Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:01 am GMT

PDB ID	:	7OA1
Title	:	Crystal structure of alfa carbonic anhydrase from Schistosoma mansoni with 4-(2-(3-(4-iodophenyl)ureido)ethyl)benzenesulfonamide
Authors	:	Angelil, A.; Ferraroni, M.
Deposited on	:	2021-04-18
Resolution	:	2.00 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:

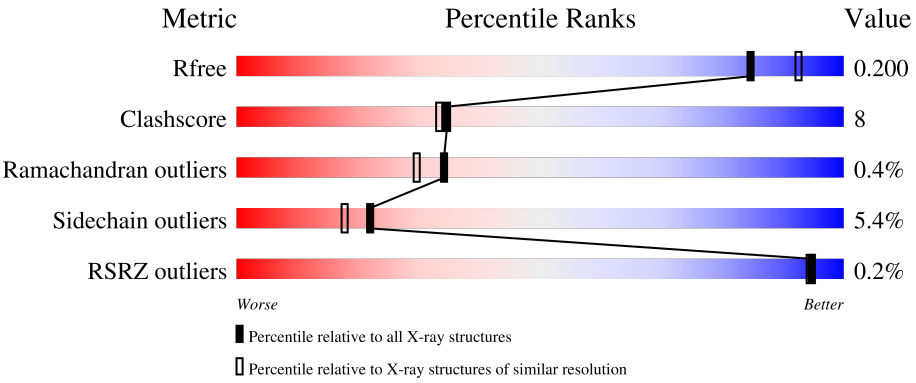
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	312	76% 12% • 11%
1	BBB	312	75% 12% • 11%
2	GGG	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4961 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	3	0
			2248	1434	382	425	7			
1	BBB	277	Total	C	N	O	S	0	3	0
			2249	1435	384	423	7			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	12	ASP	-	expression tag	UNP A0A3Q0KSG2
AAA	13	ALA	-	expression tag	UNP A0A3Q0KSG2
AAA	14	ALA	-	expression tag	UNP A0A3Q0KSG2
AAA	15	GLN	-	expression tag	UNP A0A3Q0KSG2
AAA	16	PRO	-	expression tag	UNP A0A3Q0KSG2
AAA	17	ALA	-	expression tag	UNP A0A3Q0KSG2
AAA	18	ARG	-	expression tag	UNP A0A3Q0KSG2
AAA	19	ARG	-	expression tag	UNP A0A3Q0KSG2
AAA	20	ALA	-	expression tag	UNP A0A3Q0KSG2
AAA	299	ARG	-	expression tag	UNP A0A3Q0KSG2
AAA	300	GLY	-	expression tag	UNP A0A3Q0KSG2
AAA	301	GLY	-	expression tag	UNP A0A3Q0KSG2
AAA	302	PRO	-	expression tag	UNP A0A3Q0KSG2
AAA	303	GLU	-	expression tag	UNP A0A3Q0KSG2
AAA	304	GLN	-	expression tag	UNP A0A3Q0KSG2
AAA	305	LYS	-	expression tag	UNP A0A3Q0KSG2
AAA	306	LEU	-	expression tag	UNP A0A3Q0KSG2
AAA	307	ILE	-	expression tag	UNP A0A3Q0KSG2
AAA	308	SER	-	expression tag	UNP A0A3Q0KSG2
AAA	309	GLU	-	expression tag	UNP A0A3Q0KSG2
AAA	310	GLU	-	expression tag	UNP A0A3Q0KSG2
AAA	311	ASP	-	expression tag	UNP A0A3Q0KSG2
AAA	312	LEU	-	expression tag	UNP A0A3Q0KSG2
AAA	313	ASN	-	expression tag	UNP A0A3Q0KSG2
AAA	314	SER	-	expression tag	UNP A0A3Q0KSG2

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	315	ALA	-	expression tag	UNP A0A3Q0KSG2
AAA	316	VAL	-	expression tag	UNP A0A3Q0KSG2
AAA	317	ASP	-	expression tag	UNP A0A3Q0KSG2
AAA	318	HIS	-	expression tag	UNP A0A3Q0KSG2
AAA	319	HIS	-	expression tag	UNP A0A3Q0KSG2
AAA	320	HIS	-	expression tag	UNP A0A3Q0KSG2
AAA	321	HIS	-	expression tag	UNP A0A3Q0KSG2
AAA	322	HIS	-	expression tag	UNP A0A3Q0KSG2
AAA	323	HIS	-	expression tag	UNP A0A3Q0KSG2
BBB	12	ASP	-	expression tag	UNP A0A3Q0KSG2
BBB	13	ALA	-	expression tag	UNP A0A3Q0KSG2
BBB	14	ALA	-	expression tag	UNP A0A3Q0KSG2
BBB	15	GLN	-	expression tag	UNP A0A3Q0KSG2
BBB	16	PRO	-	expression tag	UNP A0A3Q0KSG2
BBB	17	ALA	-	expression tag	UNP A0A3Q0KSG2
BBB	18	ARG	-	expression tag	UNP A0A3Q0KSG2
BBB	19	ARG	-	expression tag	UNP A0A3Q0KSG2
BBB	20	ALA	-	expression tag	UNP A0A3Q0KSG2
BBB	299	ARG	-	expression tag	UNP A0A3Q0KSG2
BBB	300	GLY	-	expression tag	UNP A0A3Q0KSG2
BBB	301	GLY	-	expression tag	UNP A0A3Q0KSG2
BBB	302	PRO	-	expression tag	UNP A0A3Q0KSG2
BBB	303	GLU	-	expression tag	UNP A0A3Q0KSG2
BBB	304	GLN	-	expression tag	UNP A0A3Q0KSG2
BBB	305	LYS	-	expression tag	UNP A0A3Q0KSG2
BBB	306	LEU	-	expression tag	UNP A0A3Q0KSG2
BBB	307	ILE	-	expression tag	UNP A0A3Q0KSG2
BBB	308	SER	-	expression tag	UNP A0A3Q0KSG2
BBB	309	GLU	-	expression tag	UNP A0A3Q0KSG2
BBB	310	GLU	-	expression tag	UNP A0A3Q0KSG2
BBB	311	ASP	-	expression tag	UNP A0A3Q0KSG2
BBB	312	LEU	-	expression tag	UNP A0A3Q0KSG2
BBB	313	ASN	-	expression tag	UNP A0A3Q0KSG2
BBB	314	SER	-	expression tag	UNP A0A3Q0KSG2
BBB	315	ALA	-	expression tag	UNP A0A3Q0KSG2
BBB	316	VAL	-	expression tag	UNP A0A3Q0KSG2
BBB	317	ASP	-	expression tag	UNP A0A3Q0KSG2
BBB	318	HIS	-	expression tag	UNP A0A3Q0KSG2
BBB	319	HIS	-	expression tag	UNP A0A3Q0KSG2
BBB	320	HIS	-	expression tag	UNP A0A3Q0KSG2
BBB	321	HIS	-	expression tag	UNP A0A3Q0KSG2
BBB	322	HIS	-	expression tag	UNP A0A3Q0KSG2

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	323	HIS	-	expression tag	UNP A0A3Q0KSG2

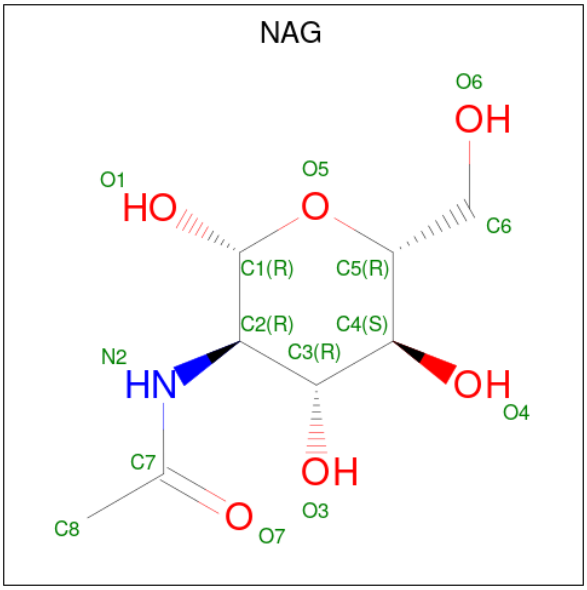
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	GGG	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

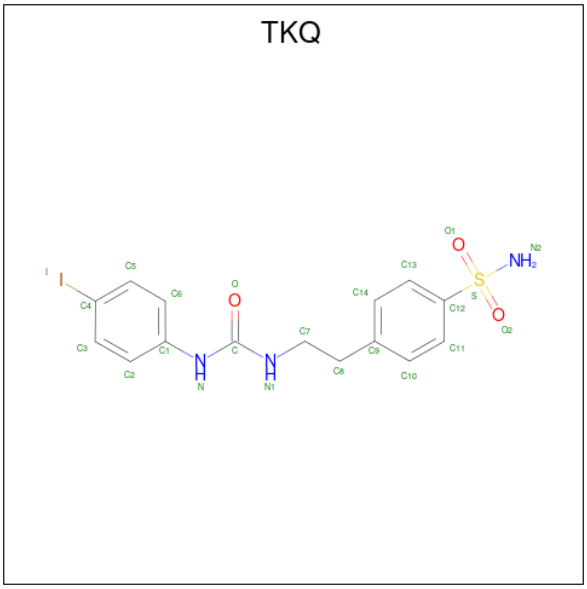
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Zn 1 1	0	0
3	BBB	1	Total Zn 1 1	0	0

- Molecule 4 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).



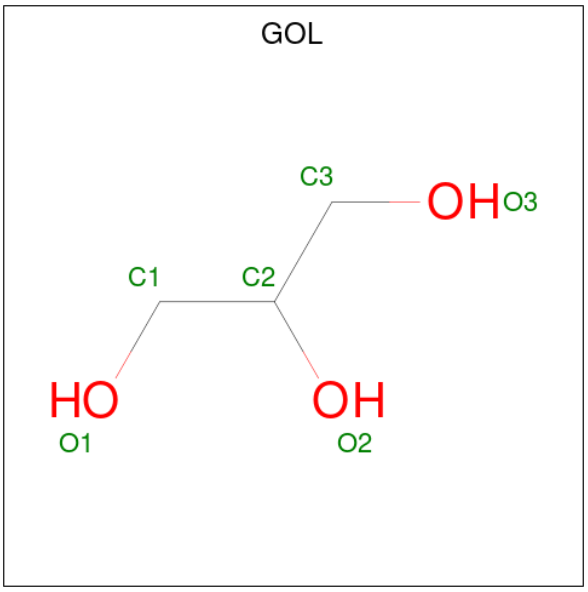
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C N O 14 8 1 5	0	0
4	AAA	1	Total C N O 14 8 1 5	0	0
4	AAA	1	Total C N O 14 8 1 5	0	0
4	BBB	1	Total C N O 14 8 1 5	0	0
4	BBB	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 1-(4-iodophenyl)-3-[2-(4-sulfamoylphenyl)ethyl]urea (three-letter code: TKQ) (formula: $C_{15}H_{16}IN_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C I N O S 23 15 1 3 3 1	0	0
5	BBB	1	Total C I N O S 23 15 1 3 3 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

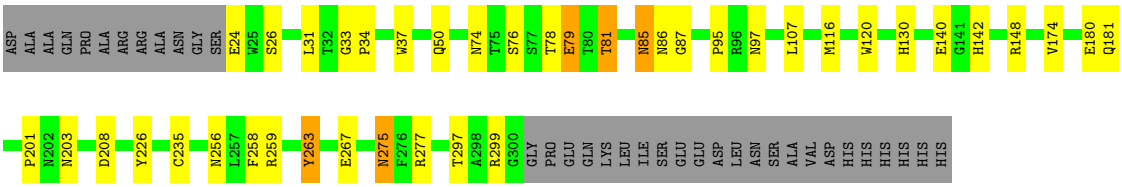
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	162	Total O 162 162	0	0
7	BBB	150	Total O 150 150	0	0

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.

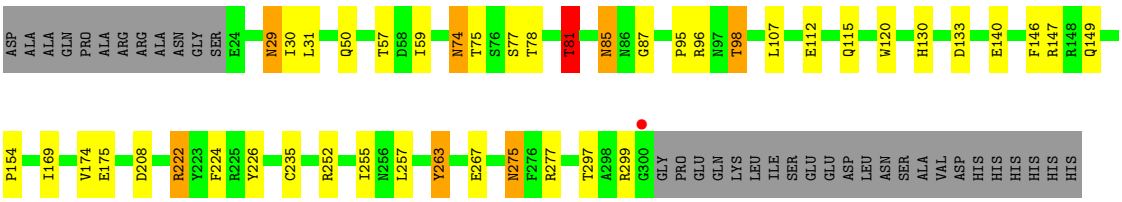
• Molecule 1: Carbonic anhydrase

Chain AAA:



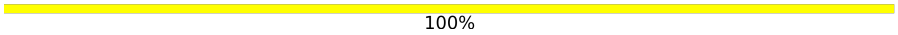
• Molecule 1: Carbonic anhydrase

Chain BBB:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GGG:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.50Å 103.50Å 133.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.63 – 2.00 89.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.63-2.00) 100.0 (89.63-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.164 , 0.194 0.174 , 0.200	Depositor DCC
R_{free} test set	2818 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.5	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	0.96	EDS
Total number of atoms	4961	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.76	1/2317 (0.0%)	0.91	0/3152
1	BBB	0.76	0/2319	0.96	4/3156 (0.1%)
All	All	0.76	1/4636 (0.0%)	0.94	4/6308 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	180	GLU	CD-OE1	6.01	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	222	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	BBB	75	THR	CA-CB-OG1	-6.68	94.97	109.00
1	BBB	222	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	BBB	81	THR	CA-CB-OG1	5.08	119.67	109.00

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	2248	0	2174	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	2249	0	2171	38	0
2	GGG	28	0	25	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	42	0	39	7	0
4	BBB	28	0	26	0	0
5	AAA	23	0	0	0	0
5	BBB	23	0	0	1	0
6	BBB	6	0	8	0	0
7	AAA	162	0	0	3	0
7	BBB	150	0	0	4	0
All	All	4961	0	4443	75	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 8.

All (75) 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:AAA:97:ASN:HB3	4:AAA:403:NAG:H83	1.54	0.88
5:BBB:405:TKQ:I	7:BBB:628:HOH:O	2.66	0.84
1:BBB:59:ILE:CG1	7:BBB:648:HOH:O	2.29	0.79
1:AAA:50:GLN:HE22	1:AAA:235:CYS:HB3	1.50	0.76
1:AAA:130:HIS:HE1	1:AAA:226:TYR:OH	1.70	0.75
1:BBB:130:HIS:HE1	1:BBB:226:TYR:OH	1.75	0.69
1:BBB:120:TRP:H	1:BBB:275:ASN:HD21	1.41	0.69
1:BBB:50:GLN:HE22	1:BBB:235:CYS:HB3	1.59	0.67
1:AAA:120:TRP:H	1:AAA:275:ASN:HD21	1.44	0.66
1:AAA:148:ARG:HH12	4:AAA:403:NAG:H81	1.61	0.66
1:BBB:95:PRO:HG2	1:BBB:98:THR:HG21	1.77	0.65
1:BBB:85:ASN:C	1:BBB:85:ASN:HD22	2.00	0.64
1:AAA:85:ASN:HD22	1:AAA:85:ASN:C	1.99	0.63
1:AAA:275:ASN:HD22	1:AAA:275:ASN:H	1.45	0.63
7:AAA:631:HOH:O	1:BBB:57:THR:HG21	1.98	0.63
1:BBB:29:ASN:HD22	1:BBB:31:LEU:H	1.43	0.63
1:BBB:96:ARG:NH1	1:BBB:112:GLU:OE2	2.32	0.62
1:AAA:120:TRP:H	1:AAA:275:ASN:ND2	1.98	0.62
1:BBB:275:ASN:HD22	1:BBB:275:ASN:H	1.48	0.61
1:AAA:50:GLN:NE2	1:AAA:277:ARG:HH12	2.00	0.60
1:BBB:147:ARG:HE	1:BBB:149:GLN:HE21	1.48	0.60
1:AAA:174:VAL:HG12	1:BBB:174:VAL:HG12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:50:GLN:HE21	1:BBB:277:ARG:HH22	1.51	0.59
1:BBB:81:THR:CG2	7:BBB:561:HOH:O	2.51	0.59
1:AAA:130:HIS:HD2	1:AAA:140:GLU:OE2	1.86	0.58
1:AAA:85:ASN:ND2	1:AAA:87:GLY:H	2.02	0.58
1:BBB:120:TRP:H	1:BBB:275:ASN:ND2	2.02	0.57
1:AAA:50:GLN:HE21	1:AAA:277:ARG:HH22	1.52	0.57
1:BBB:57:THR:HG23	1:BBB:133:ASP:OD2	2.05	0.57
1:AAA:81:THR:HG22	7:AAA:526:HOH:O	2.04	0.57
1:BBB:81:THR:HG21	1:BBB:208:ASP:OD1	2.04	0.57
1:AAA:85:ASN:HD22	1:AAA:87:GLY:H	1.54	0.56
1:AAA:81:THR:HG21	1:AAA:208:ASP:OD1	2.06	0.55
1:BBB:81:THR:HG23	7:BBB:561:HOH:O	2.05	0.55
1:BBB:175:GLU:OE2	1:BBB:252:ARG:NH1	2.41	0.54
1:BBB:85:ASN:ND2	1:BBB:87:GLY:H	2.07	0.53
1:BBB:85:ASN:HD22	1:BBB:87:GLY:H	1.56	0.53
1:AAA:275:ASN:HD22	1:AAA:275:ASN:N	2.07	0.53
1:BBB:130:HIS:HD2	1:BBB:140:GLU:OE2	1.92	0.53
1:BBB:147:ARG:HE	1:BBB:149:GLN:NE2	2.07	0.52
1:BBB:96:ARG:O	1:BBB:98:THR:HG22	2.10	0.51
1:BBB:29:ASN:ND2	1:BBB:31:LEU:H	2.08	0.51
1:BBB:77:SER:CB	1:BBB:98:THR:HB	2.41	0.51
1:AAA:79:GLU:HB3	1:AAA:95:PRO:HB3	1.93	0.50
4:AAA:402:NAG:HO4	4:AAA:404:NAG:C1	2.25	0.50
1:AAA:24:GLU:HA	1:AAA:24:GLU:OE1	2.12	0.49
1:BBB:50:GLN:NE2	1:BBB:277:ARG:HH12	2.11	0.48
1:BBB:95:PRO:O	1:BBB:98:THR:HG23	2.14	0.48
1:AAA:275:ASN:H	1:AAA:275:ASN:ND2	2.09	0.48
1:BBB:29:ASN:HD22	1:BBB:29:ASN:C	2.17	0.48
1:BBB:96:ARG:O	1:BBB:98:THR:CG2	2.62	0.48
4:AAA:402:NAG:O4	4:AAA:404:NAG:C1	2.63	0.47
1:BBB:146:PHE:CE1	1:BBB:154:PRO:HG3	2.50	0.47
1:AAA:148:ARG:NH1	4:AAA:403:NAG:H81	2.30	0.45
1:BBB:95:PRO:HG2	1:BBB:98:THR:CG2	2.45	0.45
1:AAA:116:MET:HA	1:AAA:142:HIS:O	2.18	0.44
1:BBB:30:ILE:HD12	1:BBB:31:LEU:N	2.32	0.44
1:AAA:120:TRP:CE2	1:AAA:258:PHE:HB3	2.52	0.44
1:AAA:256:ASN:HD22	1:AAA:259:ARG:HD2	1.83	0.44
1:AAA:263:TYR:CD1	1:AAA:267:GLU:HG3	2.53	0.44
1:AAA:85:ASN:C	1:AAA:85:ASN:ND2	2.70	0.43
1:AAA:34:PRO:HA	1:AAA:37:TRP:CE2	2.54	0.43
1:BBB:85:ASN:C	1:BBB:85:ASN:ND2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:252:ARG:O	1:BBB:255:ILE:HG22	2.19	0.42
1:AAA:50:GLN:HE21	1:AAA:277:ARG:HH12	1.66	0.42
1:BBB:74:ASN:C	1:BBB:74:ASN:HD22	2.23	0.42
1:AAA:79:GLU:HB3	1:AAA:95:PRO:CB	2.49	0.41
1:AAA:85:ASN:HD22	1:AAA:86:ASN:N	2.18	0.41
1:BBB:57:THR:HG22	1:BBB:224:PHE:HZ	1.84	0.41
1:AAA:97:ASN:CB	4:AAA:403:NAG:H83	2.39	0.41
1:AAA:26:SER:O	1:AAA:33:GLY:HA2	2.20	0.41
1:BBB:263:TYR:CD1	1:BBB:267:GLU:HG3	2.56	0.41
1:AAA:97:ASN:HB3	4:AAA:403:NAG:C8	2.38	0.41
1:AAA:181:GLN:NE2	1:AAA:181:GLN:HA	2.36	0.40
1:AAA:81:THR:CG2	7:AAA:526:HOH:O	2.67	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	AAA	278/312 (89%)	271 (98%)	6 (2%)	1 (0%)	34	30
1	BBB	278/312 (89%)	270 (97%)	7 (2%)	1 (0%)	34	30
All	All	556/624 (89%)	541 (97%)	13 (2%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	299	ARG
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	253/279 (91%)	239 (94%)	14 (6%)	21	17
1	BBB	251/279 (90%)	237 (94%)	14 (6%)	21	17
All	All	504/558 (90%)	476 (94%)	28 (6%)	22	17

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	31	LEU
1	AAA	74	ASN
1	AAA	76[A]	SER
1	AAA	76[B]	SER
1	AAA	78	THR
1	AAA	79	GLU
1	AAA	81	THR
1	AAA	85	ASN
1	AAA	107	LEU
1	AAA	201	PRO
1	AAA	203	ASN
1	AAA	263	TYR
1	AAA	275	ASN
1	AAA	297	THR
1	BBB	29	ASN
1	BBB	74	ASN
1	BBB	78	THR
1	BBB	81	THR
1	BBB	85	ASN
1	BBB	98	THR
1	BBB	107	LEU
1	BBB	115	GLN
1	BBB	169	ILE
1	BBB	222	ARG
1	BBB	257	LEU
1	BBB	263	TYR
1	BBB	275	ASN

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Mol	Chain	Res	Type
1	BBB	297	THR

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

2 monosaccharides 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	GGG	1	2	14,14,15	0.72	0	17,19,21	1.22	2 (11%)
2	NAG	GGG	2	2	14,14,15	0.60	0	17,19,21	1.60	2 (11%)

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	GGG	1	2	-	0/6/23/26	0/1/1/1
2	NAG	GGG	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	GGG	2	NAG	C1-O5-C5	5.10	119.11	112.19
2	GGG	1	NAG	O3-C3-C2	-2.59	104.11	109.47
2	GGG	1	NAG	O7-C7-C8	-2.16	118.04	122.06
2	GGG	2	NAG	O3-C3-C4	-2.05	105.62	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

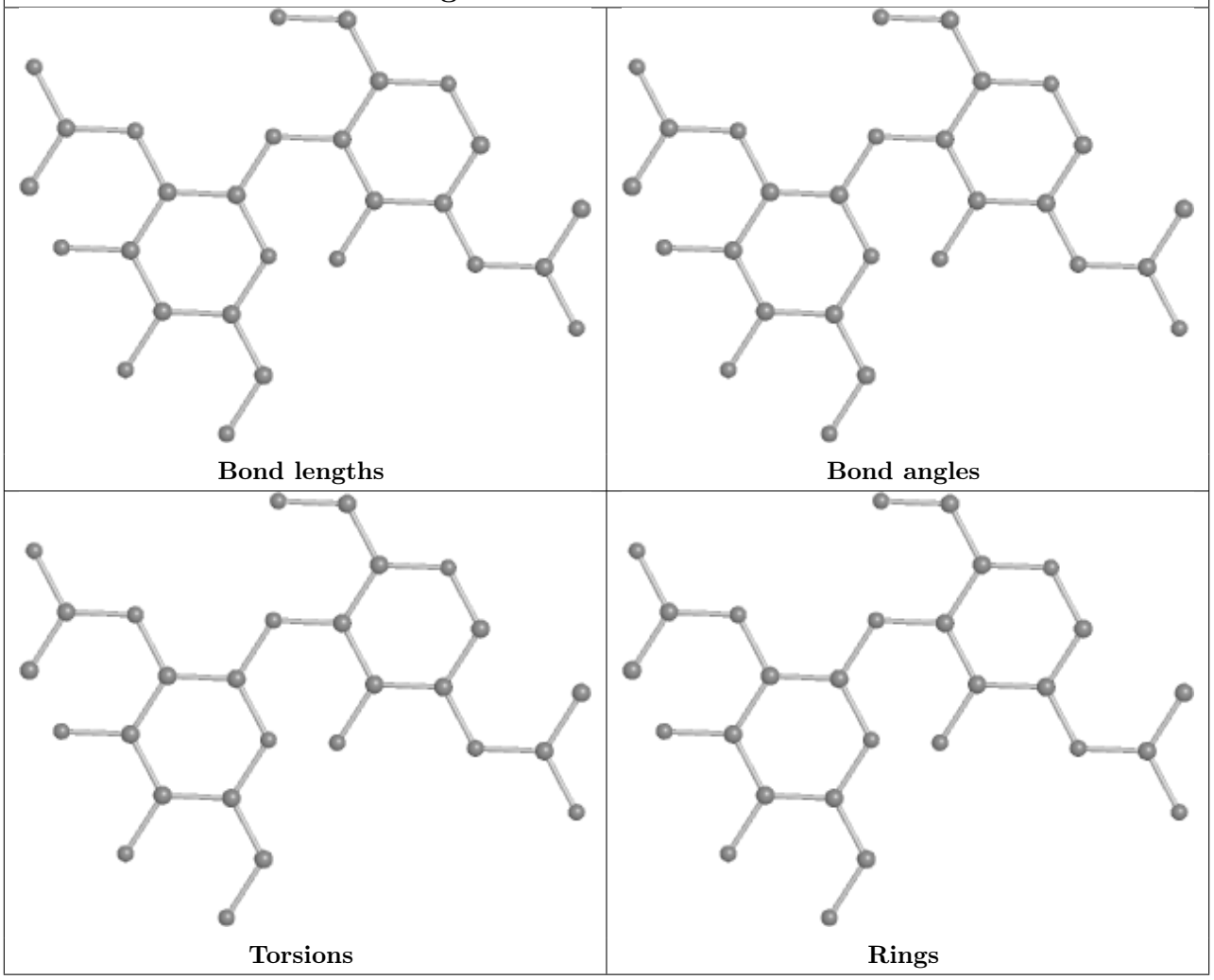
Mol	Chain	Res	Type	Atoms
2	GGG	2	NAG	C4-C5-C6-O6
2	GGG	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain GGG



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	$\#\|Z\| > 2$
6	GOL	BBB	404	-	5,5,5	0.35	0	5,5,5	1.19	0
4	NAG	AAA	404	-	14,14,15	0.49	0	17,19,21	1.55	3 (17%)
4	NAG	BBB	402	-	14,14,15	1.46	3 (21%)	17,19,21	2.99	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	AAA	402	-	14,14,15	0.61	0	17,19,21	1.94	3 (17%)
5	TKQ	AAA	405	3	24,24,24	0.45	0	33,33,33	0.63	1 (3%)
4	NAG	AAA	403	-	14,14,15	0.97	1 (7%)	17,19,21	1.65	4 (23%)
4	NAG	BBB	403	-	14,14,15	1.27	2 (14%)	17,19,21	2.56	5 (29%)
5	TKQ	BBB	405	3	24,24,24	0.45	0	33,33,33	1.13	5 (15%)

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
6	GOL	BBB	404	-	-	0/4/4/4	-
4	NAG	AAA	404	-	-	4/6/23/26	0/1/1/1
4	NAG	BBB	402	-	-	3/6/23/26	0/1/1/1
4	NAG	AAA	402	-	-	0/6/23/26	0/1/1/1
5	TKQ	AAA	405	3	-	9/16/16/16	0/2/2/2
4	NAG	AAA	403	-	-	4/6/23/26	0/1/1/1
4	NAG	BBB	403	-	-	2/6/23/26	0/1/1/1
5	TKQ	BBB	405	3	-	7/16/16/16	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	402	NAG	O5-C5	3.04	1.49	1.43
4	BBB	403	NAG	O5-C1	2.45	1.47	1.43
4	BBB	403	NAG	C1-C2	2.28	1.55	1.52
4	BBB	402	NAG	O5-C1	2.25	1.47	1.43
4	AAA	403	NAG	O5-C5	2.16	1.47	1.43
4	BBB	402	NAG	O4-C4	2.05	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	403	NAG	C1-O5-C5	8.19	123.28	112.19
4	BBB	402	NAG	C1-C2-N2	5.50	119.89	110.49
4	AAA	402	NAG	O5-C5-C6	5.25	115.43	107.20
4	BBB	402	NAG	C2-N2-C7	4.45	129.24	122.90
4	BBB	402	NAG	O7-C7-N2	-4.44	113.78	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	402	NAG	O4-C4-C5	3.75	118.61	109.30
4	BBB	403	NAG	O5-C5-C6	3.73	113.04	107.20
4	AAA	402	NAG	O5-C1-C2	3.67	117.09	111.29
4	AAA	404	NAG	C1-O5-C5	3.65	117.14	112.19
4	BBB	402	NAG	O7-C7-C8	3.52	128.60	122.06
4	BBB	402	NAG	C1-O5-C5	3.50	116.93	112.19
4	BBB	402	NAG	O5-C1-C2	-3.45	105.83	111.29
4	AAA	402	NAG	C1-O5-C5	3.41	116.81	112.19
4	AAA	403	NAG	O4-C4-C5	3.29	117.46	109.30
4	BBB	402	NAG	C3-C4-C5	-3.04	104.81	110.24
4	AAA	403	NAG	C2-N2-C7	3.03	127.21	122.90
5	BBB	405	TKQ	C1-N-C	2.91	132.57	126.61
4	AAA	404	NAG	O5-C5-C6	2.80	111.60	107.20
4	AAA	403	NAG	O7-C7-C8	-2.78	116.90	122.06
5	BBB	405	TKQ	C6-C1-N	-2.68	111.40	120.40
4	AAA	404	NAG	C8-C7-N2	2.66	120.60	116.10
4	BBB	402	NAG	C4-C3-C2	-2.66	107.13	111.02
4	BBB	403	NAG	C2-N2-C7	2.51	126.48	122.90
5	BBB	405	TKQ	N-C-N1	-2.42	109.71	113.87
4	BBB	403	NAG	O4-C4-C5	2.39	115.24	109.30
5	AAA	405	TKQ	C7-C8-C9	2.36	118.34	112.87
4	BBB	402	NAG	O3-C3-C2	-2.36	104.58	109.47
4	BBB	403	NAG	O5-C1-C2	2.30	114.92	111.29
4	AAA	403	NAG	O3-C3-C2	-2.28	104.76	109.47
5	BBB	405	TKQ	C2-C1-N	2.12	127.53	120.40
5	BBB	405	TKQ	O-C-N	2.06	127.11	123.62

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	405	TKQ	N1-C7-C8-C9
5	AAA	405	TKQ	N1-C-N-C1
5	AAA	405	TKQ	O-C-N-C1
5	BBB	405	TKQ	O-C-N1-C7
5	BBB	405	TKQ	N-C-N1-C7
5	BBB	405	TKQ	N1-C7-C8-C9
4	AAA	403	NAG	C8-C7-N2-C2
4	AAA	403	NAG	O7-C7-N2-C2
4	AAA	404	NAG	C8-C7-N2-C2
4	AAA	404	NAG	O7-C7-N2-C2
4	BBB	402	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	BBB	402	NAG	O7-C7-N2-C2
4	BBB	403	NAG	C4-C5-C6-O6
4	BBB	403	NAG	O5-C5-C6-O6
4	AAA	404	NAG	C4-C5-C6-O6
4	BBB	402	NAG	C1-C2-N2-C7
4	AAA	404	NAG	O5-C5-C6-O6
5	BBB	405	TKQ	C7-C8-C9-C14
5	BBB	405	TKQ	C7-C8-C9-C10
4	AAA	403	NAG	C4-C5-C6-O6
5	AAA	405	TKQ	N-C-N1-C7
5	AAA	405	TKQ	C7-C8-C9-C10
4	AAA	403	NAG	O5-C5-C6-O6
5	AAA	405	TKQ	C13-C12-S-O2
5	AAA	405	TKQ	C11-C12-S-O2
5	BBB	405	TKQ	C11-C12-S-O1
5	BBB	405	TKQ	C13-C12-S-O1
5	AAA	405	TKQ	O-C-N1-C7
5	AAA	405	TKQ	C7-C8-C9-C14

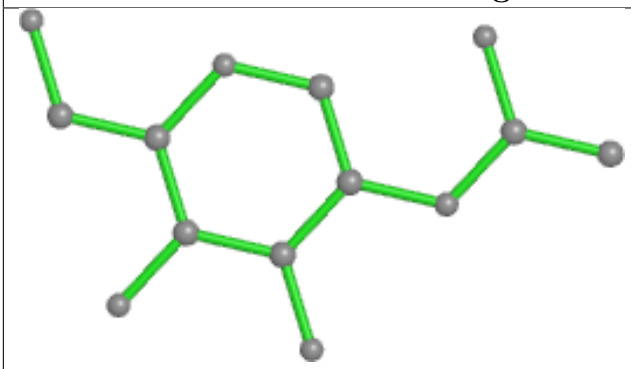
There are no ring outliers.

4 monomers are involved in 8 short contacts:

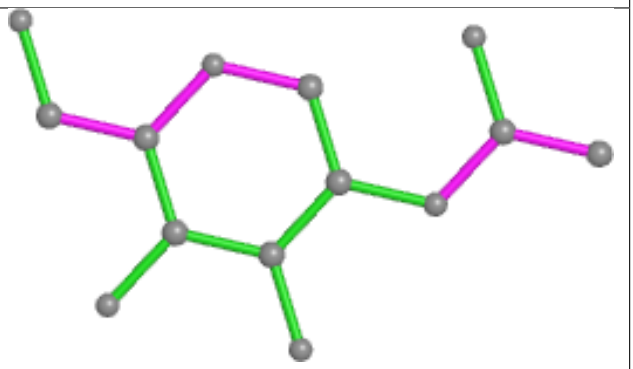
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	404	NAG	2	0
4	AAA	402	NAG	2	0
4	AAA	403	NAG	5	0
5	BBB	405	TKQ	1	0

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.

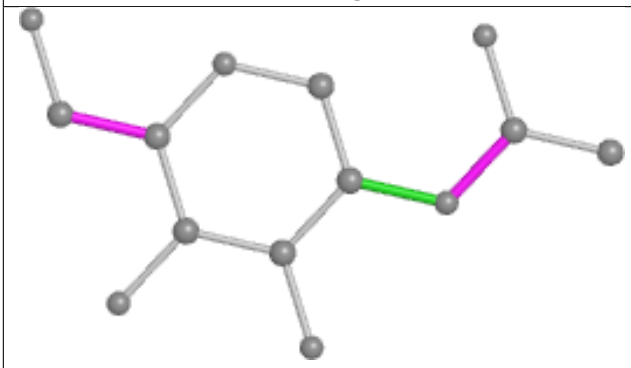
Ligand NAG AAA 404



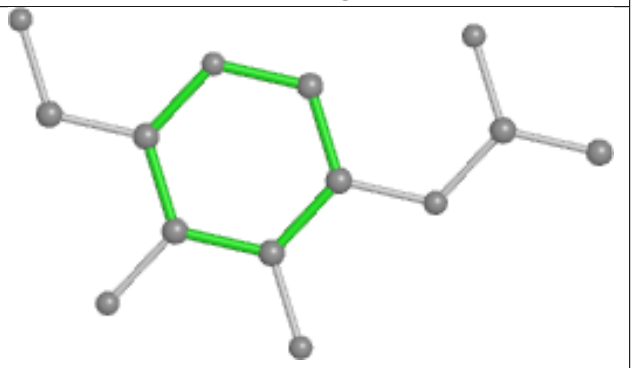
Bond lengths



Bond angles

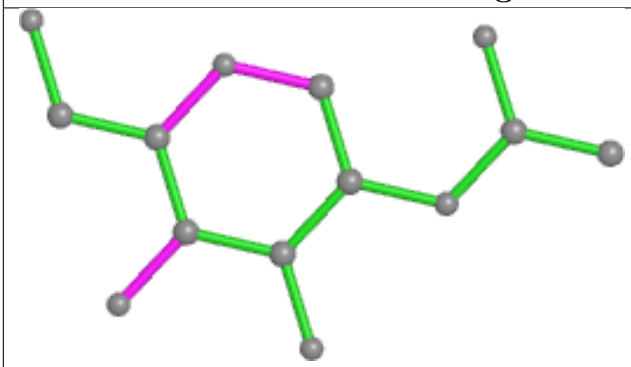


Torsions



Rings

Ligand NAG BBB 402



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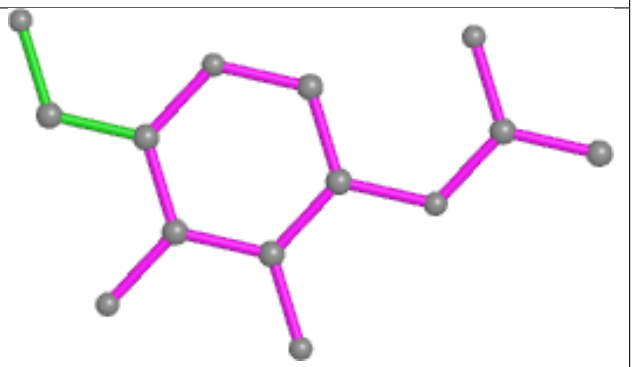

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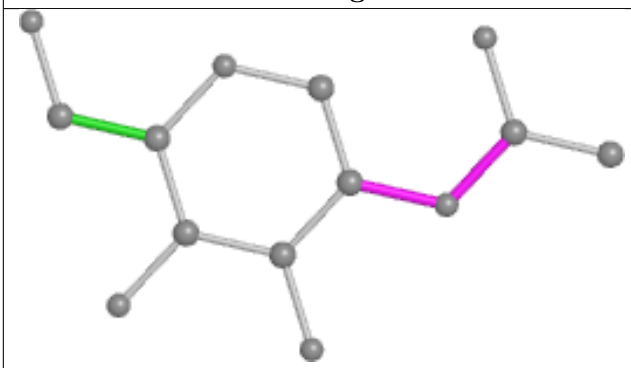

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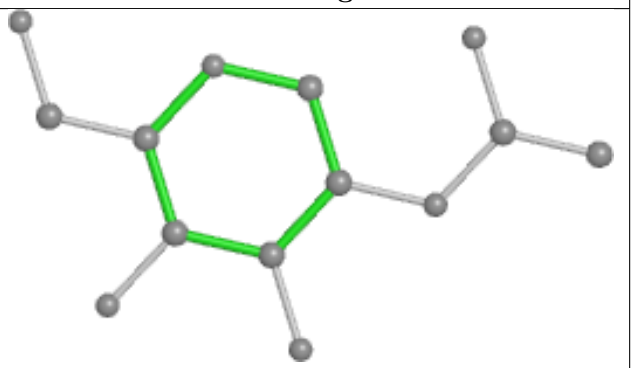
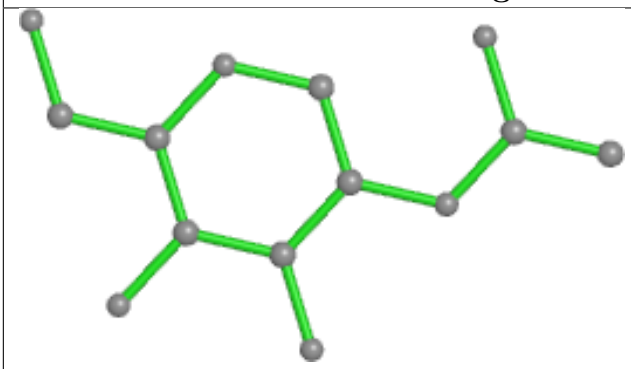
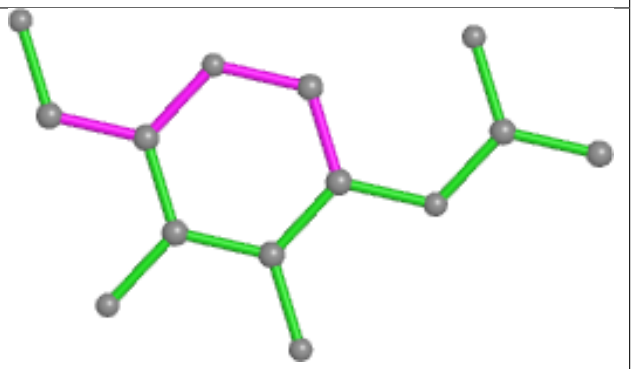


Rings

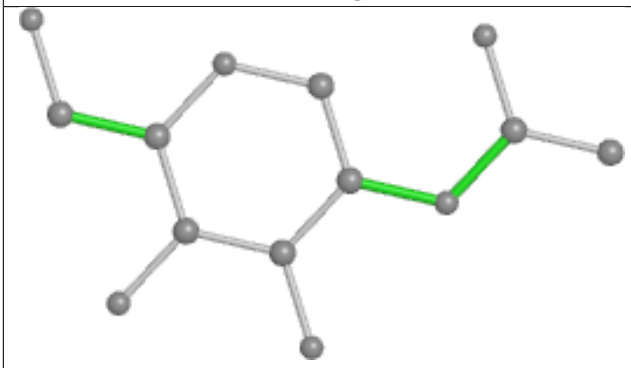
Ligand NAG AAA 402



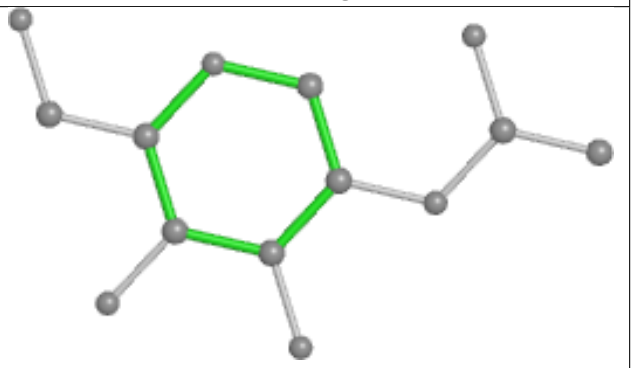
Bond lengths



Bond angles

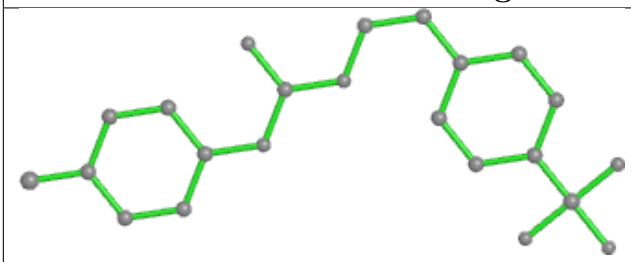


Torsions

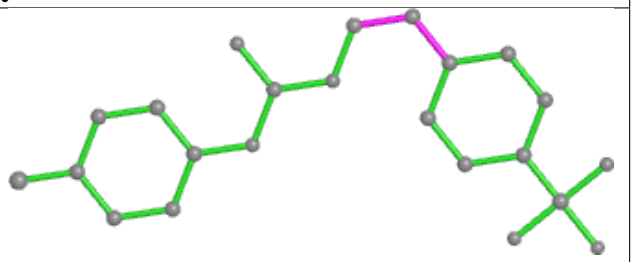


Rings

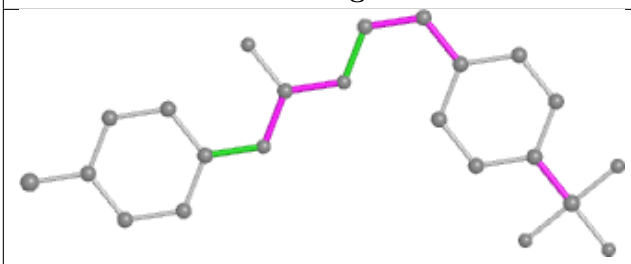
Ligand TKQ AAA 405



Bond lengths



Bond angles



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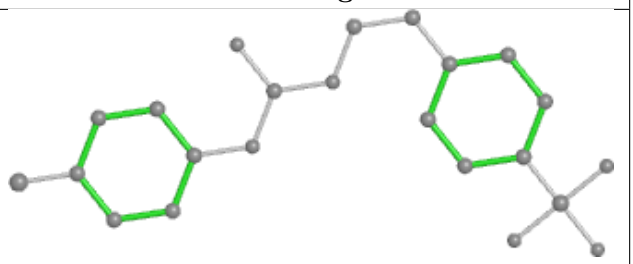
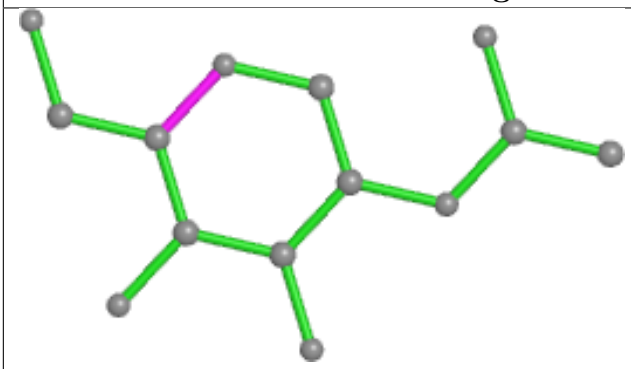
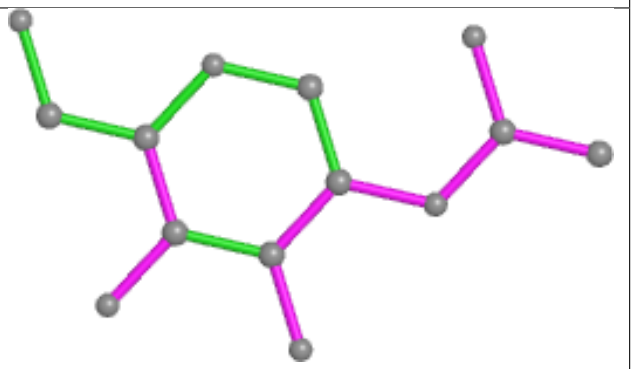


Rings

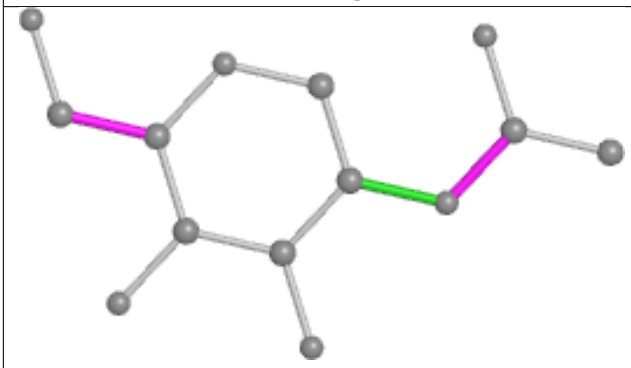
Ligand NAG AAA 403



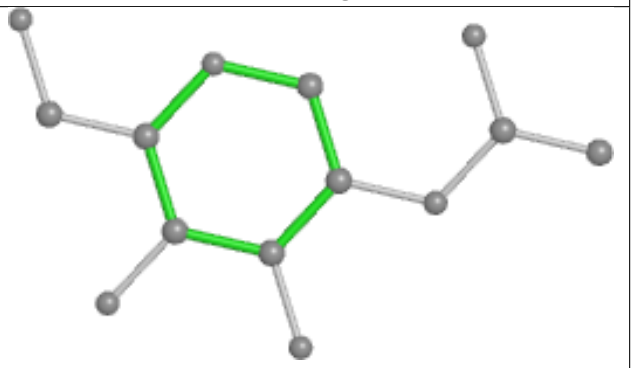
Bond lengths



Bond angles

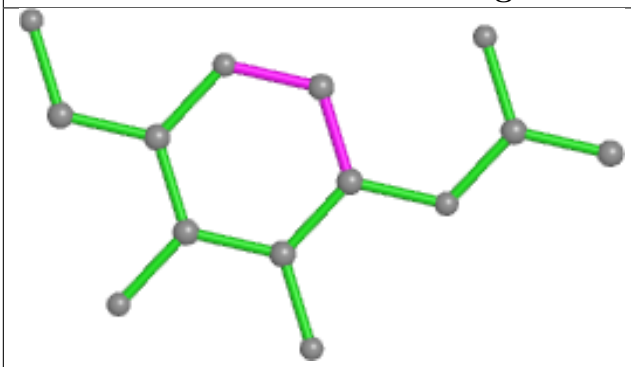


Torsions

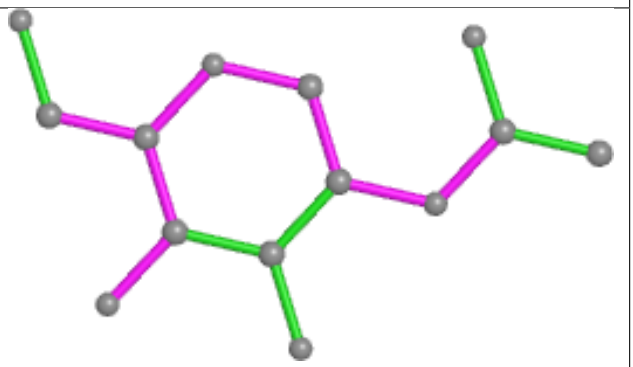


Rings

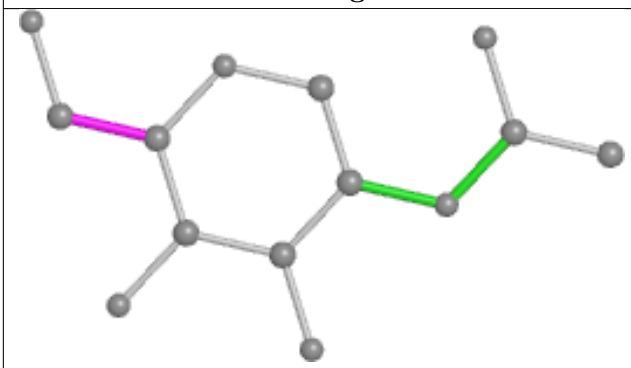
Ligand NAG BBB 403



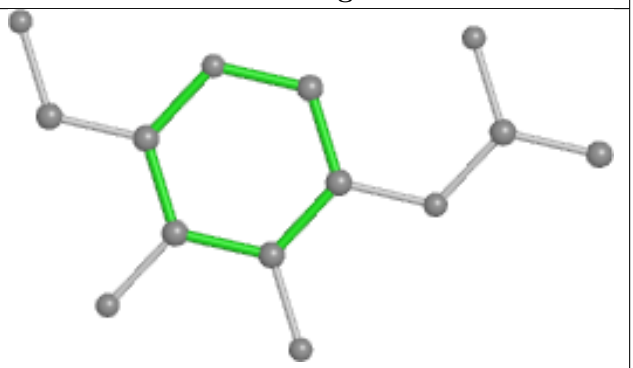
Bond lengths



Bond angles

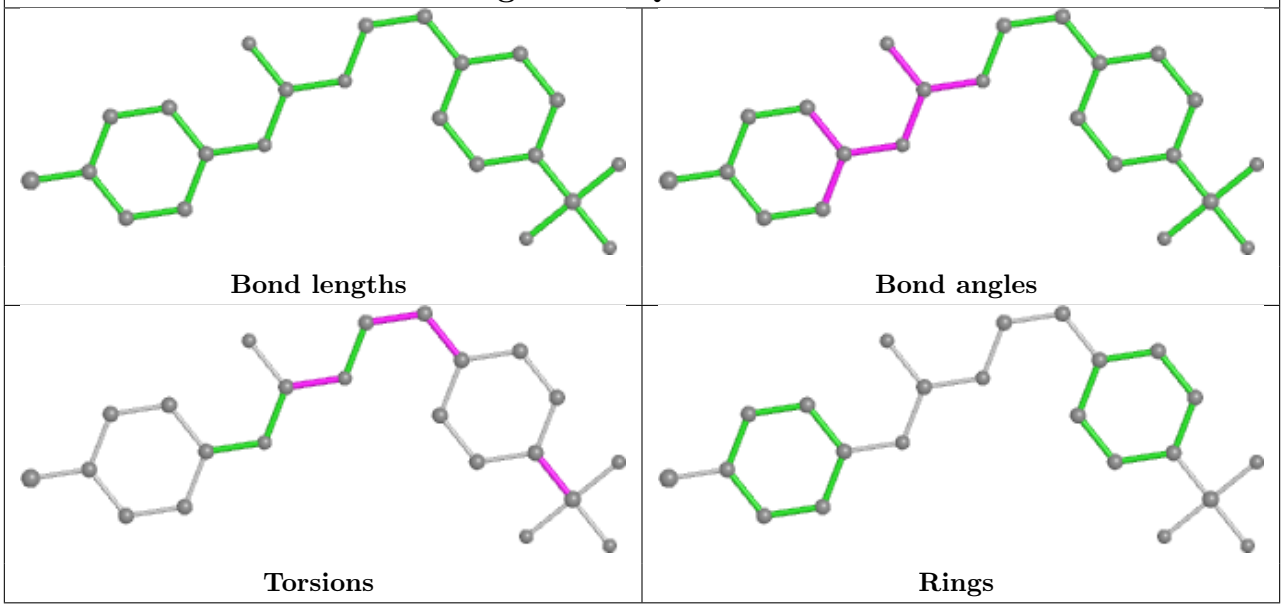


Torsions



Rings

Ligand TKQ BBB 405



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	277/312 (88%)	-0.38	0 100 100	17, 26, 48, 64	0
1	BBB	277/312 (88%)	-0.41	1 (0%) 92 92	17, 28, 49, 64	0
All	All	554/624 (88%)	-0.39	1 (0%) 95 94	17, 27, 48, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	300	GLY	2.3

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

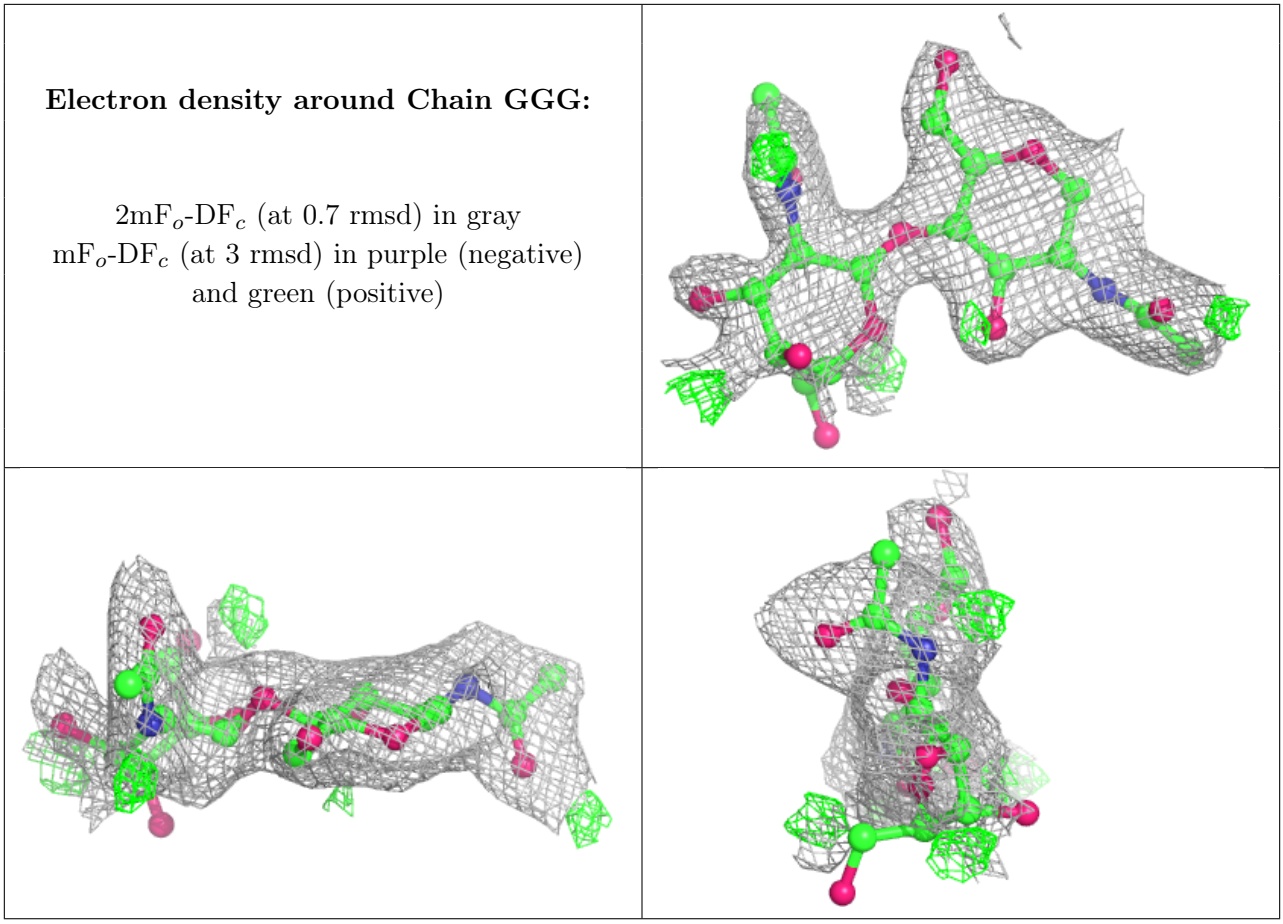
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GGG	2	14/15	0.84	0.23	51,82,95,104	0
2	NAG	GGG	1	14/15	0.91	0.11	43,51,62,65	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain GGG:

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



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.

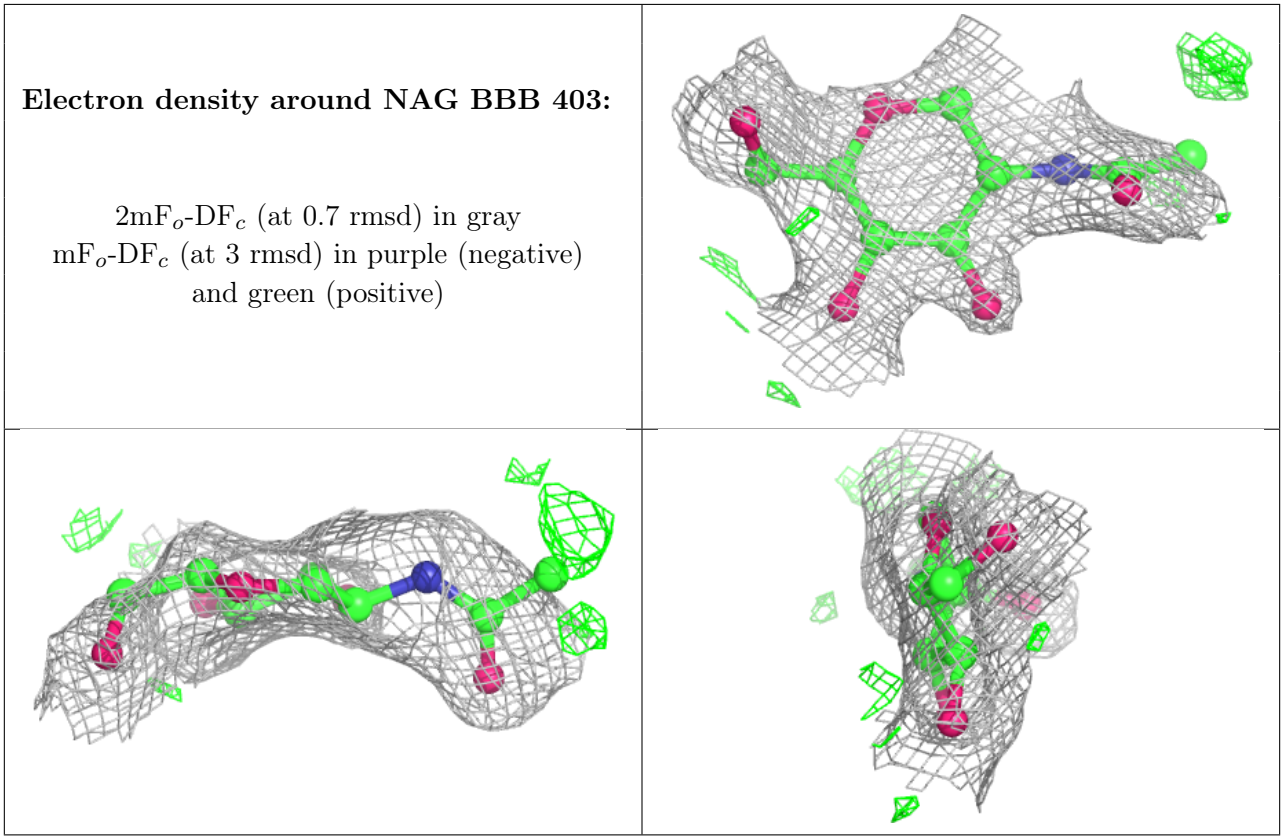
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	BBB	403	14/15	0.76	0.17	66,76,86,92	0
4	NAG	AAA	404	14/15	0.78	0.32	85,98,106,112	0
4	NAG	BBB	402	14/15	0.84	0.13	40,52,55,59	0
4	NAG	AAA	403	14/15	0.91	0.10	36,46,50,53	0
5	TKQ	BBB	405	23/23	0.92	0.25	34,52,143,293	0
5	TKQ	AAA	405	23/23	0.94	0.28	30,46,162,265	0
4	NAG	AAA	402	14/15	0.94	0.12	40,52,67,68	0
6	GOL	BBB	404	6/6	0.94	0.13	23,29,30,36	0
3	ZN	AAA	401	1/1	0.99	0.07	22,22,22,22	1
3	ZN	BBB	401	1/1	0.99	0.05	26,26,26,26	1

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.

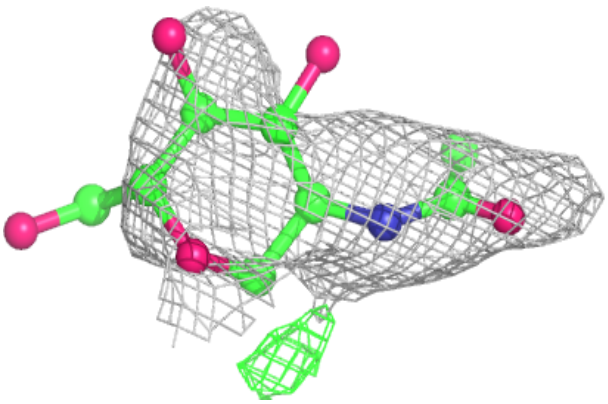
Electron density around NAG BBB 403:

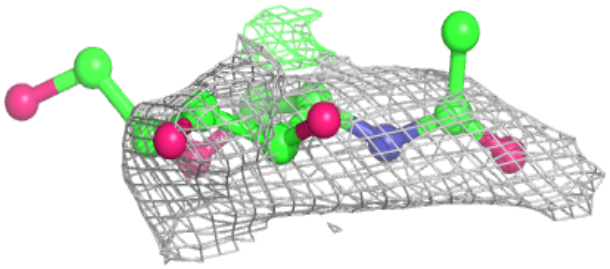
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

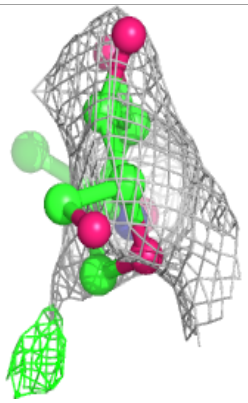


Electron density around NAG AAA 404:

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

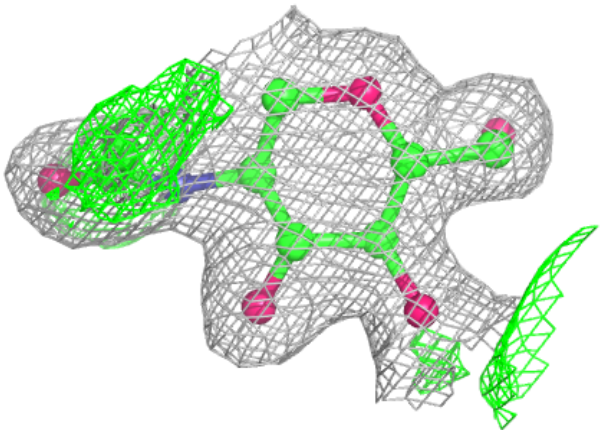


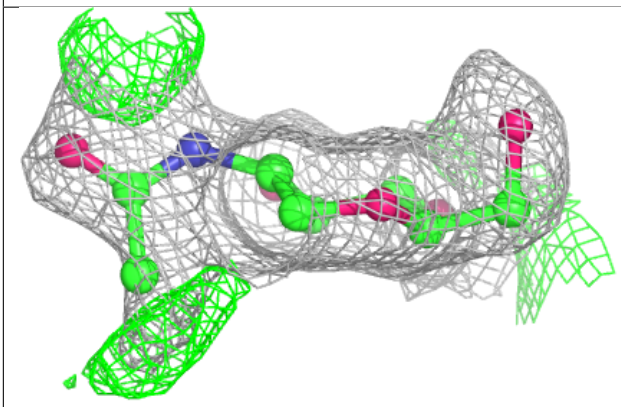


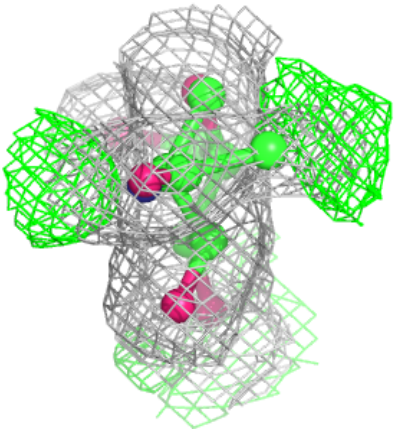


Electron density around NAG BBB 402:

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

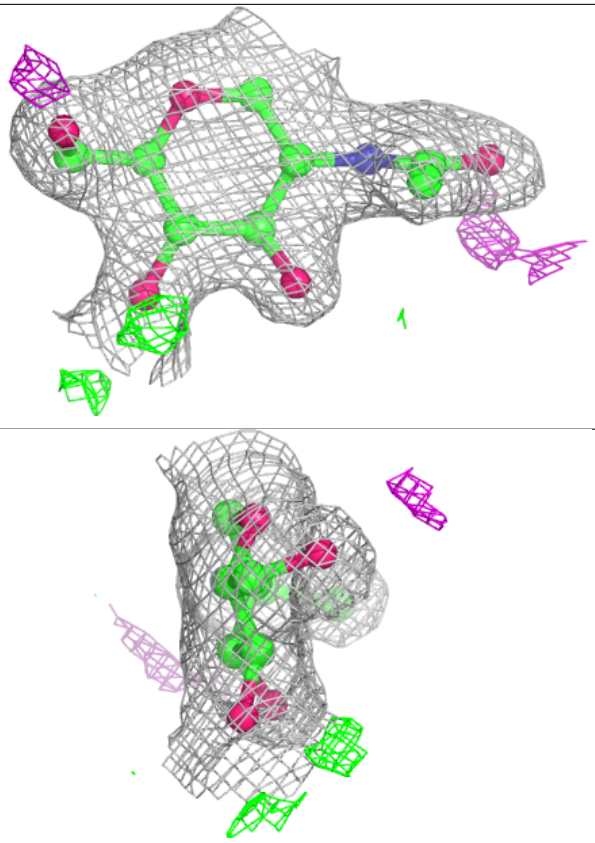






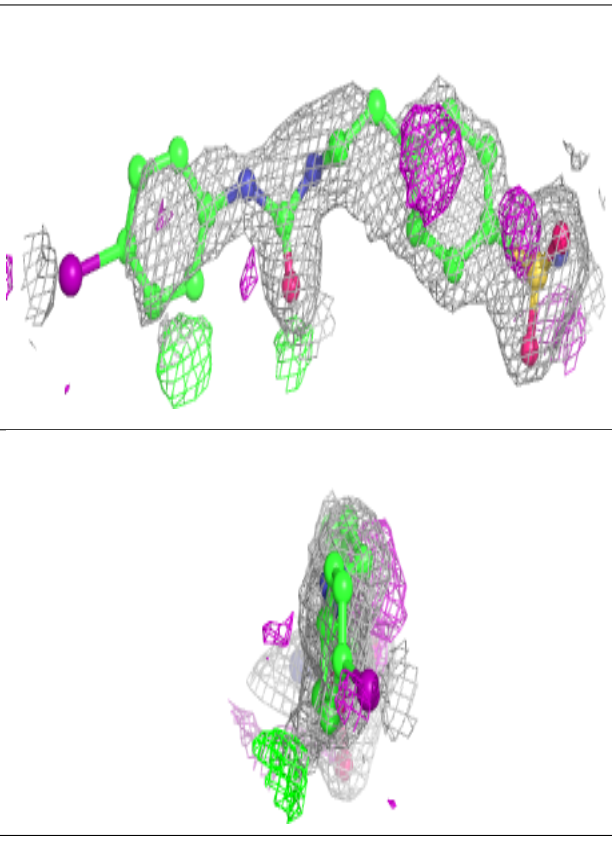
Electron density around NAG AAA 403:

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



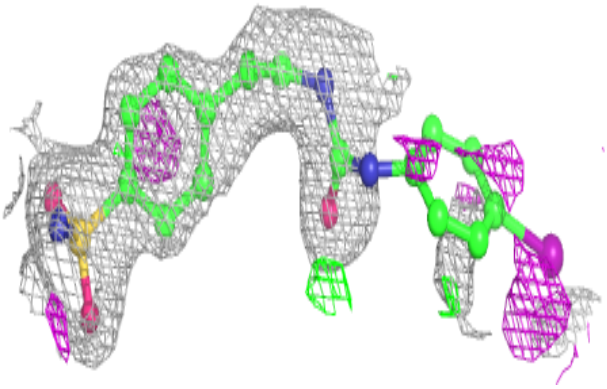
Electron density around TKQ BBB 405:

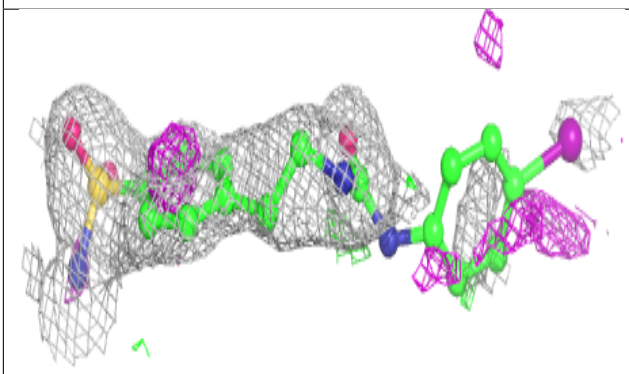
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

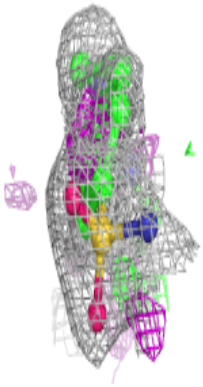


Electron density around TKQ AAA 405:

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

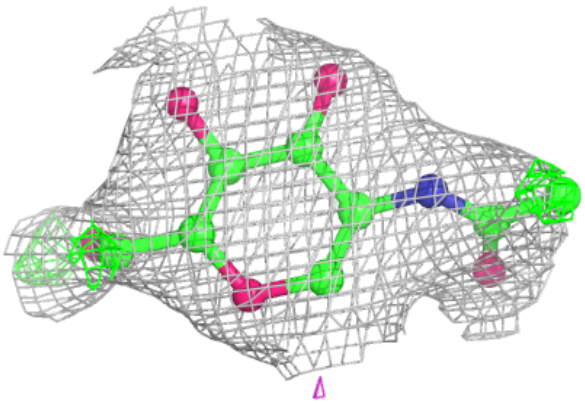


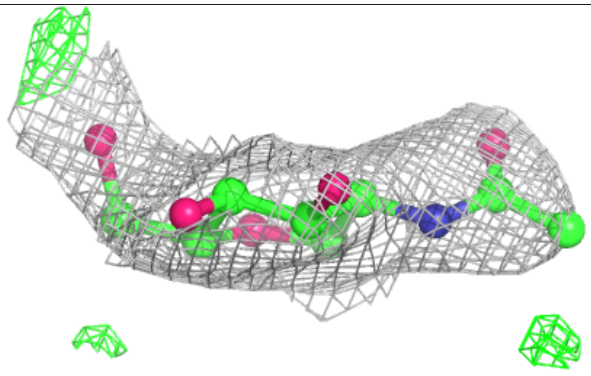


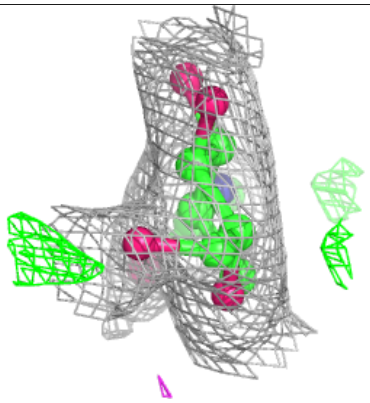


Electron density around NAG AAA 402:

$2mF_o$-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.