



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 28, 2025 – 01:34 pm BST

PDB ID : 8RTP / pdb_00008rtp
Title : Bilirubin oxidase from Myrothecium verrucaria in complex with NAD+
Authors : Svecova, L.; Koval, T.; Kolenko, P.; Ostergaard, L.H.; Dohnalek, J.
Deposited on : 2024-01-27
Resolution : 2.10 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 ⓘ 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

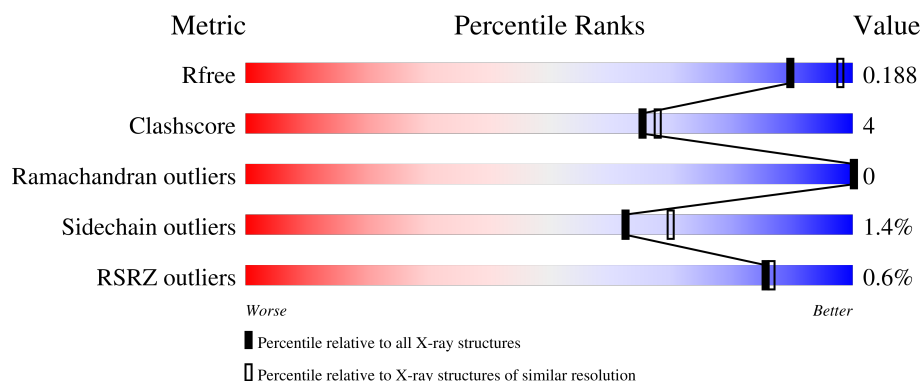
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	534	 89% 10% .
1	BBB	534	 89% 10% .
2	AeA	4	 100%
3	AiA	2	 100%
3	BeB	2	 100%

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Mol	Chain	Length	Quality of chain
3	BgB	2	 50% 50%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9877 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 Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	534	Total	C	N	O	S	0	10	0
			4303	2747	730	812	14			
1	BBB	533	Total	C	N	O	S	0	5	0
			4265	2724	725	802	14			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AeA	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

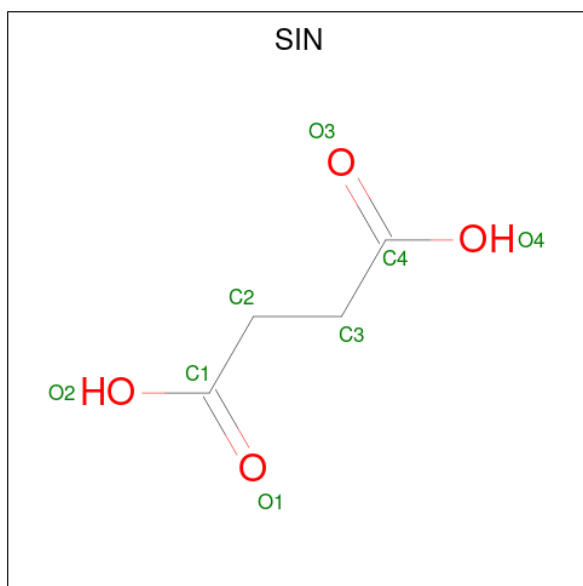


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AiA	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	BgB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

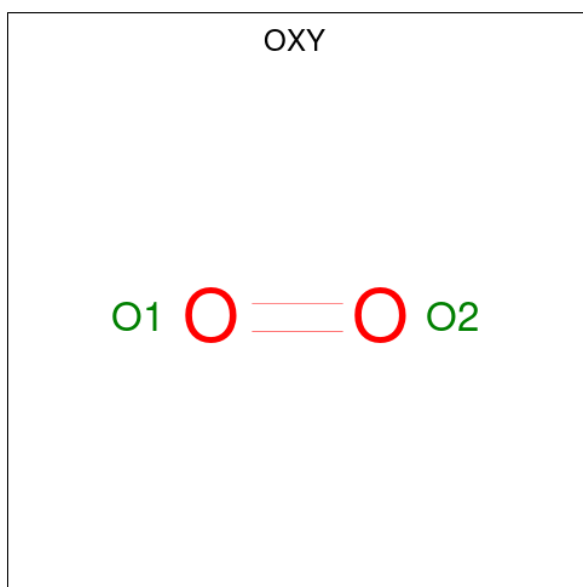
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	4	Total Cu 4 4	0	0
4	BBB	4	Total Cu 4 4	0	0

- Molecule 5 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



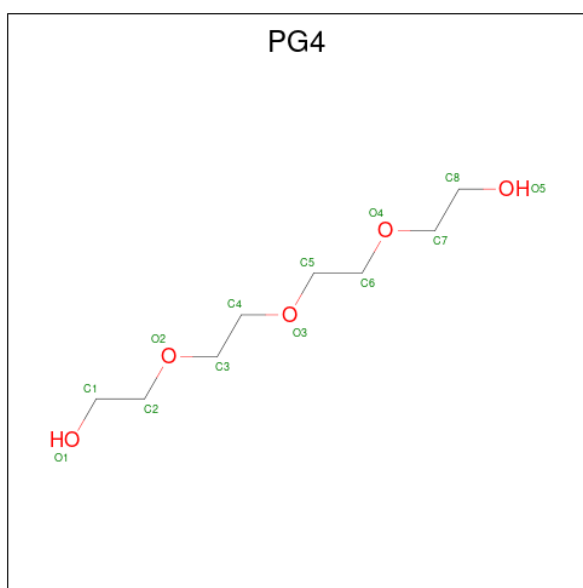
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 8 4 4	0	0
5	AAA	1	Total C O 8 4 4	0	0
5	BBB	1	Total C O 8 4 4	0	0

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			13	8	5		
7	BBB	1	Total	C	O	0	0
			13	8	5		

-
- Chemical structure of (R)-propan-2-ol (PGR). The central carbon is bonded to a methyl group (C3), a hydroxyl group (OH, O2), a hydroxymethyl group (CH₂OH, C1, O1), and a hydrogen atom (not shown). The stereochemistry is (R), indicated by the wedge bond to the hydroxyl group.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			5	3	2		

- # NAD
-
- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD). The molecule is composed of two nucleotides linked by a pyrophosphate bridge. The top nucleotide consists of a nicotinamide ring (labeled with N1A, N3A, C2A, C4A, C5A, C6A, N6A, N7A, N8A, N9A, C8A, C9A) attached to a ribose sugar (labeled with C1B, C2B, C3B, C4B, C5B, C6B, C7B, C8B, C9B). The bottom nucleotide consists of an adenine ring (labeled with N1C, N3C, C2C, C4C, C5C, C6C, N6C, N7C, N8C, N9C, C8C, C9C) attached to a ribose sugar (labeled with C1D, C2D, C3D, C4D, C5D, C6D, C7D, C8D, C9D). The two ribose sugars are linked by a pyrophosphate bridge (labeled with P1, P2, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779,

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AAA	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	BBB	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

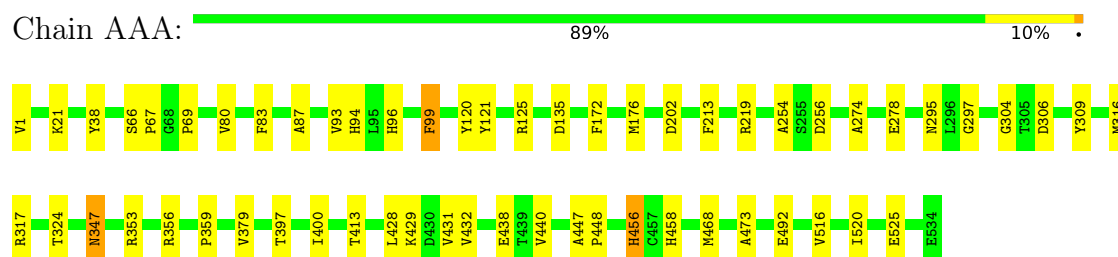
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AAA	541	Total	O	0	4
			542	542		
11	BBB	472	Total	O	0	3
			472	472		

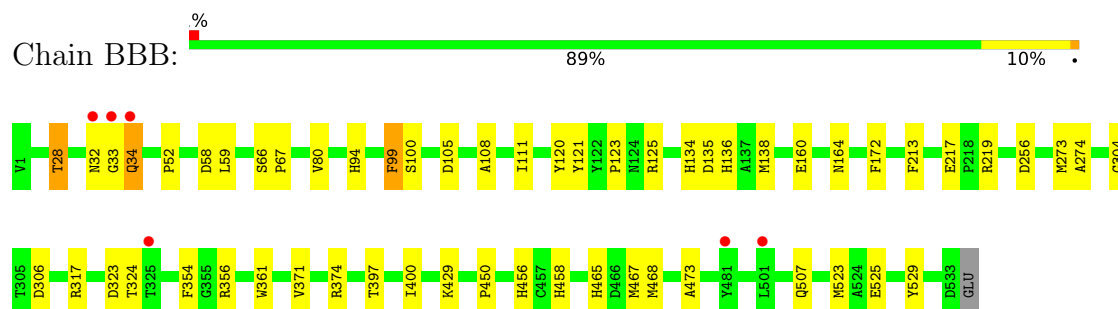
3 Residue-property plots

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: Bilirubin oxidase



- Molecule 1: Bilirubin oxidase



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BeB:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BgB:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.73Å 202.44Å 224.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.10 46.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.99-2.10) 98.7 (46.99-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.169 , 0.215 0.176 , 0.188	Depositor DCC
R_{free} test set	4435 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9877	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, OXY, NAG, SIN, NAD, PGR, MAN, PG4, GOL, BMA

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	1.08	4/4464 (0.1%)	1.28	8/6101 (0.1%)
1	BBB	1.10	2/4411 (0.0%)	1.32	6/6032 (0.1%)
All	All	1.09	6/8875 (0.1%)	1.30	14/12133 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	134	HIS	CE1-NE2	6.40	1.39	1.32
1	BBB	100	SER	C-O	5.55	1.30	1.23
1	AAA	428	LEU	C-O	5.44	1.30	1.24
1	AAA	297	GLY	C-O	5.37	1.28	1.23
1	AAA	456	HIS	C-O	5.15	1.30	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	135	ASP	CA-CB-CG	-6.13	106.47	112.60
1	BBB	99	PHE	CA-CB-CG	6.00	119.80	113.80
1	BBB	111	ILE	CA-C-N	5.96	131.41	123.00
1	BBB	111	ILE	C-N-CA	5.96	131.41	123.00
1	AAA	99	PHE	CA-CB-CG	5.87	119.67	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4303	0	4101	28	0
1	BBB	4265	0	4057	35	0
2	AeA	50	0	43	0	0
3	AiA	28	0	25	2	0
3	BeB	28	0	25	0	0
3	BgB	28	0	25	1	0
4	AAA	4	0	0	0	0
4	BBB	4	0	0	0	0
5	AAA	16	0	8	0	0
5	BBB	8	0	4	1	0
6	AAA	2	0	0	0	0
6	BBB	2	0	0	0	0
7	AAA	13	0	18	0	0
7	BBB	13	0	18	0	0
8	AAA	5	0	8	0	0
9	AAA	44	0	26	0	0
9	BBB	44	0	26	1	0
10	BBB	6	0	8	0	0
11	AAA	542	0	0	4	0
11	BBB	472	0	0	3	0
All	All	9877	0	8392	64	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 64 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:28:THR:HG22	1:BBB:33:GLY:O	1.70	0.92
1:BBB:456:HIS:HB3	1:BBB:468:MET:HG3	1.75	0.66
1:BBB:356[A]:ARG:HH21	1:BBB:356[A]:ARG:HG2	1.60	0.65
1:AAA:525[B]:GLU:OE1	3:AiA:2:NAG:H5	1.98	0.63
1:AAA:254:ALA:HB3	1:AAA:278:GLU:HB2	1.81	0.62

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	542/534 (102%)	512 (94%)	30 (6%)	0	100	100
1	BBB	536/534 (100%)	504 (94%)	32 (6%)	0	100	100
All	All	1078/1068 (101%)	1016 (94%)	62 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	463/453 (102%)	458 (99%)	5 (1%)	70	77
1	BBB	457/453 (101%)	449 (98%)	8 (2%)	54	61
All	All	920/906 (102%)	907 (99%)	13 (1%)	62	70

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	99	PHE
1	BBB	121	TYR
1	BBB	374	ARG
1	BBB	306	ASP
1	BBB	323	ASP

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 ⓘ

10 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	AeA	1	1,2	14,14,15	0.93	2 (14%)	17,19,21	1.62	5 (29%)
2	NAG	AeA	2	2	14,14,15	0.70	0	17,19,21	1.26	3 (17%)
2	BMA	AeA	3	2	11,11,12	0.79	0	15,15,17	2.17	4 (26%)
2	MAN	AeA	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.53	2 (13%)
3	NAG	AiA	1	1,3	14,14,15	1.20	1 (7%)	17,19,21	1.66	5 (29%)
3	NAG	AiA	2	3	14,14,15	0.58	0	17,19,21	1.69	3 (17%)
3	NAG	BeB	1	1,3	14,14,15	0.94	0	17,19,21	1.47	3 (17%)
3	NAG	BeB	2	3	14,14,15	0.62	0	17,19,21	1.59	4 (23%)
3	NAG	BgB	1	1,3	14,14,15	0.58	0	17,19,21	1.23	3 (17%)
3	NAG	BgB	2	3	14,14,15	0.72	0	17,19,21	1.57	3 (17%)

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	AeA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AeA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AeA	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	AeA	4	2	-	0/2/19/22	0/1/1/1
3	NAG	AiA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	AiA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BeB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BeB	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BgB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BgB	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AiA	1	NAG	C1-C2	-3.65	1.46	1.52
2	AeA	1	NAG	O5-C1	-2.25	1.40	1.43
2	AeA	4	MAN	C2-C3	2.20	1.55	1.52
2	AeA	1	NAG	C1-C2	-2.14	1.49	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AeA	3	BMA	O5-C5-C6	4.69	114.56	107.20
2	AeA	3	BMA	C3-C4-C5	3.77	116.97	110.24
2	AeA	3	BMA	C2-C3-C4	3.74	117.36	110.89
3	BeB	1	NAG	C1-C2-N2	-3.60	104.34	110.49
3	AiA	2	NAG	O7-C7-C8	-3.52	115.51	122.06

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BgB	2	NAG	O5-C5-C6-O6
3	BgB	2	NAG	C4-C5-C6-O6
3	AiA	2	NAG	O5-C5-C6-O6
3	AiA	2	NAG	C4-C5-C6-O6
3	BeB	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

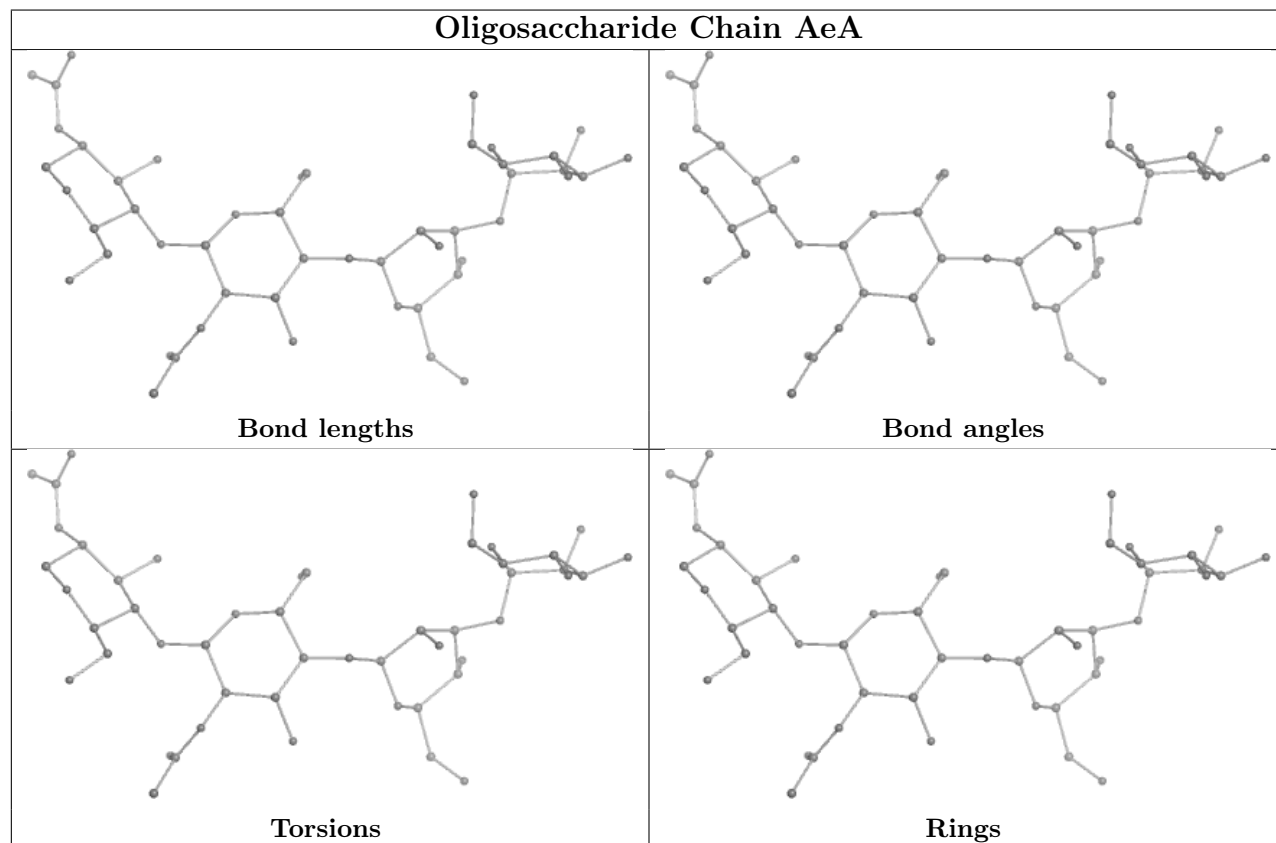
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BgB	2	NAG	1	0

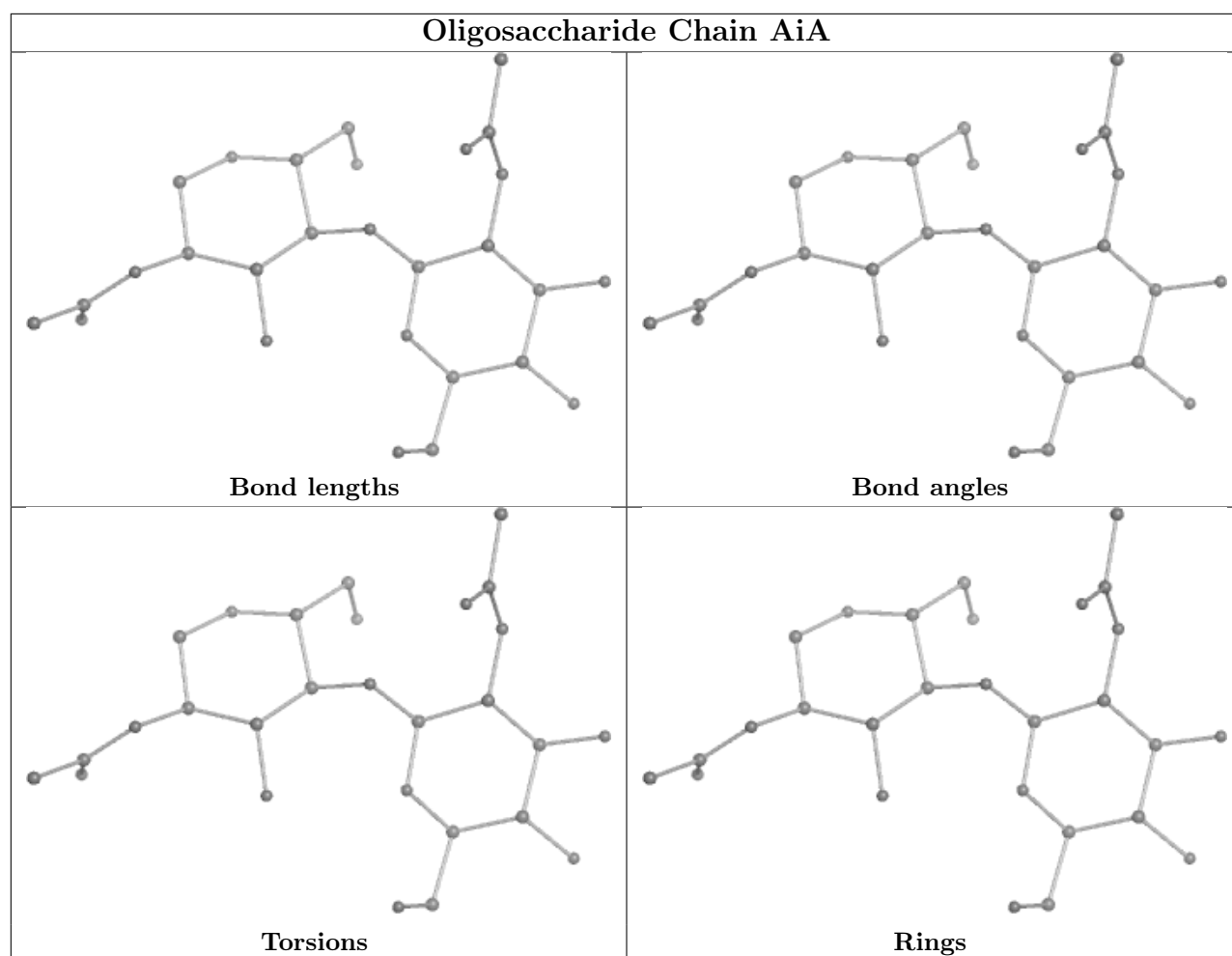
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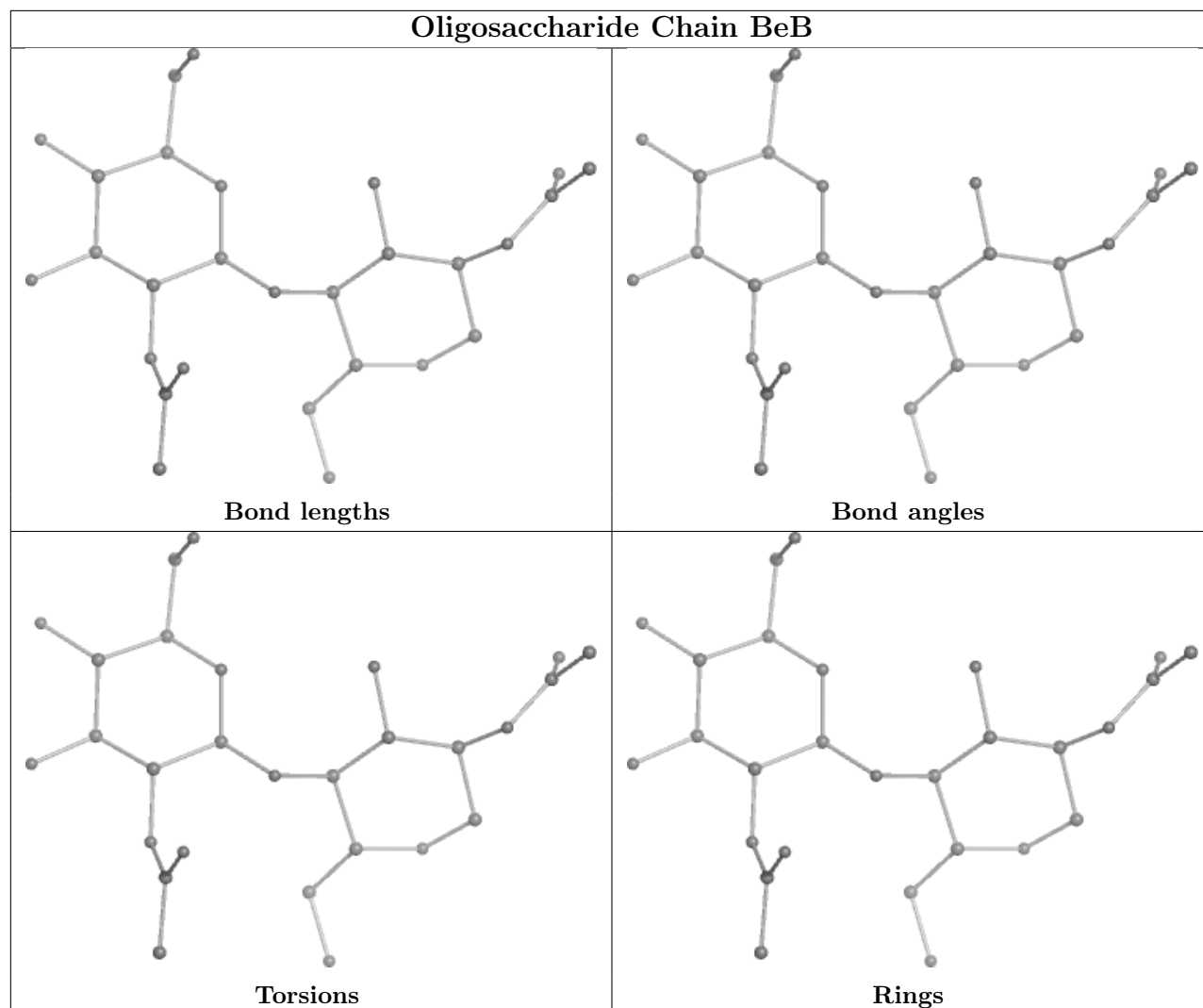
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AiA	2	NAG	1	0
3	AiA	1	NAG	1	0

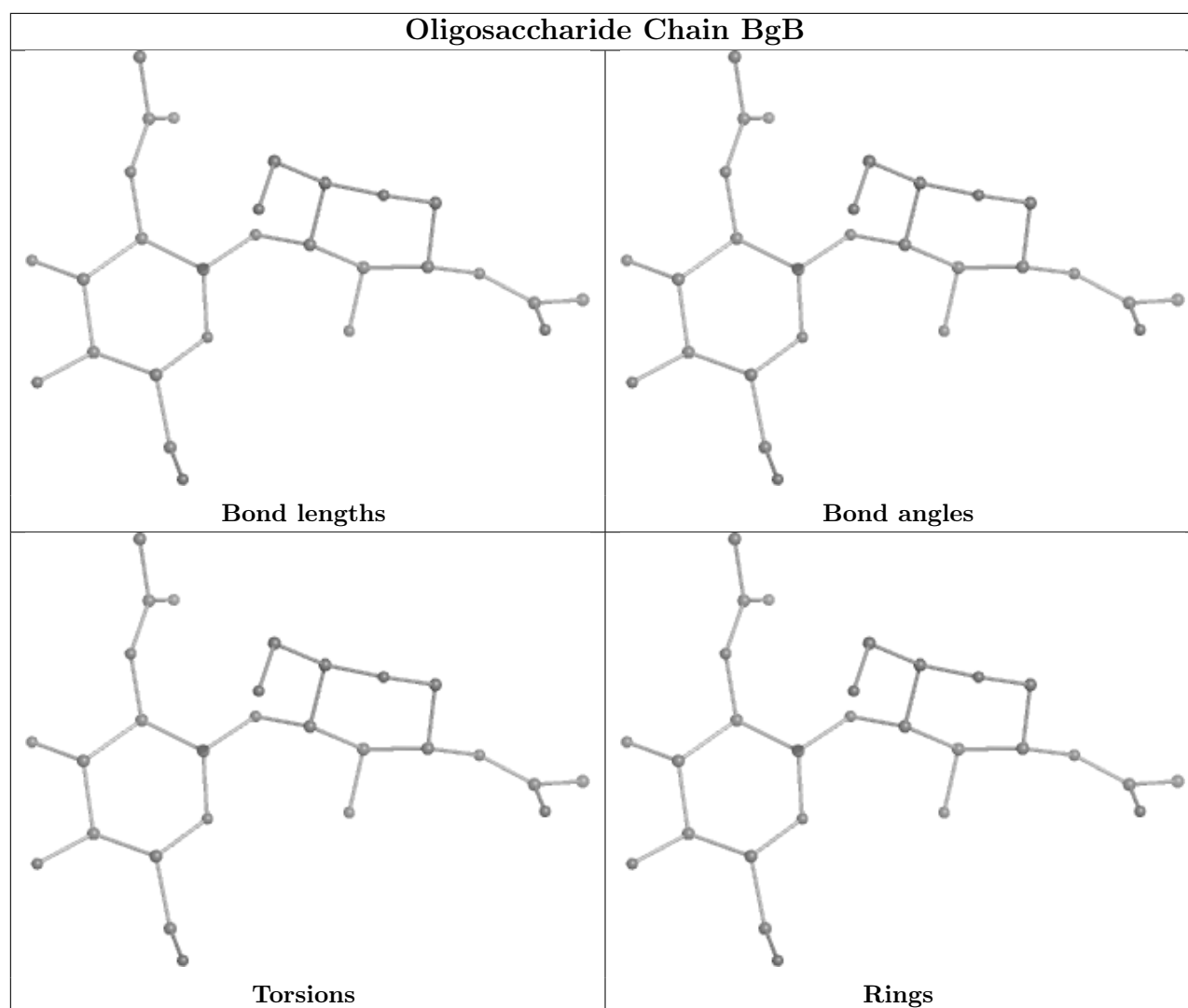
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





Oligosaccharide Chain BeB





5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	OXY	AAA	607	4	1,1,1	0.18	0	-		
8	PGR	AAA	609	-	3,4,4	0.39	0	1,4,4	0.42	0
9	NAD	AAA	610	-	42,48,48	0.67	1 (2%)	50,73,73	0.96	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PG4	BBB	607	-	12,12,12	0.44	0	11,11,11	0.22	0
5	SIN	BBB	605	-	7,7,7	1.05	0	8,8,8	1.34	1 (12%)
6	OXY	BBB	606	4	1,1,1	0.30	0	-		
7	PG4	AAA	608	-	12,12,12	0.34	0	11,11,11	0.13	0
10	GOL	BBB	608	-	5,5,5	0.14	0	5,5,5	0.35	0
5	SIN	AAA	606	-	7,7,7	1.09	0	8,8,8	1.25	0
9	NAD	BBB	609	-	42,48,48	0.66	1 (2%)	50,73,73	1.00	4 (8%)
5	SIN	AAA	605	-	7,7,7	1.01	1 (14%)	8,8,8	1.32	1 (12%)

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
8	PGR	AAA	609	-	-	1/2/2/2	-
9	NAD	AAA	610	-	-	14/26/62/62	0/5/5/5
7	PG4	BBB	607	-	-	0/10/10/10	-
5	SIN	BBB	605	-	-	0/5/5/5	-
7	PG4	AAA	608	-	-	4/10/10/10	-
10	GOL	BBB	608	-	-	2/4/4/4	-
5	SIN	AAA	606	-	-	5/5/5/5	-
9	NAD	BBB	609	-	-	5/26/62/62	0/5/5/5
5	SIN	AAA	605	-	-	1/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BBB	609	NAD	C2N-N1N	2.36	1.37	1.35
9	AAA	610	NAD	C2N-N1N	2.29	1.37	1.35
5	AAA	605	SIN	O2-C1	-2.18	1.23	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AAA	610	NAD	C6N-N1N-C2N	-3.09	119.16	121.97
9	BBB	609	NAD	O4D-C1D-C2D	-2.93	102.65	106.93
9	BBB	609	NAD	C3D-C2D-C1D	2.92	105.38	100.98
9	AAA	610	NAD	C5A-C6A-N6A	2.81	124.62	120.35
9	BBB	609	NAD	C6N-N1N-C2N	-2.67	119.54	121.97

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AAA	610	NAD	C5D-O5D-PN-O3
9	AAA	610	NAD	O4D-C1D-N1N-C2N
9	AAA	610	NAD	O4D-C1D-N1N-C6N
9	AAA	610	NAD	C2D-C1D-N1N-C2N
9	AAA	610	NAD	C2D-C1D-N1N-C6N

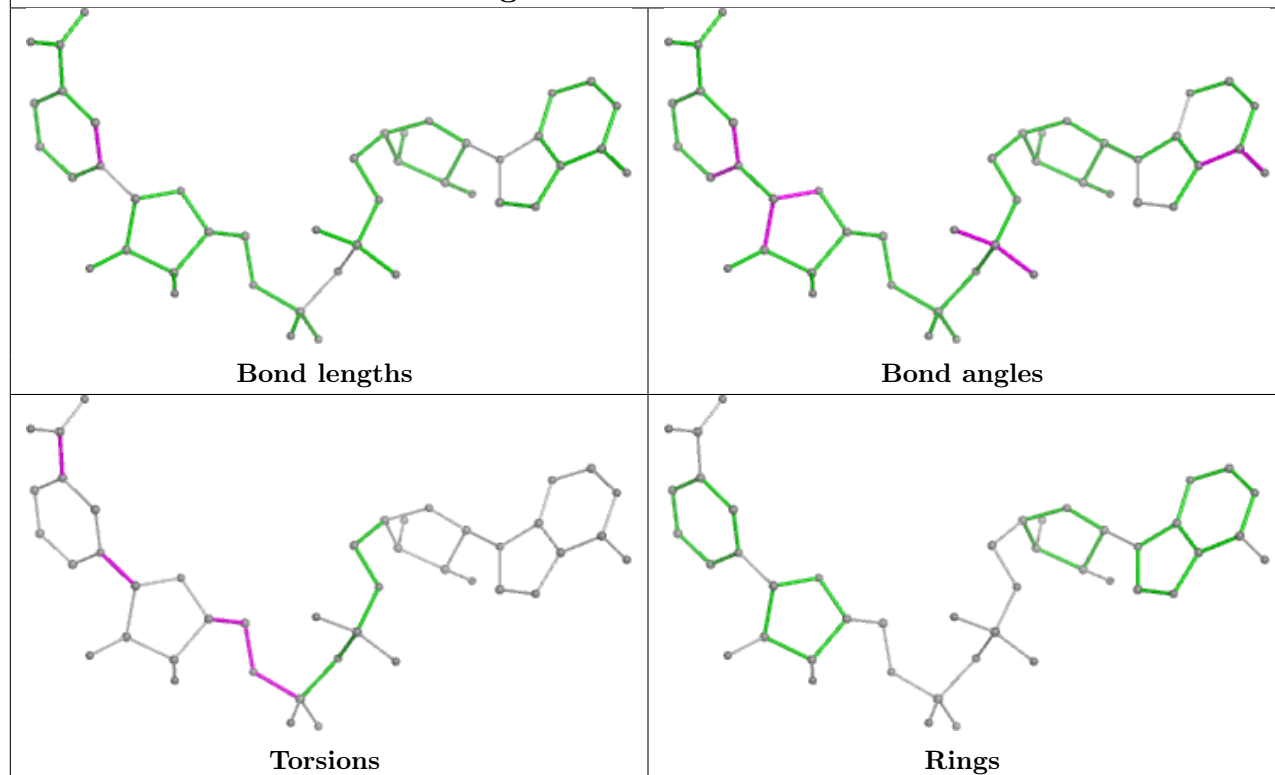
There are no ring outliers.

2 monomers are involved in 2 short contacts:

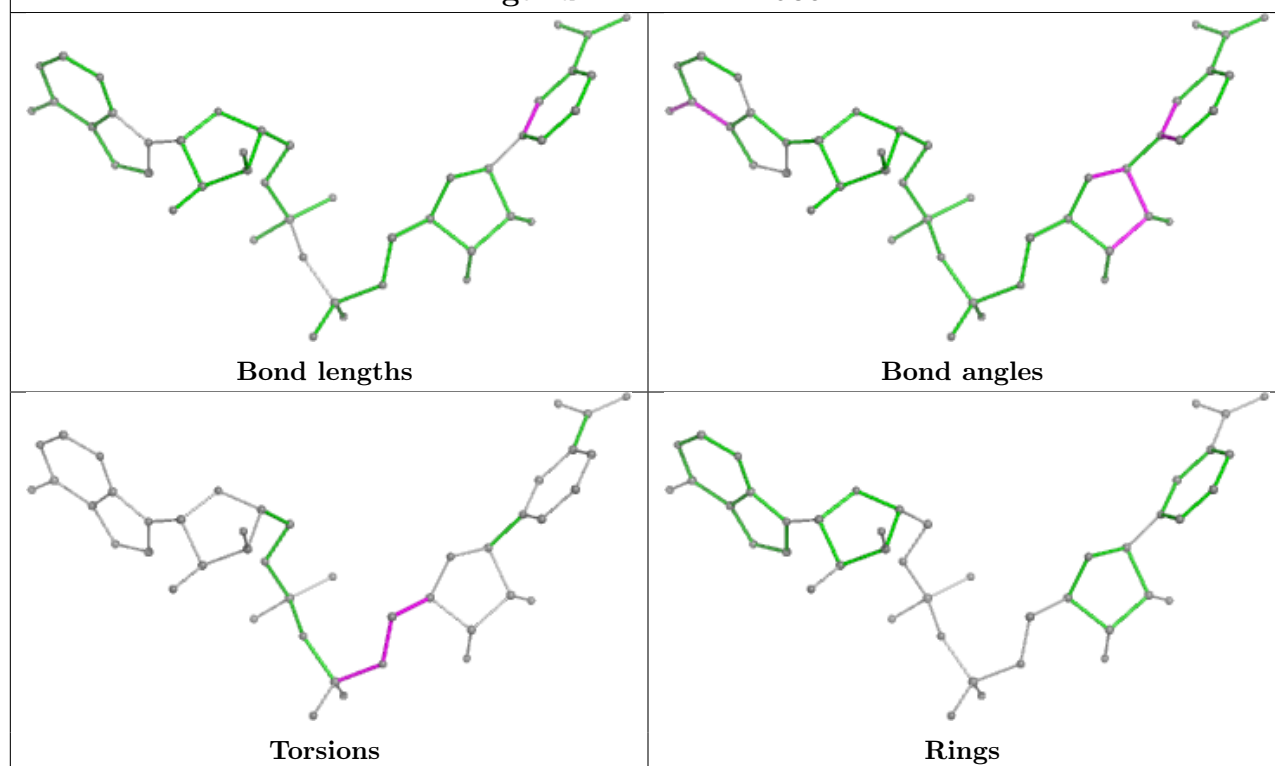
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	605	SIN	1	0
9	BBB	609	NAD	1	0

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 NAD AAA 610



Ligand NAD BBB 609



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	534/534 (100%)	-0.41	0 100 100	16, 28, 43, 63	10 (1%)
1	BBB	533/534 (99%)	-0.03	6 (1%) 77 78	21, 34, 60, 100	6 (1%)
All	All	1067/1068 (99%)	-0.22	6 (0%) 85 86	16, 31, 54, 100	16 (1%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	34	GLN	3.9
1	BBB	33	GLY	3.1
1	BBB	325	THR	3.0
1	BBB	32	ASN	2.6
1	BBB	481	TYR	2.3

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](#)

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.

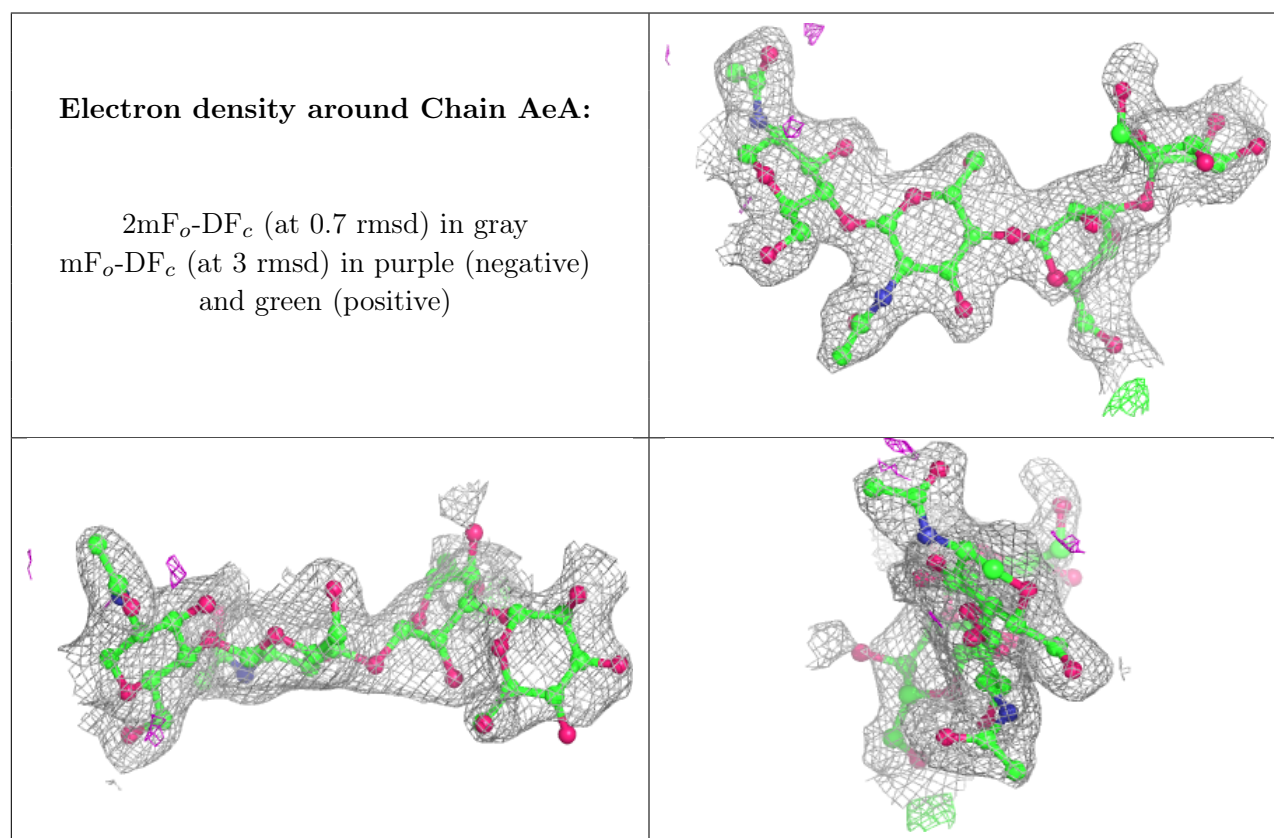
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	AeA	1	14/15	-	-	31,35,38,47	0
2	NAG	AeA	2	14/15	-	-	44,52,62,70	0
2	BMA	AeA	3	11/12	-	-	78,85,96,97	0
2	MAN	AeA	4	11/12	-	-	90,100,109,109	0
3	NAG	AiA	1	14/15	-	-	34,39,43,46	0

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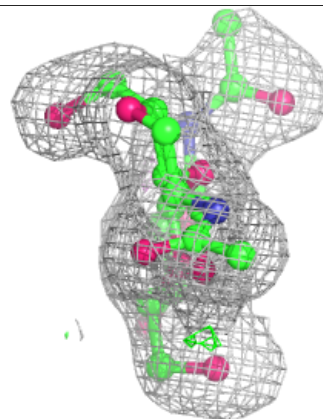
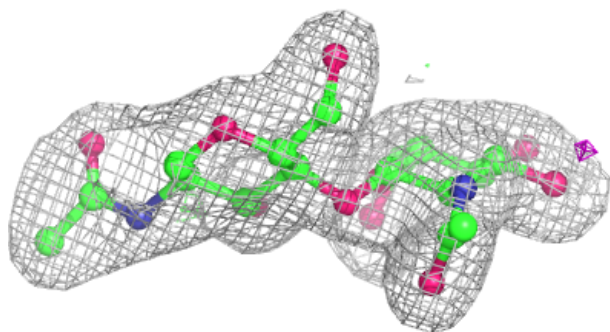
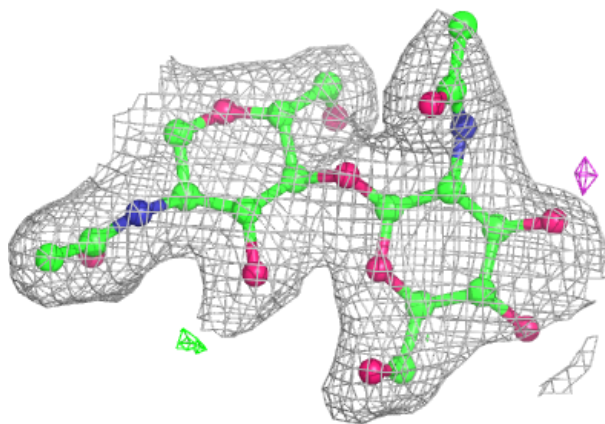
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	AiA	2	14/15	-	-	44,56,69,85	0
3	NAG	BeB	1	14/15	-	-	38,44,50,63	0
3	NAG	BeB	2	14/15	-	-	55,64,74,86	0
3	NAG	BgB	1	14/15	-	-	46,55,59,59	0
3	NAG	BgB	2	14/15	-	-	57,68,74,75	0

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.



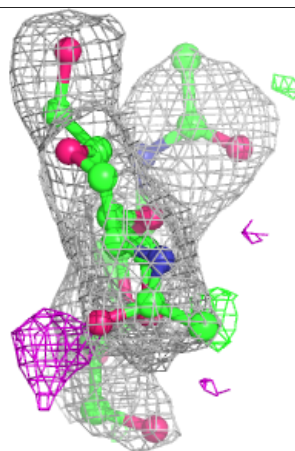
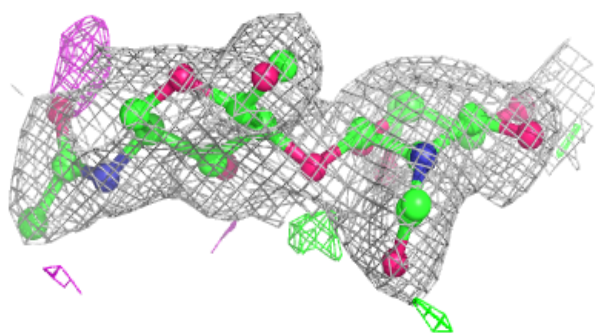
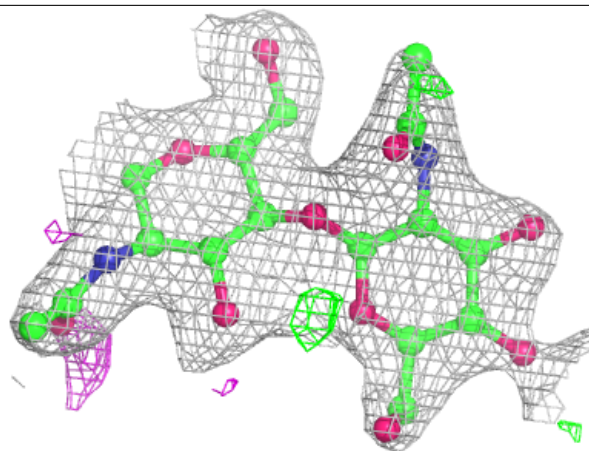
Electron density around Chain AiA:

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



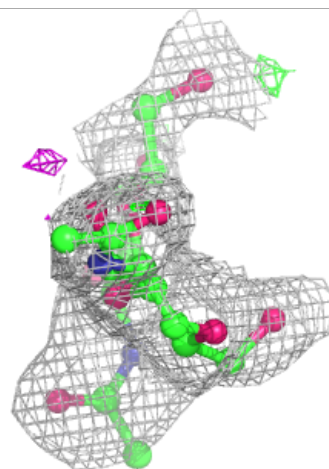
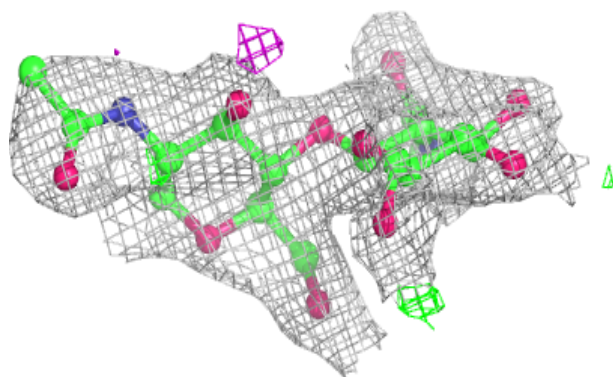
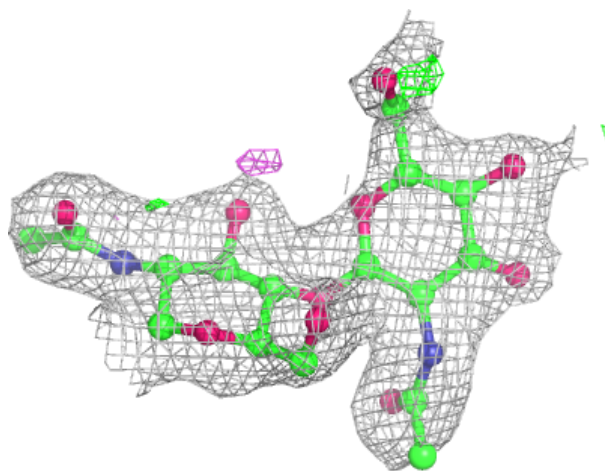
Electron density around Chain BeB:

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



Electron density around Chain BgB:

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** [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
5	SIN	AAA	606	8/8	0.83	0.14	50,62,68,70	0
9	NAD	AAA	610	44/44	0.86	0.15	33,51,109,110	44
5	SIN	BBB	605	8/8	0.87	0.12	41,51,58,60	0
8	PGR	AAA	609	5/5	0.89	0.16	47,49,52,53	0
9	NAD	BBB	609	44/44	0.90	0.14	33,50,104,108	44
10	GOL	BBB	608	6/6	0.90	0.13	61,63,68,69	0
7	PG4	BBB	607	13/13	0.92	0.10	37,39,41,41	13
7	PG4	AAA	608	13/13	0.93	0.11	43,46,51,53	13
5	SIN	AAA	605	8/8	0.96	0.06	27,30,31,35	0
6	OXY	BBB	606	2/2	0.98	0.12	24,24,24,43	0
6	OXY	AAA	607	2/2	0.99	0.04	21,21,21,28	0

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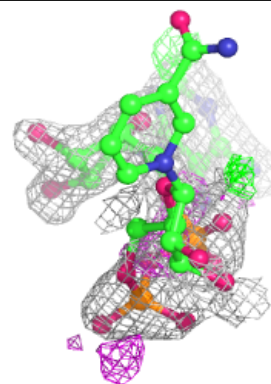
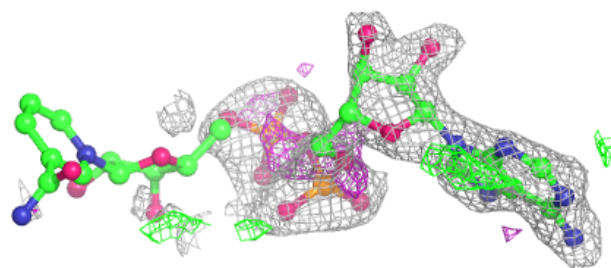
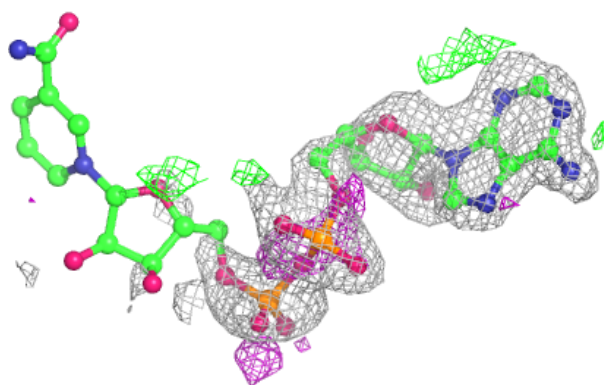
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CU	BBB	604	1/1	0.99	0.07	40,40,40,40	1
4	CU	BBB	602	1/1	1.00	0.03	35,35,35,35	0
4	CU	BBB	603	1/1	1.00	0.04	31,31,31,31	0
4	CU	AAA	601	1/1	1.00	0.03	28,28,28,28	0
4	CU	AAA	602	1/1	1.00	0.03	31,31,31,31	0
4	CU	AAA	603	1/1	1.00	0.03	31,31,31,31	0
4	CU	AAA	604	1/1	1.00	0.06	33,33,33,33	1
4	CU	BBB	601	1/1	1.00	0.02	28,28,28,28	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.

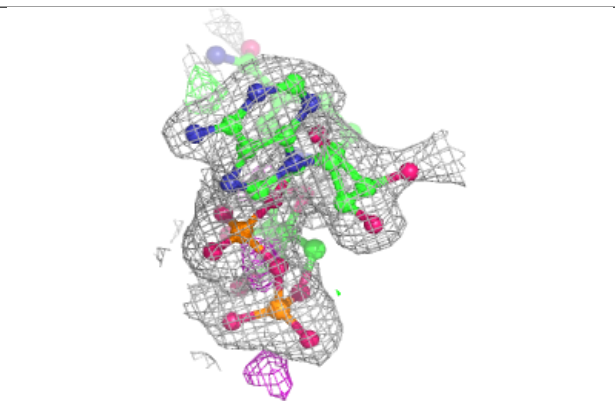
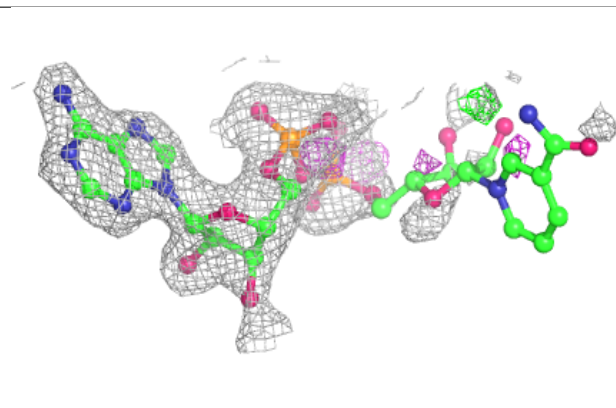
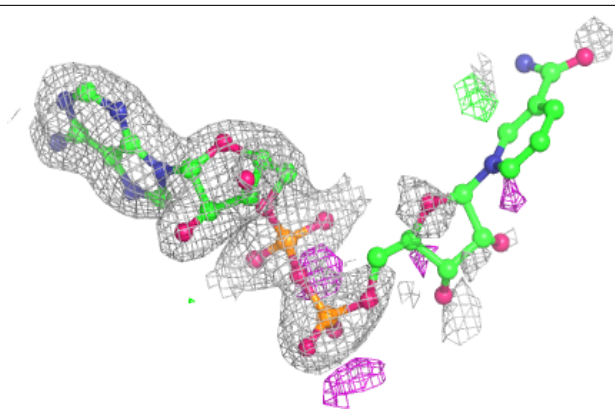
Electron density around NAD AAA 610:

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



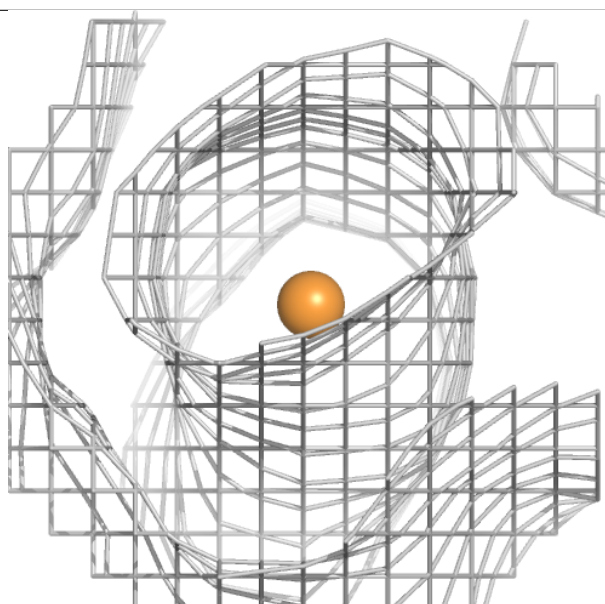
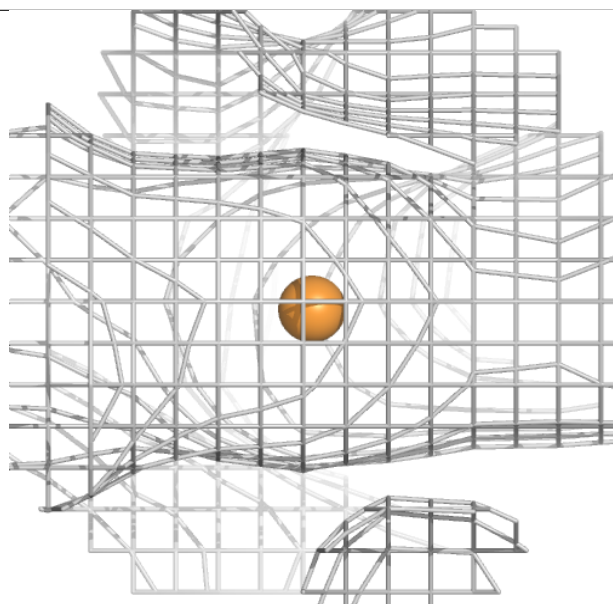
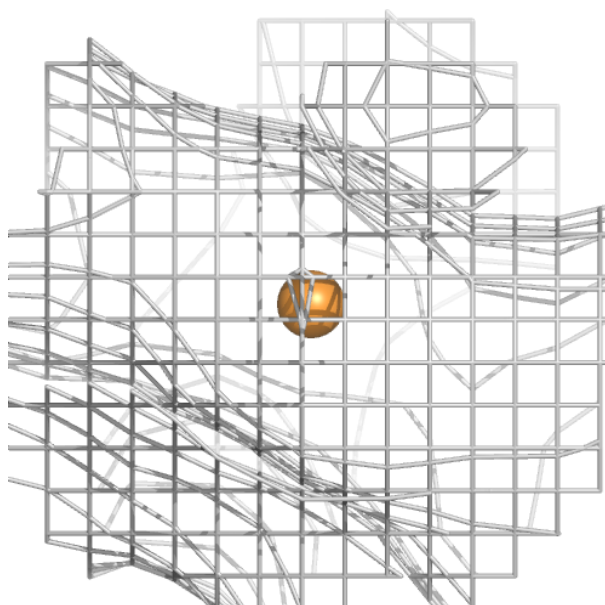
Electron density around NAD BBB 609:

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



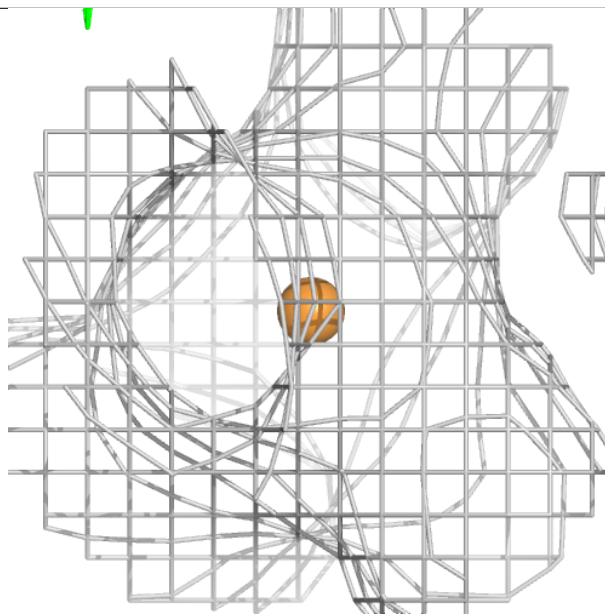
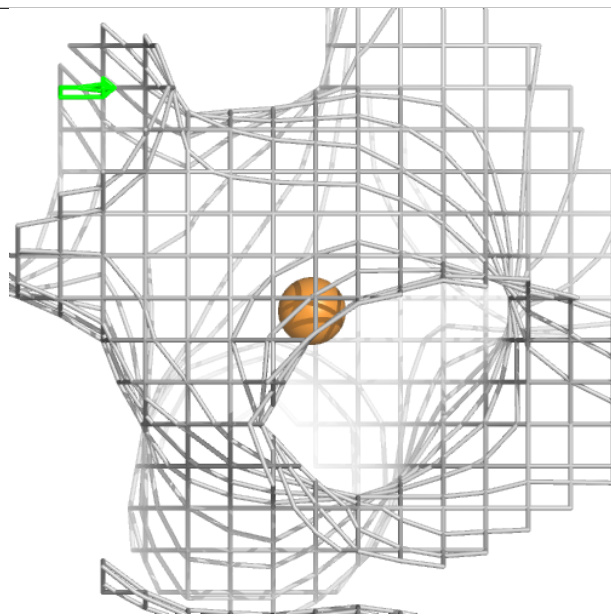
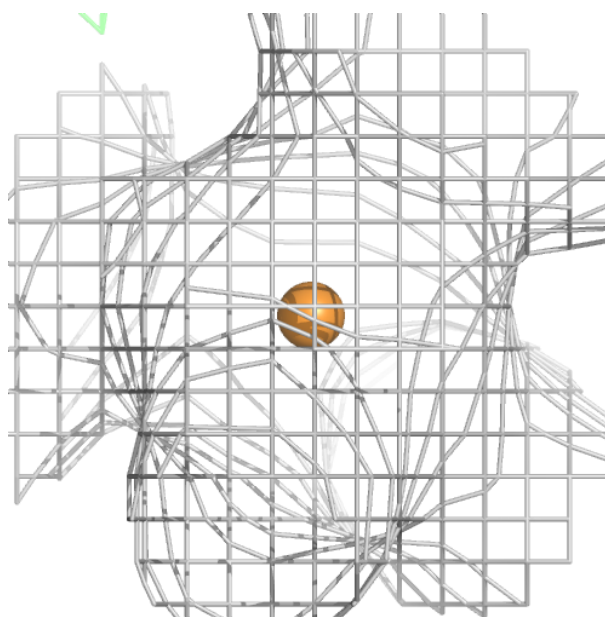
Electron density around CU BBB 604:

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



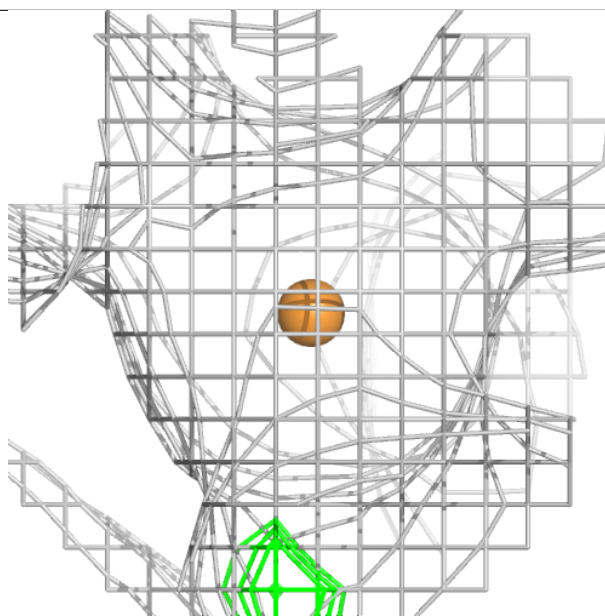
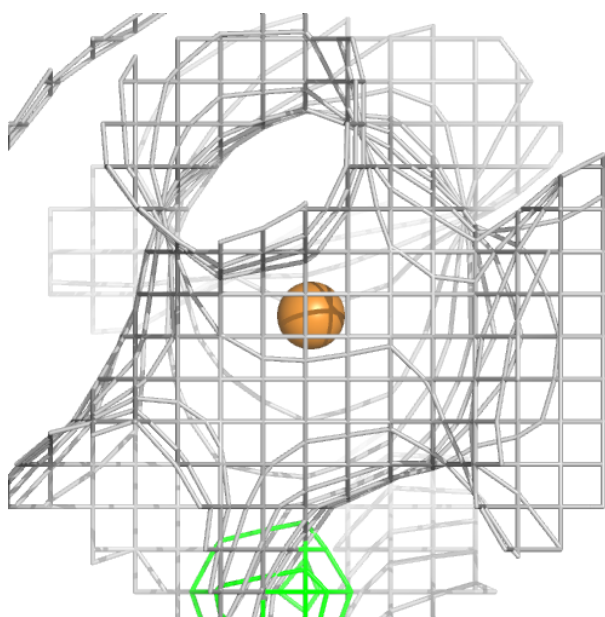
Electron density around CU BBB 602:

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



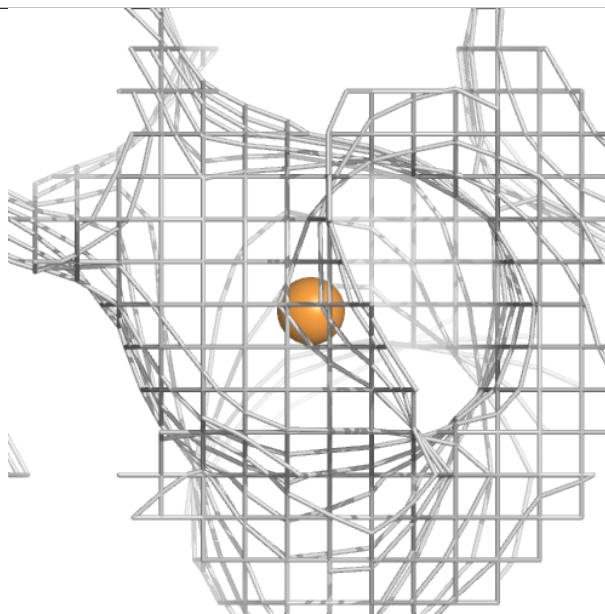
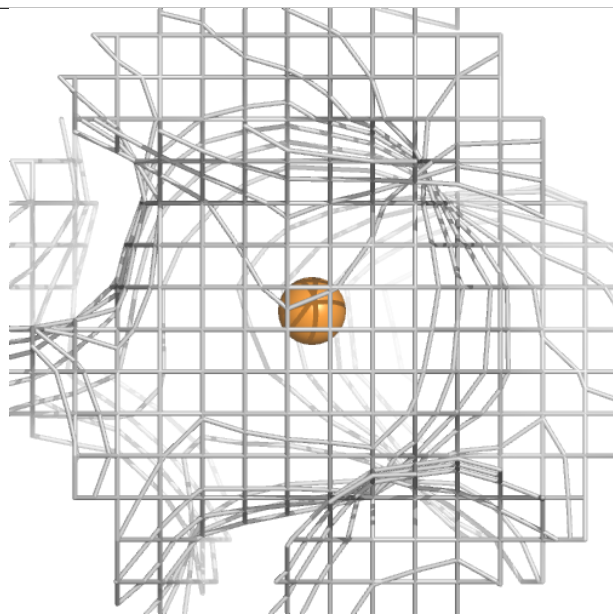
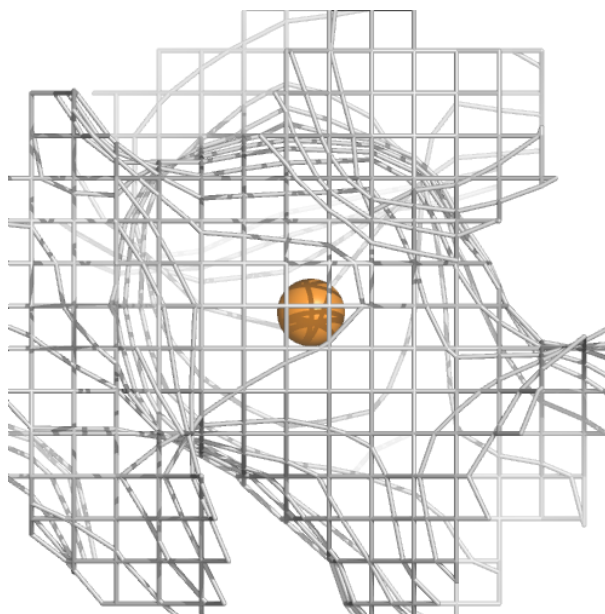
Electron density around CU BBB 603:

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



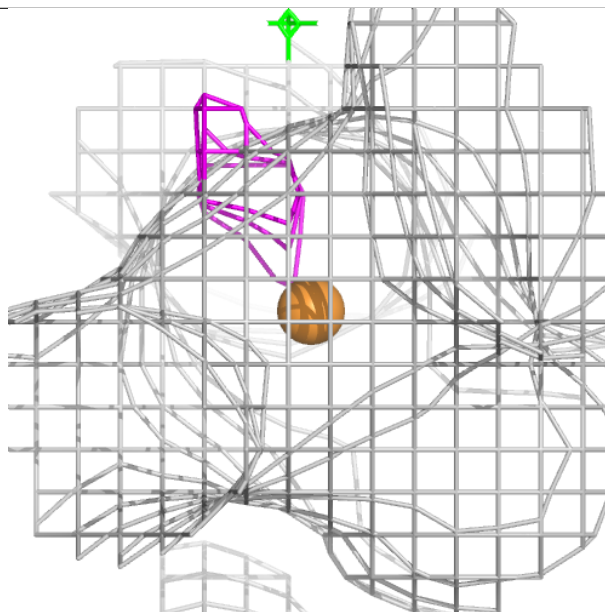
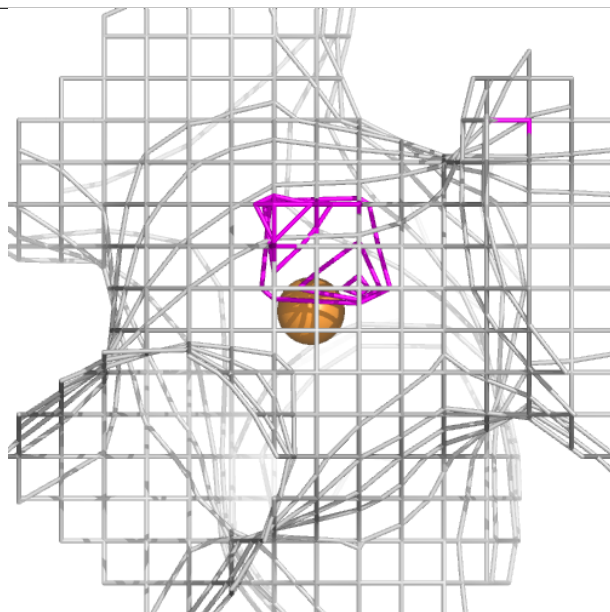
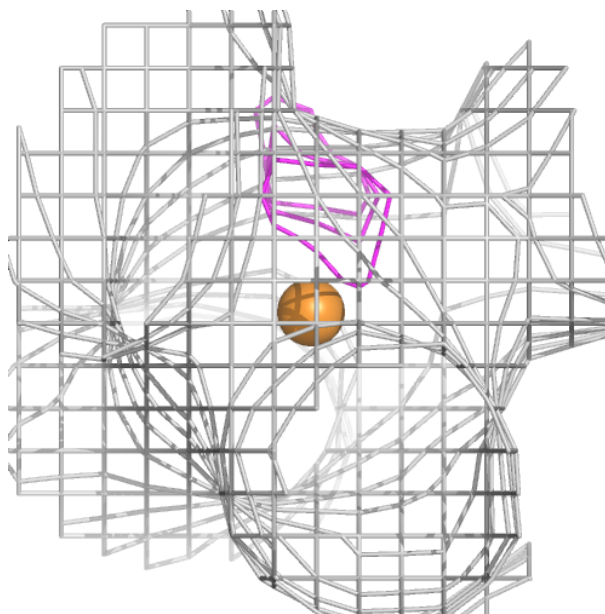
Electron density around CU AAA 601:

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



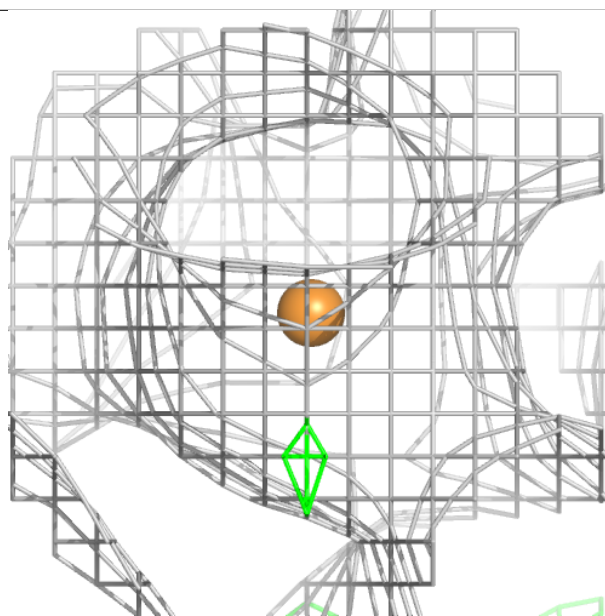
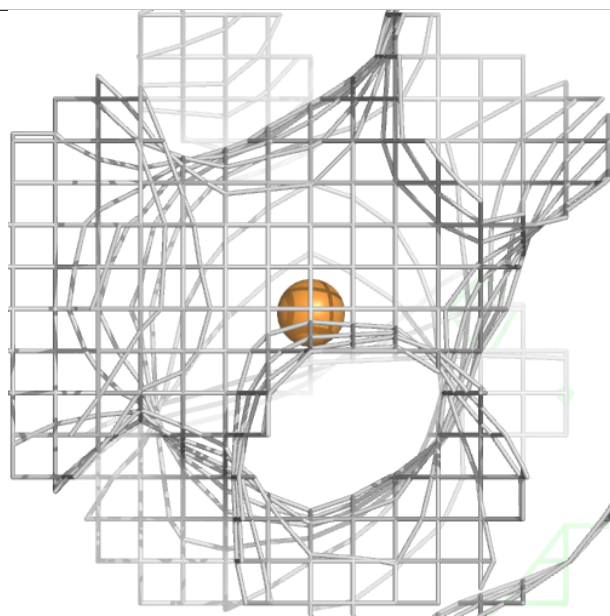
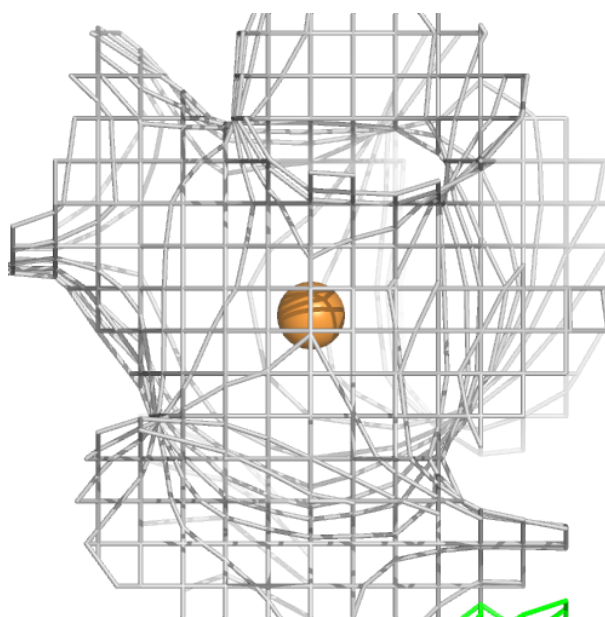
Electron density around CU AAA 602:

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



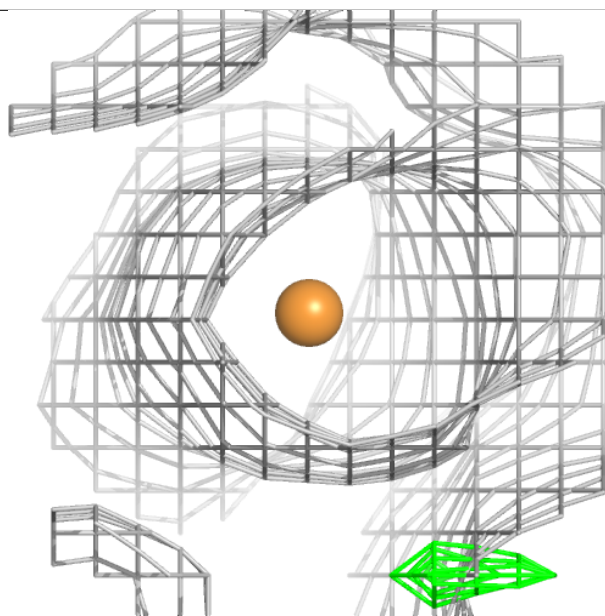
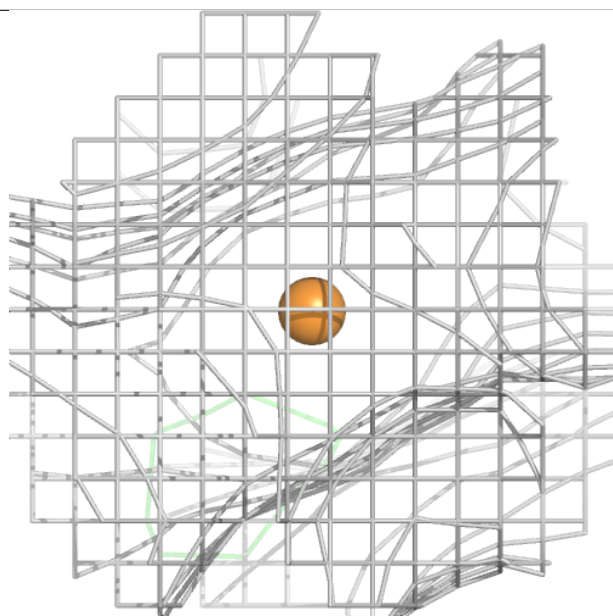
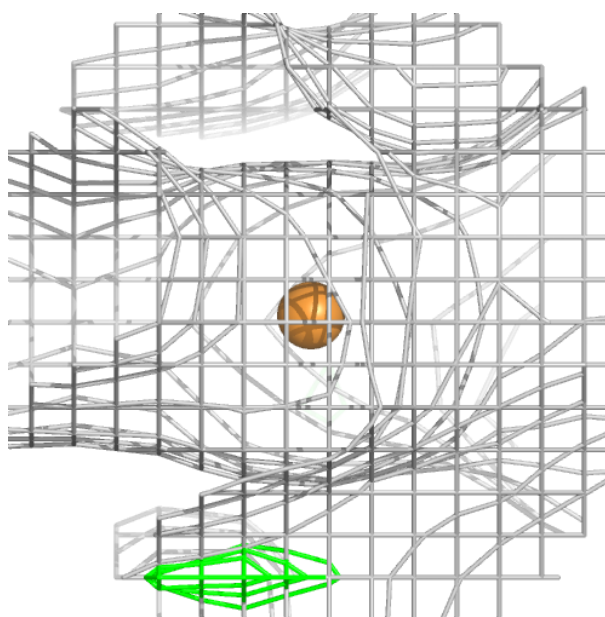
Electron density around CU AAA 603:

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



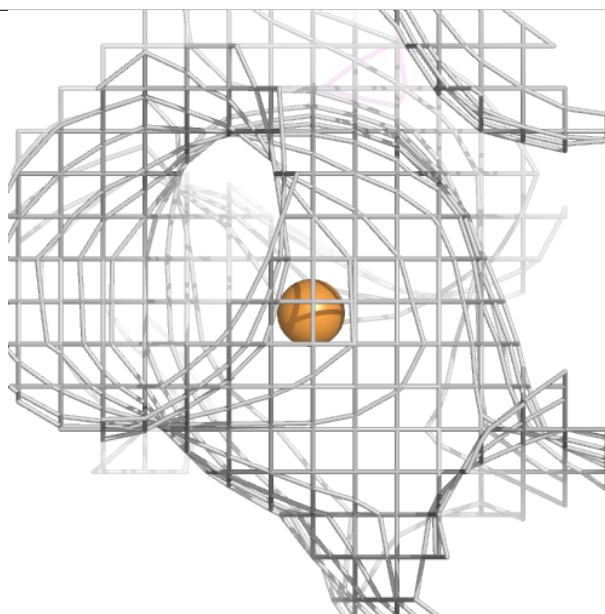
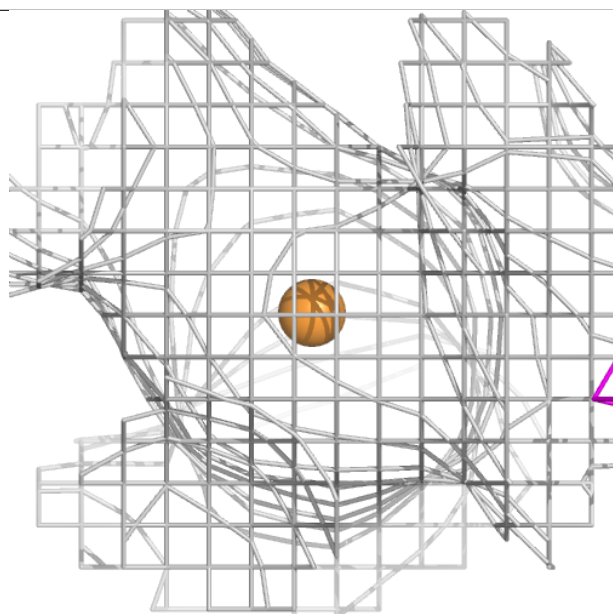
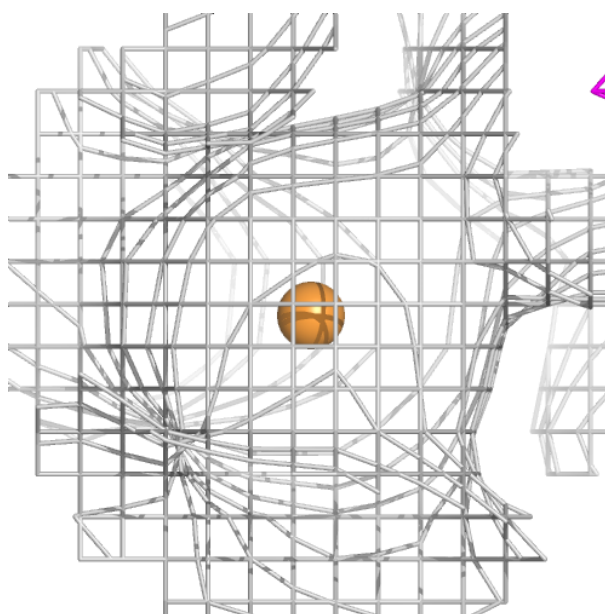
Electron density around CU AAA 604:

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



Electron density around CU BBB 601:

$2mF_o-DF_c$ (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.