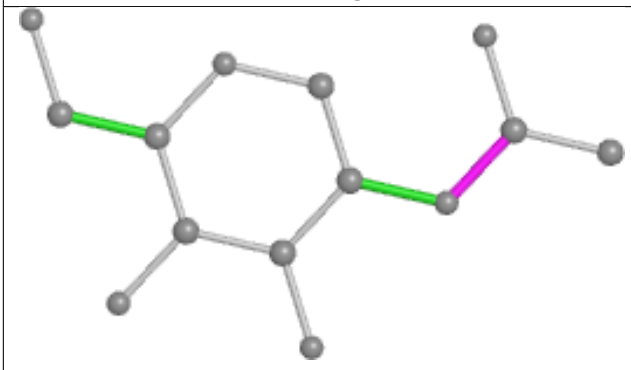
Ligand NAG C 503



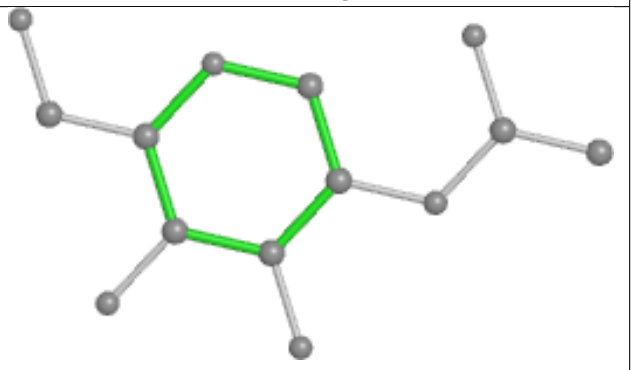
Bond lengths



Bond angles

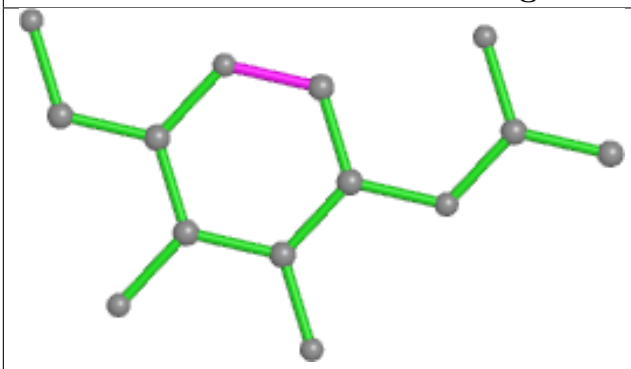


Torsions

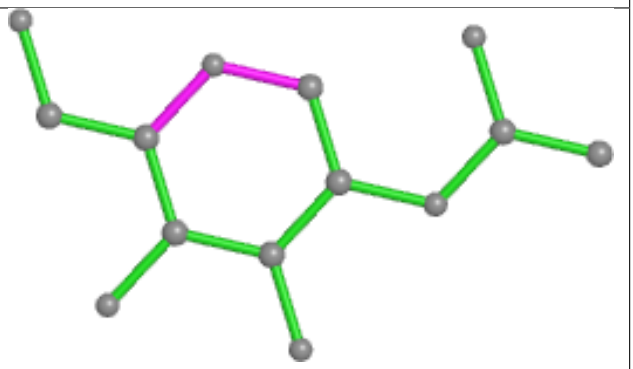


Rings

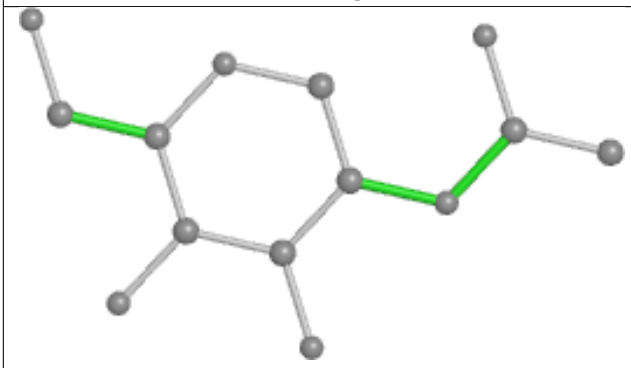
Ligand NAG A 506



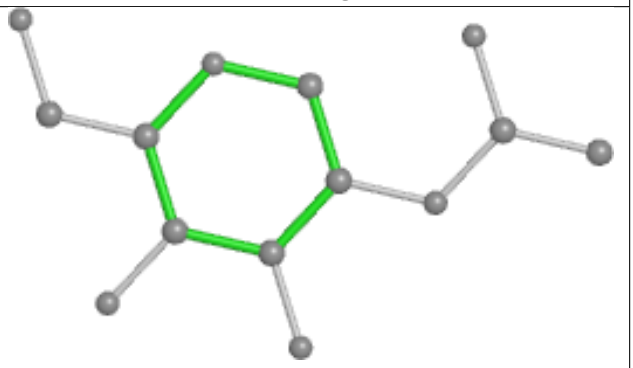
Bond lengths



Bond angles

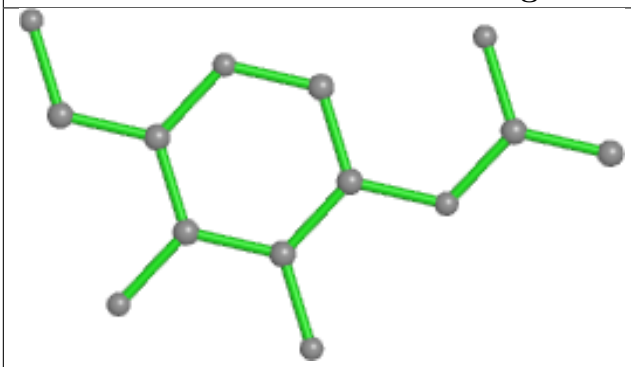


Torsions

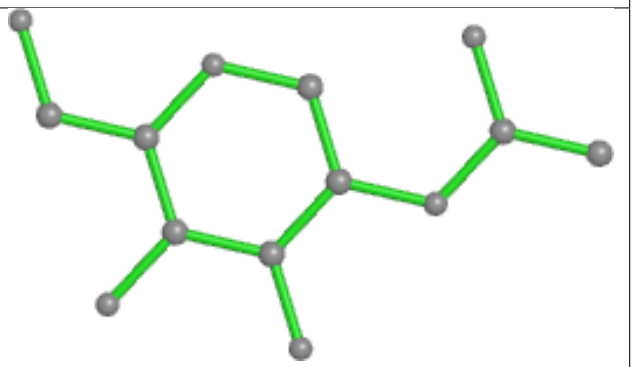


Rings

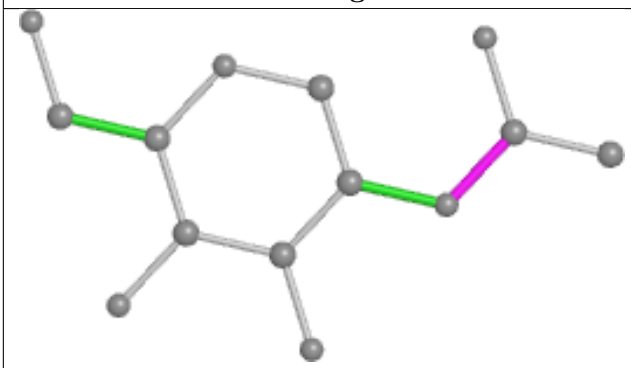
Ligand NAG B 503



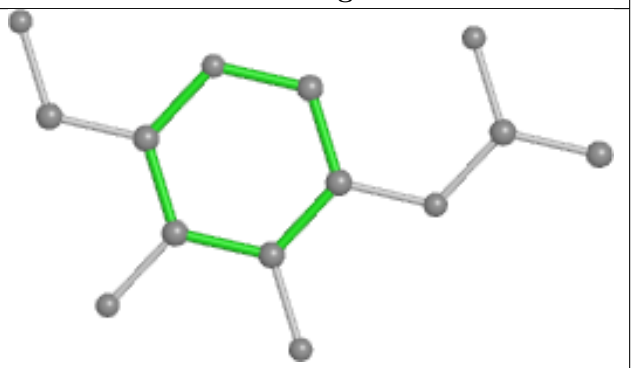
Bond lengths



Bond angles

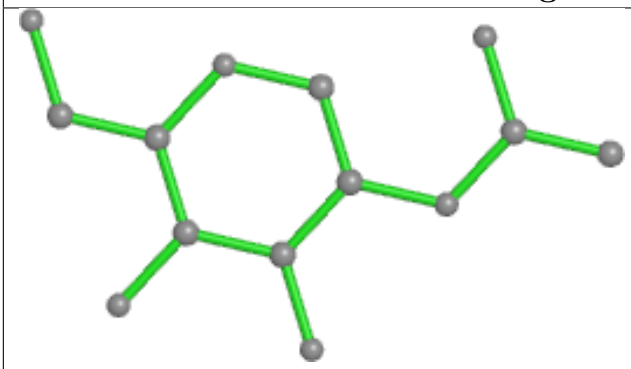


Torsions

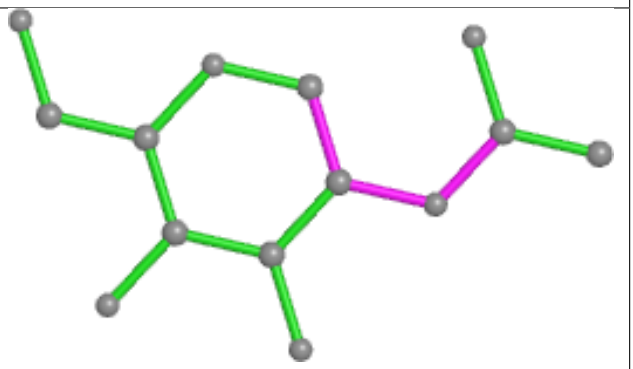


Rings

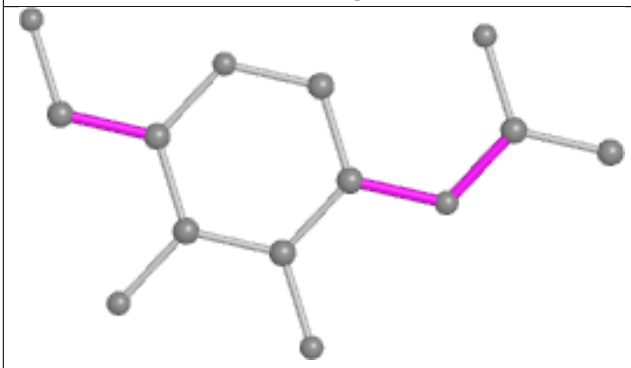
Ligand NAG E 1



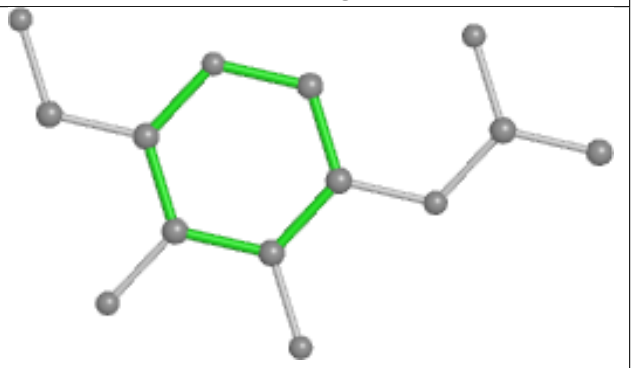
Bond lengths



Bond angles

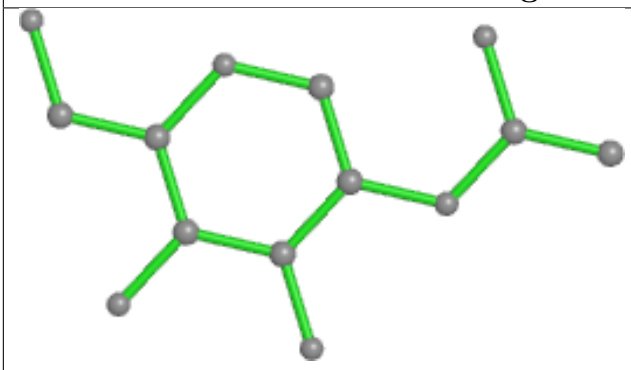


Torsions

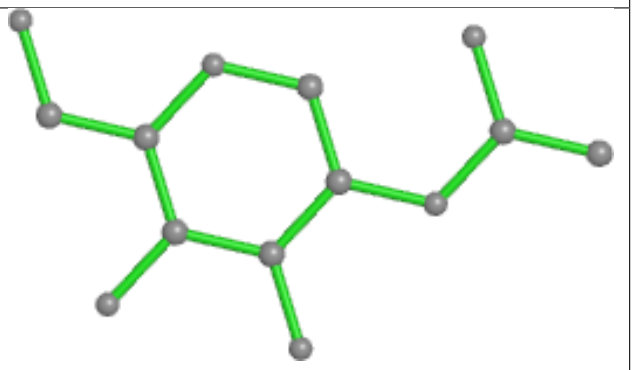


Rings

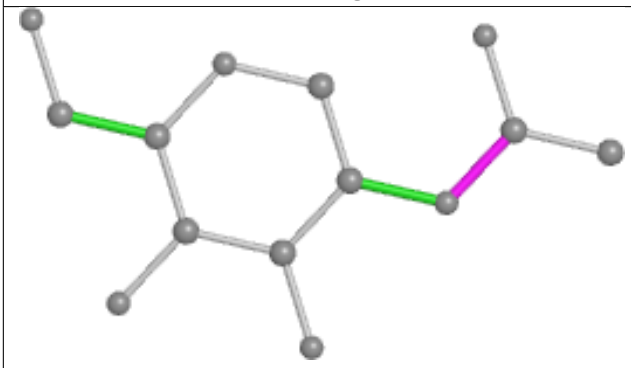
Ligand NAG B 505



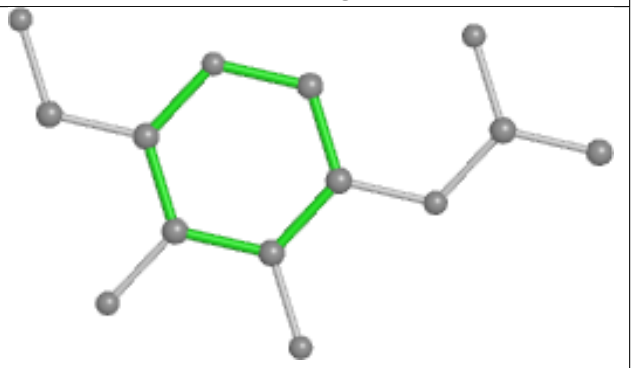
Bond lengths



Bond angles

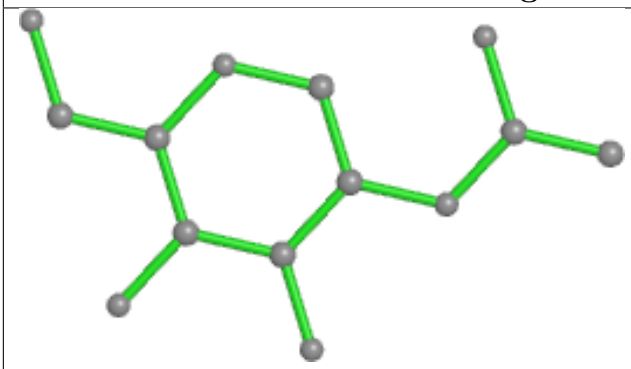


Torsions

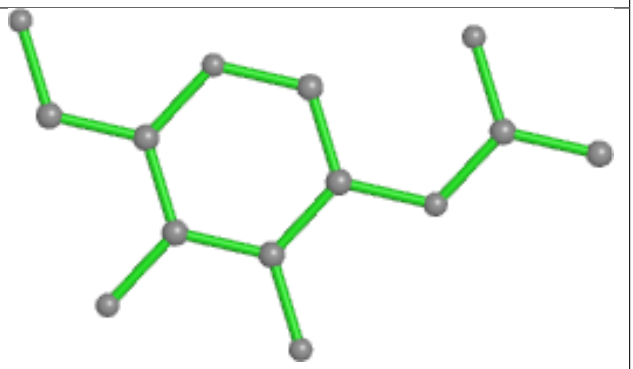


Rings

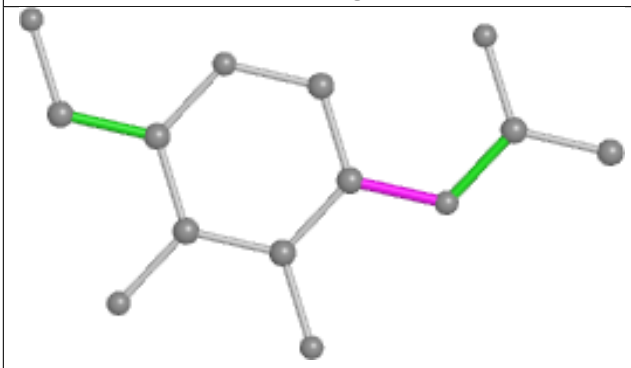
Ligand NAG C 501



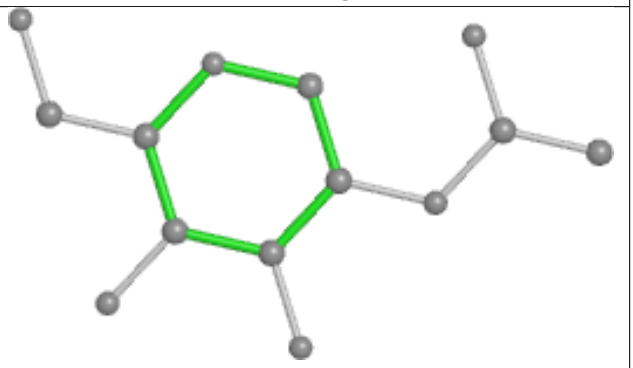
Bond lengths



Bond angles

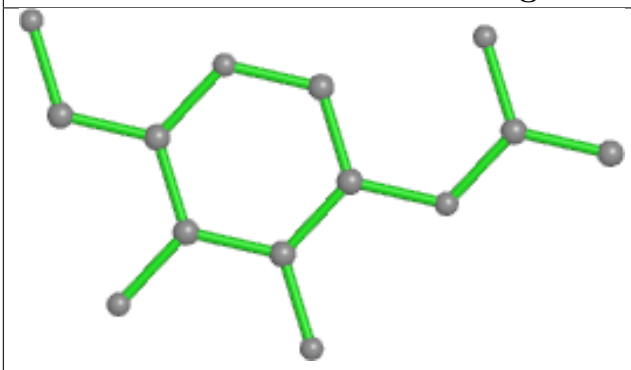


Torsions

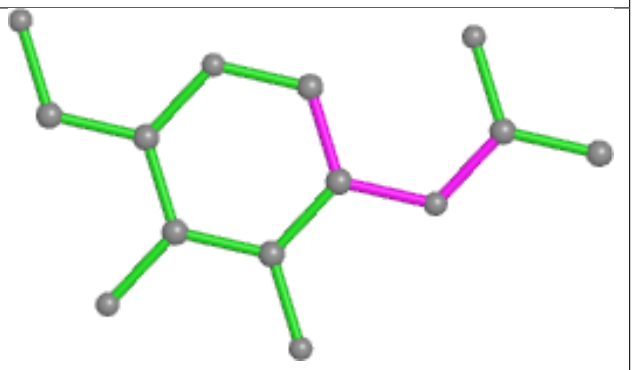


Rings

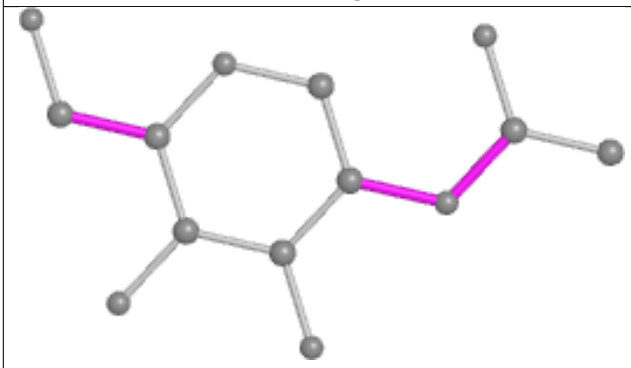
Ligand NAG D 504



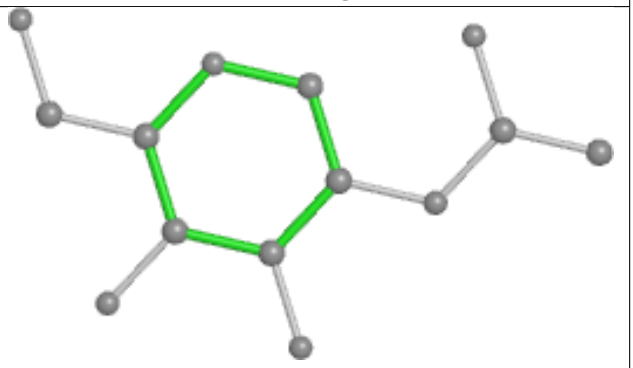
Bond lengths



Bond angles

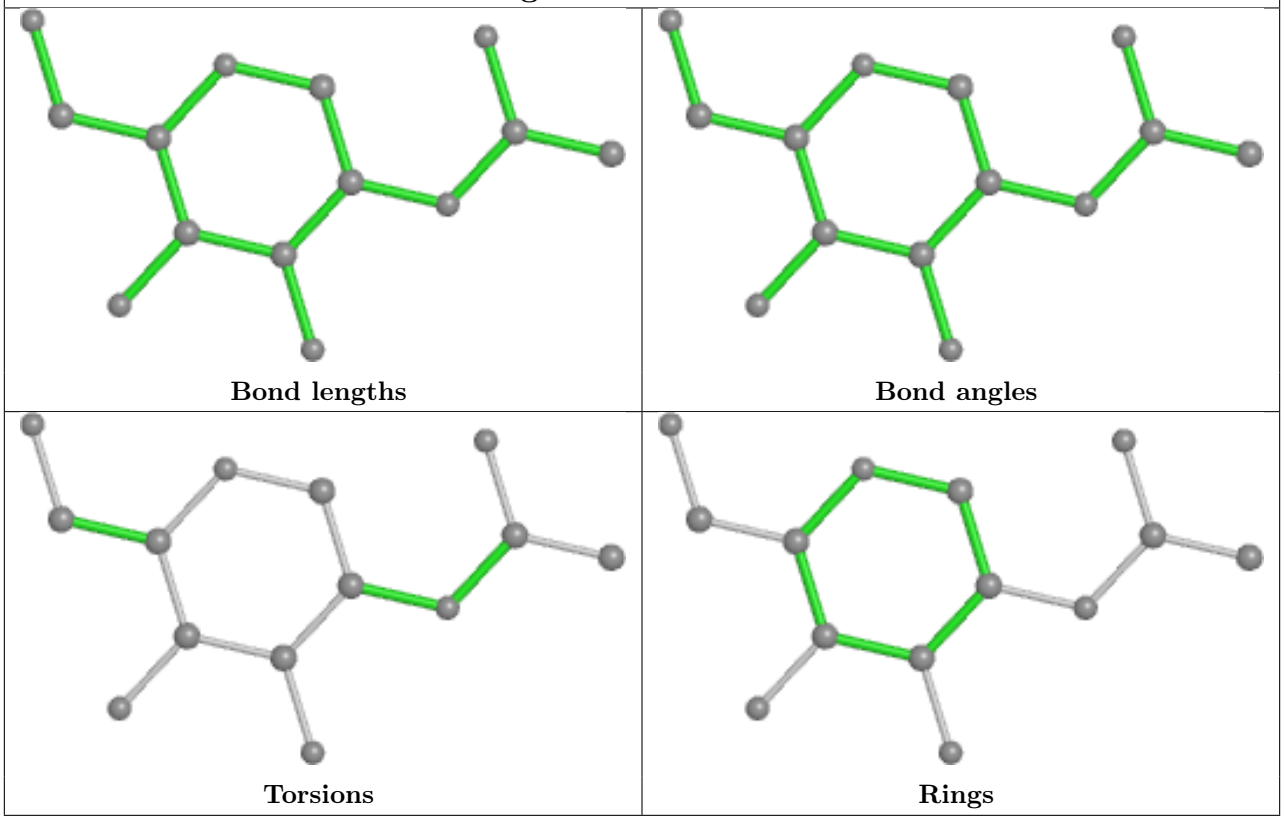


Torsions



Rings

Ligand NAG A 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	354:PRO	C	356:SER	N	4.43
1	A	354:PRO	C	356:SER	N	3.85
1	D	399:THR	C	403:TYR	N	3.85
1	B	354:PRO	C	356:SER	N	3.51
1	B	399:THR	C	403:TYR	N	3.02

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	335/362 (92%)	0.50	17 (5%)	28	34	43, 63, 88, 108	0
1	B	335/362 (92%)	0.33	8 (2%)	59	68	40, 58, 85, 109	0
1	C	335/362 (92%)	0.57	16 (4%)	30	36	45, 67, 99, 130	0
1	D	335/362 (92%)	0.41	10 (2%)	50	59	40, 61, 89, 110	0
All	All	1340/1448 (92%)	0.45	51 (3%)	40	48	40, 62, 91, 130	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	SER	7.7
1	B	404	ASN	5.4
1	A	89	VAL	5.1
1	D	354	PRO	4.8
1	C	356	SER	4.5
1	C	198	GLY	4.3
1	C	488	VAL	4.1
1	D	85	VAL	4.1
1	A	357	LYS	3.8
1	C	326	ILE	3.7
1	C	88	ASN	3.5
1	C	226	LEU	3.5
1	A	50	THR	3.4
1	A	201	ILE	3.4
1	B	240	ARG	3.3
1	C	202	THR	3.3
1	A	221	ALA	3.2
1	C	90	THR	3.2
1	A	354	PRO	3.1
1	D	87	ALA	3.0
1	D	399	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	87	ALA	2.9
1	A	87	ALA	2.8
1	D	79	PRO	2.7
1	B	61	TYR	2.7
1	C	52	LEU	2.6
1	A	356	SER	2.6
1	B	354	PRO	2.6
1	A	441	GLY	2.3
1	A	449	ILE	2.3
1	C	486	TYR	2.3
1	D	365	SER	2.3
1	C	396	ARG	2.2
1	A	198	GLY	2.2
1	A	223	PHE	2.2
1	B	295	VAL	2.2
1	C	288	LEU	2.2
1	A	444	THR	2.1
1	C	485	LYS	2.1
1	A	91	GLU	2.1
1	A	124	GLY	2.1
1	B	285	ILE	2.1
1	C	489	VAL	2.1
1	D	86	LEU	2.0
1	D	61	TYR	2.0
1	B	219	ALA	2.0
1	A	78	ASP	2.0
1	C	223	PHE	2.0
1	B	89	VAL	2.0
1	A	292	VAL	2.0
1	D	245	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 monosaccharides in this entry.

6.4 Ligands (i)

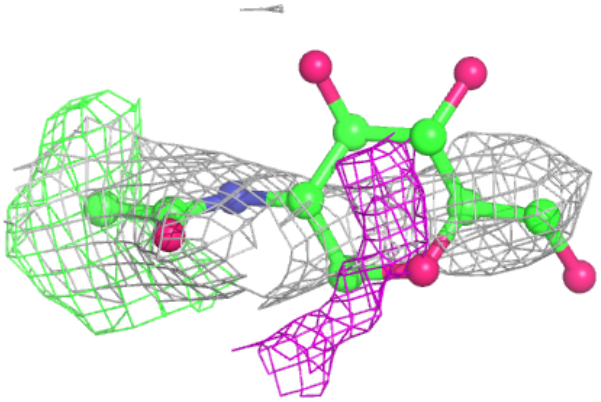
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

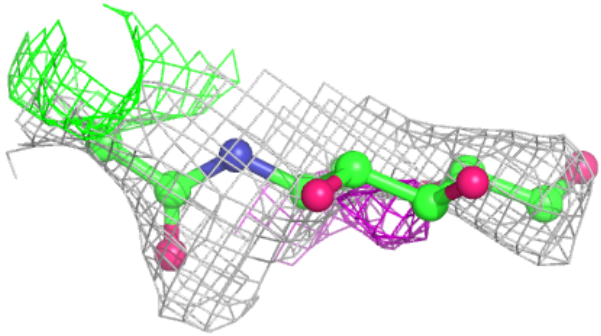
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	506	14/15	0.36	0.45	95,102,111,113	0
2	NAG	D	501	14/15	0.38	0.42	71,87,96,100	0
2	NAG	D	504	14/15	0.64	0.44	87,105,111,111	0
2	NAG	E	2	14/15	0.73	0.31	72,77,92,102	0
3	7IT	B	506	37/37	0.73	0.29	57,76,101,105	0
3	7IT	C	506	37/37	0.75	0.43	57,76,101,105	0
3	7IT	D	508	37/37	0.76	0.40	57,76,101,105	0
2	NAG	C	505	14/15	0.78	0.23	68,76,90,93	0
2	NAG	E	1	14/15	0.78	0.27	76,92,99,101	0
2	NAG	C	503	14/15	0.79	0.34	89,102,111,119	0
3	7IT	A	507	37/37	0.80	0.38	57,76,101,105	0
2	NAG	C	504	14/15	0.80	0.25	60,78,88,89	0
2	NAG	A	505	14/15	0.84	0.23	64,73,86,87	0
2	NAG	A	504	14/15	0.85	0.18	57,65,73,78	0
2	NAG	C	501	14/15	0.86	0.23	70,80,89,98	0
2	NAG	D	502	14/15	0.88	0.29	74,80,93,106	0
2	NAG	B	503	14/15	0.89	0.21	69,74,81,82	0
2	NAG	B	505	14/15	0.89	0.20	48,55,63,70	0
2	NAG	C	502	14/15	0.90	0.22	56,62,70,78	0
2	NAG	B	501	14/15	0.90	0.21	63,68,75,80	0
2	NAG	A	501	14/15	0.91	0.17	64,74,84,100	0
2	NAG	A	503	14/15	0.91	0.20	62,71,78,80	0
2	NAG	D	505	14/15	0.91	0.18	68,71,79,82	0
2	NAG	D	506	14/15	0.93	0.21	53,73,80,82	0
2	NAG	A	502	14/15	0.94	0.16	41,56,60,63	0
2	NAG	B	504	14/15	0.94	0.13	53,63,71,71	0
2	NAG	D	507	14/15	0.94	0.15	52,60,67,76	0
2	NAG	D	503	14/15	0.95	0.16	39,50,62,64	0
2	NAG	B	502	14/15	0.96	0.20	44,51,60,60	0

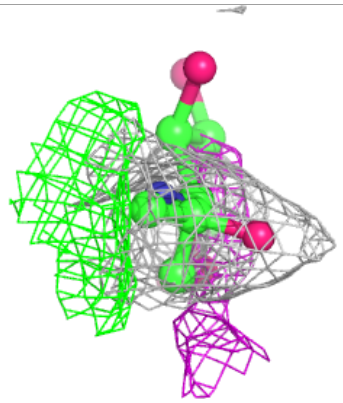
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 506:

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

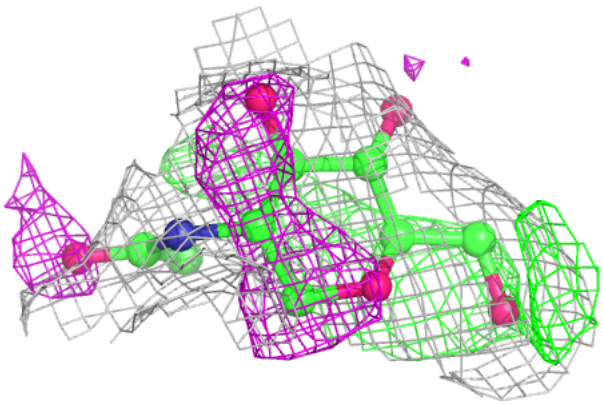


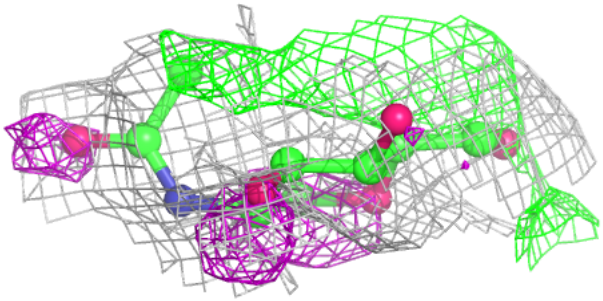


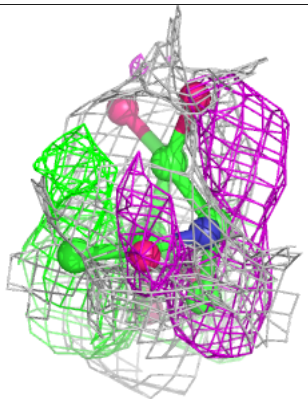


Electron density around NAG D 501:

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

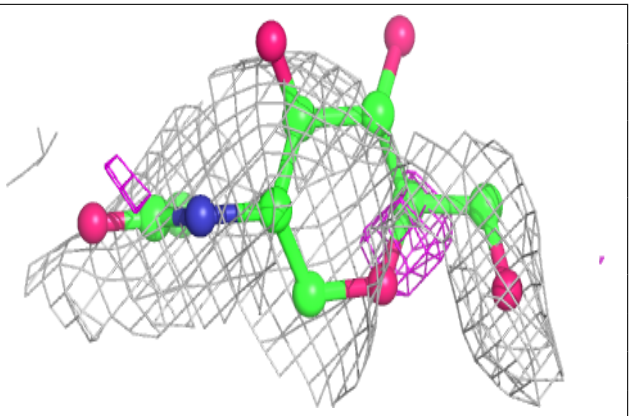


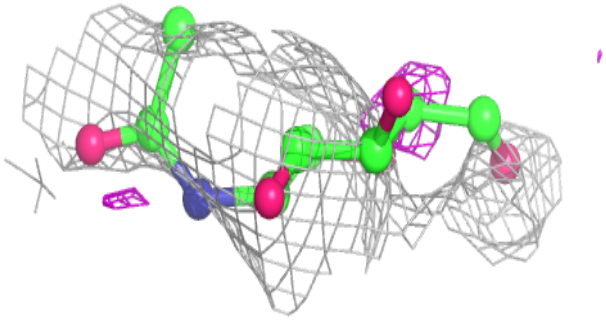


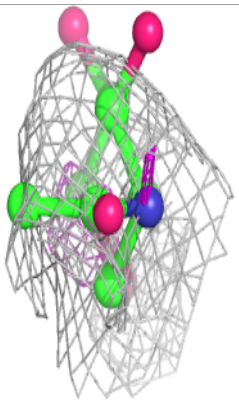


Electron density around NAG D 504:

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

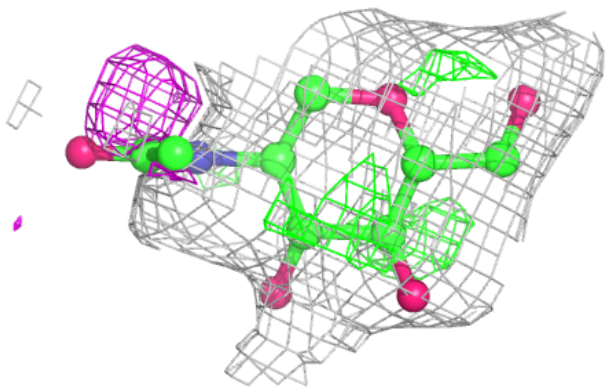


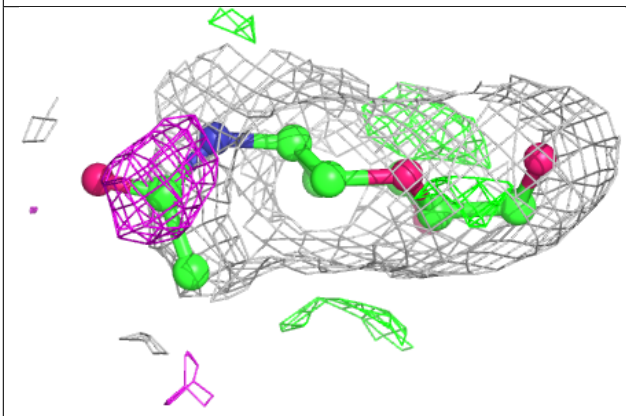


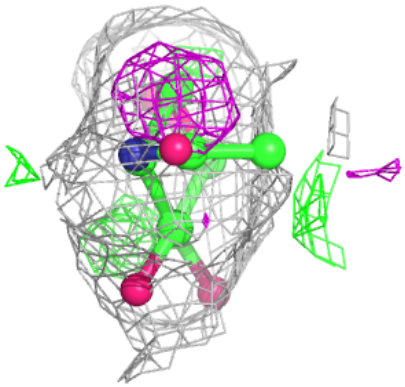


Electron density around NAG E 2:

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

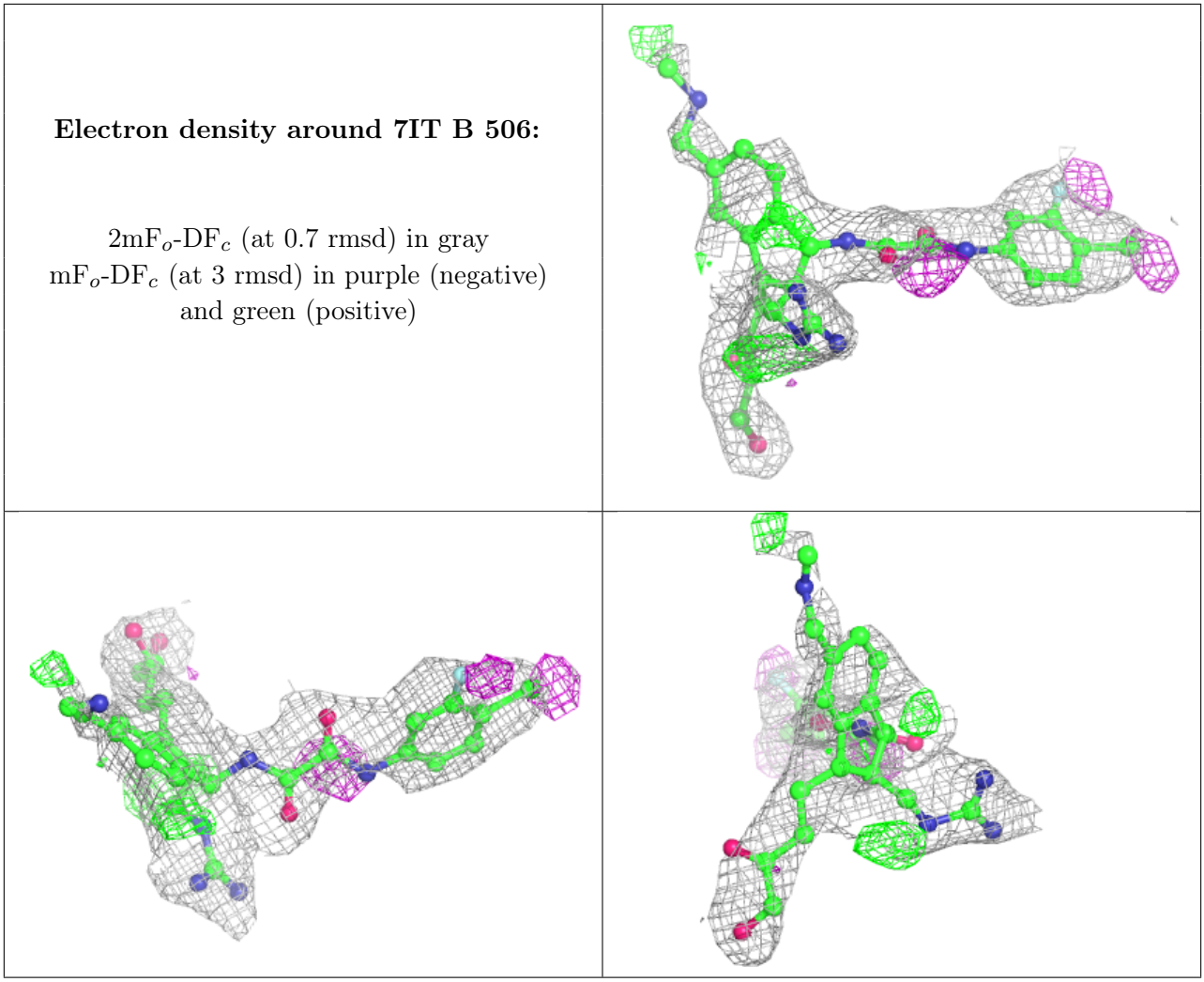






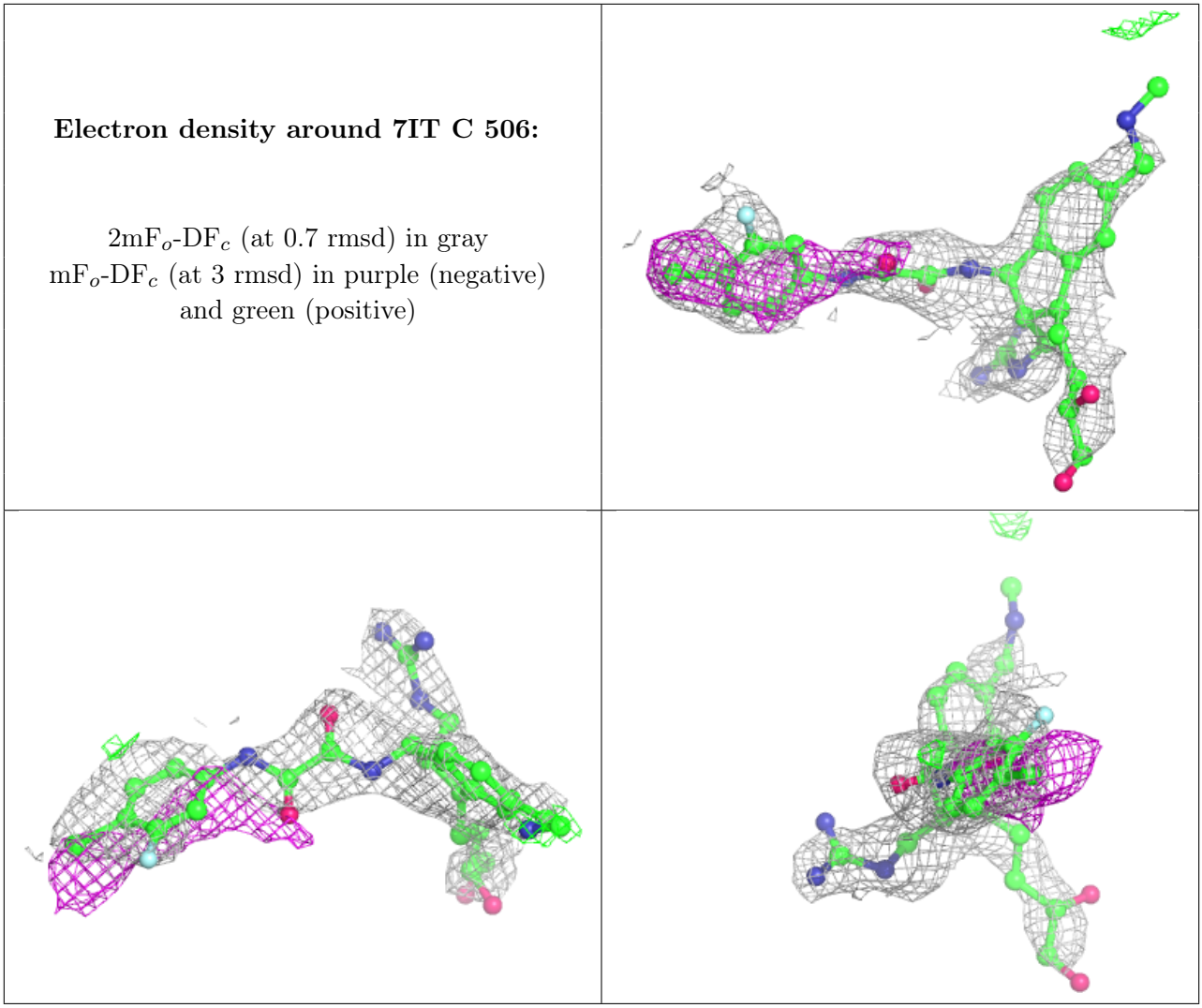
Electron density around 7IT B 506:

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



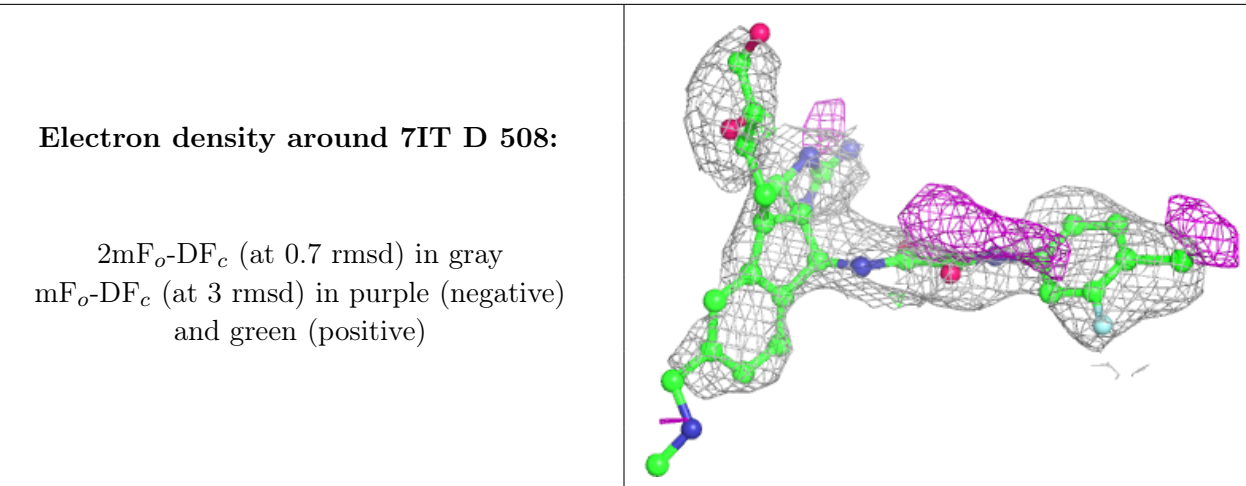
Electron density around 7IT C 506:

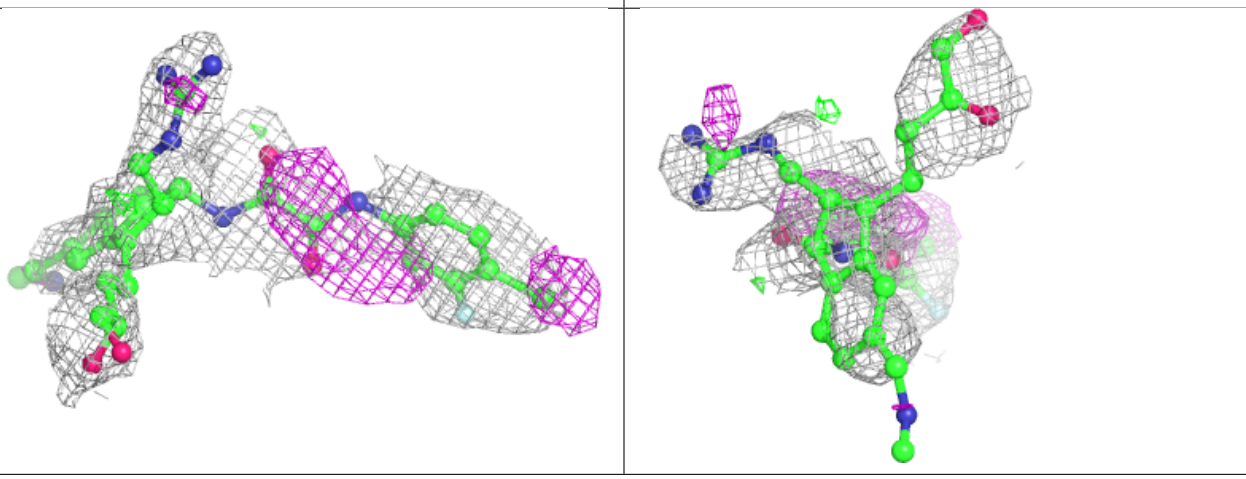
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 7IT D 508:

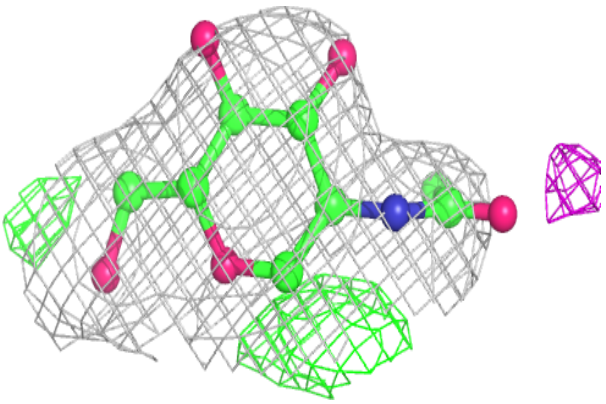
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

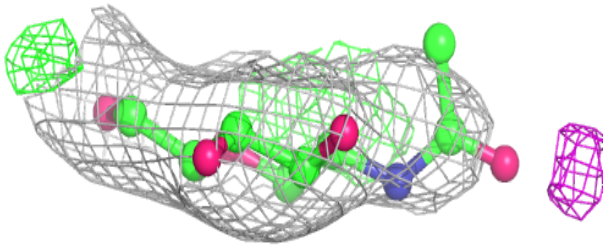


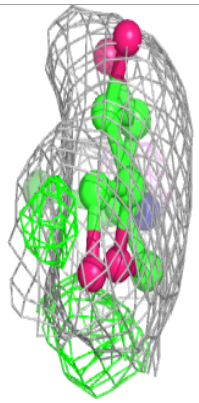


Electron density around NAG C 505:

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

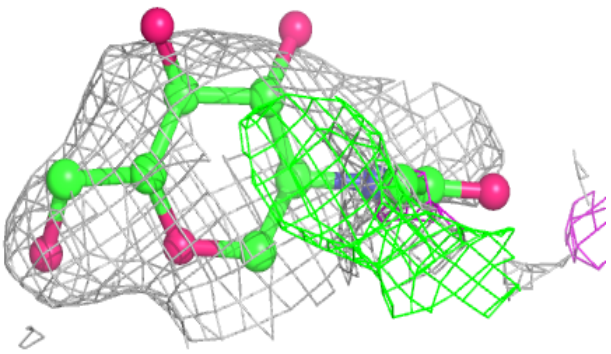


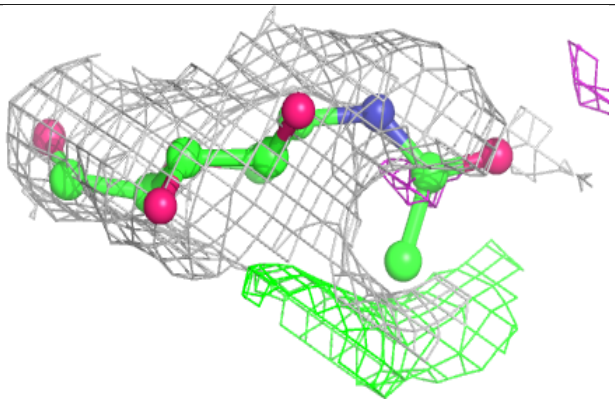


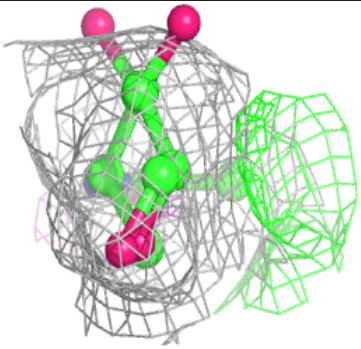


Electron density around NAG E 1:

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

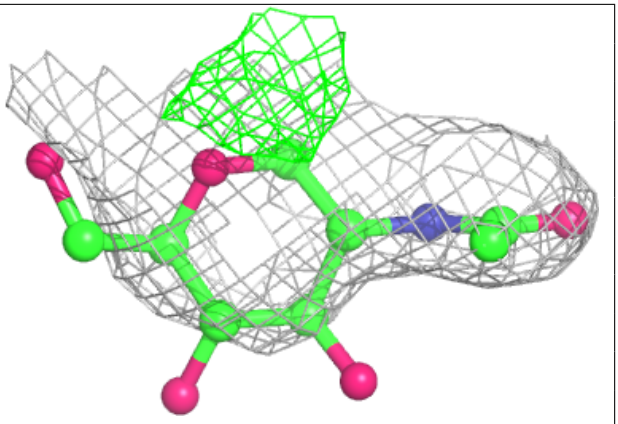


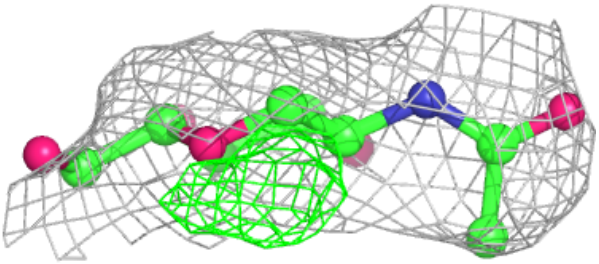


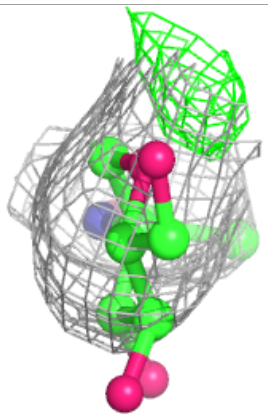


Electron density around NAG C 503:

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

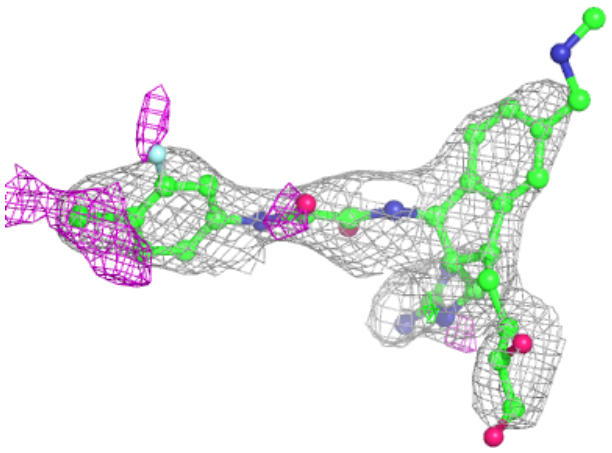


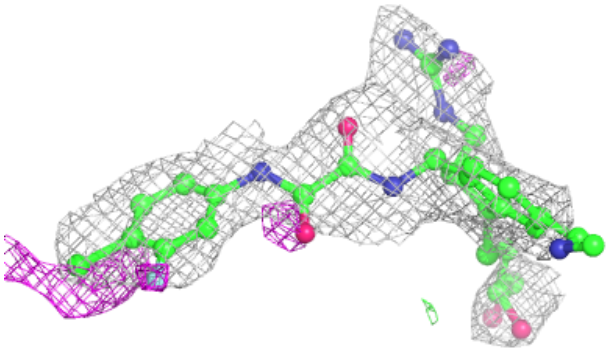


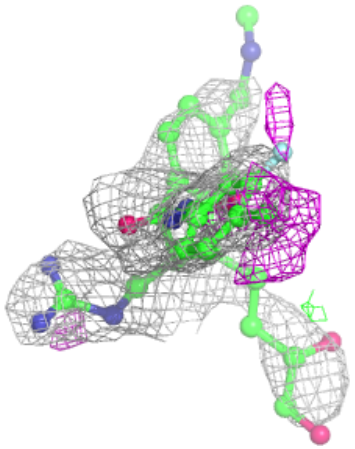


Electron density around 7IT A 507:

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

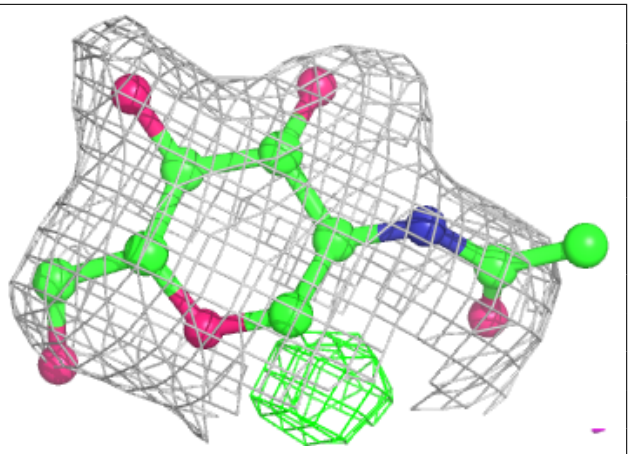


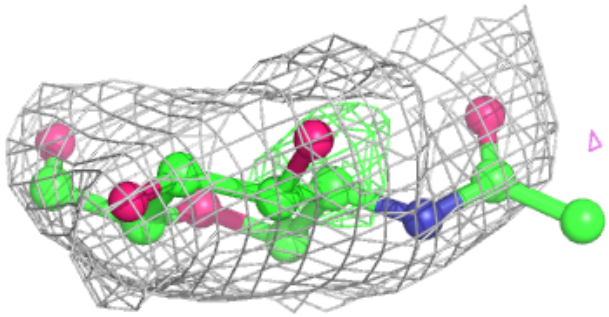


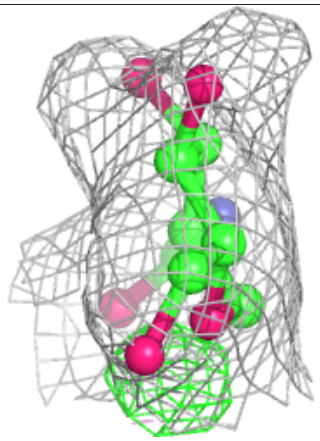


Electron density around NAG C 504:

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

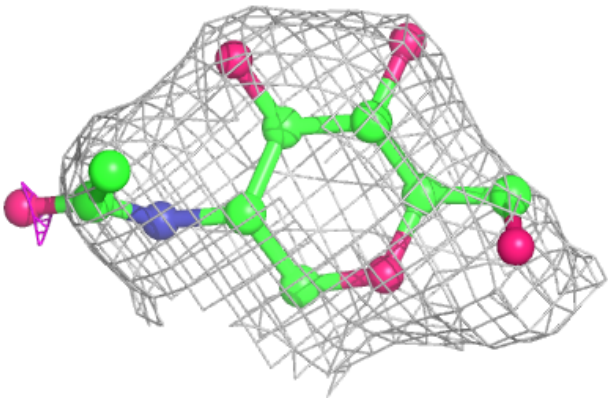


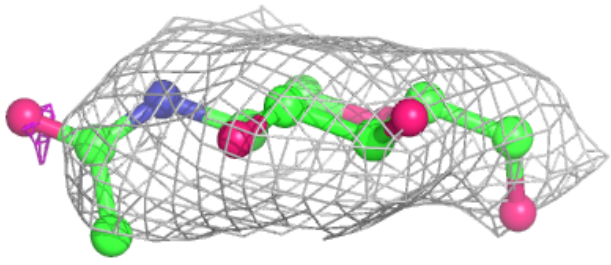


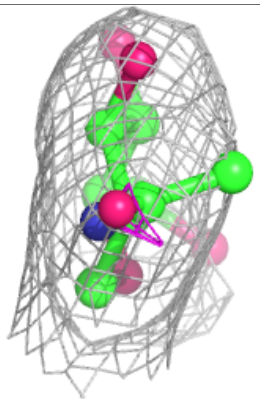


Electron density around NAG A 505:

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

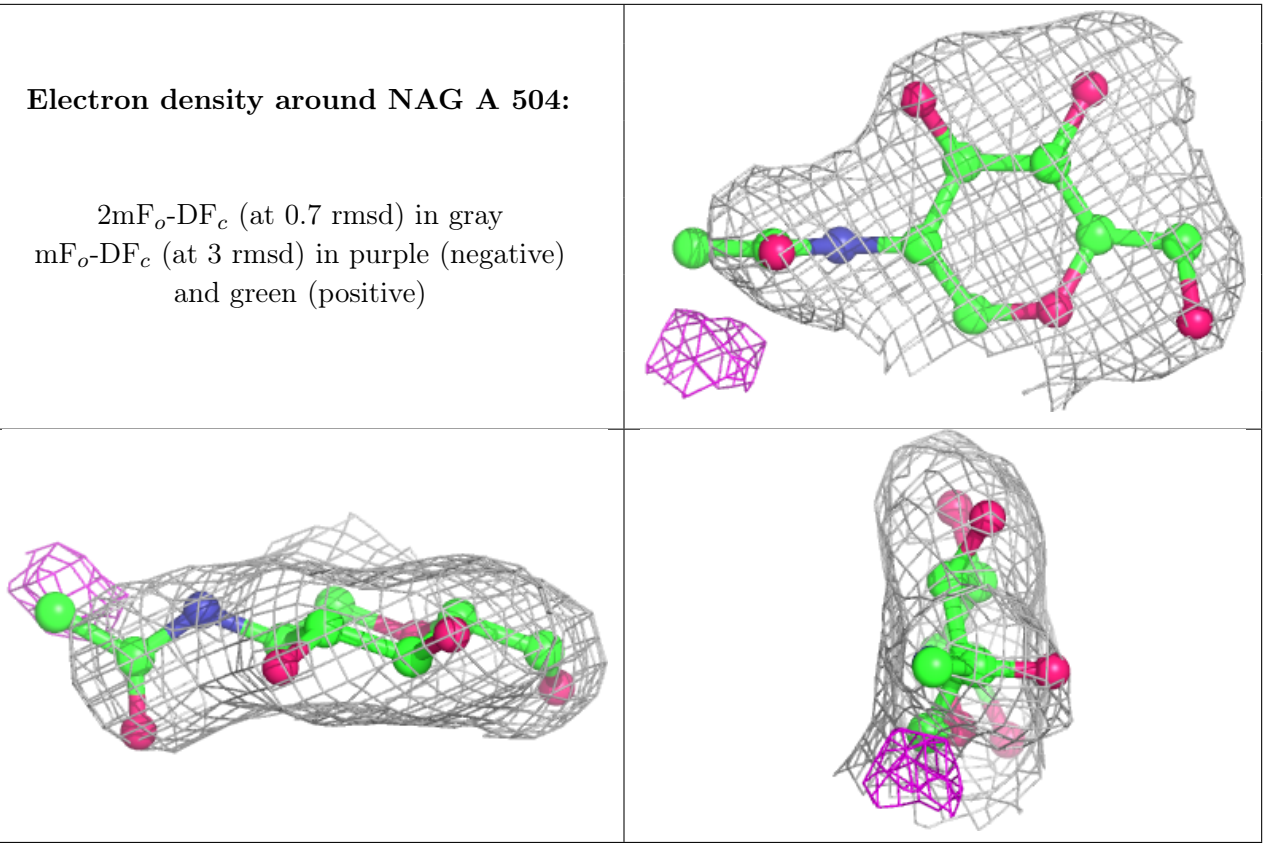






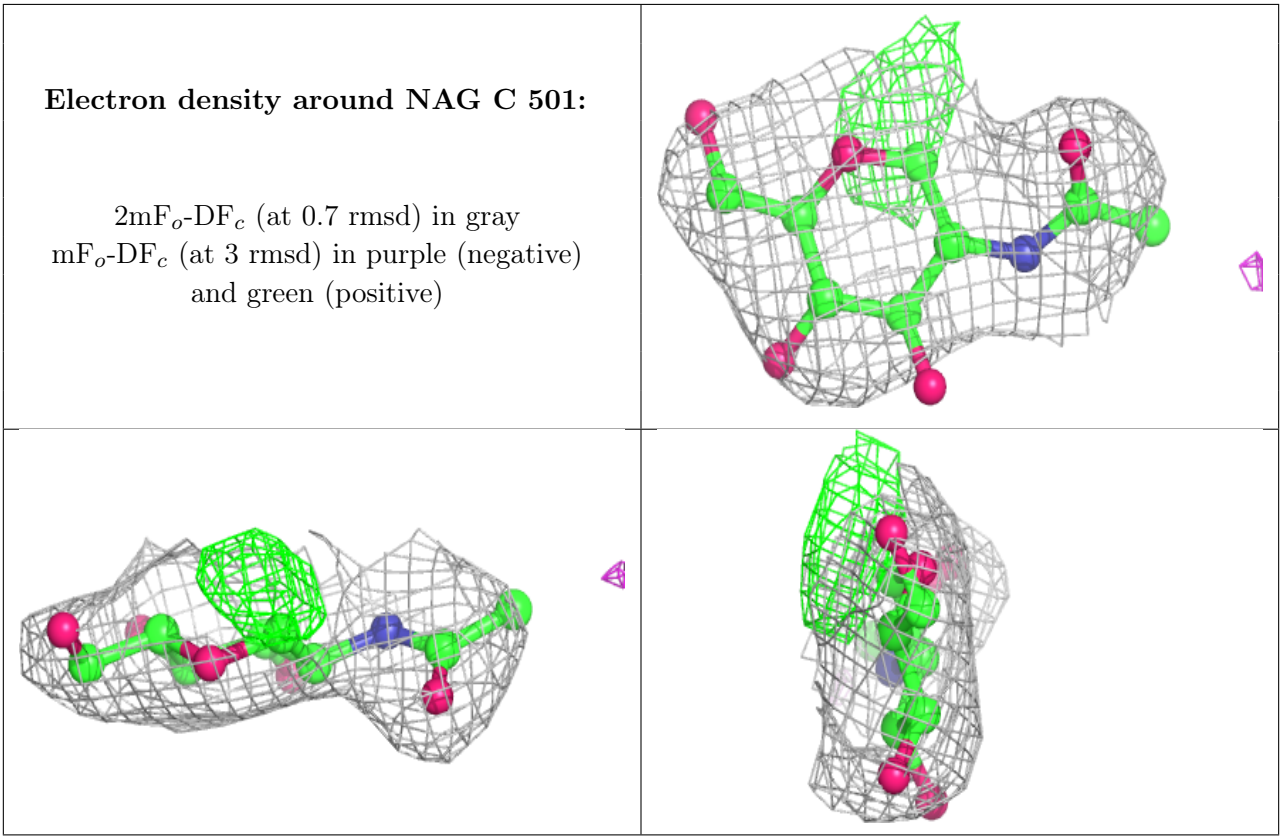
Electron density around NAG A 504:

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



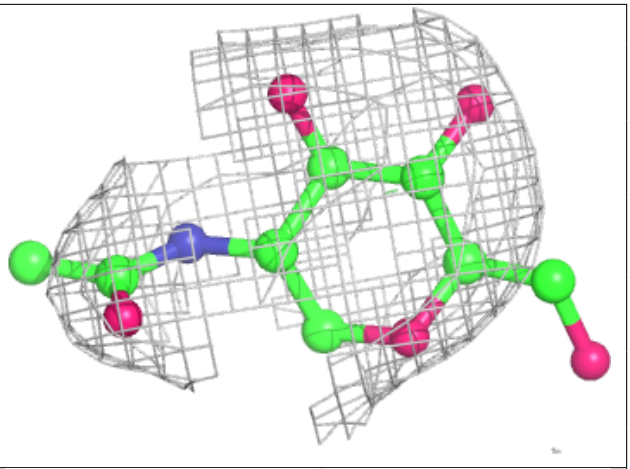
Electron density around NAG C 501:

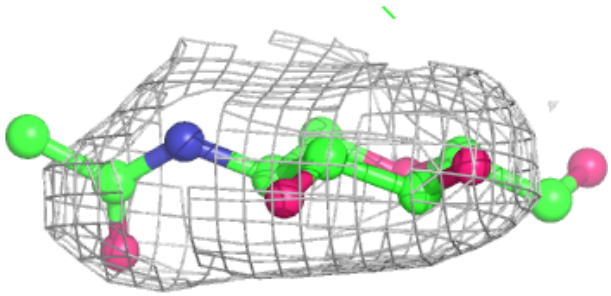
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

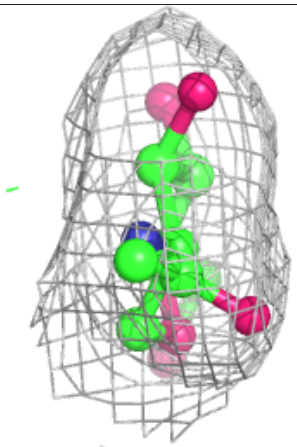


Electron density around NAG D 502:

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

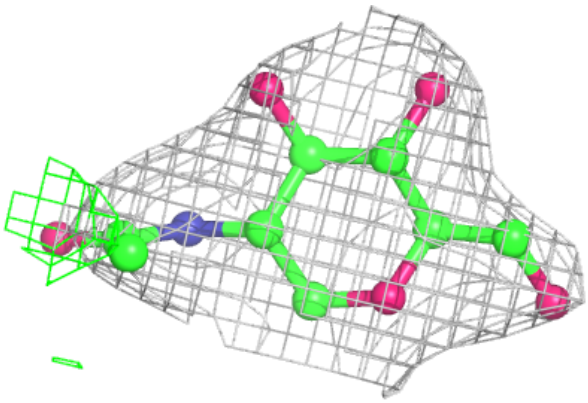


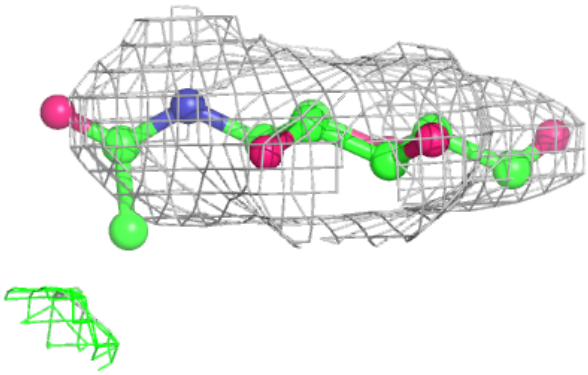


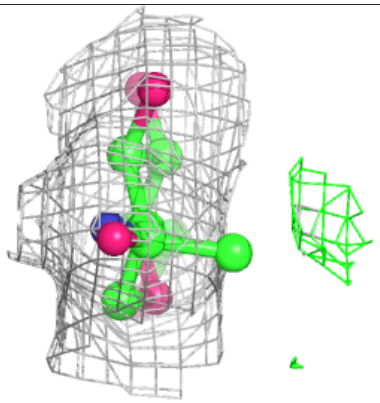


Electron density around NAG B 503:

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

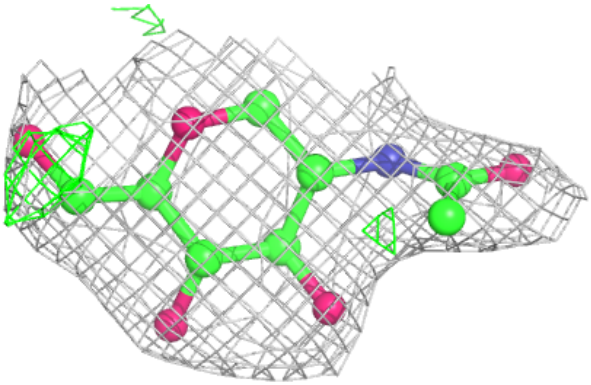


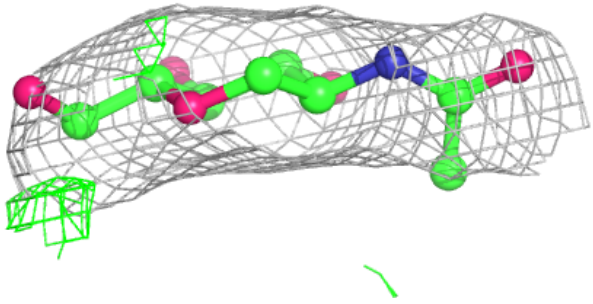


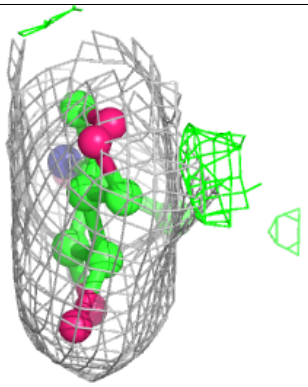


Electron density around NAG B 505:

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

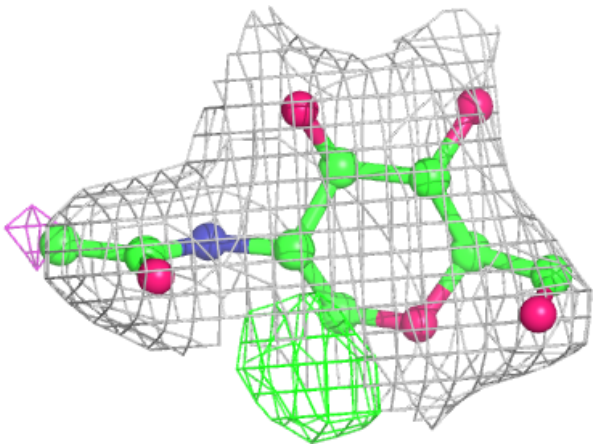


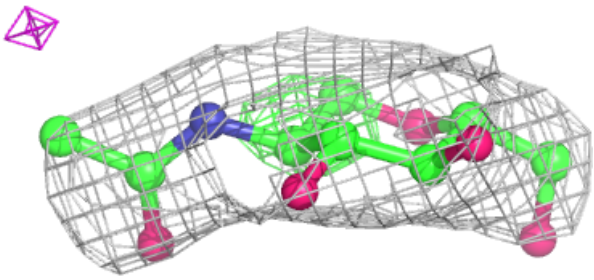


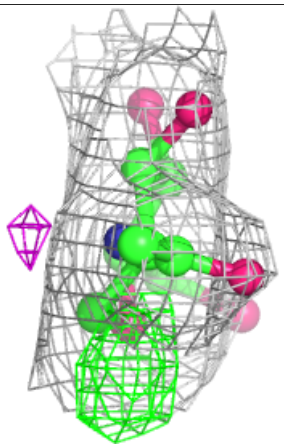


Electron density around NAG C 502:

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

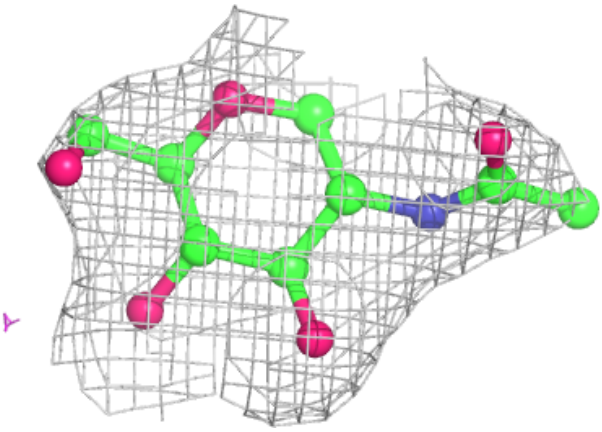


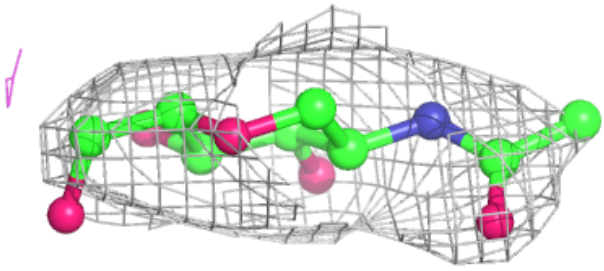


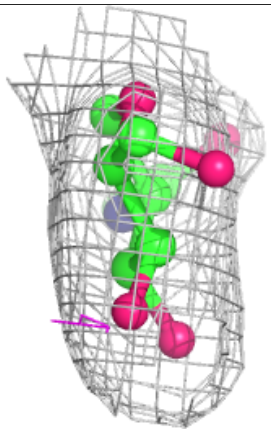


Electron density around NAG B 501:

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

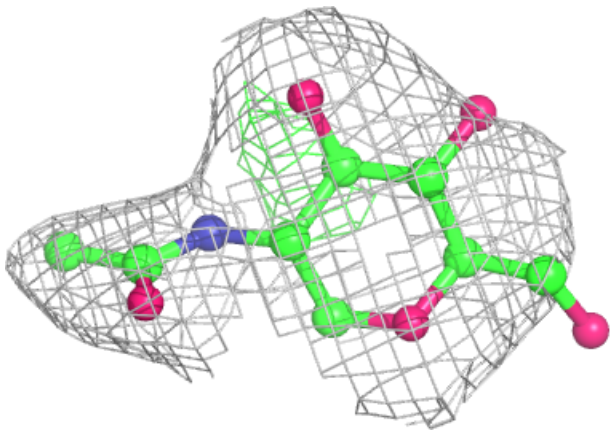


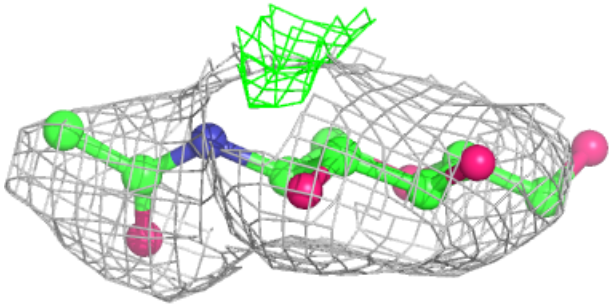


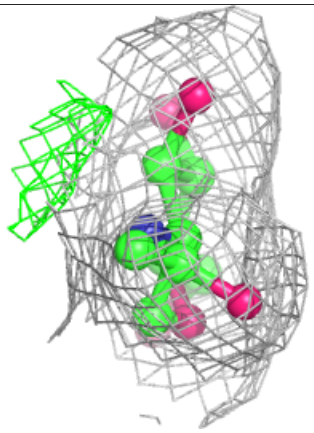


Electron density around NAG A 501:

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

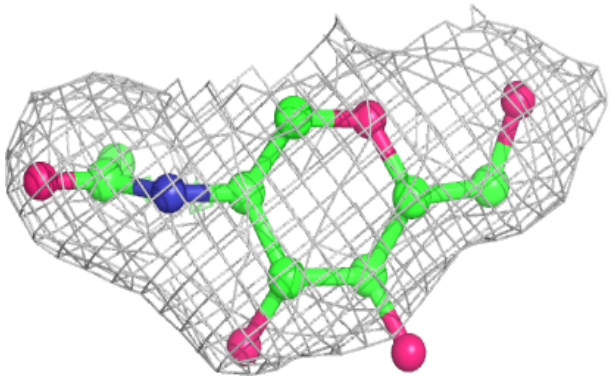


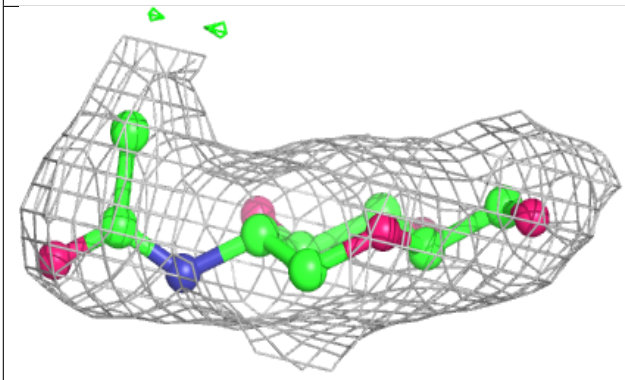


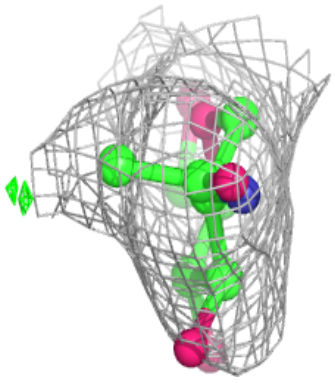


Electron density around NAG A 503:

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

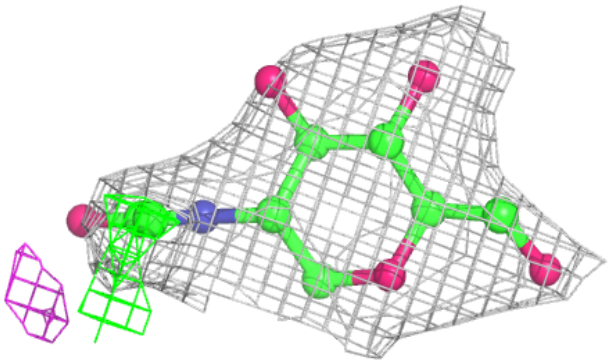


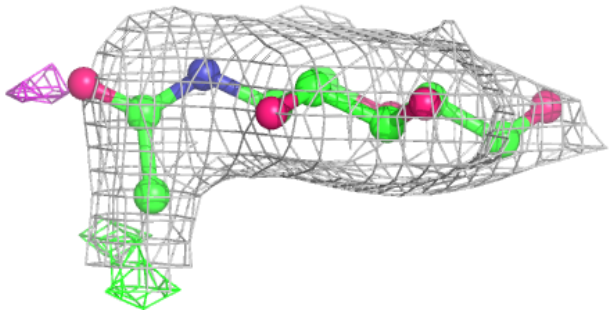


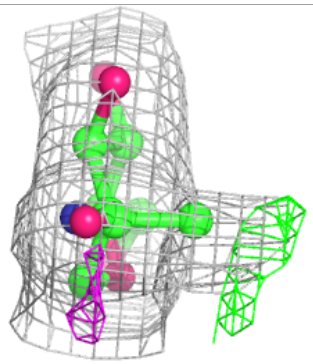


Electron density around NAG D 505:

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

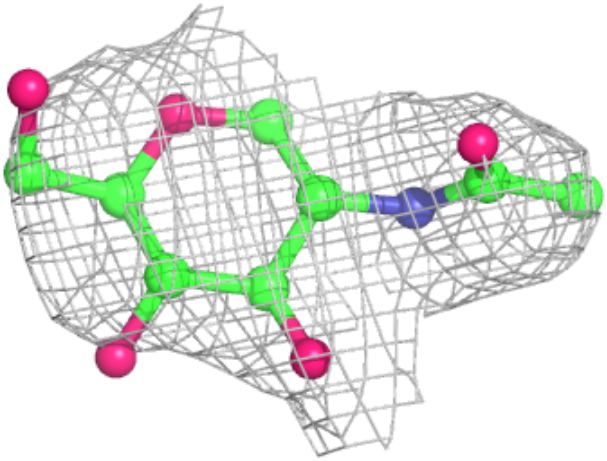


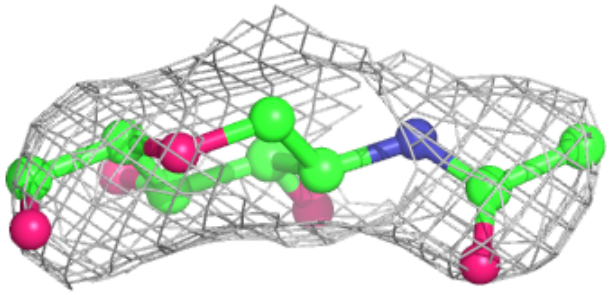


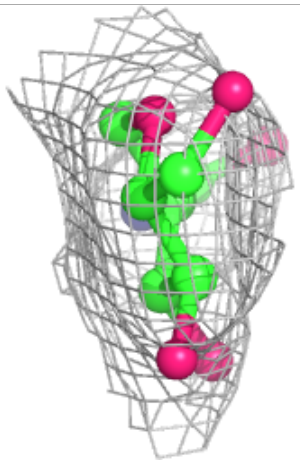


Electron density around NAG D 506:

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

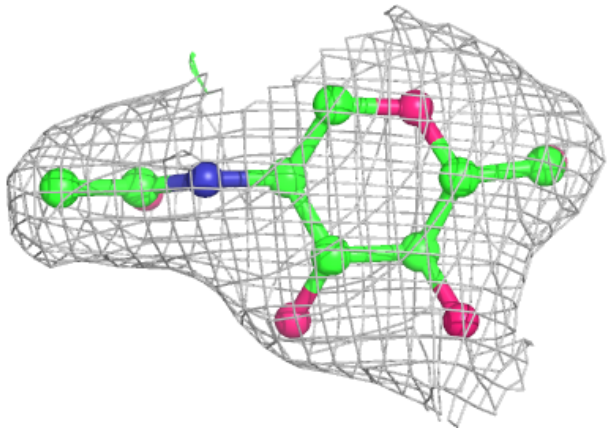


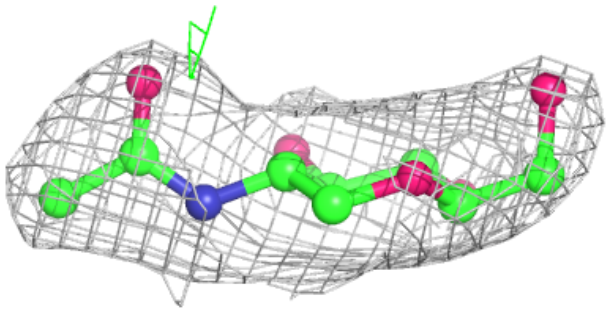


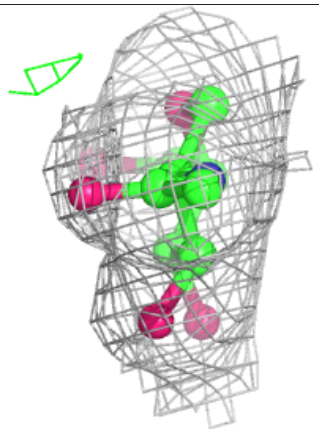


Electron density around NAG A 502:

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

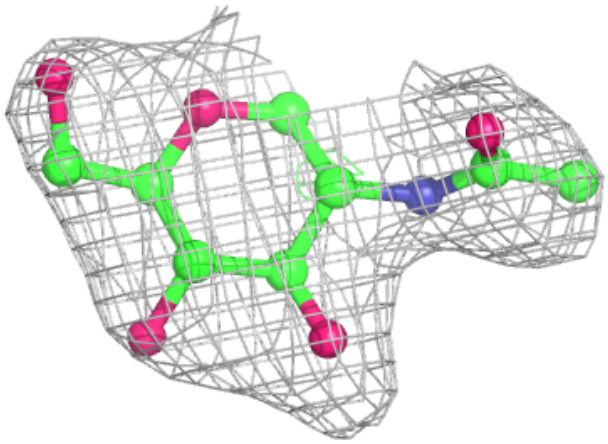


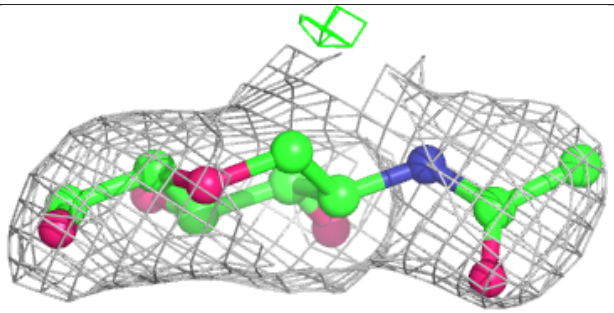


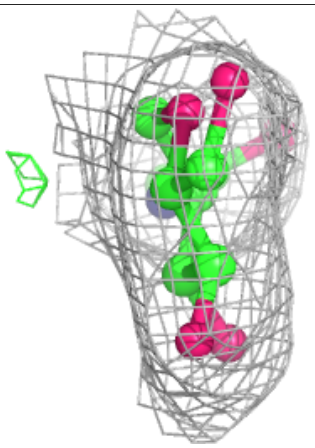


Electron density around NAG B 504:

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

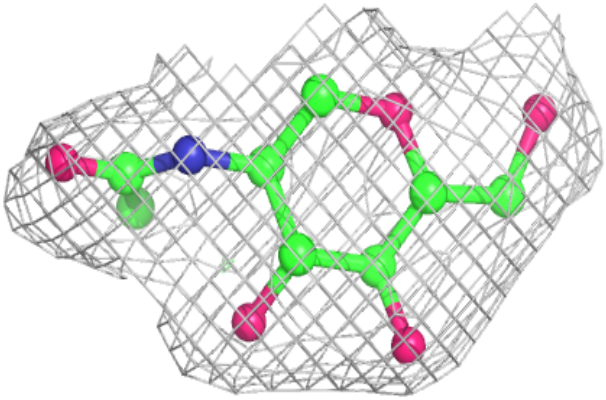


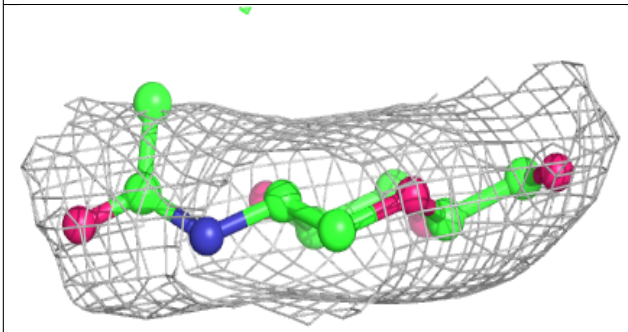


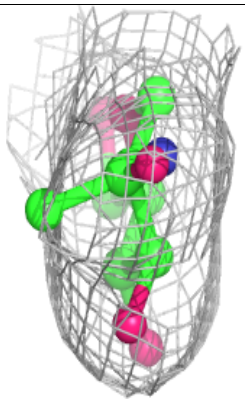


Electron density around NAG D 507:

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

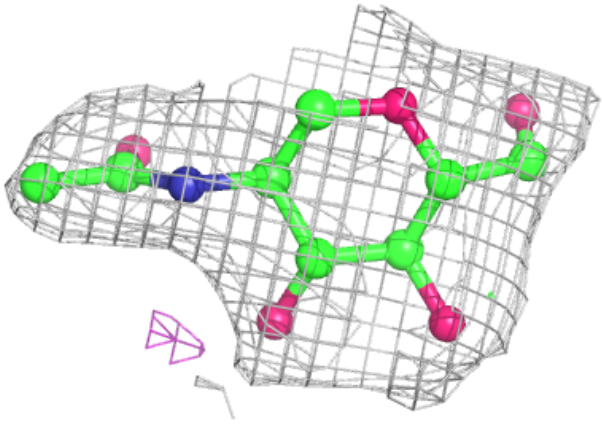


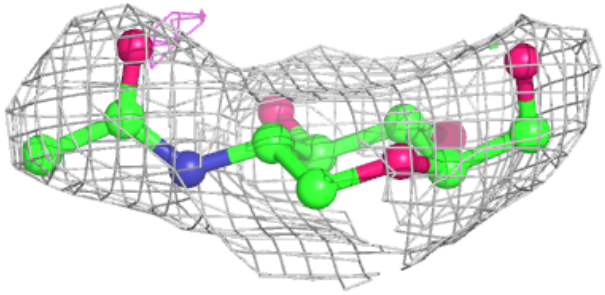


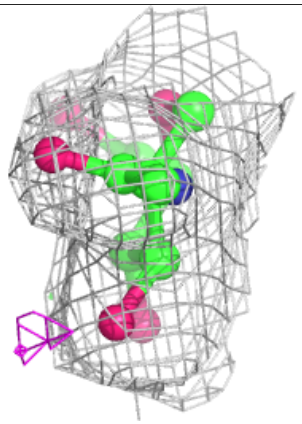


Electron density around NAG D 503:

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

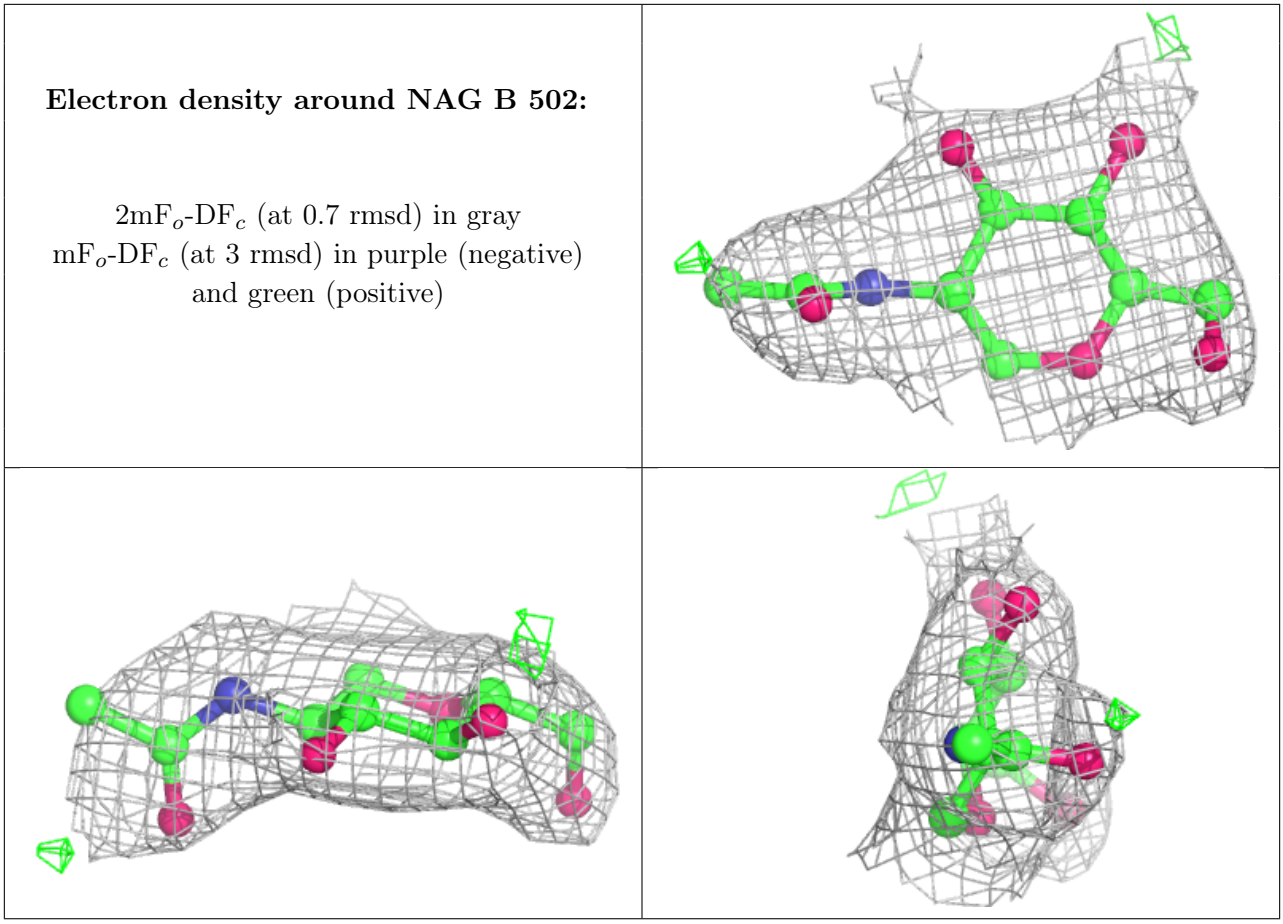






Electron density around NAG B 502:

$2mF_o$-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.