



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:47 AM UTC

PDB ID : 6TRV / pdb_00006trv
Title : Structure of SapL1 lectin in complex with alpha methyl fucoside
Authors : Martinez Alarcon, D.; Varrot, A.
Deposited on : 2019-12-19
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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

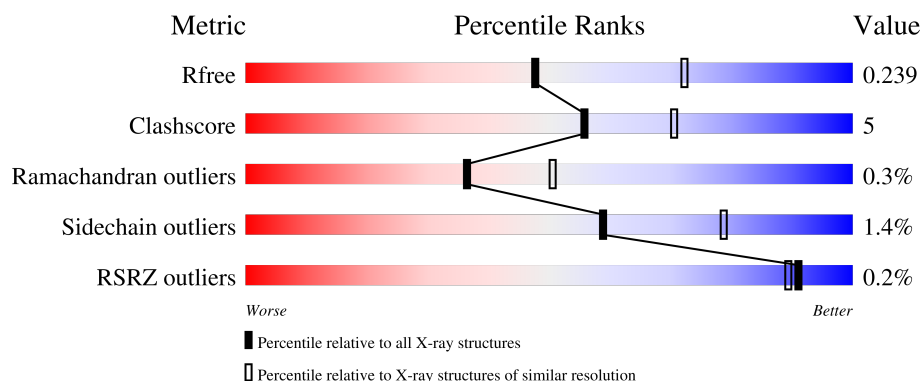
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	297	
1	BBB	297	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4777 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.

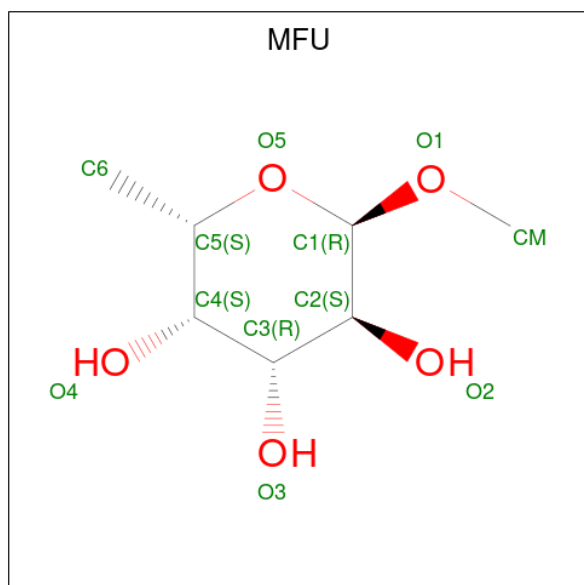
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	294	Total	C	N	O	S	0	0	0
			2222	1416	386	419	1			
1	BBB	294	Total	C	N	O	S	0	0	0
			2220	1415	385	419	1			

There are 4 discrepancies between the modelled and reference sequences:

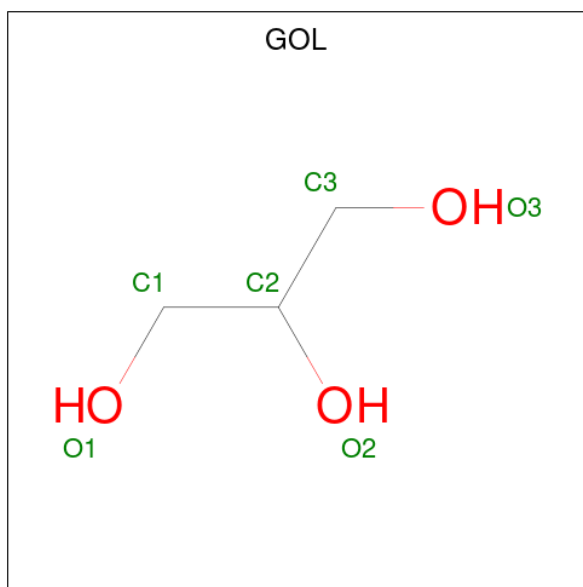
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP A0A084FYP2
AAA	0	HIS	-	expression tag	UNP A0A084FYP2
BBB	-1	GLY	-	expression tag	UNP A0A084FYP2
BBB	0	HIS	-	expression tag	UNP A0A084FYP2

- Molecule 2 is methyl α -L-fucopyranoside (CCD ID: MFU) (formula: $C_7H_{14}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 12 7 5	0	0
2	AAA	1	Total C O 12 7 5	0	0
2	AAA	1	Total C O 12 7 5	0	0
2	AAA	1	Total C O 12 7 5	0	0
2	AAA	1	Total C O 12 7 5	0	0
2	BBB	1	Total C O 12 7 5	0	0
2	BBB	1	Total C O 12 7 5	0	0
2	BBB	1	Total C O 12 7 5	0	0
2	BBB	1	Total C O 12 7 5	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



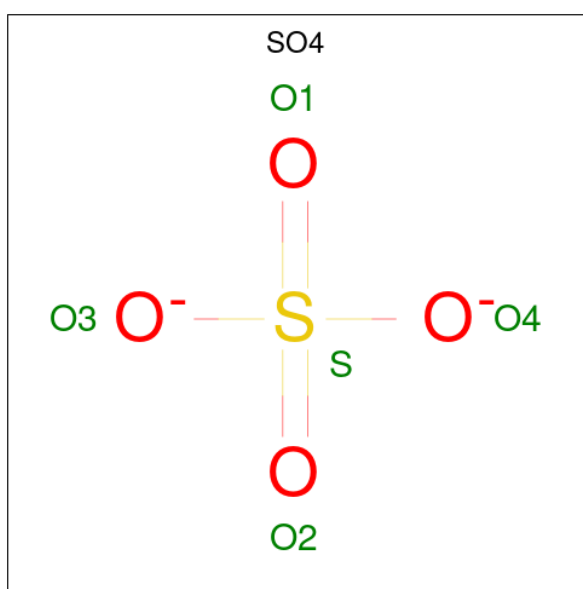
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	O	S	0	0
			5	4	1		

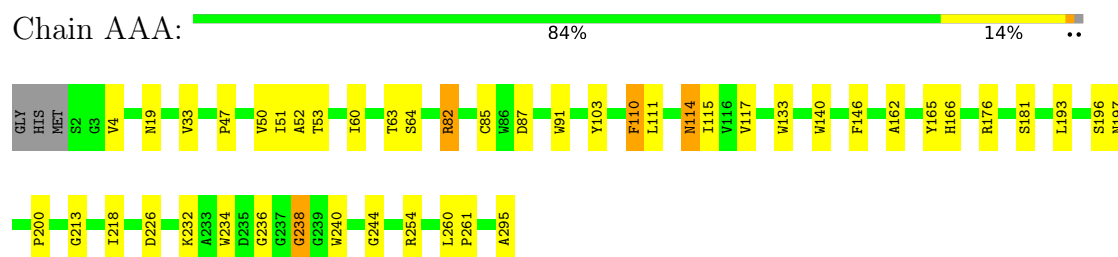
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	111	Total	O	0	2
			111	111		
5	BBB	68	Total	O	0	1
			69	69		

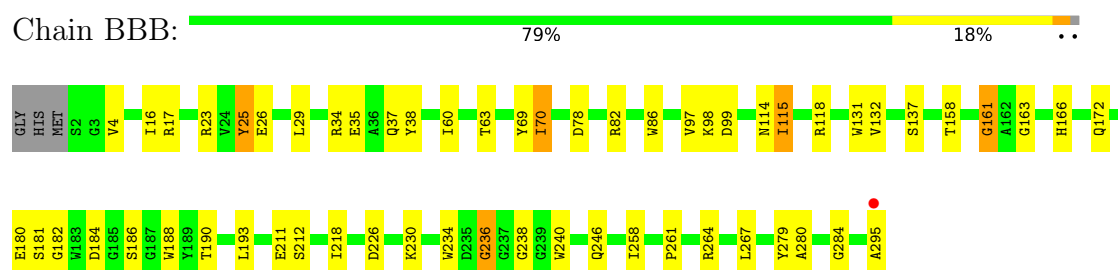
3 Residue-property plots

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.06Å 45.66Å 83.48Å 90.00° 105.05° 90.00°	Depositor
Resolution (Å)	39.99 – 2.40 39.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.99-2.40) 97.9 (39.99-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.175 , 0.240 0.183 , 0.239	Depositor DCC
R_{free} test set	1089 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.4	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	0.95	EDS
Total number of atoms	4777	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: SO4, GOL, MFU

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	1.31	10/2287 (0.4%)	1.47	10/3125 (0.3%)
1	BBB	1.26	5/2285 (0.2%)	1.44	16/3123 (0.5%)
All	All	1.29	15/4572 (0.3%)	1.45	26/6248 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	114	ASN	C-O	8.61	1.35	1.23
1	AAA	110	PHE	C-O	-7.60	1.14	1.23
1	AAA	111	LEU	C-O	7.30	1.32	1.24
1	AAA	244	GLY	C-O	-7.27	1.15	1.24
1	AAA	140	TRP	C-O	-6.78	1.16	1.24
1	BBB	70	ILE	C-O	6.57	1.30	1.24
1	BBB	284	GLY	C-O	6.35	1.29	1.23
1	BBB	218	ILE	C-O	5.97	1.30	1.24
1	AAA	166	HIS	CE1-NE2	5.94	1.38	1.32
1	AAA	181	SER	CA-CB	-5.93	1.45	1.53
1	AAA	200	PRO	C-O	-5.85	1.16	1.23
1	AAA	53	THR	C-O	-5.29	1.18	1.24
1	AAA	146	PHE	C-O	-5.17	1.17	1.24
1	BBB	180	GLU	CD-OE1	-5.11	1.15	1.25
1	BBB	280	ALA	C-O	5.02	1.30	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	238	GLY	O-C-N	6.48	128.47	122.90
1	BBB	190	THR	CA-CB-OG1	-6.31	100.14	109.60
1	BBB	236	GLY	CA-C-N	6.21	126.83	120.00
1	BBB	236	GLY	C-N-CA	6.21	126.83	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	161	GLY	CA-C-O	-5.80	117.59	122.29
1	BBB	115	ILE	O-C-N	5.61	126.67	121.96
1	AAA	226	ASP	CA-CB-CG	5.55	118.16	112.60
1	AAA	232	LYS	CA-C-O	-5.43	114.77	120.80
1	AAA	87	ASP	CA-CB-CG	5.40	118.00	112.60
1	BBB	99	ASP	CA-C-O	-5.35	115.16	121.16
1	BBB	226	ASP	CB-CA-C	5.32	119.47	111.18
1	AAA	218	ILE	CA-C-O	-5.28	114.96	120.76
1	BBB	114	ASN	CB-CA-C	5.21	120.36	110.51
1	AAA	254	ARG	N-CA-C	-5.20	104.01	110.41
1	BBB	63	THR	CB-CA-C	5.19	121.00	109.94
1	BBB	172	GLN	CB-CA-C	5.18	118.69	110.19
1	BBB	97	VAL	CA-C-O	-5.17	115.62	120.22
1	BBB	16	ILE	CA-C-O	-5.16	116.58	121.64
1	BBB	115	ILE	CA-C-O	-5.13	118.16	122.63
1	AAA	19	ASN	CB-CA-C	-5.12	110.69	116.63
1	AAA	103	TYR	CA-C-O	-5.09	113.60	119.56
1	AAA	63	THR	CB-CA-C	5.06	120.71	109.94
1	BBB	60	ILE	O-C-N	5.04	128.52	123.07
1	BBB	26	GLU	CB-CG-CD	5.04	121.17	112.60
1	BBB	25	TYR	CB-CA-C	5.02	118.43	110.19
1	AAA	82	ARG	CA-C-O	-5.02	115.67	121.49

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	2222	0	2107	17	0
1	BBB	2220	0	2100	25	0
2	AAA	60	0	67	0	0
2	BBB	48	0	56	2	0
3	AAA	24	0	25	0	0
3	BBB	18	0	24	2	0
4	AAA	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	111	0	0	2	0
5	BBB	69	0	0	0	0
All	All	4777	0	4379	42	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 (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:158:THR:OG1	3:BBB:307:GOL:H2	1.83	0.78
1:AAA:213:GLY:O	1:AAA:236:GLY:HA2	1.93	0.68
1:AAA:115:ILE:N	1:AAA:115:ILE:HD13	2.11	0.65
1:AAA:193:LEU:HD23	1:AAA:240:TRP:CD2	2.38	0.59
1:BBB:17:ARG:NH2	1:BBB:261:PRO:HD2	2.22	0.55
1:BBB:29:LEU:C	1:BBB:29:LEU:HD12	2.33	0.53
1:BBB:35:GLU:HG2	1:BBB:37:GLN:HE21	1.73	0.53
1:BBB:38:TYR:CE2	2:BBB:304:MFU:H5	2.44	0.52
1:BBB:193:LEU:HD23	1:BBB:240:TRP:CD2	2.45	0.52
1:AAA:234:TRP:CZ2	1:AAA:238:GLY:HA3	2.45	0.51
1:BBB:234:TRP:CZ2	2:BBB:302:MFU:H5	2.47	0.50
1:BBB:69:TYR:CE2	1:BBB:115:ILE:HD11	2.47	0.50
1:BBB:166:HIS:ND1	1:BBB:184:ASP:OD1	2.37	0.49
1:AAA:114:ASN:HB2	5:AAA:427:HOH:O	2.12	0.49
1:BBB:4:VAL:HB	1:BBB:295:ALA:HB2	1.95	0.48
1:AAA:85:CYS:O	1:AAA:91:TRP:HA	2.14	0.48
1:AAA:33:VAL:HG13	1:AAA:60:ILE:HD13	1.96	0.47
1:BBB:98:LYS:HD2	1:BBB:131:TRP:CH2	2.49	0.47
1:BBB:267:LEU:C	1:BBB:267:LEU:HD12	2.39	0.47
1:BBB:234:TRP:CE2	1:BBB:238:GLY:HA2	2.49	0.47
1:AAA:114:ASN:C	1:AAA:115:ILE:HD13	2.40	0.47
1:BBB:182:GLY:O	1:BBB:188:TRP:HA	2.14	0.47
1:BBB:70:ILE:HB	1:BBB:86:TRP:HB3	1.97	0.46
1:AAA:47:PRO:O	1:AAA:50:VAL:HG23	2.14	0.46
1:AAA:4:VAL:HB	1:AAA:295:ALA:HB2	1.97	0.46
1:BBB:161:GLY:HA2	1:BBB:211:GLU:OE1	2.15	0.46
1:BBB:234:TRP:CZ2	1:BBB:238:GLY:HA2	2.51	0.45
1:AAA:162:ALA:HA	1:AAA:165:TYR:CD1	2.51	0.45
1:AAA:260:LEU:HG	1:AAA:261:PRO:HA	1.98	0.45
1:BBB:17:ARG:HD3	1:BBB:258:ILE:HD12	1.99	0.44
1:BBB:115:ILE:HD13	1:BBB:115:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:51:ILE:O	1:AAA:52:ALA:HB2	2.17	0.43
1:AAA:133:TRP:C	1:AAA:133:TRP:CD1	2.96	0.43
1:BBB:78:ASP:OD2	1:BBB:82:ARG:NH2	2.47	0.43
1:AAA:110:PHE:CE1	1:AAA:117:VAL:HG22	2.53	0.42
1:BBB:23:ARG:HH21	3:BBB:305:GOL:H31	1.85	0.42
1:BBB:230:LYS:HE3	1:BBB:246:GLN:OE1	2.19	0.41
1:AAA:196:SER:O	1:AAA:197:ASN:C	2.63	0.41
1:AAA:82:ARG:NH1	5:AAA:411:HOH:O	2.53	0.41
1:BBB:25:TYR:HA	1:BBB:34:ARG:O	2.22	0.40
1:BBB:264:ARG:HA	1:BBB:279:TYR:O	2.21	0.40
1:BBB:118:ARG:CZ	1:BBB:132:VAL:HG13	2.51	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	292/297 (98%)	280 (96%)	12 (4%)	0	100	100
1	BBB	292/297 (98%)	277 (95%)	13 (4%)	2 (1%)	18	28
All	All	584/594 (98%)	557 (95%)	25 (4%)	2 (0%)	36	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	236	GLY
1	BBB	163	GLY

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	216/221 (98%)	214 (99%)	2 (1%)	70	85
1	BBB	215/221 (97%)	211 (98%)	4 (2%)	50	71
All	All	431/442 (98%)	425 (99%)	6 (1%)	59	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	64	SER
1	AAA	176	ARG
1	BBB	137	SER
1	BBB	181	SER
1	BBB	186	SER
1	BBB	212	SER

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands 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	MFU	AAA	305	-	12,12,12	2.56	5 (41%)	17,17,17	1.18	1 (5%)
2	MFU	BBB	302	-	12,12,12	1.31	1 (8%)	17,17,17	1.02	1 (5%)
2	MFU	AAA	302	-	12,12,12	1.24	2 (16%)	17,17,17	1.01	1 (5%)
3	GOL	AAA	306	-	5,5,5	0.21	0	5,5,5	0.42	0
3	GOL	BBB	306	-	5,5,5	0.40	0	5,5,5	0.24	0
2	MFU	BBB	304	-	12,12,12	2.87	3 (25%)	17,17,17	1.17	2 (11%)
2	MFU	AAA	304	-	12,12,12	1.71	2 (16%)	17,17,17	1.31	2 (11%)
3	GOL	AAA	307	-	5,5,5	0.51	0	5,5,5	0.31	0
3	GOL	BBB	305	-	5,5,5	0.24	0	5,5,5	0.22	0
2	MFU	AAA	301	-	12,12,12	1.00	0	17,17,17	1.04	1 (5%)
4	SO4	AAA	310	-	4,4,4	2.40	2 (50%)	6,6,6	0.20	0
2	MFU	AAA	303	-	12,12,12	0.92	0	17,17,17	1.11	3 (17%)
3	GOL	AAA	309	-	5,5,5	0.42	0	5,5,5	0.81	0
3	GOL	AAA	308	-	5,5,5	0.53	0	5,5,5	0.90	0
2	MFU	BBB	303	-	12,12,12	1.31	0	17,17,17	1.53	3 (17%)
3	GOL	BBB	307	-	5,5,5	0.41	0	5,5,5	0.55	0
2	MFU	BBB	301	-	12,12,12	1.36	1 (8%)	17,17,17	1.21	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MFU	AAA	305	-	-	2/2/22/22	0/1/1/1
2	MFU	BBB	302	-	-	0/2/22/22	0/1/1/1
2	MFU	AAA	302	-	-	0/2/22/22	0/1/1/1
3	GOL	AAA	306	-	-	2/4/4/4	-
3	GOL	BBB	306	-	-	2/4/4/4	-
2	MFU	BBB	304	-	-	0/2/22/22	0/1/1/1
2	MFU	AAA	304	-	-	0/2/22/22	0/1/1/1
3	GOL	AAA	307	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	BBB	305	-	-	0/4/4/4	-
2	MFU	AAA	301	-	-	2/2/22/22	0/1/1/1
2	MFU	AAA	303	-	-	0/2/22/22	0/1/1/1
3	GOL	AAA	309	-	-	4/4/4/4	-
3	GOL	AAA	308	-	-	4/4/4/4	-
2	MFU	BBB	303	-	-	2/2/22/22	0/1/1/1
3	GOL	BBB	307	-	-	2/4/4/4	-
2	MFU	BBB	301	-	-	0/2/22/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	304	MFU	O1-C1	8.04	1.53	1.40
2	AAA	305	MFU	O1-C1	6.09	1.50	1.40
2	AAA	305	MFU	C4-C5	4.14	1.62	1.52
2	BBB	304	MFU	O1-CM	3.70	1.55	1.42
2	AAA	304	MFU	O1-C1	3.54	1.46	1.40
2	BBB	301	MFU	O1-C1	3.03	1.45	1.40
2	BBB	302	MFU	O1-C1	2.97	1.45	1.40
4	AAA	310	SO4	O1-S	2.91	1.62	1.44
4	AAA	310	SO4	O2-S	2.80	1.61	1.44
2	BBB	304	MFU	O5-C1	2.73	1.48	1.41
2	AAA	304	MFU	O2-C2	2.70	1.49	1.43
2	AAA	302	MFU	O3-C3	2.57	1.49	1.43
2	AAA	305	MFU	O2-C2	2.55	1.49	1.43
2	AAA	305	MFU	O5-C1	2.21	1.47	1.41
2	AAA	305	MFU	O5-C5	2.09	1.49	1.44
2	AAA	302	MFU	O4-C4	2.01	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	303	MFU	CM-O1-C1	-4.64	106.20	113.26
2	AAA	304	MFU	O1-C1-C2	-4.21	103.29	108.14
2	AAA	301	MFU	CM-O1-C1	-3.37	108.14	113.26
2	AAA	305	MFU	C6-C5-C4	2.70	118.02	113.08
2	BBB	303	MFU	O1-C1-C2	-2.65	105.08	108.14
2	BBB	301	MFU	CM-O1-C1	-2.62	109.27	113.26
2	BBB	301	MFU	O1-C1-C2	-2.57	105.18	108.14
2	BBB	303	MFU	C6-C5-C4	2.43	117.53	113.08
2	AAA	304	MFU	O5-C1-O1	2.25	116.17	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	303	MFU	CM-O1-C1	-2.22	109.89	113.26
2	AAA	302	MFU	O5-C5-C4	-2.17	105.65	109.55
2	BBB	304	MFU	C4-C3-C2	-2.15	107.06	110.83
2	AAA	303	MFU	C3-C4-C5	-2.15	106.55	109.81
2	BBB	302	MFU	O2-C2-C1	2.03	114.90	110.08
2	AAA	303	MFU	O1-C1-C2	-2.02	105.80	108.14
2	BBB	304	MFU	C3-C4-C5	-2.02	106.74	109.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	MFU	C2-C1-O1-CM
2	AAA	301	MFU	O5-C1-O1-CM
3	AAA	307	GOL	O1-C1-C2-O2
3	AAA	307	GOL	O1-C1-C2-C3
3	AAA	308	GOL	O1-C1-C2-C3
3	AAA	308	GOL	C1-C2-C3-O3
3	AAA	308	GOL	O2-C2-C3-O3
3	AAA	309	GOL	O1-C1-C2-C3
3	AAA	309	GOL	C1-C2-C3-O3
2	BBB	303	MFU	C2-C1-O1-CM
2	AAA	305	MFU	C2-C1-O1-CM
2	BBB	303	MFU	O5-C1-O1-CM
3	AAA	306	GOL	O1-C1-C2-C3
3	BBB	306	GOL	O1-C1-C2-C3
3	AAA	306	GOL	O1-C1-C2-O2
3	AAA	308	GOL	O1-C1-C2-O2
3	AAA	309	GOL	O1-C1-C2-O2
3	AAA	309	GOL	O2-C2-C3-O3
3	BBB	306	GOL	O1-C1-C2-O2
2	AAA	305	MFU	O5-C1-O1-CM
3	BBB	307	GOL	O2-C2-C3-O3
3	BBB	307	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

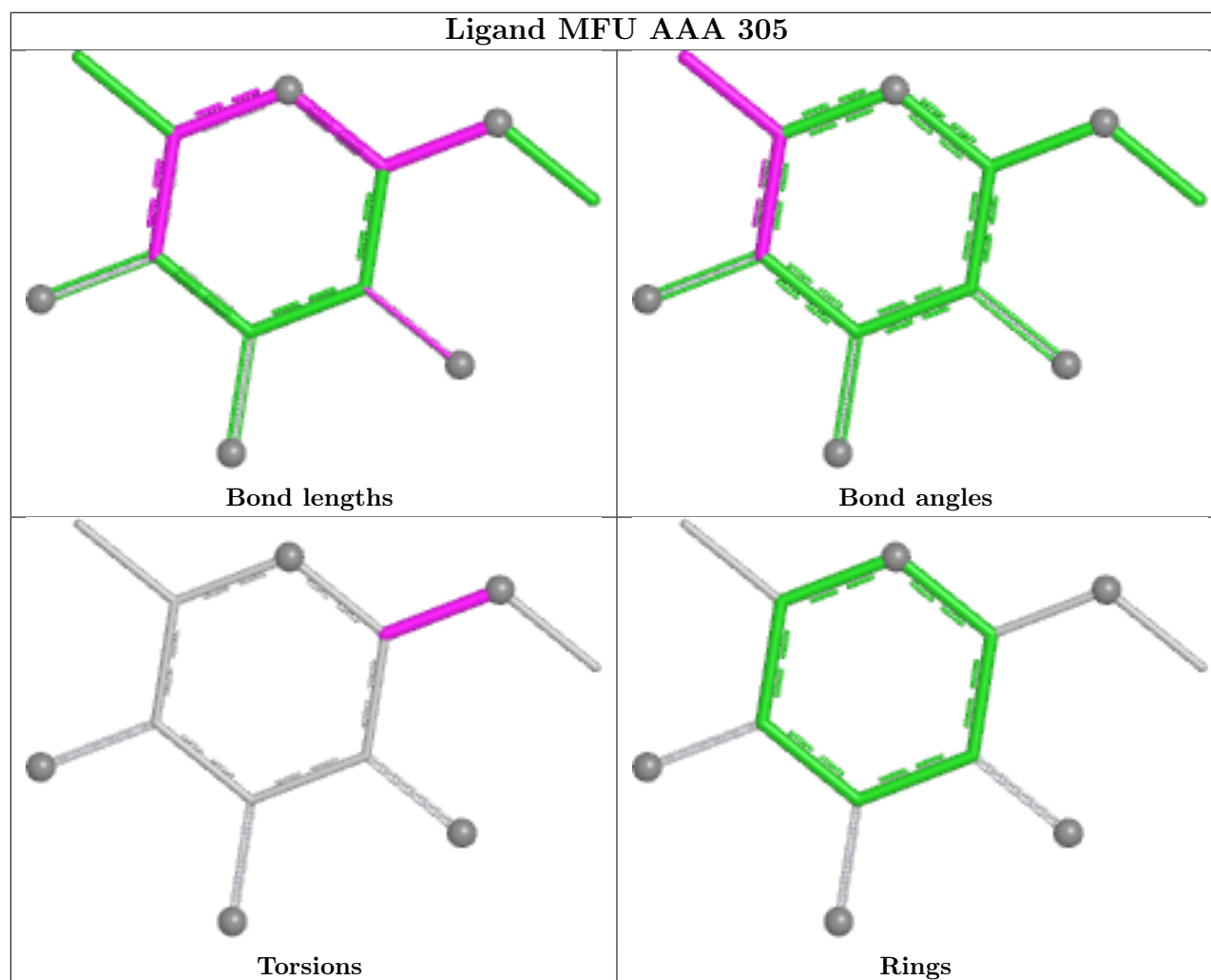
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	302	MFU	1	0
2	BBB	304	MFU	1	0

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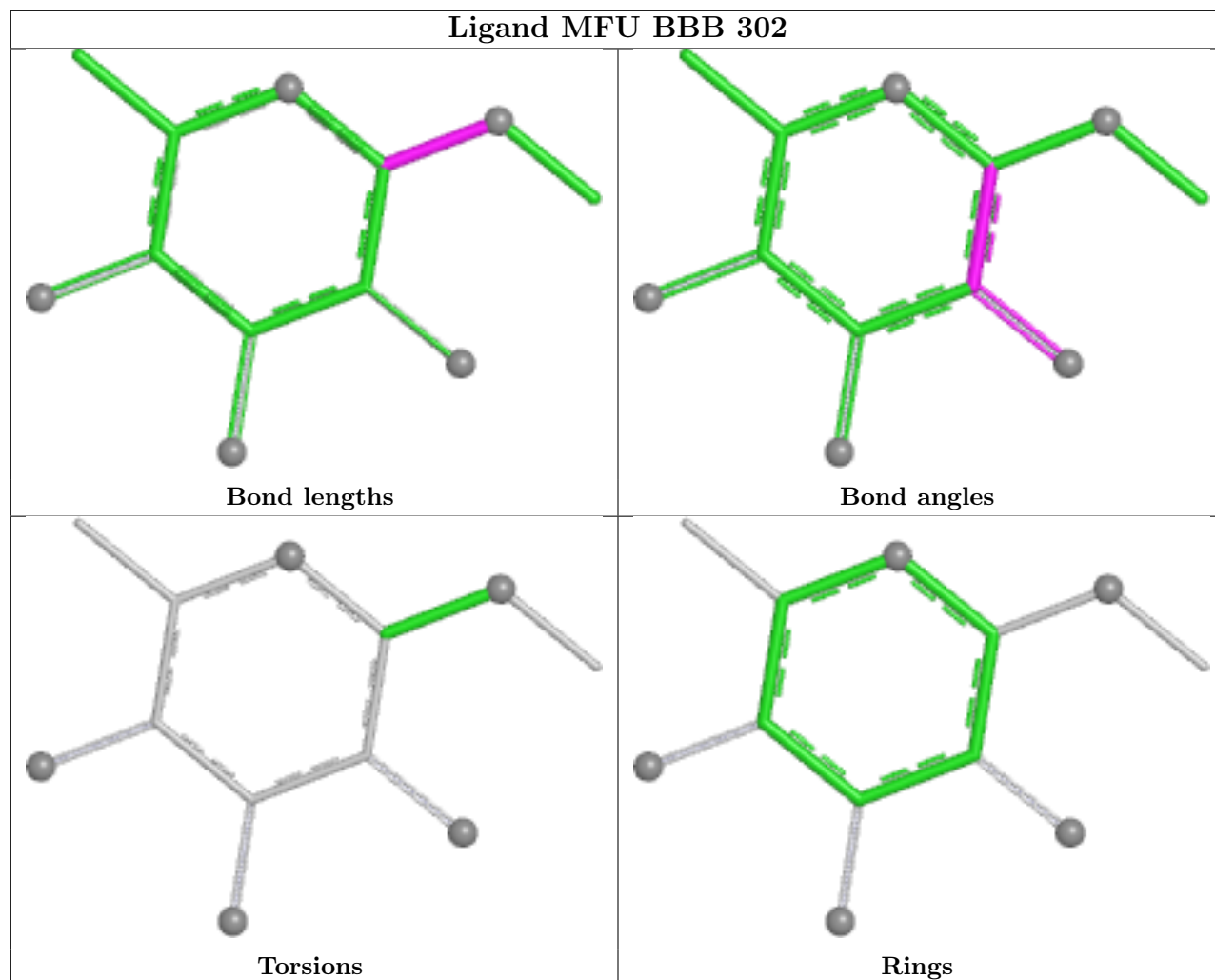
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	305	GOL	1	0
3	BBB	307	GOL	1	0

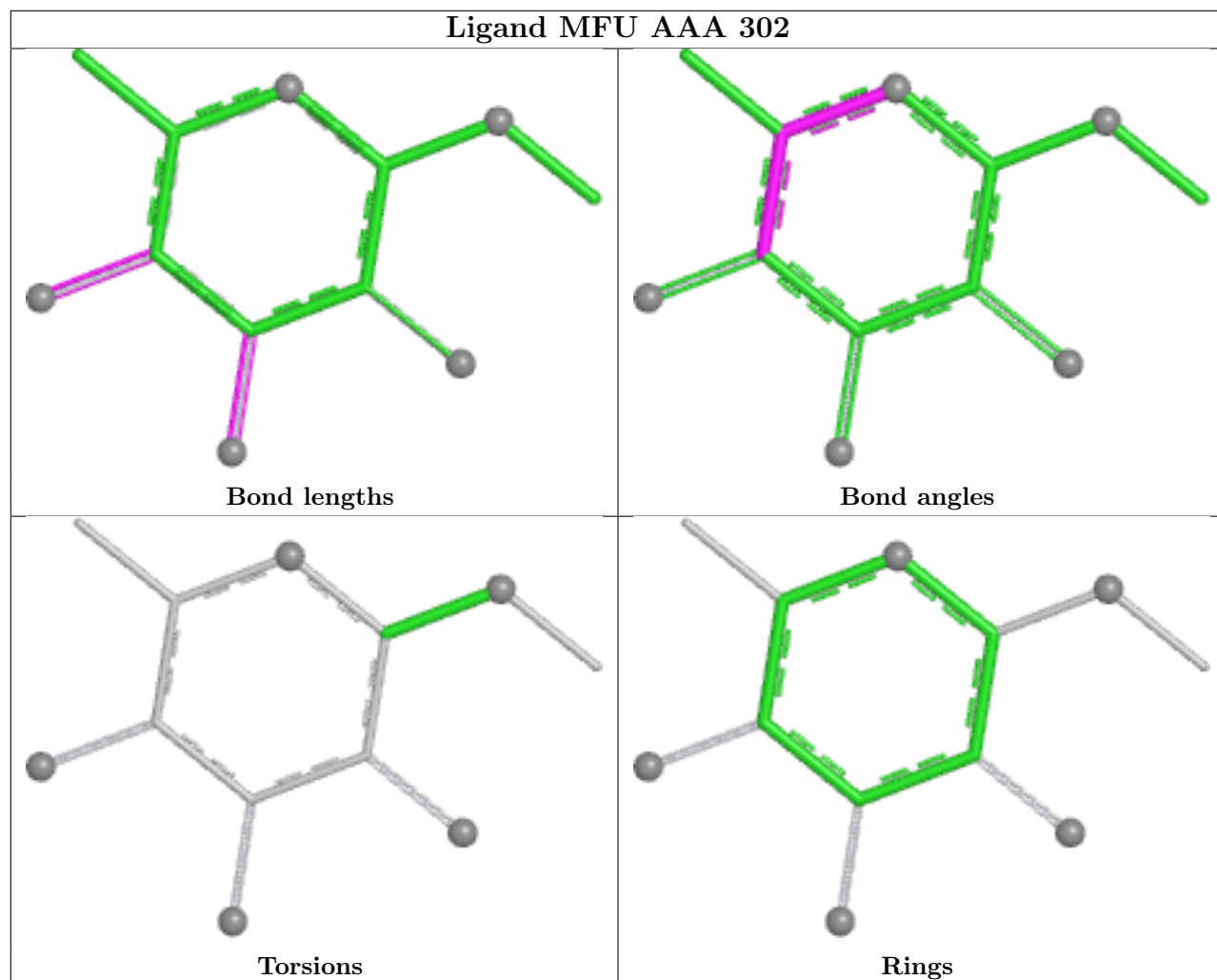
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



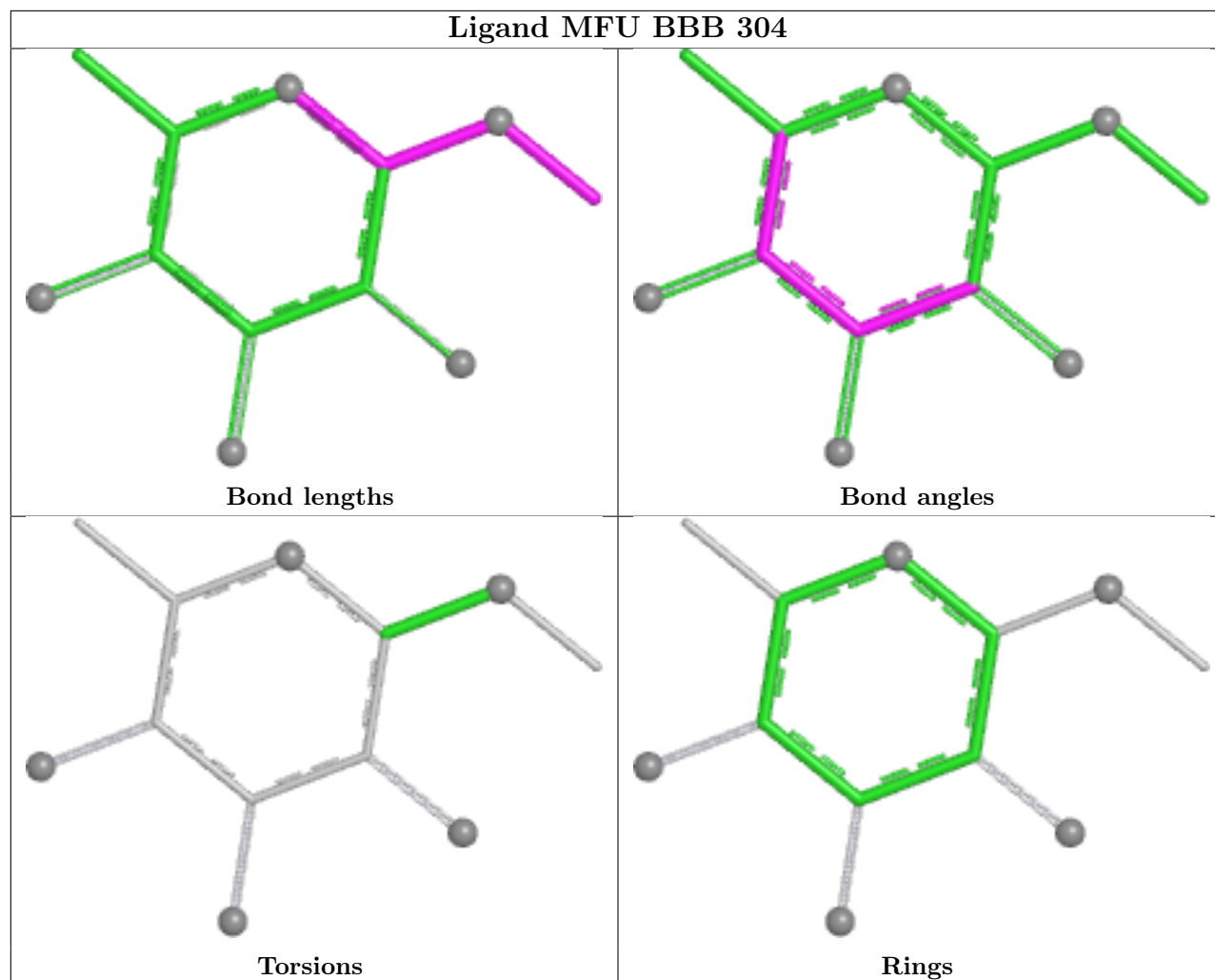
Ligand MFU BBB 302



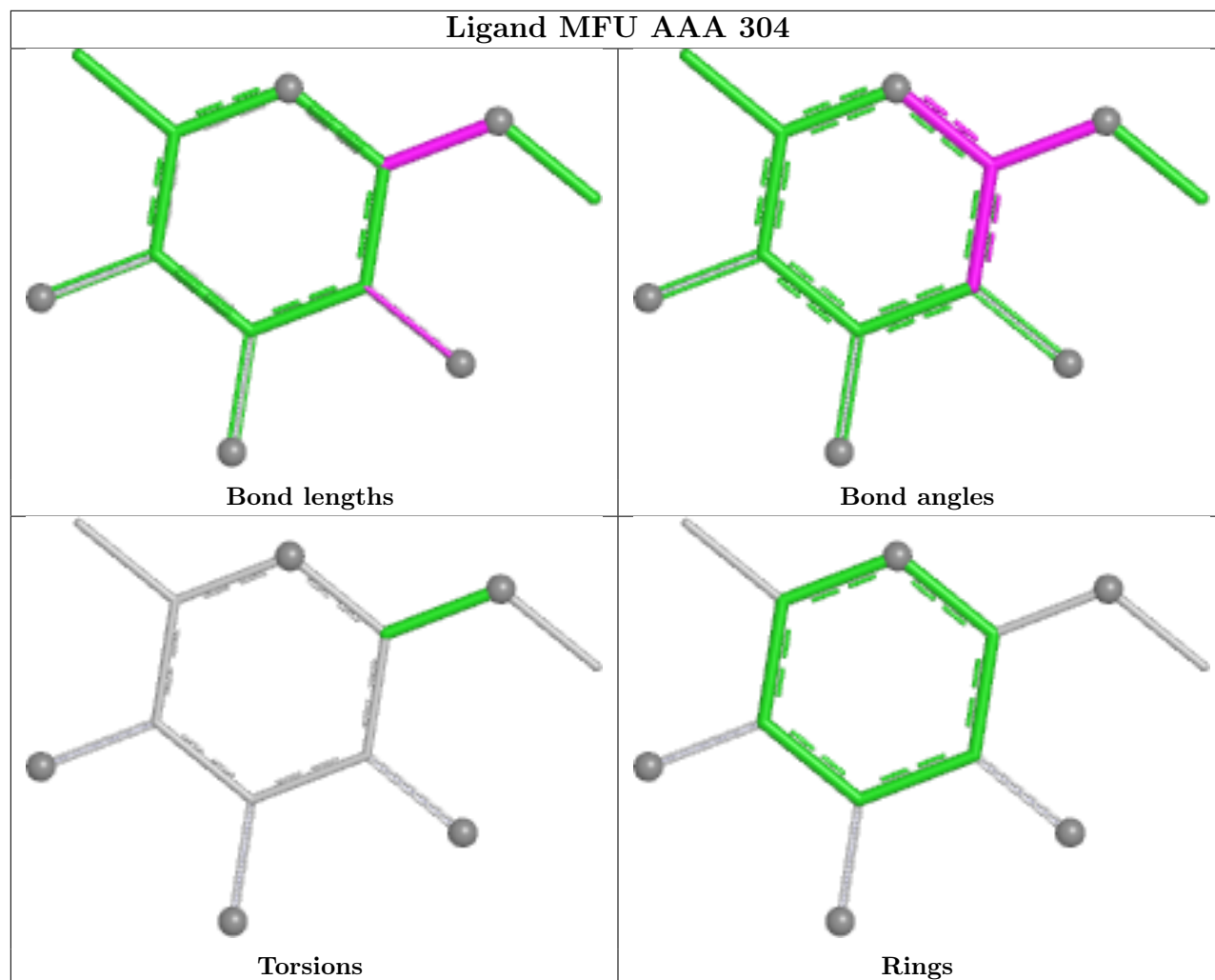
Ligand MFU AAA 302



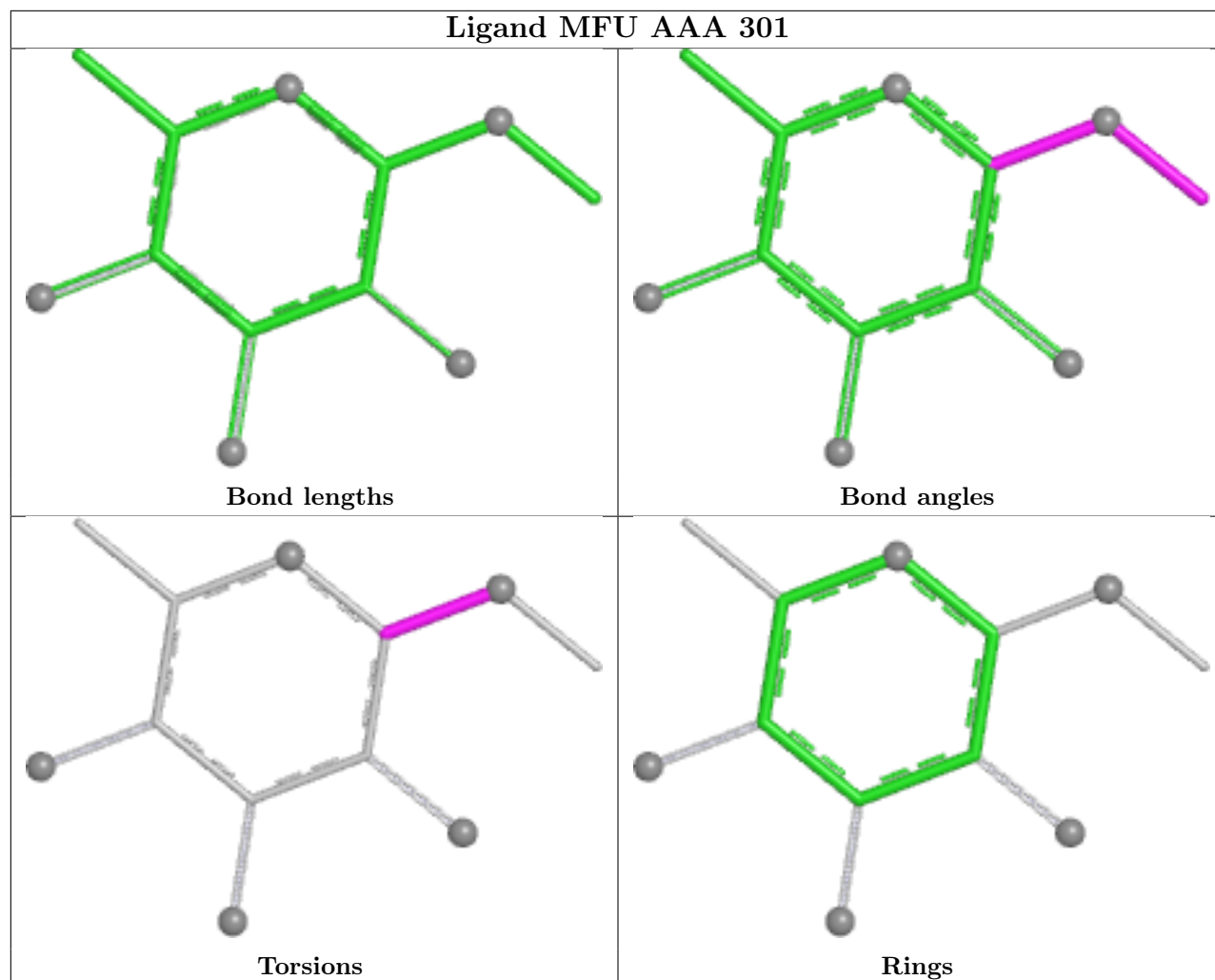
Ligand MFU BBB 304



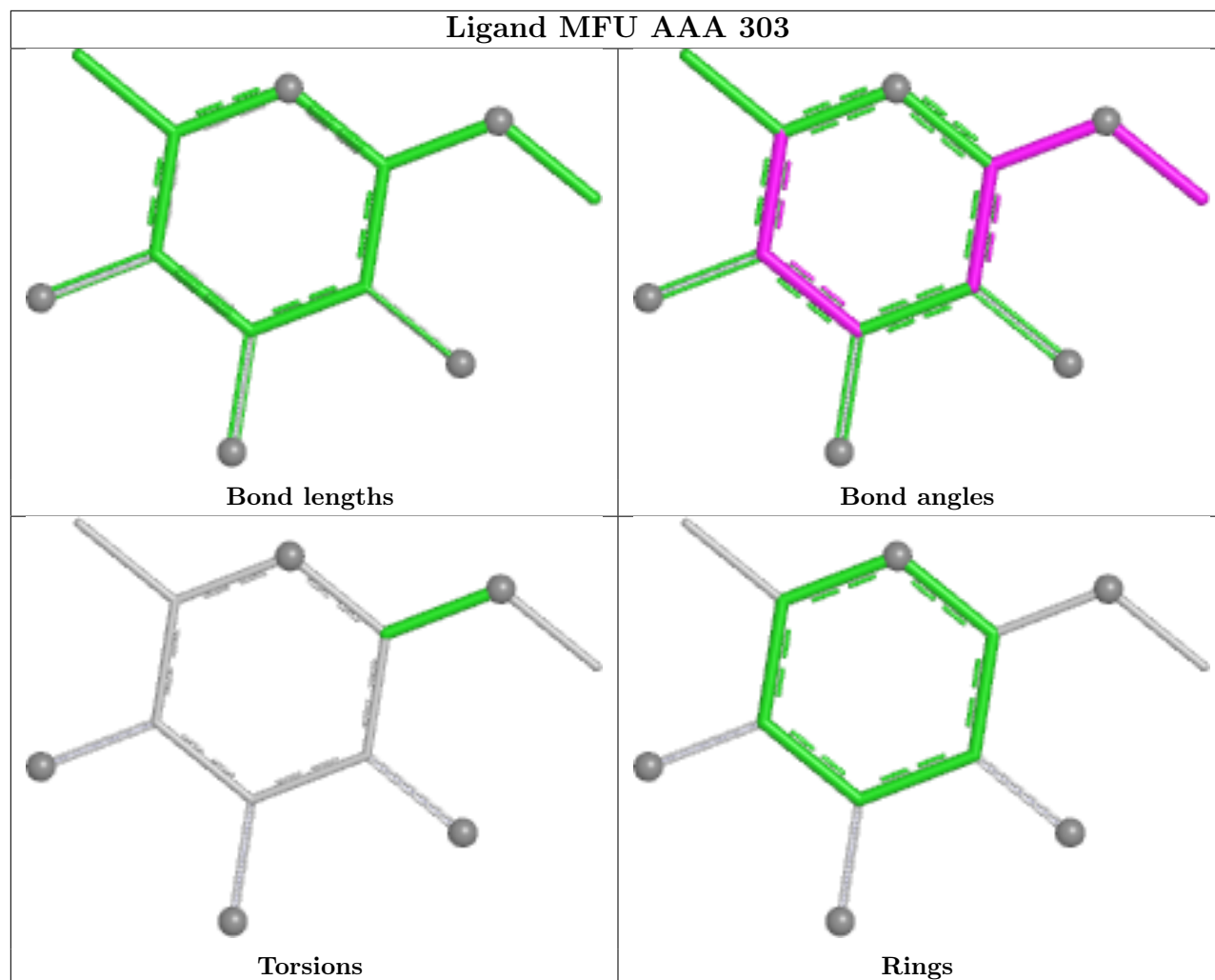
Ligand MFU AAA 304



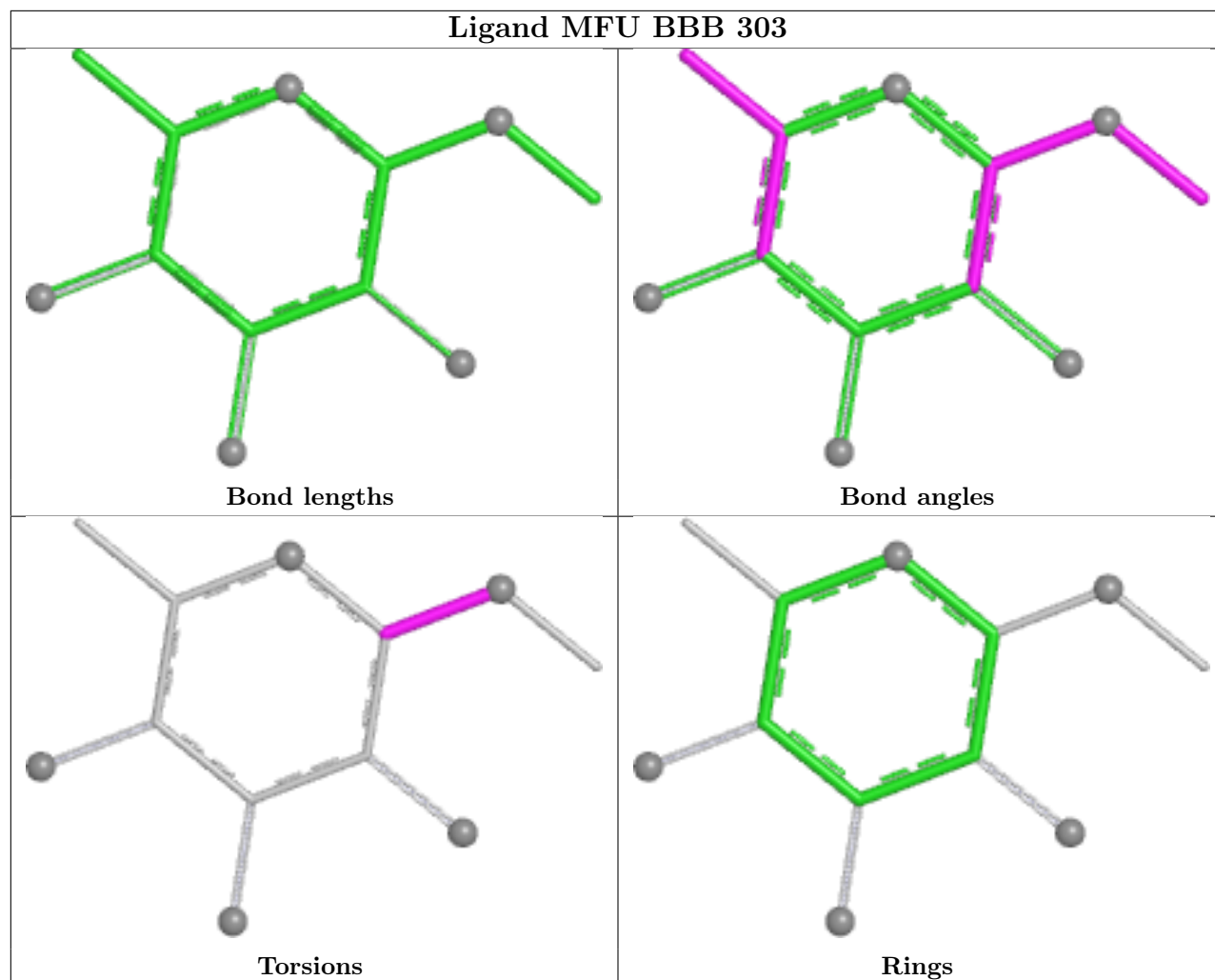
Ligand MFU AAA 301

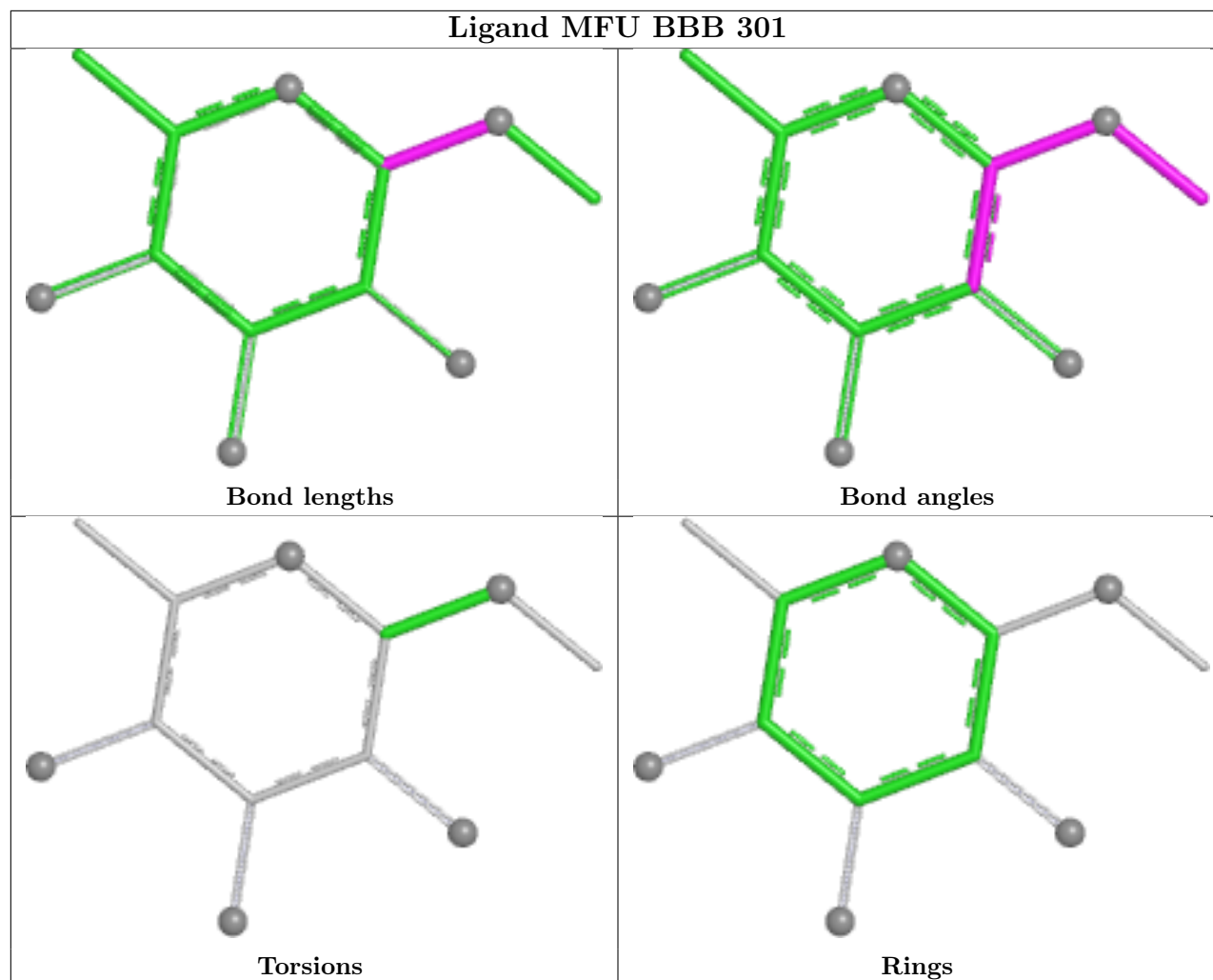


Ligand MFU AAA 303



Ligand MFU BBB 303





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	294/297 (98%)	-0.74	0	100 100	22, 31, 44, 65	0
1	BBB	294/297 (98%)	-0.49	1 (0%)	90 88	29, 39, 56, 74	0
All	All	588/594 (98%)	-0.61	1 (0%)	91 89	22, 35, 53, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	295	ALA	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MFU	BBB	304	12/12	0.82	0.12	31,40,56,59	0
3	GOL	BBB	305	6/6	0.84	0.11	34,45,47,48	0
3	GOL	BBB	307	6/6	0.84	0.11	42,46,47,49	0
2	MFU	AAA	301	12/12	0.88	0.14	28,31,37,37	12

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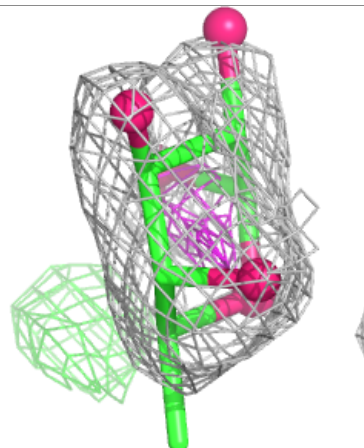
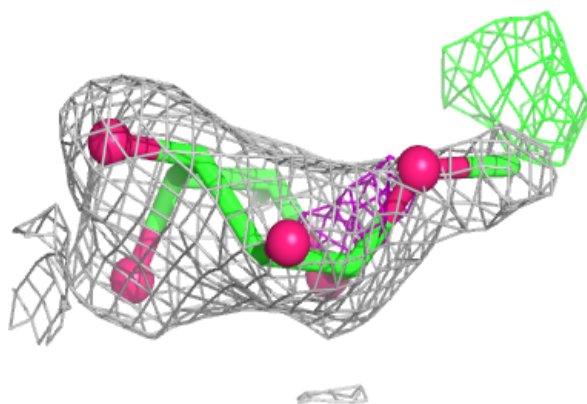
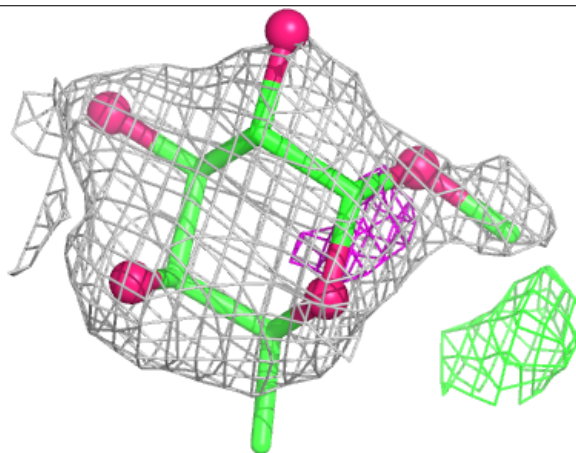
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	BBB	306	6/6	0.89	0.09	31,32,35,37	0
3	GOL	AAA	308	6/6	0.90	0.10	35,36,39,45	0
3	GOL	AAA	307	6/6	0.91	0.10	27,34,35,38	0
4	SO4	AAA	310	5/5	0.91	0.14	37,38,40,46	0
2	MFU	AAA	305	12/12	0.94	0.08	25,38,41,42	0
3	GOL	AAA	309	6/6	0.94	0.09	33,35,36,42	0
2	MFU	BBB	302	12/12	0.94	0.08	27,30,35,40	0
2	MFU	BBB	301	12/12	0.96	0.06	29,31,36,38	0
3	GOL	AAA	306	6/6	0.96	0.07	31,32,36,37	6
2	MFU	BBB	303	12/12	0.96	0.07	27,28,33,46	0
2	MFU	AAA	303	12/12	0.98	0.05	21,22,27,33	0
2	MFU	AAA	304	12/12	0.98	0.05	24,26,28,30	0
2	MFU	AAA	302	12/12	0.98	0.04	23,26,28,30	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.

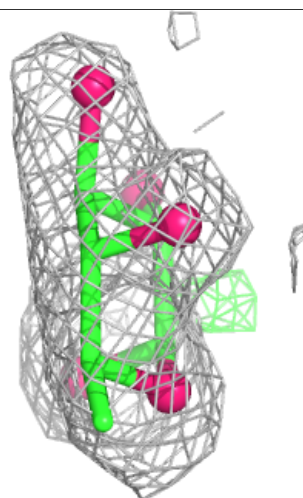
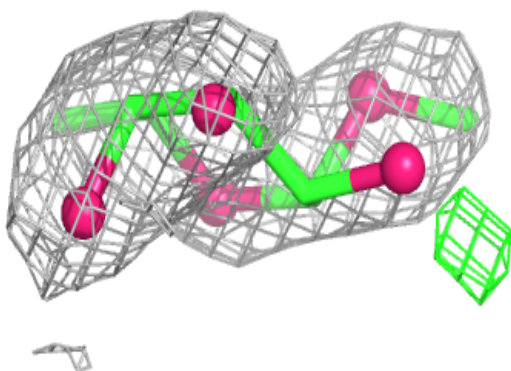
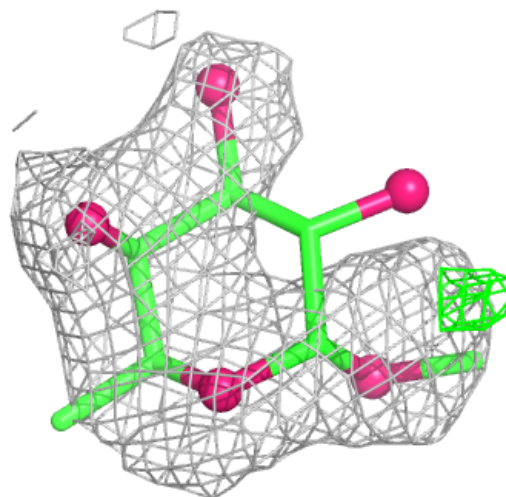
Electron density around MFU BBB 304:

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



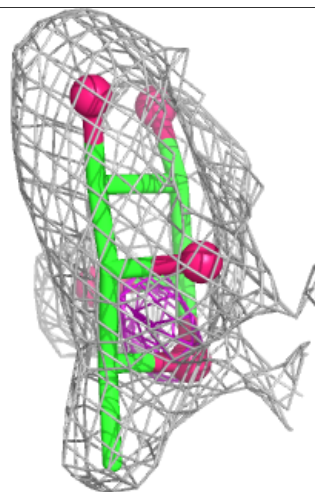
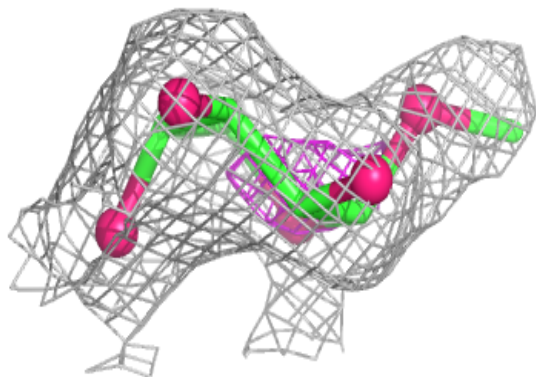
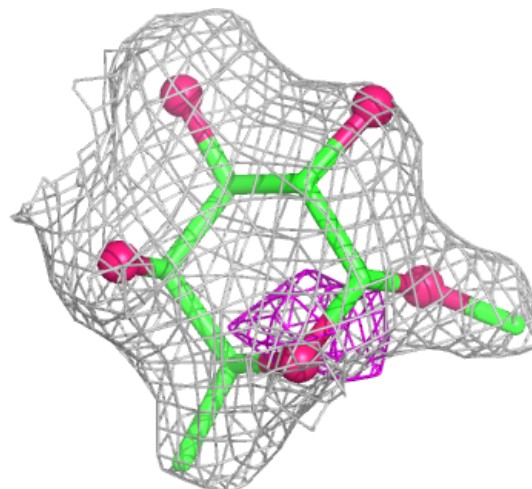
Electron density around MFU AAA 301:

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



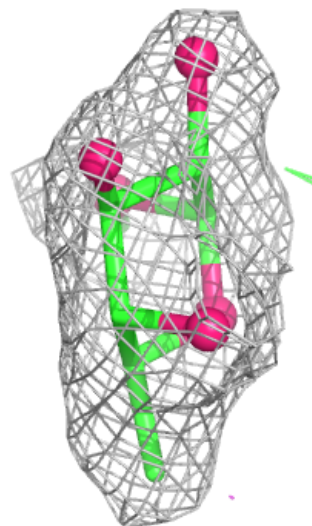
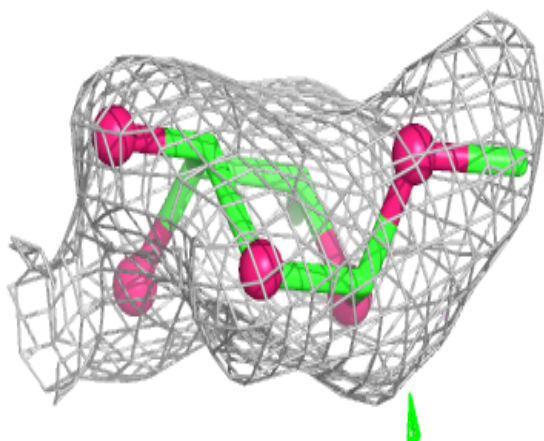
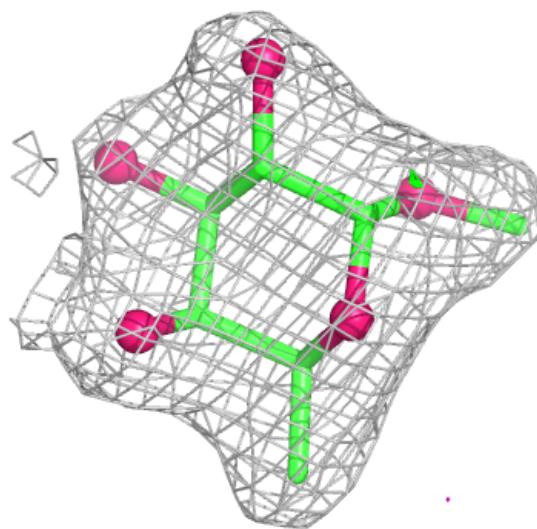
Electron density around MFU AAA 305:

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



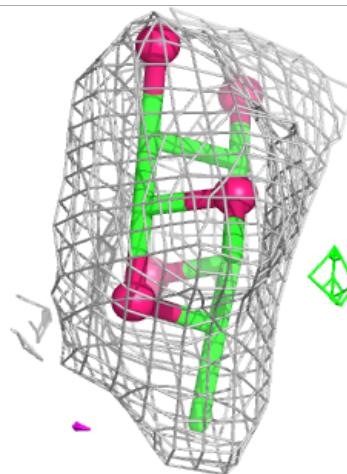
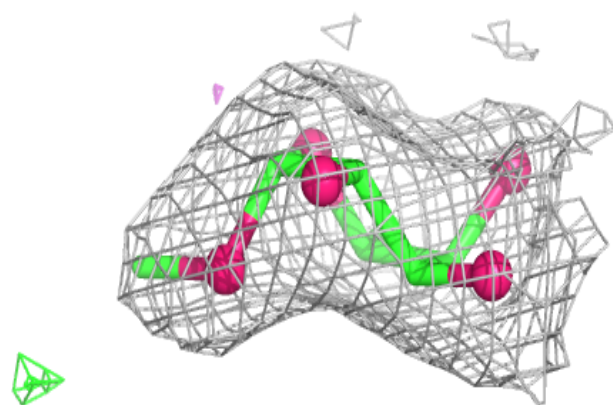
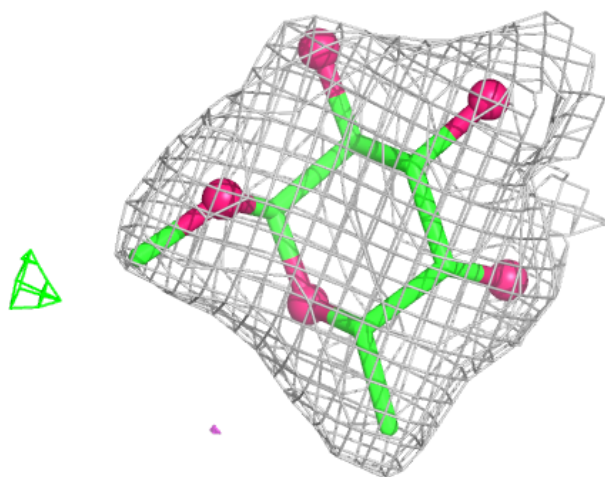
Electron density around MFU BBB 302:

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



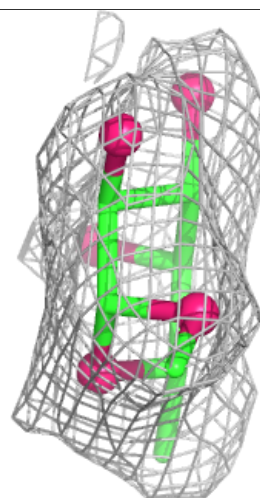
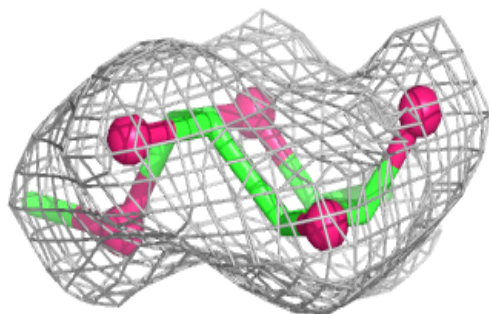
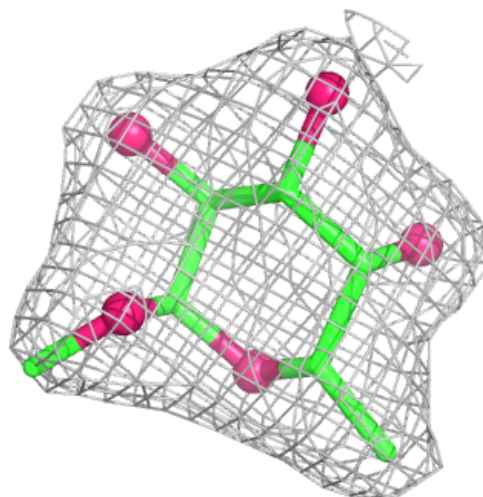
Electron density around MFU BBB 301:

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



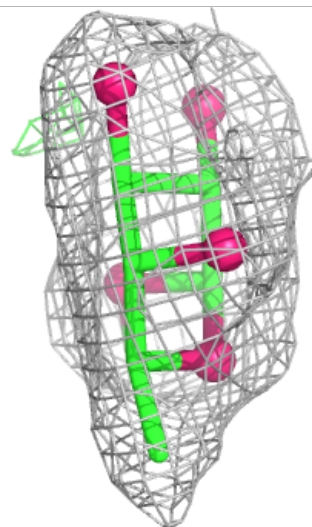
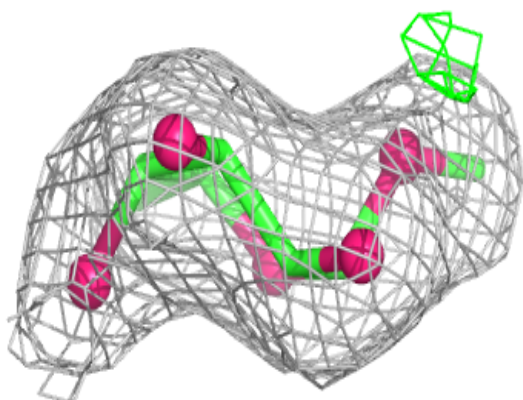
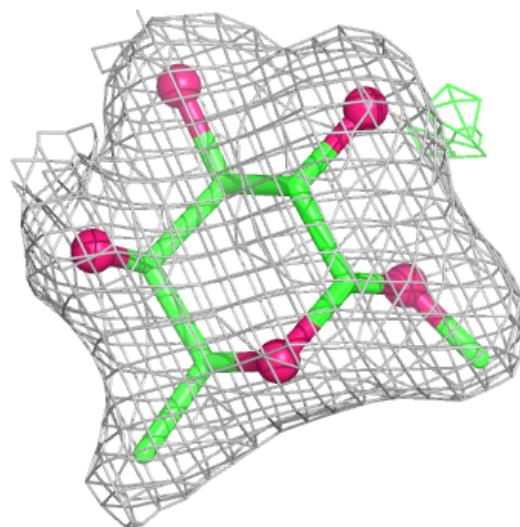
Electron density around MFU BBB 303:

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



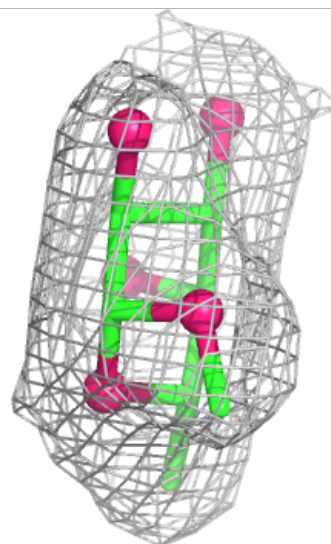
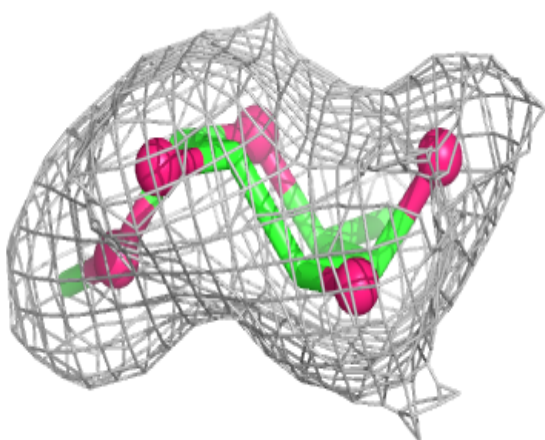
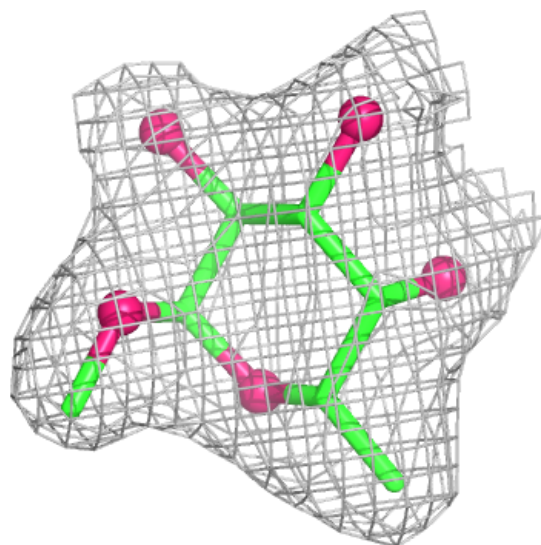
Electron density around MFU AAA 303:

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



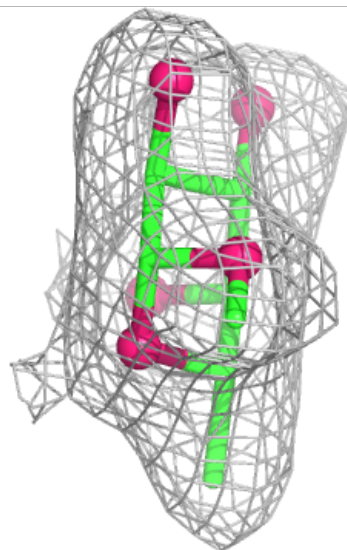
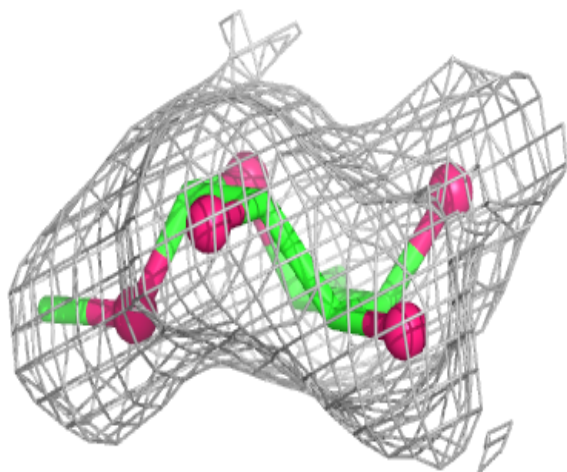
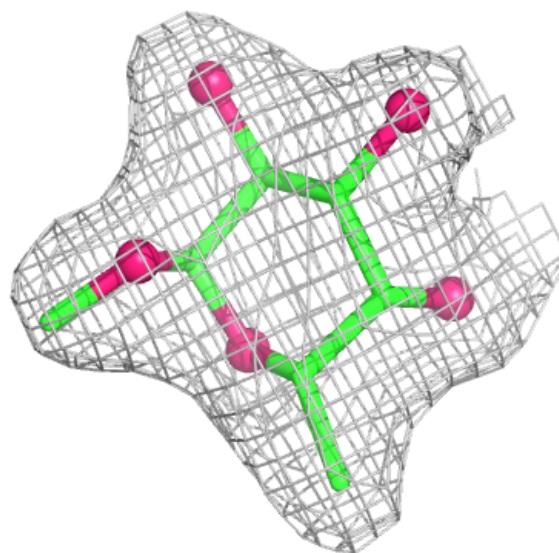
Electron density around MFU AAA 304:

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



Electron density around MFU AAA 302:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.