



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:04 AM UTC

PDB ID : 5C65 / pdb_00005c65
Title : Structure of the human glucose transporter GLUT3 / SLC2A3
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Deposited on : 2015-06-22
Resolution : 2.65 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](#) ①) 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

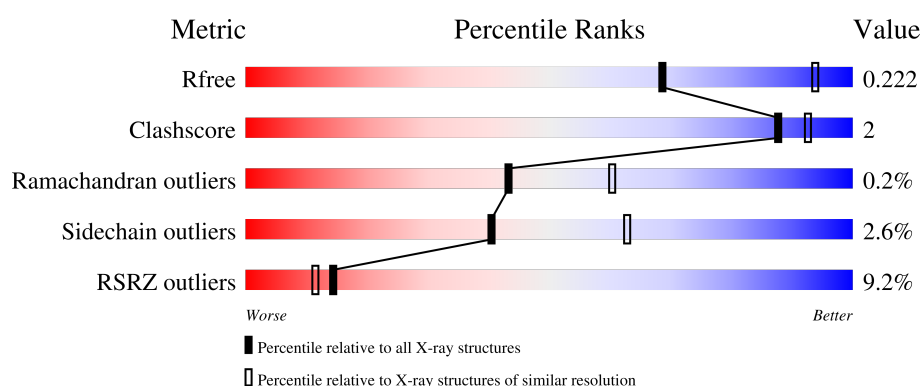
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	A	481	8% 87% 7% • 5%
1	B	481	9% 88% 5% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7231 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 Solute carrier family 2, facilitated glucose transporter member 3.

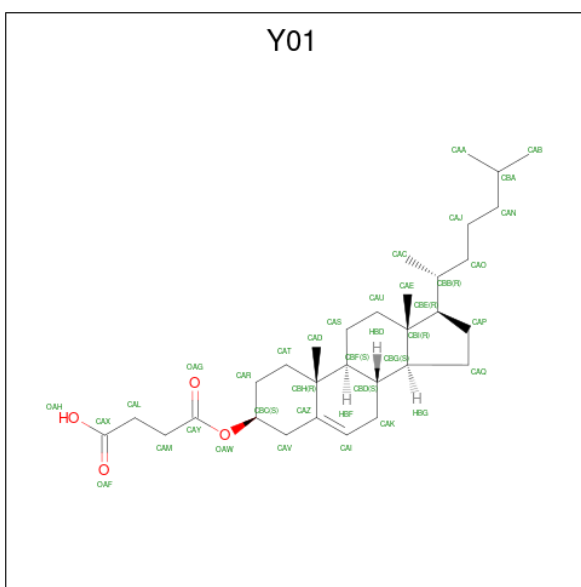
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3443	2274	548	601	20			
1	B	452	Total	C	N	O	S	0	0	0
			3343	2201	532	592	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLN	ASN	engineered mutation	UNP P11169
A	475	ALA	-	expression tag	UNP P11169
A	476	GLU	-	expression tag	UNP P11169
A	477	ASN	-	expression tag	UNP P11169
A	478	LEU	-	expression tag	UNP P11169
A	479	TYR	-	expression tag	UNP P11169
A	480	PHE	-	expression tag	UNP P11169
A	481	GLN	-	expression tag	UNP P11169
B	43	GLN	ASN	engineered mutation	UNP P11169
B	475	ALA	-	expression tag	UNP P11169
B	476	GLU	-	expression tag	UNP P11169
B	477	ASN	-	expression tag	UNP P11169
B	478	LEU	-	expression tag	UNP P11169
B	479	TYR	-	expression tag	UNP P11169
B	480	PHE	-	expression tag	UNP P11169
B	481	GLN	-	expression tag	UNP P11169

- Molecule 2 is Octyl Glucose Neopentyl Glycol (CCD ID: 37X) (formula: C₂₇H₅₂O₁₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 35	C 31	O 4	0	0
3	B	1	Total 35	C 31	O 4	0	0

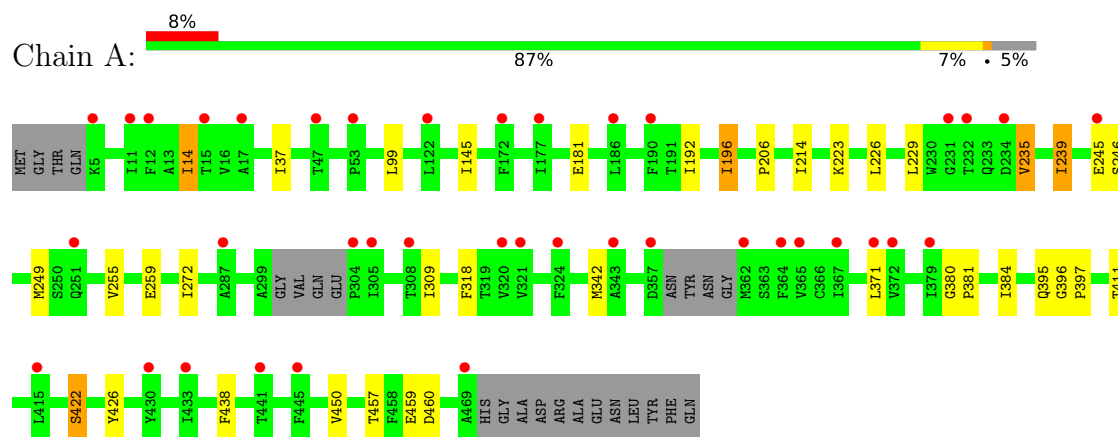
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	9	Total O 9 9	0	0

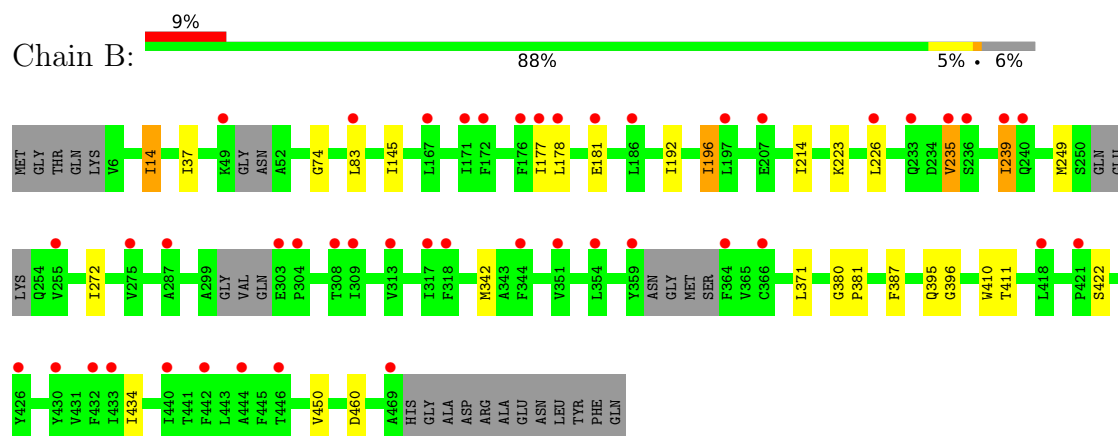
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Solute carrier family 2, facilitated glucose transporter member 3



- Molecule 1: Solute carrier family 2, facilitated glucose transporter member 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.55Å 116.03Å 99.75Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 40.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.65) 99.7 (40.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.205 , 0.223 (Not available) , 0.222	Depositor DCC
R_{free} test set	2010 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7231	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: 37X, Y01

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	A	0.84	1/3519 (0.0%)	1.41	5/4782 (0.1%)
1	B	0.84	0/3413	1.42	4/4646 (0.1%)
All	All	0.84	1/6932 (0.0%)	1.42	9/9428 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ILE	CA-CB	5.68	1.56	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	438	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	318	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	235	VAL	CA-C-N	5.62	127.81	120.28
1	A	235	VAL	C-N-CA	5.62	127.81	120.28
1	B	235	VAL	CA-C-N	5.36	127.46	120.28
1	B	235	VAL	C-N-CA	5.36	127.46	120.28
1	B	387	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	460	ASP	CA-CB-CG	5.29	117.89	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	0	3502	17	0
1	B	3343	0	3324	14	0
2	A	231	0	303	0	0
2	B	117	0	156	4	0
3	A	35	0	49	1	0
3	B	35	0	49	1	0
4	A	18	0	0	0	0
4	B	9	0	0	0	0
All	All	7231	0	7383	29	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 2.

All (29) 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:B:214:ILE:HD13	1:B:395:GLN:HG3	1.75	0.67
1:A:214:ILE:HD13	1:A:395:GLN:HG3	1.78	0.65
1:B:83:LEU:HD11	2:B:503:37X:H51	1.85	0.57
1:B:226:LEU:HD23	1:B:235:VAL:HB	1.88	0.55
1:A:192:ILE:HG21	1:B:196:ILE:HD13	1.89	0.54
1:A:411:THR:HB	3:A:507:Y01:HAQ2	1.90	0.54
1:A:196:ILE:HD13	1:B:192:ILE:HG21	1.91	0.53
1:A:214:ILE:HG23	1:A:246:SER:HA	1.92	0.50
1:A:99:LEU:HG	2:B:501:37X:H19	1.92	0.50
1:A:226:LEU:HD23	1:A:235:VAL:HB	1.94	0.48
1:B:411:THR:HB	3:B:504:Y01:HAQ2	1.94	0.48
1:A:206:PRO:HG3	1:A:229:LEU:HD21	1.97	0.47
1:A:422:SER:O	1:A:426:TYR:HD2	1.97	0.47
1:B:83:LEU:HD21	2:B:503:37X:H52	1.98	0.46
1:A:14:ILE:HG13	1:A:145:ILE:HD11	1.98	0.45
1:B:14:ILE:HG13	1:B:145:ILE:HD11	1.99	0.45
1:A:99:LEU:HG	2:B:501:37X:CBD	2.47	0.45
1:B:272:ILE:HG23	1:B:450:VAL:HG22	1.99	0.44
1:B:249:MET:HE3	1:B:396:GLY:HA2	2.00	0.43
1:A:272:ILE:HG23	1:A:450:VAL:HG22	2.00	0.43
1:A:342:MET:CE	1:A:381:PRO:HG2	2.49	0.43
1:B:342:MET:CE	1:B:381:PRO:HG2	2.49	0.42
1:A:457:THR:HG22	1:A:459:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LYS:HA	1:B:239:ILE:HD11	2.02	0.41
1:A:249:MET:HE3	1:A:396:GLY:HA2	2.02	0.41
1:B:177:ILE:HG22	1:B:178:LEU:HG	2.02	0.41
1:A:223:LYS:HA	1:A:239:ILE:HD11	2.03	0.41
1:A:255:VAL:HG11	1:A:397:PRO:HB3	2.03	0.40
1:B:74:GLY:HA3	1:B:410:TRP:CE3	2.56	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	A	451/481 (94%)	441 (98%)	9 (2%)	1 (0%)	43	60
1	B	442/481 (92%)	433 (98%)	8 (2%)	1 (0%)	43	60
All	All	893/962 (93%)	874 (98%)	17 (2%)	2 (0%)	43	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	GLY
1	B	380	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	A	361/397 (91%)	351 (97%)	10 (3%)	38	60
1	B	340/397 (86%)	332 (98%)	8 (2%)	43	65
All	All	701/794 (88%)	683 (97%)	18 (3%)	40	63

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

Mol	Chain	Res	Type
1	A	14	ILE
1	A	37	ILE
1	A	181	GLU
1	A	196	ILE
1	A	239	ILE
1	A	245	GLU
1	A	259	GLU
1	A	309	ILE
1	A	371	LEU
1	A	422	SER
1	B	14	ILE
1	B	37	ILE
1	B	181	GLU
1	B	196	ILE
1	B	239	ILE
1	B	371	LEU
1	B	422	SER
1	B	434	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	315	ASN
1	A	409	ASN
1	A	413	ASN
1	B	315	ASN
1	B	409	ASN
1	B	413	ASN

5.3.3 RNA ⓘ

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](#)

11 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	37X	A	504	-	40,40,40	0.32	0	48,54,54	0.59	1 (2%)
2	37X	B	502	-	40,40,40	0.25	0	48,54,54	0.59	2 (4%)
2	37X	A	503	-	40,40,40	0.24	0	48,54,54	0.67	2 (4%)
2	37X	A	505	-	40,40,40	0.30	0	48,54,54	0.88	3 (6%)
2	37X	B	501	-	40,40,40	0.26	0	48,54,54	0.67	2 (4%)
2	37X	A	506	-	40,40,40	0.28	0	48,54,54	0.52	1 (2%)
2	37X	A	502	-	40,40,40	0.23	0	48,54,54	1.05	3 (6%)
2	37X	A	501	-	37,37,40	0.25	0	45,51,54	1.04	2 (4%)
2	37X	B	503	-	40,40,40	0.26	0	48,54,54	0.52	0
3	Y01	A	507	-	38,38,38	0.43	0	57,57,57	0.54	0
3	Y01	B	504	-	38,38,38	0.39	0	57,57,57	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	37X	A	504	-	-	7/30/70/70	0/2/2/2
2	37X	B	502	-	-	7/30/70/70	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	37X	A	503	-	-	6/30/70/70	0/2/2/2
2	37X	A	505	-	-	13/30/70/70	0/2/2/2
2	37X	B	501	-	-	9/30/70/70	0/2/2/2
2	37X	A	506	-	-	4/30/70/70	0/2/2/2
2	37X	A	502	-	-	11/30/70/70	0/2/2/2
2	37X	A	501	-	-	8/27/67/70	0/2/2/2
2	37X	B	503	-	-	11/30/70/70	0/2/2/2
3	Y01	A	507	-	-	5/19/77/77	0/4/4/4
3	Y01	B	504	-	-	7/19/77/77	0/4/4/4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	37X	CBS-O1-C1	4.80	125.49	113.31
2	A	501	37X	CBS-O1-C1	4.43	124.55	113.31
2	A	501	37X	CBT-OBV-CCJ	3.89	123.19	113.31
2	A	505	37X	CBT-CCM-CBS	-3.83	90.89	109.56
2	A	502	37X	CBT-OBV-CCJ	3.42	121.98	113.31
2	A	505	37X	CBT-OBV-CCJ	3.25	121.56	113.31
2	A	503	37X	CBT-OBV-CCJ	3.18	121.37	113.31
2	B	501	37X	CBS-O1-C1	3.15	121.30	113.31
2	A	504	37X	CBS-O1-C1	3.11	121.19	113.31
2	A	502	37X	CBR-CCM-CBQ	-3.05	104.29	109.96
2	A	506	37X	CBS-O1-C1	2.51	119.69	113.31
2	B	502	37X	CBT-OBV-CCJ	2.48	119.60	113.31
2	A	503	37X	CBS-O1-C1	2.47	119.57	113.31
2	A	505	37X	CBS-O1-C1	2.27	119.07	113.31
2	B	502	37X	CBS-O1-C1	2.24	118.99	113.31
2	B	501	37X	CBT-CCM-CBS	2.16	120.11	109.56

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	37X	O5-C1-O1-CBS
2	A	501	37X	O1-CBS-CCM-CBQ
2	A	501	37X	O1-CBS-CCM-CBR
2	A	502	37X	O5-C1-O1-CBS

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Mol	Chain	Res	Type	Atoms
2	A	502	37X	CBK-CBQ-CCM-CBR
2	A	502	37X	CBK-CBQ-CCM-CBS
2	A	502	37X	CBK-CBQ-CCM-CBT
2	A	502	37X	OBX-CCJ-OBV-CBT
2	A	503	37X	O5-C1-O1-CBS
2	A	503	37X	OBX-CCJ-OBV-CBT
2	A	505	37X	O5-C1-O1-CBS
2	A	505	37X	OBX-CCJ-OBV-CBT
2	A	505	37X	CCL-CCJ-OBV-CBT
2	B	501	37X	O5-C1-O1-CBS
2	B	501	37X	OBV-CBT-CCM-CBQ
2	B	501	37X	OBV-CBT-CCM-CBR
2	B	502	37X	O1-CBS-CCM-CBQ
2	B	502	37X	O1-CBS-CCM-CBR
2	B	503	37X	O1-CBS-CCM-CBQ
2	B	503	37X	O1-CBS-CCM-CBR
2	B	501	37X	C4-C5-C6-O6
2	B	503	37X	OBX-CCJ-OBV-CBT
2	B	501	37X	OBV-CBT-CCM-CBS
2	A	505	37X	OAL-CBP-CCF-OBX
2	B	503	37X	O1-CBS-CCM-CBT
2	A	503	37X	CCL-CCJ-OBV-CBT
2	B	503	37X	CCL-CCJ-OBV-CBT
2	A	502	37X	O5-C5-C6-O6
2	B	501	37X	O5-C5-C6-O6
2	B	502	37X	O1-CBS-CCM-CBT
3	B	504	Y01	CAO-CAJ-CAN-CBA
2	B	501	37X	CBI-CBK-CBQ-CCM
2	B	503	37X	CBJ-CBL-CBR-CCM
3	B	504	Y01	CAX-CAL-CAM-CAY
3	A	507	Y01	CAJ-CAO-CBB-CBE
3	B	504	Y01	CAJ-CAO-CBB-CBE
3	A	507	Y01	CAO-CAJ-CAN-CBA
2	A	504	37X	C2-C1-O1-CBS
2	A	502	37X	CBJ-CBL-CBR-CCM
2	A	501	37X	OBX-CCJ-OBV-CBT
2	A	504	37X	O5-C1-O1-CBS
2	A	506	37X	CBJ-CBL-CBR-CCM
2	A	501	37X	O1-CBS-CCM-CBT
2	B	503	37X	CBG-CBI-CBK-CBQ
2	B	502	37X	O5-C5-C6-O6
2	A	502	37X	CBH-CBJ-CBL-CBR

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Mol	Chain	Res	Type	Atoms
2	A	505	37X	CBG-CBI-CBK-CBQ
3	A	507	Y01	CAJ-CAO-CBB-CAC
2	A	506	37X	CBH-CBJ-CBL-CBR
2	A	505	37X	CBL-CBR-CCM-CBT
2	B	503	37X	O5-C5-C6-O6
2	A	503	37X	CBF-CBH-CBJ-CBL
2	A	505	37X	CBH-CBJ-CBL-CBR
2	A	504	37X	O5-C5-C6-O6
3	B	504	Y01	CAJ-CAO-CBB-CAC
2	B	503	37X	OAL-CBP-CCF-OBX
2	A	502	37X	C4-C5-C6-O6
2	A	505	37X	OAL-CBP-CCF-CCQ
2	A	501	37X	CBE-CBG-CBI-CBK
2	B	501	37X	CBC-CBE-CBG-CBI
2	A	504	37X	CBC-CBE-CBG-CBI
2	A	502	37X	CBF-CBH-CBJ-CBL
2	A	506	37X	CBG-CBI-CBK-CBQ
2	A	504	37X	OBV-CBT-CCM-CBS
2	A	501	37X	OBV-CBT-CCM-CBQ
2	A	501	37X	OBV-CBT-CCM-CBR
2	A	503	37X	O1-CBS-CCM-CBQ
2	A	503	37X	O1-CBS-CCM-CBR
2	A	504	37X	OBV-CBT-CCM-CBR
2	A	505	37X	O1-CBS-CCM-CBQ
2	A	505	37X	O1-CBS-CCM-CBR
2	A	504	37X	CBE-CBG-CBI-CBK
2	B	501	37X	CBJ-CBL-CBR-CCM
2	B	503	37X	CBH-CBJ-CBL-CBR
2	A	505	37X	O1-CBS-CCM-CBT
2	B	503	37X	CBE-CBG-CBI-CBK
2	B	502	37X	OBX-CCJ-OBV-CBT
2	A	505	37X	CBE-CBG-CBI-CBK
3	A	507	Y01	CAM-CAL-CAX-OAH
3	A	507	Y01	CAM-CAL-CAX-OAF
2	B	502	37X	CBH-CBJ-CBL-CBR
3	B	504	Y01	CAM-CAL-CAX-OAH
3	B	504	Y01	CAM-CAL-CAX-OAF
2	A	502	37X	O1-CBS-CCM-CBQ
2	A	505	37X	OBV-CBT-CCM-CBR
2	A	506	37X	O1-CBS-CCM-CBR
2	B	502	37X	OBV-CBT-CCM-CBQ
3	B	504	Y01	CAL-CAM-CAY-OAW

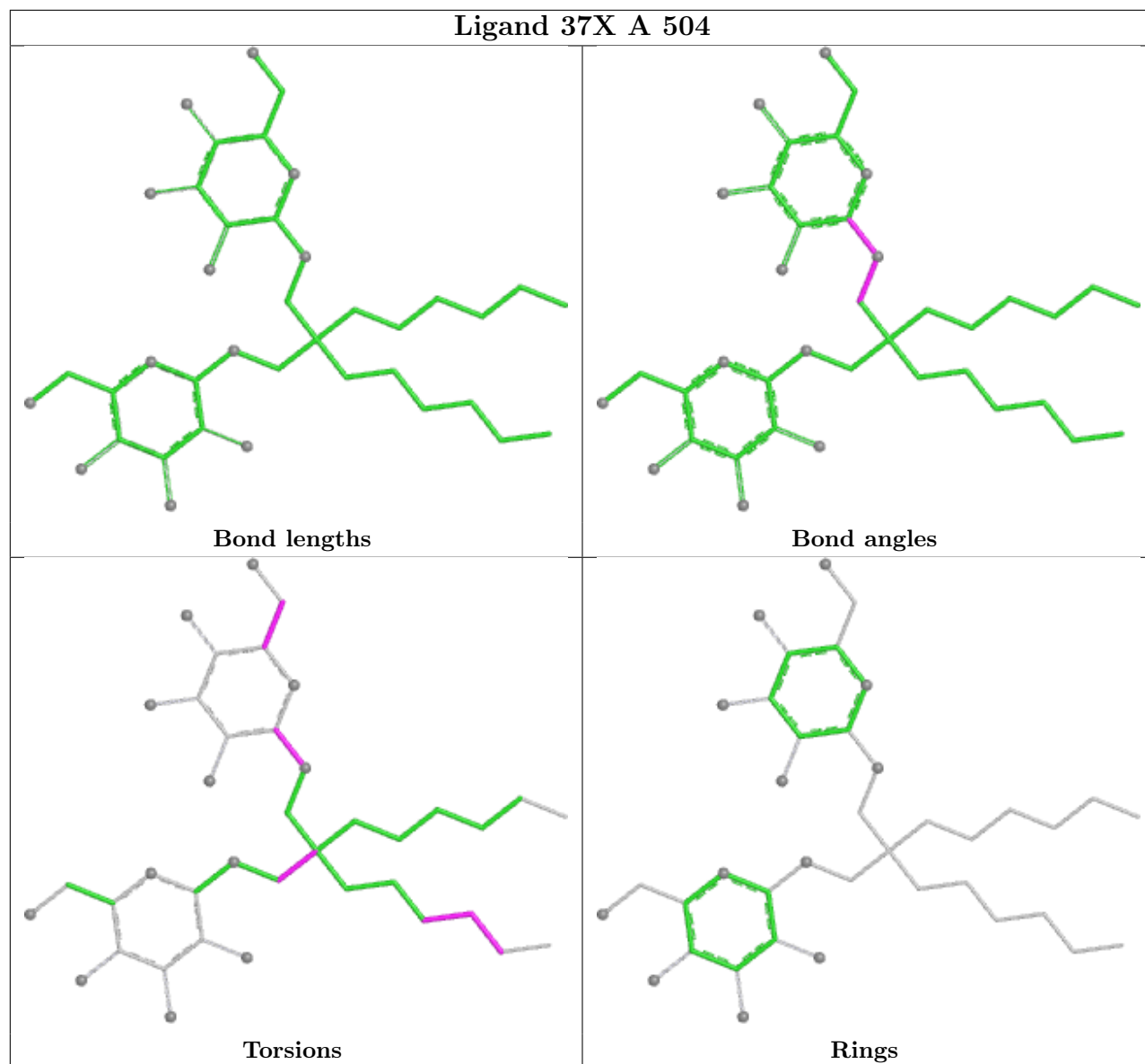
There are no ring outliers.

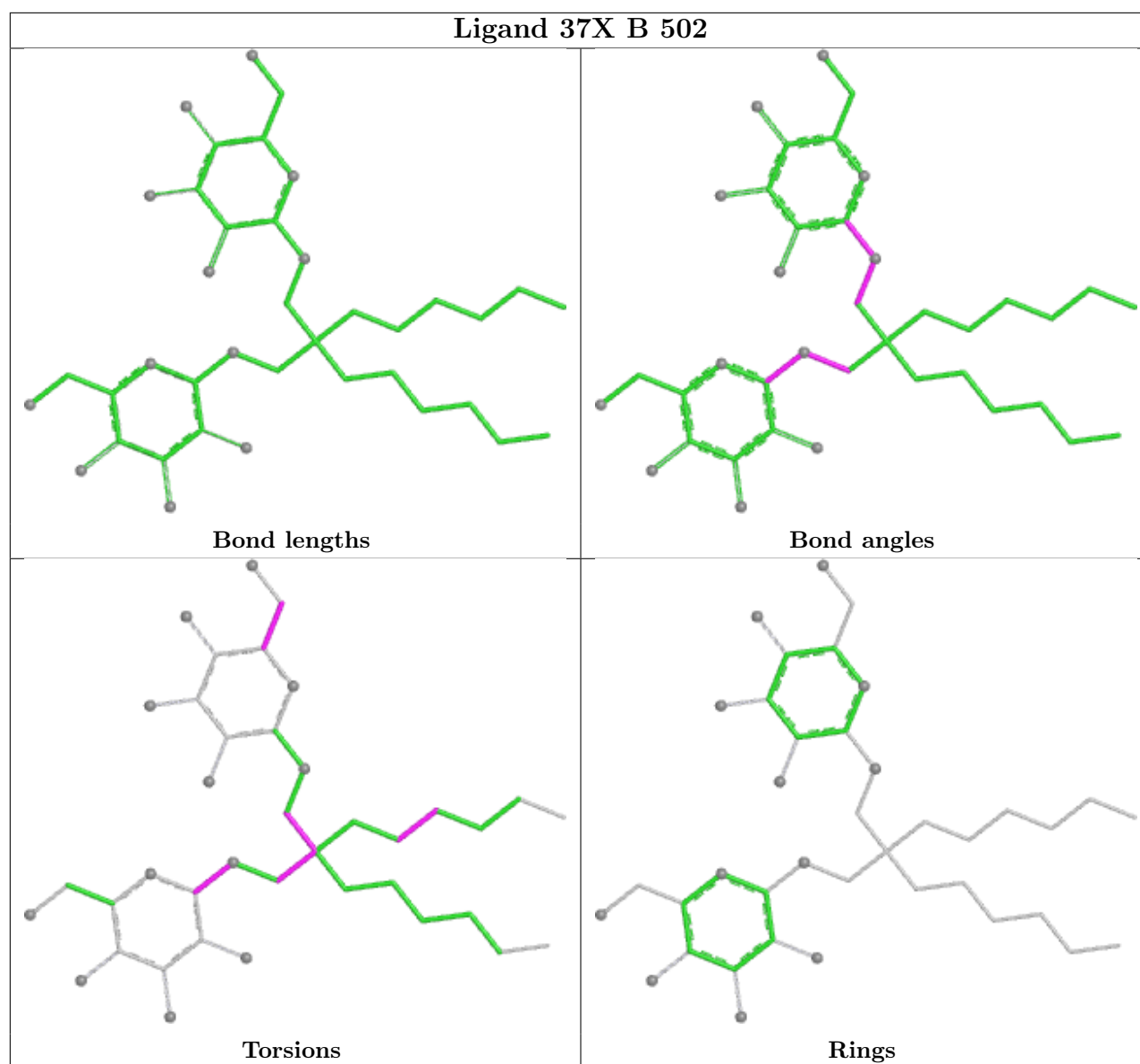
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	37X	2	0
2	B	503	37X	2	0
3	A	507	Y01	1	0
3	B	504	Y01	1	0

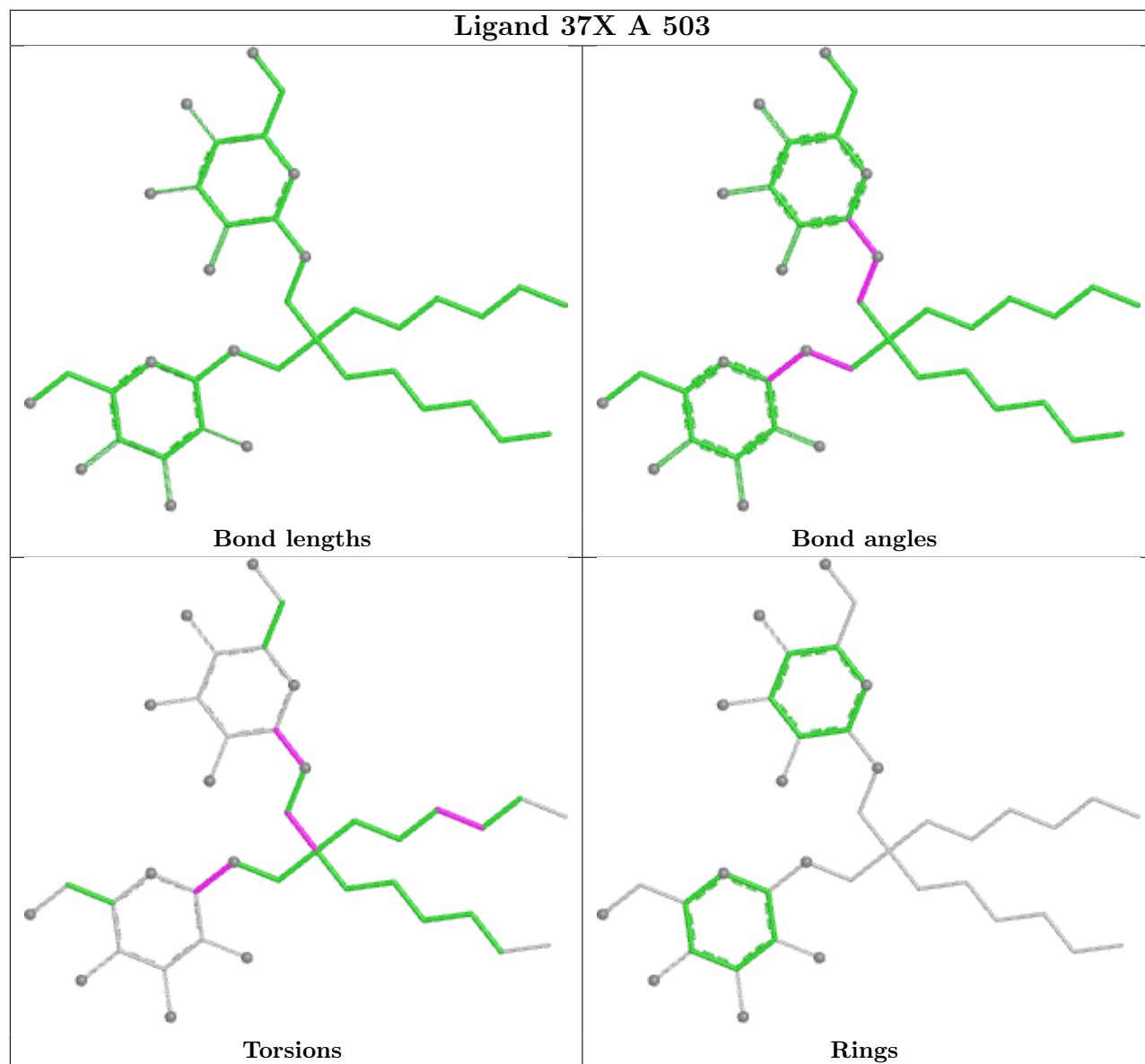
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 37X A 504

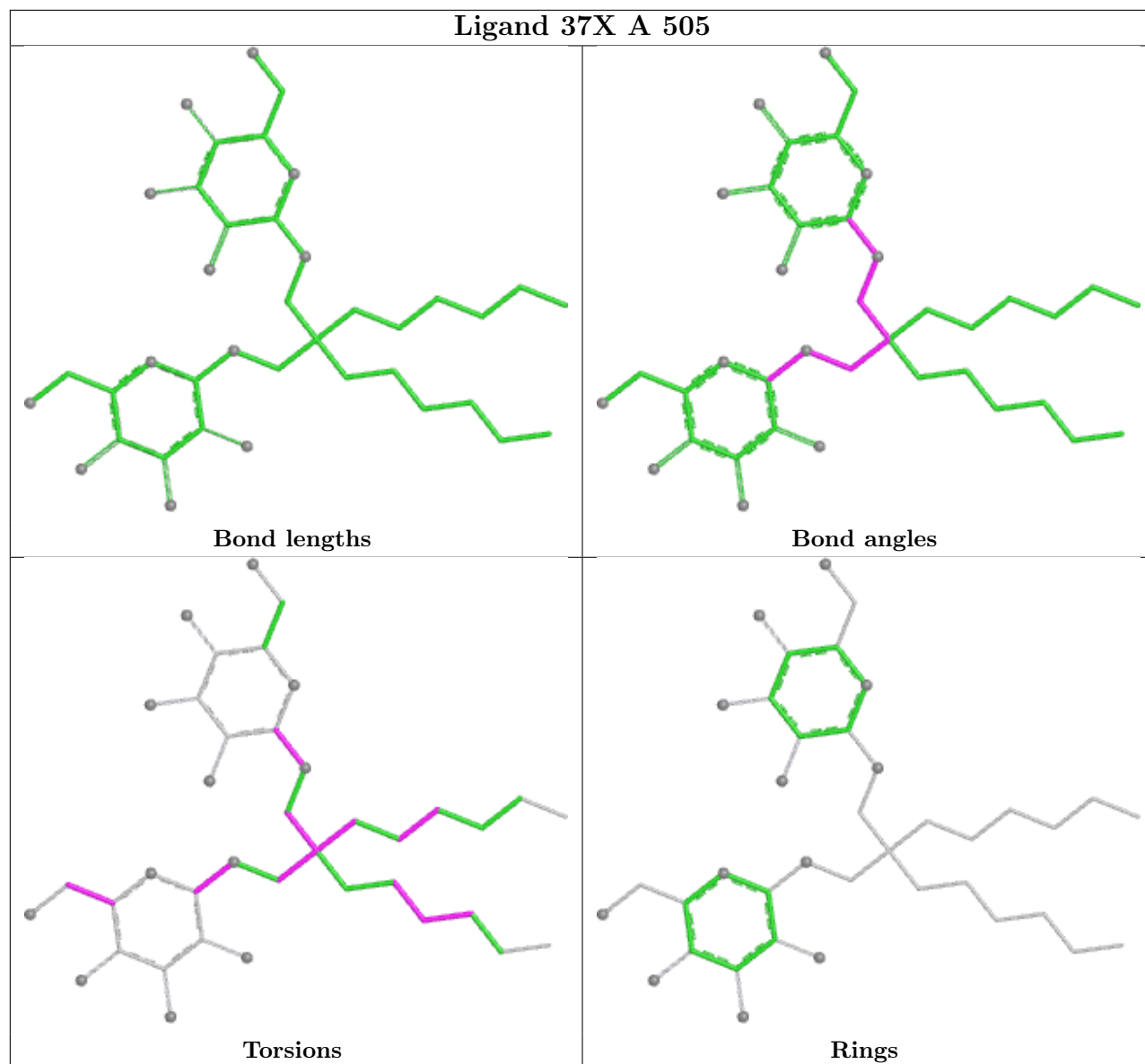


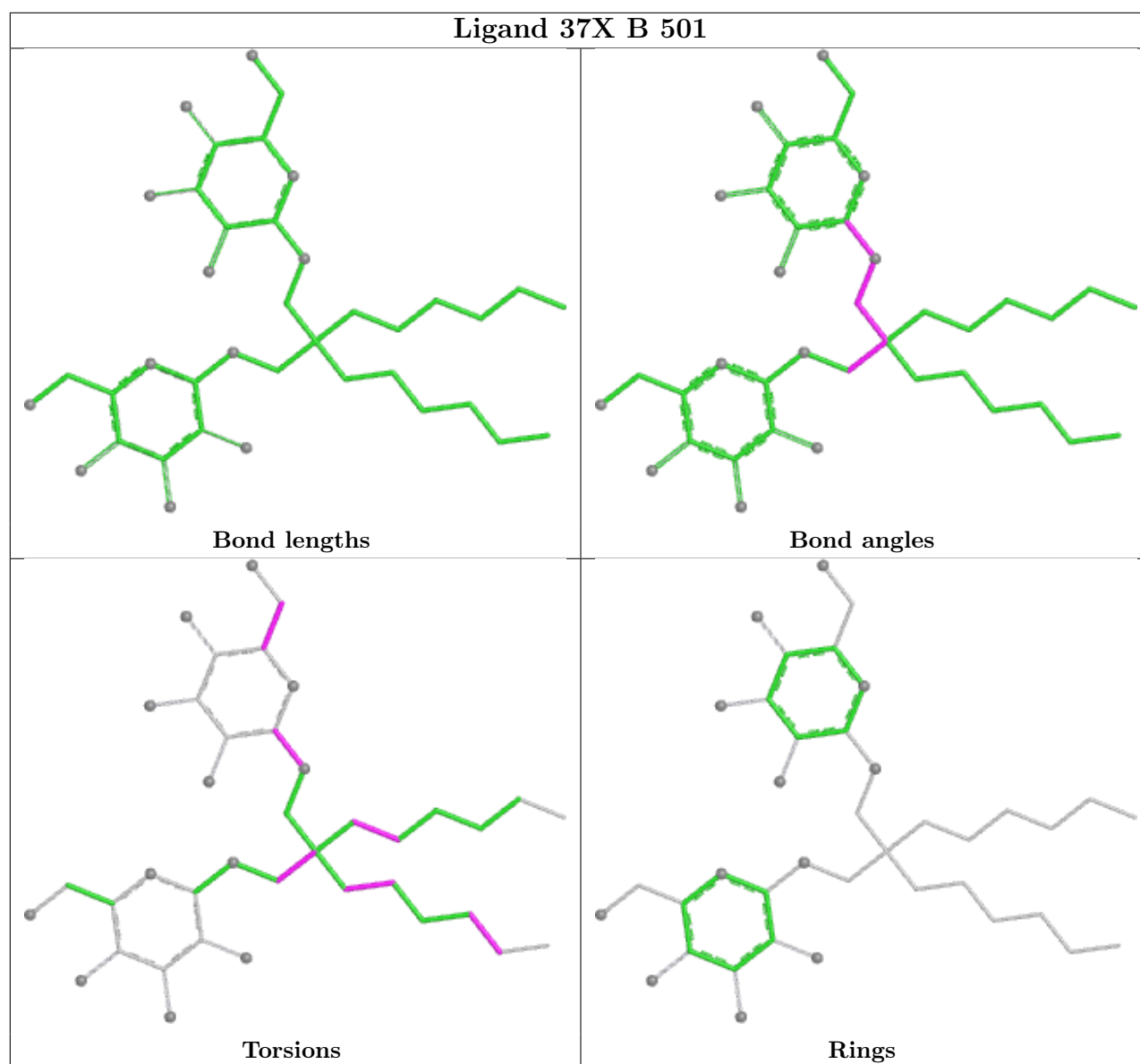


Ligand 37X A 503

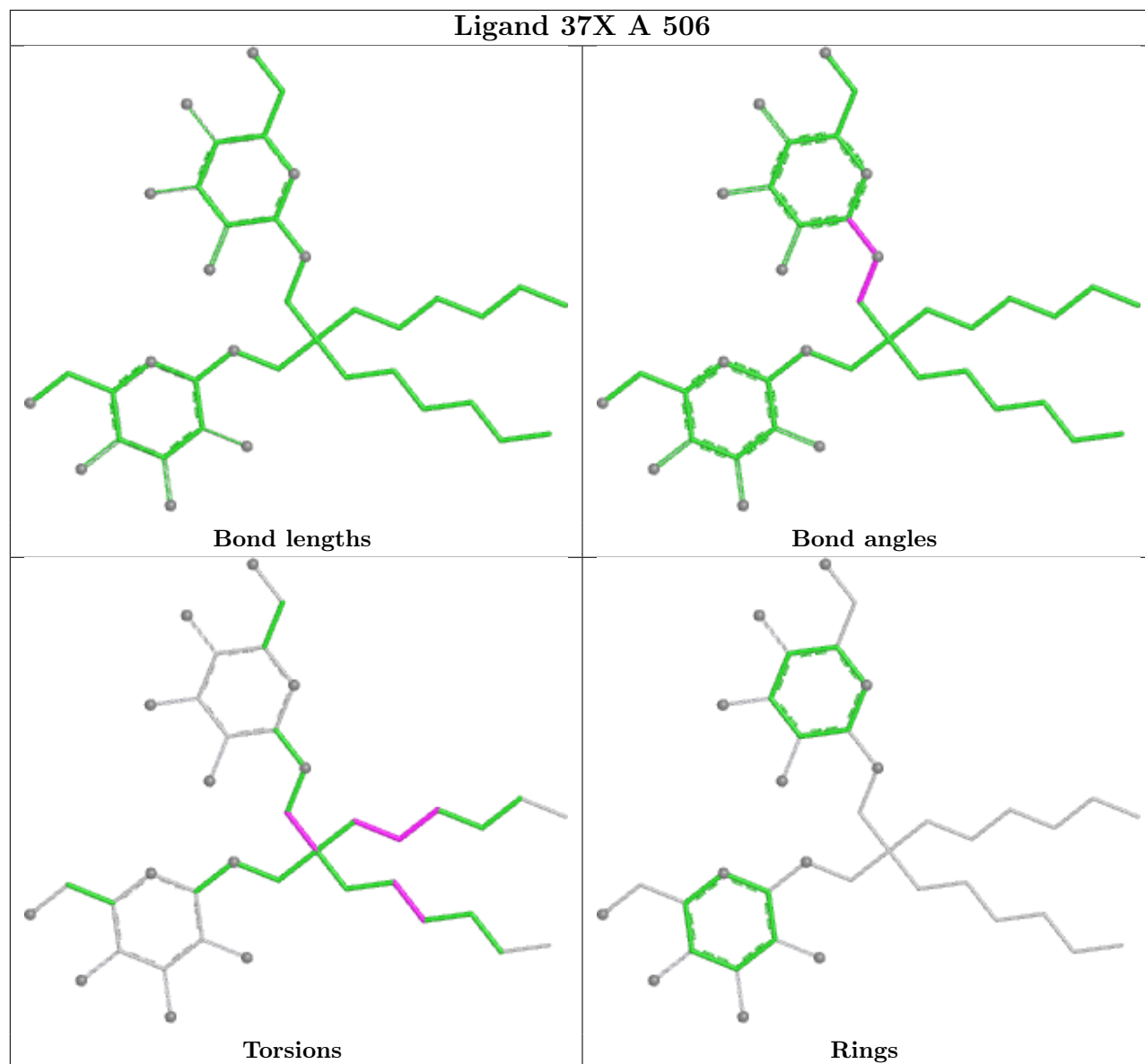


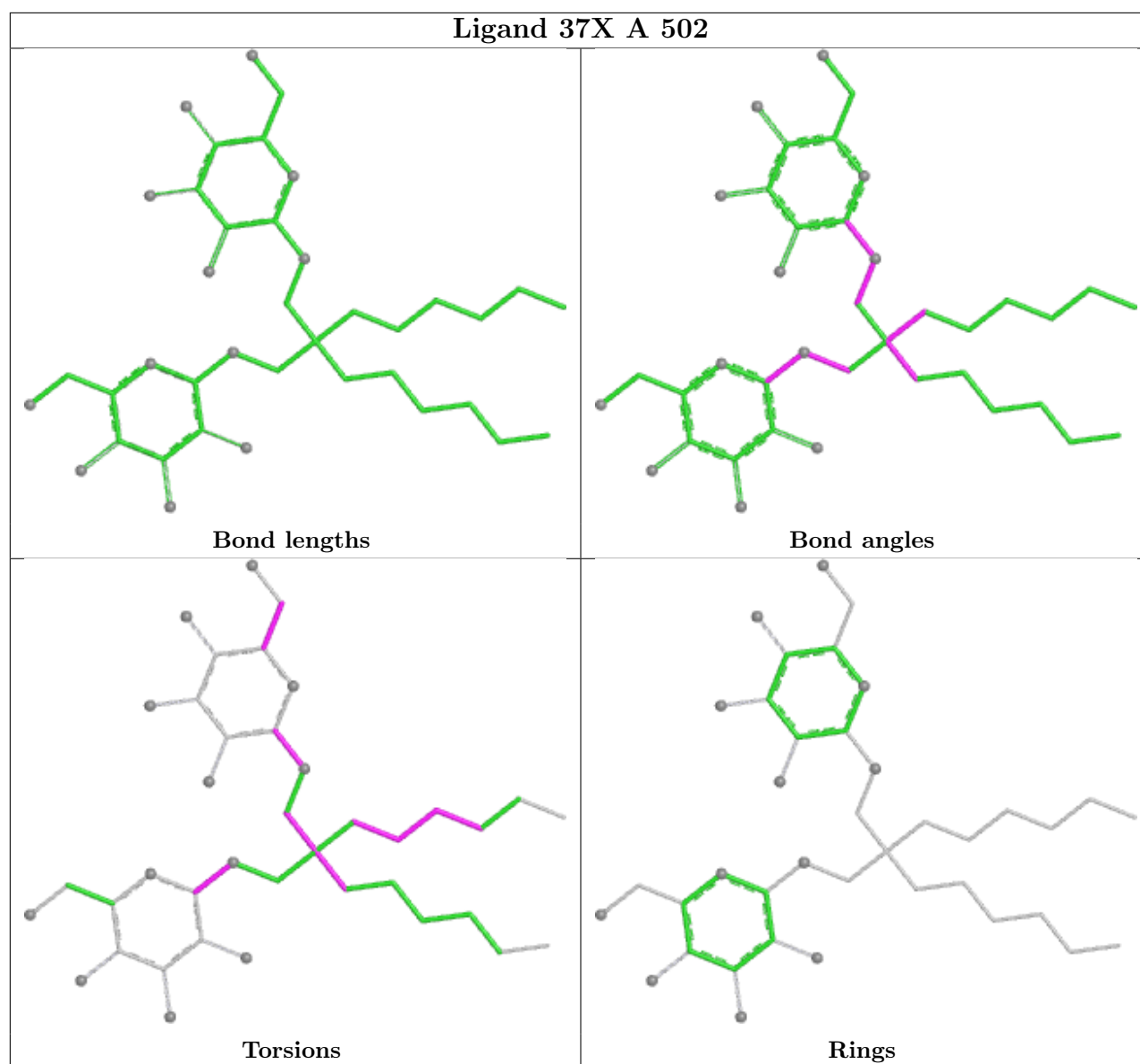
Ligand 37X A 505



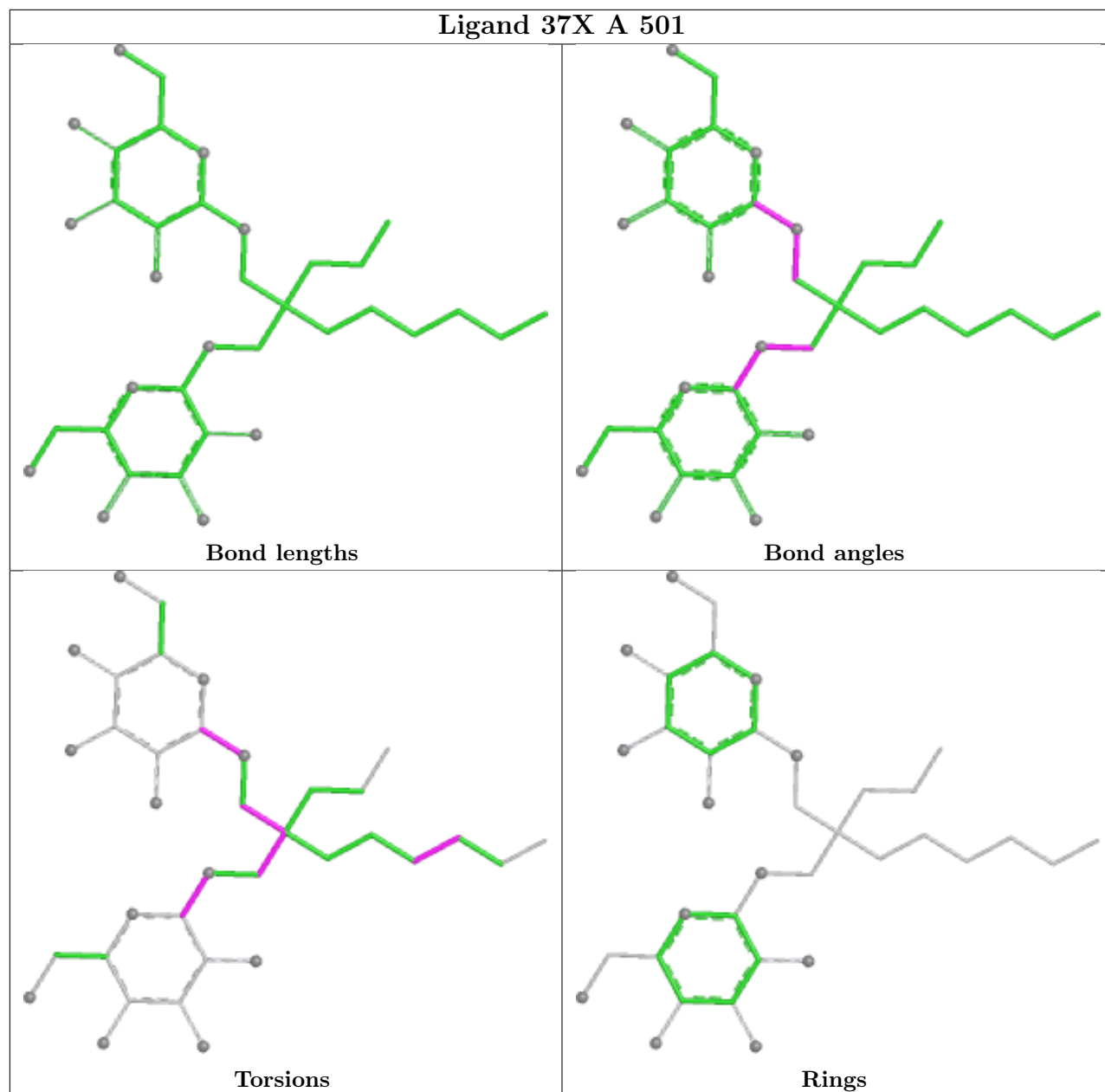


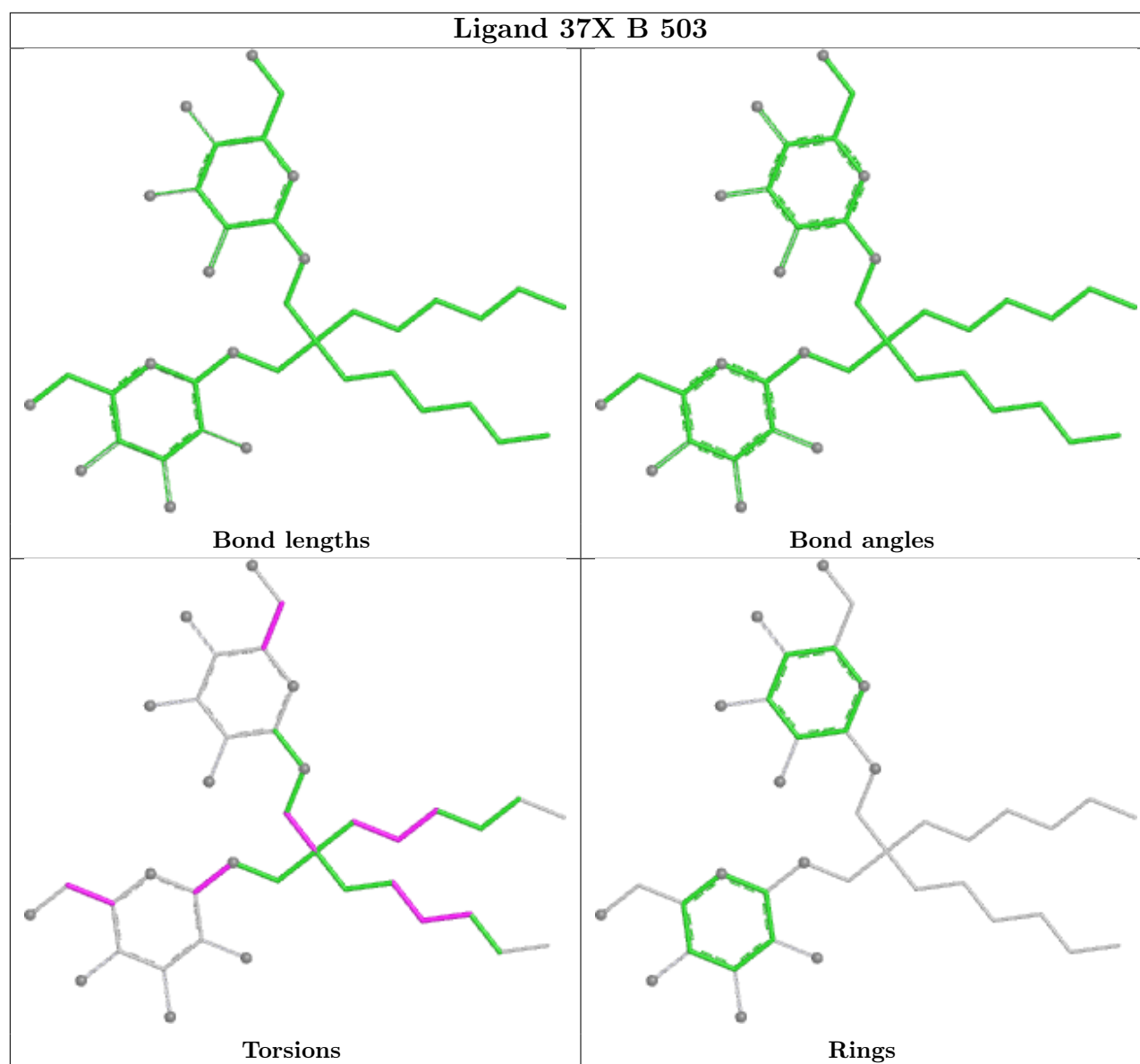
Ligand 37X A 506

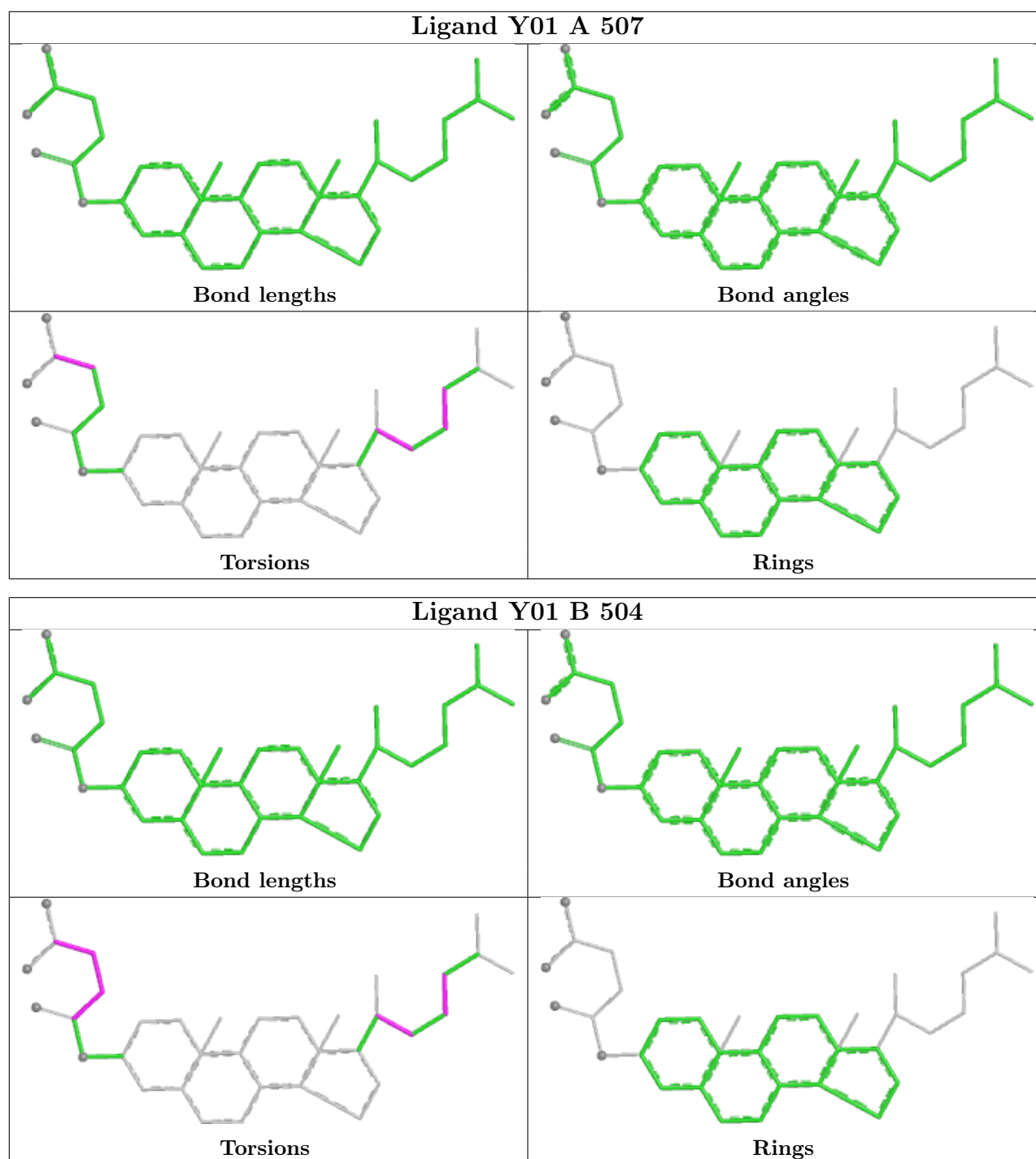




Ligand 37X A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	457/481 (95%)	0.43	39 (8%) 16 12	61, 88, 133, 181	0
1	B	452/481 (93%)	0.59	45 (9%) 12 10	66, 108, 164, 220	0
All	All	909/962 (94%)	0.51	84 (9%) 14 11	61, 96, 152, 220	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ILE	5.6
1	A	15	THR	4.6
1	B	177	ILE	4.5
1	B	359	TYR	4.2
1	A	172	PHE	4.2
1	B	366	CYS	4.1
1	A	305	ILE	4.0
1	A	186	LEU	4.0
1	B	171	ILE	3.9
1	B	317	ILE	3.8
1	A	287	ALA	3.8
1	A	190	PHE	3.6
1	A	357	ASP	3.5
1	B	172	PHE	3.5
1	A	324	PHE	3.5
1	A	430	TYR	3.4
1	B	442	PHE	3.4
1	A	12	PHE	3.4
1	B	313	VAL	3.4
1	B	430	TYR	3.3
1	B	351	VAL	3.3
1	B	303	GLU	3.1
1	B	236	SER	3.1
1	B	275	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	433	ILE	3.0
1	A	47	THR	3.0
1	B	207	GLU	2.9
1	B	308	THR	2.9
1	A	234	ASP	2.8
1	B	426	TYR	2.8
1	A	320	VAL	2.8
1	A	251	GLN	2.8
1	B	421	PRO	2.8
1	A	231	GLY	2.8
1	A	304	PRO	2.7
1	B	226	LEU	2.7
1	B	418	LEU	2.7
1	A	122	LEU	2.7
1	A	245	GLU	2.7
1	B	287	ALA	2.6
1	B	364	PHE	2.6
1	B	469	ALA	2.6
1	B	432	PHE	2.6
1	B	304	PRO	2.5
1	B	255	VAL	2.5
1	A	415	LEU	2.5
1	A	232	THR	2.4
1	A	441	THR	2.4
1	A	364	PHE	2.4
1	A	371	LEU	2.4
1	A	5	LYS	2.4
1	A	11	ILE	2.3
1	A	379	ILE	2.3
1	B	235	VAL	2.3
1	A	362	MET	2.3
1	B	178	LEU	2.3
1	B	233	GLN	2.3
1	A	365	VAL	2.3
1	B	444	ALA	2.2
1	B	83	LEU	2.2
1	B	197	LEU	2.2
1	A	445	PHE	2.2
1	A	308	THR	2.2
1	B	354	LEU	2.2
1	A	433	ILE	2.2
1	A	343	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	2.2
1	B	181	GLU	2.2
1	B	49	LYS	2.2
1	B	167	LEU	2.2
1	B	318	PHE	2.2
1	A	321	VAL	2.1
1	B	239	ILE	2.1
1	B	344	PHE	2.1
1	A	469	ALA	2.1
1	B	309	ILE	2.1
1	B	176	PHE	2.1
1	A	17	ALA	2.0
1	B	440	ILE	2.0
1	A	53	PRO	2.0
1	B	446	THR	2.0
1	B	240	GLN	2.0
1	A	367	ILE	2.0
1	A	372	VAL	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](#)

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	37X	A	506	39/39	0.62	0.21	123,158,161,161	0
2	37X	A	502	39/39	0.84	0.14	95,101,116,118	0
2	37X	A	505	39/39	0.86	0.14	103,112,128,130	0
3	Y01	B	504	35/35	0.87	0.18	142,151,158,159	0
2	37X	B	501	39/39	0.89	0.13	94,99,102,108	0

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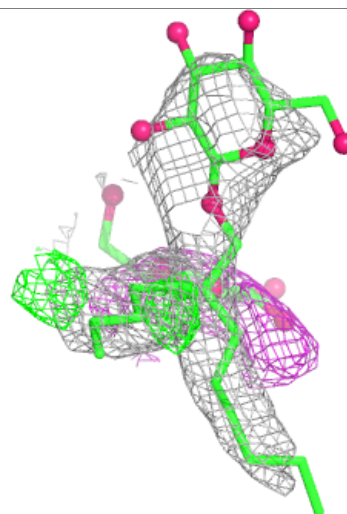
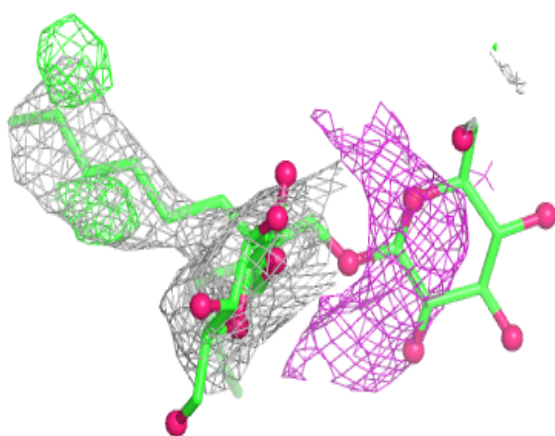
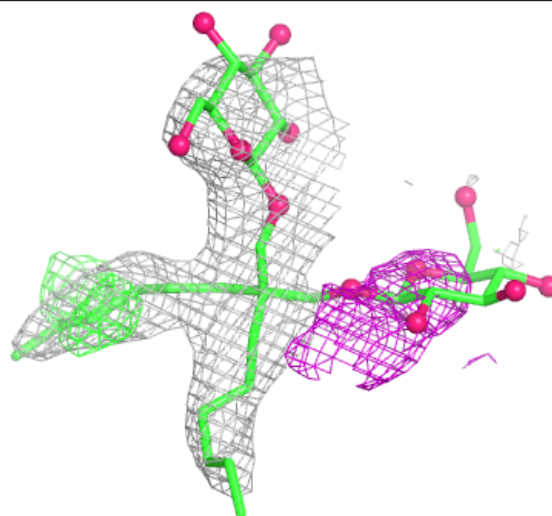
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	37X	A	503	39/39	0.89	0.13	98,119,145,146	0
2	37X	B	503	39/39	0.90	0.12	110,136,153,154	0
2	37X	A	504	39/39	0.90	0.13	101,137,144,147	0
3	Y01	A	507	35/35	0.91	0.18	122,130,140,142	0
2	37X	B	502	39/39	0.91	0.15	115,148,153,154	0
2	37X	A	501	36/39	0.92	0.10	86,95,106,112	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.

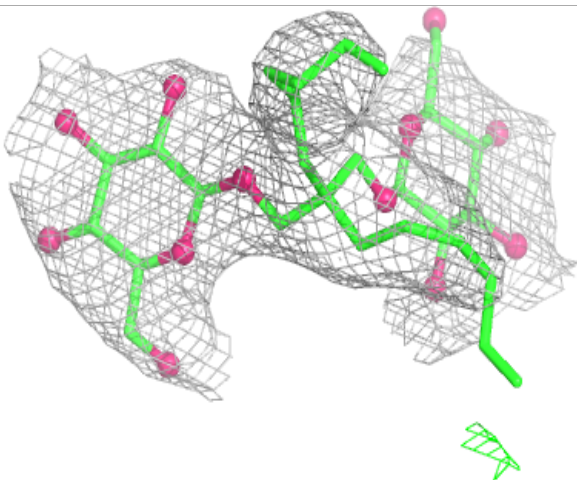
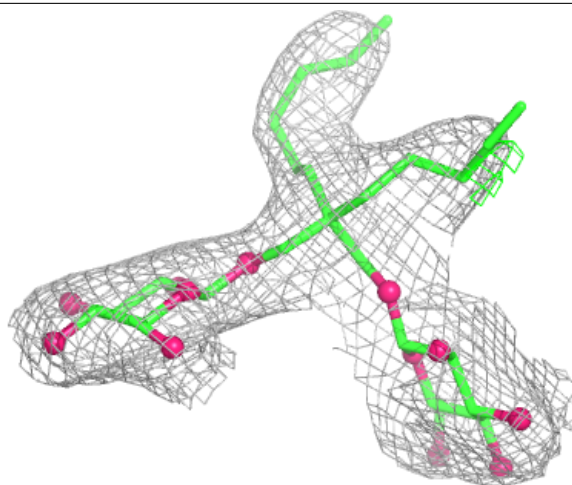
Electron density around 37X A 506:

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



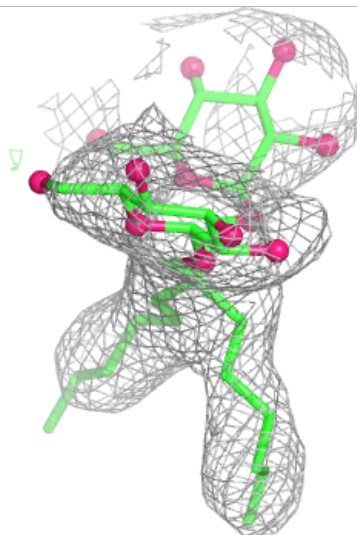
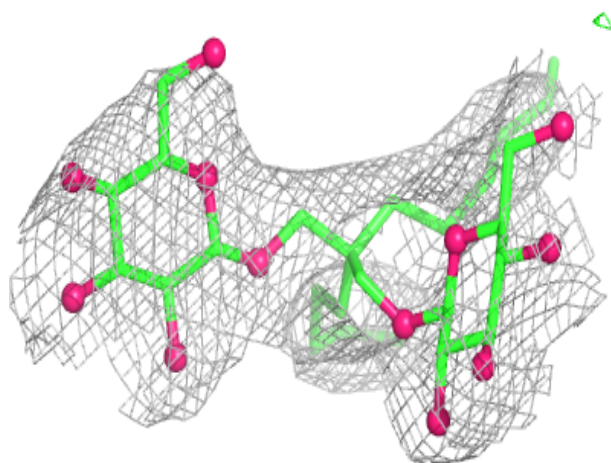
Electron density around 37X A 502:

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



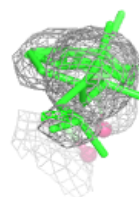
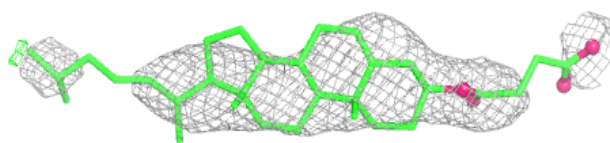
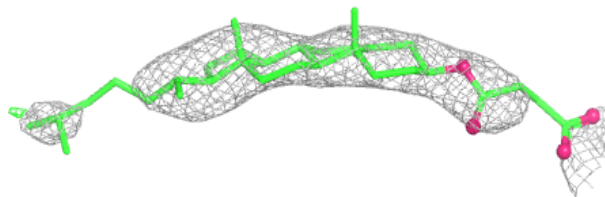
Electron density around 37X A 505:

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



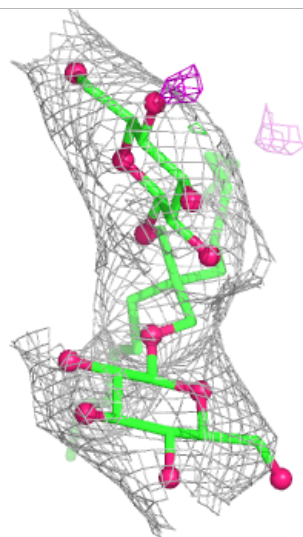
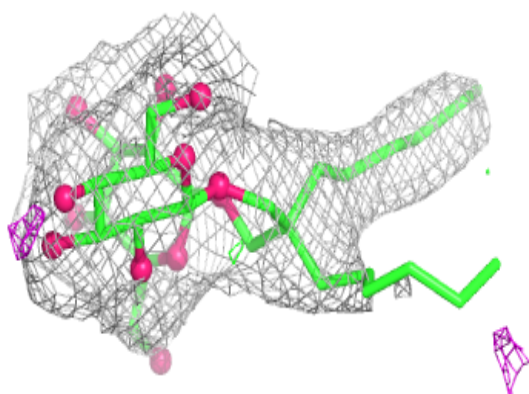
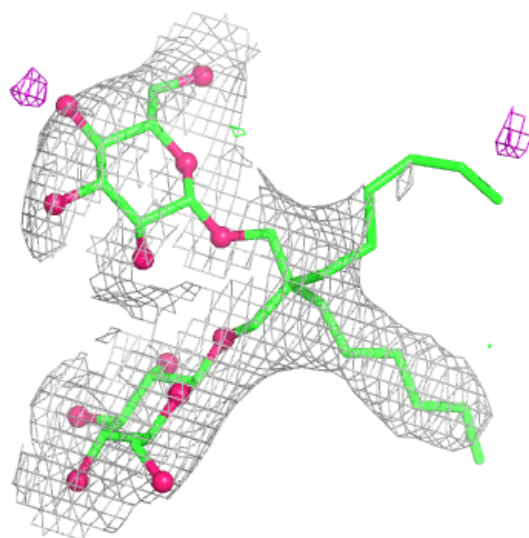
Electron density around Y01 B 504:

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



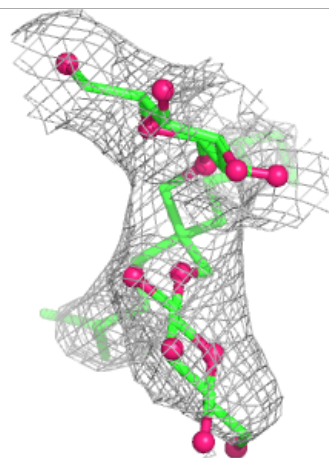
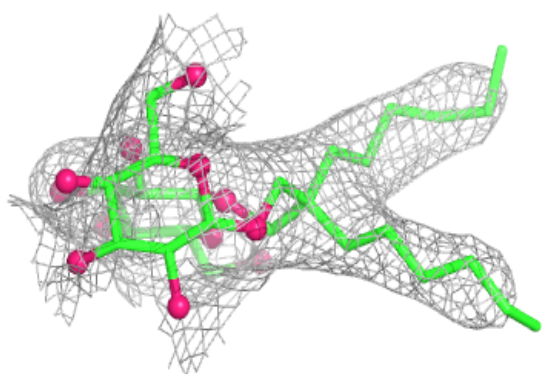
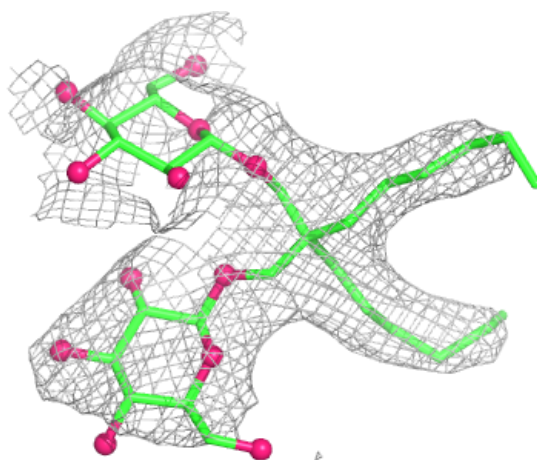
Electron density around 37X B 501:

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



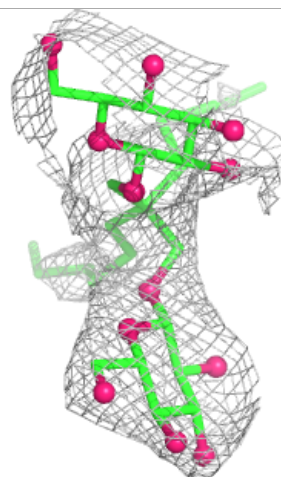
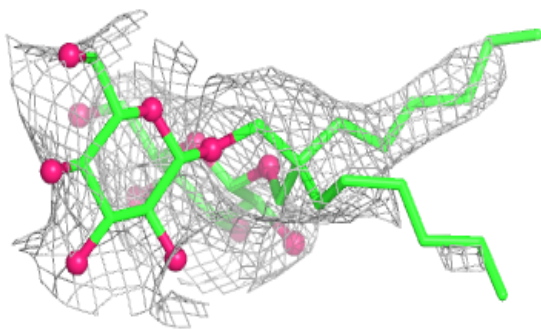
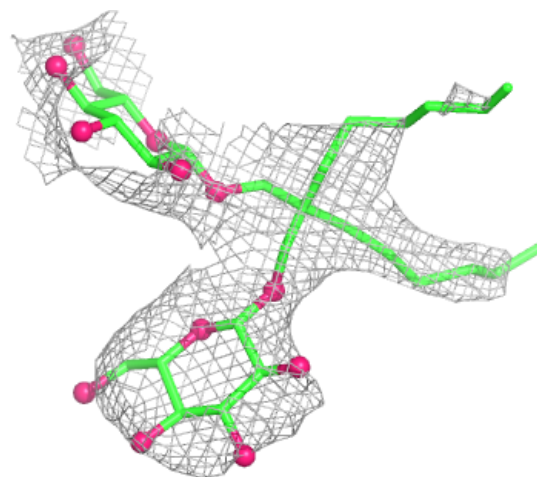
Electron density around 37X A 503:

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



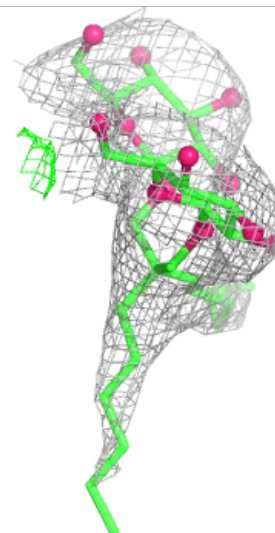
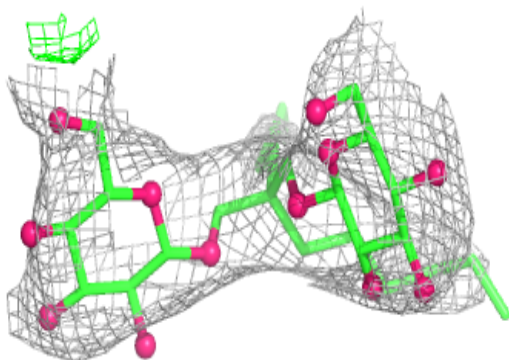
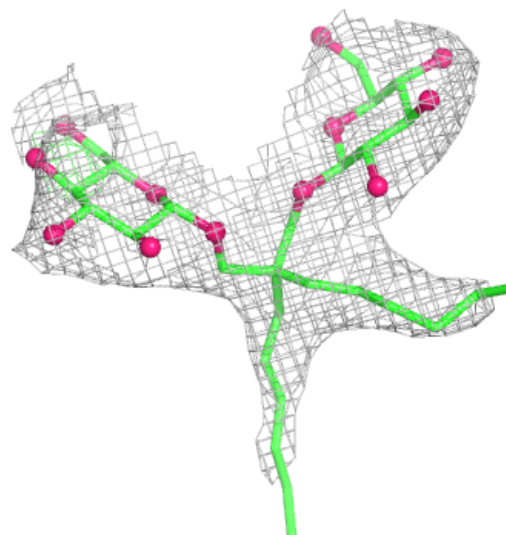
Electron density around 37X B 503:

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



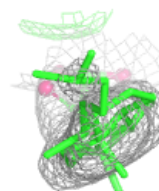
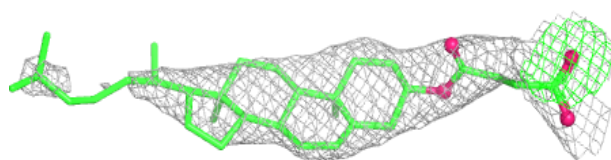
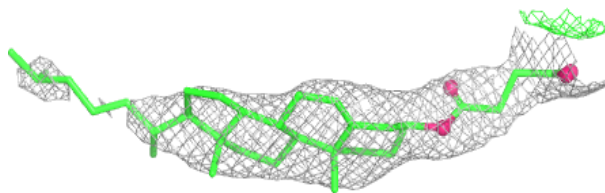
Electron density around 37X A 504:

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



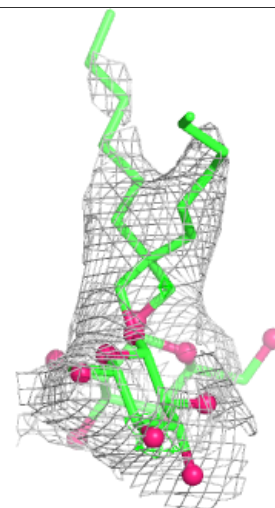
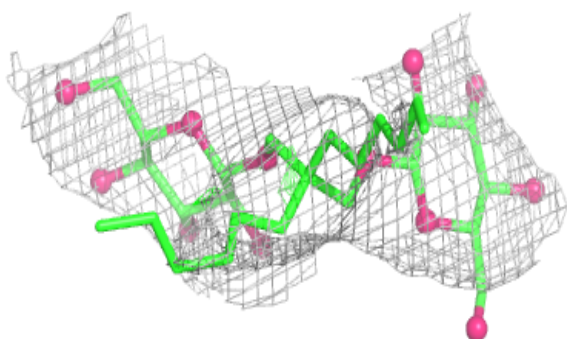
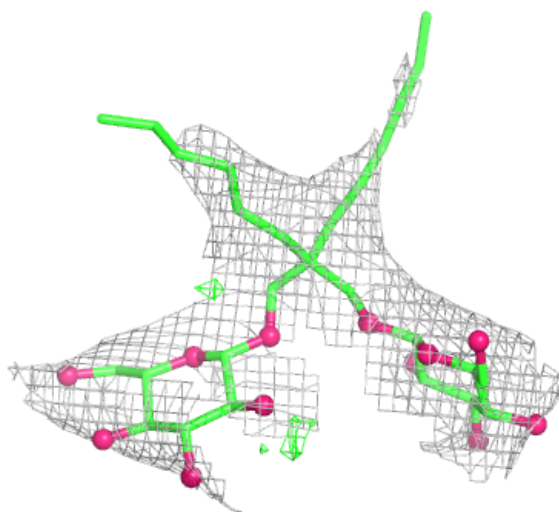
Electron density around Y01 A 507:

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



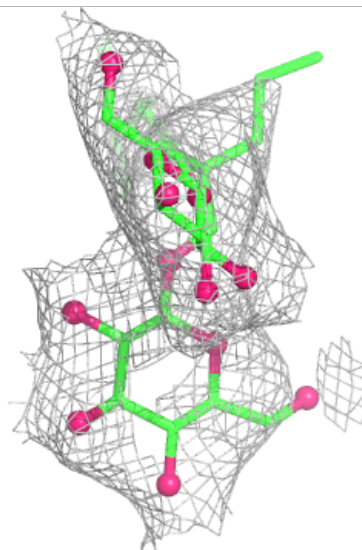
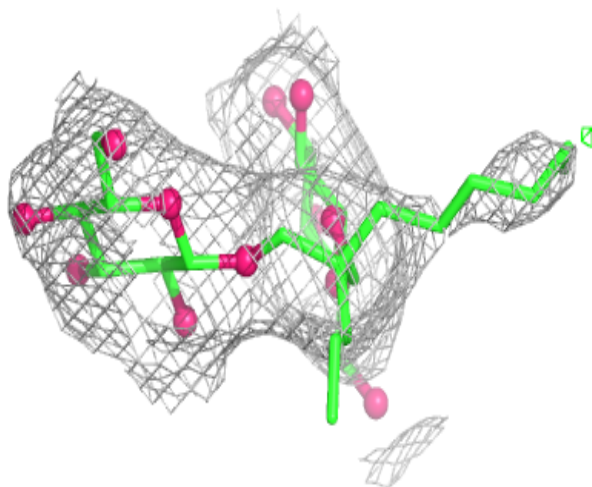
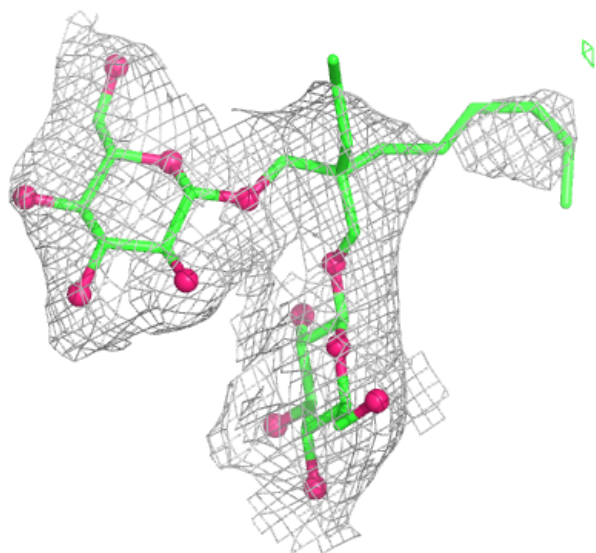
Electron density around 37X B 502:

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



Electron density around 37X A 501:

$2mF_o-DF_c$ (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.