



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:12 PM UTC

PDB ID : 7PRI / pdb_00007pri
Title : Carbonic Anhydrase from Schistosoma Mansoni in complex with clorsulon
Authors : Angeli, A.; Ferraroni, M.
Deposited on : 2021-09-21
Resolution : 1.68 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

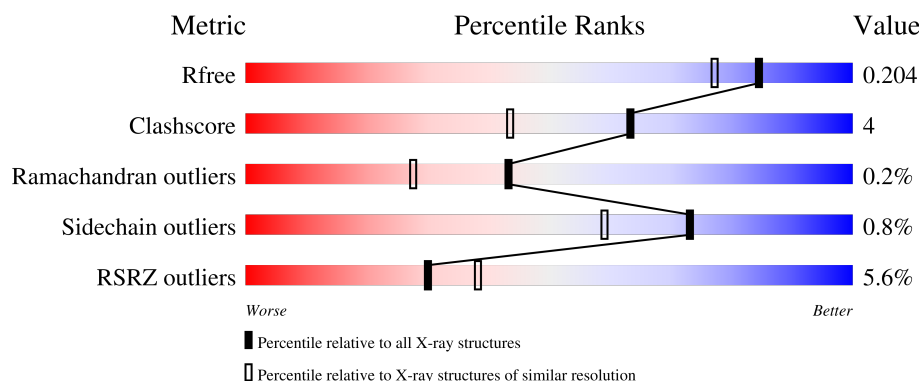
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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

Mol	Chain	Length	Quality of chain
1	AAA	280	
1	BBB	280	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4998 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
			2259	1441	386	425	7			
1	BBB	277	Total	C	N	O	S	0	0	0
			2247	1433	385	422	7			

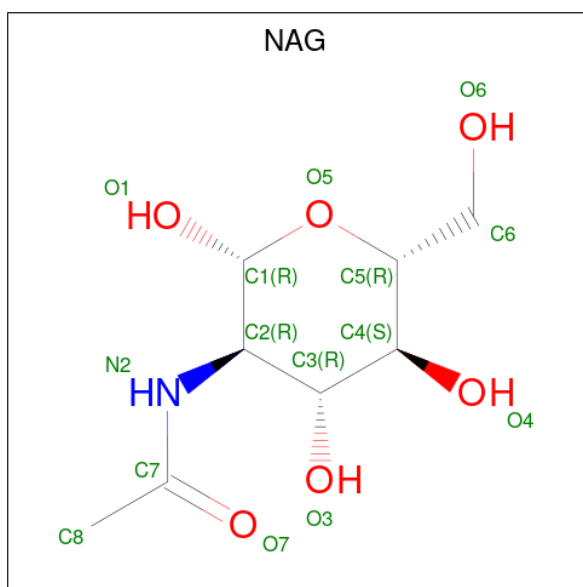
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	299	ARG	-	expression tag	UNP A0A3Q0KSG2
AAA	300	GLY	-	expression tag	UNP A0A3Q0KSG2
BBB	299	ARG	-	expression tag	UNP A0A3Q0KSG2
BBB	300	GLY	-	expression tag	UNP A0A3Q0KSG2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

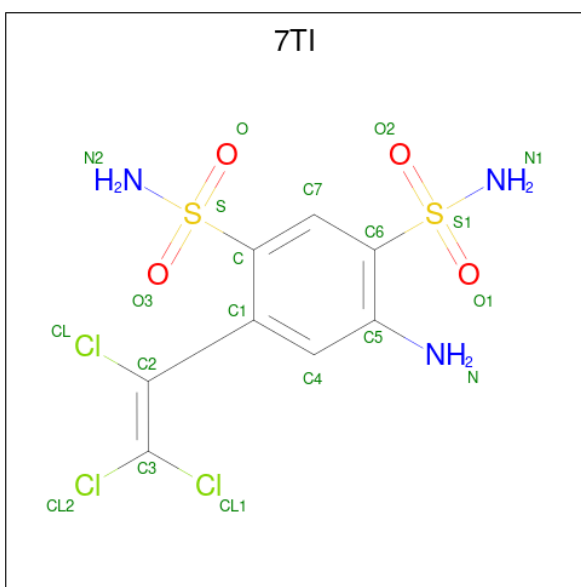
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Zn	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



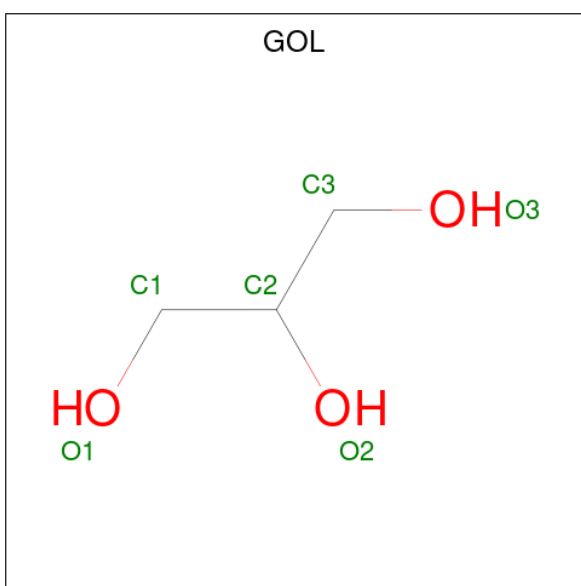
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
3	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
3	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
3	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
3	BBB	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 4-azanyl-6-[1,2,2-tris(chloranyl)ethenyl]benzene-1,3-disulfonamide (CCD ID: 7TI) (formula: C₈H₈Cl₃N₃O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	AAA	1	Total	C	Cl	N	O	S	0	0
			20	8	3	3	4	2		
4	BBB	1	Total	C	Cl	N	O	S	0	0
			20	8	3	3	4	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

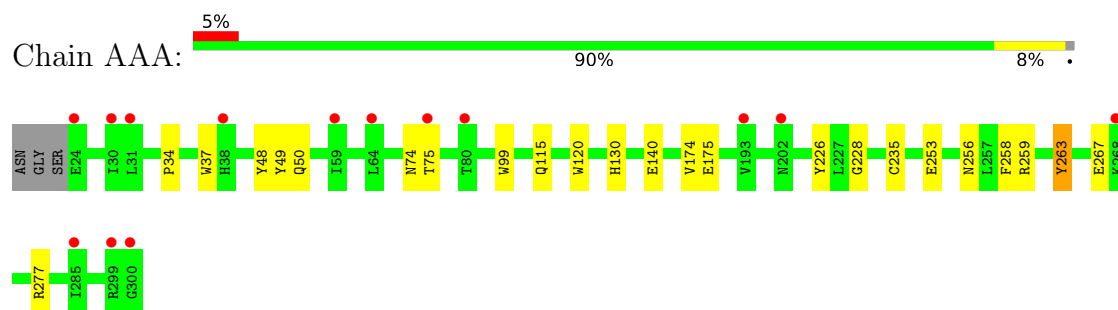
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	190	Total 190	O 190	0	0
6	BBB	184	Total 184	O 184	0	0

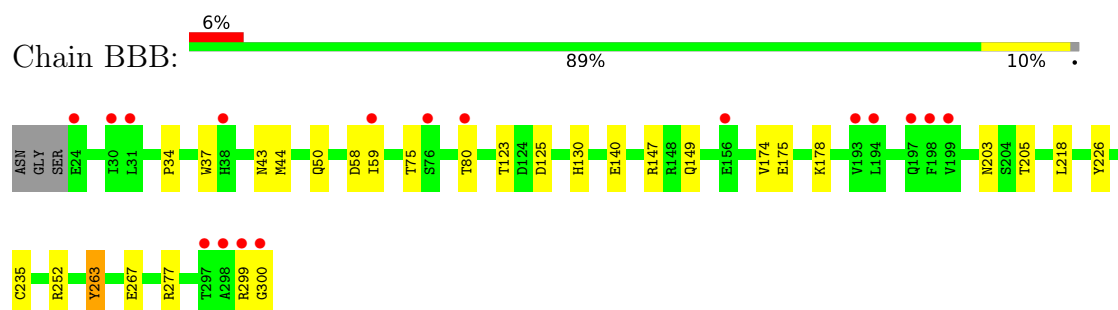
3 Residue-property plots [i](#)

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



- Molecule 1: Carbonic anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.80Å 103.80Å 132.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.89 – 1.68 89.89 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.89-1.68) 99.7 (89.89-1.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.195 0.178 , 0.204	Depositor DCC
R_{free} test set	4543 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7TI, GOL, NAG, ZN

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	1.07	1/2325 (0.0%)	1.21	4/3163 (0.1%)
1	BBB	1.06	1/2307 (0.0%)	1.21	2/3139 (0.1%)
All	All	1.06	2/4632 (0.0%)	1.21	6/6302 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	59	ILE	C-O	6.17	1.31	1.24
1	AAA	228	GLY	C-O	5.62	1.29	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	75	THR	CA-CB-OG1	-10.04	94.55	109.60
1	BBB	75	THR	CA-CB-OG1	-8.85	96.32	109.60
1	AAA	74	ASN	CA-C-N	5.50	128.21	120.28
1	AAA	74	ASN	C-N-CA	5.50	128.21	120.28
1	BBB	58	ASP	CA-CB-CG	5.16	117.76	112.60
1	AAA	99	TRP	O-C-N	5.03	129.77	123.23

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	2259	0	2194	14	0
1	BBB	2247	0	2180	20	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	28	0	26	0	0
3	BBB	42	0	39	4	0
4	AAA	20	0	0	1	0
4	BBB	20	0	0	0	0
5	BBB	6	0	8	0	0
6	AAA	190	0	0	2	0
6	BBB	184	0	0	2	0
All	All	4998	0	4447	35	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.

All (35) 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:203:ASN:HD21	3:BBB:405:NAG:C1	1.38	1.35
1:AAA:50:GLN:HE22	1:AAA:235:CYS:HB3	1.49	0.77
1:BBB:130:HIS:HE1	1:BBB:226:TYR:OH	1.72	0.71
1:AAA:130:HIS:HE1	1:AAA:226:TYR:OH	1.75	0.70
1:BBB:50:GLN:HE22	1:BBB:235:CYS:HB3	1.56	0.69
1:BBB:175:GLU:OE2	1:BBB:252:ARG:NH2	2.28	0.67
1:AAA:253[B]:GLU:HG3	6:AAA:551:HOH:O	1.98	0.63
1:AAA:174:VAL:HG12	1:BBB:174:VAL:HG12	1.83	0.61
1:AAA:175:GLU:HG2	6:BBB:561:HOH:O	2.00	0.60
1:BBB:203:ASN:HD21	3:BBB:405:NAG:C2	2.11	0.58
4:AAA:404:7TI:N2	4:AAA:404:7TI:CL	2.74	0.57
1:AAA:50:GLN:HE21	1:AAA:277:ARG:HH22	1.52	0.57
1:BBB:50:GLN:HE21	1:BBB:277:ARG:HH22	1.55	0.55
1:AAA:130:HIS:HD2	1:AAA:140:GLU:OE2	1.90	0.54
1:AAA:50:GLN:NE2	1:AAA:277:ARG:HH12	2.05	0.54
1:BBB:130:HIS:HD2	1:BBB:140:GLU:OE2	1.91	0.53
1:BBB:50:GLN:NE2	1:BBB:277:ARG:HH12	2.09	0.50
1:BBB:203:ASN:CG	3:BBB:405:NAG:C1	2.86	0.48
1:BBB:263:TYR:CD1	1:BBB:267:GLU:HG3	2.49	0.48
1:BBB:123:THR:OG1	1:BBB:125:ASP:OD1	2.32	0.45
1:AAA:120:TRP:CE2	1:AAA:258:PHE:HB3	2.50	0.45
1:AAA:48:TYR:HE1	1:AAA:49:TYR:CZ	2.35	0.45
1:BBB:263:TYR:CG	1:BBB:267:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:130:HIS:CE1	1:BBB:226:TYR:OH	2.62	0.43
1:BBB:80:THR:OG1	1:BBB:205:THR:HG23	2.18	0.43
3:BBB:403:NAG:H83	6:BBB:618:HOH:O	2.16	0.43
1:AAA:263:TYR:CD1	1:AAA:267:GLU:HG3	2.54	0.43
1:BBB:147:ARG:HE	1:BBB:149:GLN:HE21	1.68	0.42
1:AAA:256:ASN:HD22	1:AAA:259:ARG:HD2	1.85	0.42
1:BBB:34:PRO:HA	1:BBB:37:TRP:CE2	2.55	0.42
1:BBB:43:ASN:HA	1:BBB:44:MET:HA	1.87	0.41
1:AAA:34:PRO:HA	1:AAA:37:TRP:CE2	2.56	0.41
1:AAA:256:ASN:ND2	1:AAA:259:ARG:HH11	2.19	0.41
6:AAA:541:HOH:O	1:BBB:300:GLY:C	2.63	0.41
1:BBB:218:LEU:HD12	1:BBB:218:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	277/280 (99%)	267 (96%)	10 (4%)	0	100	100
1	BBB	275/280 (98%)	269 (98%)	5 (2%)	1 (0%)	30	13
All	All	552/560 (99%)	536 (97%)	15 (3%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	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	253/253 (100%)	251 (99%)	2 (1%)	73	59
1	BBB	251/253 (99%)	249 (99%)	2 (1%)	73	59
All	All	504/506 (100%)	500 (99%)	4 (1%)	73	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	115	GLN
1	AAA	263	TYR
1	BBB	178	LYS
1	BBB	263	TYR

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 oligosaccharides 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	AAA	402	1	14,14,15	1.13	1 (7%)	17,19,21	1.36	3 (17%)
3	NAG	BBB	405	1	14,14,15	0.92	0	17,19,21	1.82	3 (17%)
4	7TI	AAA	404	2	19,20,20	1.03	2 (10%)	28,32,32	0.69	1 (3%)
3	NAG	BBB	404	1	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
4	7TI	BBB	406	2	19,20,20	1.14	2 (10%)	28,32,32	0.99	1 (3%)
5	GOL	BBB	401	-	5,5,5	0.55	0	5,5,5	1.36	1 (20%)
3	NAG	BBB	403	1	14,14,15	1.09	1 (7%)	17,19,21	1.96	5 (29%)
3	NAG	AAA	403	1	14,14,15	1.11	2 (14%)	17,19,21	3.28	8 (47%)

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	AAA	402	1	-	0/6/23/26	0/1/1/1
3	NAG	BBB	405	1	-	0/6/23/26	0/1/1/1
4	7TI	AAA	404	2	-	2/20/20/20	0/1/1/1
3	NAG	BBB	404	1	-	0/6/23/26	0/1/1/1
4	7TI	BBB	406	2	-	3/20/20/20	0/1/1/1
5	GOL	BBB	401	-	-	0/4/4/4	-
3	NAG	BBB	403	1	-	2/6/23/26	0/1/1/1
3	NAG	AAA	403	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	406	7TI	C-S	2.75	1.81	1.77
4	AAA	404	7TI	C-S	2.73	1.81	1.77
4	AAA	404	7TI	C2-CL	2.36	1.79	1.74
3	AAA	402	NAG	O5-C5	2.34	1.48	1.43
3	AAA	403	NAG	C6-C5	2.17	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	406	7TI	O1-S1	2.12	1.47	1.43
3	BBB	403	NAG	C4-C5	2.11	1.57	1.53
3	AAA	403	NAG	O5-C5	2.01	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	403	NAG	C1-O5-C5	10.71	126.53	112.19
3	BBB	405	NAG	C1-O5-C5	4.73	118.52	112.19
3	BBB	403	NAG	O7-C7-C8	-4.17	114.63	122.05
3	BBB	403	NAG	C8-C7-N2	4.04	122.82	116.12
3	BBB	403	NAG	C2-N2-C7	4.04	128.31	122.90
3	AAA	403	NAG	C2-N2-C7	3.49	127.58	122.90
3	AAA	403	NAG	C3-C4-C5	3.41	116.42	110.23
3	BBB	405	NAG	C1-C2-N2	3.37	115.75	110.43
3	AAA	402	NAG	C2-N2-C7	3.35	127.38	122.90
3	AAA	403	NAG	O5-C1-C2	3.07	116.05	111.29
3	AAA	403	NAG	C4-C3-C2	2.97	115.37	111.02
3	AAA	403	NAG	C6-C5-C4	-2.69	106.41	113.02
3	AAA	403	NAG	O6-C6-C5	2.59	120.14	111.33
3	BBB	403	NAG	C3-C4-C5	-2.36	105.95	110.23
4	BBB	406	7TI	O1-S1-N1	-2.34	103.98	107.35
3	BBB	404	NAG	C8-C7-N2	-2.32	112.27	116.12
3	AAA	402	NAG	O5-C1-C2	-2.31	107.72	111.29
3	BBB	405	NAG	O7-C7-C8	-2.28	117.99	122.05
3	AAA	403	NAG	O3-C3-C4	-2.26	105.04	110.38
3	AAA	402	NAG	O4-C4-C5	2.25	114.86	109.32
4	AAA	404	7TI	O-S-N2	2.17	110.48	107.35
5	BBB	401	GOL	O2-C2-C3	2.17	118.16	109.18
3	BBB	403	NAG	O4-C4-C5	2.10	114.51	109.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	403	NAG	C4-C5-C6-O6
3	AAA	403	NAG	O5-C5-C6-O6
3	BBB	403	NAG	C8-C7-N2-C2
3	BBB	403	NAG	O7-C7-N2-C2
4	BBB	406	7TI	C5-C6-S1-O1
4	AAA	404	7TI	C5-C6-S1-O2
4	BBB	406	7TI	C7-C6-S1-O1

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Mol	Chain	Res	Type	Atoms
4	AAA	404	7TI	C7-C6-S1-O2
4	BBB	406	7TI	C1-C-S-N2

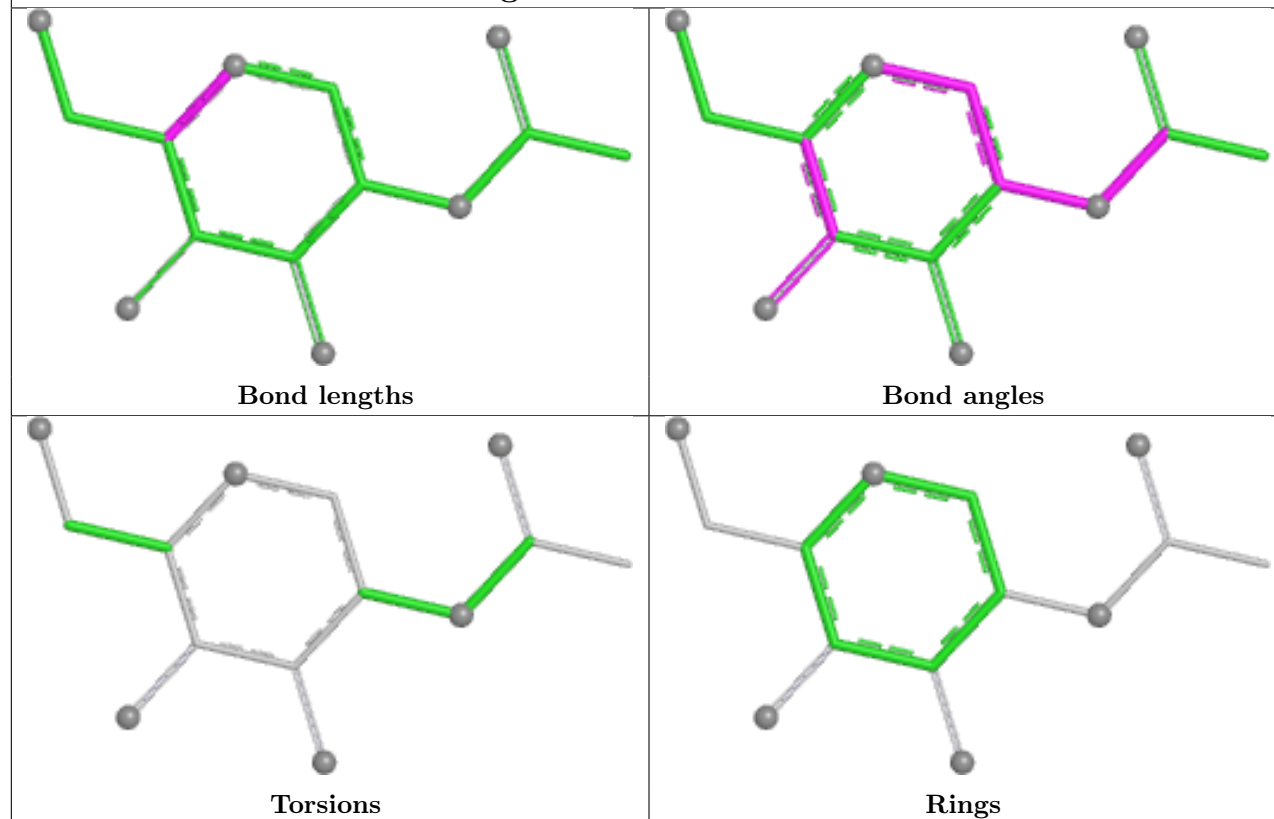
There are no ring outliers.

3 monomers are involved in 5 short contacts:

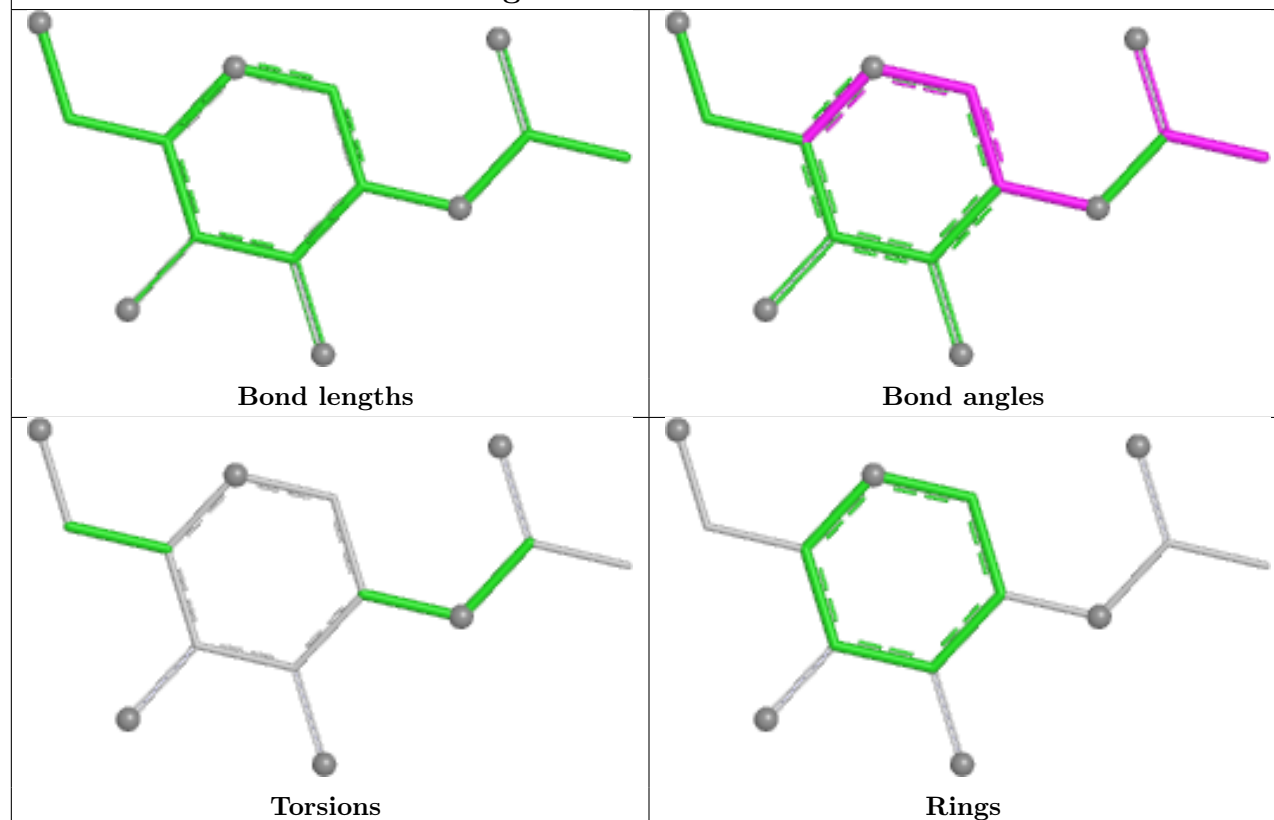
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	405	NAG	3	0
4	AAA	404	7TI	1	0
3	BBB	403	NAG	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

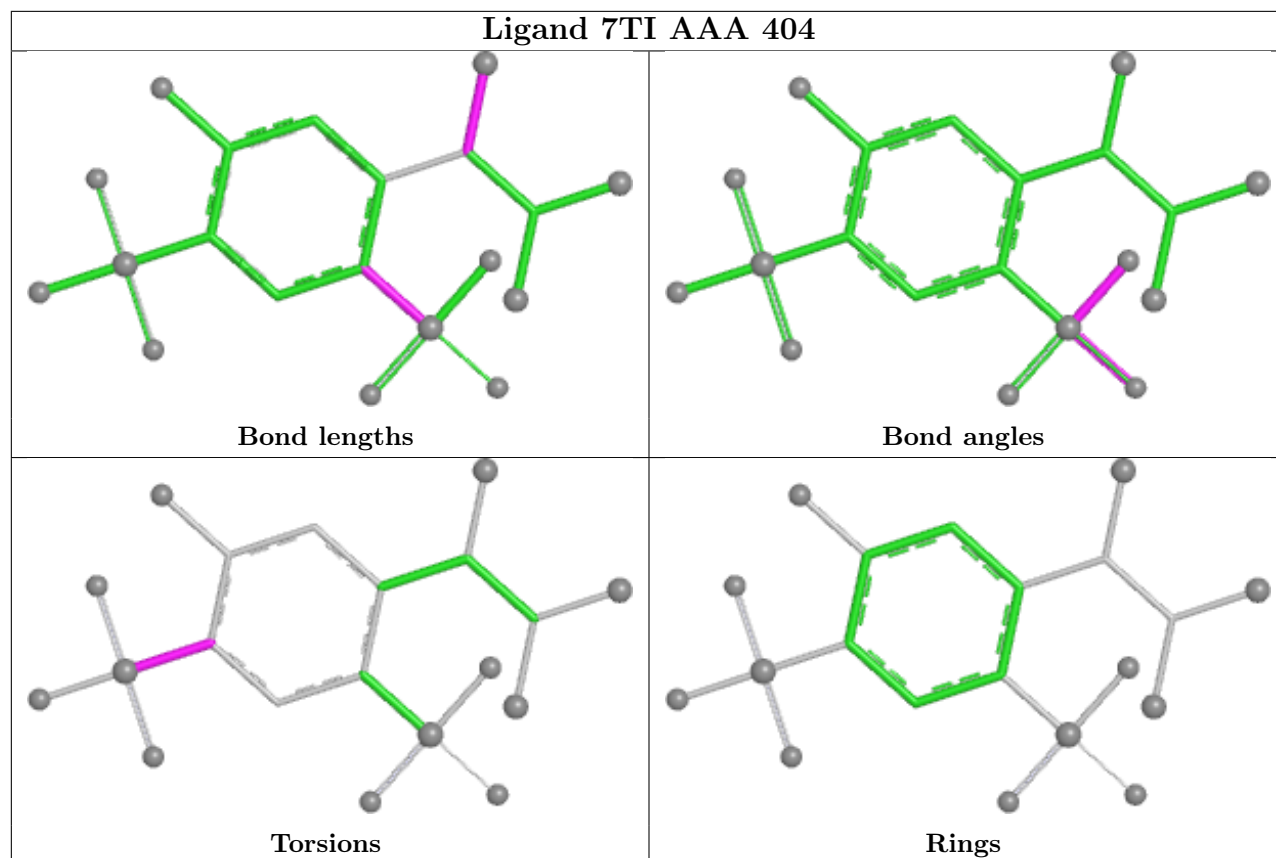
Ligand NAG AAA 402



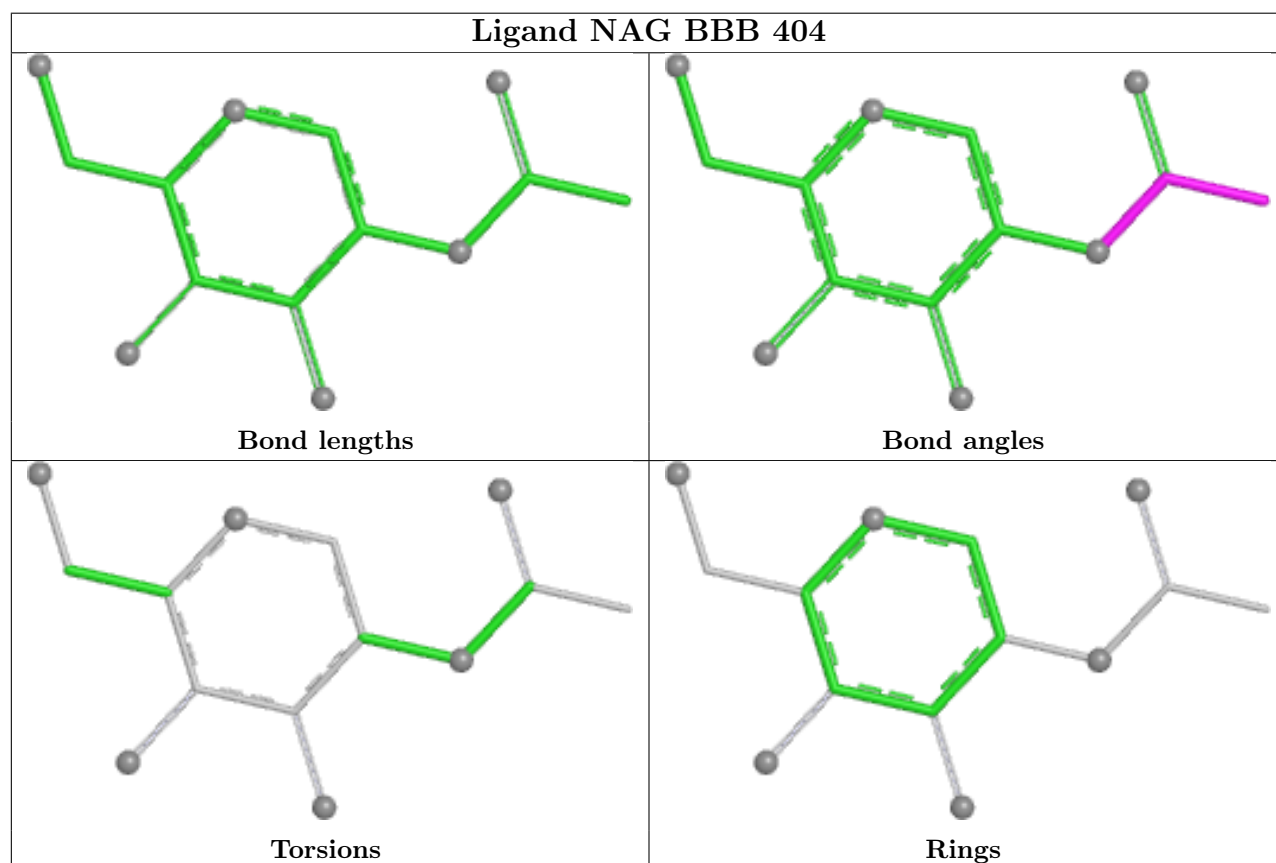
Ligand NAG BBB 405



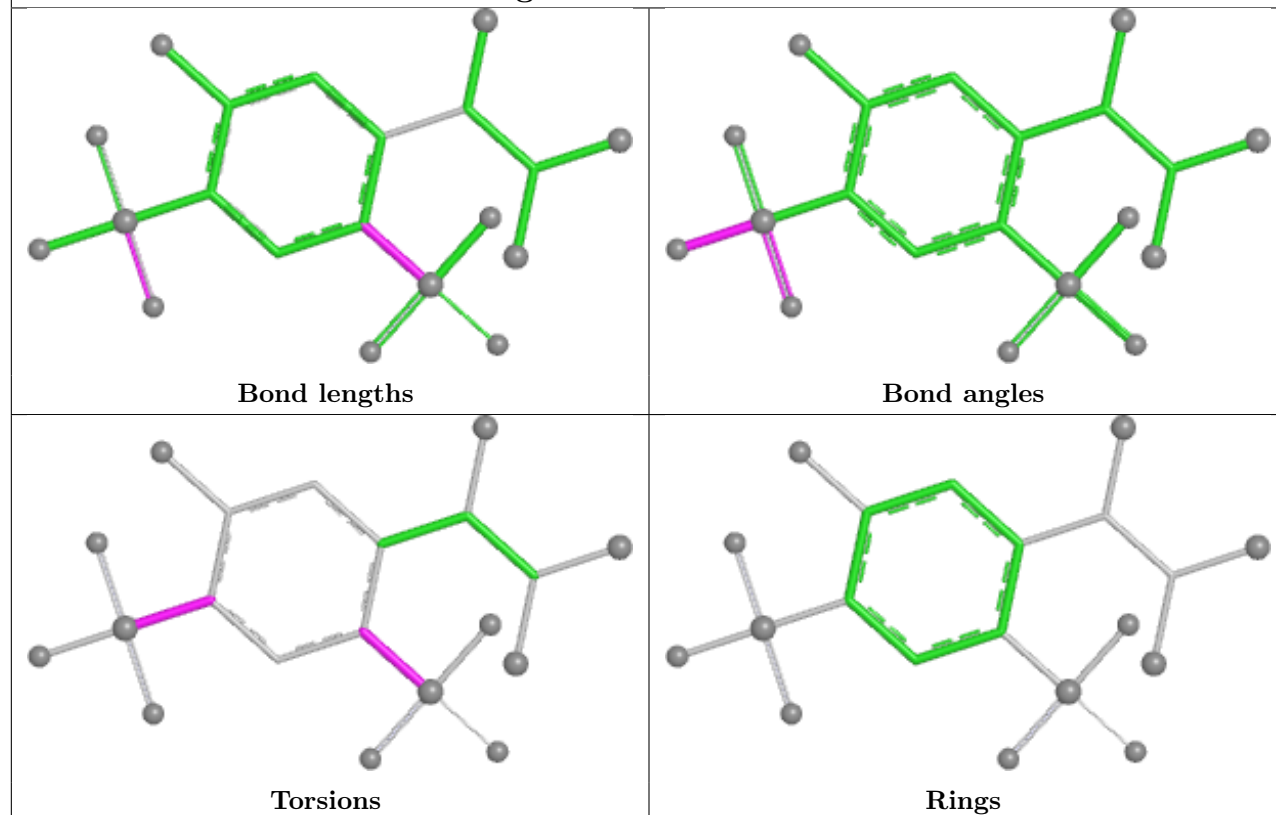
Ligand 7TI AAA 404



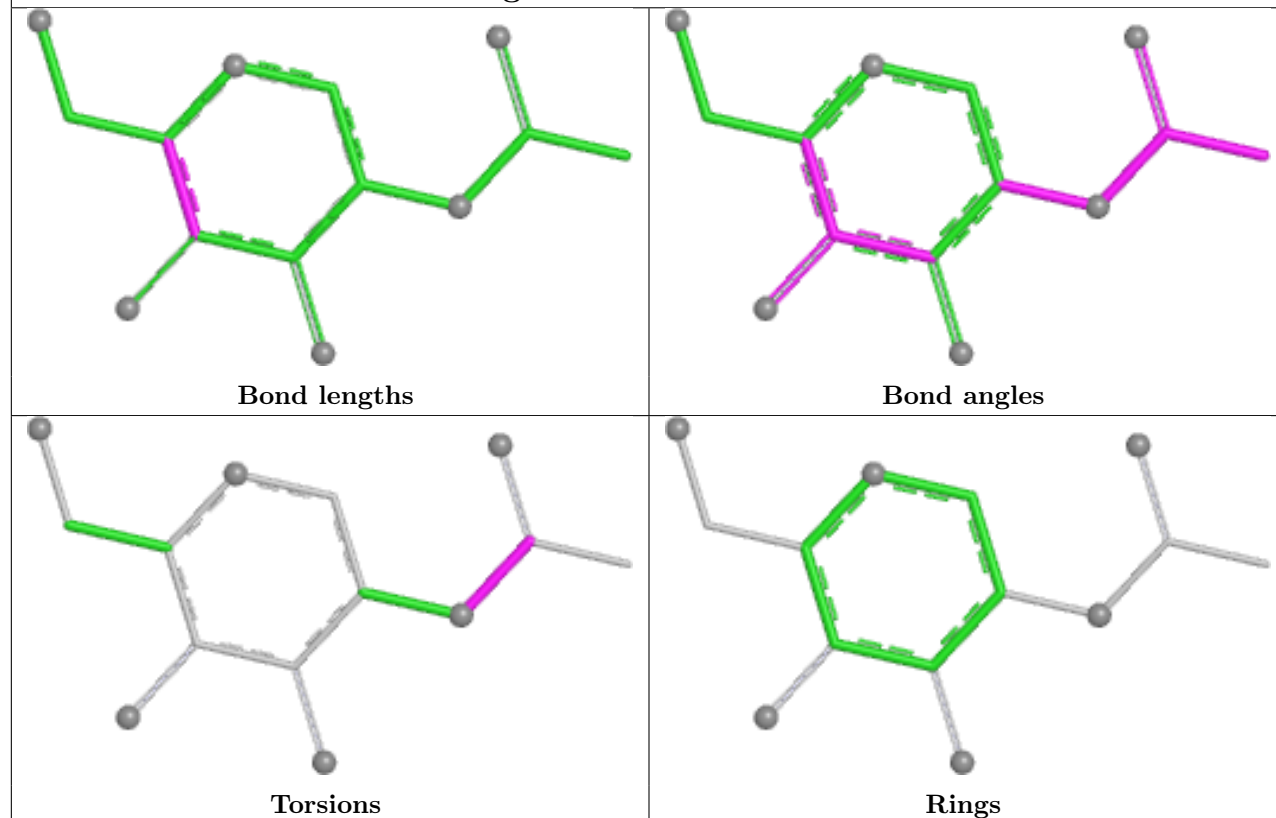
Ligand NAG BBB 404

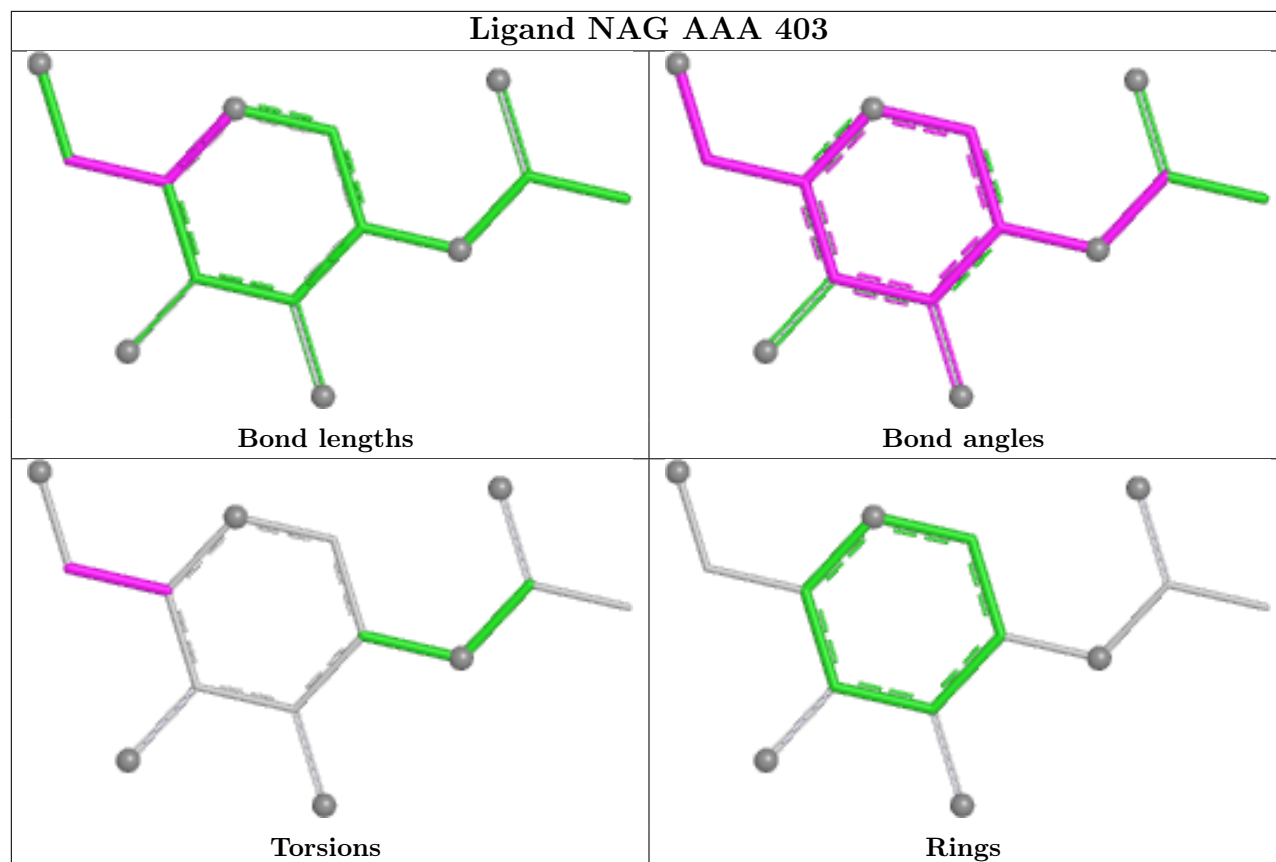


Ligand 7TI BBB 406



Ligand NAG BBB 403





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	AAA	277/280 (98%)	0.09	14 (5%)	33 42	13, 20, 38, 61	2 (0%)
1	BBB	277/280 (98%)	0.21	17 (6%)	27 35	13, 22, 40, 65	0
All	All	554/560 (98%)	0.15	31 (5%)	30 38	13, 21, 39, 65	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	300	GLY	5.6
1	AAA	31	LEU	4.6
1	AAA	30	ILE	4.3
1	AAA	285	ILE	4.2
1	AAA	300	GLY	4.1
1	AAA	24	GLU	3.8
1	AAA	299	ARG	3.6
1	BBB	31	LEU	3.5
1	BBB	24	GLU	3.4
1	BBB	38	HIS	3.1
1	BBB	59	ILE	3.0
1	BBB	199	VAL	2.9
1	AAA	59	ILE	2.9
1	BBB	30	ILE	2.8
1	AAA	64	LEU	2.6
1	AAA	268	LYS	2.6
1	AAA	80	THR	2.6
1	BBB	298	ALA	2.6
1	AAA	75	THR	2.5
1	BBB	80	THR	2.5
1	BBB	197	GLN	2.4
1	AAA	193	VAL	2.4
1	BBB	193	VAL	2.4
1	BBB	194	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	38	HIS	2.2
1	BBB	156	GLU	2.2
1	AAA	202	ASN	2.2
1	BBB	76	SER	2.1
1	BBB	297	THR	2.1
1	BBB	299	ARG	2.0
1	BBB	198	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

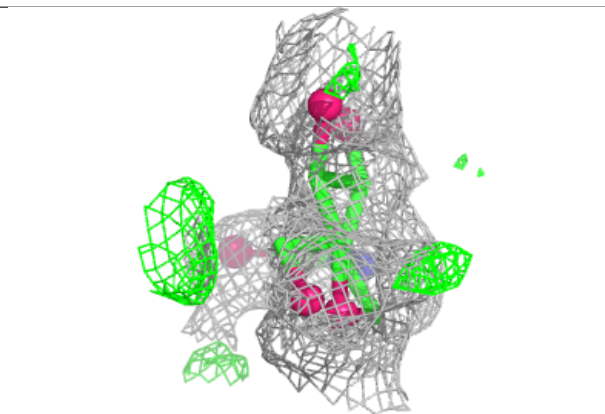
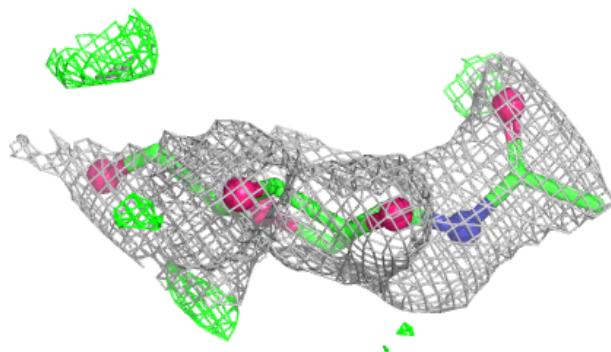
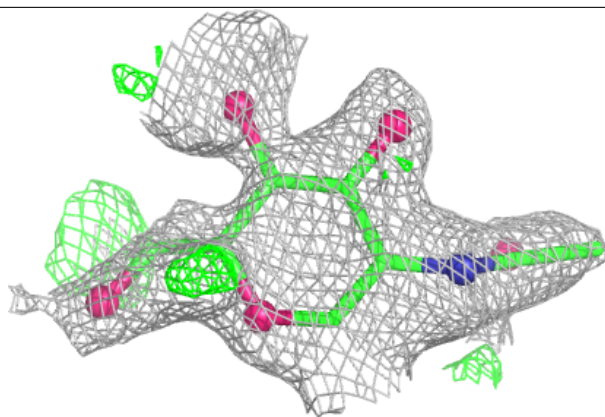
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	BBB	405	14/15	0.65	0.20	60,68,75,77	0
3	NAG	AAA	403	14/15	0.79	0.18	36,46,56,57	0
3	NAG	BBB	403	14/15	0.81	0.14	35,42,47,48	0
3	NAG	AAA	402	14/15	0.86	0.13	31,35,43,43	0
3	NAG	BBB	404	14/15	0.89	0.11	34,37,43,43	0
5	GOL	BBB	401	6/6	0.93	0.11	18,25,26,31	0
4	7TI	BBB	406	20/20	0.95	0.12	18,32,77,100	0
4	7TI	AAA	404	20/20	0.95	0.12	17,28,69,83	0
2	ZN	AAA	401	1/1	1.00	0.02	15,15,15,15	0
2	ZN	BBB	402	1/1	1.00	0.02	17,17,17,17	0

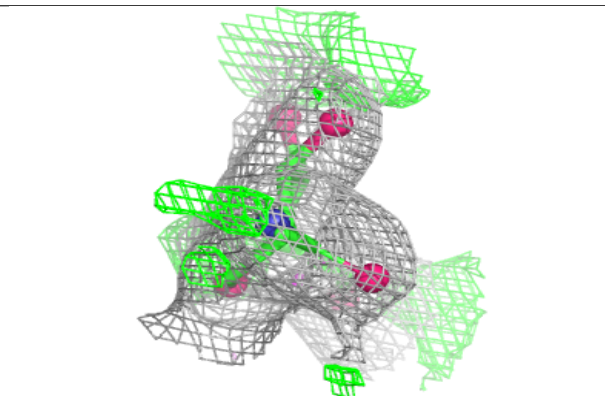
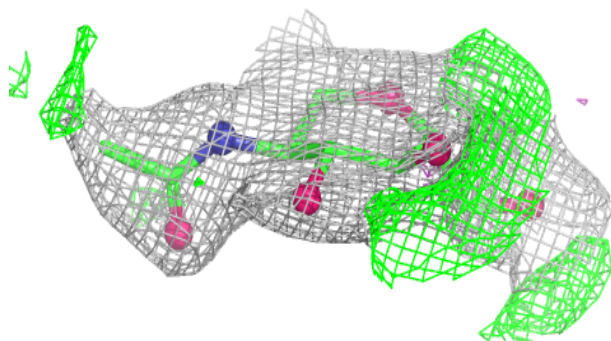
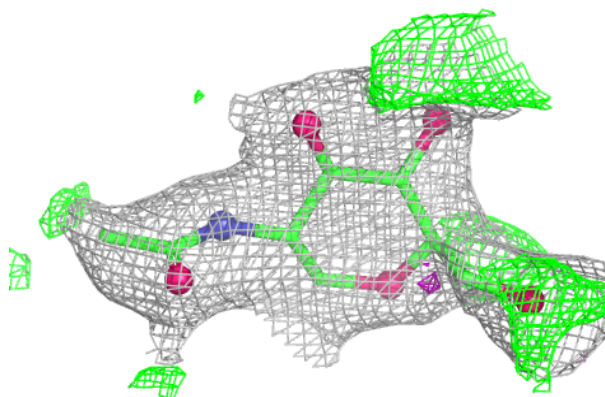
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG BBB 405:

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

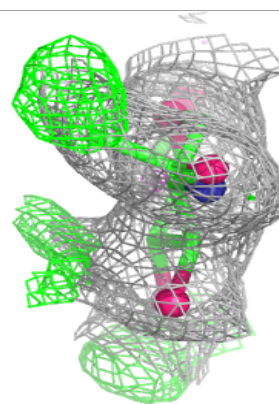
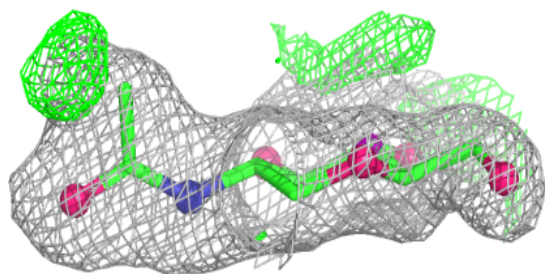
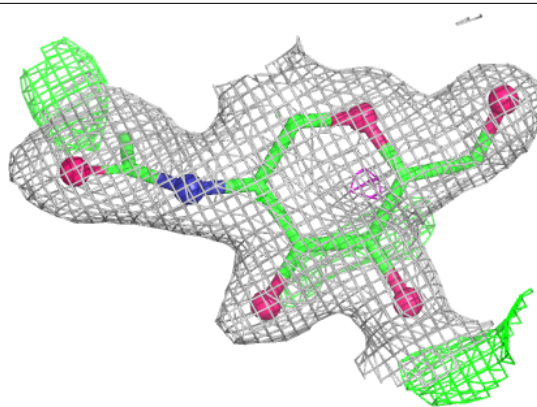
**Electron density around NAG AAA 403:**

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



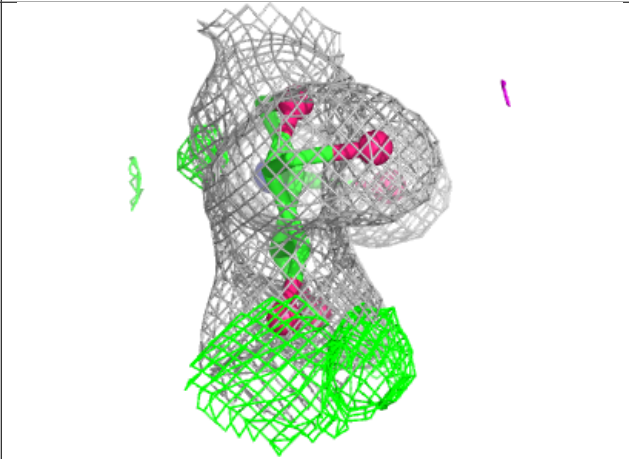
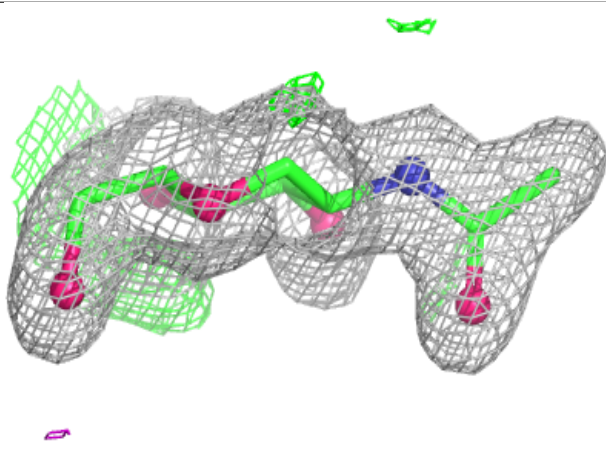
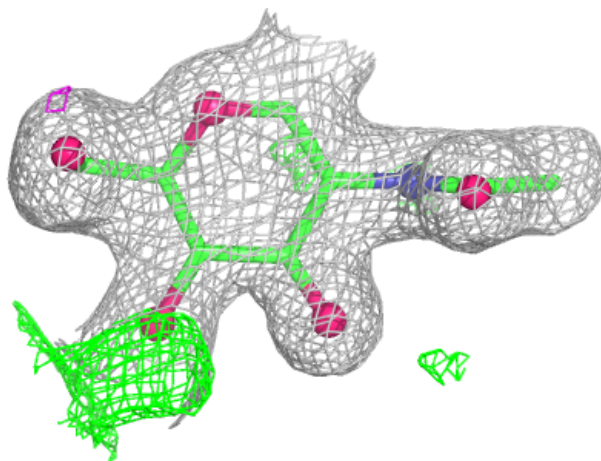
Electron density around NAG BBB 403:

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



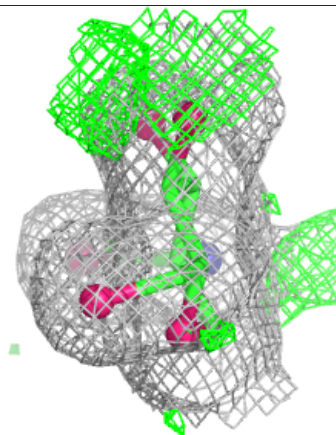
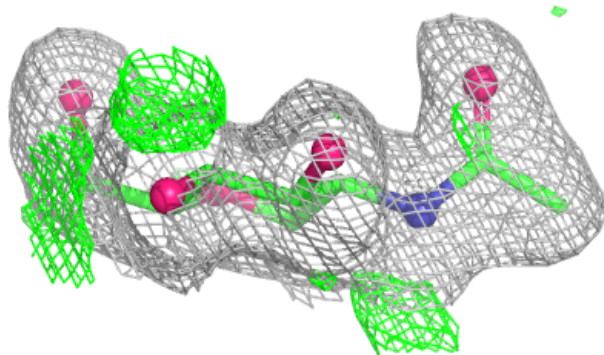
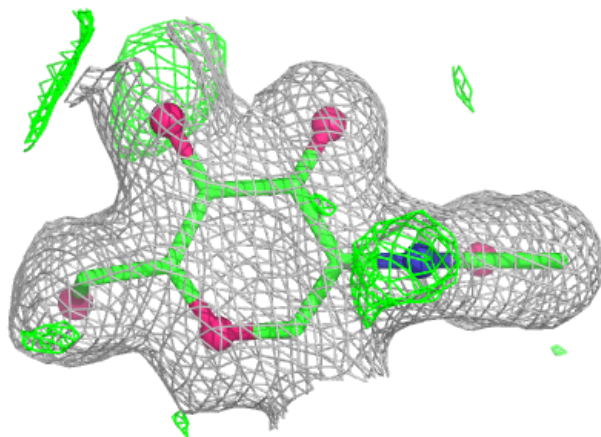
Electron density around NAG AAA 402:

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



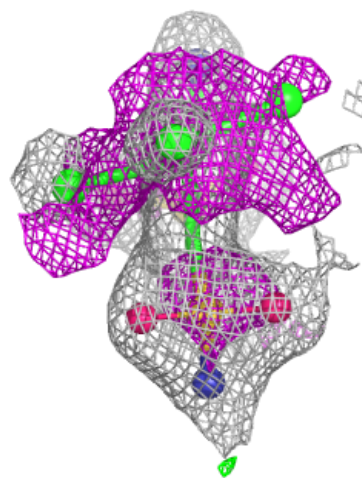
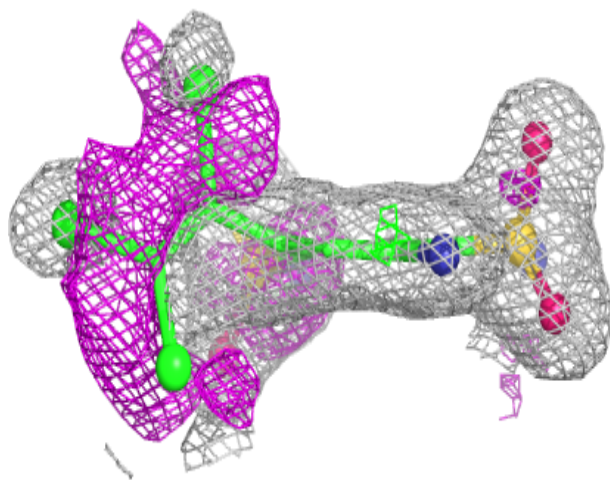
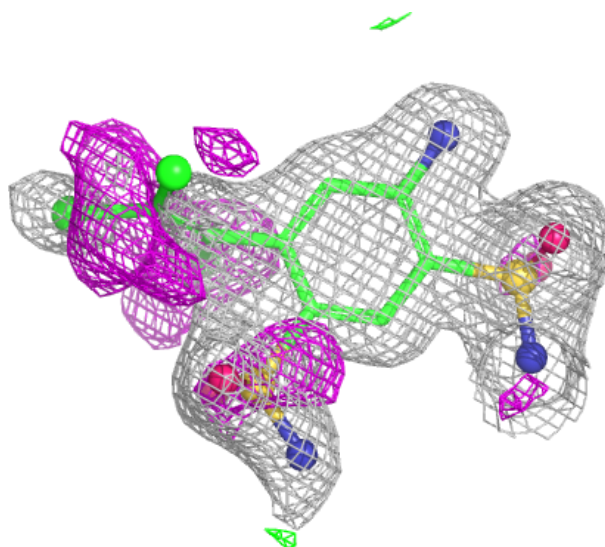
Electron density around NAG BBB 404:

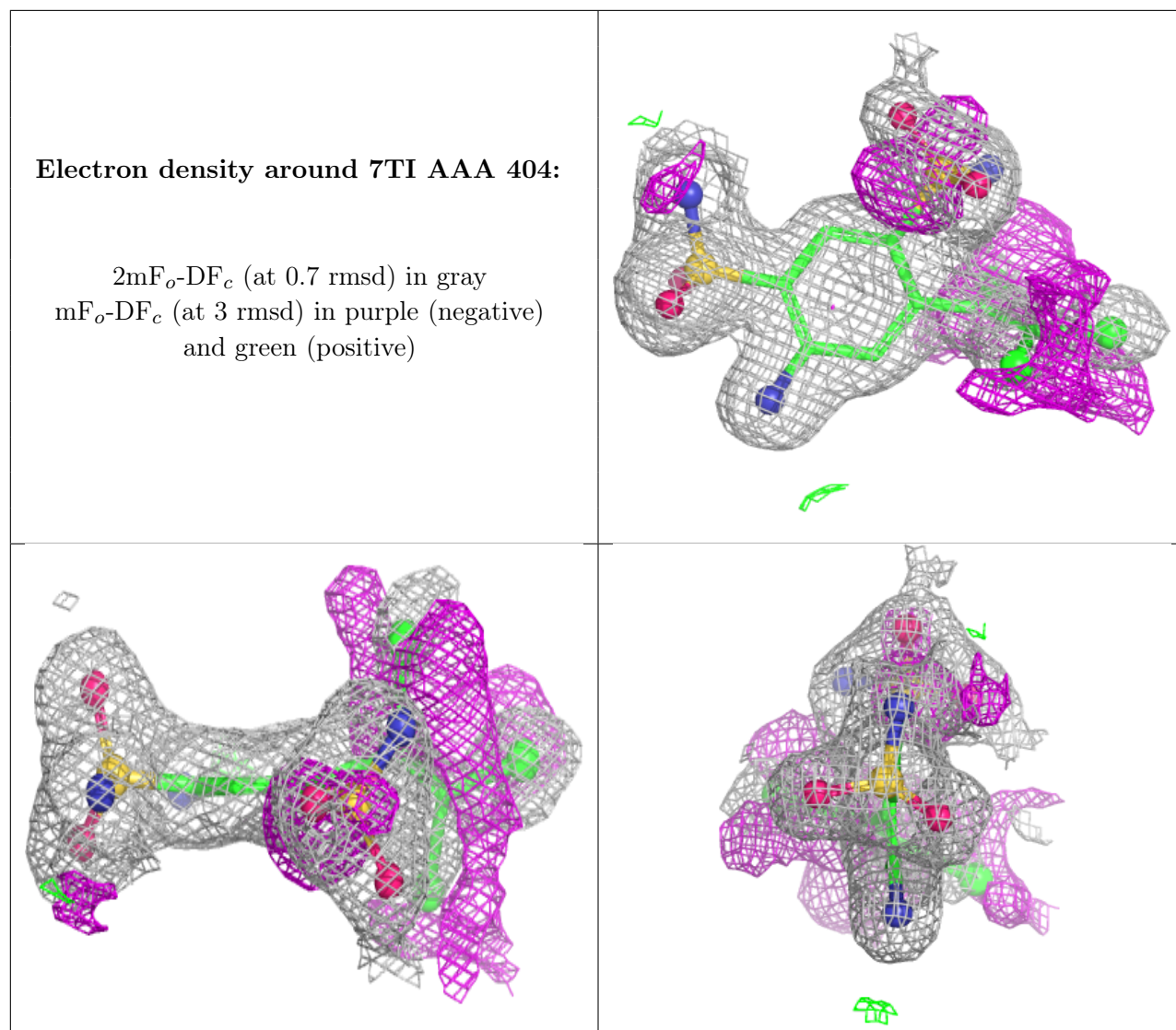
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7TI 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.