



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:41 pm BST

PDB ID : 8RTO / pdb_00008rto
Title : Bilirubin oxidase from Myrothecium verrucaria in complex with ATP
Authors : Svecova, L.; Koval, T.; Kolenko, P.; Ostergaard, L.H.; Dohnalek, J.
Deposited on : 2024-01-27
Resolution : 2.40 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
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

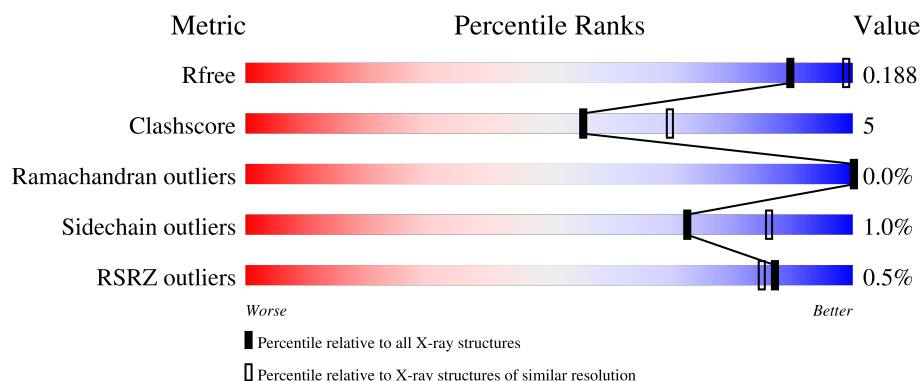
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	 87% 12% .
1	BBB	534	 87% 13%
1	CCC	534	 83% 16% .
1	DDD	534	 86% 13% .
2	AeA	3	 100%

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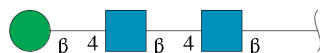
Mol	Chain	Length	Quality of chain
2	BeB	3	 67% 33%
3	AhA	2	 50% 50%
3	BhB	2	 100%
3	CeC	2	 100%
3	CgC	2	 100%
3	DeD	2	 50% 50%
3	DgD	2	 100%

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 4257	C 2718	N 721	O 804	S 14	0	2	0
1	BBB	534	Total 4251	C 2714	N 721	O 802	S 14	0	1	0
1	CCC	533	Total 4255	C 2718	N 723	O 800	S 14	0	3	0
1	DDD	534	Total 4243	C 2709	N 718	O 802	S 14	0	0	0

- Molecule 2 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
2	AeA	3	Total 39	C 22	N 2	O 15	0	0	0
2	BeB	3	Total 39	C 22	N 2	O 15	0	0	0

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

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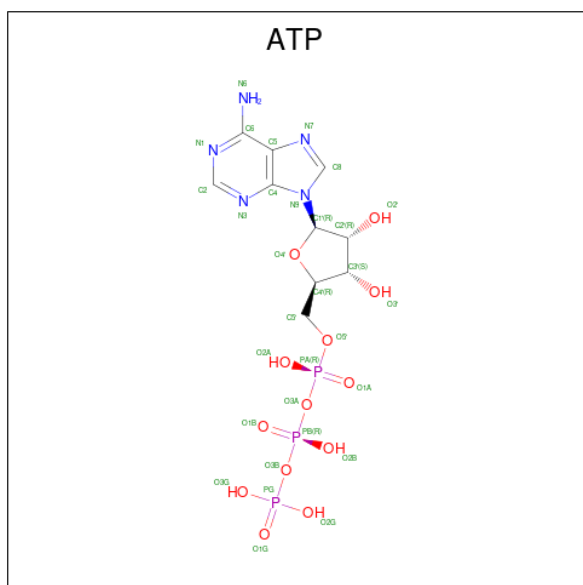
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	BhB	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	CeC	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	CgC	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	DeD	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	DgD	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

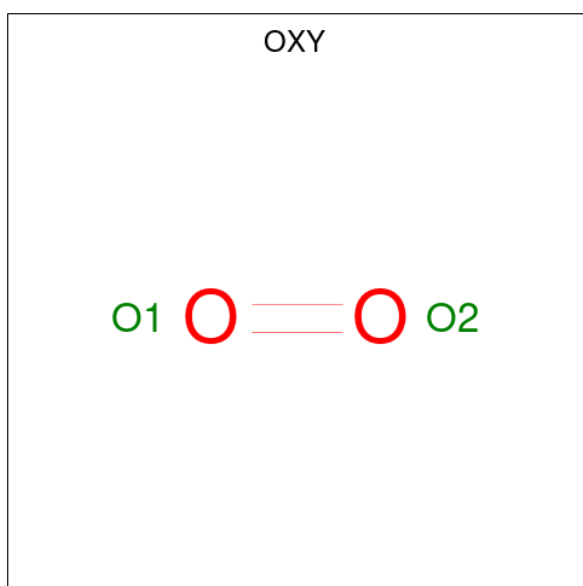
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	4	Total	Cu	0	0
			4	4		
4	BBB	4	Total	Cu	0	0
			4	4		
4	CCC	4	Total	Cu	0	0
			4	4		
4	DDD	4	Total	Cu	0	0
			4	4		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	P	0	1
			44	10	5	23	6		
5	BBB	1	Total	C	N	O	P	0	1
			44	10	5	23	6		
5	CCC	1	Total	C	N	O	P	0	1
			44	10	5	23	6		
5	DDD	1	Total	C	N	O	P	0	1
			44	10	5	23	6		

- 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		
6	CCC	1	Total	O	0	0
			2	2		
6	DDD	1	Total	O	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	2	Total	Cl	0	0
			2	2		
7	CCC	2	Total	Cl	0	0
			2	2		

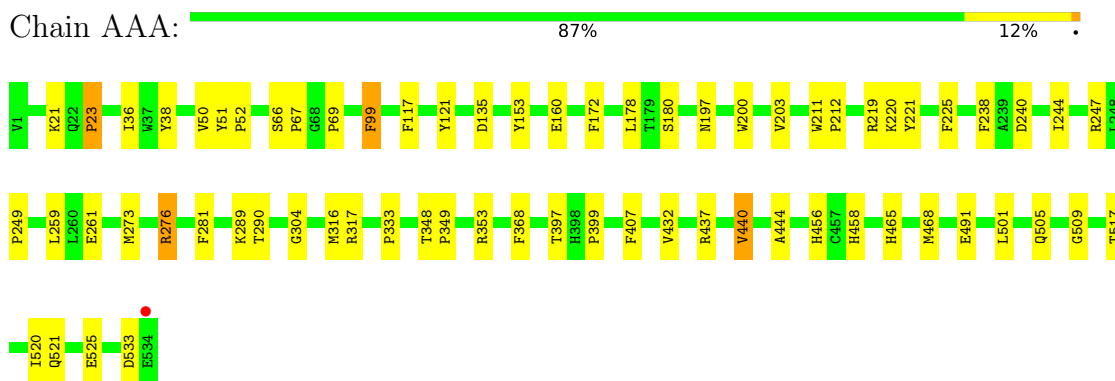
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	456	Total 456	O 456	0	0
8	BBB	292	Total 292	O 292	0	0
8	CCC	346	Total 347	O 347	0	1
8	DDD	371	Total 371	O 371	0	0

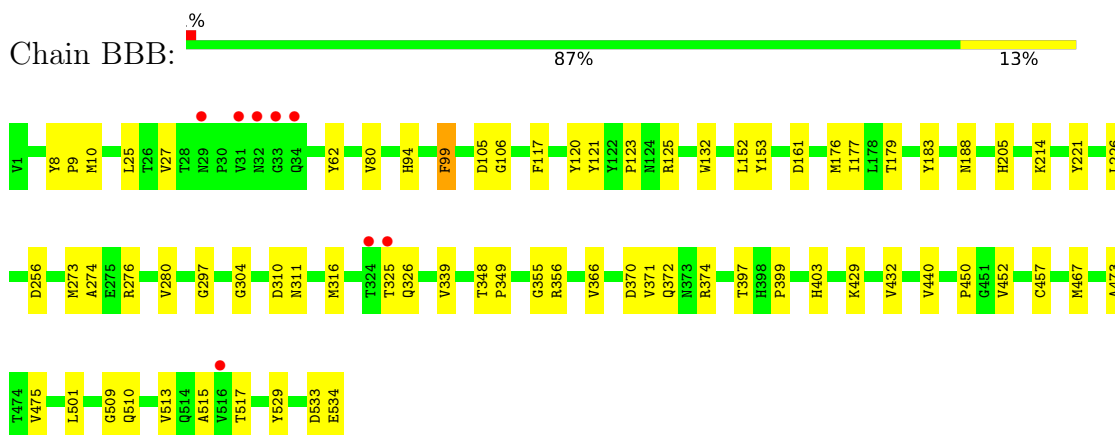
3 Residue-property plots

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.

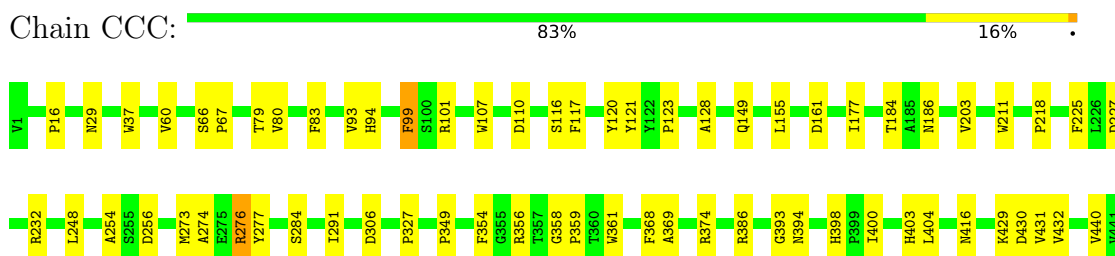
• Molecule 1: Bilirubin oxidase



• Molecule 1: Bilirubin oxidase



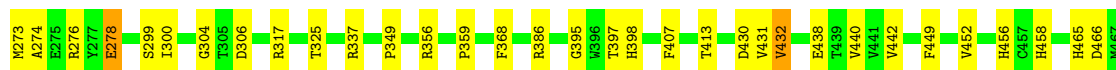
• Molecule 1: Bilirubin oxidase





- Molecule 1: Bilirubin oxidase

Chain DDD: 86% 13%



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

Chain AeA: 100%



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

Chain BeB: 67% 33%



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

Chain AhA: 50% 50%




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

Chain BhB: 100%




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

Chain CeC:  100%

NAG1
NAG2

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

Chain CgC:  100%

NAG1
NAG2

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

Chain DeD:  50% 50%

NAG1
NAG2

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

Chain DgD:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.47Å 204.73Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.50 – 2.40 46.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.8 (46.50-2.40) 89.8 (46.50-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.170 , 0.224 0.176 , 0.188	Depositor DCC
R_{free} test set	5384 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18922	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.60% 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: ATP, OXY, NAG, CL, BMA, CU

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	1.17	7/4394 (0.2%)	1.41	12/6008 (0.2%)
1	BBB	1.13	2/4385 (0.0%)	1.39	11/5996 (0.2%)
1	CCC	1.16	5/4395 (0.1%)	1.40	11/6010 (0.2%)
1	DDD	1.12	2/4374 (0.0%)	1.38	8/5982 (0.1%)
All	All	1.15	16/17548 (0.1%)	1.40	42/23996 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	149	GLN	C-O	7.16	1.31	1.23
1	DDD	432	VAL	C-O	6.11	1.30	1.24
1	AAA	23	PRO	C-O	-6.04	1.16	1.23
1	AAA	178	LEU	C-O	5.99	1.31	1.23
1	AAA	465	HIS	CE1-NE2	5.64	1.38	1.32
1	AAA	197	ASN	C-O	5.61	1.28	1.23
1	AAA	36	ILE	C-O	5.51	1.30	1.24
1	CCC	227	ASP	C-O	5.31	1.30	1.23
1	BBB	355	GLY	C-O	5.29	1.27	1.23
1	CCC	116	SER	C-O	5.26	1.30	1.23
1	AAA	221	TYR	C-O	5.19	1.30	1.24
1	DDD	398	HIS	CE1-NE2	5.12	1.37	1.32
1	AAA	247	ARG	C-O	5.10	1.30	1.24
1	CCC	398	HIS	CE1-NE2	5.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	177	ILE	C-O	5.04	1.30	1.23
1	BBB	297	GLY	C-O	5.03	1.28	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	99	PHE	CA-CB-CG	7.24	121.04	113.80
1	AAA	153	TYR	CB-CA-C	6.55	119.89	110.79
1	DDD	99	PHE	CA-CB-CG	6.28	120.08	113.80
1	AAA	533	ASP	CA-CB-CG	6.11	118.71	112.60
1	DDD	407	PHE	CA-CB-CG	6.10	119.90	113.80
1	BBB	501	LEU	CA-C-N	6.04	126.81	119.99
1	BBB	501	LEU	C-N-CA	6.04	126.81	119.99
1	CCC	99	PHE	CA-CB-CG	5.83	119.63	113.80
1	AAA	440	VAL	CA-C-O	-5.77	114.24	120.36
1	BBB	339	VAL	N-CA-CB	5.76	115.44	110.08
1	AAA	509	GLY	CA-C-N	5.71	128.50	120.28
1	AAA	509	GLY	C-N-CA	5.71	128.50	120.28
1	CCC	184	THR	CA-CB-OG1	-5.65	101.13	109.60
1	CCC	161	ASP	CA-CB-CG	5.58	118.18	112.60
1	BBB	99	PHE	CA-CB-CG	5.55	119.35	113.80
1	CCC	369	ALA	CA-C-O	-5.53	114.01	120.20
1	AAA	135	ASP	CA-CB-CG	-5.49	107.11	112.60
1	CCC	502	GLY	CA-C-N	5.49	129.05	120.82
1	CCC	502	GLY	C-N-CA	5.49	129.05	120.82
1	DDD	509	GLY	CA-C-N	5.49	127.90	120.38
1	DDD	509	GLY	C-N-CA	5.49	127.90	120.38
1	CCC	448	PRO	N-CA-CB	-5.41	96.65	102.60
1	AAA	238	PHE	CA-CB-CG	5.37	119.17	113.80
1	DDD	28	THR	CA-CB-OG1	-5.30	101.65	109.60
1	BBB	153	TYR	CB-CA-C	5.23	118.27	111.42
1	AAA	261	GLU	CB-CG-CD	5.21	121.45	112.60
1	CCC	349	PRO	CB-CA-C	-5.19	104.31	111.21
1	AAA	50	VAL	N-CA-C	-5.18	105.79	110.82
1	DDD	278	GLU	CB-CA-C	5.18	118.29	109.80
1	BBB	62	TYR	CB-CA-C	5.17	117.61	110.16
1	BBB	310	ASP	CA-CB-CG	5.17	117.77	112.60
1	CCC	521	GLN	CA-C-N	5.15	127.13	120.44
1	CCC	521	GLN	C-N-CA	5.15	127.13	120.44
1	BBB	370	ASP	CA-C-N	5.11	127.19	120.60
1	BBB	370	ASP	C-N-CA	5.11	127.19	120.60
1	BBB	161	ASP	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	501	LEU	CA-C-N	5.07	125.72	119.99
1	DDD	501	LEU	C-N-CA	5.07	125.72	119.99
1	BBB	371	VAL	N-CA-CB	-5.03	104.92	110.51
1	AAA	491	GLU	CA-C-N	5.01	127.31	120.54
1	AAA	491	GLU	C-N-CA	5.01	127.31	120.54
1	CCC	416	ASN	N-CA-C	-5.00	106.43	112.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	458	HIS	Peptide

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	4257	0	4038	29	0
1	BBB	4251	0	4032	34	0
1	CCC	4255	0	4045	52	0
1	DDD	4243	0	4019	42	0
2	AeA	39	0	34	0	0
2	BeB	39	0	34	1	0
3	AhA	28	0	25	1	0
3	BhB	28	0	25	0	0
3	CeC	28	0	25	0	0
3	CgC	28	0	25	0	0
3	DeD	28	0	25	1	0
3	DgD	28	0	25	0	0
4	AAA	4	0	0	0	0
4	BBB	4	0	0	0	0
4	CCC	4	0	0	0	0
4	DDD	4	0	0	0	0
5	AAA	44	0	4	1	0
5	BBB	44	0	4	0	0
5	CCC	44	0	4	4	0
5	DDD	44	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AAA	2	0	0	0	0
6	BBB	2	0	0	0	0
6	CCC	2	0	0	0	0
6	DDD	2	0	0	1	0
7	AAA	2	0	0	0	0
7	CCC	2	0	0	0	0
8	AAA	456	0	0	2	0
8	BBB	292	0	0	3	0
8	CCC	347	0	0	5	0
8	DDD	371	0	0	1	0
All	All	18922	0	16368	155	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 5.

All (155) 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:DDD:11:PHE:CD2	1:DDD:317:ARG:HD2	2.26	0.70
1:DDD:83:PHE:CG	1:DDD:93:VAL:HG21	2.29	0.67
1:DDD:70:THR:CG2	1:DDD:154:MET:HE2	2.25	0.66
1:DDD:356:ARG:NH1	1:DDD:359:PRO:HA	2.12	0.65
1:BBB:152:LEU:HG	1:BBB:177:ILE:HD11	1.78	0.64
1:BBB:176:MET:HE1	1:BBB:316:MET:SD	2.40	0.61
1:AAA:304:GLY:HA2	1:AAA:397:THR:HG21	1.83	0.61
1:CCC:394:ASN:N	5:CCC:605[A]:ATP:O2A	2.27	0.60
1:BBB:356[A]:ARG:NH2	8:BBB:704:HOH:O	2.34	0.59
1:BBB:94:HIS:HB2	1:BBB:105:ASP:O	2.04	0.58
1:CCC:123:PRO:HB3	1:CCC:529:TYR:CG	2.39	0.57
1:DDD:70:THR:HG21	1:DDD:154:MET:HE2	1.87	0.57
1:BBB:432:VAL:HG21	1:BBB:440:VAL:HG11	1.85	0.57
1:AAA:21:LYS:HB2	1:AAA:69:PRO:HB2	1.87	0.56
1:AAA:437:ARG:NH2	5:AAA:605[B]:ATP:O1G	2.38	0.56
1:BBB:304:GLY:HA2	1:BBB:397:THR:HG21	1.86	0.56
1:DDD:432:VAL:HG21	1:DDD:440:VAL:HG11	1.88	0.56
1:AAA:240:ASP:OD2	1:AAA:289:LYS:HE2	2.06	0.56
1:CCC:60:VAL:HB	8:CCC:737:HOH:O	2.06	0.55
1:AAA:517:THR:O	1:AAA:521:GLN:HG3	2.06	0.55
1:BBB:325:THR:HG22	1:BBB:326:GLN:HG3	1.87	0.55
1:BBB:372:GLN:NE2	8:BBB:708:HOH:O	2.39	0.55
1:DDD:456:HIS:HB3	1:DDD:468:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:393:GLY:HA2	5:CCC:605[B]:ATP:O2A	2.07	0.54
1:DDD:213:PHE:HA	1:DDD:317:ARG:O	2.08	0.54
1:AAA:203:VAL:HA	1:AAA:211:TRP:CH2	2.42	0.54
1:AAA:160:GLU:HG3	1:AAA:259:LEU:HD11	1.90	0.54
1:CCC:519:ARG:O	1:CCC:523:MET:HG3	2.08	0.54
1:CCC:80:VAL:HA	1:CCC:120:TYR:O	2.07	0.54
1:AAA:38:TYR:CD1	1:AAA:520:ILE:HD11	2.43	0.53
1:CCC:500:GLU:O	1:CCC:503:GLU:HB2	2.07	0.53
1:AAA:525[B]:GLU:OE1	3:AhA:2:NAG:H5	2.08	0.53
1:CCC:532:ALA:O	1:CCC:533:ASP:HB2	2.08	0.53
1:AAA:117:PHE:C	1:AAA:117:PHE:CD1	2.87	0.52
1:AAA:456:HIS:HB3	1:AAA:468:MET:HG3	1.91	0.52
1:BBB:366:VAL:HG11	1:BBB:374:ARG:HA	1.92	0.52
1:BBB:273:MET:O	1:BBB:274:ALA:HB3	2.09	0.52
1:DDD:123:PRO:HB3	1:DDD:529:TYR:CG	2.45	0.52
1:DDD:507:GLN:HG2	8:DDD:892:HOH:O	2.09	0.51
1:CCC:203:VAL:HA	1:CCC:211:TRP:CH2	2.45	0.51
1:CCC:368:PHE:O	1:CCC:374:ARG:HD3	2.09	0.51
1:DDD:181:LYS:HB2	1:DDD:205:HIS:CE1	2.46	0.51
1:DDD:32:ASN:CG	1:DDD:34:GLN:HG3	2.36	0.51
1:BBB:25:LEU:CD1	1:BBB:27:VAL:HG23	2.41	0.50
1:CCC:368:PHE:HB2	1:CCC:468:MET:HB3	1.93	0.50
1:BBB:125:ARG:NH1	1:BBB:533:ASP:OD1	2.45	0.50
1:DDD:117:PHE:C	1:DDD:117:PHE:CD1	2.90	0.50
1:CCC:218:PRO:HB2	1:CCC:284:SER:HA	1.93	0.50
1:DDD:299:SER:C	1:DDD:300:ILE:HD12	2.37	0.49
1:DDD:465:HIS:HA	1:DDD:466:ASP:HB2	1.94	0.49
1:BBB:94:HIS:HB2	1:BBB:106:GLY:HA3	1.94	0.49
1:BBB:117:PHE:C	1:BBB:117:PHE:CD1	2.90	0.49
1:BBB:256:ASP:HB2	1:BBB:429:LYS:HA	1.94	0.49
1:DDD:273:MET:O	1:DDD:274:ALA:HB3	2.12	0.49
1:DDD:11:PHE:CG	1:DDD:317:ARG:HD2	2.49	0.48
1:BBB:450:PRO:HB3	1:BBB:475:VAL:HG13	1.94	0.48
1:CCC:16:PRO:HB2	8:CCC:993:HOH:O	2.14	0.48
1:DDD:259:LEU:HB2	1:DDD:337:ARG:HG2	1.95	0.48
1:BBB:452:VAL:HG21	2:BeB:1:NAG:H82	1.95	0.48
1:CCC:386:ARG:HA	1:CCC:442:VAL:O	2.14	0.48
1:CCC:481:TYR:HA	8:CCC:924:HOH:O	2.14	0.48
1:AAA:172:PHE:CE1	1:AAA:219:ARG:HD3	2.48	0.48
1:DDD:300:ILE:HD12	1:DDD:300:ILE:N	2.29	0.48
1:CCC:517:THR:O	1:CCC:521:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:273:MET:O	1:CCC:274:ALA:HB3	2.14	0.47
1:BBB:123:PRO:HB3	1:BBB:529:TYR:CG	2.49	0.47
1:CCC:256:ASP:HB2	1:CCC:429:LYS:HA	1.96	0.47
1:CCC:356[B]:ARG:HD2	1:CCC:361:TRP:CH2	2.49	0.47
1:AAA:249:PRO:HD2	8:AAA:766:HOH:O	2.13	0.47
1:AAA:368:PHE:HB2	1:AAA:468:MET:HB3	1.96	0.47
1:CCC:356[A]:ARG:NH1	1:CCC:359:PRO:HA	2.30	0.47
1:AAA:273:MET:HE2	1:AAA:399:PRO:HG3	1.97	0.47
1:AAA:432:VAL:HG21	1:AAA:440:VAL:HG11	1.96	0.46
1:CCC:186:ASN:ND2	8:CCC:731:HOH:O	2.48	0.46
1:BBB:132:TRP:CE3	1:BBB:226:LEU:HD21	2.51	0.46
1:DDD:386:ARG:HA	1:DDD:442:VAL:O	2.15	0.46
1:BBB:8:TYR:CG	1:BBB:9:PRO:HD2	2.50	0.46
1:DDD:138:MET:HG3	1:DDD:139:HIS:CD2	2.50	0.46
1:DDD:452:VAL:HG21	3:DeD:1:NAG:H82	1.96	0.46
1:CCC:83:PHE:CG	1:CCC:93:VAL:HG21	2.50	0.46
1:CCC:507:GLN:HG2	8:CCC:755:HOH:O	2.14	0.46
1:DDD:94:HIS:ND1	1:DDD:105:ASP:O	2.48	0.46
1:CCC:394:ASN:N	5:CCC:605[B]:ATP:O2A	2.40	0.45
1:DDD:80:VAL:HA	1:DDD:120:TYR:O	2.16	0.45
1:BBB:513:VAL:O	1:BBB:517:THR:OG1	2.20	0.45
1:CCC:117:PHE:CD1	1:CCC:117:PHE:C	2.94	0.45
1:CCC:29:ASN:OD1	1:CCC:29:ASN:C	2.59	0.45
1:DDD:83:PHE:CD1	1:DDD:93:VAL:HG21	2.51	0.45
1:CCC:450:PRO:HB3	1:CCC:475:VAL:HG13	1.98	0.45
1:AAA:407:PHE:HB3	1:AAA:444:ALA:HB2	1.99	0.45
1:AAA:290:THR:HG21	1:AAA:317:ARG:HD3	1.99	0.44
1:BBB:450:PRO:HA	1:BBB:473:ALA:O	2.17	0.44
1:DDD:135:ASP:O	1:DDD:141:THR:HG23	2.17	0.44
1:BBB:509:GLY:O	1:BBB:515:ALA:CB	2.66	0.44
1:BBB:214:LYS:HG3	8:BBB:851:HOH:O	2.17	0.44
1:CCC:107:TRP:CZ3	1:CCC:452:VAL:HG12	2.53	0.44
1:AAA:66:SER:HA	1:AAA:67:PRO:C	2.43	0.44
1:DDD:94:HIS:CD2	6:DDD:606:OXY:O2	2.71	0.44
1:CCC:432:VAL:HG21	1:CCC:440:VAL:HG11	1.99	0.43
1:DDD:449:PHE:CZ	1:DDD:532:ALA:HB2	2.53	0.43
1:CCC:393:GLY:HA2	5:CCC:605[A]:ATP:O2A	2.18	0.43
1:DDD:413:THR:O	1:DDD:438:GLU:HA	2.18	0.43
1:BBB:457:CYS:HB2	1:BBB:467:MET:SD	2.58	0.43
1:CCC:356[B]:ARG:NH1	1:CCC:358:GLY:O	2.51	0.43
1:DDD:254:ALA:HB3	1:DDD:278:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:225:PHE:O	1:AAA:276:ARG:HA	2.18	0.43
1:AAA:353[A]:ARG:HD3	8:AAA:937:HOH:O	2.17	0.43
1:BBB:80:VAL:HA	1:BBB:120:TYR:O	2.19	0.43
1:DDD:368:PHE:HB2	1:DDD:468:MET:HB3	2.01	0.43
1:DDD:304:GLY:HA2	1:DDD:397:THR:HG21	2.01	0.43
1:DDD:248:LEU:HA	1:DDD:249:PRO:HD3	1.85	0.42
1:CCC:274:ALA:HB2	1:CCC:458:HIS:CG	2.54	0.42
1:CCC:356[B]:ARG:NH2	1:CCC:359:PRO:HA	2.34	0.42
1:CCC:94:HIS:CE1	1:CCC:403:HIS:CE1	3.08	0.42
1:BBB:10:MET:HE1	1:BBB:311:ASN:HB3	2.02	0.42
1:BBB:179:THR:OG1	1:BBB:205:HIS:HB2	2.20	0.42
1:BBB:356[A]:ARG:HH21	1:BBB:356[A]:ARG:HG2	1.85	0.42
1:DDD:160:GLU:HG3	1:DDD:259:LEU:HD11	2.01	0.42
1:DDD:500:GLU:O	1:DDD:503:GLU:HB2	2.19	0.42
1:CCC:101:ARG:HG2	1:CCC:529:TYR:CE1	2.55	0.42
1:CCC:403:HIS:O	1:CCC:404:LEU:HB3	2.20	0.42
1:DDD:532:ALA:O	1:DDD:533:ASP:C	2.63	0.42
1:CCC:456:HIS:HB3	1:CCC:468:MET:HG3	2.02	0.41
1:AAA:51:TYR:O	1:AAA:52:PRO:C	2.62	0.41
1:AAA:220:LYS:HA	1:AAA:281:PHE:O	2.19	0.41
1:AAA:501:LEU:HG	1:AAA:505:GLN:NE2	2.35	0.41
1:BBB:273:MET:HE2	1:BBB:399:PRO:HG3	2.01	0.41
1:CCC:465:HIS:N	1:CCC:466:ASP:HA	2.35	0.41
1:CCC:110:ASP:O	1:CCC:110:ASP:CG	2.63	0.41
1:BBB:94:HIS:CE1	1:BBB:403:HIS:CE1	3.09	0.41
1:CCC:254:ALA:O	1:CCC:277:TYR:HA	2.21	0.41
1:CCC:403:HIS:CE1	1:CCC:454:MET:HE3	2.55	0.41
1:BBB:348:THR:HA	1:BBB:349:PRO:HD3	1.94	0.41
1:CCC:37:TRP:HB2	1:CCC:79:THR:HG22	2.03	0.41
1:AAA:348:THR:HA	1:AAA:349:PRO:HD3	1.97	0.41
1:CCC:356[B]:ARG:HD2	1:CCC:361:TRP:CZ3	2.55	0.41
1:DDD:349:PRO:HA	1:DDD:386:ARG:O	2.21	0.41
1:AAA:333:PRO:HB3	1:CCC:327:PRO:HB3	2.02	0.41
1:BBB:221:TYR:O	1:BBB:280:VAL:HA	2.21	0.41
1:CCC:232:ARG:HA	1:CCC:306:ASP:OD2	2.21	0.41
1:CCC:248:LEU:CD1	1:CCC:291:ILE:HD12	2.50	0.41
1:DDD:87:ALA:O	1:DDD:114:PRO:HB3	2.19	0.41
1:BBB:183:TYR:HA	1:BBB:188:ASN:O	2.21	0.41
1:CCC:354:PHE:CE1	1:CCC:400:ILE:HD12	2.55	0.41
1:DDD:274:ALA:HB2	1:DDD:458:HIS:CG	2.56	0.40
1:AAA:212:PRO:O	1:AAA:316:MET:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:66:SER:HA	1:CCC:67:PRO:C	2.44	0.40
1:AAA:180:SER:OG	1:AAA:200:TRP:O	2.37	0.40
1:AAA:23:PRO:HG2	1:DDD:325:THR:HG21	2.02	0.40
1:CCC:225:PHE:O	1:CCC:276:ARG:HA	2.22	0.40
1:CCC:128:ALA:HA	1:CCC:155:LEU:O	2.22	0.40
1:CCC:430:ASP:OD1	1:CCC:431:VAL:HG23	2.21	0.40
1:DDD:430:ASP:OD1	1:DDD:431:VAL:HG23	2.21	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	534/534 (100%)	502 (94%)	32 (6%)	0	100	100
1	BBB	533/534 (100%)	497 (93%)	36 (7%)	0	100	100
1	CCC	534/534 (100%)	496 (93%)	37 (7%)	1 (0%)	44	59
1	DDD	532/534 (100%)	502 (94%)	30 (6%)	0	100	100
All	All	2133/2136 (100%)	1997 (94%)	135 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	510	GLN

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	455/453 (100%)	451 (99%)	4 (1%)	75	88
1	BBB	454/453 (100%)	449 (99%)	5 (1%)	70	84
1	CCC	455/453 (100%)	452 (99%)	3 (1%)	81	91
1	DDD	453/453 (100%)	447 (99%)	6 (1%)	65	81
All	All	1817/1812 (100%)	1799 (99%)	18 (1%)	73	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	99	PHE
1	AAA	121	TYR
1	AAA	244	ILE
1	AAA	276	ARG
1	BBB	99	PHE
1	BBB	121	TYR
1	BBB	276	ARG
1	BBB	510	GLN
1	BBB	534	GLU
1	CCC	99	PHE
1	CCC	121	TYR
1	CCC	276	ARG
1	DDD	99	PHE
1	DDD	121	TYR
1	DDD	205	HIS
1	DDD	266	THR
1	DDD	276	ARG
1	DDD	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 ⓘ

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

5.5 Carbohydrates ⓘ

18 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	0.65	0	17,19,21	1.98	5 (29%)
2	NAG	AeA	2	2	14,14,15	1.06	0	17,19,21	1.77	4 (23%)
2	BMA	AeA	3	2	11,11,12	1.10	1 (9%)	15,15,17	2.00	3 (20%)
3	NAG	AhA	1	1,3	14,14,15	0.52	0	17,19,21	1.57	2 (11%)
3	NAG	AhA	2	3	14,14,15	1.02	0	17,19,21	1.73	4 (23%)
2	NAG	BeB	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	2.20	7 (41%)
2	NAG	BeB	2	2	14,14,15	0.73	0	17,19,21	1.45	2 (11%)
2	BMA	BeB	3	2	11,11,12	0.88	0	15,15,17	1.56	3 (20%)
3	NAG	BhB	1	1,3	14,14,15	0.56	0	17,19,21	1.34	3 (17%)
3	NAG	BhB	2	3	14,14,15	0.83	0	17,19,21	1.48	3 (17%)
3	NAG	CeC	1	1,3	14,14,15	0.80	0	17,19,21	1.50	3 (17%)
3	NAG	CeC	2	3	14,14,15	1.12	1 (7%)	17,19,21	2.40	3 (17%)
3	NAG	CgC	1	1,3	14,14,15	0.68	0	17,19,21	1.67	4 (23%)
3	NAG	CgC	2	3	14,14,15	0.92	0	17,19,21	1.69	4 (23%)
3	NAG	DeD	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.94	6 (35%)
3	NAG	DeD	2	3	14,14,15	1.19	2 (14%)	17,19,21	2.34	5 (29%)
3	NAG	DgD	1	1,3	14,14,15	0.73	0	17,19,21	1.41	1 (5%)
3	NAG	DgD	2	3	14,14,15	1.02	1 (7%)	17,19,21	2.38	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	-	2/6/23/26	0/1/1/1
2	NAG	AeA	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	AeA	3	2	-	0/2/19/22	0/1/1/1
3	NAG	AhA	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	AhA	2	3	-	2/6/23/26	0/1/1/1
2	NAG	BeB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BeB	2	2	-	2/6/23/26	0/1/1/1
2	BMA	BeB	3	2	-	2/2/19/22	0/1/1/1
3	NAG	BhB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BhB	2	3	-	0/6/23/26	0/1/1/1
3	NAG	CeC	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	CeC	2	3	-	1/6/23/26	0/1/1/1
3	NAG	CgC	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	CgC	2	3	-	2/6/23/26	0/1/1/1
3	NAG	DeD	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	DeD	2	3	-	2/6/23/26	0/1/1/1
3	NAG	DgD	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	DgD	2	3	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DeD	2	NAG	C4-C5	2.72	1.58	1.53
2	BeB	1	NAG	O5-C1	-2.53	1.39	1.43
2	AeA	3	BMA	C4-C5	2.43	1.58	1.53
3	CeC	2	NAG	O4-C4	2.29	1.48	1.43
3	DeD	1	NAG	C4-C5	2.16	1.57	1.53
3	DeD	2	NAG	O4-C4	2.10	1.47	1.43
3	DgD	2	NAG	O4-C4	2.01	1.47	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CeC	2	NAG	C1-O5-C5	8.42	123.60	112.19
2	AeA	3	BMA	C3-C4-C5	5.28	119.65	110.24
3	DgD	2	NAG	O5-C1-C2	-5.08	103.27	111.29
3	DeD	2	NAG	O5-C5-C6	-4.90	99.52	107.20
3	DeD	2	NAG	C1-O5-C5	4.86	118.78	112.19
2	BeB	1	NAG	O5-C5-C6	-4.70	99.83	107.20
3	DgD	2	NAG	C1-O5-C5	4.50	118.28	112.19
2	AeA	1	NAG	O5-C1-C2	-4.39	104.36	111.29
3	AhA	2	NAG	C1-O5-C5	4.09	117.73	112.19
3	CgC	2	NAG	O4-C4-C5	3.90	118.97	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DgD	2	NAG	C3-C4-C5	-3.71	103.63	110.24
3	DeD	2	NAG	O4-C4-C5	3.71	118.50	109.30
2	AeA	2	NAG	O5-C1-C2	-3.69	105.46	111.29
3	DgD	1	NAG	O5-C1-C2	-3.66	105.51	111.29
3	AhA	1	NAG	O7-C7-N2	3.66	128.67	121.95
2	AeA	1	NAG	O4-C4-C3	-3.65	101.92	110.35
3	DeD	1	NAG	O4-C4-C5	3.52	118.05	109.30
3	DeD	1	NAG	O5-C5-C6	-3.43	101.82	107.20
3	DeD	1	NAG	O4-C4-C3	-3.42	102.45	110.35
3	AhA	1	NAG	C8-C7-N2	-3.33	110.46	116.10
2	BeB	2	NAG	C4-C3-C2	3.28	115.82	111.02
2	BeB	1	NAG	O7-C7-N2	3.24	127.90	121.95
3	DgD	2	NAG	O4-C4-C5	3.21	117.28	109.30
2	BeB	3	BMA	O2-C2-C1	3.21	115.72	109.15
2	BeB	1	NAG	C1-O5-C5	3.20	116.53	112.19
3	DgD	2	NAG	C2-N2-C7	-3.17	118.39	122.90
3	CeC	2	NAG	O4-C4-C3	3.15	117.63	110.35
3	CeC	1	NAG	O5-C1-C2	-3.13	106.34	111.29
2	BeB	3	BMA	O5-C5-C6	3.13	112.11	107.20
3	CgC	1	NAG	O5-C5-C6	3.03	111.95	107.20
3	BhB	2	NAG	O4-C4-C5	3.01	116.77	109.30
3	DeD	2	NAG	C4-C3-C2	-2.98	106.65	111.02
3	AhA	2	NAG	O4-C4-C3	2.92	117.09	110.35
2	BeB	1	NAG	C8-C7-N2	-2.91	111.18	116.10
3	CgC	2	NAG	C1-C2-N2	2.91	115.45	110.49
3	BhB	2	NAG	O5-C5-C6	2.89	111.73	107.20
3	CgC	1	NAG	C3-C4-C5	2.86	115.33	110.24
3	CeC	1	NAG	O5-C5-C4	-2.84	103.92	110.83
3	CeC	1	NAG	O4-C4-C5	2.84	116.34	109.30
2	AeA	2	NAG	O4-C4-C5	2.77	116.18	109.30
2	AeA	3	BMA	O4-C4-C3	-2.75	103.98	110.35
3	DeD	2	NAG	O5-C5-C4	2.74	117.50	110.83
2	AeA	2	NAG	C1-O5-C5	2.61	115.73	112.19
2	AeA	2	NAG	O5-C5-C6	-2.60	103.13	107.20
3	CgC	1	NAG	C2-N2-C7	-2.59	119.21	122.90
2	BeB	1	NAG	C2-N2-C7	2.59	126.59	122.90
3	DeD	1	NAG	C6-C5-C4	2.54	118.96	113.00
2	BeB	1	NAG	O4-C4-C3	-2.54	104.47	110.35
3	CgC	2	NAG	C2-N2-C7	2.54	126.52	122.90
3	BhB	1	NAG	O3-C3-C2	-2.53	104.22	109.47
2	AeA	3	BMA	C1-O5-C5	2.46	115.52	112.19
3	AhA	2	NAG	O5-C1-C2	-2.44	107.43	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BhB	1	NAG	O5-C1-C2	-2.39	107.52	111.29
2	AeA	1	NAG	C2-N2-C7	-2.38	119.51	122.90
3	BhB	2	NAG	C1-O5-C5	2.34	115.36	112.19
3	CeC	2	NAG	C6-C5-C4	-2.31	107.60	113.00
2	AeA	1	NAG	C6-C5-C4	2.28	118.35	113.00
3	DeD	1	NAG	O7-C7-C8	2.26	126.25	122.06
2	BeB	3	BMA	C3-C4-C5	2.24	114.23	110.24
3	BhB	1	NAG	C1-C2-N2	2.22	114.29	110.49
3	DeD	1	NAG	O3-C3-C4	2.17	115.38	110.35
3	CgC	2	NAG	O4-C4-C3	-2.12	105.44	110.35
2	BeB	1	NAG	C6-C5-C4	2.12	117.97	113.00
3	DgD	2	NAG	O7-C7-C8	-2.08	118.19	122.06
2	BeB	2	NAG	O4-C4-C5	2.07	114.44	109.30
3	CgC	1	NAG	O7-C7-C8	2.04	125.86	122.06
2	AeA	1	NAG	C4-C3-C2	2.03	113.99	111.02
3	AhA	2	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (19) torsion outliers are listed below:

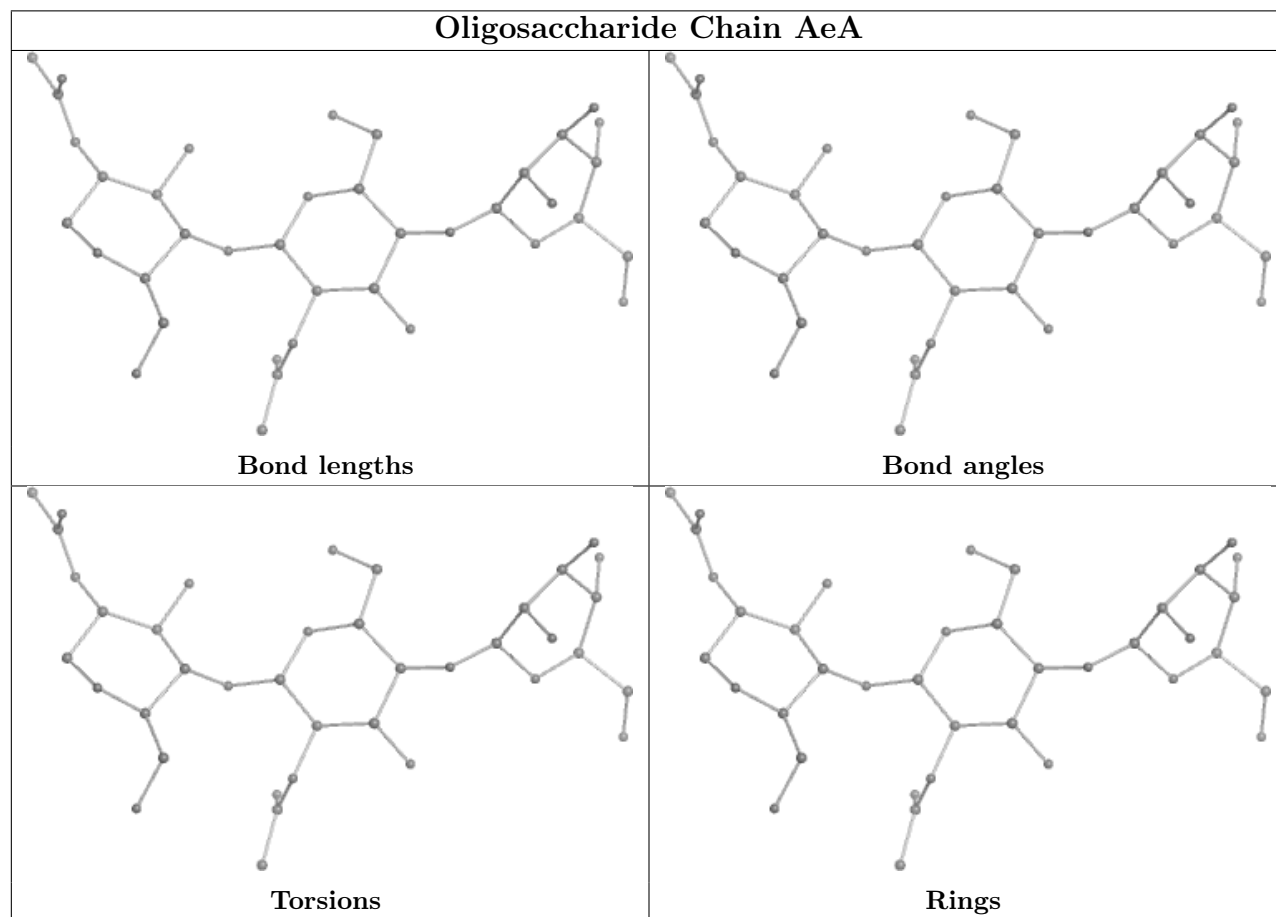
Mol	Chain	Res	Type	Atoms
3	DeD	2	NAG	C4-C5-C6-O6
2	AeA	2	NAG	O5-C5-C6-O6
3	DgD	2	NAG	O5-C5-C6-O6
3	DeD	2	NAG	O5-C5-C6-O6
2	AeA	2	NAG	C4-C5-C6-O6
3	CgC	2	NAG	O5-C5-C6-O6
3	DgD	2	NAG	C4-C5-C6-O6
2	BeB	2	NAG	O5-C5-C6-O6
3	CgC	2	NAG	C4-C5-C6-O6
2	BeB	2	NAG	C4-C5-C6-O6
2	BeB	3	BMA	C4-C5-C6-O6
3	AhA	2	NAG	O5-C5-C6-O6
2	BeB	3	BMA	O5-C5-C6-O6
3	AhA	2	NAG	C4-C5-C6-O6
2	AeA	1	NAG	C4-C5-C6-O6
3	CeC	2	NAG	C4-C5-C6-O6
2	AeA	1	NAG	O5-C5-C6-O6
3	AhA	1	NAG	C4-C5-C6-O6
3	DgD	1	NAG	C4-C5-C6-O6

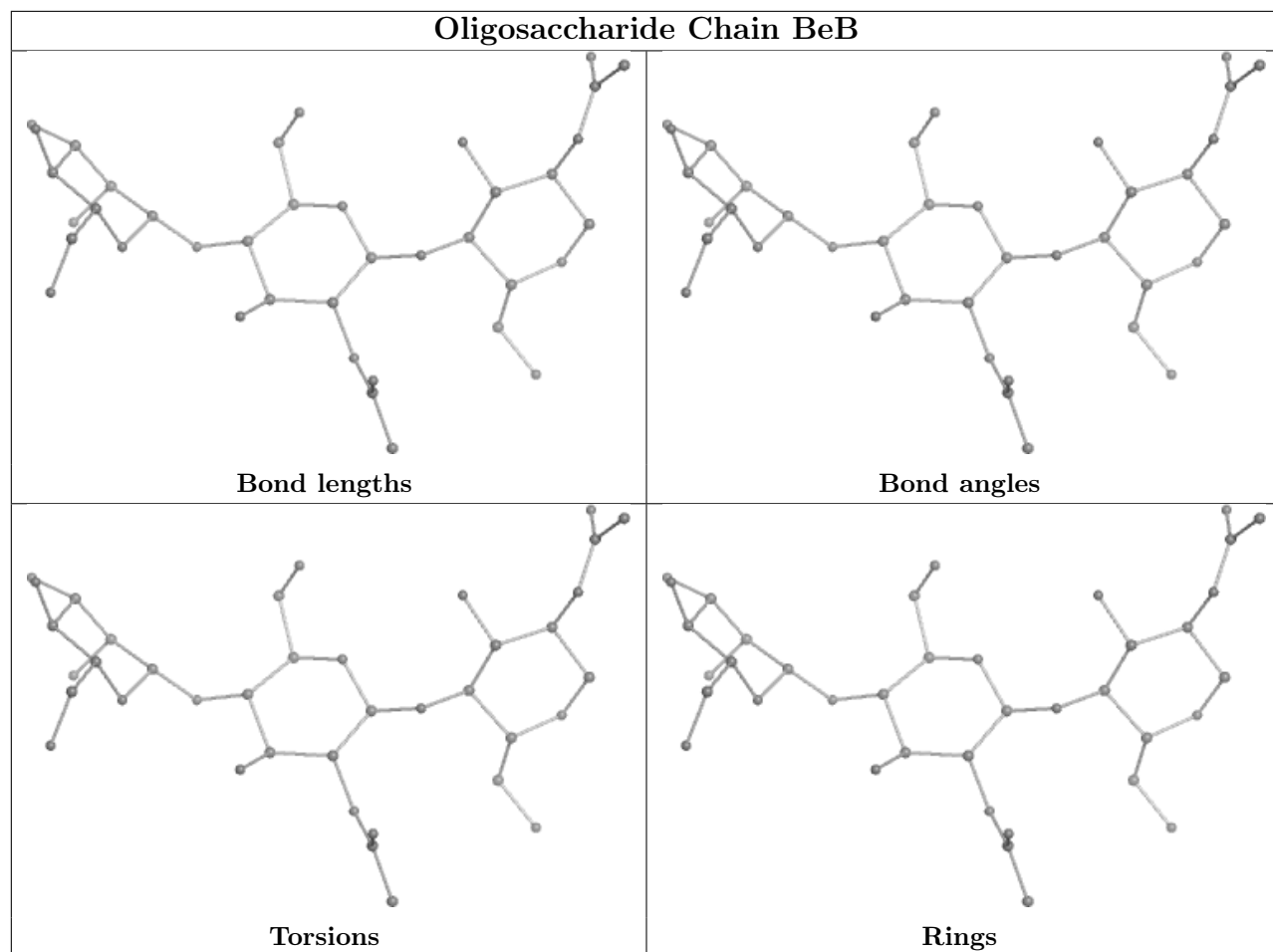
There are no ring outliers.

3 monomers are involved in 3 short contacts:

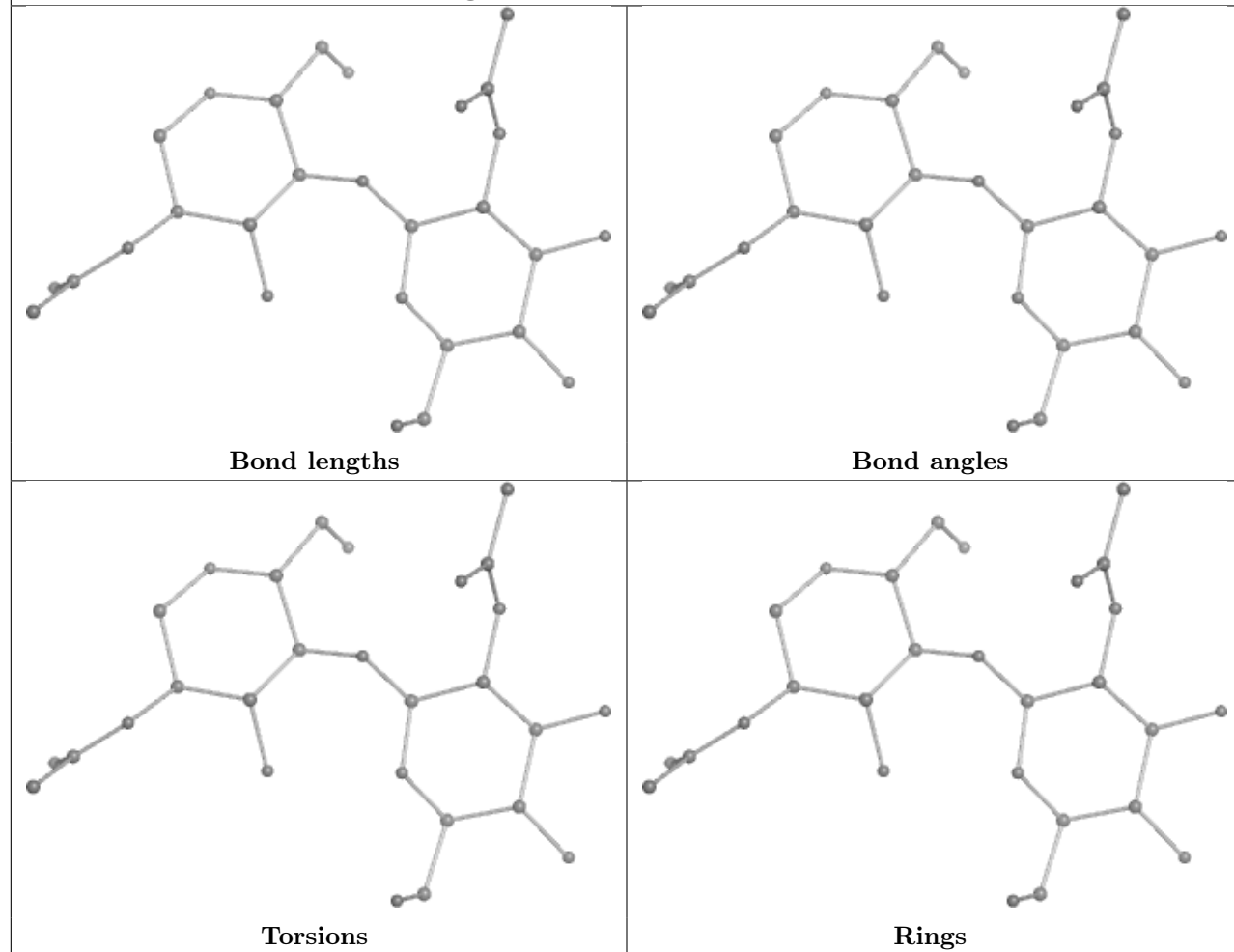
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AhA	2	NAG	1	0
2	BeB	1	NAG	1	0
3	DeD	1	NAG	1	0

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

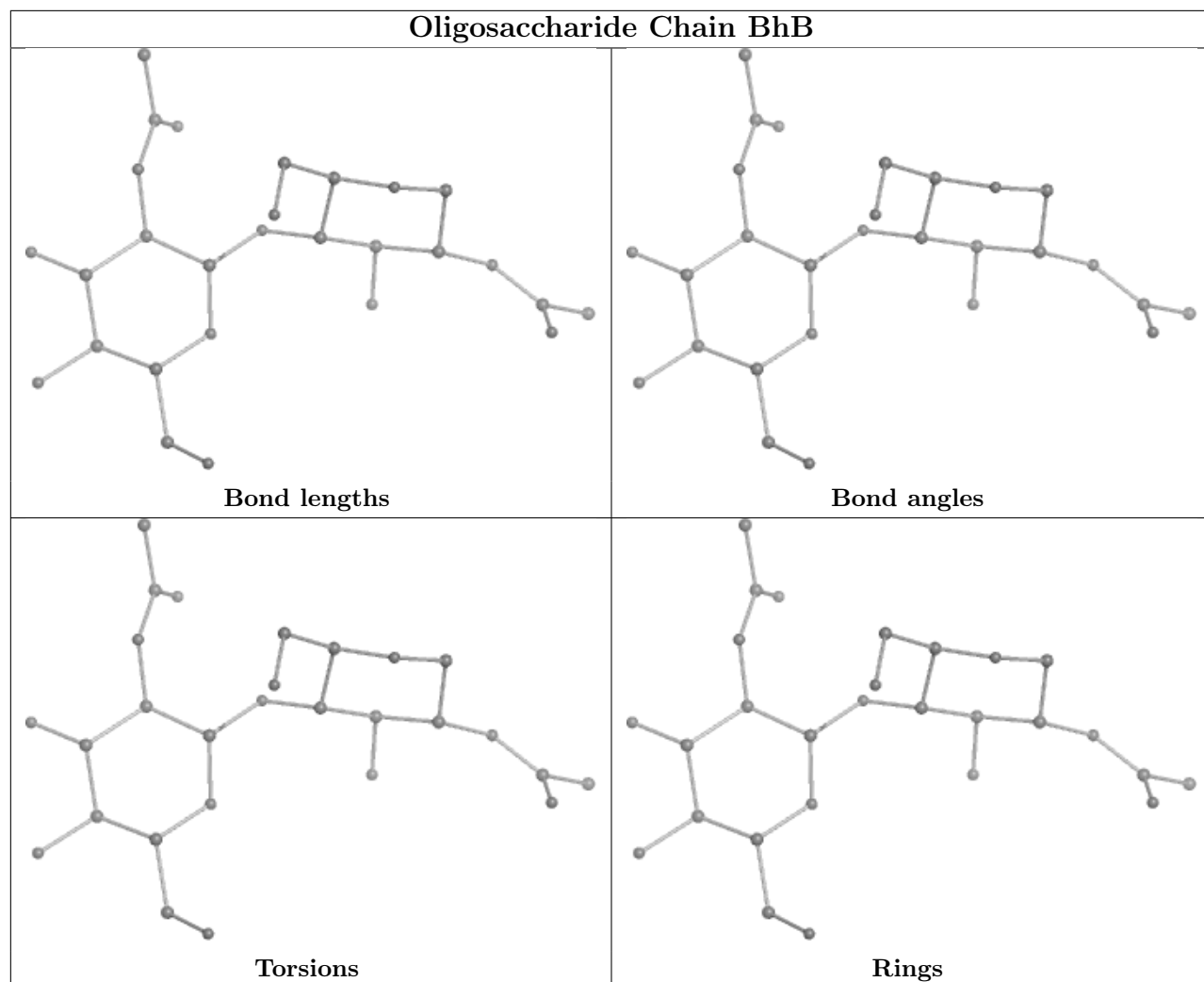


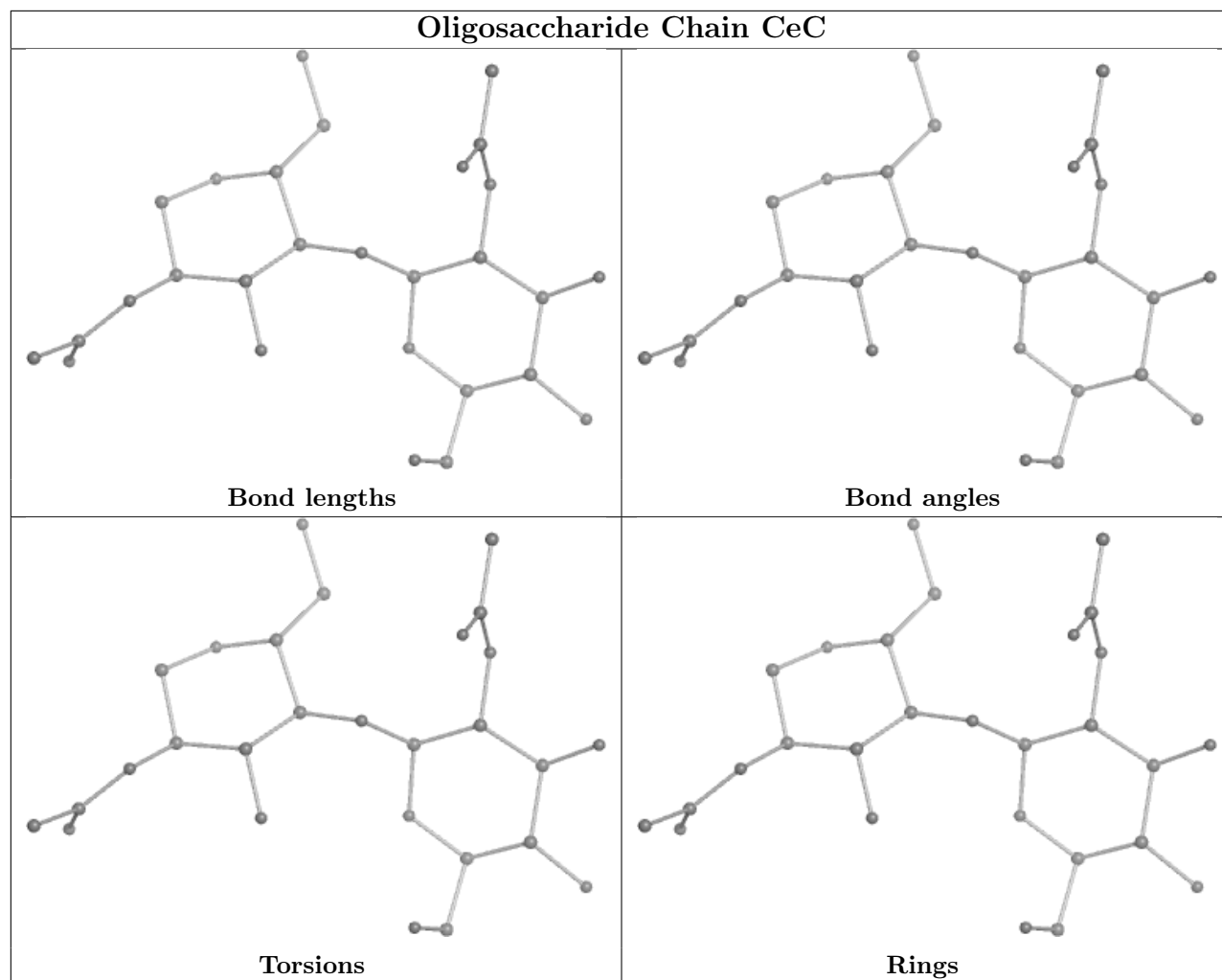


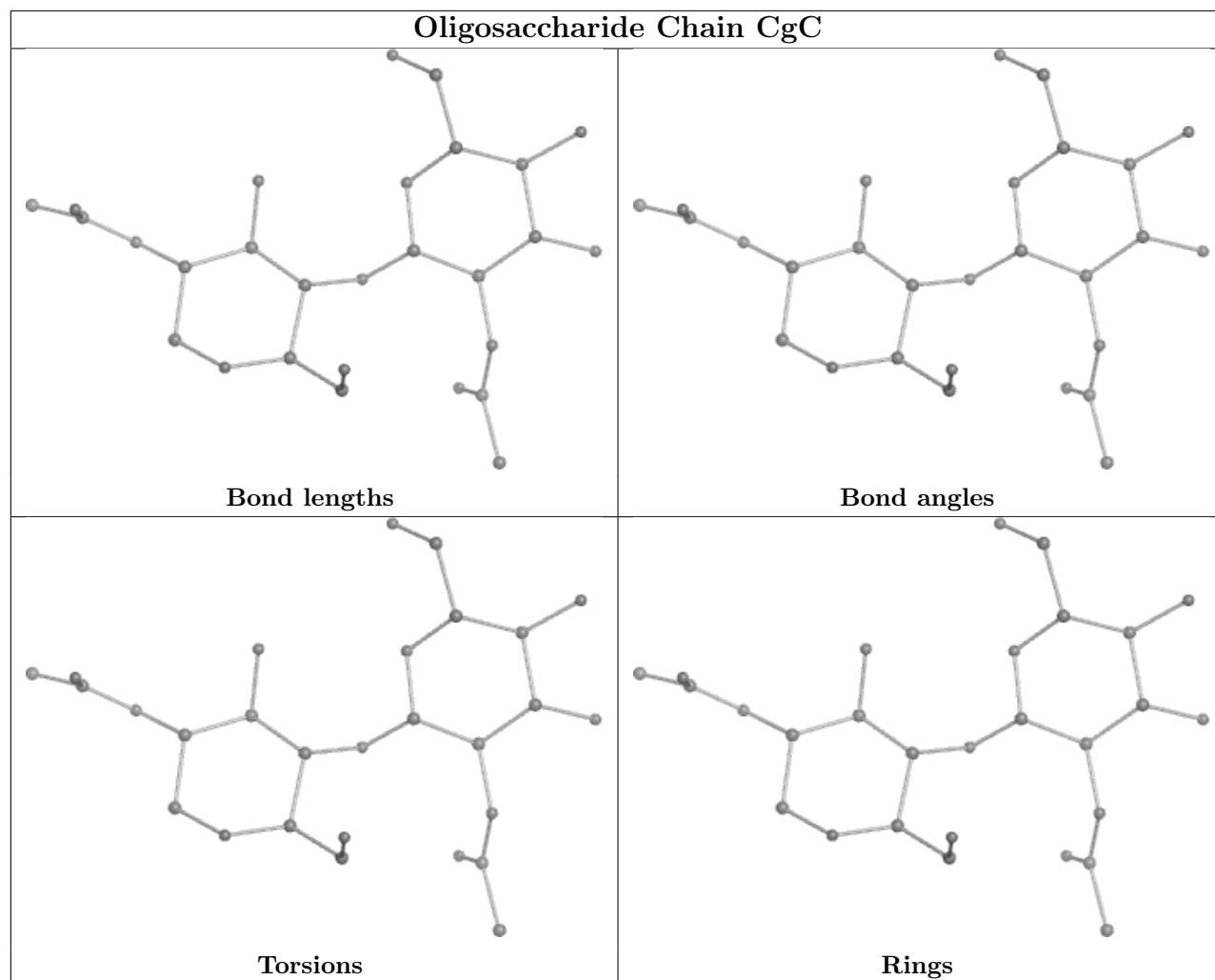
Oligosaccharide Chain AhA

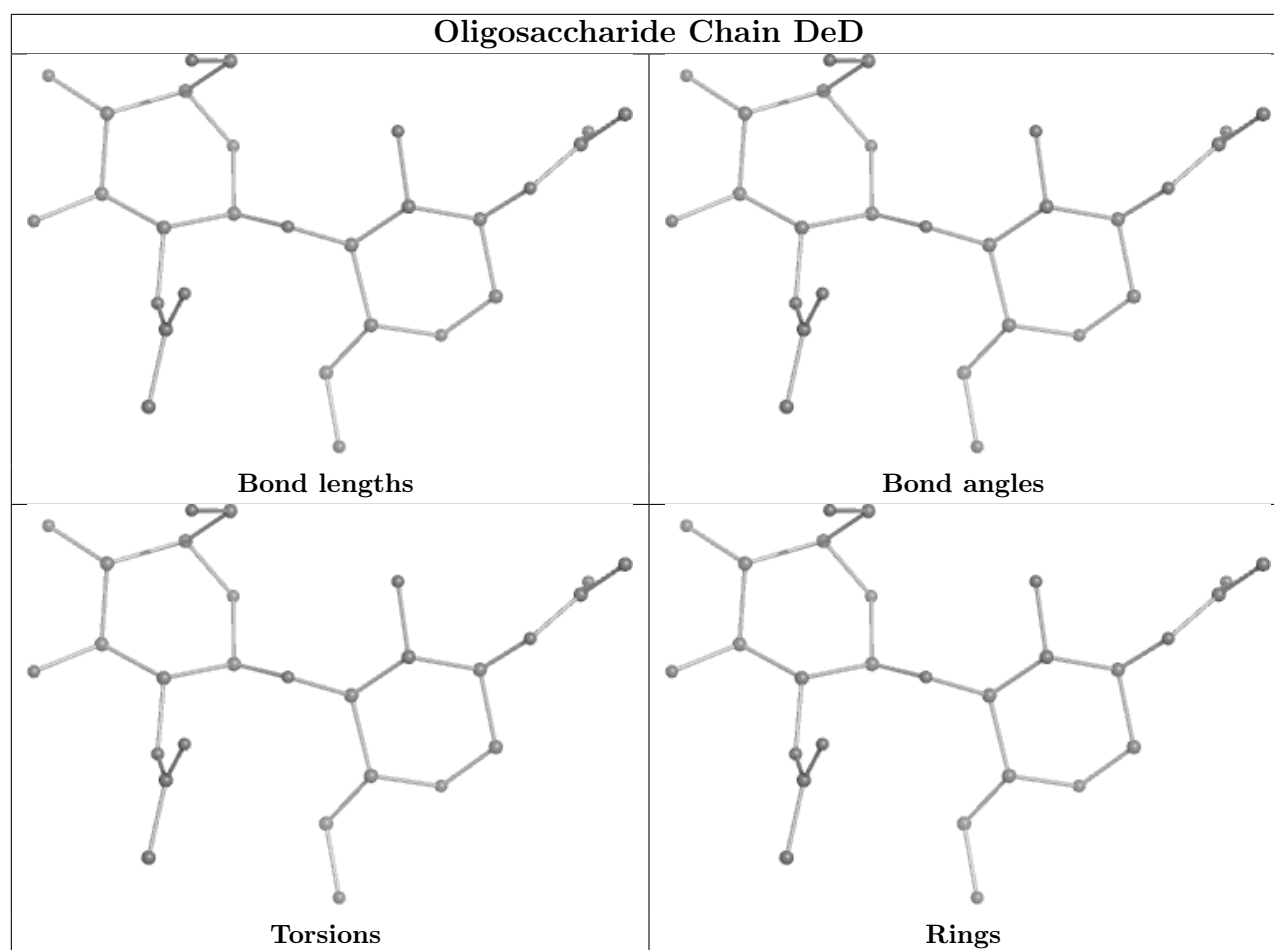


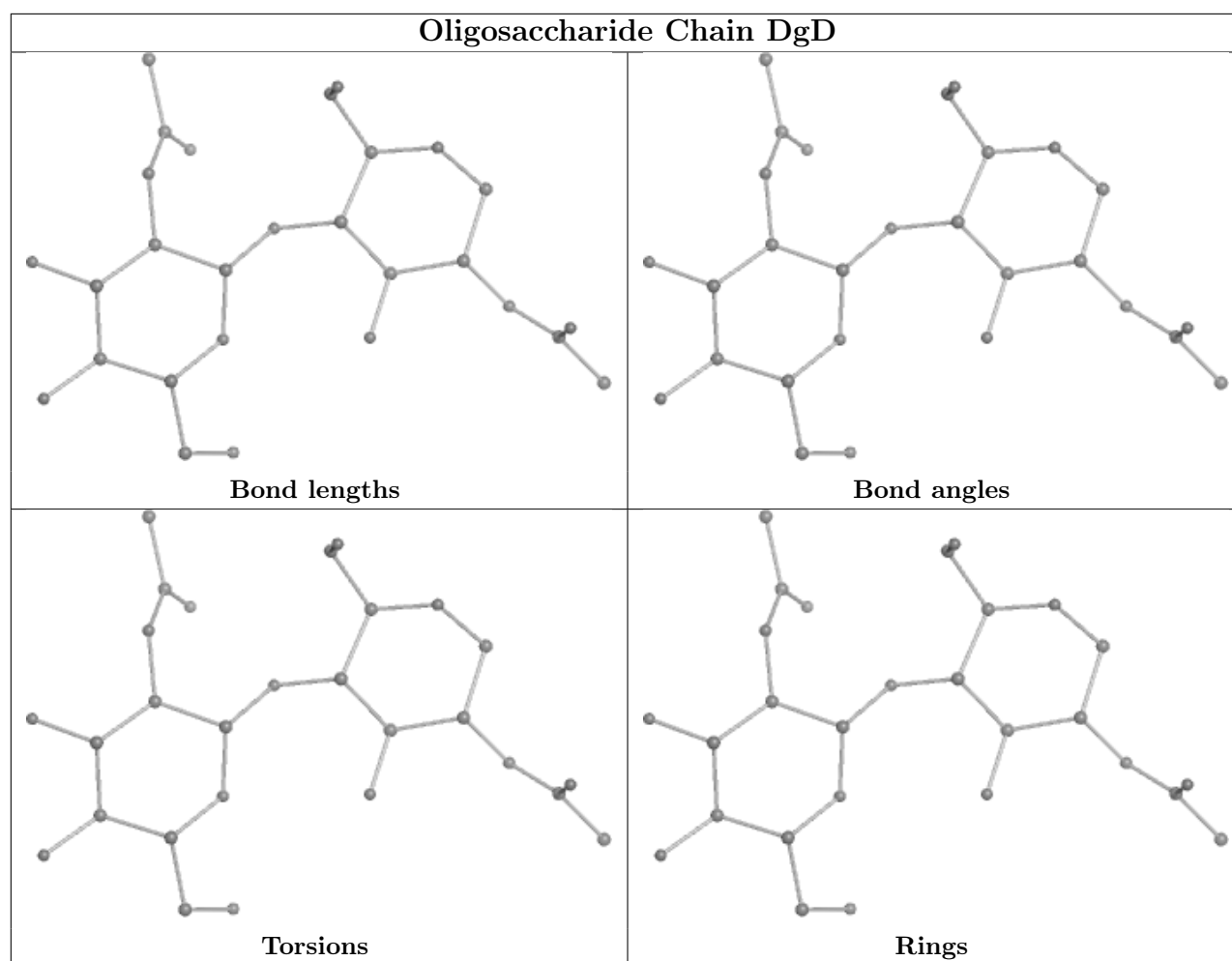
Oligosaccharide Chain BhB











5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 20 are monoatomic - leaving 12 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	$\# Z > 2$
5	ATP	CCC	605[A]	-	26,33,33	0.66	0	31,52,52	0.95	1 (3%)
5	ATP	BBB	605[B]	-	26,33,33	0.68	0	31,52,52	0.77	1 (3%)
6	OXY	BBB	606	4	1,1,1	0.34	0	-		
5	ATP	AAA	605[A]	-	26,33,33	0.62	0	31,52,52	1.02	2 (6%)
5	ATP	DDD	605[B]	-	26,33,33	0.68	0	31,52,52	0.79	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OXY	DDD	606	4	1,1,1	0.20	0	-		
5	ATP	CCC	605[B]	-	26,33,33	0.67	0	31,52,52	0.98	1 (3%)
5	ATP	AAA	605[B]	-	26,33,33	0.60	0	31,52,52	0.89	1 (3%)
5	ATP	DDD	605[A]	-	26,33,33	0.65	0	31,52,52	0.76	1 (3%)
6	OXY	CCC	606	4	1,1,1	0.28	0	-		
6	OXY	AAA	606	4	1,1,1	0.28	0	-		
5	ATP	BBB	605[A]	-	26,33,33	0.70	0	31,52,52	0.86	1 (3%)

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
5	ATP	CCC	605[A]	-	-	6/18/38/38	0/3/3/3
5	ATP	BBB	605[B]	-	-	5/18/38/38	0/3/3/3
5	ATP	AAA	605[A]	-	-	2/18/38/38	0/3/3/3
5	ATP	DDD	605[B]	-	-	1/18/38/38	0/3/3/3
5	ATP	CCC	605[B]	-	-	3/18/38/38	0/3/3/3
5	ATP	AAA	605[B]	-	-	0/18/38/38	0/3/3/3
5	ATP	DDD	605[A]	-	-	0/18/38/38	0/3/3/3
5	ATP	BBB	605[A]	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	CCC	605[A]	ATP	C5-C6-N6	3.06	125.00	120.35
5	CCC	605[B]	ATP	C5-C6-N6	3.06	125.00	120.35
5	AAA	605[A]	ATP	PA-O3A-PB	2.74	142.22	132.83
5	AAA	605[A]	ATP	C5-C6-N6	2.67	124.42	120.35
5	AAA	605[B]	ATP	C5-C6-N6	2.67	124.42	120.35
5	DDD	605[A]	ATP	C5-C6-N6	2.25	123.78	120.35
5	DDD	605[B]	ATP	C5-C6-N6	2.25	123.78	120.35
5	BBB	605[A]	ATP	C5-C6-N6	2.02	123.43	120.35
5	BBB	605[B]	ATP	C5-C6-N6	2.02	123.43	120.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BBB	605[A]	ATP	C5'-O5'-PA-O1A
5	BBB	605[A]	ATP	C5'-O5'-PA-O2A
5	BBB	605[A]	ATP	C5'-O5'-PA-O3A
5	BBB	605[A]	ATP	O4'-C4'-C5'-O5'
5	BBB	605[B]	ATP	C5'-O5'-PA-O1A
5	BBB	605[B]	ATP	C5'-O5'-PA-O2A
5	BBB	605[B]	ATP	C5'-O5'-PA-O3A
5	BBB	605[B]	ATP	O4'-C4'-C5'-O5'
5	CCC	605[A]	ATP	C5'-O5'-PA-O1A
5	CCC	605[A]	ATP	C5'-O5'-PA-O2A
5	CCC	605[A]	ATP	C5'-O5'-PA-O3A
5	CCC	605[B]	ATP	C5'-O5'-PA-O3A
5	BBB	605[A]	ATP	C3'-C4'-C5'-O5'
5	BBB	605[B]	ATP	C3'-C4'-C5'-O5'
5	AAA	605[A]	ATP	PG-O3B-PB-O2B
5	DDD	605[B]	ATP	PA-O3A-PB-O1B
5	CCC	605[B]	ATP	C5'-O5'-PA-O1A
5	CCC	605[B]	ATP	C5'-O5'-PA-O2A
5	CCC	605[A]	ATP	PG-O3B-PB-O2B
5	AAA	605[A]	ATP	PG-O3B-PB-O1B
5	CCC	605[A]	ATP	PG-O3B-PB-O1B
5	CCC	605[A]	ATP	PB-O3A-PA-O2A

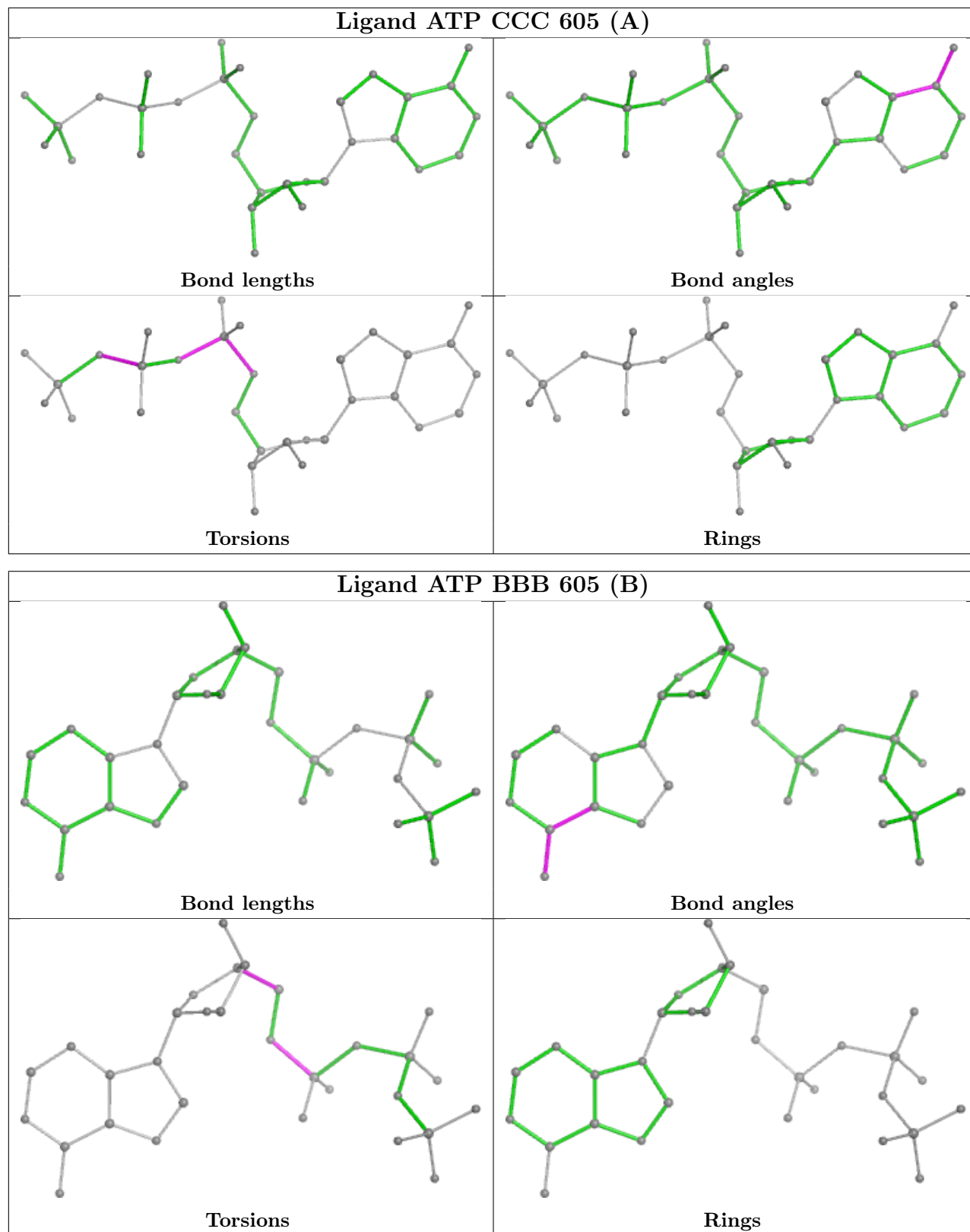
There are no ring outliers.

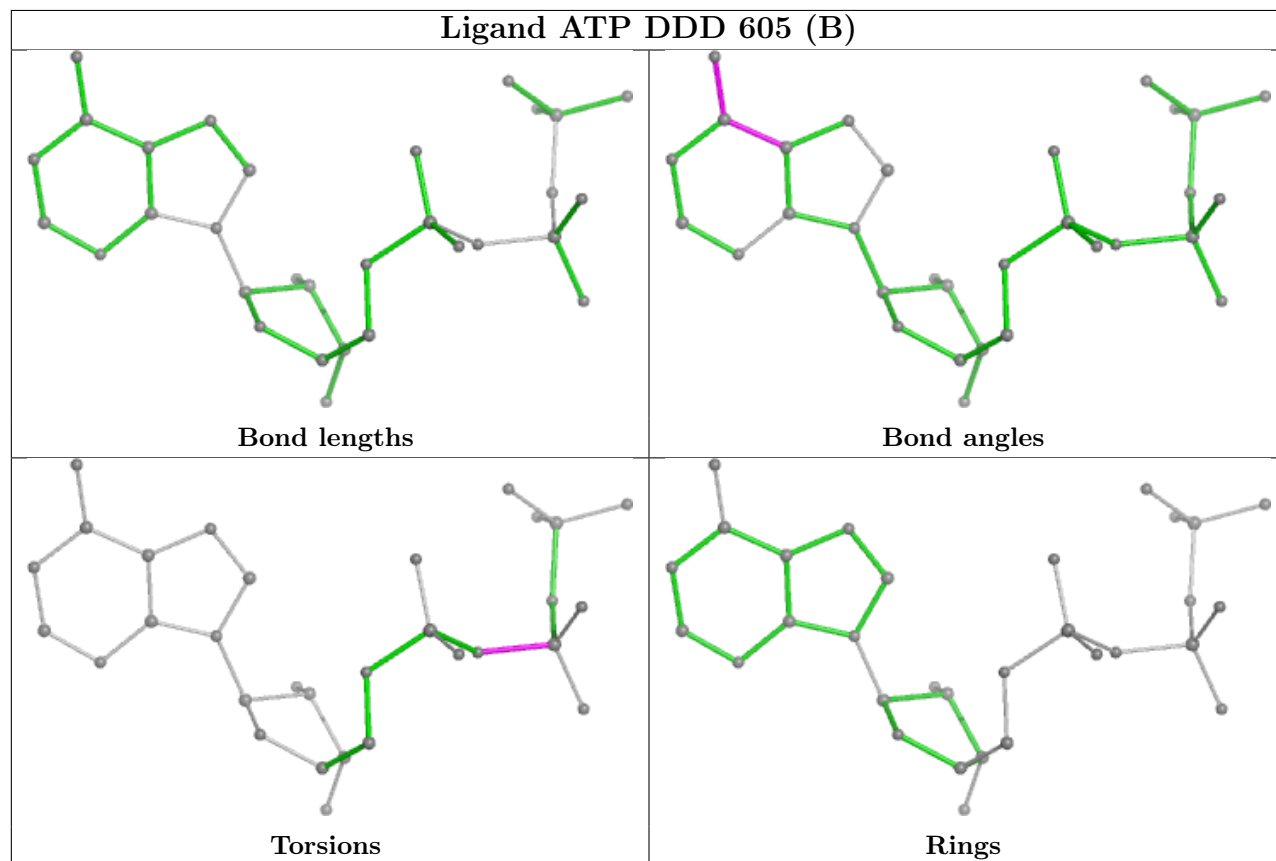
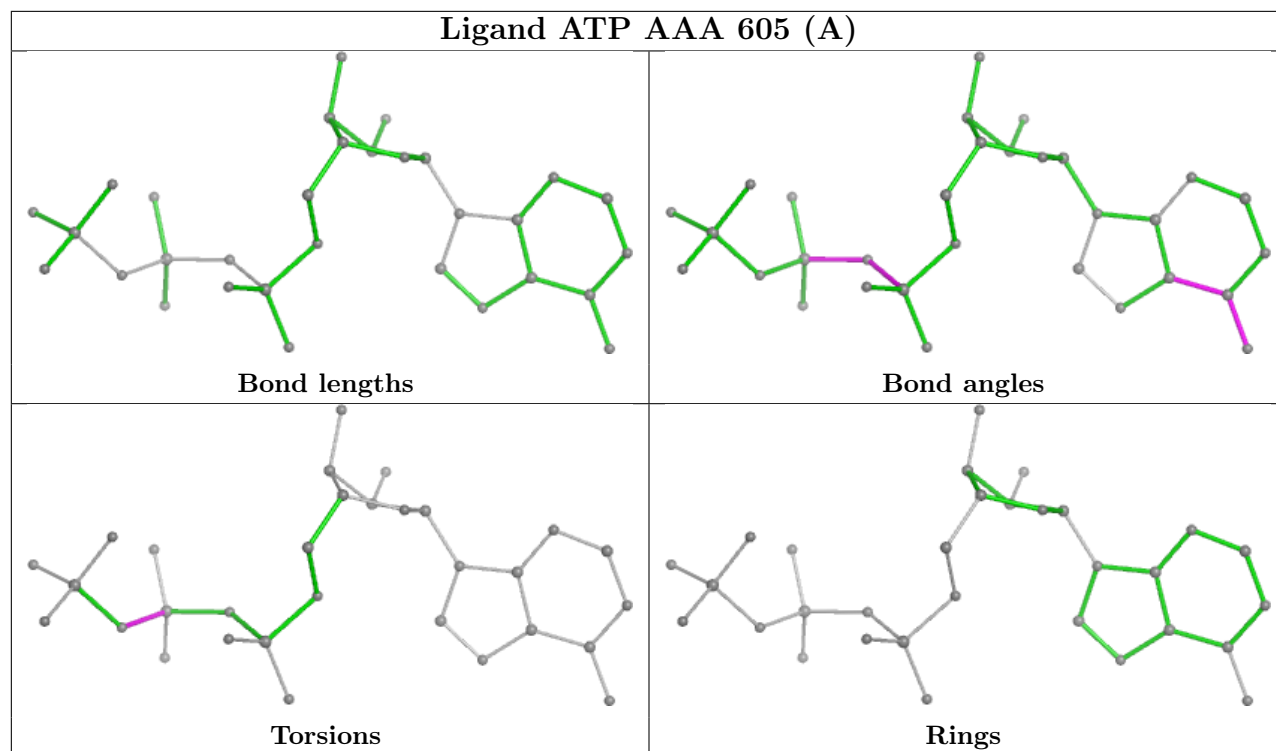
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	605[A]	ATP	2	0
6	DDD	606	OXY	1	0
5	CCC	605[B]	ATP	2	0
5	AAA	605[B]	ATP	1	0

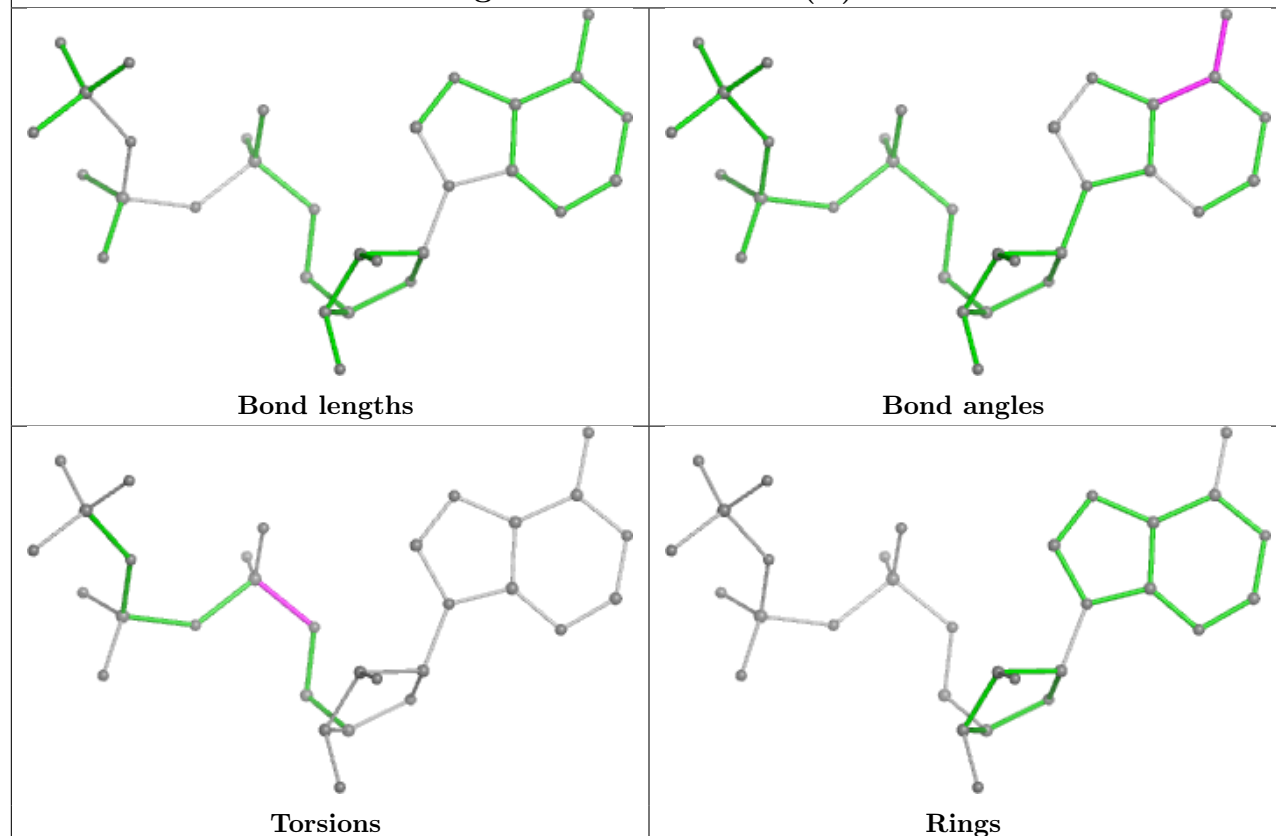
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

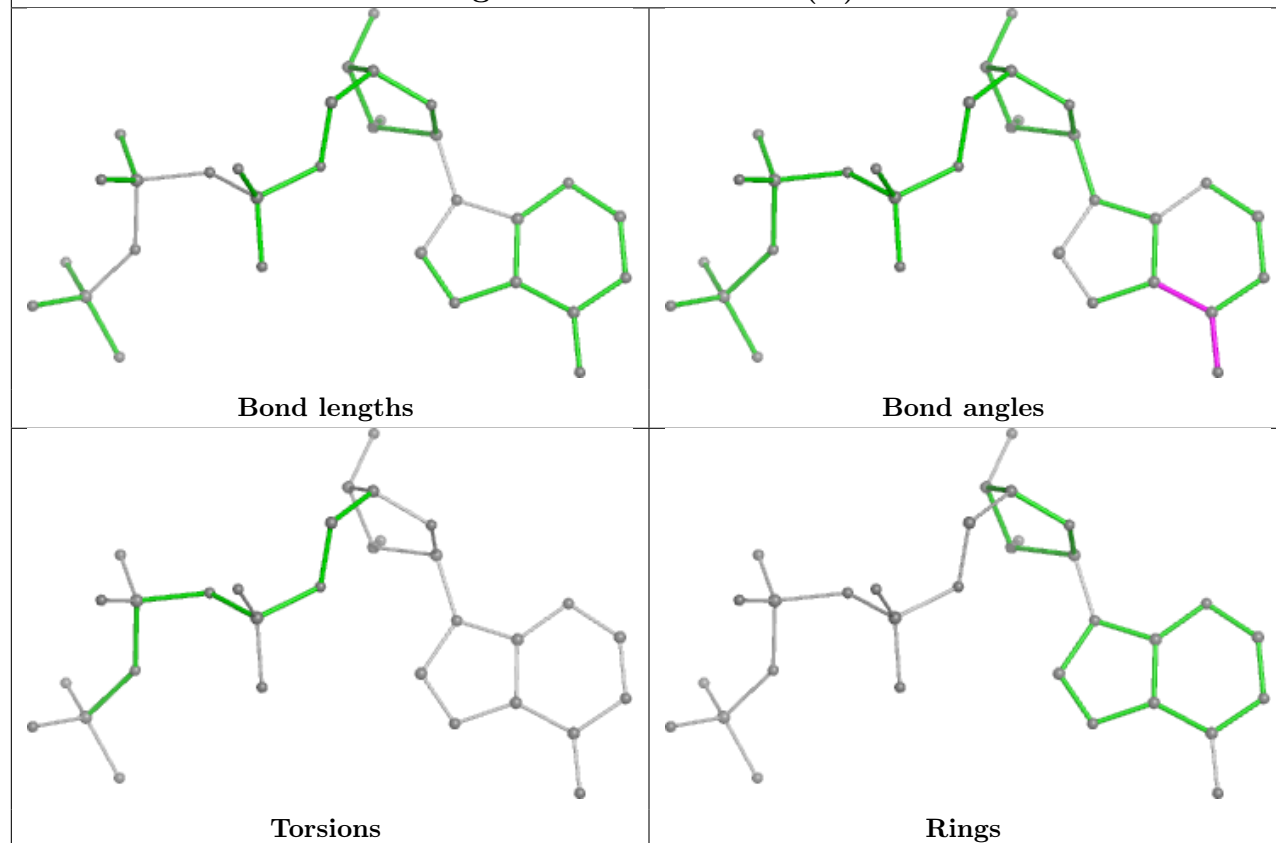


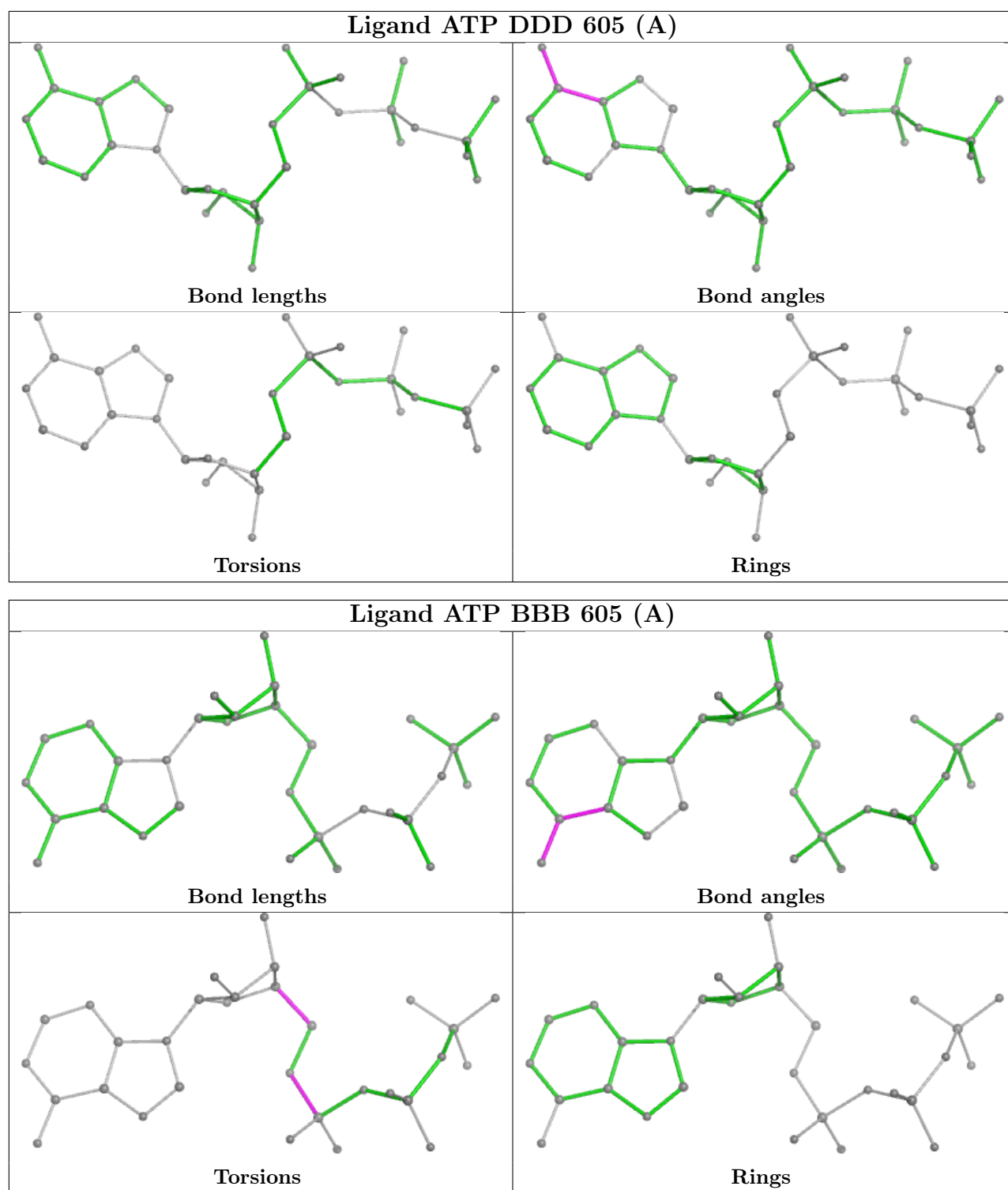


Ligand ATP CCC 605 (B)



Ligand ATP AAA 605 (B)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.67	1 (0%) 92 90	11, 21, 39, 84	3 (0%)
1	BBB	534/534 (100%)	-0.20	8 (1%) 71 68	16, 33, 65, 92	2 (0%)
1	CCC	533/534 (99%)	-0.40	0 100 100	17, 27, 50, 76	4 (0%)
1	DDD	534/534 (100%)	-0.49	2 (0%) 89 87	16, 27, 48, 79	1 (0%)
All	All	2135/2136 (99%)	-0.44	11 (0%) 87 85	11, 26, 53, 92	10 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	32	ASN	3.7
1	BBB	31	VAL	3.1
1	BBB	33	GLY	2.8
1	AAA	534	GLU	2.7
1	BBB	516	VAL	2.7
1	DDD	534	GLU	2.5
1	BBB	325	THR	2.3
1	BBB	34	GLN	2.2
1	BBB	324	THR	2.1
1	BBB	29	ASN	2.1
1	DDD	497	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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,

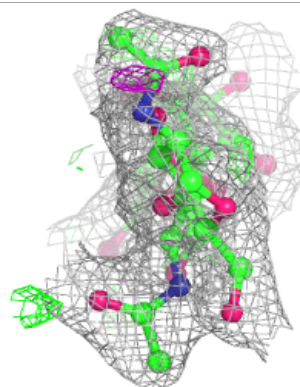
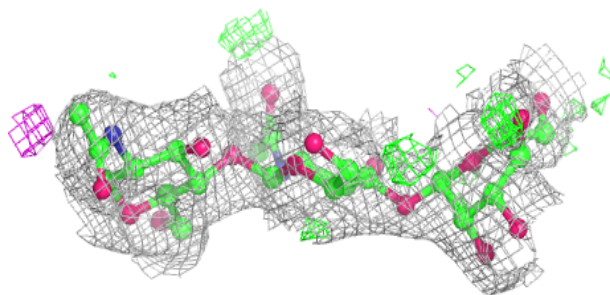
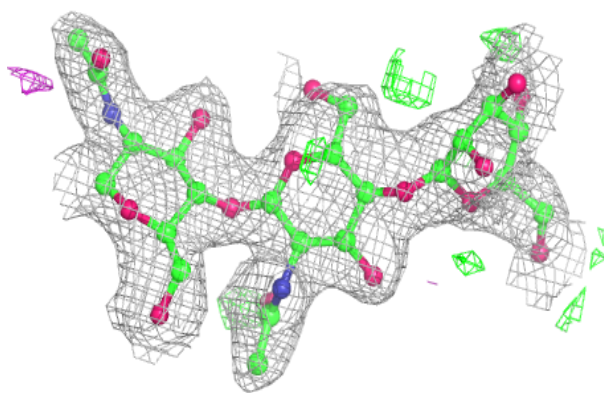
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	AeA	1	14/15	-	-	26,28,34,35	0
2	NAG	AeA	2	14/15	-	-	37,48,60,67	0
2	BMA	AeA	3	11/12	-	-	58,69,74,75	0
2	NAG	BeB	1	14/15	-	-	32,39,44,51	0
2	NAG	BeB	2	14/15	-	-	48,63,75,86	0
2	BMA	BeB	3	11/12	-	-	93,101,112,113	0
3	NAG	AhA	1	14/15	-	-	23,27,30,30	0
3	NAG	AhA	2	14/15	-	-	35,37,41,43	0
3	NAG	BhB	1	14/15	-	-	50,59,63,67	0
3	NAG	BhB	2	14/15	-	-	56,71,80,84	0
3	NAG	CeC	1	14/15	-	-	27,32,37,43	0
3	NAG	CeC	2	14/15	-	-	42,58,69,71	0
3	NAG	CgC	1	14/15	-	-	30,36,40,44	0
3	NAG	CgC	2	14/15	-	-	42,48,62,62	0
3	NAG	DeD	1	14/15	-	-	30,38,42,47	0
3	NAG	DeD	2	14/15	-	-	51,63,77,82	0
3	NAG	DgD	1	14/15	-	-	30,32,39,44	0
3	NAG	DgD	2	14/15	-	-	43,49,63,66	0

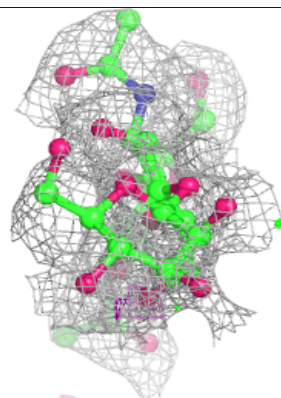
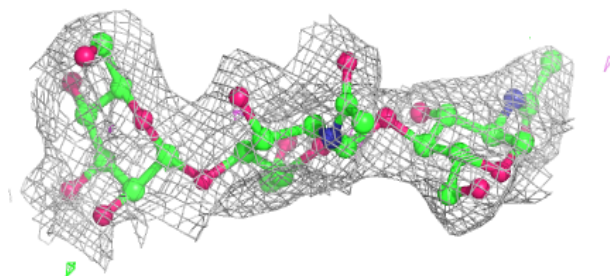
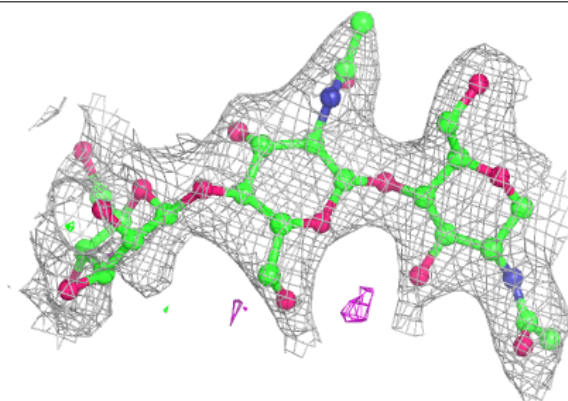
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

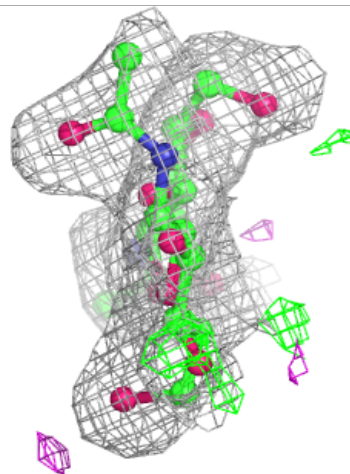
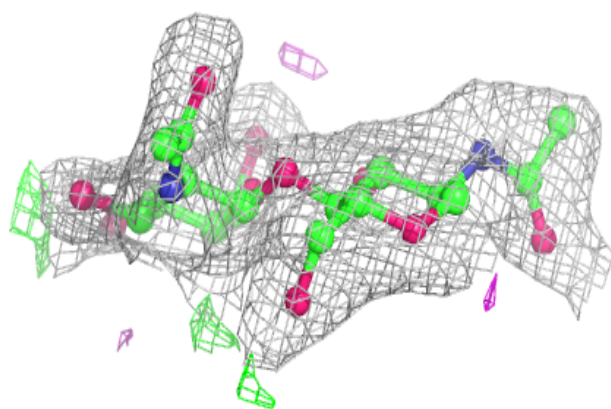
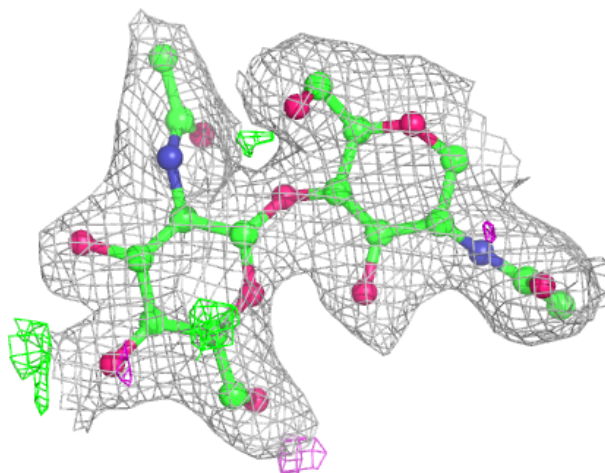
**Electron density around Chain BeB:**

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



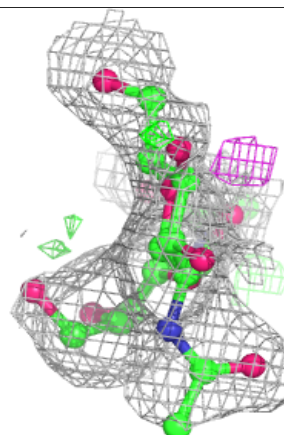
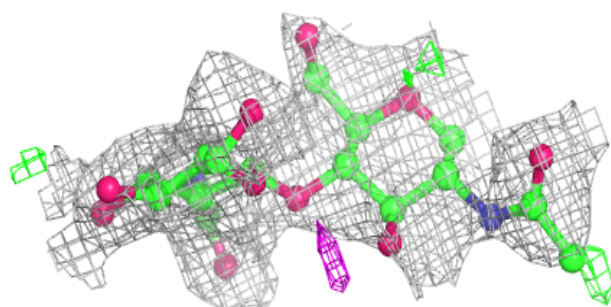
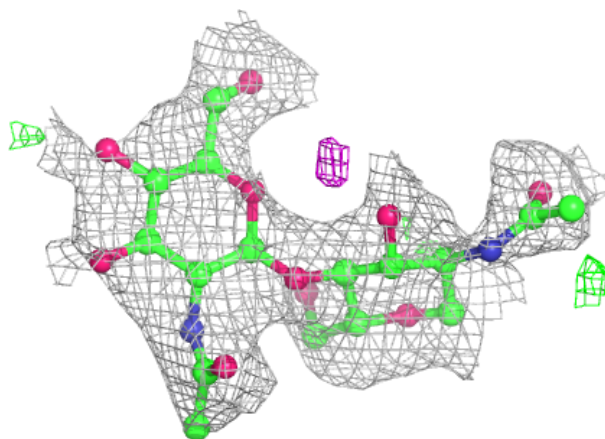
Electron density around Chain AhA:

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

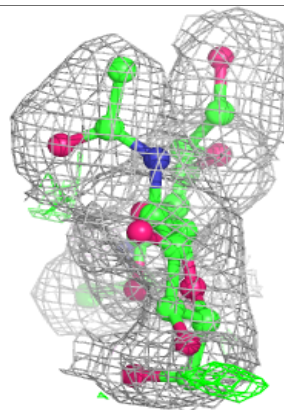
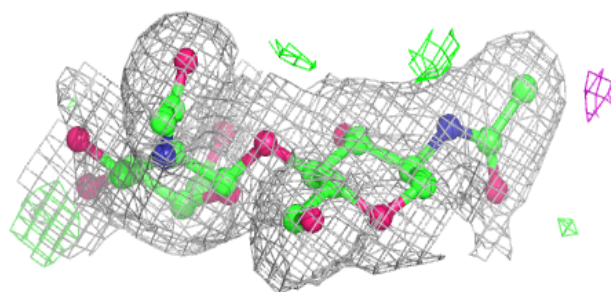
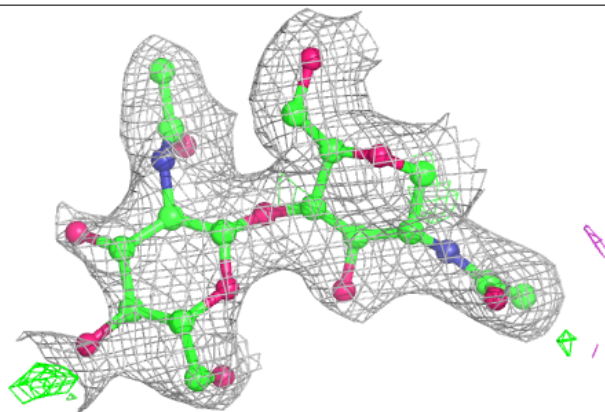


Electron density around Chain BhB:

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

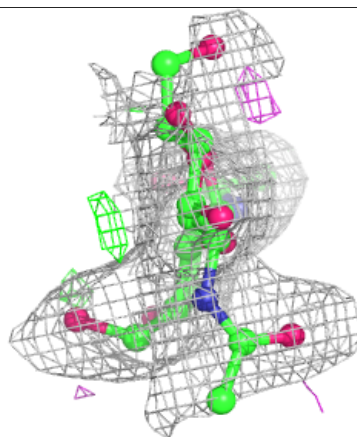
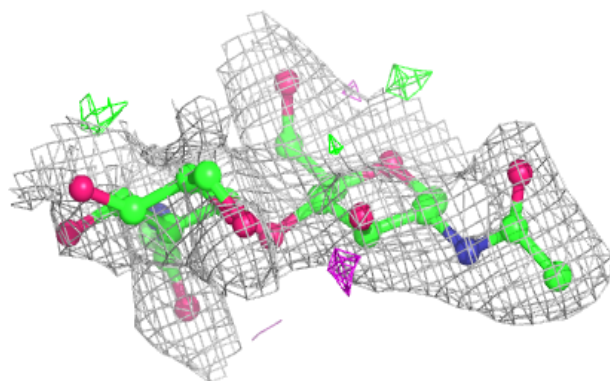
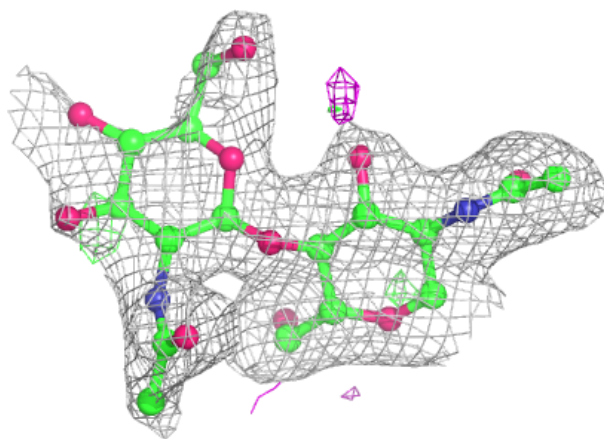
**Electron density around Chain CeC:**

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



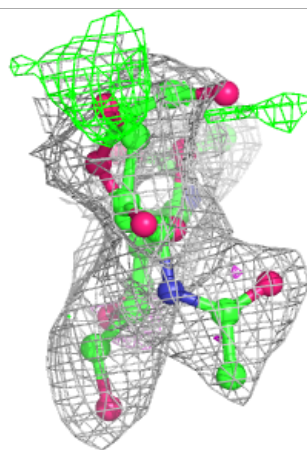
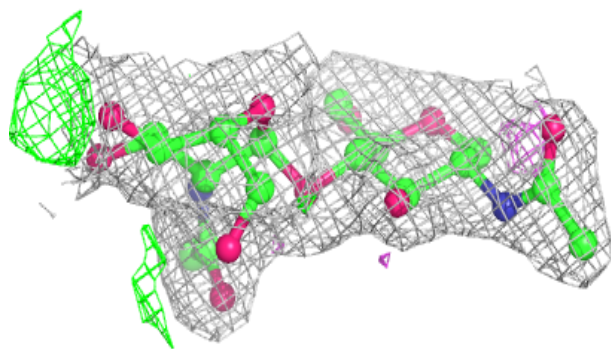
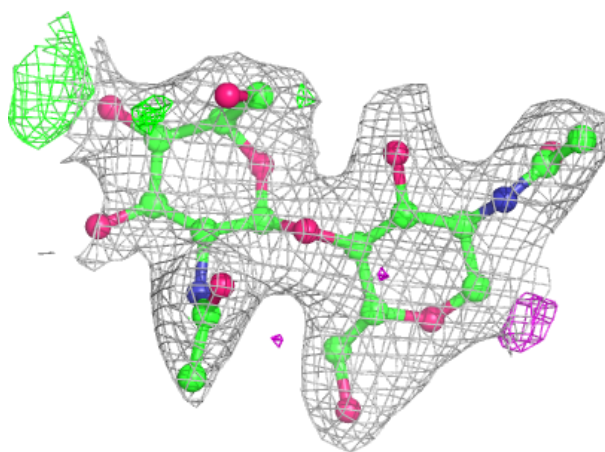
Electron density around Chain CgC:

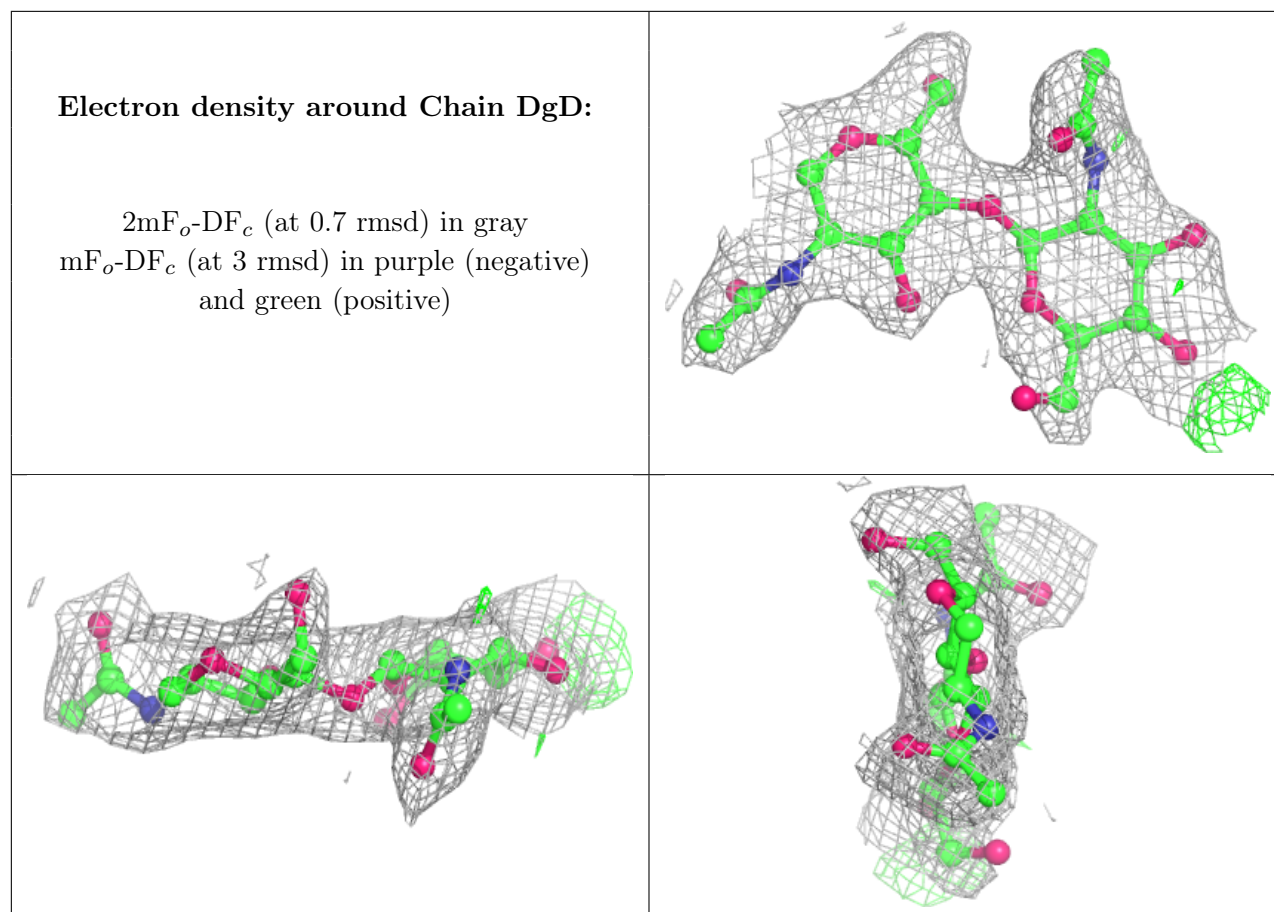
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain DeD:

$2mF_o-DF_c$ (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	ATP	CCC	605[A]	31/31	0.86	0.14	51,64,76,80	13
5	ATP	CCC	605[B]	31/31	0.86	0.14	36,53,67,69	13
5	ATP	BBB	605[A]	31/31	0.87	0.11	35,54,71,77	13
5	ATP	BBB	605[B]	31/31	0.87	0.11	47,59,71,77	13
5	ATP	AAA	605[A]	31/31	0.89	0.12	43,53,65,65	13
5	ATP	AAA	605[B]	31/31	0.89	0.12	40,50,63,65	13
5	ATP	DDD	605[A]	31/31	0.90	0.10	46,59,66,69	13
5	ATP	DDD	605[B]	31/31	0.90	0.10	38,57,66,69	13
7	CL	CCC	607	1/1	0.94	0.09	54,54,54,54	0
7	CL	AAA	608	1/1	0.95	0.14	64,64,64,64	0
7	CL	AAA	607	1/1	0.96	0.09	52,52,52,52	0
7	CL	CCC	608	1/1	0.97	0.10	49,49,49,49	0

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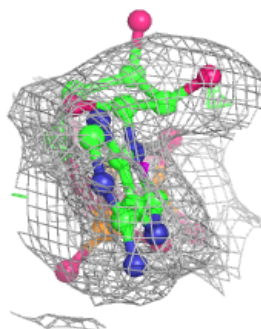
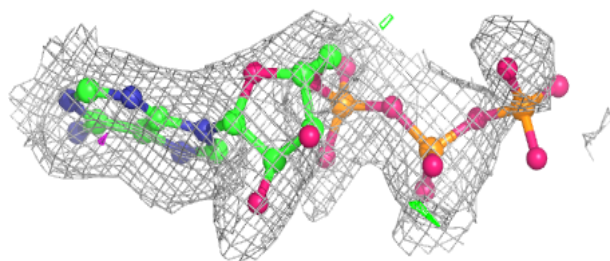
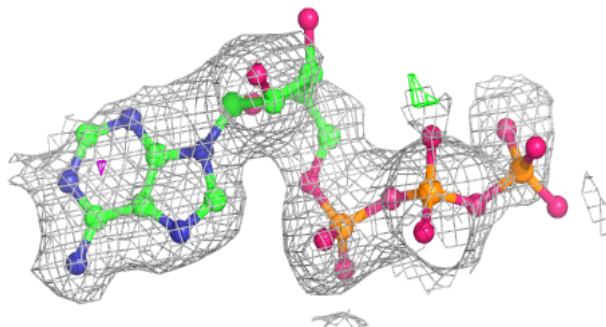
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	OXY	DDD	606	2/2	0.98	0.07	28,28,28,31	0
4	CU	DDD	602	1/1	0.99	0.02	30,30,30,30	0
6	OXY	BBB	606	2/2	0.99	0.04	21,21,21,24	0
6	OXY	CCC	606	2/2	0.99	0.08	25,25,25,28	0
4	CU	BBB	604	1/1	0.99	0.05	44,44,44,44	0
4	CU	AAA	604	1/1	1.00	0.07	32,32,32,32	0
4	CU	BBB	601	1/1	1.00	0.02	30,30,30,30	0
4	CU	BBB	602	1/1	1.00	0.03	31,31,31,31	0
4	CU	BBB	603	1/1	1.00	0.03	32,32,32,32	0
4	CU	AAA	601	1/1	1.00	0.04	21,21,21,21	0
4	CU	CCC	601	1/1	1.00	0.04	28,28,28,28	0
4	CU	CCC	602	1/1	1.00	0.04	23,23,23,23	0
6	OXY	AAA	606	2/2	1.00	0.05	23,23,23,25	0
4	CU	CCC	603	1/1	1.00	0.05	27,27,27,27	0
4	CU	CCC	604	1/1	1.00	0.07	39,39,39,39	0
4	CU	DDD	601	1/1	1.00	0.02	27,27,27,27	0
4	CU	AAA	602	1/1	1.00	0.02	22,22,22,22	0
4	CU	DDD	603	1/1	1.00	0.02	30,30,30,30	0
4	CU	DDD	604	1/1	1.00	0.07	31,31,31,31	0
4	CU	AAA	603	1/1	1.00	0.01	19,19,19,19	0

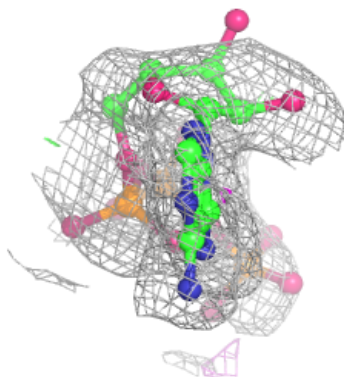
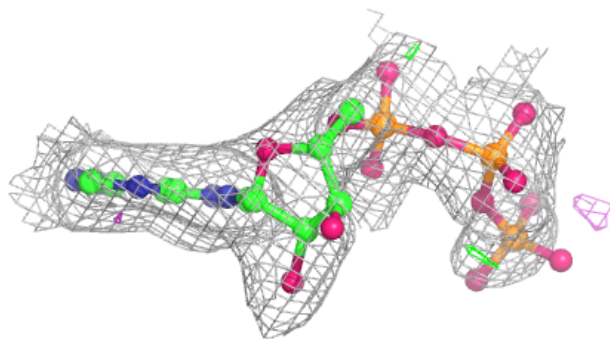
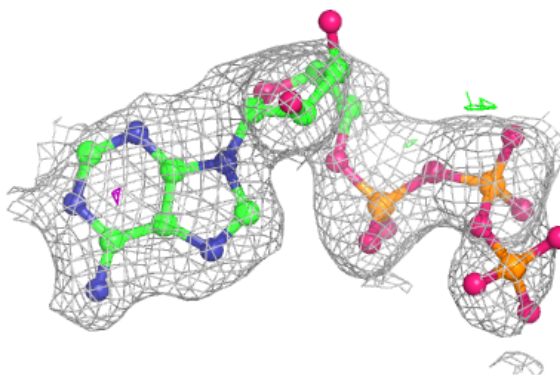
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP CCC 605 (A):

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

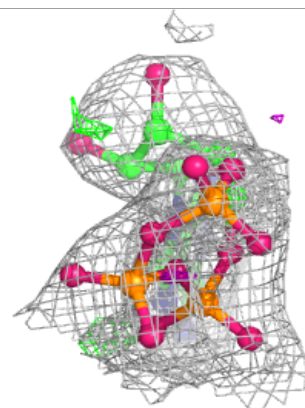
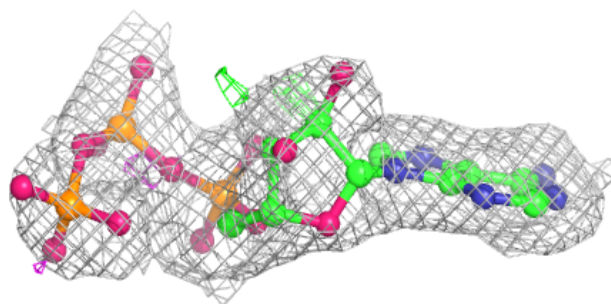
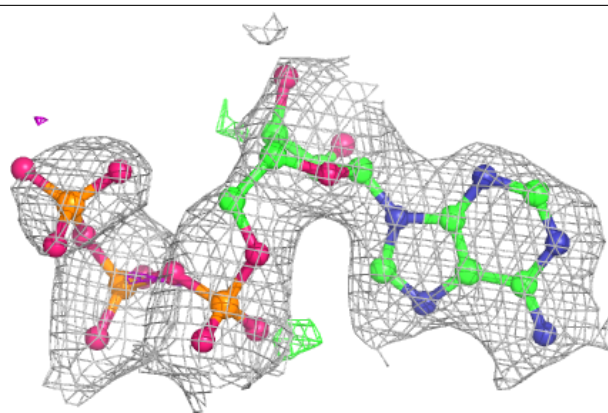
**Electron density around ATP CCC 605 (B):**

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

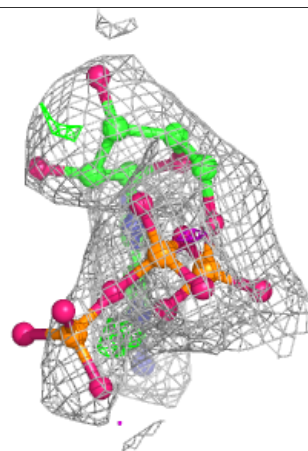
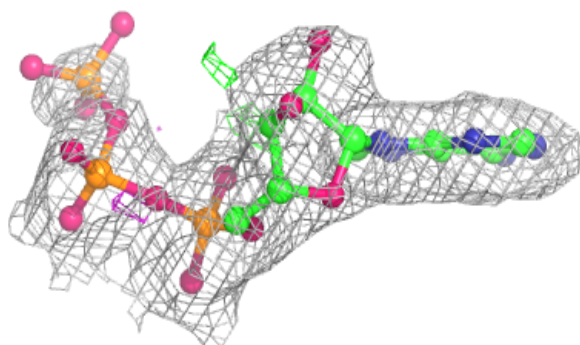
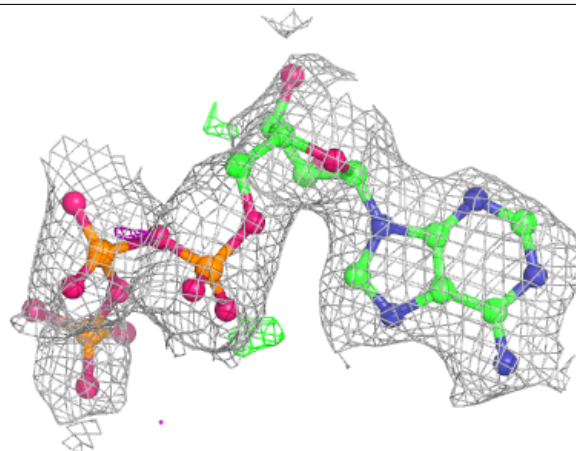


Electron density around ATP BBB 605 (A):

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

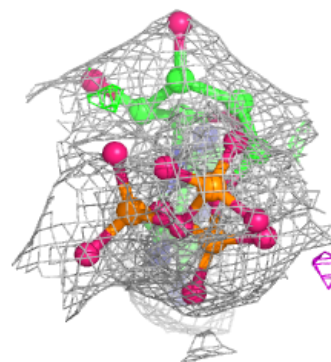
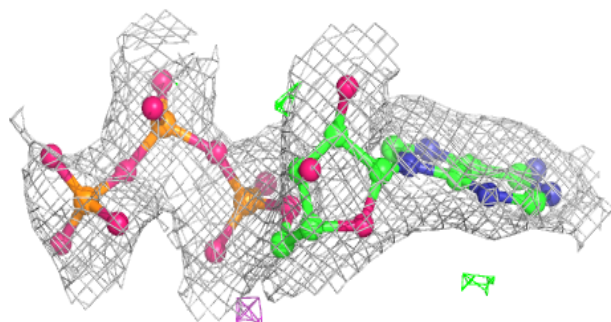
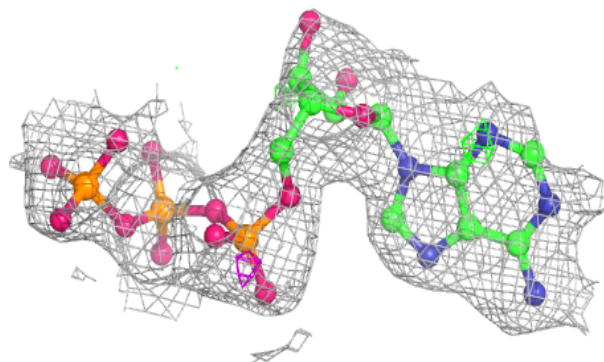
**Electron density around ATP BBB 605 (B):**

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

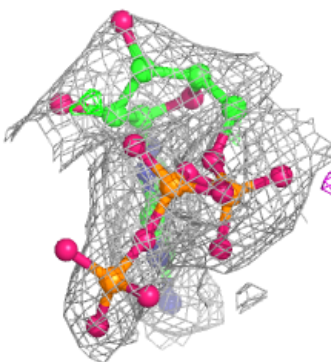
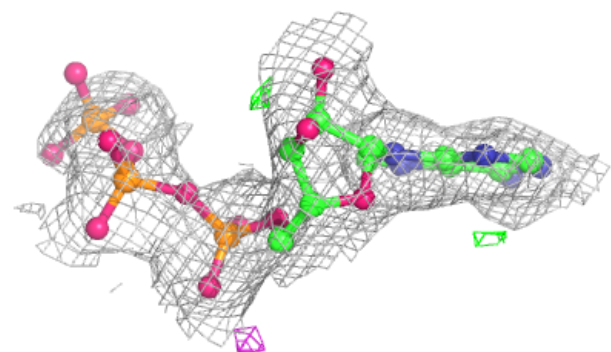
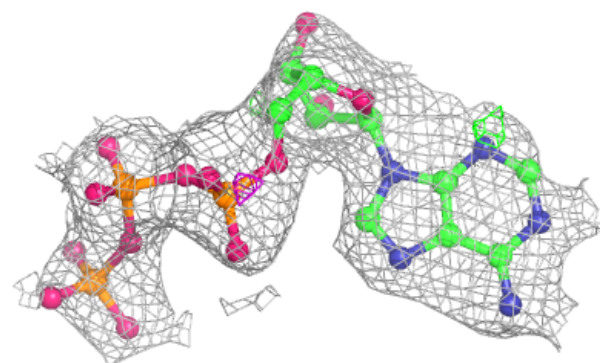


Electron density around ATP AAA 605 (A):

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

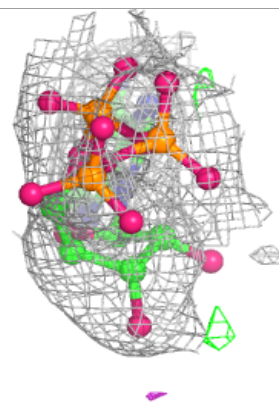
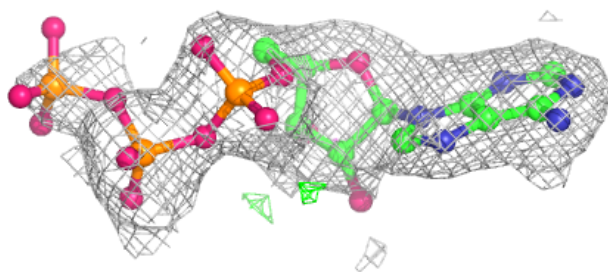
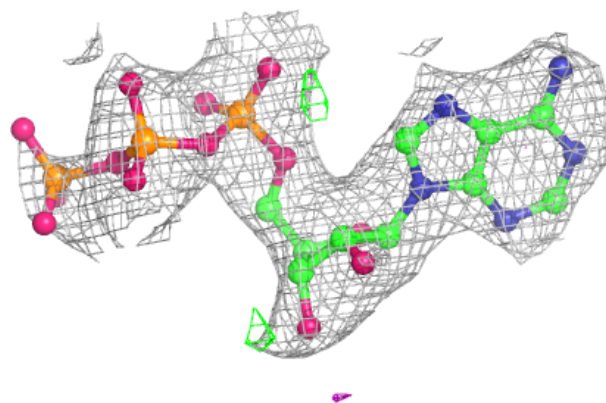
**Electron density around ATP AAA 605 (B):**

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

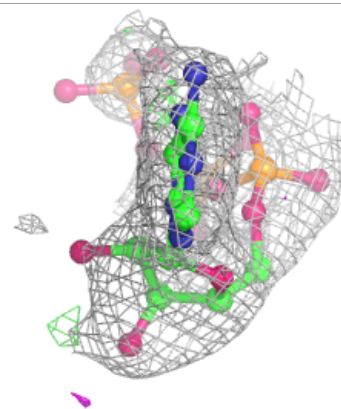
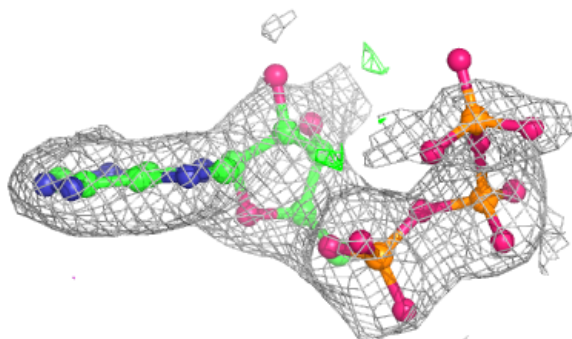
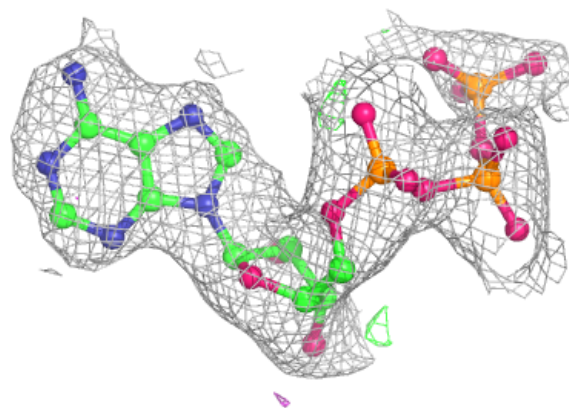


Electron density around ATP DDD 605 (A):

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

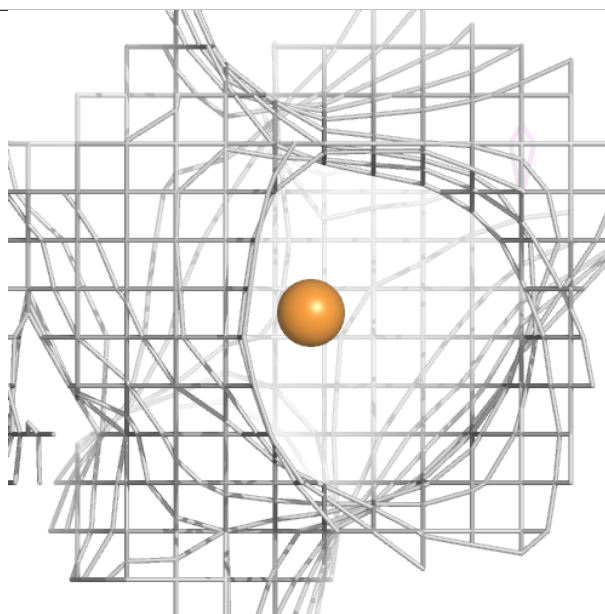
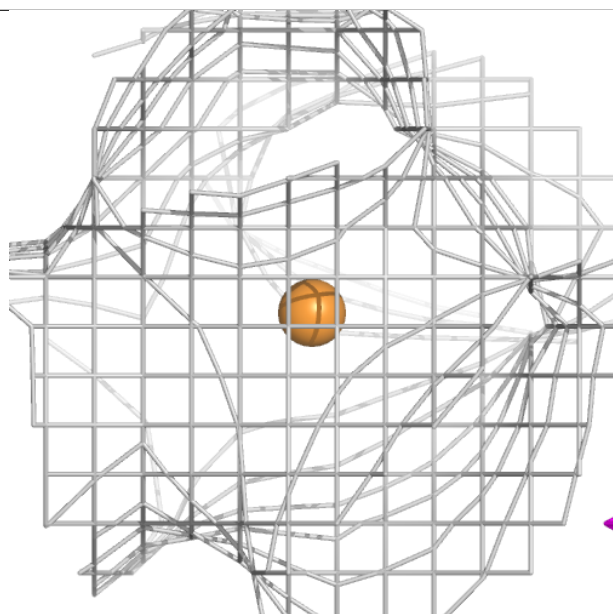
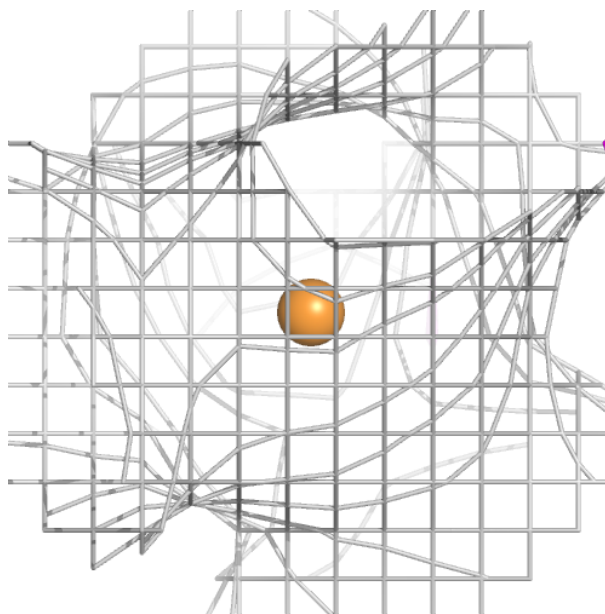
**Electron density around ATP DDD 605 (B):**

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



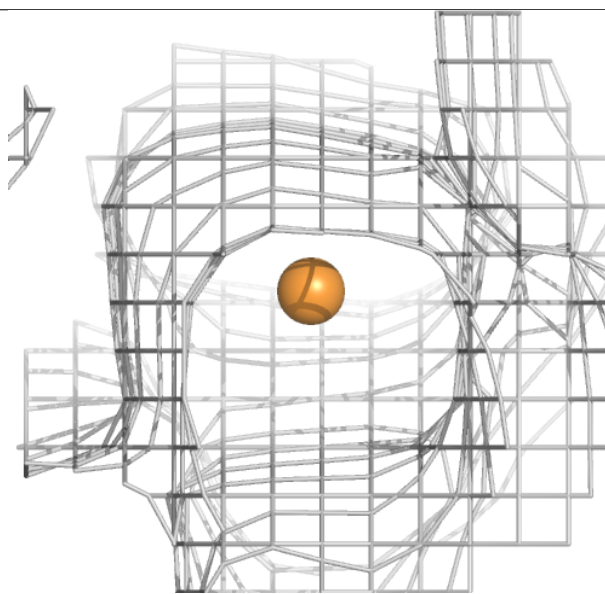
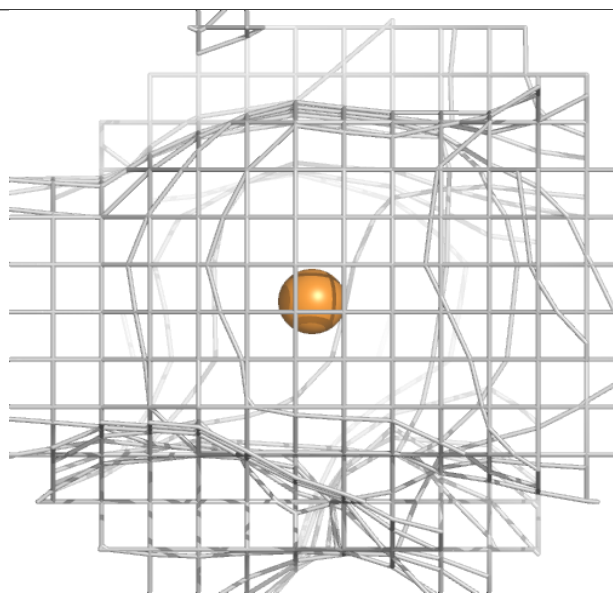
Electron density around CU DDD 602:

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



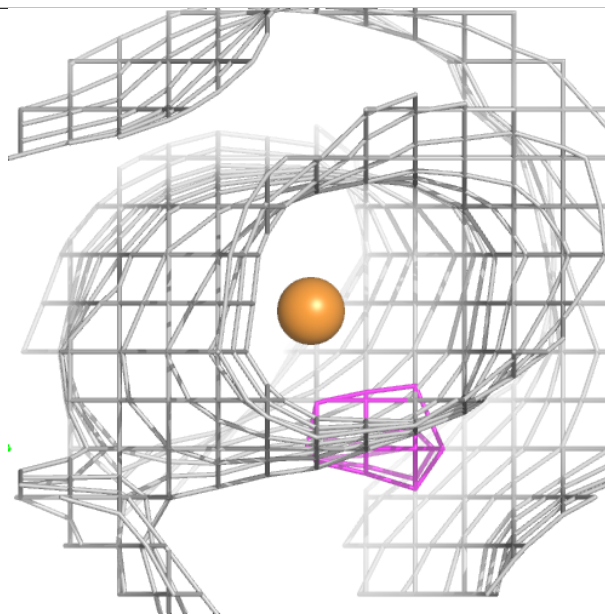
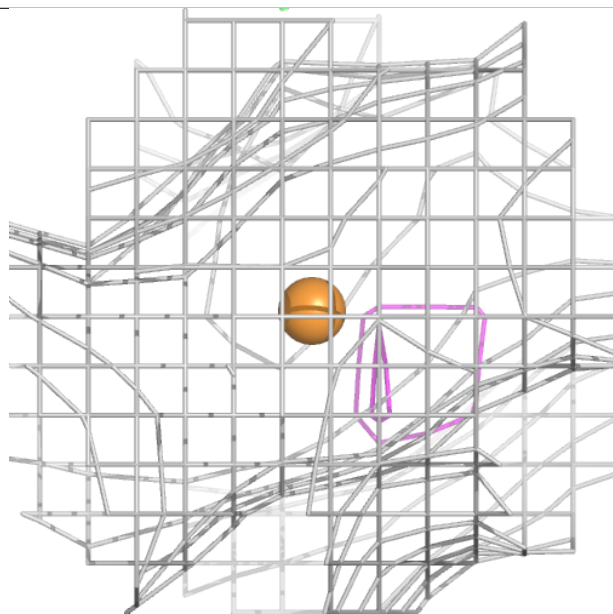
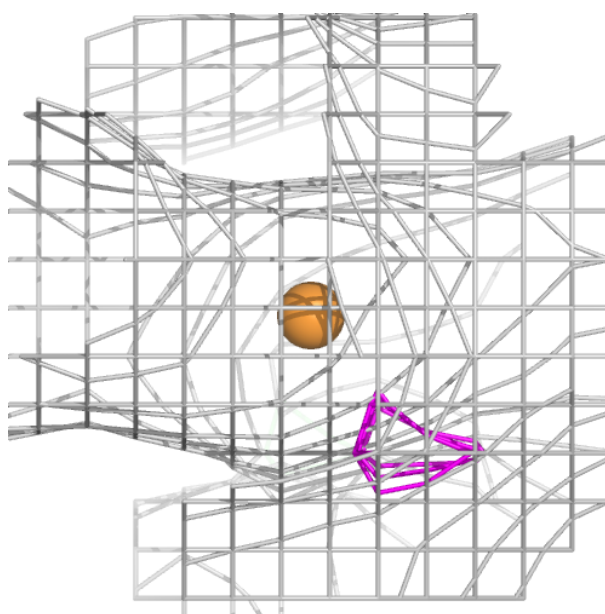
Electron density around CU BBB 604:

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



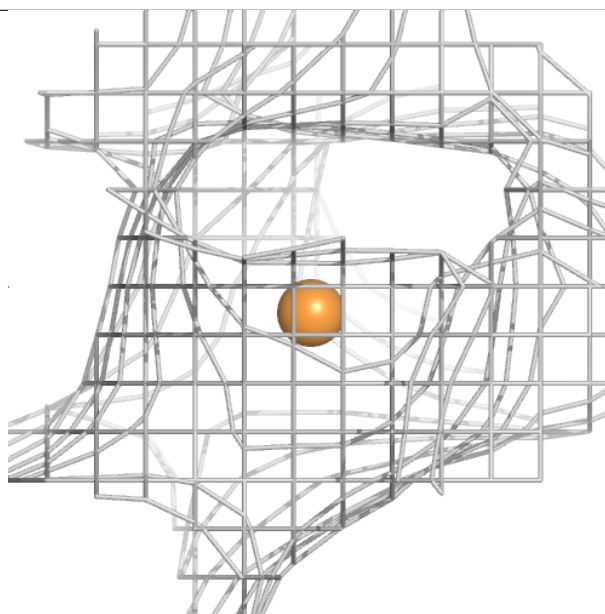
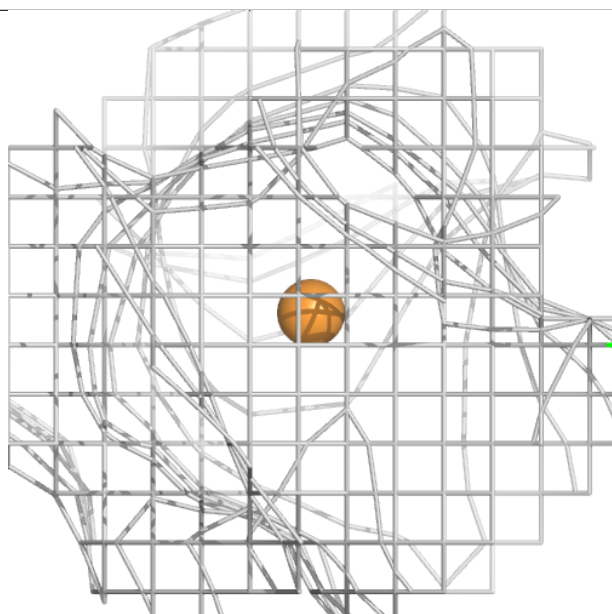
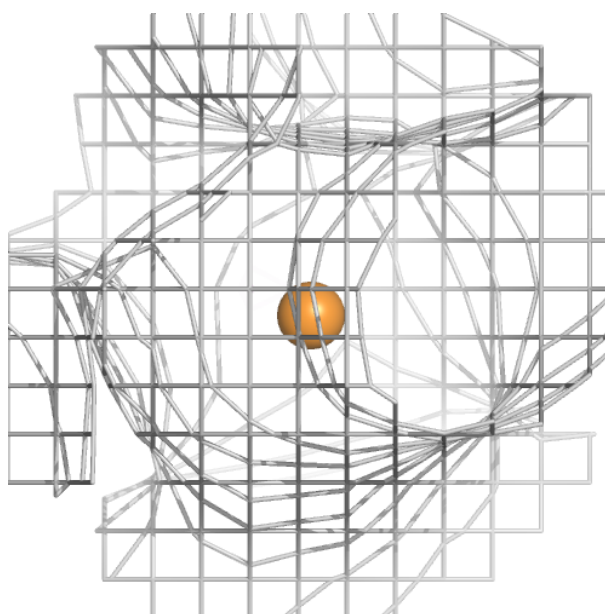
Electron density around CU AAA 604:

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



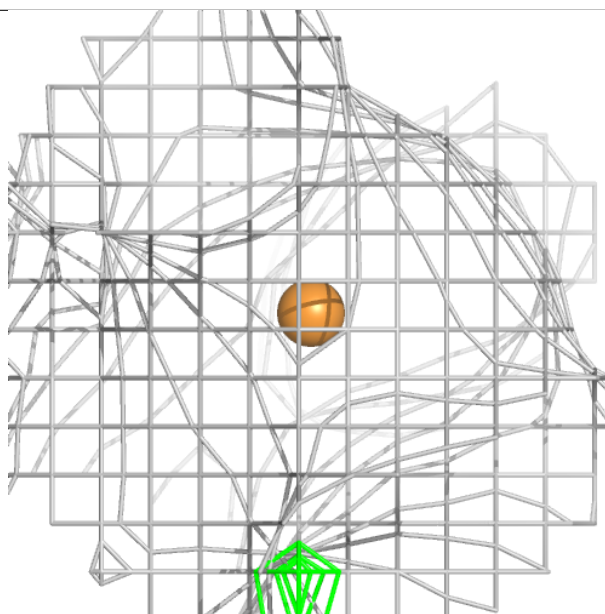
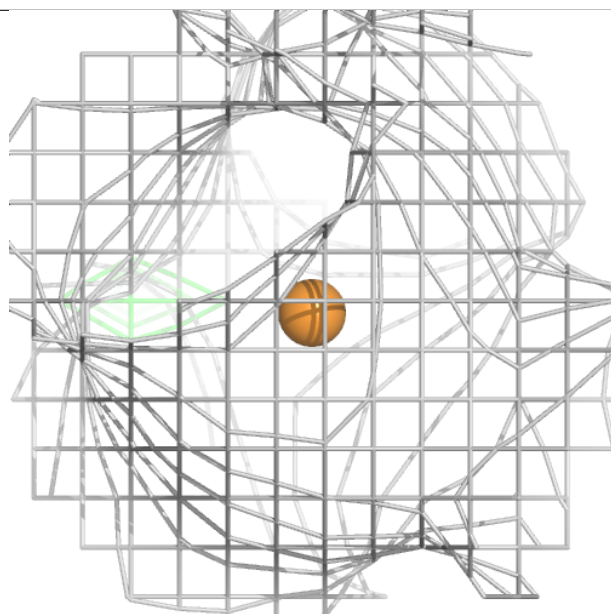
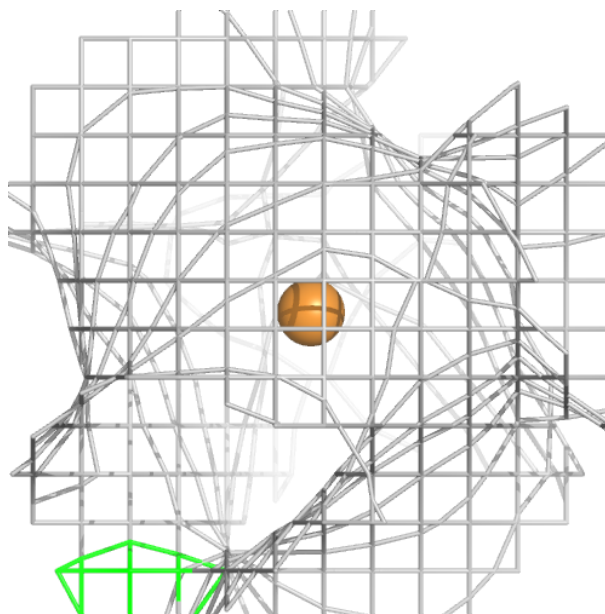
Electron density around CU BBB 601:

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



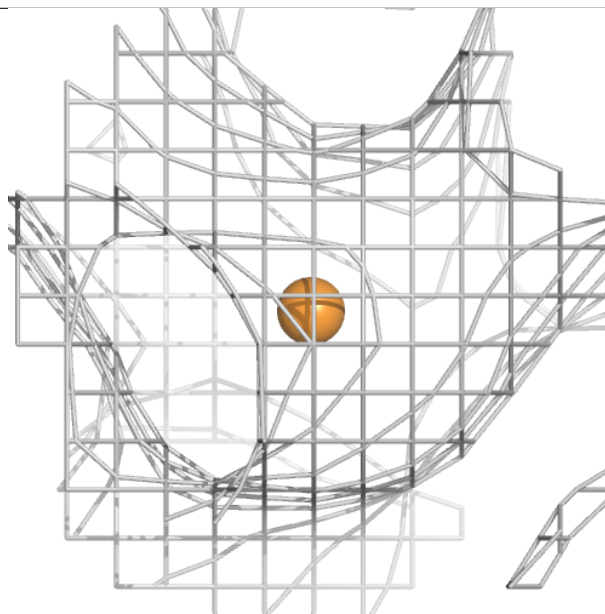
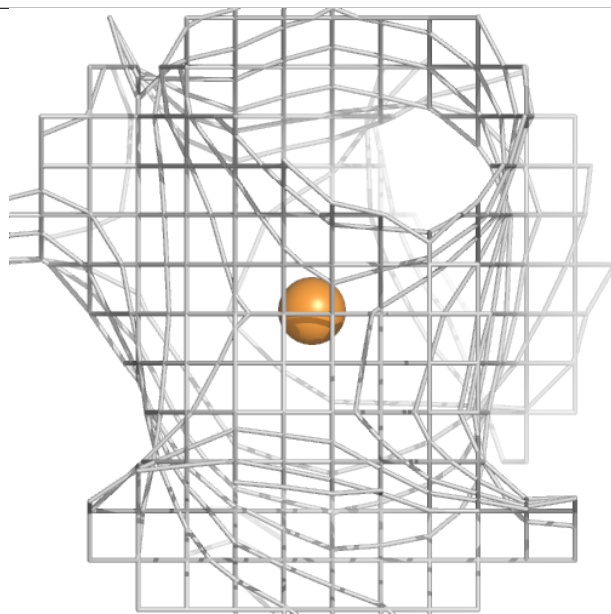
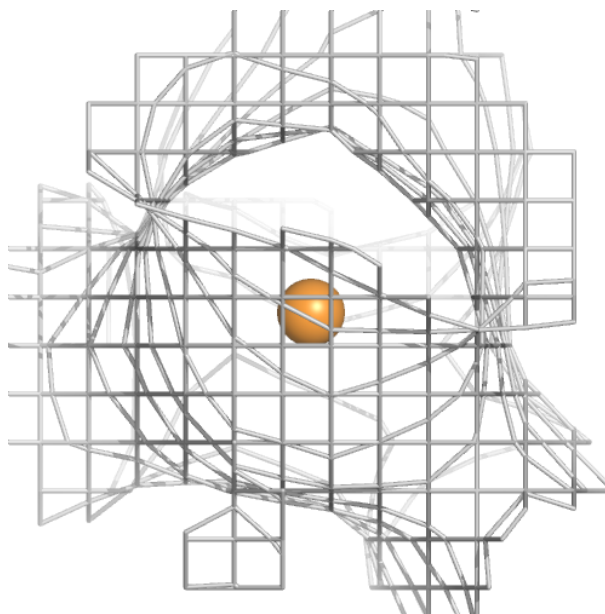
Electron density around CU BBB 602:

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



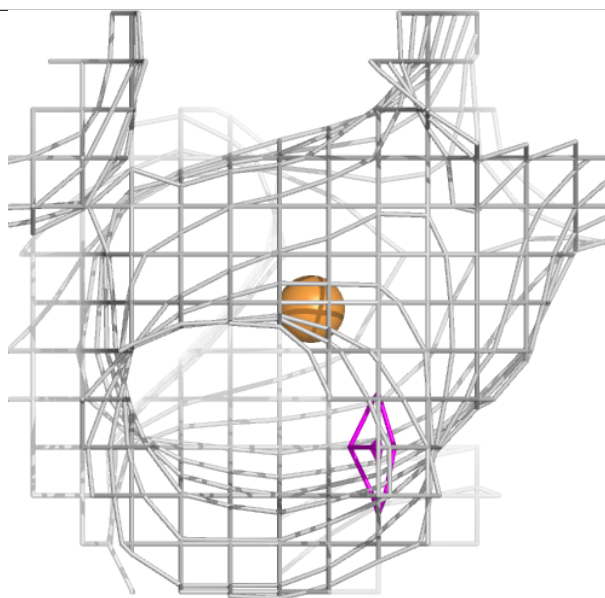
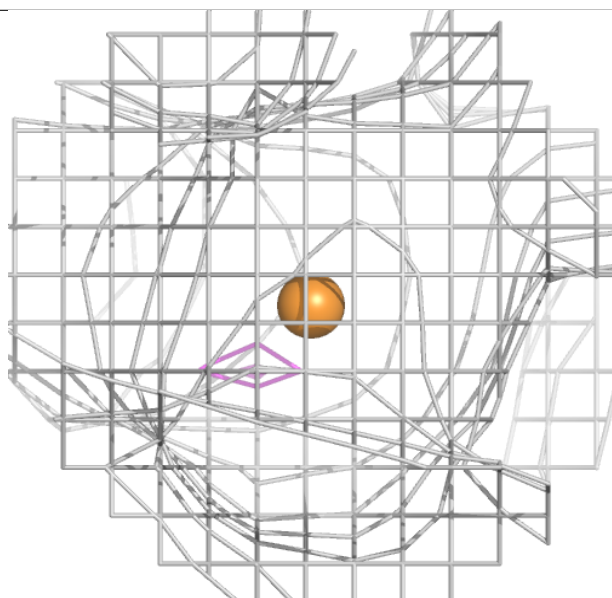
Electron density around CU BBB 603:

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



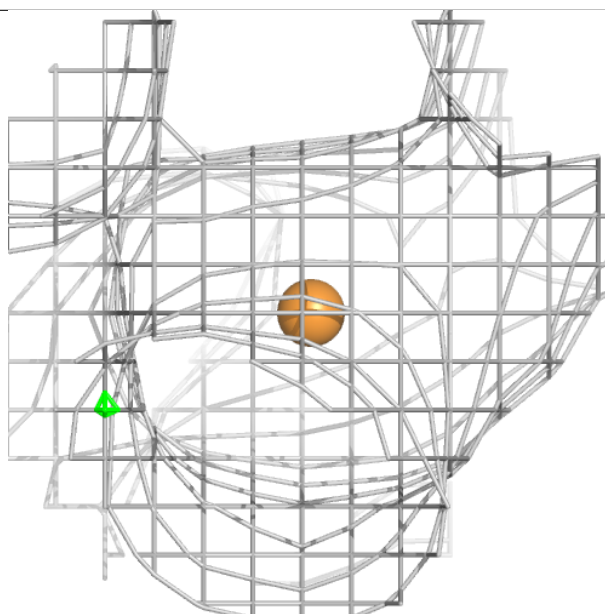
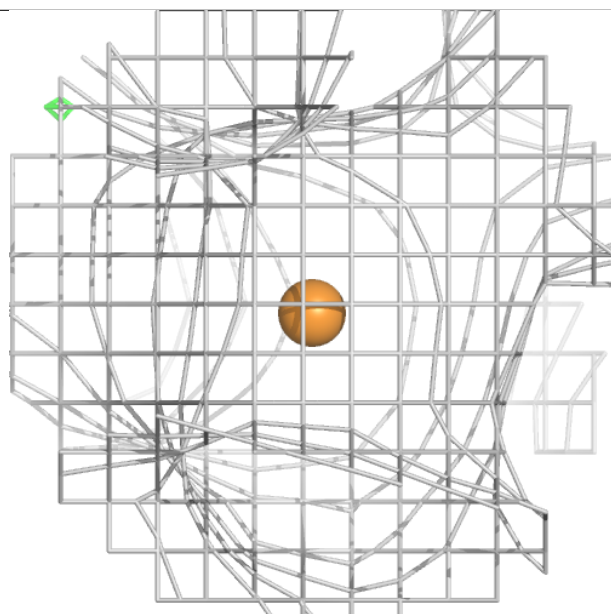
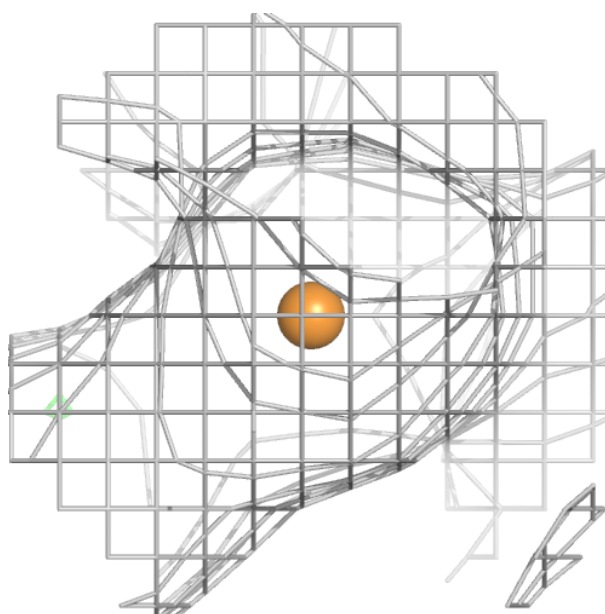
Electron density around CU AAA 601:

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



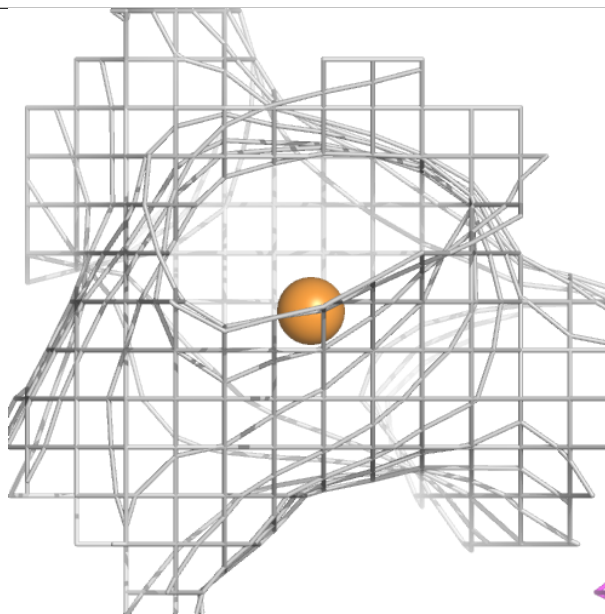
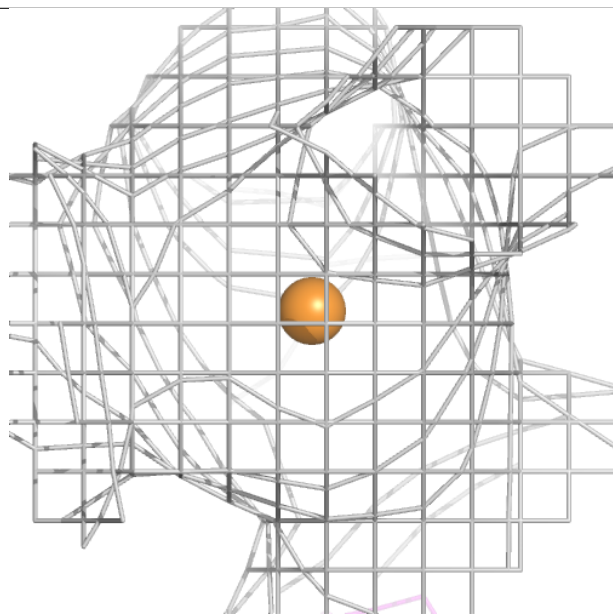
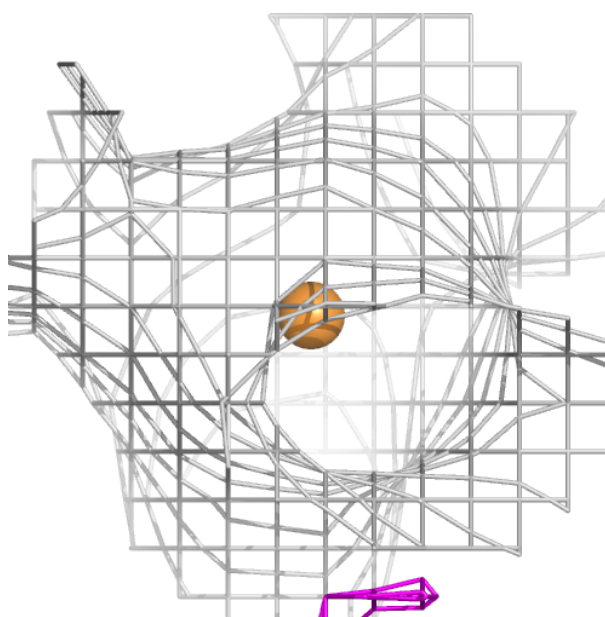
Electron density around CU CCC 601:

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



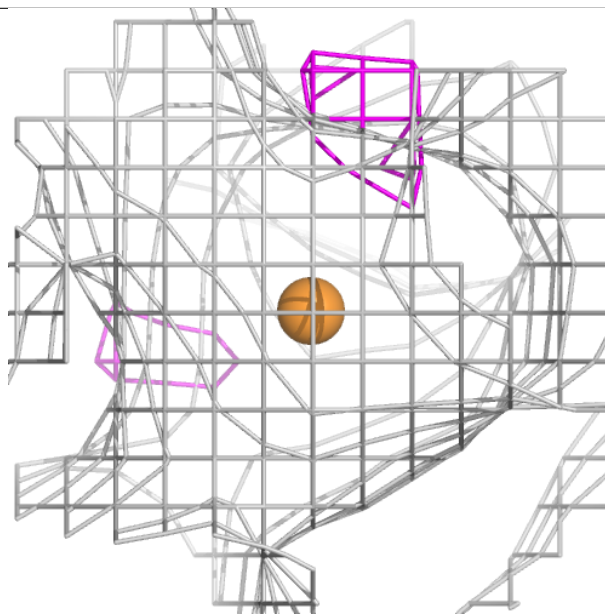
Electron density around CU CCC 602:

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and green (positive)



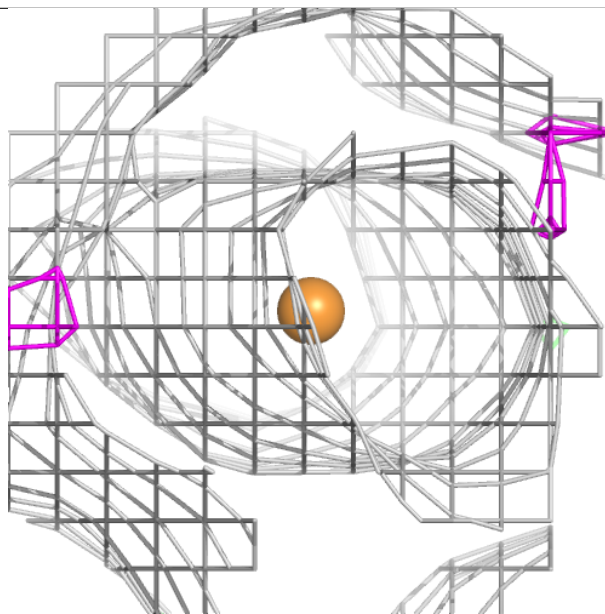
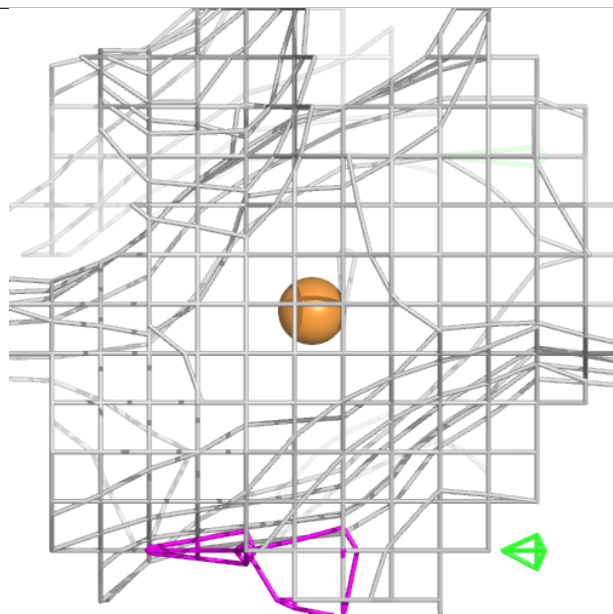
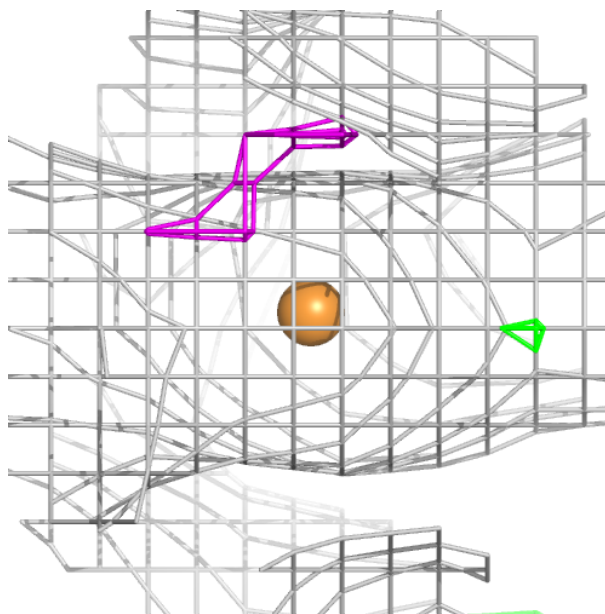
Electron density around CU CCC 603:

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



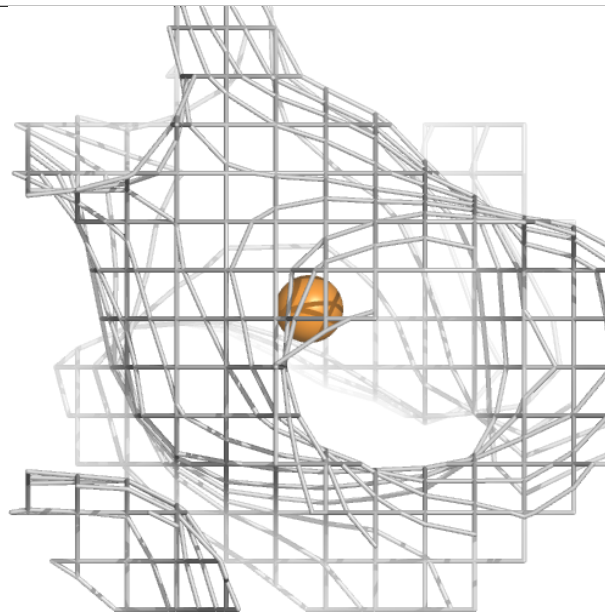
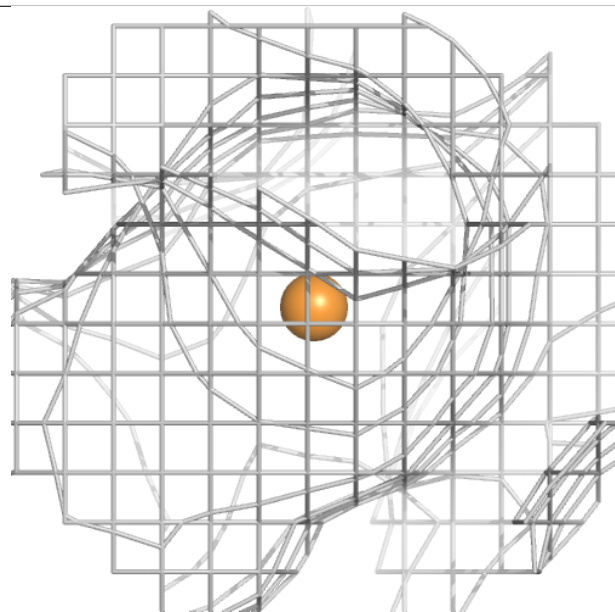
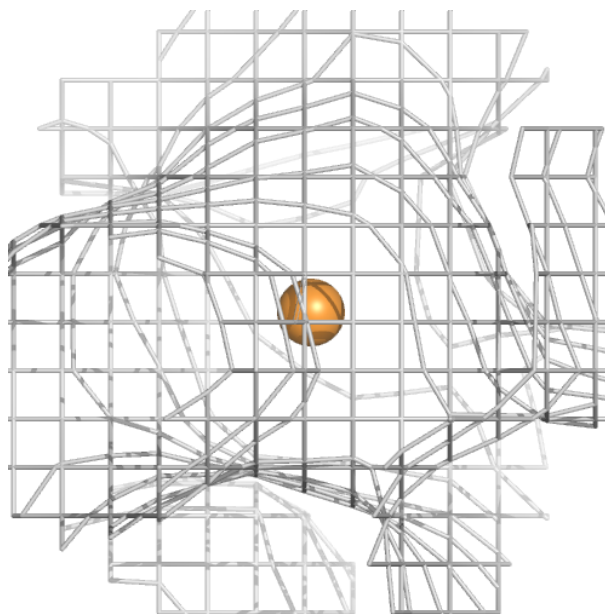
Electron density around CU CCC 604:

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and green (positive)



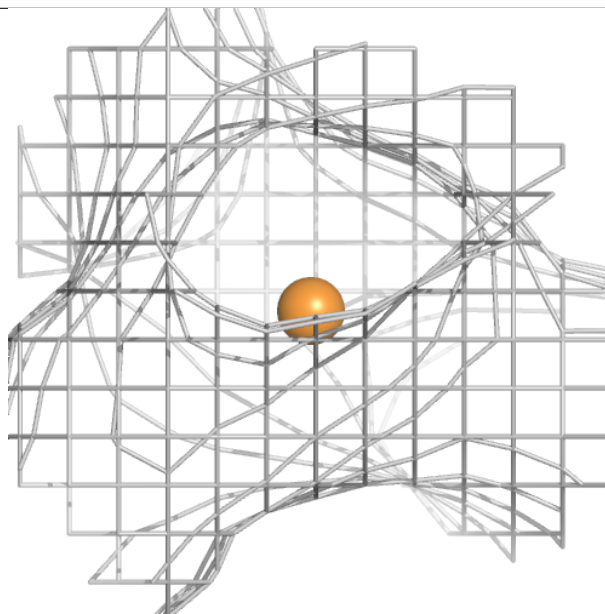
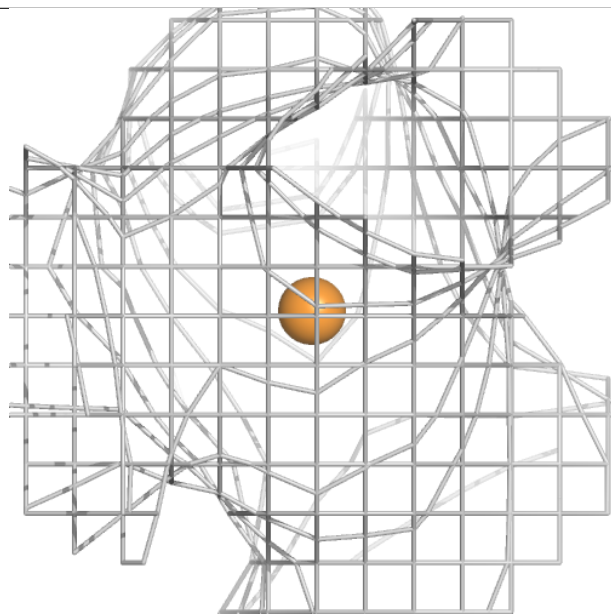
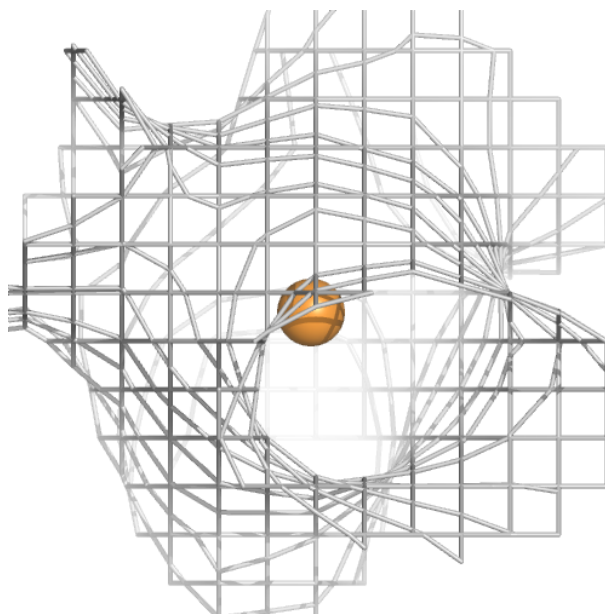
Electron density around CU DDD 601:

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



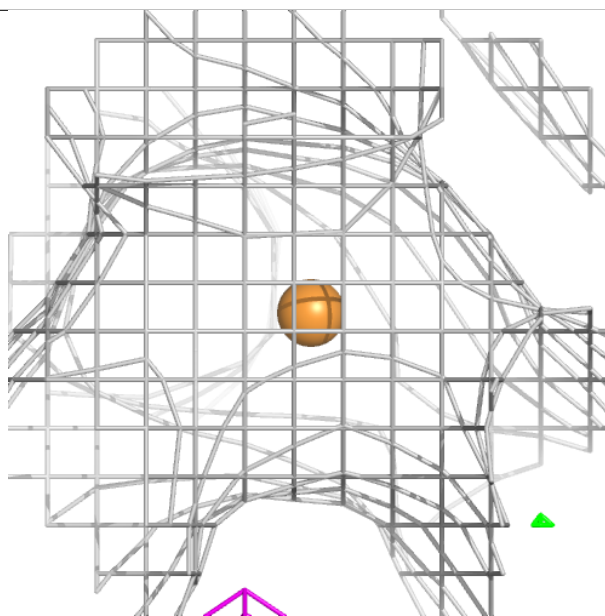
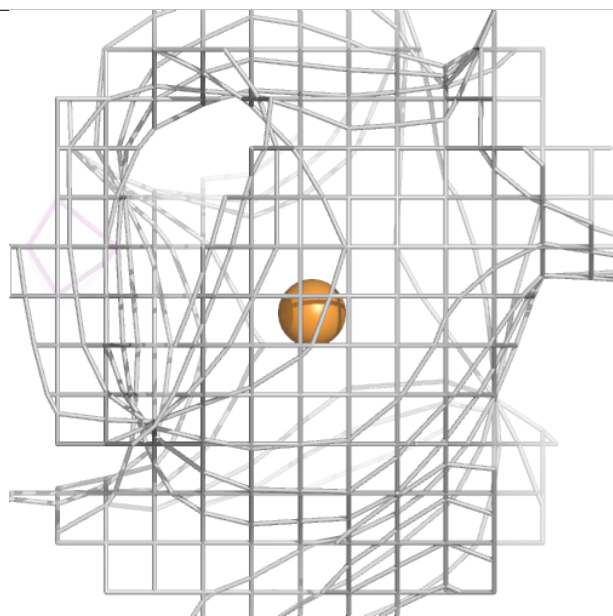
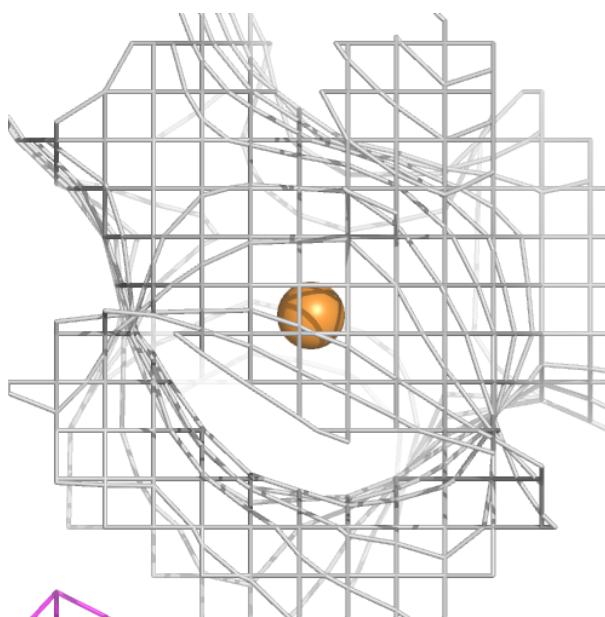
Electron density around CU AAA 602:

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



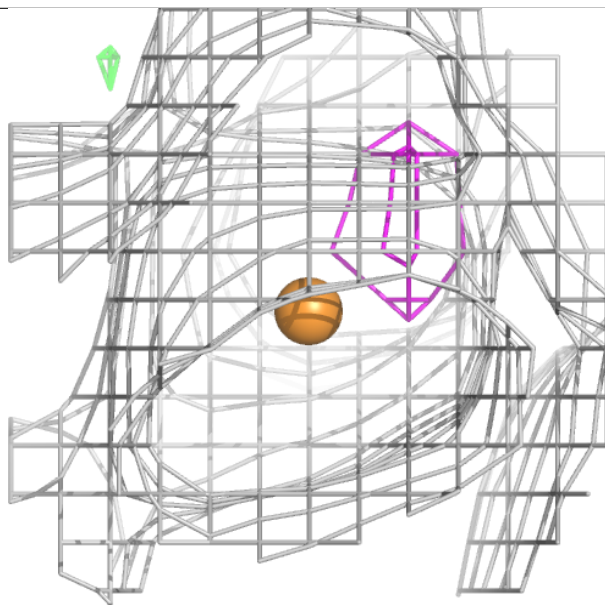
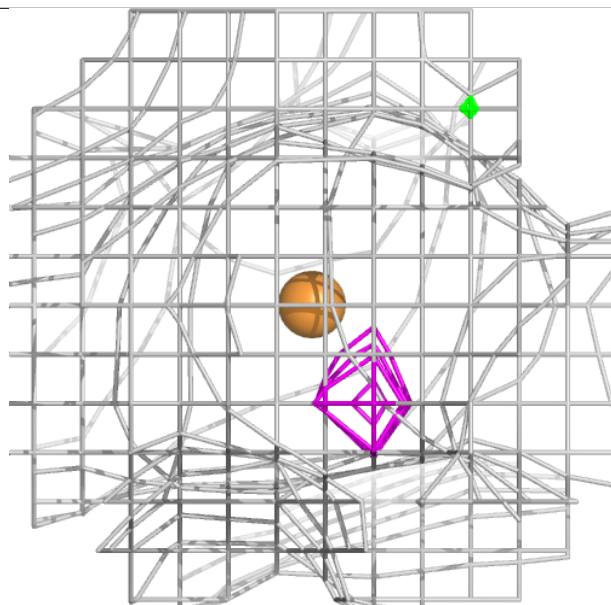
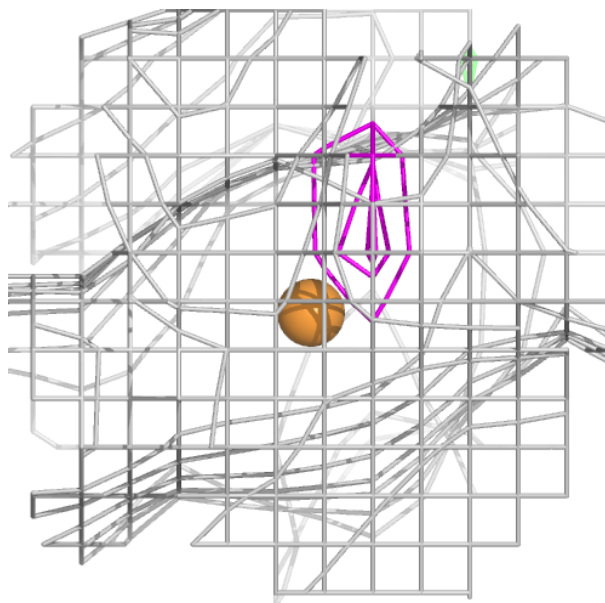
Electron density around CU DDD 603:

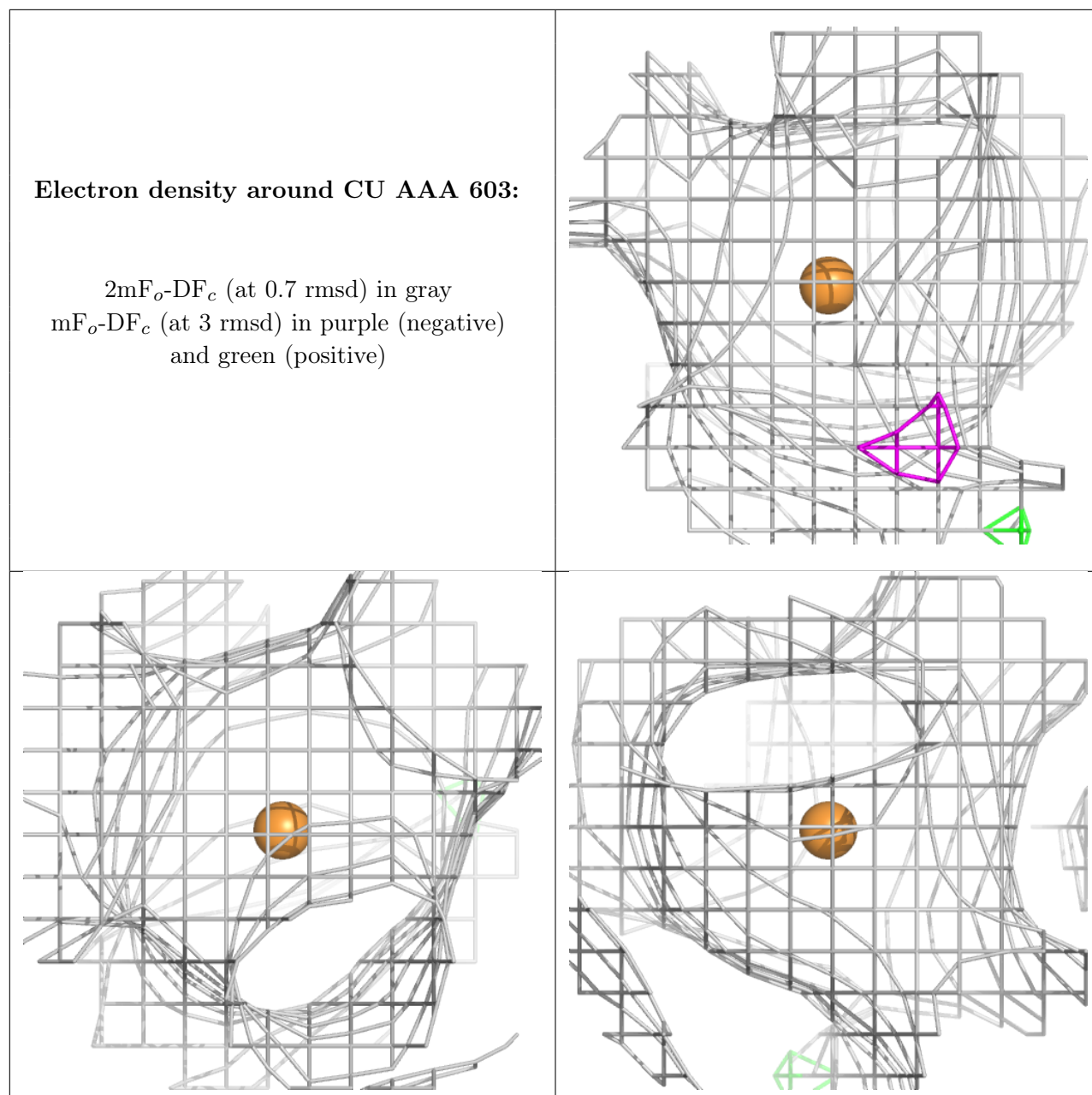
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU DDD 604:

$2mF_o-DF_c$ (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.