wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 10:20 pm BST

PDB ID	:	7YZH
Title	:	Schistosoma Mansoni Carbonic Anhydrase in complex with 4-oxo-N-(4-sulfamoylphenethyl)-1,3,4,6,7,11b-hexahydro-2H-pyrazino[2,1-a]isoquinoline-2-carbothioamide
Authors	:	Angeli, A.; Ferraroni, M.
Deposited on	:	2022-02-20
Resolution	:	1.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

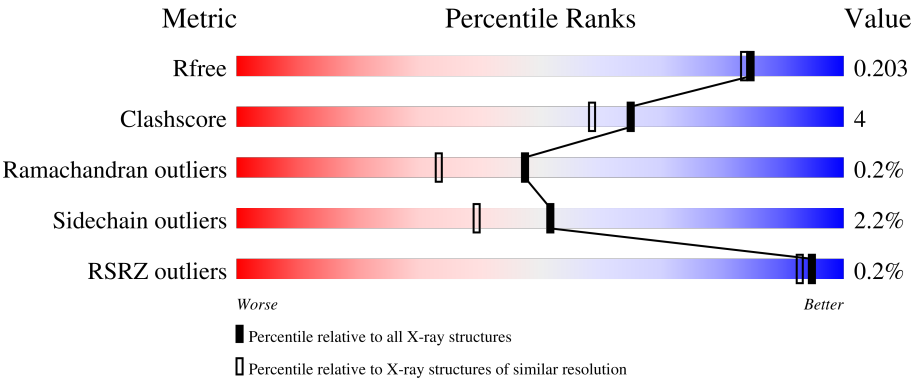
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	AAA	323	79% 6% • 14%
1	BBB	323	77% 8% • 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HFF	AAA	404	X	-	-	-
4	HFF	BBB	406	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5006 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 Carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	277	Total	C	N	O	S	0	2	0
			2250	1434	385	424	7			
1	BBB	276	Total	C	N	O	S	0	4	0
			2247	1435	383	422	7			

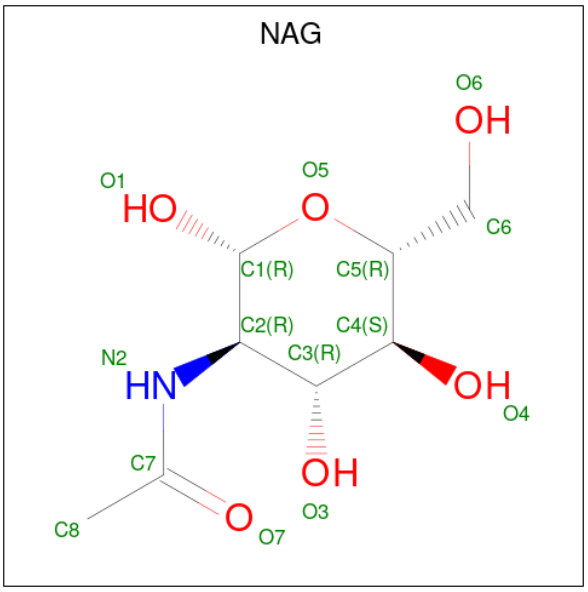
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	299	ARG	SER	conflict	UNP A0A3Q0KSG2
BBB	299	ARG	SER	conflict	UNP A0A3Q0KSG2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

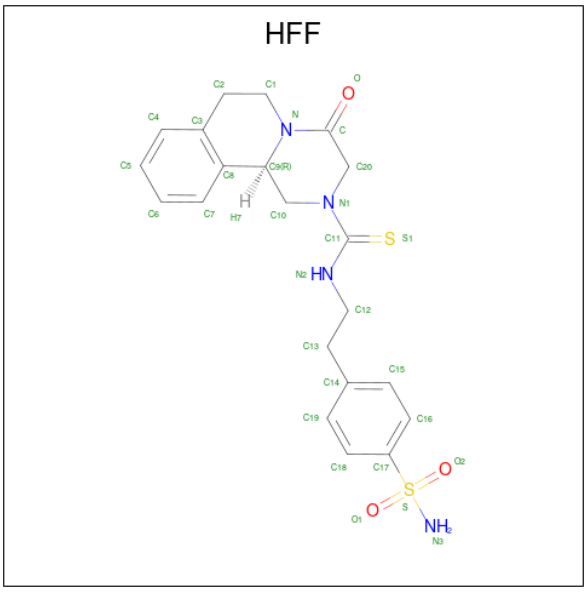
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Zn	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 3 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).



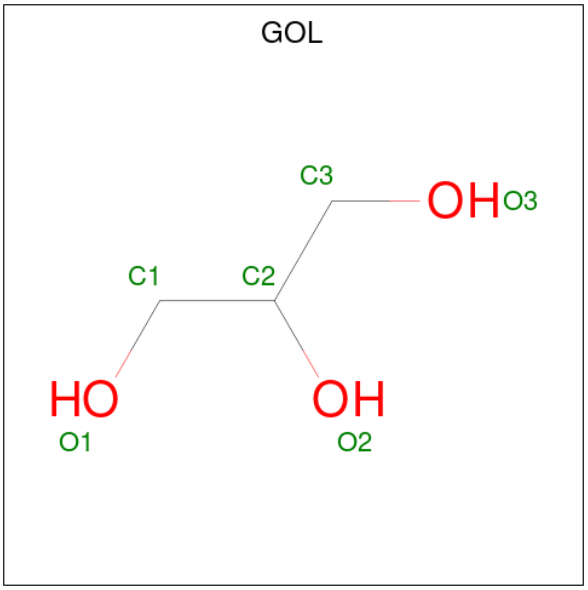
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O 14 8 1 5	0	0
3	AAA	1	Total C N O 14 8 1 5	0	0
3	BBB	1	Total C N O 14 8 1 5	0	0
3	BBB	1	Total C N O 14 8 1 5	0	0
3	BBB	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 4-oxo-N-(4-sulfamoylphenethyl)-1,3,4,6,7,11b-hexahydro-2H-pyrazino[2,1-a]isoquinoline-2-carbothioamide (three-letter code: HFF) (formula: $C_{21}H_{24}N_4O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	S	0	0
			30	21	4	3	2		
4	BBB	1	Total	C	N	O	S	0	0
			30	21	4	3	2		

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



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

- Molecule 6 is water.

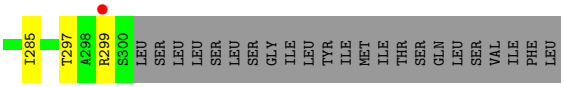
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	195	Total O 195 195	0	0
6	BBB	176	Total O 176 176	0	0

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: Carbonic anhydrase

Chain AAA:



- Molecule 1: Carbonic anhydrase

Chain BBB:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.83Å 103.83Å 133.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 1.79 89.92 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-1.79) 100.0 (89.92-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.198 0.178 , 0.203	Depositor DCC
R_{free} test set	3862 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5006	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: HFF, GOL, ZN, NAG

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	AAA	0.77	1/2316 (0.0%)	0.89	0/3150
1	BBB	0.76	0/2320	0.88	1/3158 (0.0%)
All	All	0.76	1/4636 (0.0%)	0.89	1/6308 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	180	GLU	CD-OE1	5.53	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	299	ARG	CA-C-O	-5.87	107.78	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2250	0	2171	10	0
1	BBB	2247	0	2173	27	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	28	0	25	0	0
3	BBB	42	0	39	9	0
4	AAA	30	0	0	0	0
4	BBB	30	0	0	0	0
5	BBB	6	0	8	0	0
6	AAA	195	0	0	0	0
6	BBB	176	0	0	3	0
All	All	5006	0	4416	37	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 4.

The worst 5 of 37 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:BBB:74:ASN:HD21	3:BBB:402:NAG:C1	0.96	1.59
1:BBB:74:ASN:ND2	3:BBB:402:NAG:C1	1.79	1.39
1:BBB:203:ASN:HD21	3:BBB:404:NAG:C1	1.47	1.27
1:BBB:203:ASN:ND2	3:BBB:404:NAG:C1	2.28	0.96
1:BBB:203:ASN:HD21	3:BBB:404:NAG:C2	1.96	0.77

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	AAA	277/323 (86%)	267 (96%)	9 (3%)	1 (0%)	34 21
1	BBB	278/323 (86%)	270 (97%)	8 (3%)	0	100 100
All	All	555/646 (86%)	537 (97%)	17 (3%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	299	ARG

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	AAA	252/295 (85%)	247 (98%)	5 (2%)	55 44
1	BBB	252/295 (85%)	246 (98%)	6 (2%)	49 36
All	All	504/590 (85%)	493 (98%)	11 (2%)	52 39

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	178	LYS
1	BBB	263	TYR
1	BBB	297	THR
1	BBB	275	ASN
1	AAA	297	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NAG	BBB	403	1	14,14,15	1.09	2 (14%)	17,19,21	1.88	4 (23%)
3	NAG	AAA	402	-	14,14,15	1.15	1 (7%)	17,19,21	3.33	6 (35%)
4	HFF	BBB	406	2	33,33,33	0.60	0	47,48,48	0.70	2 (4%)
5	GOL	BBB	401	-	5,5,5	0.42	0	5,5,5	0.69	0
3	NAG	BBB	402	-	14,14,15	1.21	1 (7%)	17,19,21	1.68	4 (23%)
3	NAG	BBB	404	-	14,14,15	0.76	0	17,19,21	1.48	5 (29%)
3	NAG	AAA	403	1	14,14,15	1.19	1 (7%)	17,19,21	1.52	4 (23%)
4	HFF	AAA	404	2	33,33,33	0.80	1 (3%)	47,48,48	0.64	1 (2%)

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
3	NAG	BBB	403	1	-	2/6/23/26	0/1/1/1
3	NAG	AAA	402	-	-	3/6/23/26	0/1/1/1
4	HFF	BBB	406	2	1/1/6/7	4/16/41/41	0/4/4/4
5	GOL	BBB	401	-	-	0/4/4/4	-
3	NAG	BBB	402	-	-	0/6/23/26	0/1/1/1
3	NAG	BBB	404	-	-	0/6/23/26	0/1/1/1
3	NAG	AAA	403	1	-	2/6/23/26	0/1/1/1
4	HFF	AAA	404	2	1/1/6/7	4/16/41/41	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	NAG	O5-C5	2.52	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	404	HFF	O2-S	-2.41	1.39	1.43
3	AAA	403	NAG	O5-C5	2.35	1.48	1.43
3	BBB	403	NAG	C4-C5	2.10	1.57	1.53
3	BBB	403	NAG	O5-C1	2.06	1.47	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	402	NAG	C2-N2-C7	9.17	135.96	122.90
3	AAA	402	NAG	O7-C7-N2	-5.36	112.10	121.95
3	AAA	402	NAG	C8-C7-N2	5.31	125.08	116.10
3	AAA	402	NAG	C1-C2-N2	-4.63	102.58	110.49
3	BBB	403	NAG	C8-C7-N2	4.31	123.40	116.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AAA	404	HFF	C9
4	BBB	406	HFF	C9

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	NAG	C3-C2-N2-C7
4	AAA	404	HFF	N1-C11-N2-C12
3	AAA	403	NAG	O5-C5-C6-O6
3	AAA	403	NAG	C4-C5-C6-O6
3	AAA	402	NAG	C8-C7-N2-C2

There are no ring outliers.

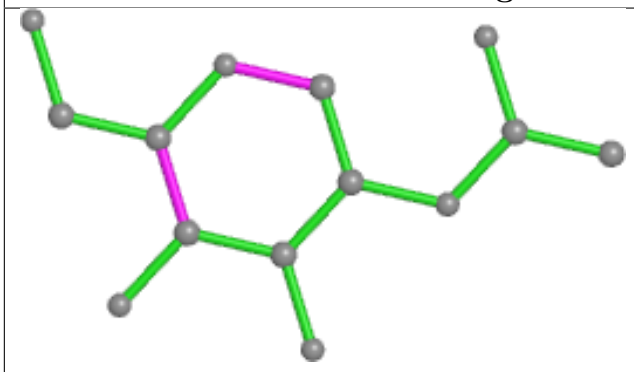
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	403	NAG	1	0
3	BBB	402	NAG	5	0
3	BBB	404	NAG	3	0

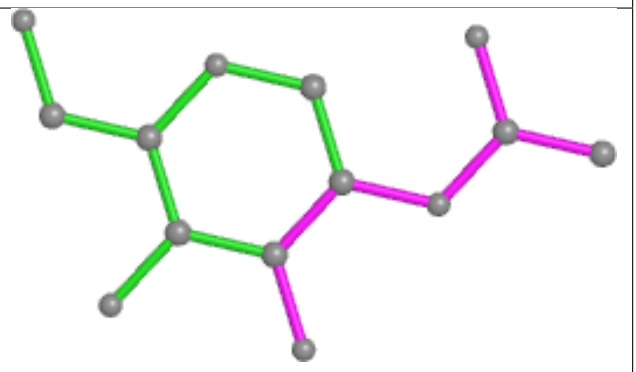
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

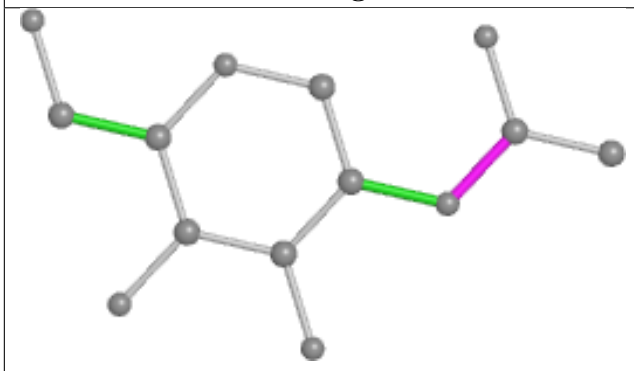
Ligand NAG BBB 403



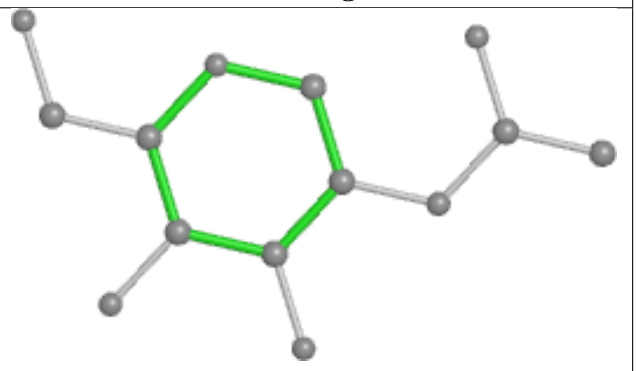
Bond lengths



Bond angles

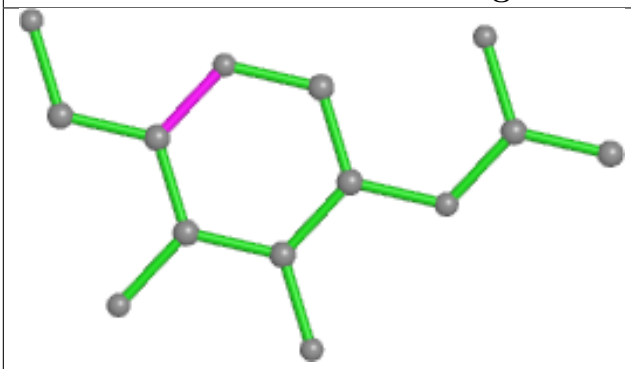


Torsions

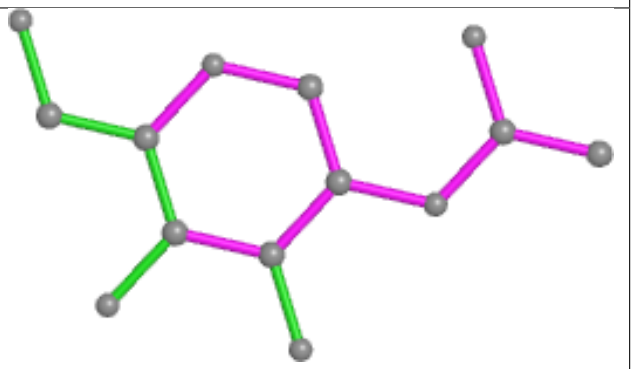


Rings

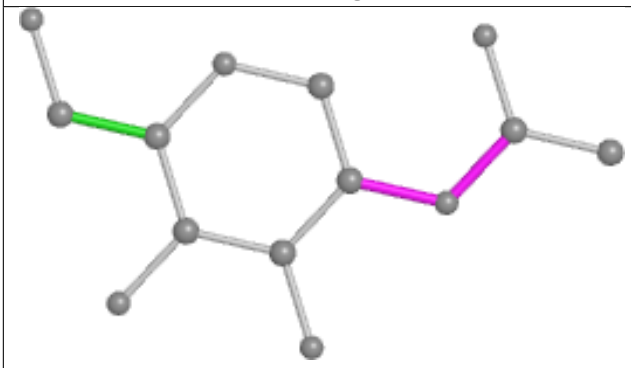
Ligand NAG AAA 402



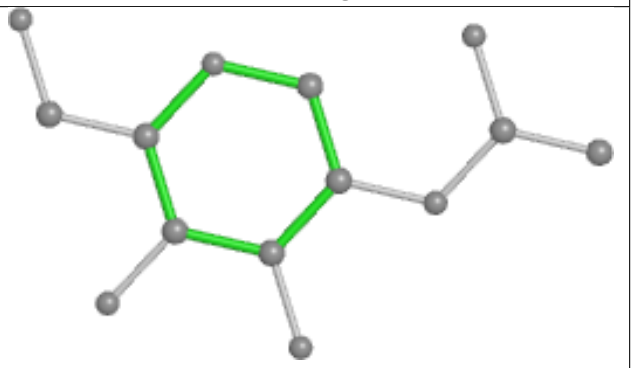
Bond lengths



Bond angles

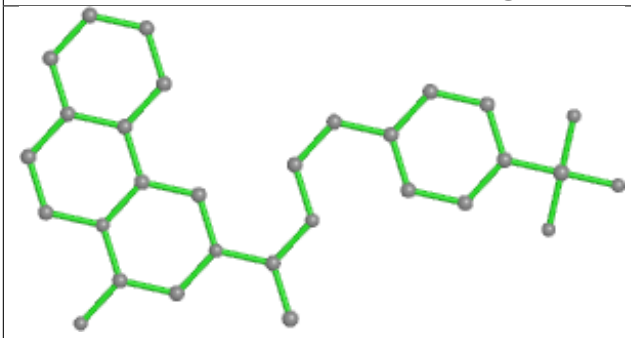


Torsions

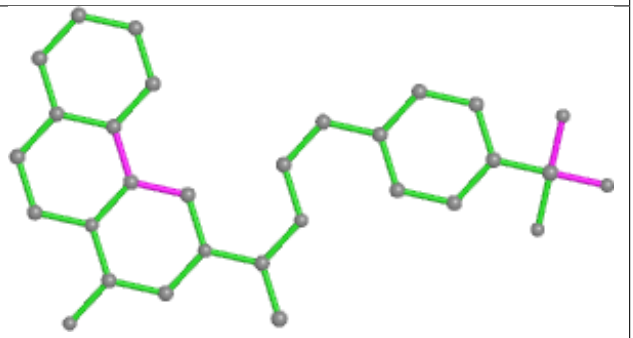


Rings

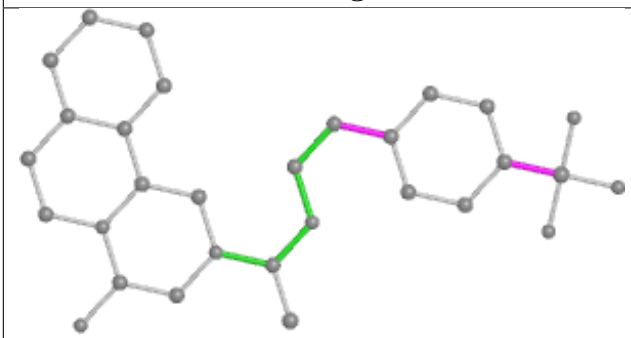
Ligand HFF BBB 406



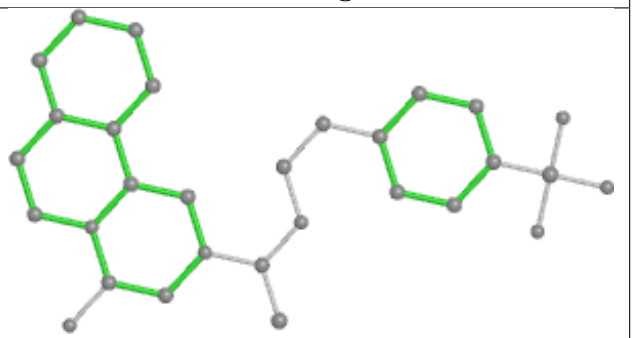
Bond lengths



Bond angles

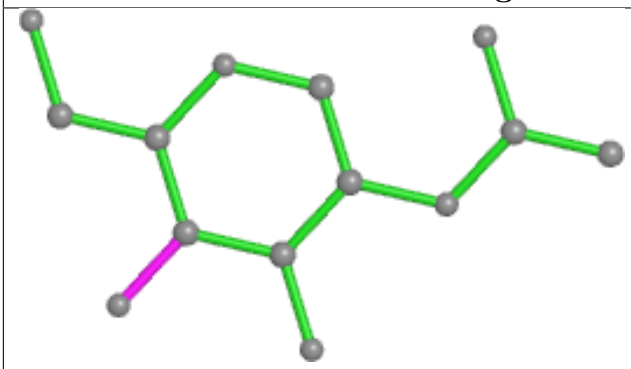


Torsions

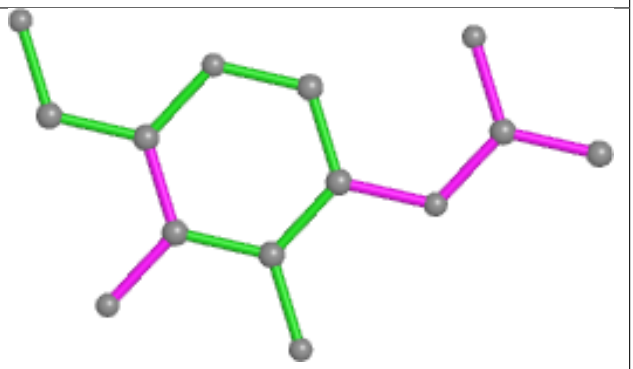


Rings

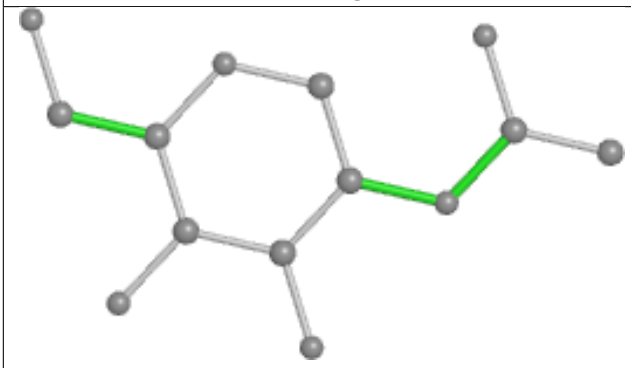
Ligand NAG BBB 402



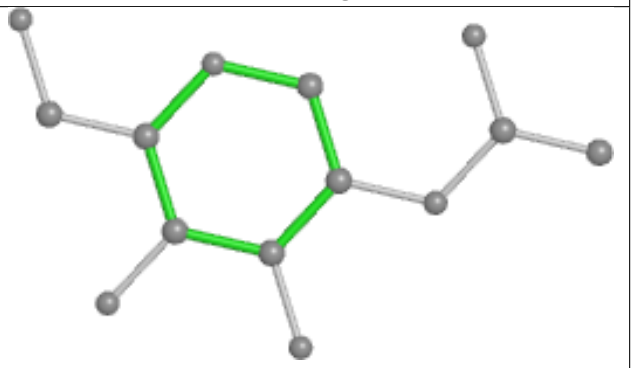
Bond lengths



Bond angles

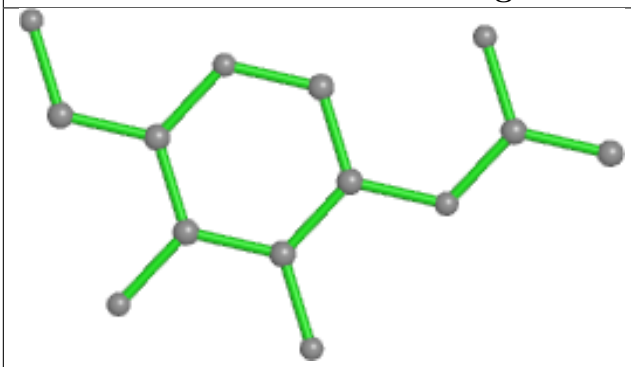


Torsions

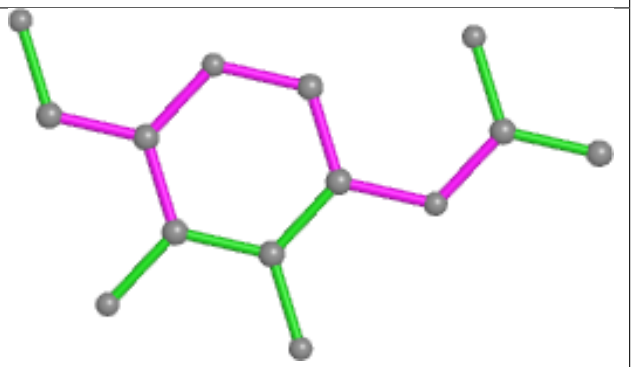


Rings

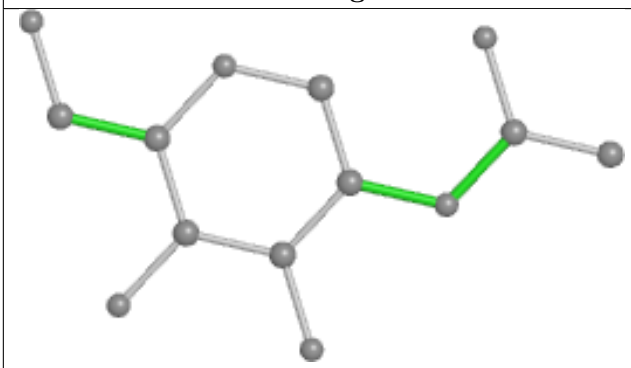
Ligand NAG BBB 404



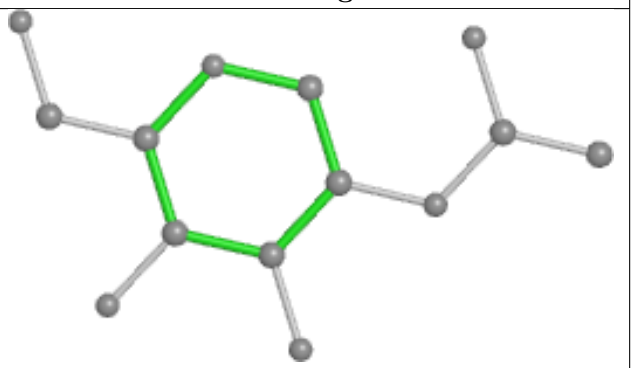
Bond lengths



Bond angles

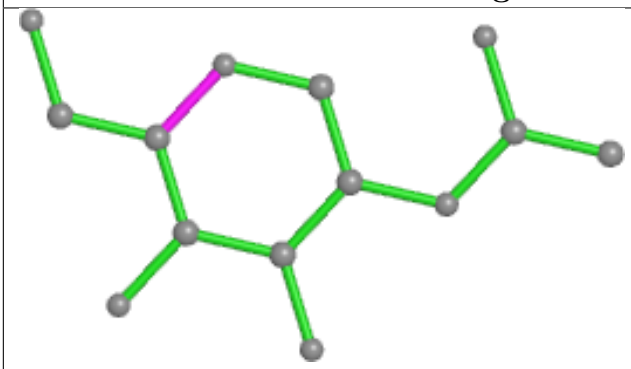


Torsions

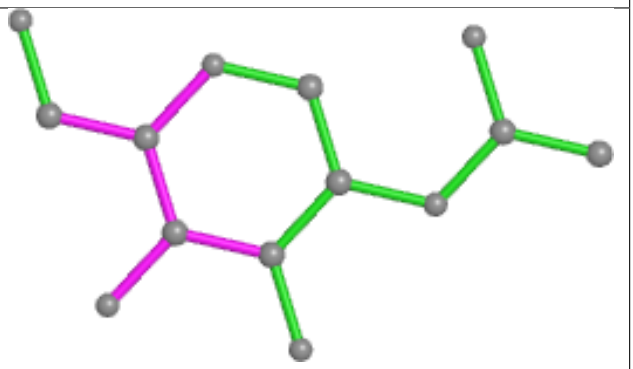


Rings

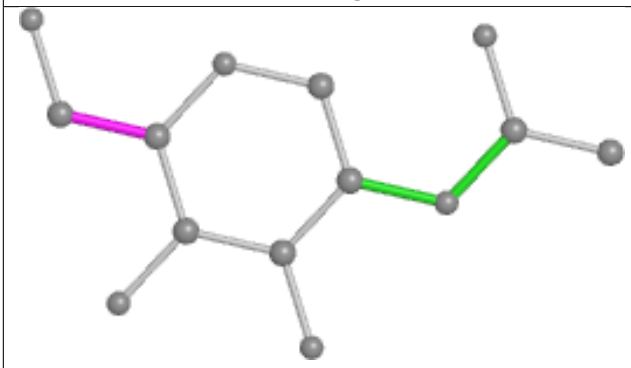
Ligand NAG AAA 403



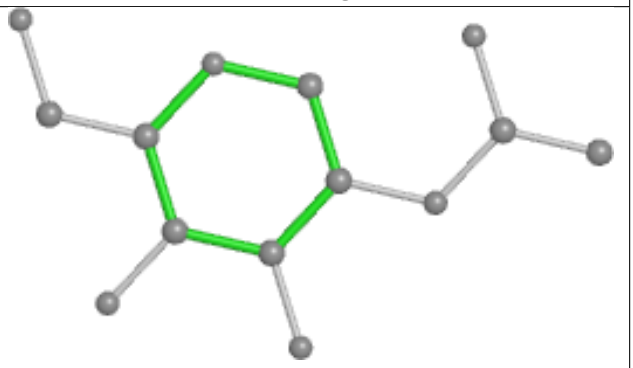
Bond lengths



Bond angles

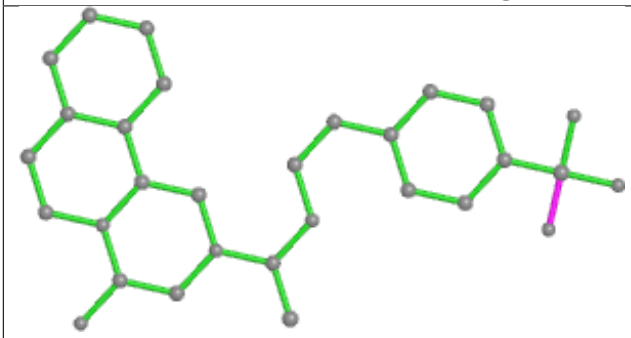


Torsions

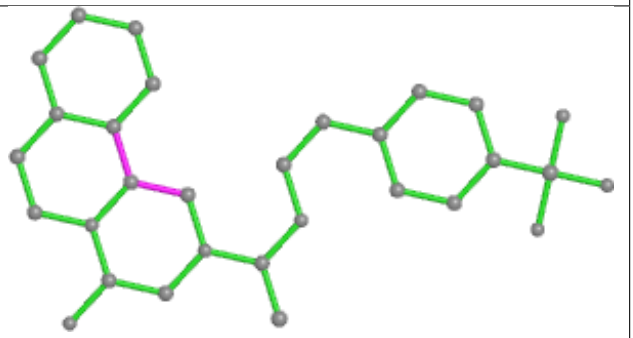


Rings

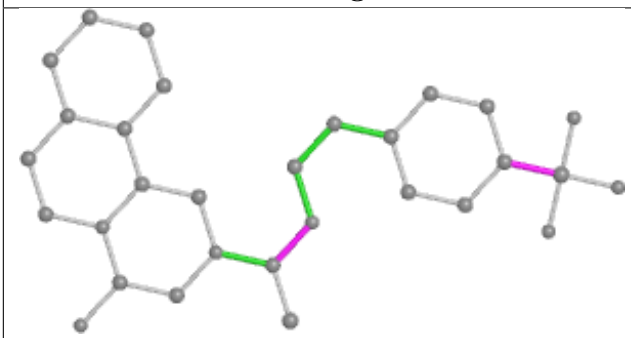
Ligand HFF AAA 404



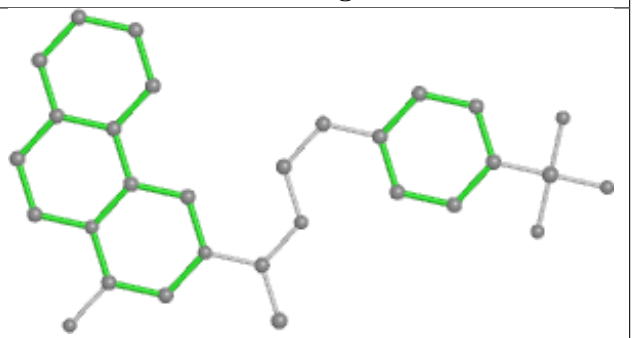
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	AAA	277/323 (85%)	-0.20	1 (0%) 92 90	21, 29, 49, 73	0
1	BBB	276/323 (85%)	-0.23	0 100 100	21, 31, 51, 68	0
All	All	553/646 (85%)	-0.21	1 (0%) 95 93	21, 30, 50, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	299	ARG	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	NAG	BBB	404	14/15	0.68	0.18	74,93,101,102	0
3	NAG	AAA	403	14/15	0.87	0.11	40,50,59,60	0
3	NAG	AAA	402	14/15	0.88	0.13	45,56,67,77	0
3	NAG	BBB	402	14/15	0.90	0.09	44,48,55,57	0

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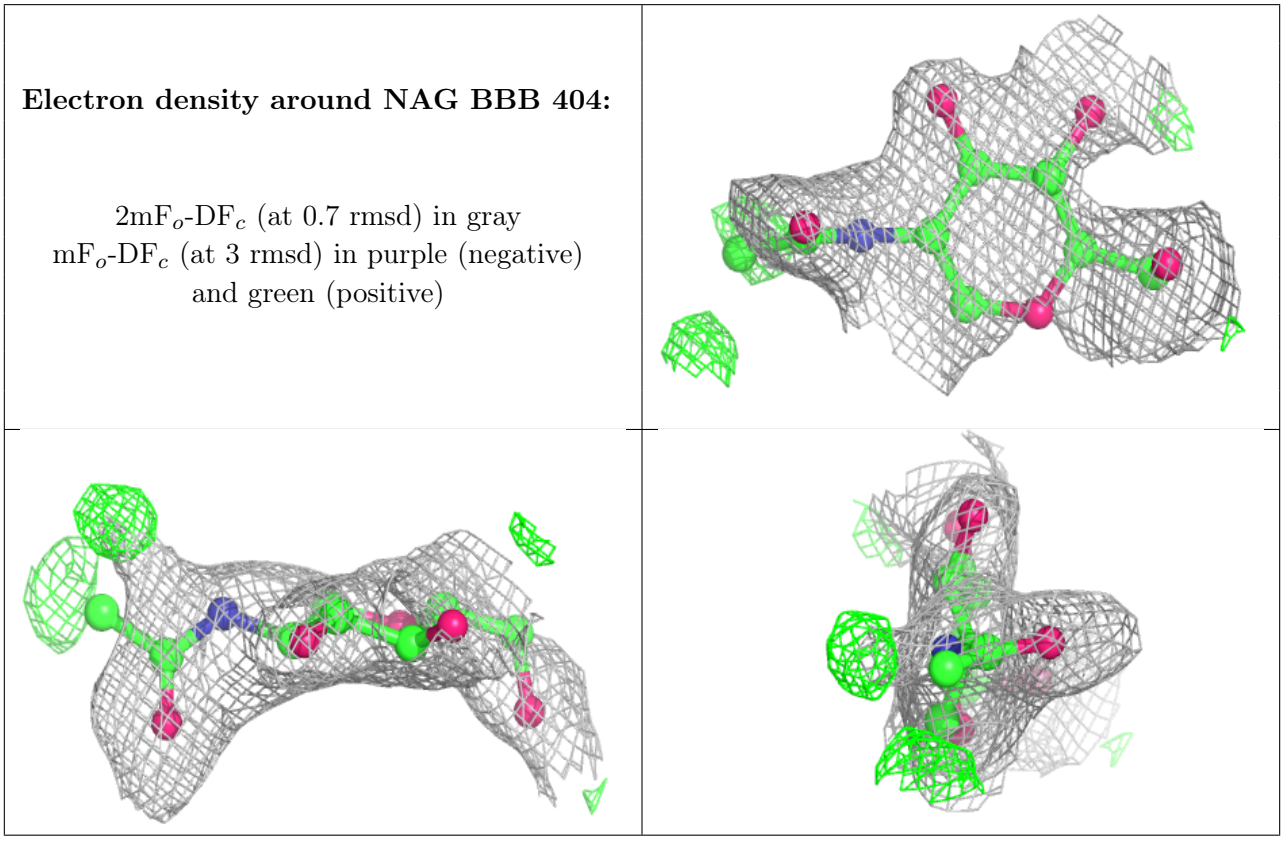
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	BBB	403	14/15	0.91	0.10	41,53,63,64	0
5	GOL	BBB	401	6/6	0.92	0.12	25,37,40,40	0
4	HFF	BBB	406	30/30	0.93	0.27	35,75,108,110	0
4	HFF	AAA	404	30/30	0.94	0.25	31,64,100,104	0
2	ZN	AAA	401	1/1	1.00	0.04	30,30,30,30	0
2	ZN	BBB	405	1/1	1.00	0.03	34,34,34,34	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.

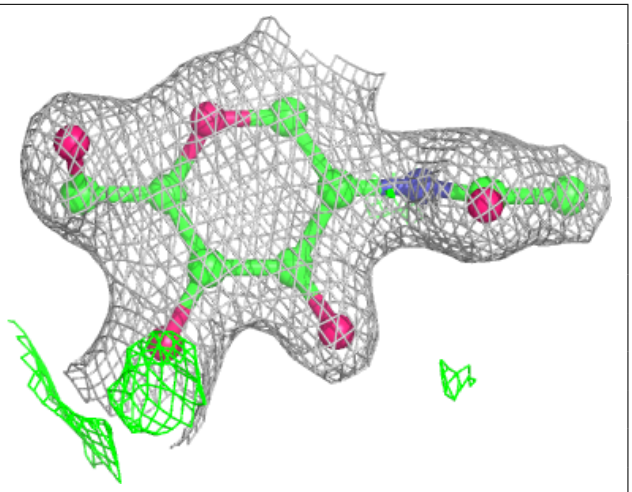
Electron density around NAG BBB 404:

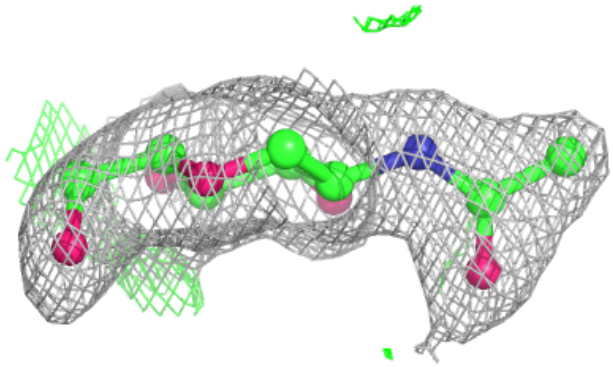
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

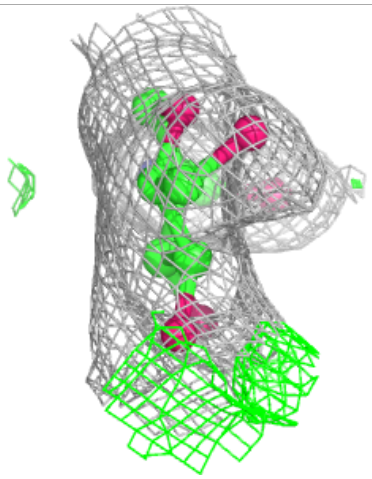


Electron density around NAG AAA 403:

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

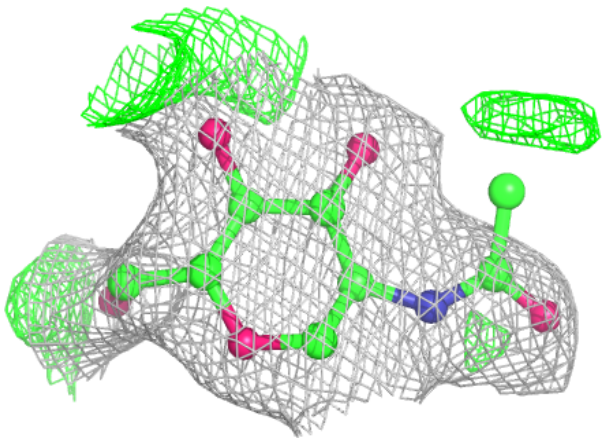


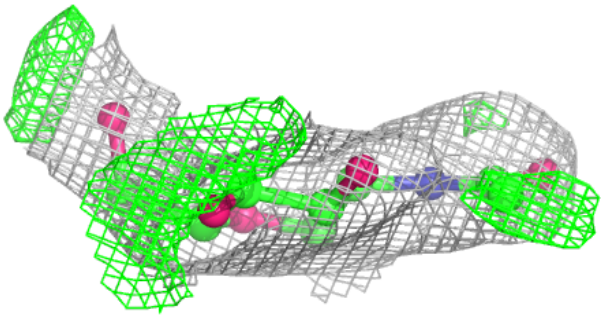


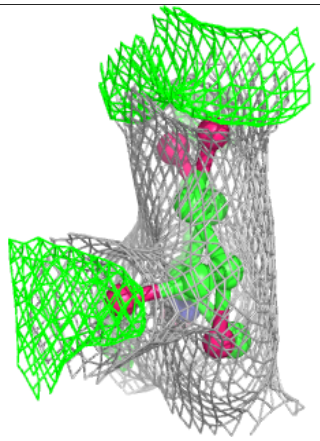


Electron density around NAG AAA 402:

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

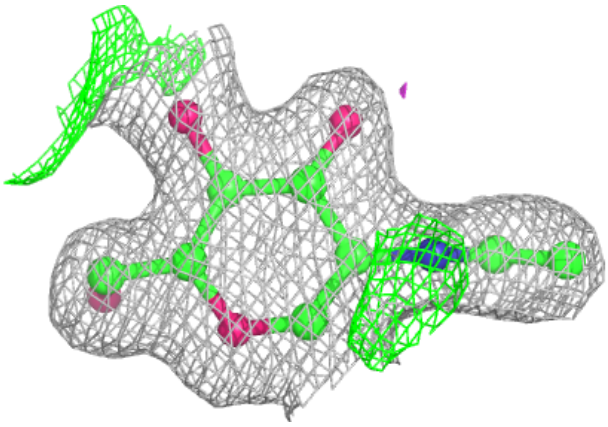


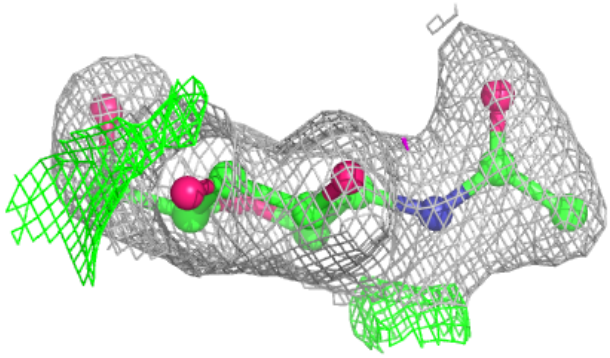


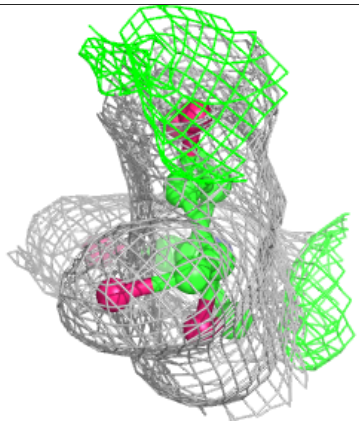


Electron density around NAG BBB 402:

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

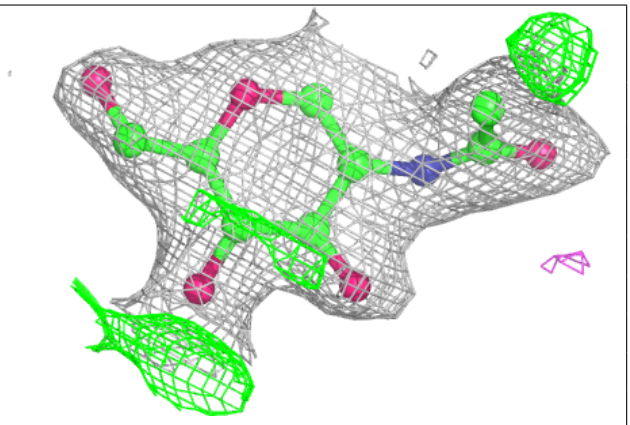


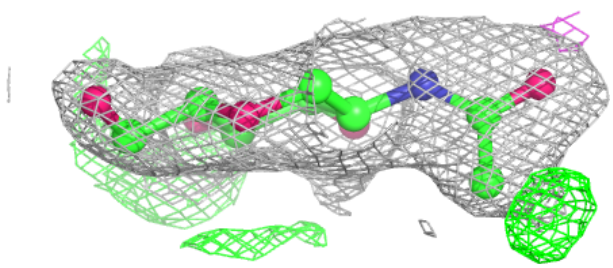


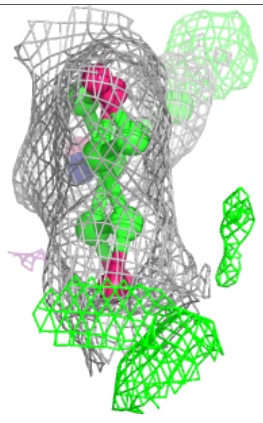


Electron density around NAG BBB 403:

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

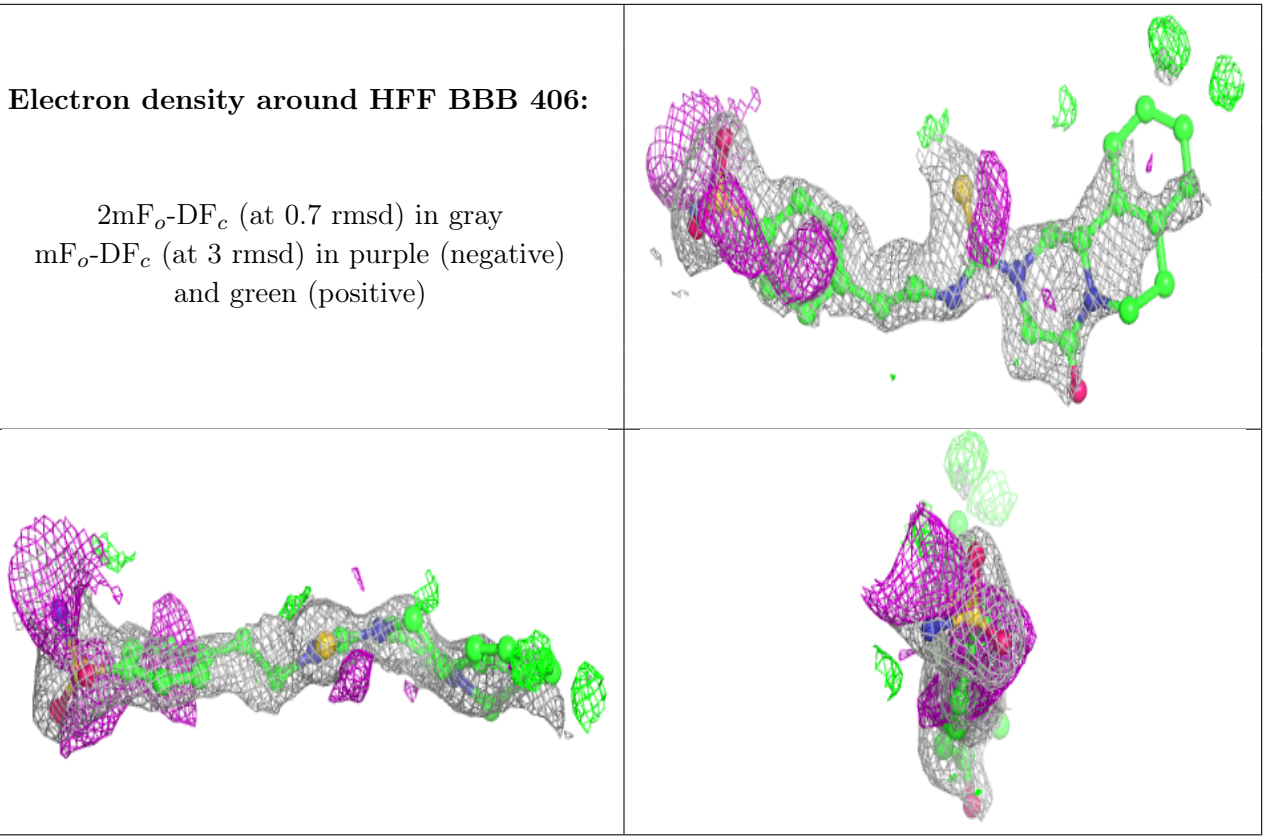






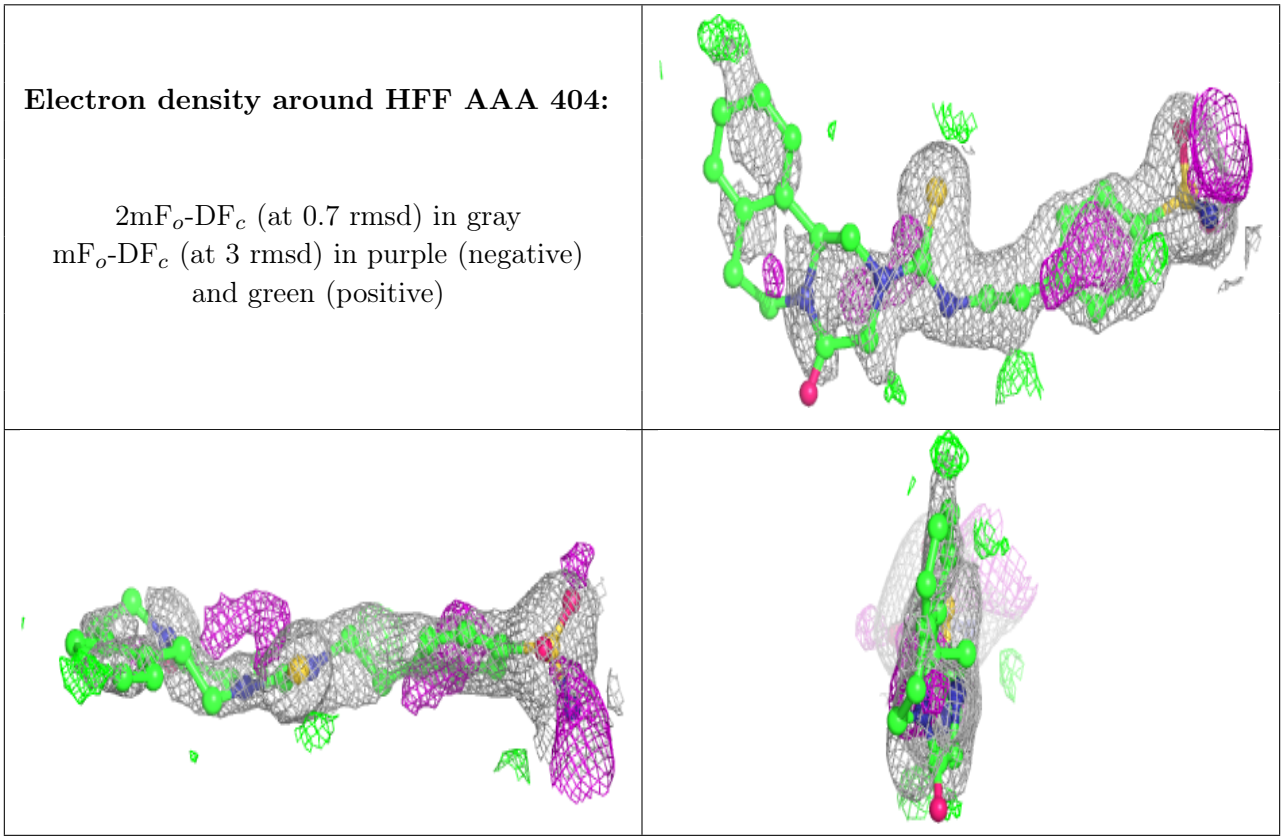
Electron density around HFF BBB 406:

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



Electron density around HFF AAA 404:

$2mF_o$-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.