



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:34 pm BST

PDB ID : 8RTQ / pdb_00008rtq
Title : Bilirubin oxidase from Myrothecium verrucaria with G395T mutation
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 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
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

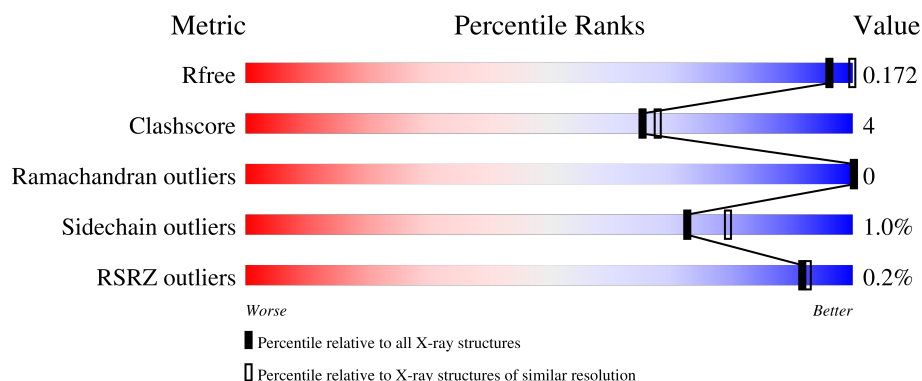
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





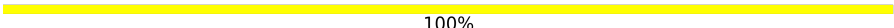
The reported resolution of this entry is 2.10 Å.

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.



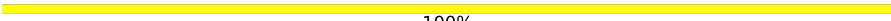
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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% 11%
1	BBB	534	 92% 7%
2	AeA	4	 25% 75%
3	AiA	2	 50% 50%
3	BhB	2	 100%

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Mol	Chain	Length	Quality of chain
4	BeB	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	BBB	610	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10072 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	15	0
			4336	2774	733	815	14			
1	BBB	534	Total	C	N	O	S	0	14	0
			4328	2764	733	817	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	395	THR	GLY	engineered mutation	UNP Q12737
BBB	395	THR	GLY	engineered mutation	UNP Q12737

- 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.



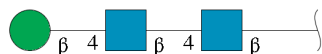
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AeA	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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	BhB	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

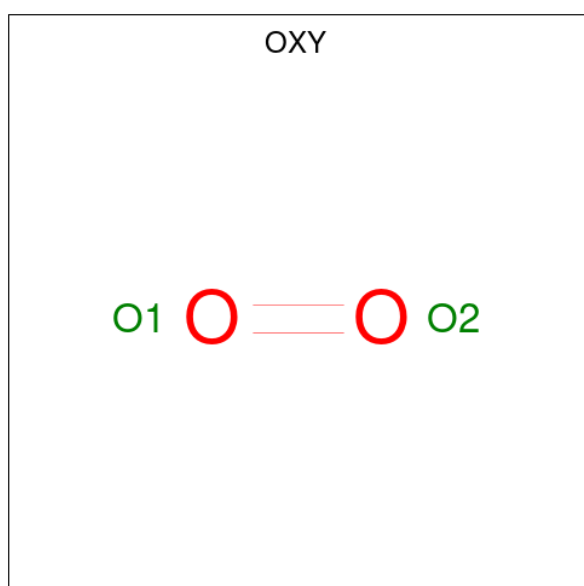


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	BeB	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

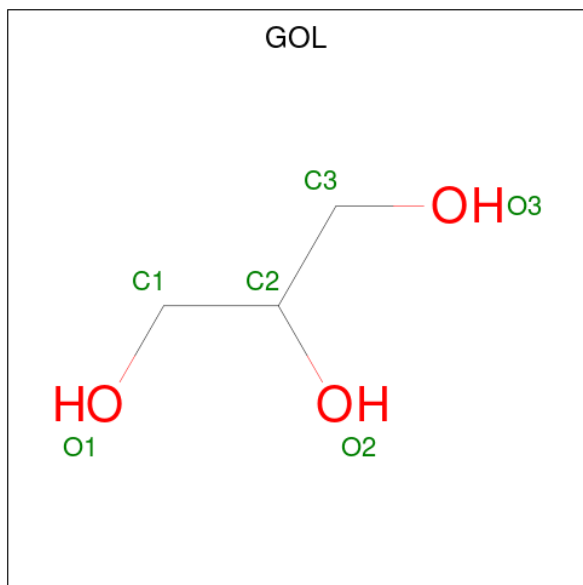
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	4	Total	Cu	0	0
			4	4		
5	BBB	4	Total	Cu	0	0
			4	4		

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



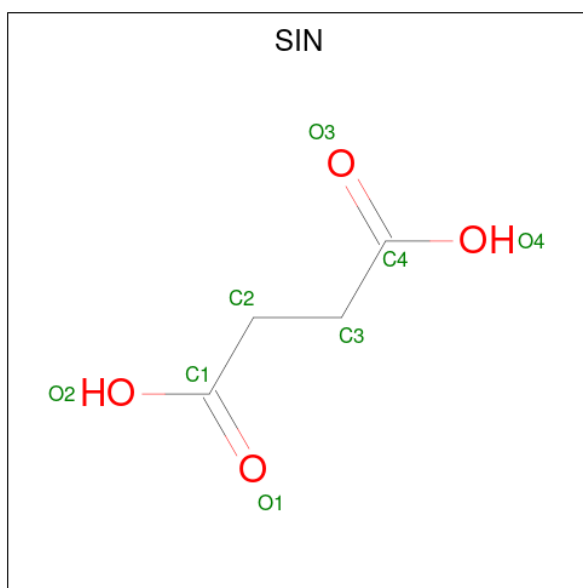
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total O 2 2	0	0
6	BBB	1	Total O 2 2	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	BBB	4	Total Cl 4 4	0	0

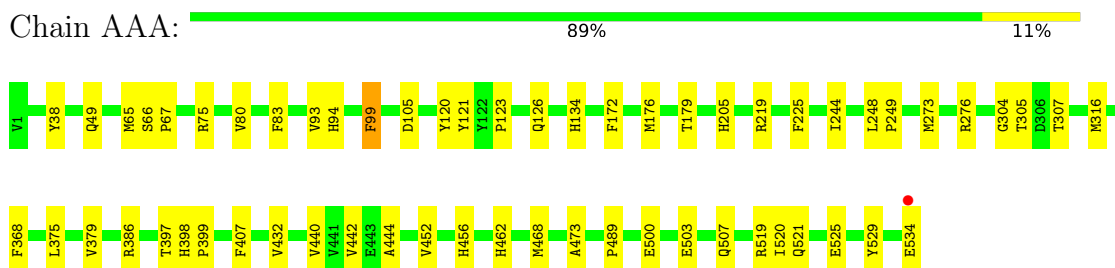
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	574	Total O 574 574	0	7
10	BBB	565	Total O 565 565	0	1

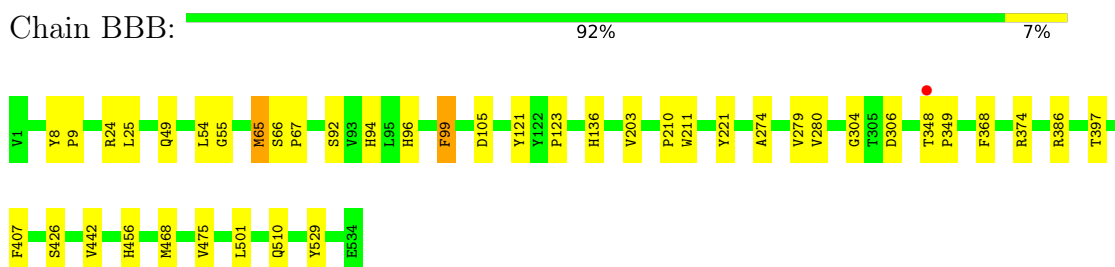
3 Residue-property plots

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 BhB:  100%

MAG1
MAG2

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

Chain BeB:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.22Å 200.68Å 216.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.10 47.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.66-2.10) 95.3 (47.66-2.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.153 , 0.197 0.162 , 0.172	Depositor DCC
R_{free} test set	4026 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10072	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: CU, NAG, SME, MAN, CL, SIN, BMA, OXY, GOL

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	1.03	3/4502 (0.1%)	1.22	1/6151 (0.0%)
1	BBB	1.03	1/4491 (0.0%)	1.22	5/6139 (0.1%)
All	All	1.03	4/8993 (0.0%)	1.22	6/12290 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	134	HIS	C-O	6.54	1.31	1.23
1	AAA	398	HIS	CE1-NE2	6.03	1.38	1.32
1	AAA	462	HIS	CE1-NE2	5.31	1.37	1.32
1	BBB	279	VAL	C-O	5.25	1.29	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	99	PHE	CA-CB-CG	6.04	119.84	113.80
1	BBB	99	PHE	CA-CB-CG	5.51	119.31	113.80
1	BBB	407	PHE	CA-CB-CG	5.28	119.08	113.80
1	BBB	501	LEU	CA-C-N	5.16	125.82	119.99
1	BBB	501	LEU	C-N-CA	5.16	125.82	119.99
1	BBB	510	GLN	CB-CA-C	5.10	119.81	110.11

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	4336	0	4159	31	0
1	BBB	4328	0	4133	28	0
2	AeA	50	0	43	0	0
3	AiA	28	0	25	1	0
3	BhB	28	0	25	0	0
4	BeB	39	0	34	0	0
5	AAA	4	0	0	0	0
5	BBB	4	0	0	0	0
6	AAA	2	0	0	0	0
6	BBB	2	0	0	0	0
7	AAA	36	0	48	5	0
7	BBB	24	0	32	5	0
8	AAA	24	0	12	3	0
8	BBB	24	0	12	0	0
9	BBB	4	0	0	0	0
10	AAA	574	0	0	8	0
10	BBB	565	0	0	2	0
All	All	10072	0	8523	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.

All (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)
7:AAA:610:GOL:H12	10:AAA:1071:HOH:O	1.62	0.98
1:AAA:525[B]:GLU:HG3	10:AAA:701:HOH:O	1.82	0.79
1:BBB:65:SME:HE3	10:BBB:792:HOH:O	1.82	0.79
1:AAA:489:PRO:HD2	8:AAA:613:SIN:O1	1.94	0.67
1:AAA:65:SME:HE3	10:AAA:769:HOH:O	1.98	0.62
1:BBB:475:VAL:HA	7:BBB:610:GOL:H31	1.82	0.61
7:AAA:607:GOL:H32	10:AAA:836:HOH:O	2.02	0.59
1:AAA:452:VAL:HG11	8:AAA:613:SIN:H32	1.87	0.57
1:AAA:534:GLU:HA	1:AAA:534:GLU:OE1	2.03	0.57
1:AAA:507:GLN:HG2	10:AAA:865:HOH:O	2.06	0.56
1:BBB:123:PRO:HB3	1:BBB:529:TYR:CG	2.42	0.55
1:BBB:475:VAL:CB	7:BBB:610:GOL:H31	2.38	0.54
8:AAA:613:SIN:H21	10:AAA:1099:HOH:O	2.06	0.54
1:AAA:273:MET:HE2	1:AAA:399:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:75[B]:ARG:HD2	1:AAA:126:GLN:O	2.08	0.53
1:AAA:407:PHE:HB3	1:AAA:444:ALA:HB2	1.91	0.53
1:AAA:305:THR:O	7:AAA:607:GOL:H11	2.08	0.52
1:AAA:38:TYR:CD1	1:AAA:520[A]:ILE:HD11	2.44	0.52
1:BBB:24:ARG:O	1:BBB:25[B]:LEU:HD13	2.09	0.52
1:BBB:49[A]:GLN:NE2	1:BBB:55:GLY:O	2.44	0.51
1:BBB:475:VAL:CA	7:BBB:610:GOL:H31	2.41	0.50
1:BBB:475:VAL:HG12	7:BBB:610:GOL:H31	1.93	0.49
1:BBB:456:HIS:HB3	1:BBB:468:MET:HG3	1.95	0.49
1:AAA:83:PHE:CG	1:AAA:93:VAL:HG21	2.48	0.49
1:BBB:348:THR:HG22	10:BBB:1003:HOH:O	2.13	0.49
1:AAA:456:HIS:HB3	1:AAA:468:MET:HG3	1.94	0.48
1:BBB:221:TYR:O	1:BBB:280:VAL:HA	2.13	0.48
1:BBB:8:TYR:CD2	1:BBB:9:PRO:HD2	2.50	0.47
1:BBB:304:GLY:HA2	1:BBB:397:THR:HG21	1.97	0.47
1:BBB:49[A]:GLN:NE2	1:BBB:54:LEU:O	2.48	0.46
1:AAA:66:SER:HA	1:AAA:67:PRO:C	2.39	0.46
10:AAA:701:HOH:O	3:AIa:2:NAG:H5	2.14	0.46
1:AAA:304:GLY:HA2	1:AAA:397:THR:HG21	1.98	0.46
1:AAA:386:ARG:HA	1:AAA:442:VAL:O	2.17	0.45
1:BBB:123:PRO:HB3	1:BBB:529:TYR:CD1	2.52	0.45
1:AAA:94:HIS:ND1	1:AAA:105:ASP:O	2.48	0.44
1:AAA:521:GLN:O	1:AAA:525[A]:GLU:HG2	2.17	0.44
1:BBB:203:VAL:HA	1:BBB:211:TRP:CH2	2.53	0.44
1:BBB:96:HIS:CE1	1:BBB:274:ALA:HB1	2.52	0.44
1:BBB:92:SER:O	1:BBB:136:HIS:N	2.51	0.44
1:BBB:426:SER:OG	7:BBB:612:GOL:H2	2.18	0.43
1:AAA:80:VAL:HA	1:AAA:120:TYR:O	2.16	0.43
1:AAA:248:LEU:HA	1:AAA:249:PRO:HD3	1.91	0.43
7:AAA:612:GOL:H11	10:AAA:1150:HOH:O	2.18	0.43
1:AAA:176:MET:HE1	1:AAA:316:MET:SD	2.59	0.42
1:AAA:500:GLU:O	1:AAA:503[A]:GLU:HB2	2.19	0.42
1:BBB:66:SER:HA	1:BBB:67:PRO:C	2.44	0.42
1:AAA:276:ARG:N	1:AAA:276:ARG:HD3	2.34	0.42
1:AAA:307:THR:HA	7:AAA:607:GOL:H31	2.02	0.41
1:BBB:8:TYR:CG	1:BBB:9:PRO:HD2	2.55	0.41
1:BBB:386:ARG:HA	1:BBB:442:VAL:O	2.19	0.41
1:AAA:432:VAL:HG21	1:AAA:440:VAL:HG11	2.02	0.41
1:AAA:379:VAL:O	1:AAA:473:ALA:HA	2.20	0.41
1:AAA:123:PRO:HB3	1:AAA:529:TYR:CG	2.56	0.41
1:AAA:172:PHE:CE1	1:AAA:219:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:348:THR:HA	1:BBB:349:PRO:HD3	1.96	0.41
1:BBB:368:PHE:HB2	1:BBB:468:MET:HB3	2.02	0.41
1:BBB:94:HIS:ND1	1:BBB:105:ASP:O	2.54	0.41
1:BBB:210:PRO:O	1:BBB:211:TRP:C	2.63	0.41
1:BBB:368:PHE:O	1:BBB:374:ARG:HD3	2.20	0.41
1:AAA:225:PHE:O	1:AAA:276:ARG:HA	2.20	0.41
1:AAA:179:THR:OG1	1:AAA:205:HIS:HB2	2.21	0.40
1:AAA:368:PHE:HB2	1:AAA:468:MET:HB3	2.04	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	546/534 (102%)	523 (96%)	23 (4%)	0	100	100
1	BBB	545/534 (102%)	518 (95%)	27 (5%)	0	100	100
All	All	1091/1068 (102%)	1041 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	468/453 (103%)	459 (98%)	9 (2%)	52	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BBB	467/453 (103%)	464 (99%)	3 (1%)	84	89
All	All	935/906 (103%)	923 (99%)	12 (1%)	73	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	49[A]	GLN
1	AAA	49[B]	GLN
1	AAA	99	PHE
1	AAA	121	TYR
1	AAA	244	ILE
1	AAA	375[A]	LEU
1	AAA	375[B]	LEU
1	AAA	519[A]	ARG
1	AAA	519[B]	ARG
1	BBB	99	PHE
1	BBB	121	TYR
1	BBB	306	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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SME	AAA	65	1	7,8,9	0.80	0	4,9,11	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SME	BBB	65	1	7,8,9	0.87	1 (14%)	4,9,11	1.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SME	AAA	65	1	-	1/6/7/9	-
1	SME	BBB	65	1	-	1/6/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	65	SME	OE-S	2.00	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	65	SME	CB-CG-S-CE
1	AAA	65	SME	CB-CG-S-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	65	SME	1	0
1	BBB	65	SME	1	0

5.5 Carbohydrates

11 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	2,1	14,14,15	1.34	2 (14%)	17,19,21	1.53	2 (11%)
2	NAG	AeA	2	2	14,14,15	0.68	0	17,19,21	1.50	3 (17%)
2	BMA	AeA	3	2	11,11,12	0.66	0	15,15,17	1.24	0
2	MAN	AeA	4	2	11,11,12	0.64	0	15,15,17	1.65	3 (20%)
3	NAG	AiA	1	3,1	14,14,15	0.66	0	17,19,21	1.07	2 (11%)
3	NAG	AiA	2	3	14,14,15	0.78	0	17,19,21	2.84	7 (41%)
4	NAG	BeB	1	4,1	14,14,15	0.80	0	17,19,21	1.37	2 (11%)
4	NAG	BeB	2	4	14,14,15	0.86	0	17,19,21	1.20	1 (5%)
4	BMA	BeB	3	4	11,11,12	1.01	0	15,15,17	1.39	3 (20%)
3	NAG	BhB	1	3,1	14,14,15	0.78	0	17,19,21	1.22	1 (5%)
3	NAG	BhB	2	3	14,14,15	0.79	0	17,19,21	1.92	6 (35%)

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	2,1	-	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
2	MAN	AeA	4	2	-	2/2/19/22	0/1/1/1
3	NAG	AiA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AiA	2	3	-	1/6/23/26	0/1/1/1
4	NAG	BeB	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	BeB	2	4	-	0/6/23/26	0/1/1/1
4	BMA	BeB	3	4	-	0/2/19/22	0/1/1/1
3	NAG	BhB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BhB	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AeA	1	NAG	C2-N2	-3.25	1.40	1.46
2	AeA	1	NAG	C1-C2	-2.08	1.49	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AiA	2	NAG	C1-C2-N2	7.04	122.51	110.49
3	AiA	2	NAG	C1-O5-C5	5.90	120.19	112.19
2	AeA	1	NAG	C2-N2-C7	-4.15	116.99	122.90
3	BhB	2	NAG	C3-C4-C5	-3.90	103.29	110.24
3	AiA	2	NAG	C2-N2-C7	-3.86	117.40	122.90
3	AiA	2	NAG	O3-C3-C2	-3.75	101.70	109.47
2	AeA	2	NAG	C1-O5-C5	-3.58	107.34	112.19
3	BhB	2	NAG	O4-C4-C5	3.52	118.04	109.30
3	BhB	2	NAG	O5-C1-C2	-3.44	105.86	111.29
4	BeB	1	NAG	O4-C4-C3	-3.41	102.46	110.35
2	AeA	4	MAN	C3-C4-C5	3.41	116.32	110.24
2	AeA	4	MAN	C2-C3-C4	3.21	116.46	110.89
2	AeA	1	NAG	O4-C4-C3	-2.90	103.64	110.35
2	AeA	2	NAG	C2-N2-C7	-2.87	118.81	122.90
2	AeA	4	MAN	C1-C2-C3	2.76	113.06	109.67
3	BhB	1	NAG	O5-C5-C6	2.64	111.34	107.20
4	BeB	3	BMA	O5-C5-C6	2.63	111.33	107.20
4	BeB	3	BMA	O5-C1-C2	-2.53	106.86	110.77
3	BhB	2	NAG	C8-C7-N2	-2.46	111.93	116.10
4	BeB	1	NAG	C1-C2-N2	-2.45	106.30	110.49
2	AeA	2	NAG	O5-C1-C2	-2.44	107.43	111.29
3	AiA	2	NAG	C6-C5-C4	-2.34	107.53	113.00
4	BeB	2	NAG	O5-C5-C6	-2.29	103.61	107.20
3	AiA	1	NAG	C1-C2-N2	-2.29	106.57	110.49
4	BeB	3	BMA	C3-C4-C5	2.27	114.29	110.24
3	AiA	2	NAG	O5-C5-C6	2.26	110.75	107.20
3	BhB	2	NAG	C1-C2-N2	2.25	114.33	110.49
3	AiA	2	NAG	O5-C5-C4	2.05	115.81	110.83
3	AiA	1	NAG	C8-C7-N2	-2.05	112.64	116.10
3	BhB	2	NAG	O3-C3-C4	-2.02	105.67	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

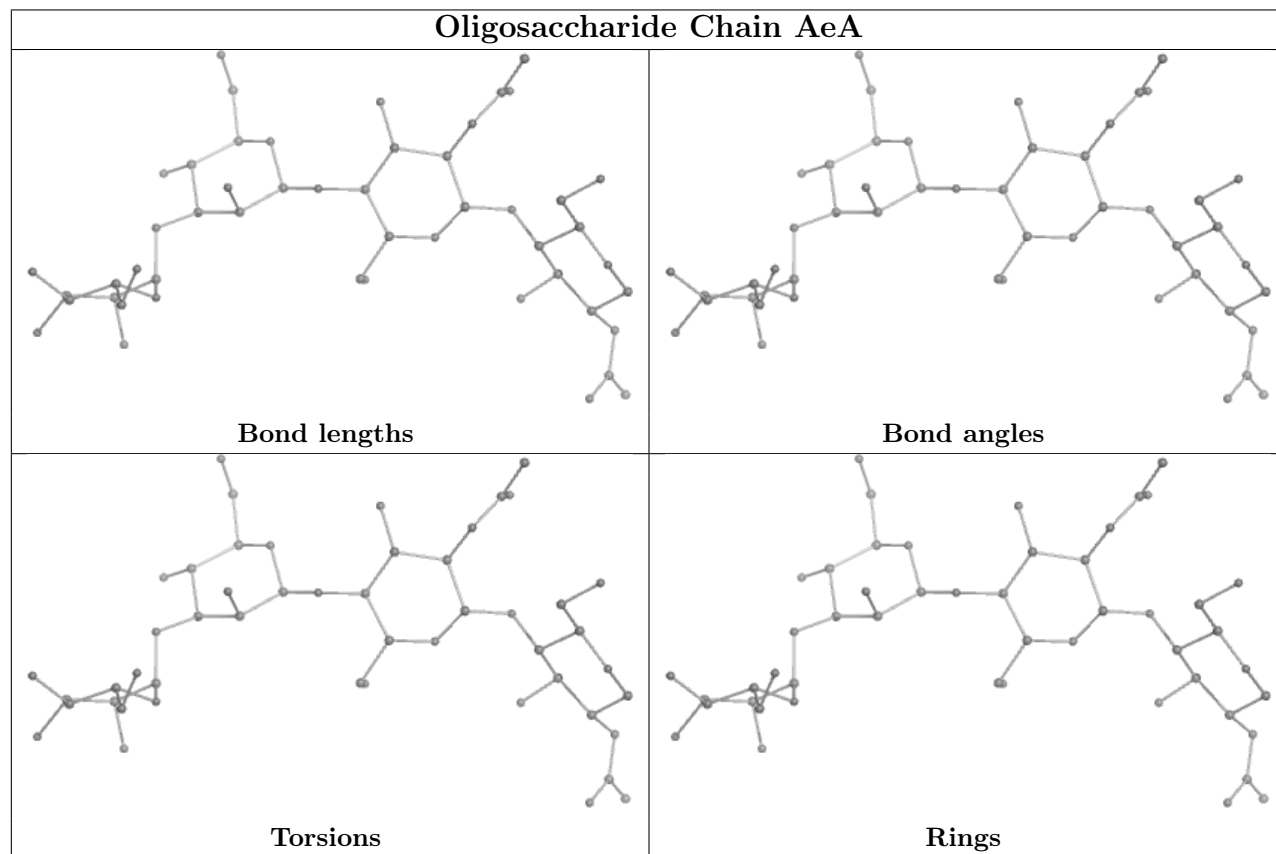
Mol	Chain	Res	Type	Atoms
2	AeA	4	MAN	C4-C5-C6-O6
2	AeA	4	MAN	O5-C5-C6-O6
3	AiA	2	NAG	C8-C7-N2-C2

There are no ring outliers.

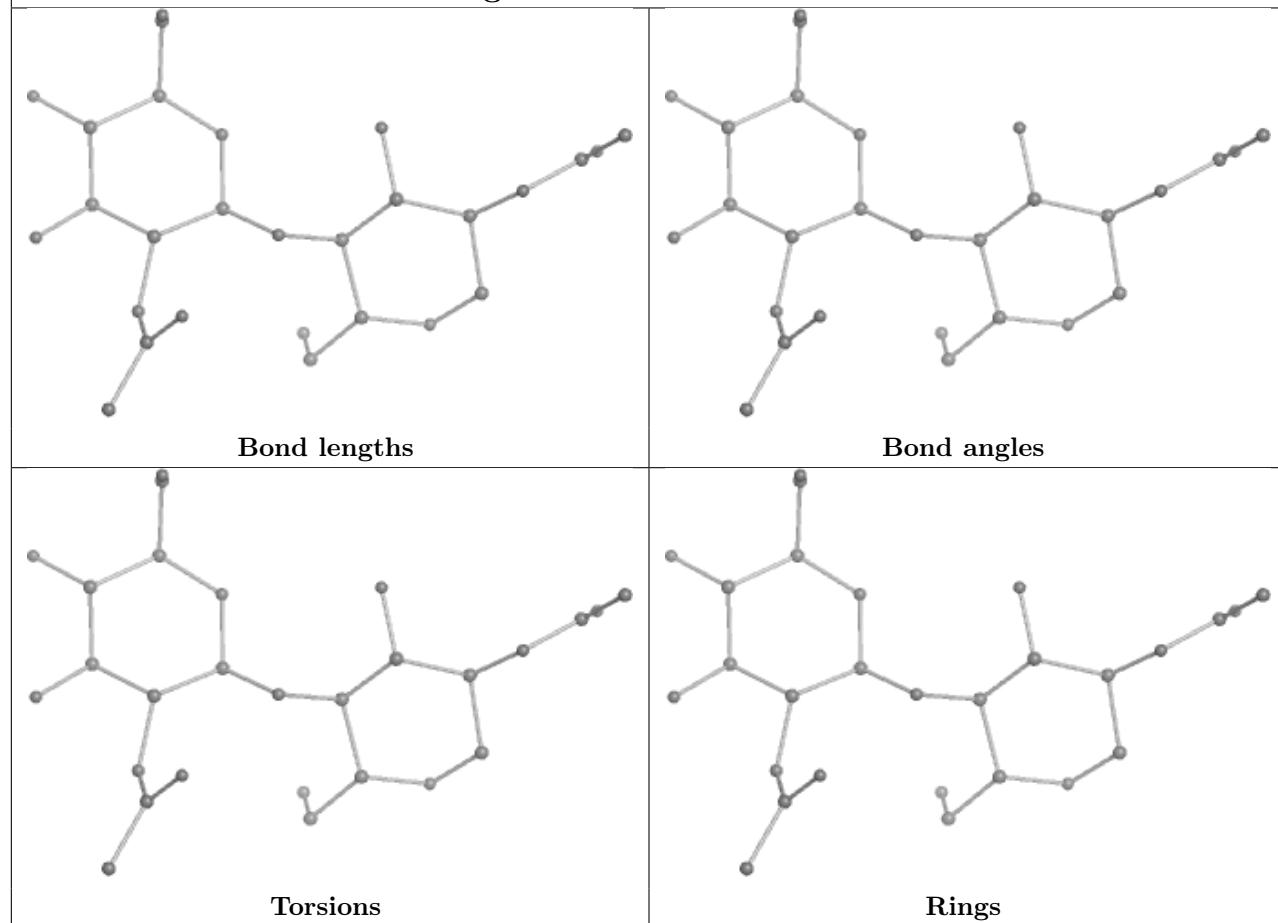
1 monomer is involved in 1 short contact:

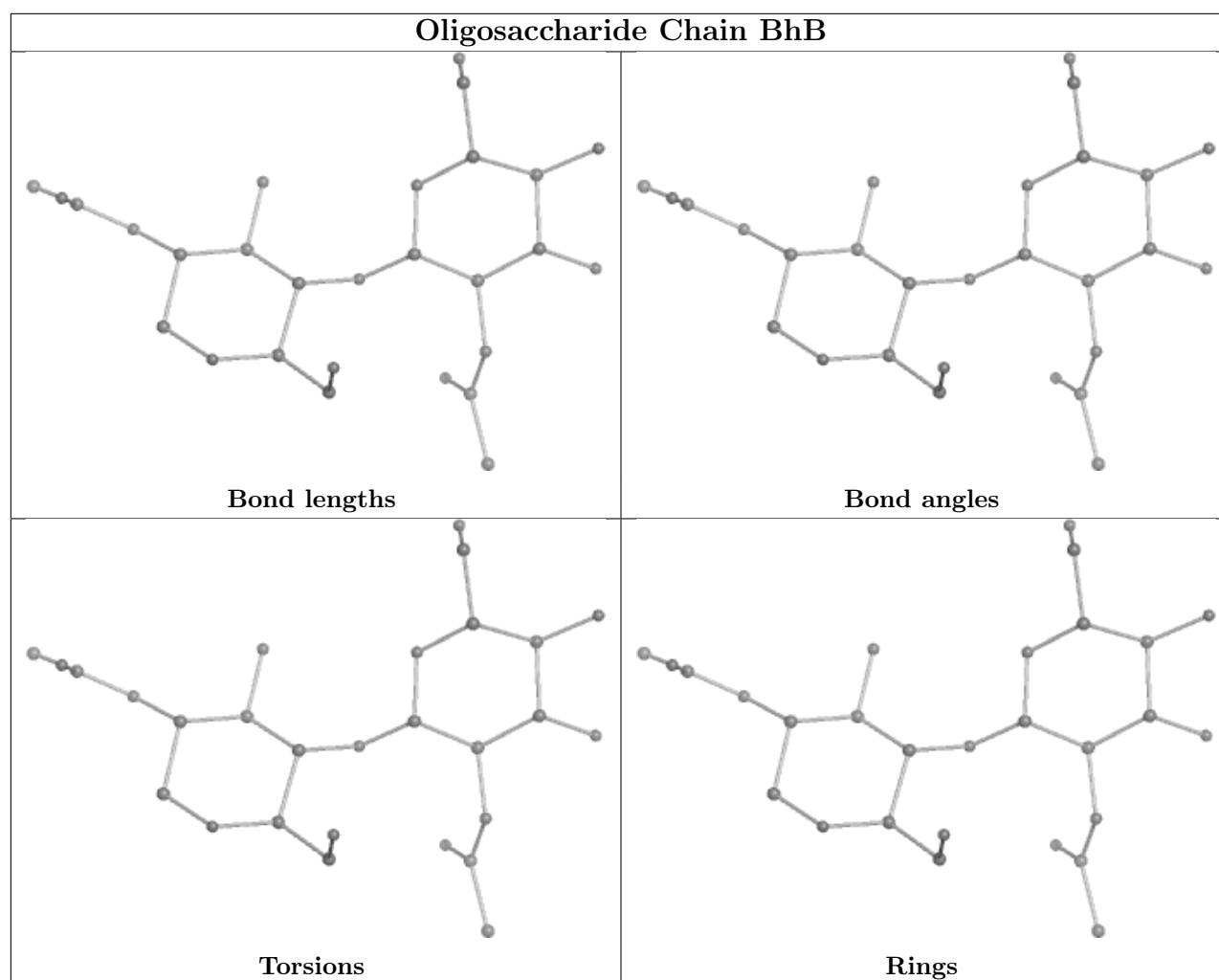
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AiA	2	NAG	1	0

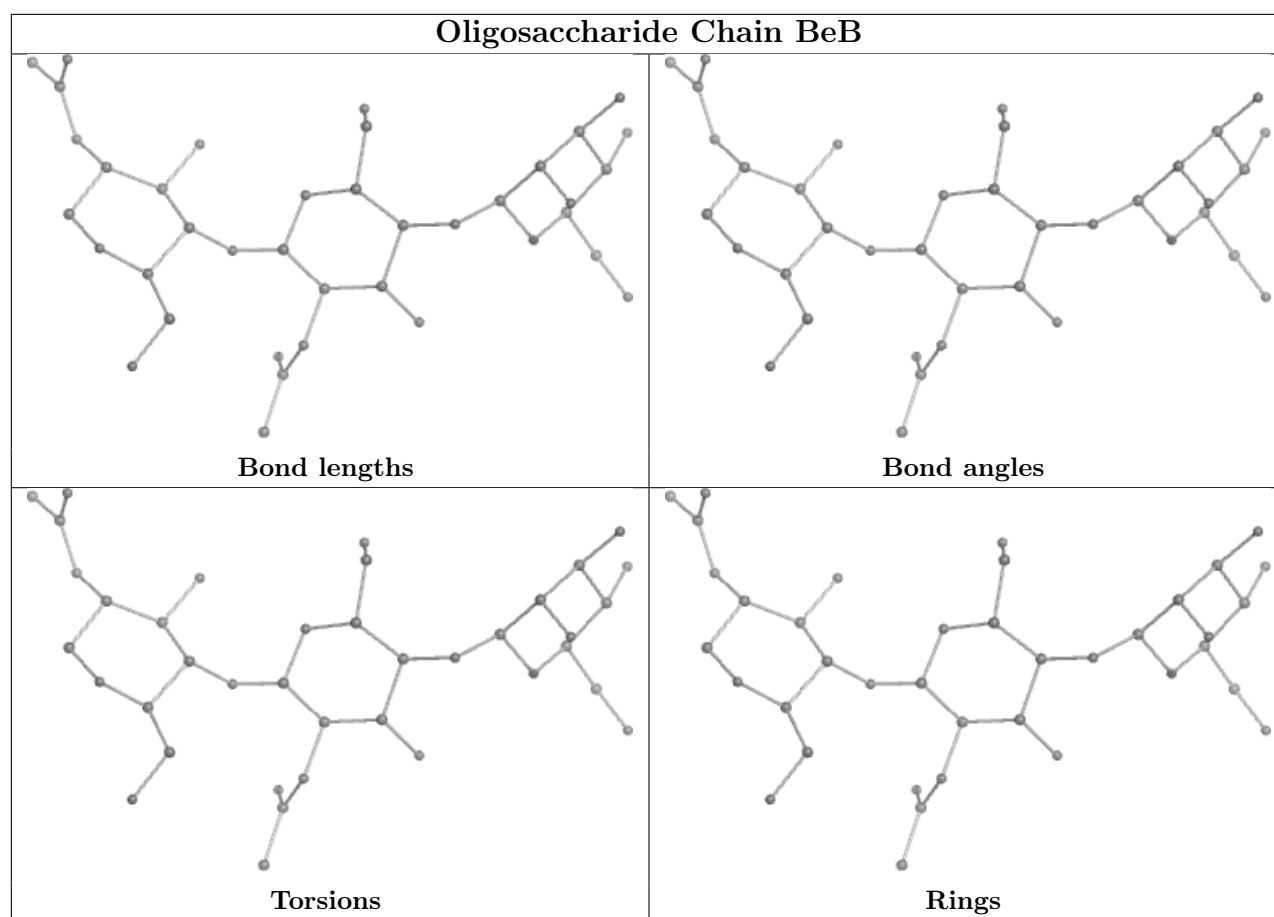
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain AiA







5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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	$\# Z > 2$
7	GOL	AAA	607	-	5,5,5	0.22	0	5,5,5	0.58	0
8	SIN	BBB	611	-	7,7,7	1.26	0	8,8,8	0.88	0
6	OXY	BBB	605	5	1,1,1	0.54	0	-		
7	GOL	AAA	610	-	5,5,5	0.39	0	5,5,5	0.82	0
7	GOL	BBB	606	-	5,5,5	0.13	0	5,5,5	0.34	0
8	SIN	AAA	613	-	7,7,7	0.85	0	8,8,8	1.46	1 (12%)
8	SIN	BBB	609	-	7,7,7	1.45	1 (14%)	8,8,8	1.27	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	AAA	612	-	5,5,5	0.11	0	5,5,5	0.32	0
7	GOL	BBB	612	-	5,5,5	0.24	0	5,5,5	0.48	0
8	SIN	AAA	608	-	7,7,7	1.12	0	8,8,8	1.00	0
7	GOL	BBB	610	-	5,5,5	0.23	0	5,5,5	0.64	0
7	GOL	AAA	614	-	5,5,5	0.30	0	5,5,5	0.72	0
7	GOL	BBB	607	-	5,5,5	0.25	0	5,5,5	0.40	0
8	SIN	AAA	609	-	7,7,7	1.78	1 (14%)	8,8,8	1.59	2 (25%)
8	SIN	BBB	608	-	7,7,7	1.15	0	8,8,8	0.95	0
7	GOL	AAA	611	-	5,5,5	0.24	0	5,5,5	0.54	0
6	OXY	AAA	605	5	1,1,1	0.67	0	-		
7	GOL	AAA	606	-	5,5,5	0.11	0	5,5,5	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	AAA	607	-	-	0/4/4/4	-
8	SIN	BBB	611	-	-	3/5/5/5	-
7	GOL	AAA	610	-	-	4/4/4/4	-
8	SIN	AAA	613	-	-	2/5/5/5	-
7	GOL	BBB	606	-	-	4/4/4/4	-
8	SIN	BBB	609	-	-	0/5/5/5	-
7	GOL	AAA	612	-	-	3/4/4/4	-
7	GOL	BBB	612	-	-	2/4/4/4	-
8	SIN	AAA	608	-	-	2/5/5/5	-
7	GOL	BBB	610	-	-	2/4/4/4	-
7	GOL	AAA	614	-	-	2/4/4/4	-
7	GOL	BBB	607	-	-	2/4/4/4	-
8	SIN	AAA	609	-	-	3/5/5/5	-
8	SIN	BBB	608	-	-	0/5/5/5	-
7	GOL	AAA	611	-	-	2/4/4/4	-
7	GOL	AAA	606	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AAA	609	SIN	O1-C1	2.75	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BBB	609	SIN	O4-C4	-2.00	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AAA	609	SIN	C3-C2-C1	3.76	121.70	113.60
8	BBB	609	SIN	C2-C3-C4	2.59	119.18	113.60
8	AAA	613	SIN	O3-C4-C3	-2.35	115.55	123.08
8	BBB	609	SIN	C3-C2-C1	2.18	118.30	113.60
8	AAA	609	SIN	C2-C3-C4	2.01	117.92	113.60

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AAA	610	GOL	C1-C2-C3-O3
7	AAA	612	GOL	O1-C1-C2-O2
7	AAA	612	GOL	O1-C1-C2-C3
7	BBB	606	GOL	O1-C1-C2-C3
7	BBB	606	GOL	C1-C2-C3-O3
7	BBB	607	GOL	C1-C2-C3-O3
7	BBB	607	GOL	O2-C2-C3-O3
7	BBB	612	GOL	C1-C2-C3-O3
8	AAA	609	SIN	C1-C2-C3-C4
8	BBB	611	SIN	C1-C2-C3-C4
7	AAA	611	GOL	C1-C2-C3-O3
7	AAA	612	GOL	C1-C2-C3-O3
7	AAA	614	GOL	C1-C2-C3-O3
7	BBB	610	GOL	C1-C2-C3-O3
7	AAA	610	GOL	O2-C2-C3-O3
7	AAA	611	GOL	O2-C2-C3-O3
7	AAA	614	GOL	O2-C2-C3-O3
7	BBB	606	GOL	O2-C2-C3-O3
7	BBB	612	GOL	O2-C2-C3-O3
7	AAA	610	GOL	O1-C1-C2-O2
7	BBB	606	GOL	O1-C1-C2-O2
7	BBB	610	GOL	O2-C2-C3-O3
8	BBB	611	SIN	O1-C1-C2-C3
8	AAA	613	SIN	O2-C1-C2-C3
8	AAA	613	SIN	O1-C1-C2-C3
8	BBB	611	SIN	O2-C1-C2-C3
8	AAA	608	SIN	C2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
7	AAA	610	GOL	O1-C1-C2-C3
8	AAA	609	SIN	C2-C3-C4-O4
8	AAA	608	SIN	C2-C3-C4-O4
8	AAA	609	SIN	C2-C3-C4-O3
7	AAA	606	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	607	GOL	3	0
7	AAA	610	GOL	1	0
8	AAA	613	SIN	3	0
7	AAA	612	GOL	1	0
7	BBB	612	GOL	1	0
7	BBB	610	GOL	4	0

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	533/534 (99%)	-0.73	1 (0%) 92 92	9, 18, 31, 69	16 (3%)
1	BBB	533/534 (99%)	-0.63	1 (0%) 92 92	11, 21, 34, 61	14 (2%)
All	All	1066/1068 (99%)	-0.68	2 (0%) 92 92	9, 19, 33, 69	30 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	534	GLU	2.2
1	BBB	348	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SME	AAA	65	9/10	0.98	0.06	18,19,25,27	0
1	SME	BBB	65	9/10	0.98	0.05	19,20,25,27	0

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	-	-	19,21,27,30	0

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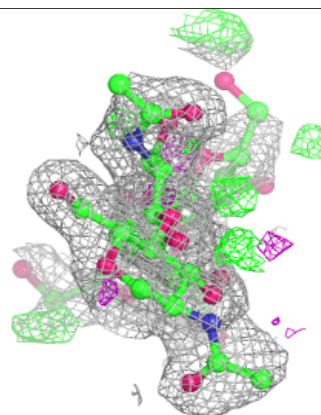
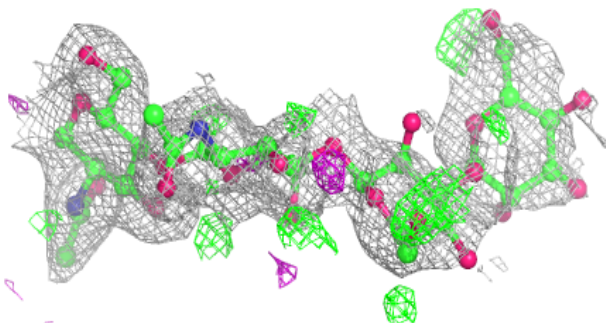
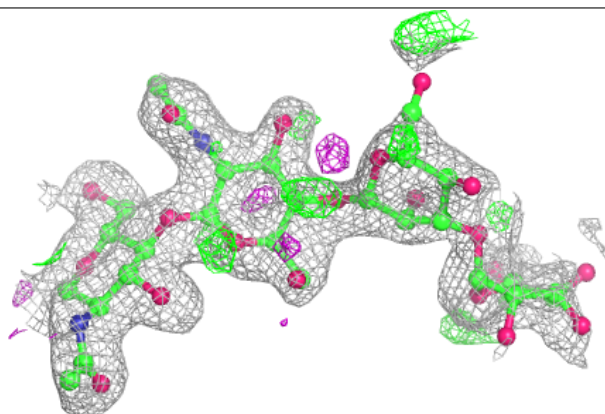
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	AeA	2	14/15	-	-	32,46,58,73	0
2	BMA	AeA	3	11/12	-	-	84,90,98,98	0
2	MAN	AeA	4	11/12	-	-	80,94,98,98	0
3	NAG	AiA	1	14/15	-	-	19,23,27,27	0
3	NAG	AiA	2	14/15	-	-	36,47,60,60	0
3	NAG	BhB	1	14/15	-	-	23,24,28,31	0
3	NAG	BhB	2	14/15	-	-	38,48,58,65	0
4	NAG	BeB	1	14/15	-	-	21,25,28,31	0
4	NAG	BeB	2	14/15	-	-	37,43,54,67	0
4	BMA	BeB	3	11/12	-	-	66,77,82,83	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.

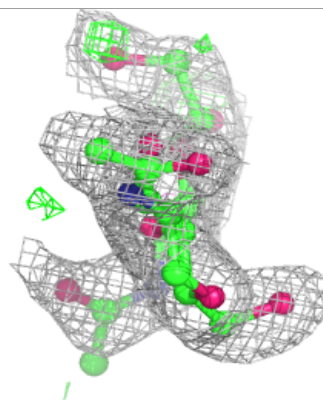
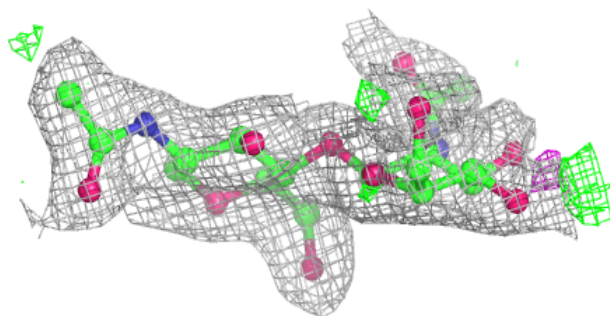
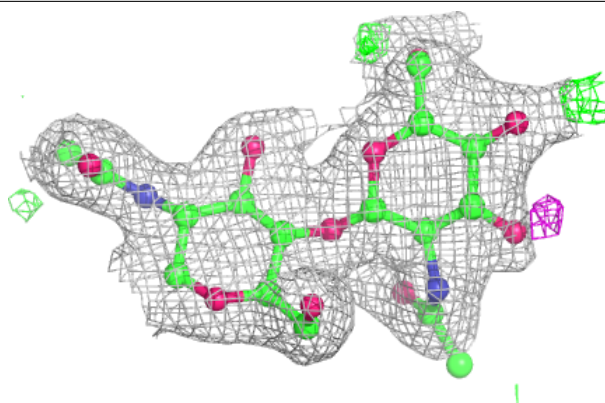
Electron density around Chain AeA:

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

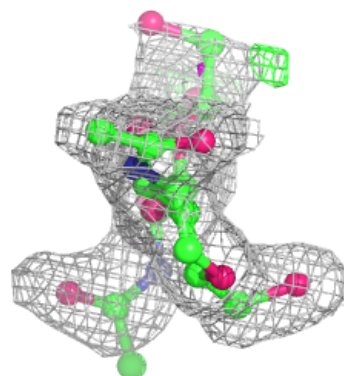
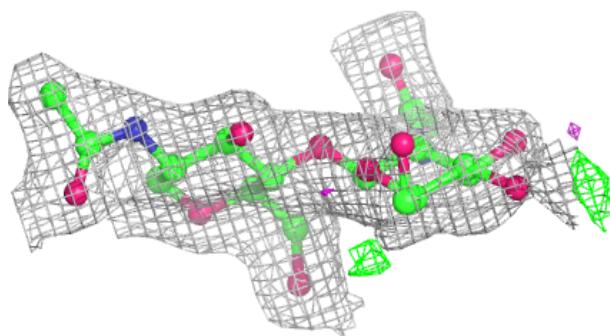
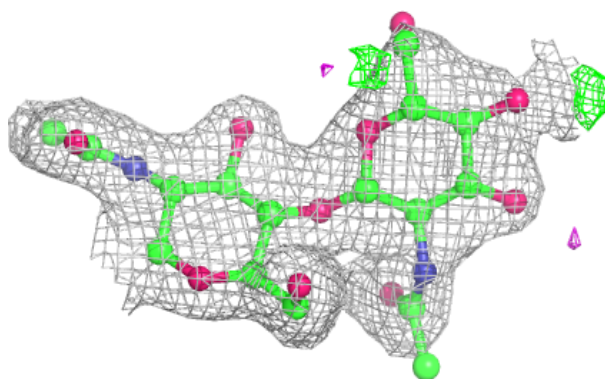


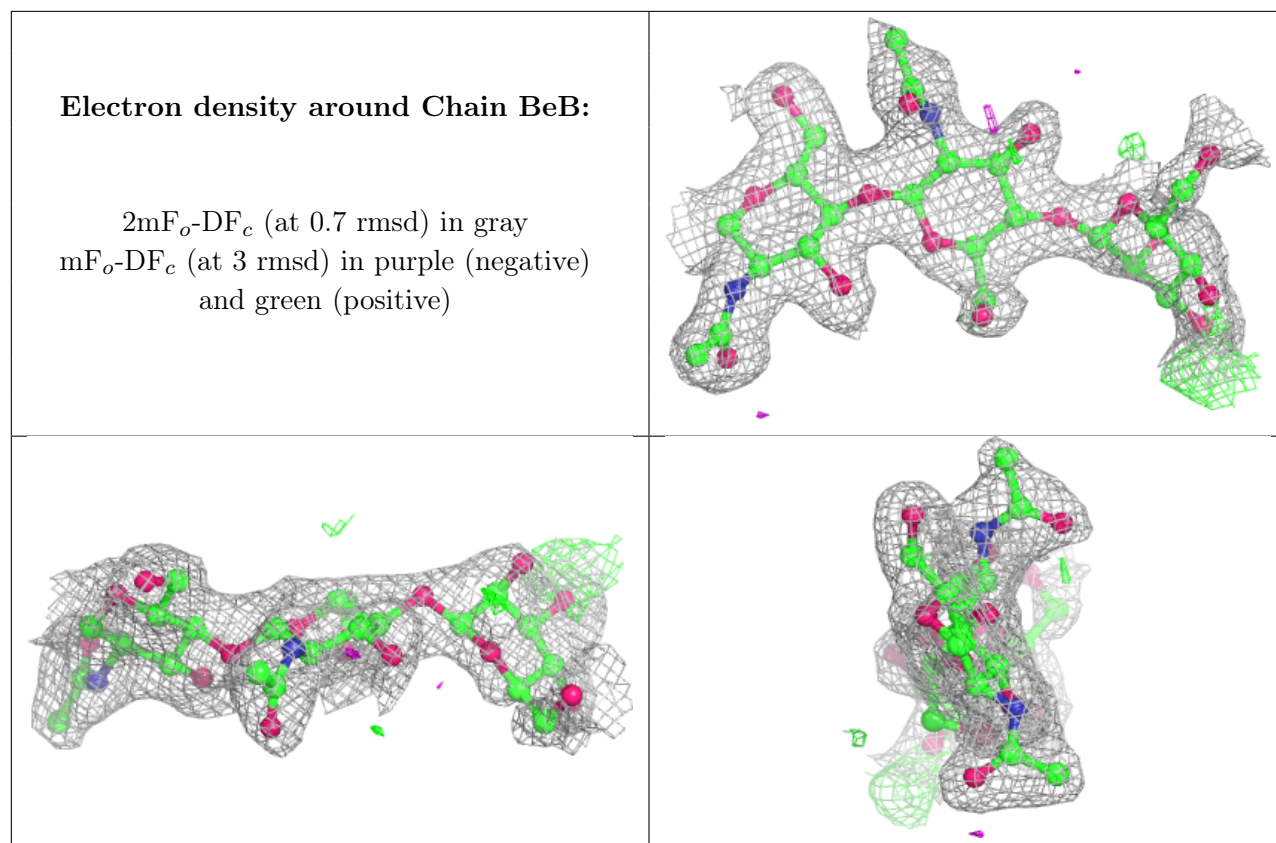
Electron density around Chain AiA:

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

**Electron density around Chain BhB:**

$2mF_o-DF_c$ (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
8	SIN	BBB	609	8/8	0.85	0.13	26,31,38,40	0
8	SIN	AAA	609	8/8	0.87	0.13	21,29,32,36	0
7	GOL	AAA	606	6/6	0.87	0.15	50,52,57,57	0
7	GOL	AAA	614	6/6	0.89	0.14	36,45,47,48	0
8	SIN	AAA	613	8/8	0.89	0.14	37,43,52,53	0
7	GOL	BBB	610	6/6	0.89	0.13	39,44,46,47	0
7	GOL	AAA	610	6/6	0.90	0.14	33,42,45,50	0
7	GOL	BBB	607	6/6	0.90	0.14	34,41,43,44	0
8	SIN	BBB	611	8/8	0.90	0.13	38,48,56,58	0
7	GOL	AAA	611	6/6	0.93	0.11	37,43,45,46	0
7	GOL	BBB	612	6/6	0.93	0.12	35,47,48,49	0
7	GOL	AAA	612	6/6	0.93	0.10	42,52,54,59	0
9	CL	BBB	614	1/1	0.93	0.11	57,57,57,57	0
7	GOL	AAA	607	6/6	0.94	0.11	34,40,43,43	0

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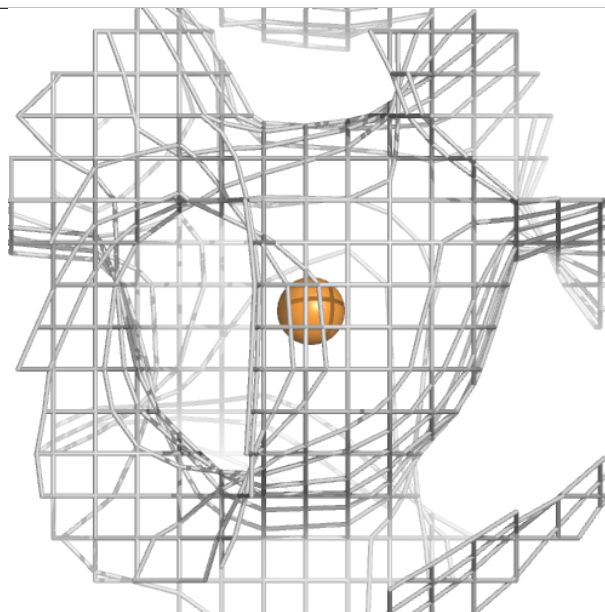
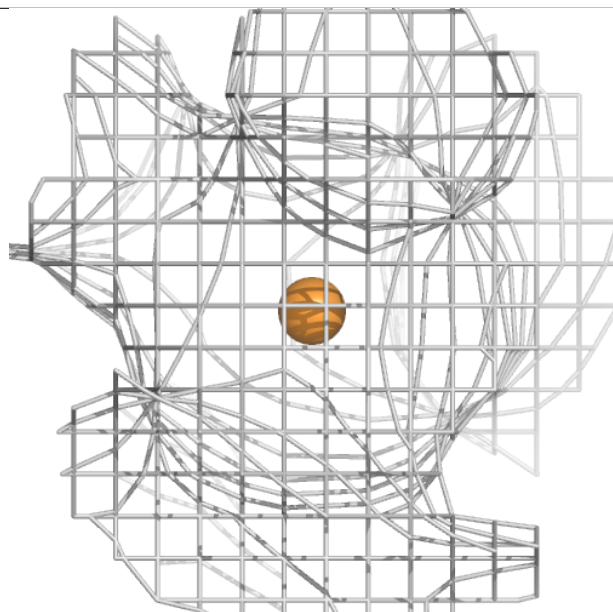
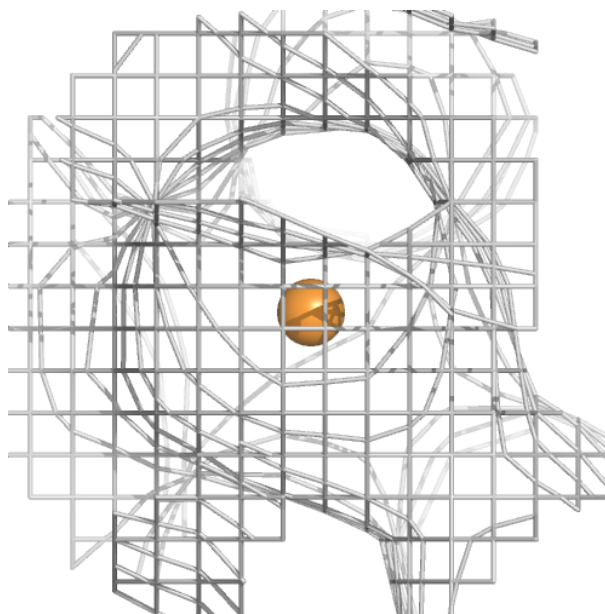
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	BBB	606	6/6	0.95	0.07	30,35,36,37	0
9	CL	BBB	613	1/1	0.96	0.09	58,58,58,58	0
8	SIN	BBB	608	8/8	0.96	0.08	22,26,34,37	0
9	CL	BBB	616	1/1	0.96	0.07	55,55,55,55	0
9	CL	BBB	615	1/1	0.97	0.08	60,60,60,60	0
8	SIN	AAA	608	8/8	0.97	0.05	19,20,23,26	0
6	OXY	AAA	605	2/2	0.99	0.04	9,9,9,9	0
6	OXY	BBB	605	2/2	0.99	0.04	13,13,13,13	0
5	CU	BBB	603	1/1	1.00	0.01	19,19,19,19	0
5	CU	BBB	604	1/1	1.00	0.03	21,21,21,21	0
5	CU	AAA	601	1/1	1.00	0.01	16,16,16,16	0
5	CU	AAA	602	1/1	1.00	0.01	18,18,18,18	0
5	CU	AAA	603	1/1	1.00	0.01	16,16,16,16	0
5	CU	AAA	604	1/1	1.00	0.01	18,18,18,18	0
5	CU	BBB	601	1/1	1.00	0.01	17,17,17,17	0
5	CU	BBB	602	1/1	1.00	0.01	18,18,18,18	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.

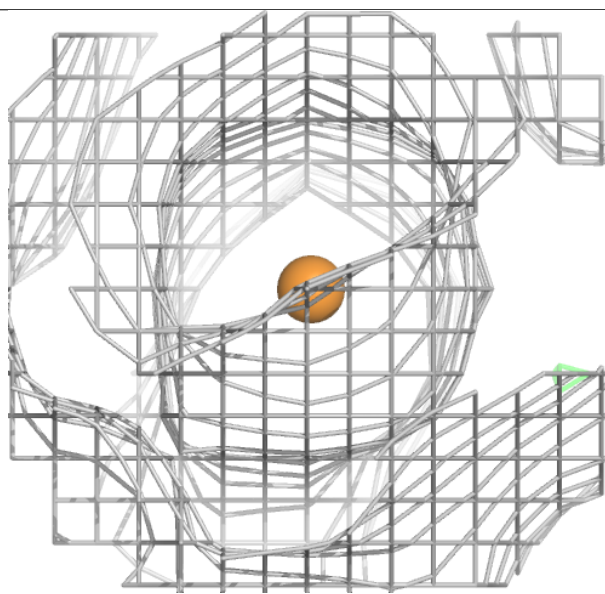
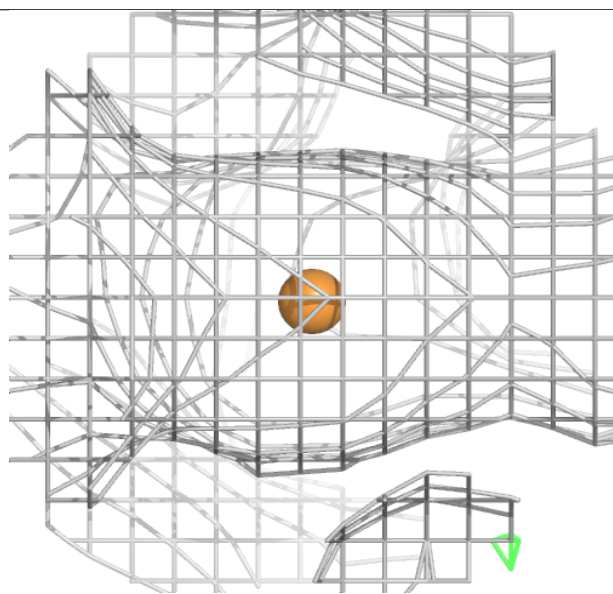
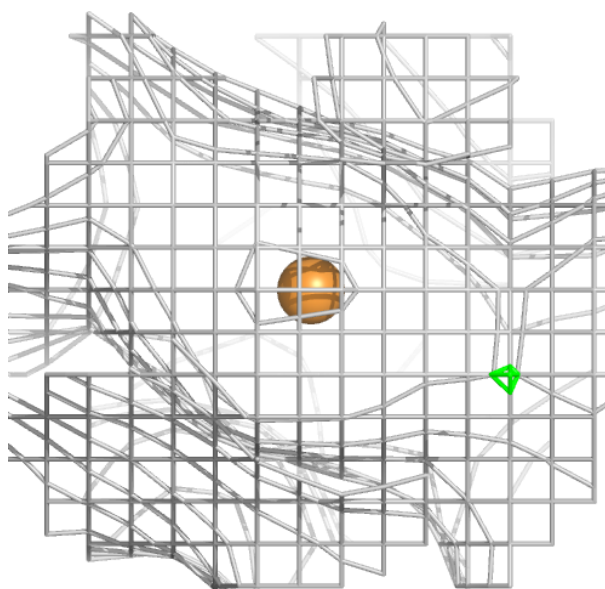
Electron density around CU BBB 603:

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



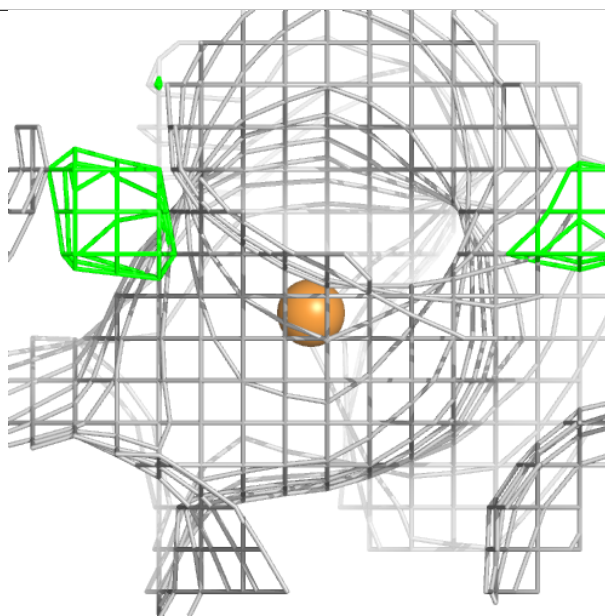
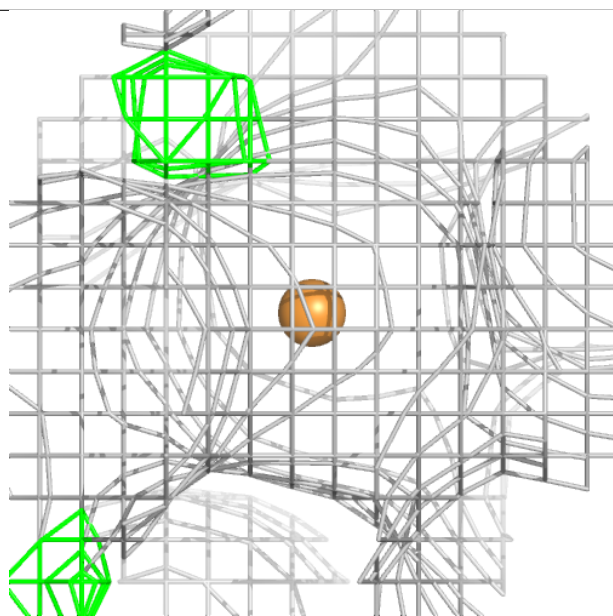
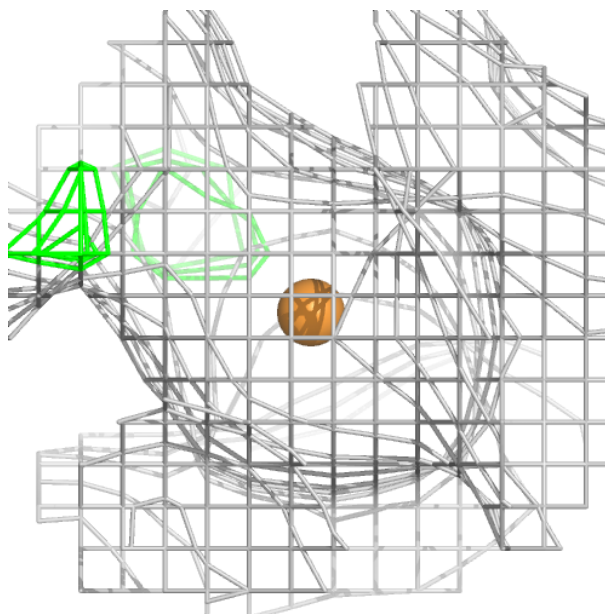
Electron density around CU BBB 604:

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



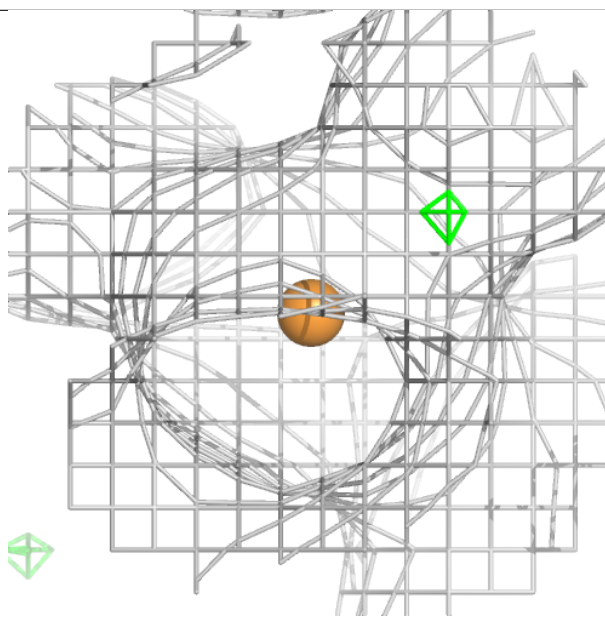
Electron density around CU AAA 601:

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



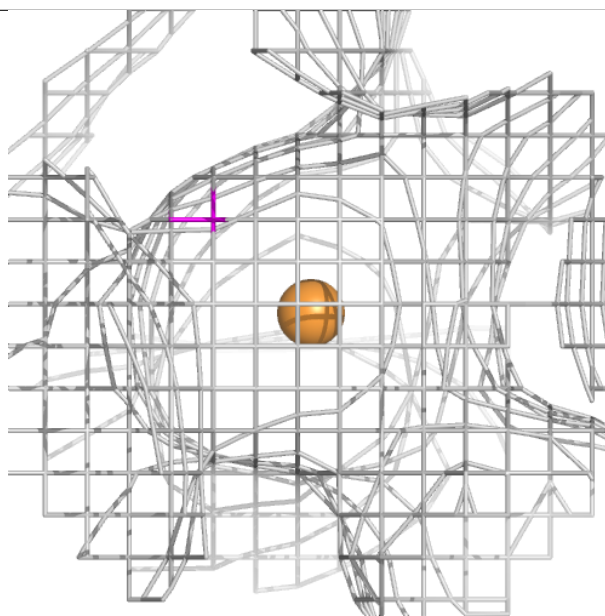
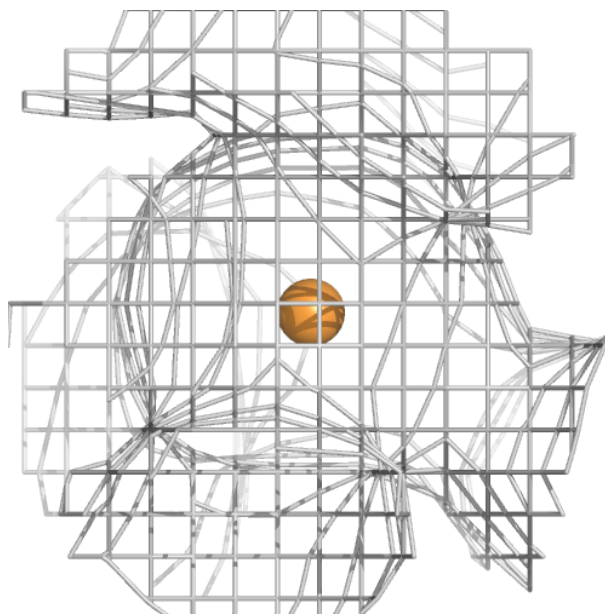
Electron density around CU AAA 602:

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



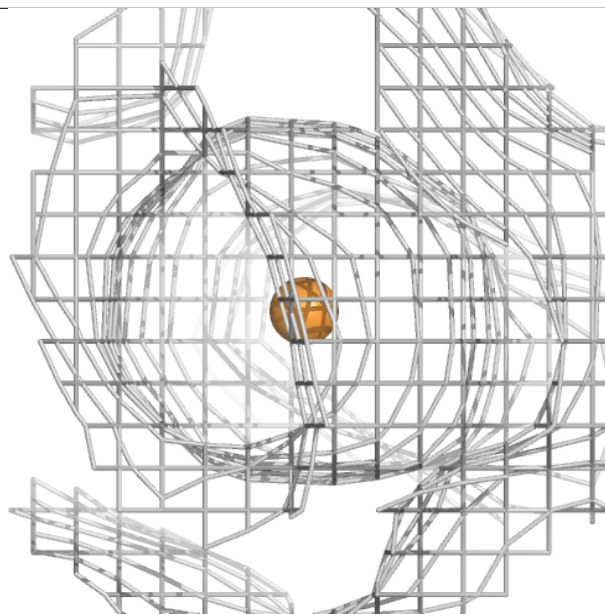
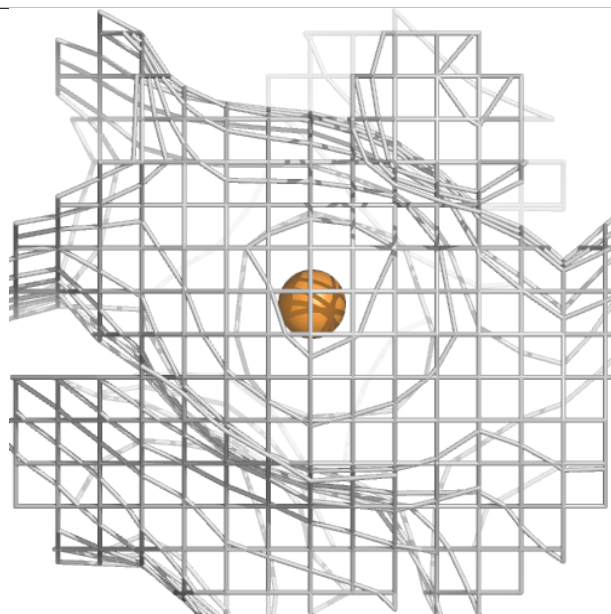
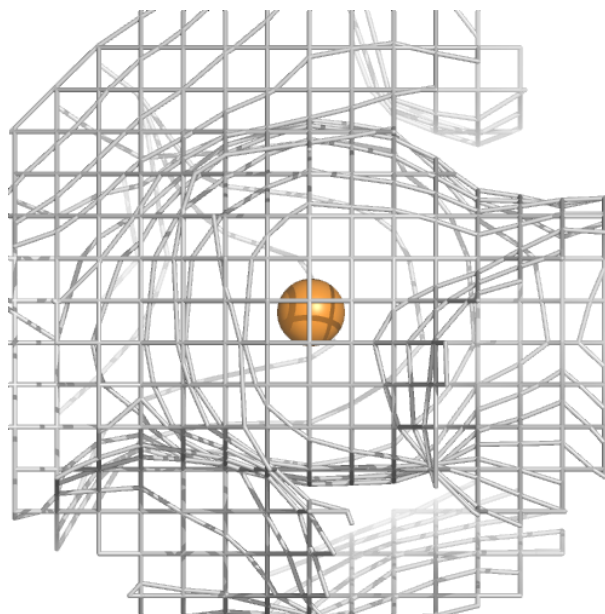
Electron density around CU AAA 603:

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



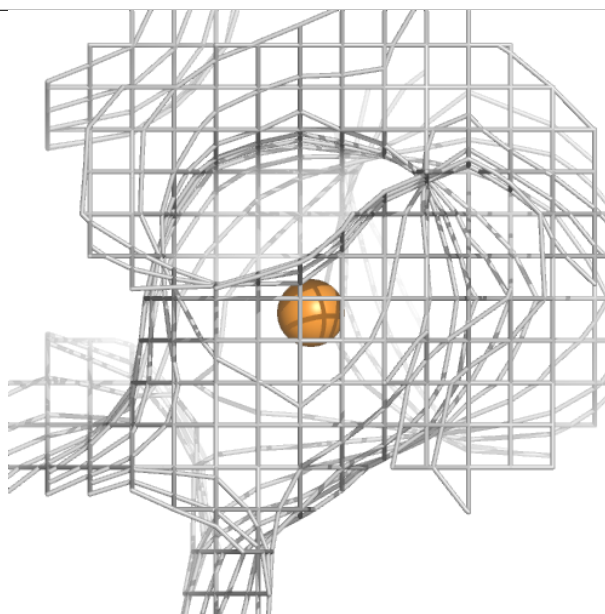
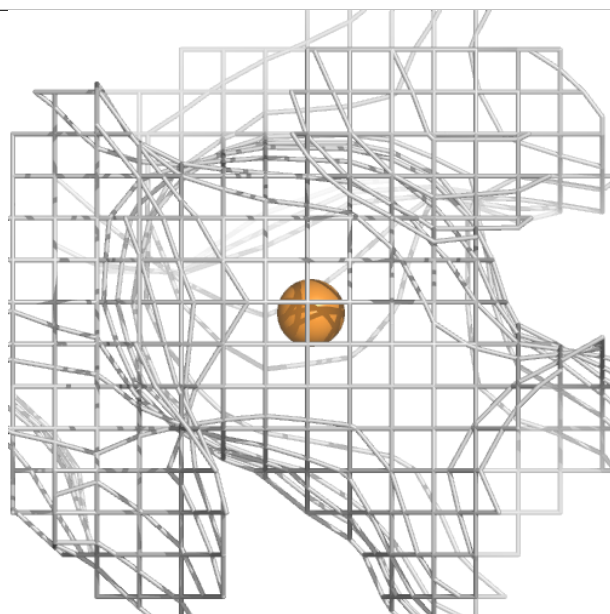
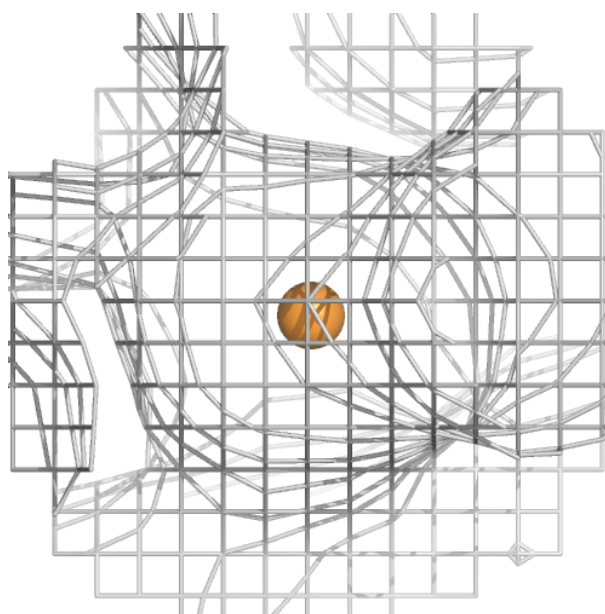
Electron density around CU AAA 604:

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



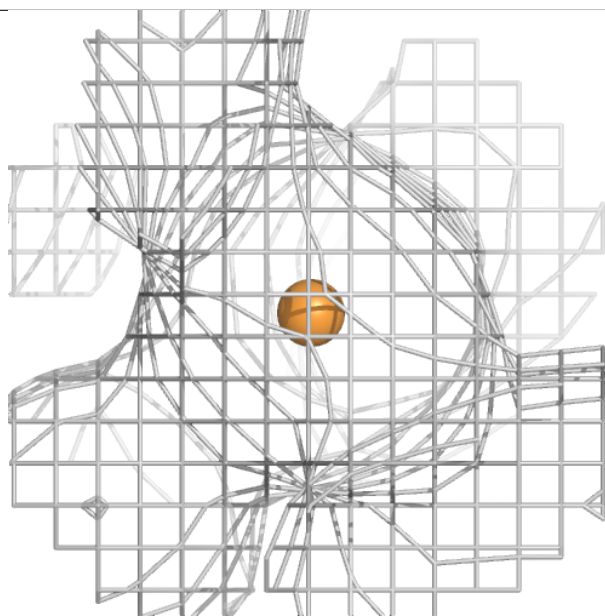
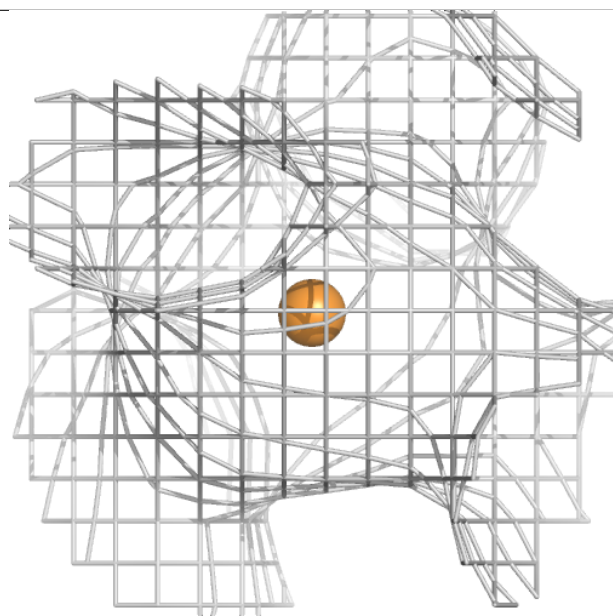
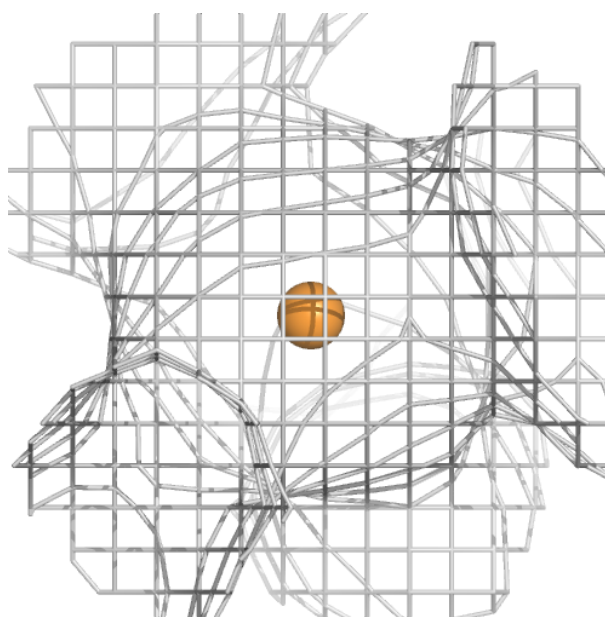
Electron density around CU BBB 601:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.