Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	5C65
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 following versions of software and data (see references ⓘ) were used in the production of this report:

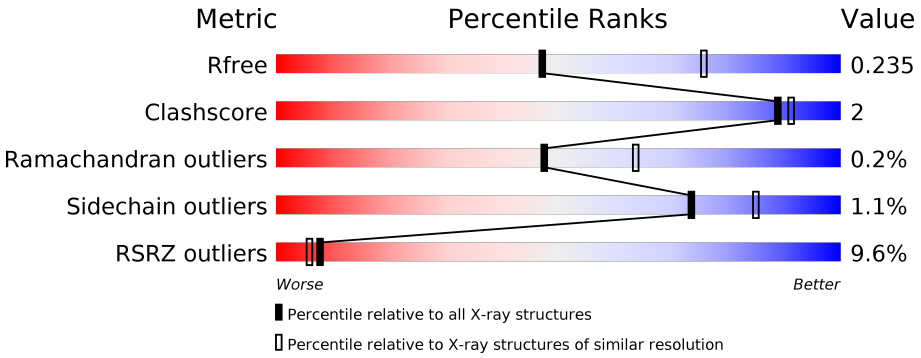
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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 <=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	6% 89% 5% 5%
1	B	481	12% 89% · 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	37X	A	506	-	-	-	X

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.

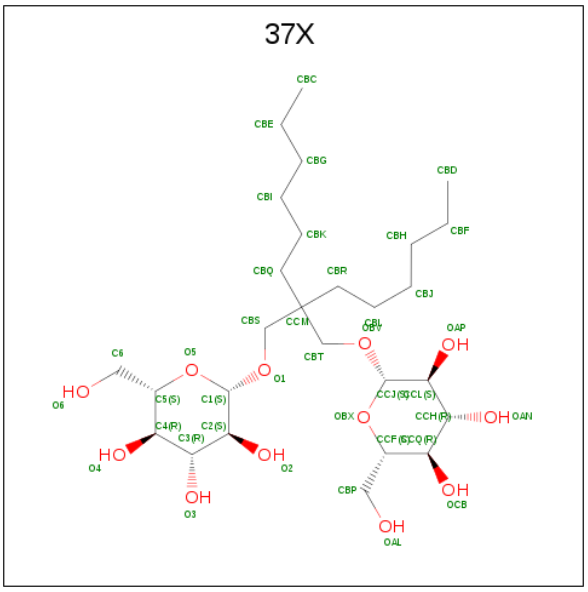
- Molecule 1 is a protein called Solute carrier family 2, facilitated glucose transporter member 3.

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:

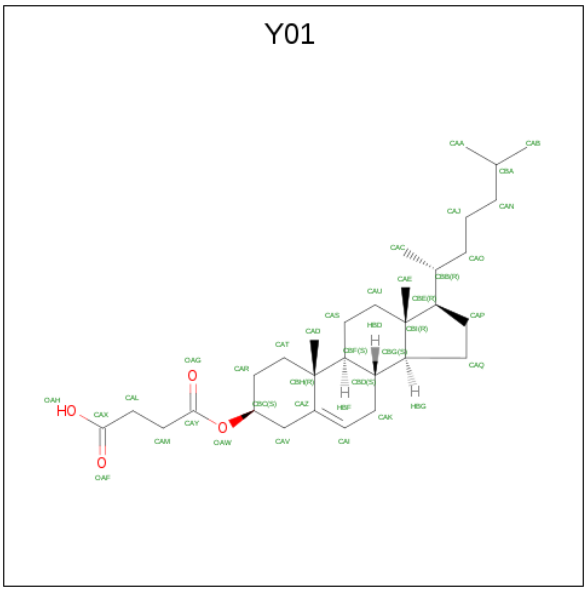
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLN	ASN	engineered mutation	UNP P11169
A	475	ALA	-	expression tag	UNP P11169
A	476	GLU	-	expression tag	UNP P11169
A	477	ASN	-	expression tag	UNP P11169
A	478	LEU	-	expression tag	UNP P11169
A	479	TYR	-	expression tag	UNP P11169
A	480	PHE	-	expression 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 (three-letter code: 37X) (formula: $C_{27}H_{52}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 36 24 12	0	0
2	A	1	Total C O 39 27 12	0	0
2	A	1	Total C O 39 27 12	0	0
2	A	1	Total C O 39 27 12	0	0
2	A	1	Total C O 39 27 12	0	0
2	A	1	Total C O 39 27 12	0	0
2	B	1	Total C O 39 27 12	0	0
2	B	1	Total C O 39 27 12	0	0
2	B	1	Total C O 39 27 12	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



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

- Molecule 4 is water.

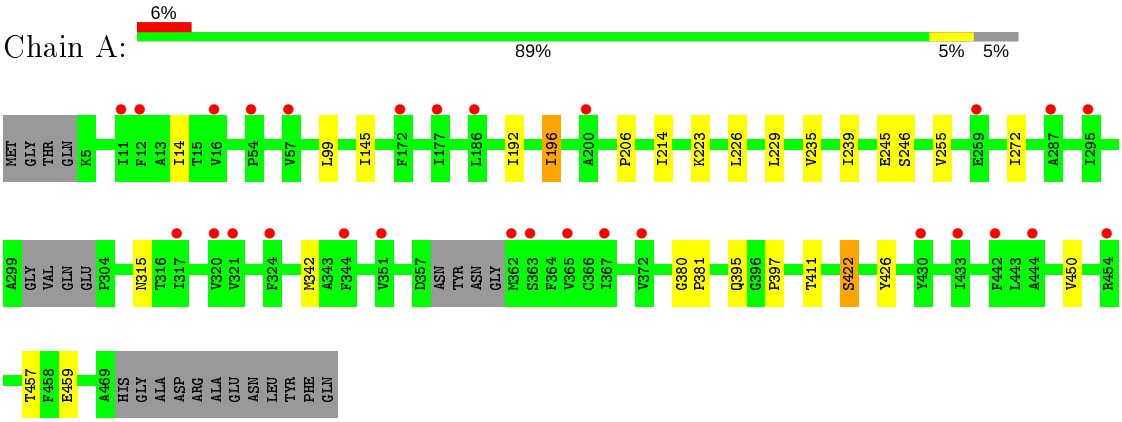
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

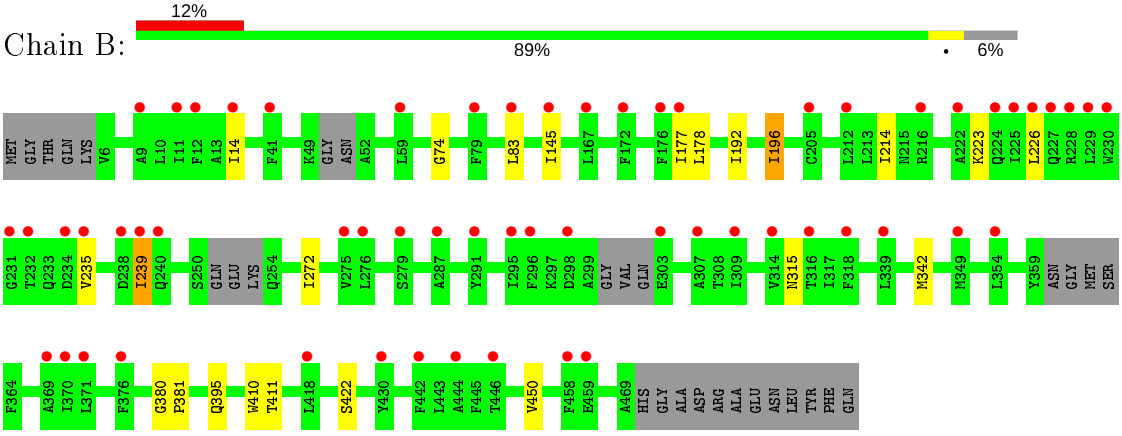
- Molecule 1: Solute carrier family 2, facilitated glucose transporter member 3

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

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 73.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.65) 99.8 (73.71-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.205 , 0.223 0.214 , 0.235	Depositor DCC
R_{free} test set	2006 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)	0.33 , 89.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.47	0/3519	0.60	0/4782
1	B	0.46	0/3413	0.60	0/4646
All	All	0.47	0/6932	0.60	0/9428

There are no bond length outliers.

There are no bond angle outliers.

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	A	3443	0	3502	16	0
1	B	3343	0	3324	13	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	27	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 (27) 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: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
1:B:223:LYS:HA	1:B:239:ILE:HD11	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%)	47	64
1	B	442/481 (92%)	433 (98%)	8 (2%)	1 (0%)	47	64
All	All	893/962 (93%)	874 (98%)	17 (2%)	2 (0%)	47	64

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%)	357 (99%)	4 (1%)	73	85
1	B	340/397 (86%)	336 (99%)	4 (1%)	71	84
All	All	701/794 (88%)	693 (99%)	8 (1%)	73	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ILE
1	A	245	GLU
1	A	315	ASN
1	A	422	SER
1	B	196	ILE
1	B	239	ILE
1	B	315	ASN
1	B	422	SER

Some 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	505	-	40,40,40	0.30	0	52,54,54	0.96	4 (7%)
2	37X	B	501	-	40,40,40	0.26	0	52,54,54	0.75	3 (5%)
2	37X	A	501	-	37,37,40	0.25	0	49,51,54	1.03	2 (4%)
2	37X	A	506	-	40,40,40	0.28	0	52,54,54	0.55	1 (1%)
2	37X	A	502	-	40,40,40	0.23	0	52,54,54	1.14	4 (7%)
3	Y01	B	504	-	35,38,38	0.39	0	54,57,57	0.48	0
2	37X	B	503	-	40,40,40	0.26	0	52,54,54	0.59	0
3	Y01	A	507	-	35,38,38	0.44	0	54,57,57	0.56	0
2	37X	A	504	-	40,40,40	0.32	0	52,54,54	0.70	1 (1%)
2	37X	A	503	-	40,40,40	0.24	0	52,54,54	0.65	2 (3%)
2	37X	B	502	-	40,40,40	0.25	0	52,54,54	0.61	2 (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
2	37X	A	505	-	-	13/30/70/70	0/2/2/2
2	37X	B	501	-	-	10/30/70/70	0/2/2/2
2	37X	A	501	-	-	8/27/67/70	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
3	Y01	B	504	-	-	6/17/77/77	0/4/4/4
2	37X	B	503	-	-	11/30/70/70	0/2/2/2
3	Y01	A	507	-	-	3/17/77/77	0/4/4/4
2	37X	A	504	-	-	7/30/70/70	0/2/2/2
2	37X	A	503	-	-	6/30/70/70	0/2/2/2
2	37X	B	502	-	-	7/30/70/70	0/2/2/2

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	37X	CBS-O1-C1	4.67	125.49	113.36
2	A	501	37X	CBS-O1-C1	4.30	124.55	113.36
2	A	502	37X	CBQ-CCM-CBS	4.04	118.98	109.40
2	A	501	37X	CBT-OBV-CCJ	3.78	123.19	113.36
2	A	505	37X	CBT-CCM-CBS	-3.67	90.89	109.57
2	A	502	37X	CBT-OBV-CCJ	3.32	121.98	113.36
2	A	505	37X	CBT-OBV-CCJ	3.15	121.56	113.36
2	A	503	37X	CBT-OBV-CCJ	3.08	121.37	113.36
2	B	501	37X	CBS-O1-C1	3.05	121.30	113.36
2	A	502	37X	CBR-CCM-CBQ	-3.03	104.29	109.97
2	A	504	37X	CBS-O1-C1	3.01	121.19	113.36
2	A	505	37X	CBQ-CCM-CBT	2.91	116.29	109.40
2	A	506	37X	CBS-O1-C1	2.43	119.69	113.36
2	B	502	37X	CBT-OBV-CCJ	2.40	119.60	113.36
2	A	503	37X	CBS-O1-C1	2.39	119.57	113.36
2	A	505	37X	CBS-O1-C1	2.19	119.07	113.36
2	B	502	37X	CBS-O1-C1	2.17	118.99	113.36
2	B	501	37X	CBT-CCM-CBS	2.07	120.11	109.57
2	B	501	37X	CBQ-CCM-CBT	-2.07	104.50	109.40

There are no chirality outliers.

All (86) torsion outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atoms
3	B	504	Y01	CAL-CAM-CAY-OAG

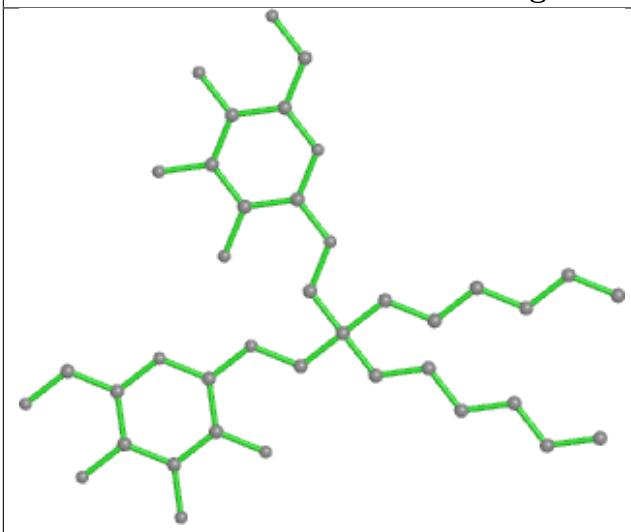
There are no ring outliers.

4 monomers are involved in 6 short contacts:

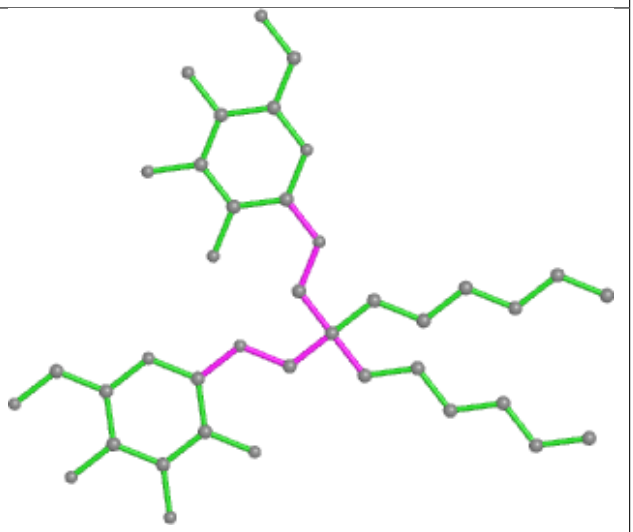
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	37X	2	0
3	B	504	Y01	1	0
2	B	503	37X	2	0
3	A	507	Y01	1	0

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 then 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.

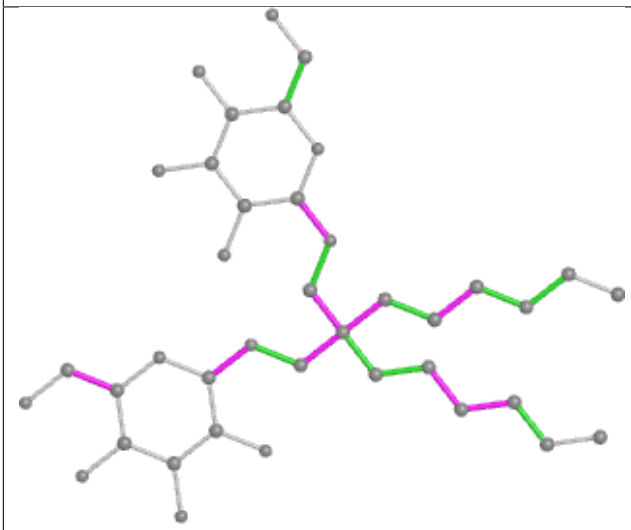
Ligand 37X A 505



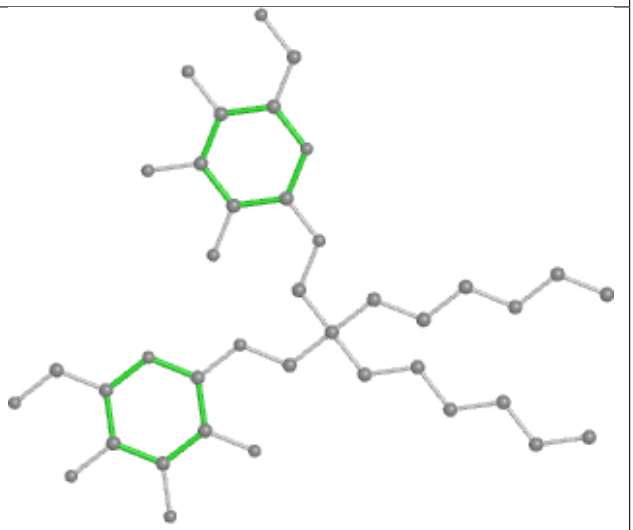
Bond lengths



Bond angles

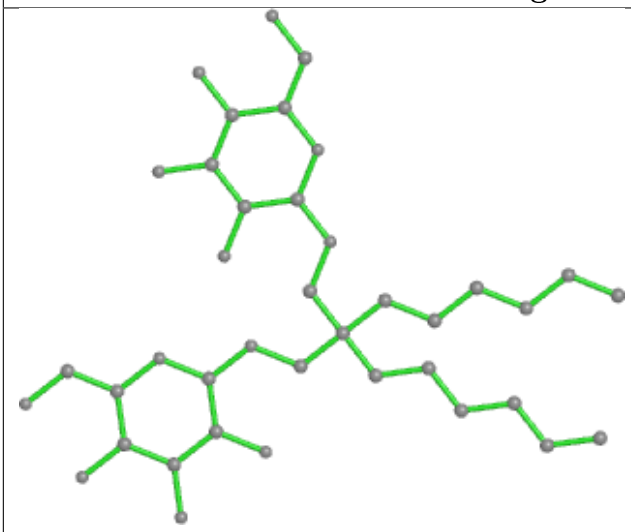


Torsions

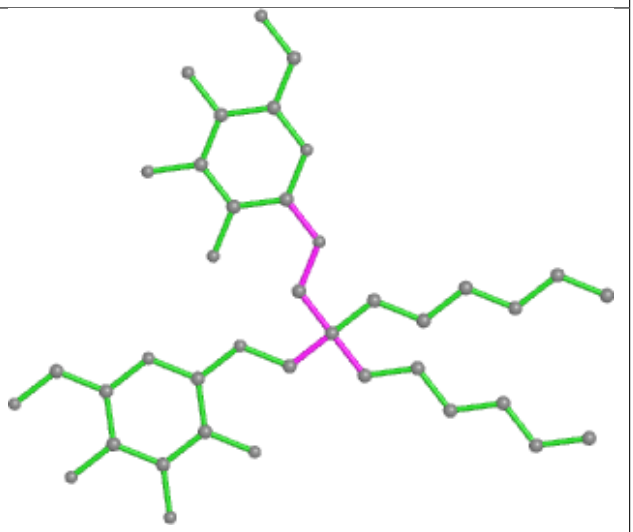


Rings

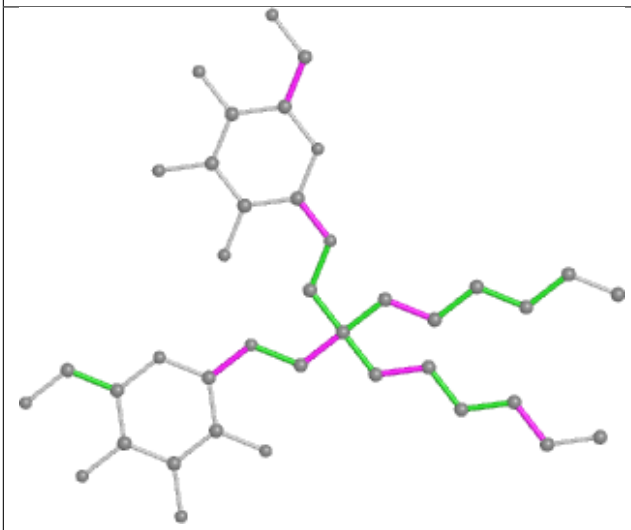
Ligand 37X B 501



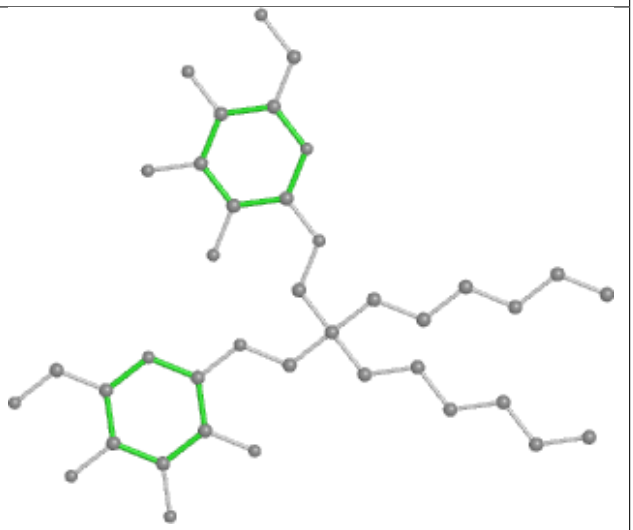
Bond lengths



Bond angles

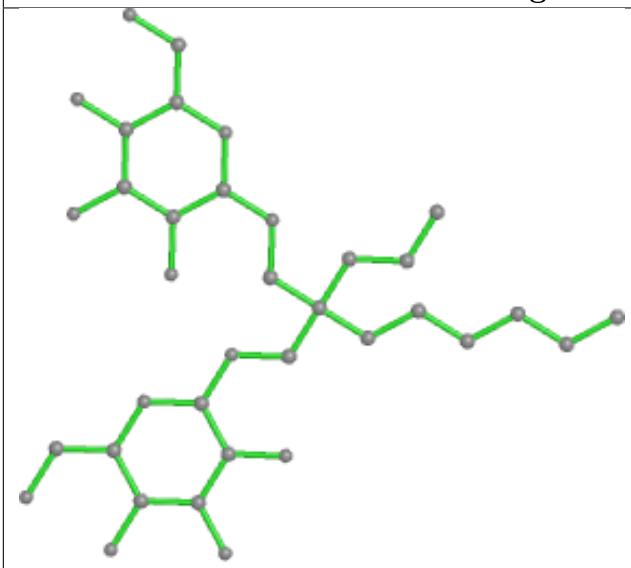


Torsions

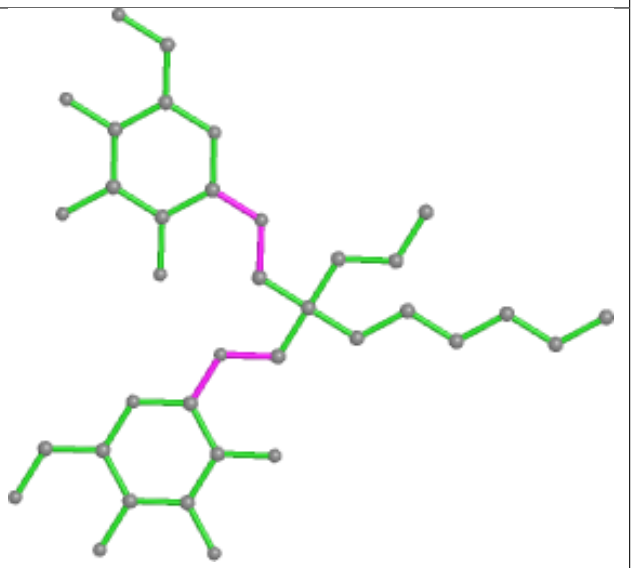


Rings

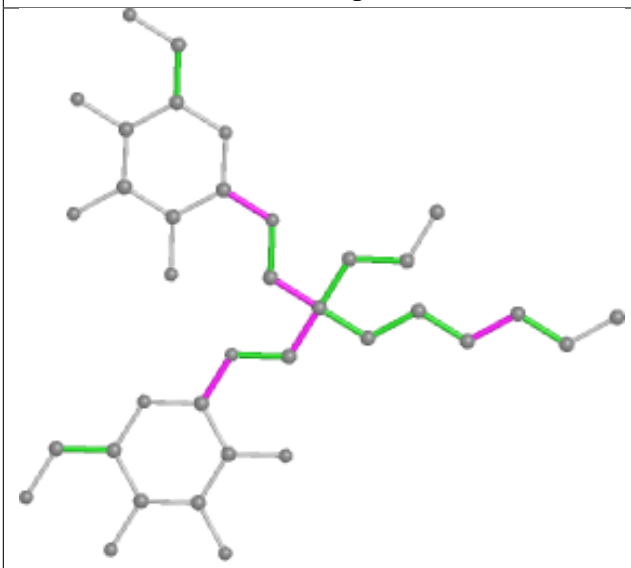
Ligand 37X A 501



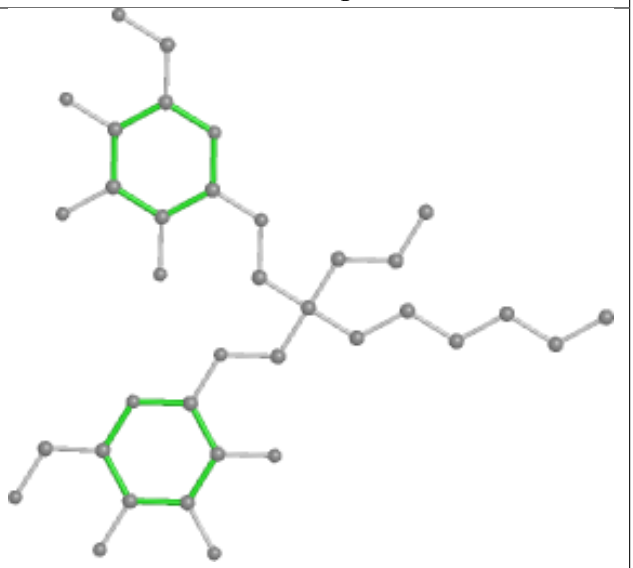
Bond lengths



Bond angles

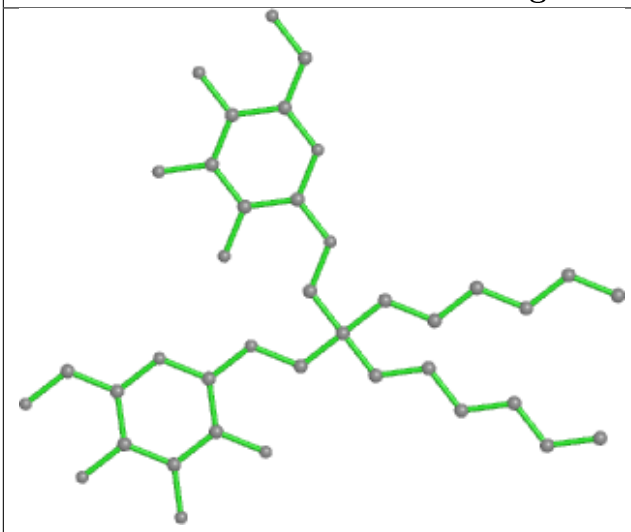


Torsions

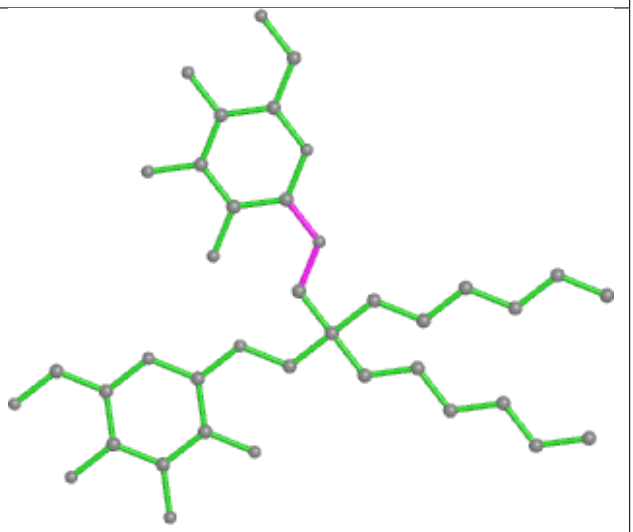


Rings

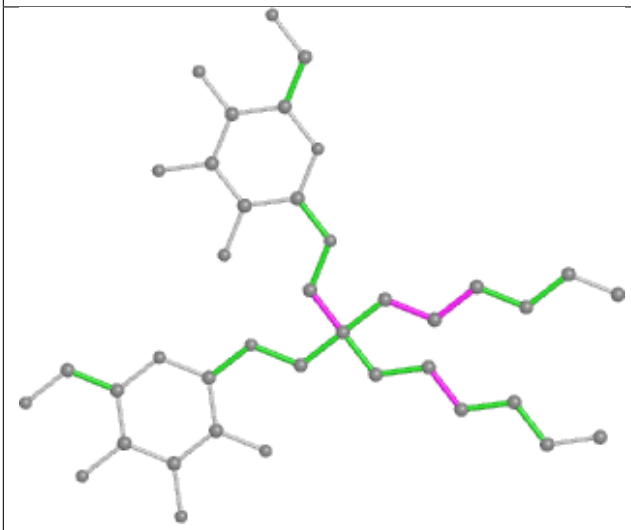
Ligand 37X A 506



Bond lengths



Bond angles



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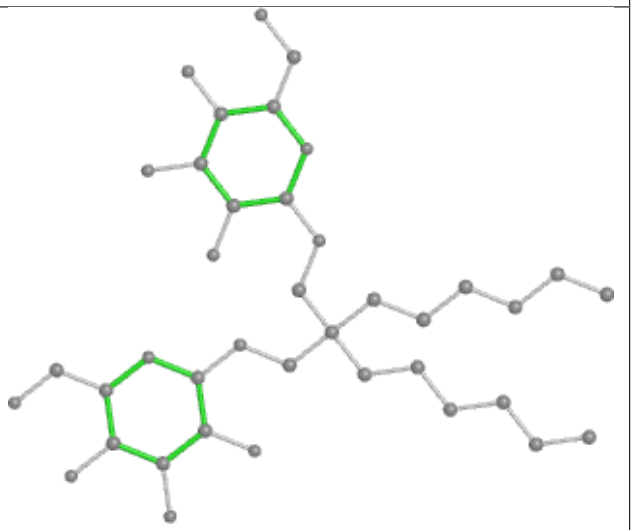
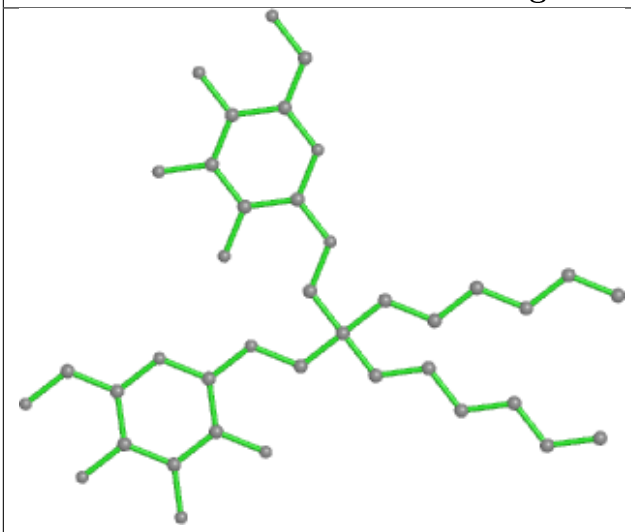
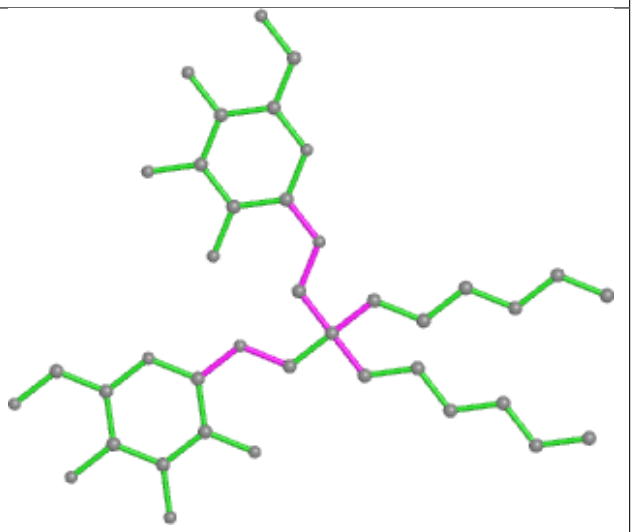


Rings

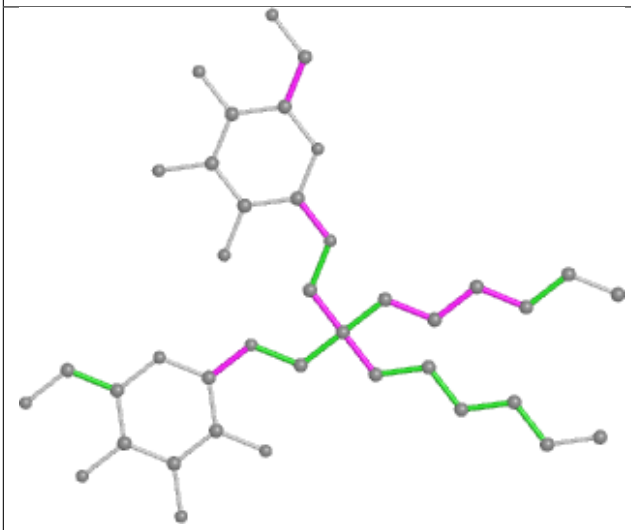
Ligand 37X A 502



Bond lengths



Bond angles



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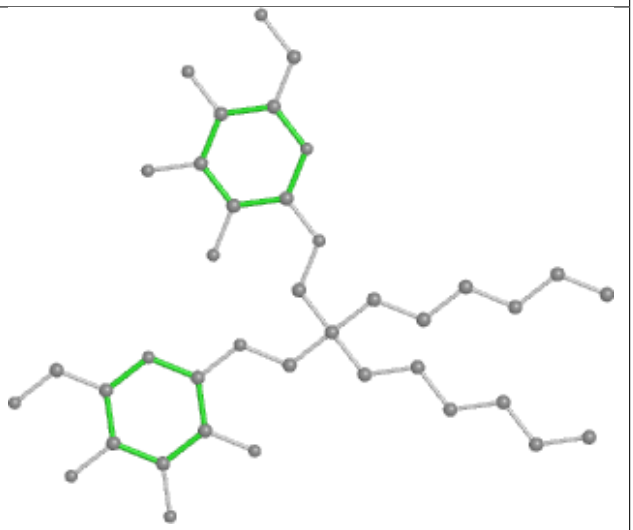
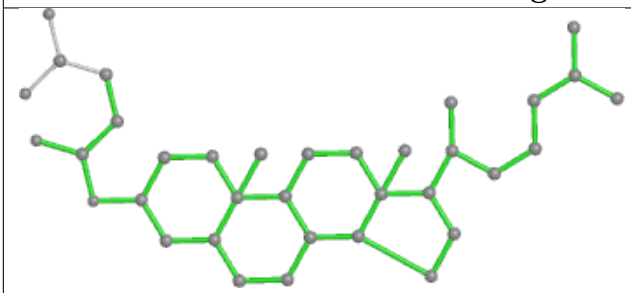
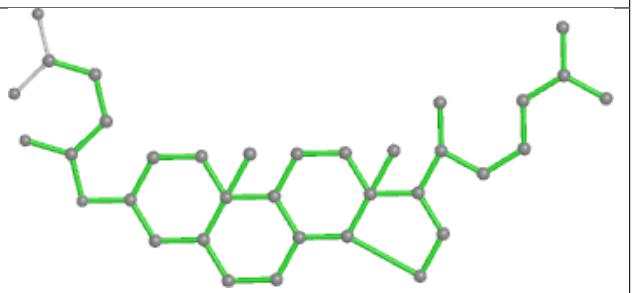


Rings

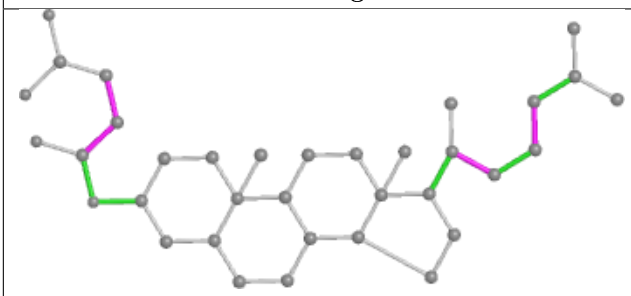
Ligand Y01 B 504



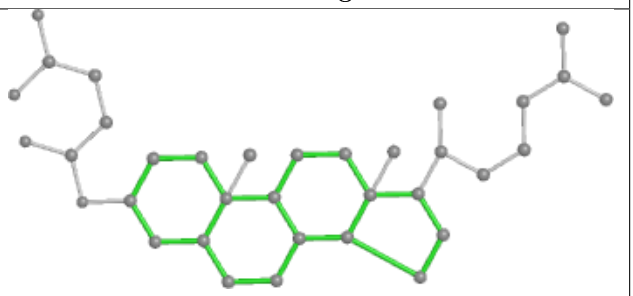
Bond lengths



Bond angles

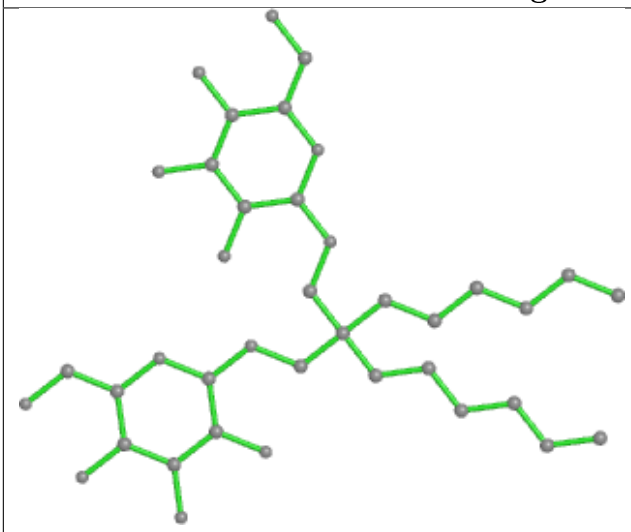


Torsions

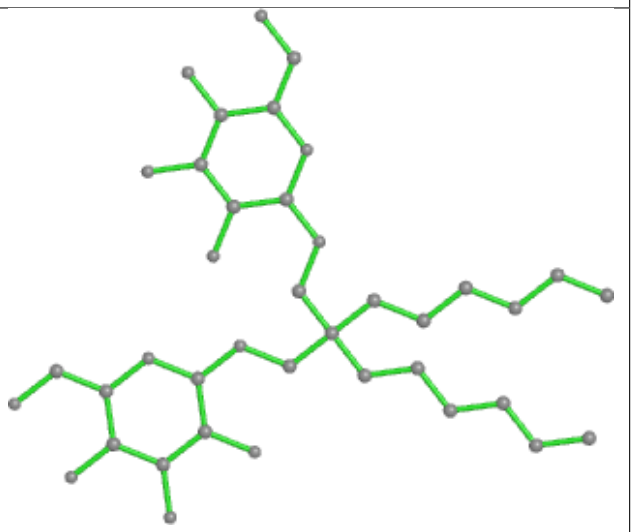


Rings

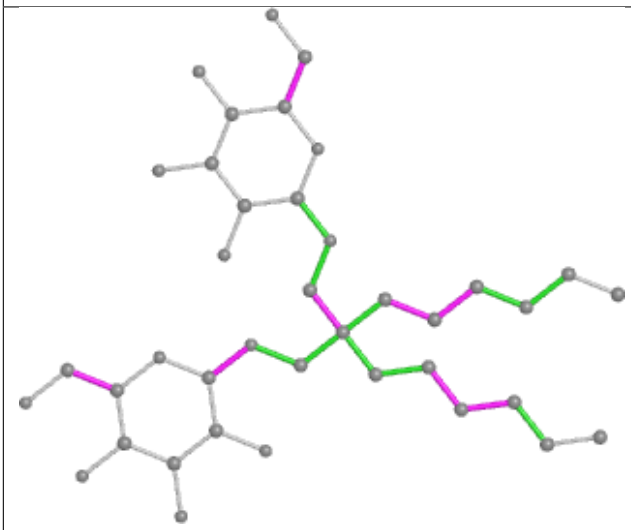
Ligand 37X B 503



Bond lengths



Bond angles



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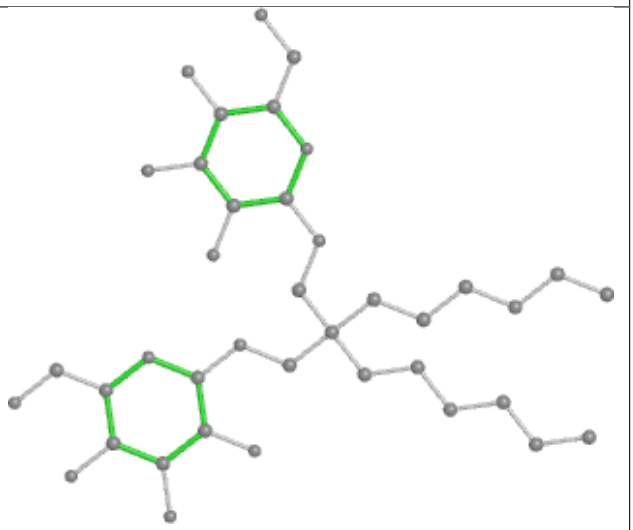
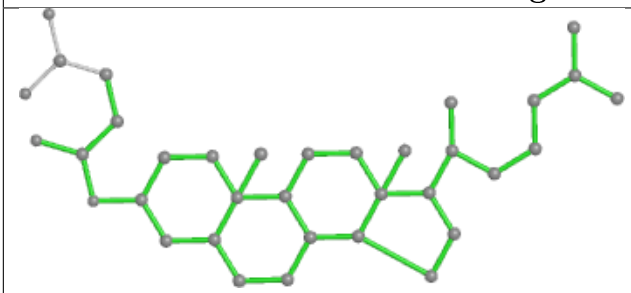
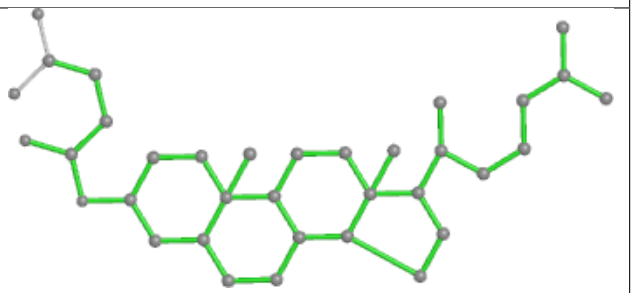


Rings

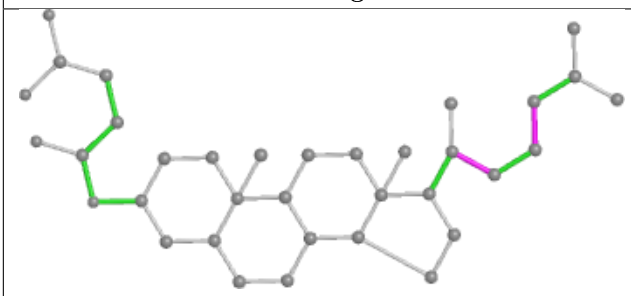
Ligand Y01 A 507



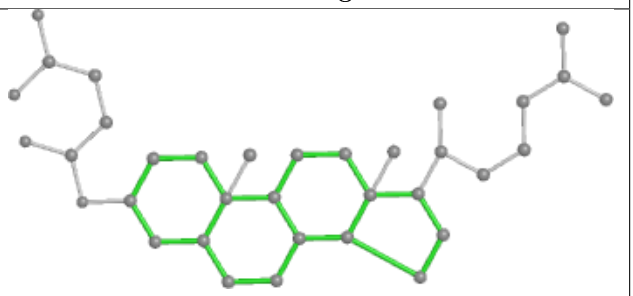
Bond lengths



Bond angles

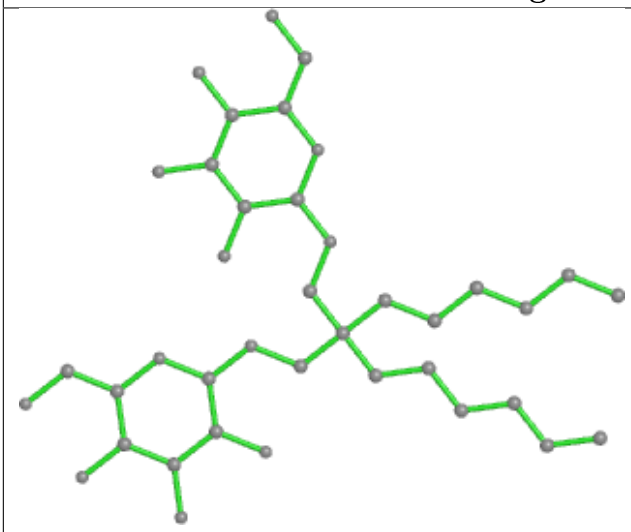


Torsions

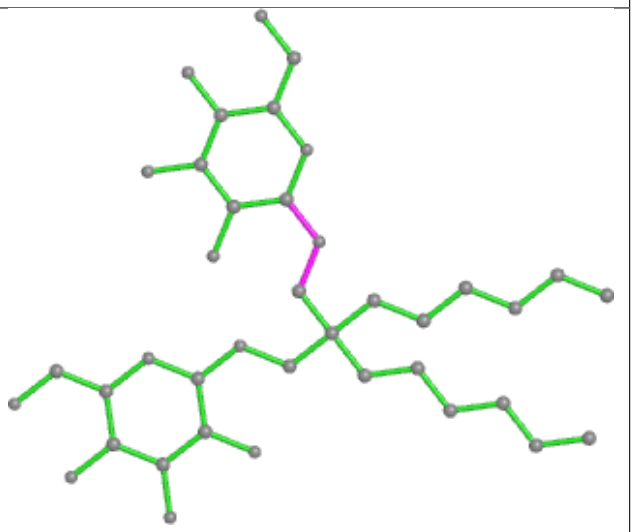


Rings

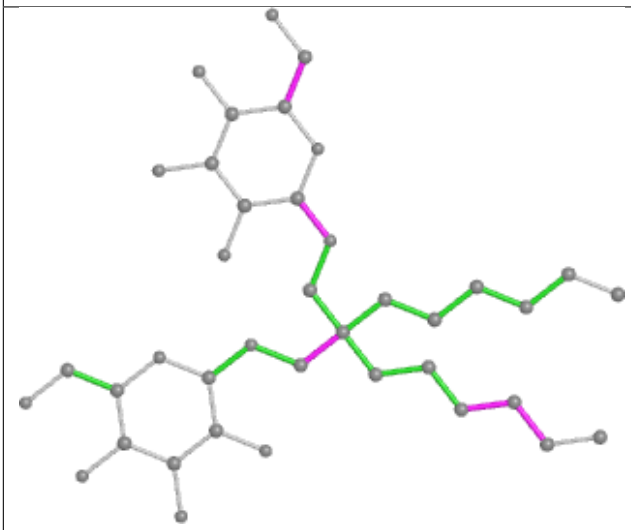
Ligand 37X A 504



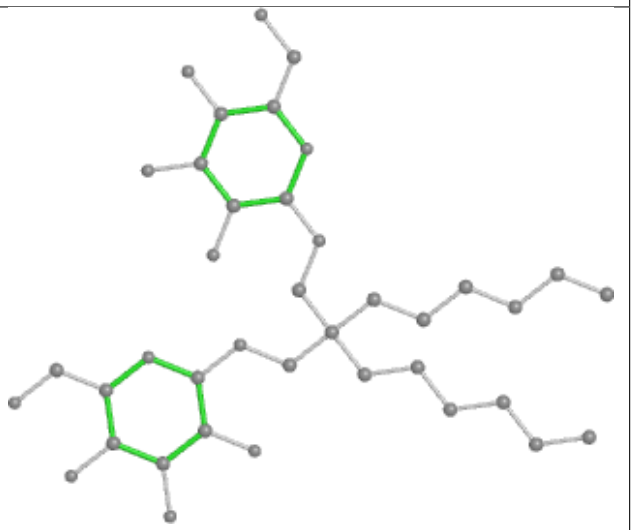
Bond lengths



Bond angles

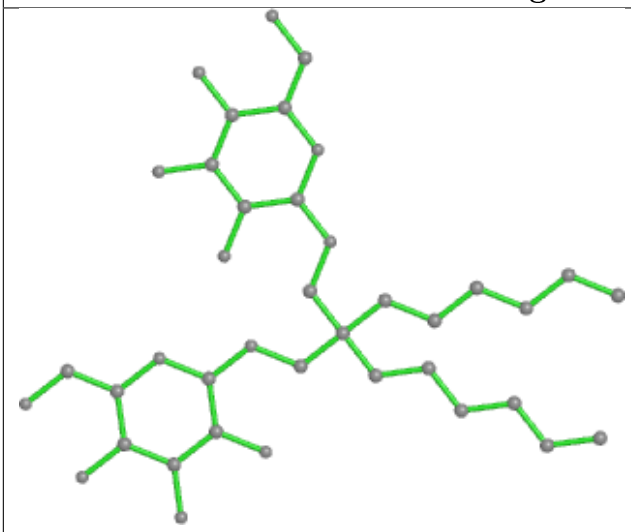


Torsions

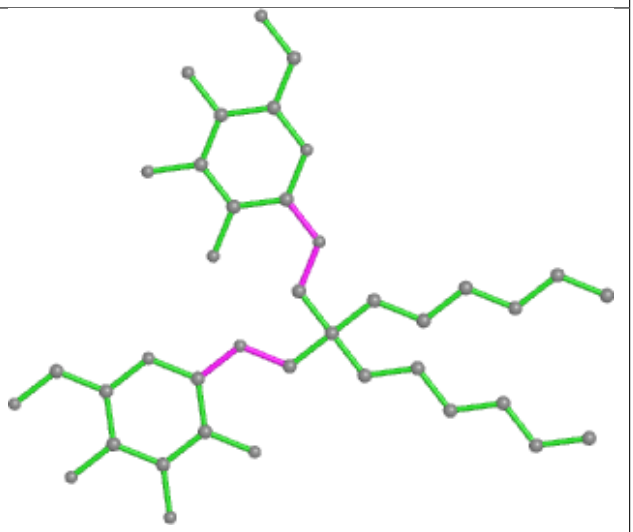


Rings

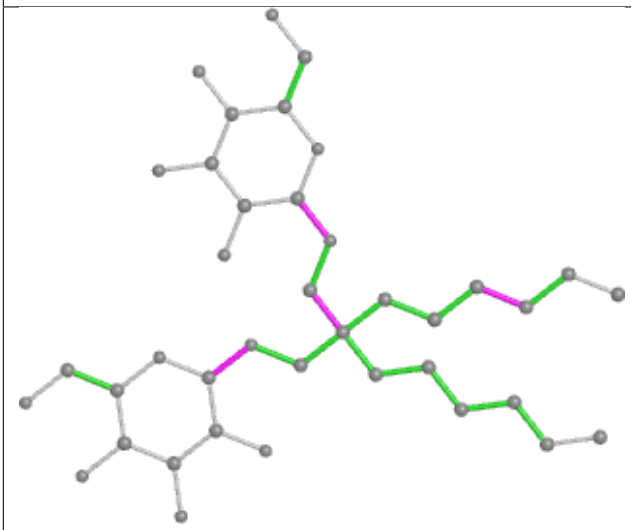
Ligand 37X A 503



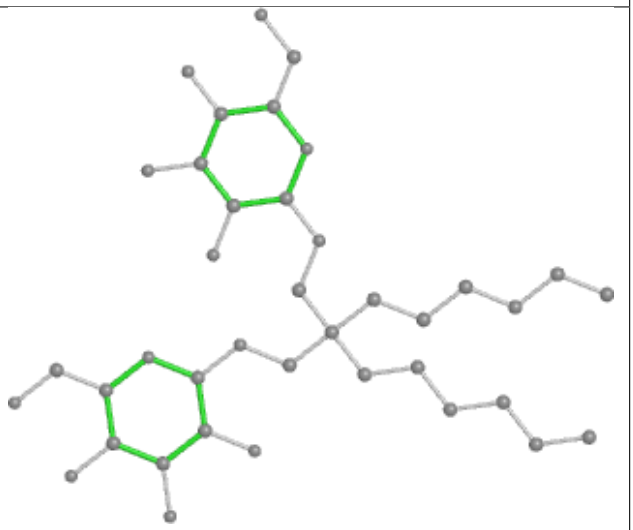
Bond lengths



Bond angles

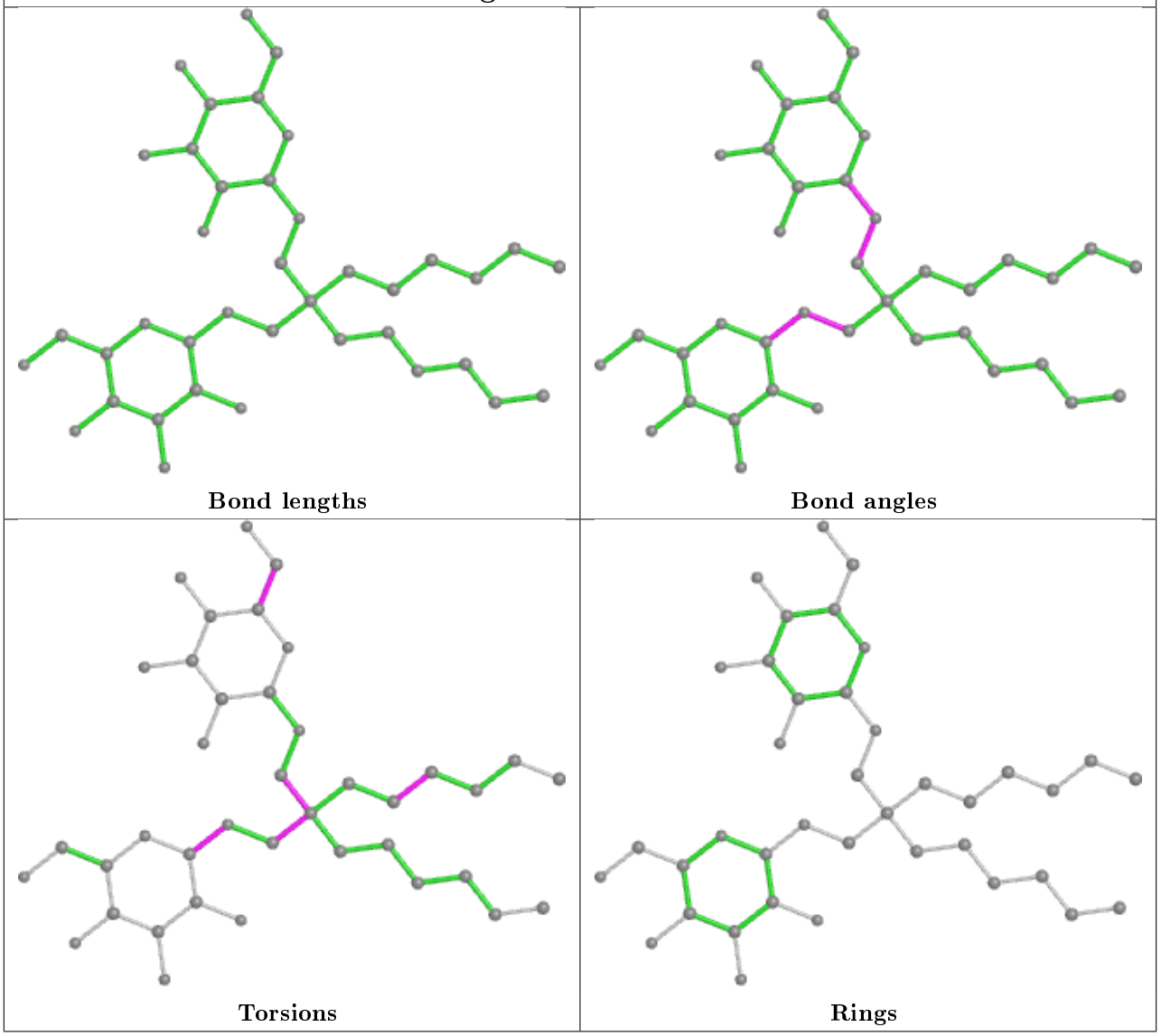


Torsions



Rings

Ligand 37X B 502



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

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, 95^{th} 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%)	0.69	28 (6%) 21 18	61, 88, 133, 181	0
1	B	452/481 (93%)	0.81	59 (13%) 3 2	66, 108, 164, 220	0
All	All	909/962 (94%)	0.75	87 (9%) 8 6	61, 96, 152, 220	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	VAL	6.5
1	B	442	PHE	5.9
1	B	295	ILE	5.6
1	A	363	SER	5.1
1	B	83	LEU	5.0
1	B	225	ILE	4.9
1	B	239	ILE	4.8
1	A	324	PHE	4.8
1	B	430	TYR	4.3
1	A	362	MET	4.2
1	B	176	PHE	4.0
1	B	177	ILE	3.9
1	A	177	ILE	3.9
1	A	57	VAL	3.9
1	B	369	ALA	3.9
1	A	351	VAL	3.6
1	B	291	TYR	3.6
1	B	226	LEU	3.5
1	B	12	PHE	3.5
1	B	231	GLY	3.4
1	B	232	THR	3.4
1	B	228	ARG	3.4
1	B	418	LEU	3.4
1	B	446	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	318	PHE	3.3
1	B	11	ILE	3.3
1	A	430	TYR	3.2
1	B	275	VAL	3.2
1	B	234	ASP	3.2
1	B	9	ALA	3.2
1	A	12	PHE	3.0
1	B	354	LEU	3.0
1	B	238	ASP	3.0
1	A	200	ALA	3.0
1	B	459	GLU	3.0
1	A	444	ALA	2.9
1	B	316	THR	2.9
1	B	205	CYS	2.9
1	A	11	ILE	2.8
1	A	295	ILE	2.8
1	A	367	ILE	2.8
1	B	309	ILE	2.8
1	B	444	ALA	2.8
1	A	16	VAL	2.7
1	B	172	PHE	2.7
1	B	279	SER	2.7
1	A	317	ILE	2.6
1	A	344	PHE	2.6
1	A	365	VAL	2.6
1	B	212	LEU	2.6
1	B	240	GLN	2.6
1	B	376	PHE	2.6
1	B	216	ARG	2.5
1	B	307	ALA	2.5
1	B	303	GLU	2.5
1	A	320	VAL	2.4
1	B	296	PHE	2.4
1	B	79	PHE	2.4
1	B	229	LEU	2.4
1	B	145	ILE	2.4
1	B	298	ASP	2.3
1	B	458	PHE	2.3
1	A	54	PRO	2.3
1	B	287	ALA	2.3
1	B	370	ILE	2.3
1	B	222	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	349	MET	2.3
1	A	287	ALA	2.3
1	A	442	PHE	2.2
1	A	321	VAL	2.2
1	B	224	GLN	2.2
1	B	227	GLN	2.1
1	A	259	GLU	2.1
1	B	14	ILE	2.1
1	B	41	PHE	2.1
1	B	59	LEU	2.1
1	B	276	LEU	2.1
1	B	339	LEU	2.1
1	A	186	LEU	2.1
1	B	314	VAL	2.1
1	A	172	PHE	2.1
1	A	454	ARG	2.1
1	B	167	LEU	2.1
1	A	372	VAL	2.1
1	B	371	LEU	2.0
1	A	433	ILE	2.0
1	B	230	TRP	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 carbohydrates 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, 95^{th} 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	0.50	0.40	123,158,161,161	0
3	Y01	B	504	35/35	0.76	0.34	142,151,158,159	0

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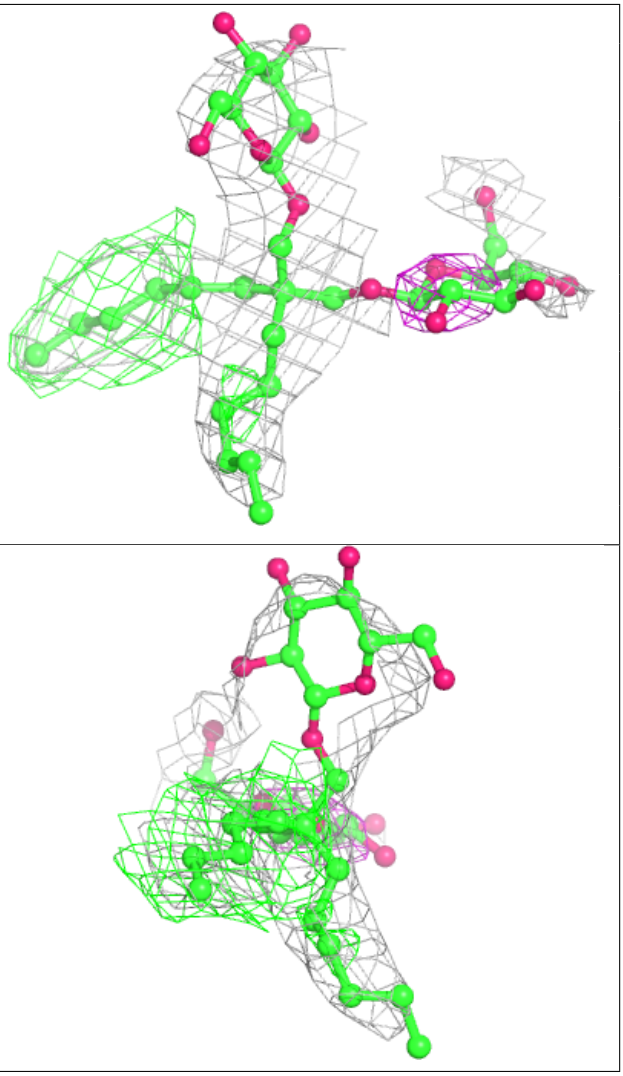
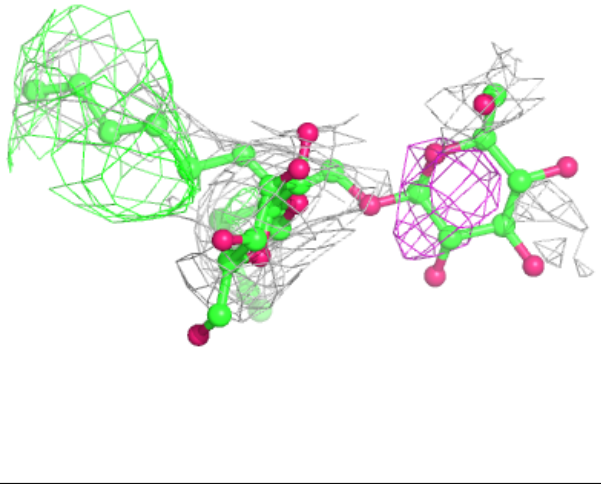
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	Y01	A	507	35/35	0.79	0.37	122,130,140,142	0
2	37X	A	504	39/39	0.80	0.31	101,137,144,147	0
2	37X	A	503	39/39	0.80	0.44	98,119,145,146	0
2	37X	B	503	39/39	0.82	0.28	110,136,153,154	0
2	37X	A	505	39/39	0.83	0.27	103,112,128,130	0
2	37X	B	502	39/39	0.85	0.26	115,148,153,154	0
2	37X	A	502	39/39	0.87	0.29	95,101,116,118	0
2	37X	A	501	36/39	0.89	0.22	86,95,106,112	0
2	37X	B	501	39/39	0.91	0.28	94,99,102,108	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:

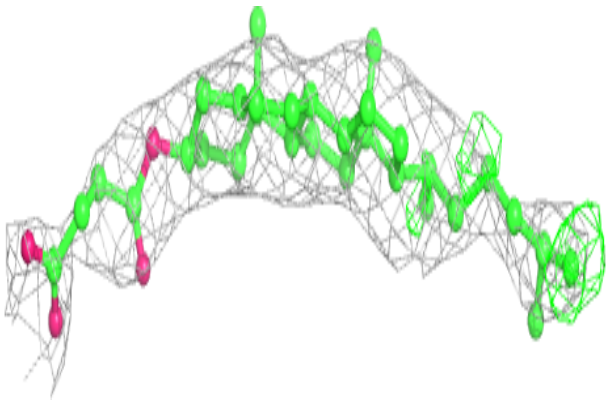
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

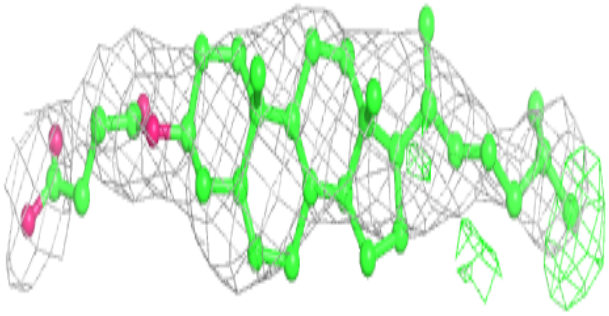


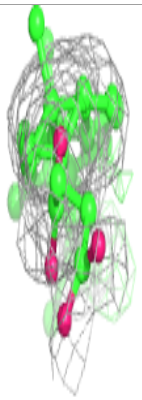


Electron density around Y01 B 504:

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

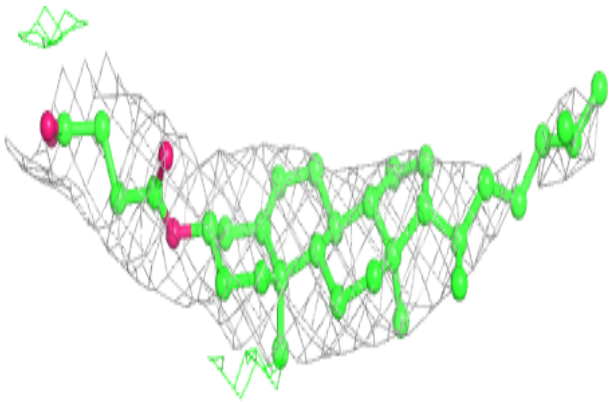


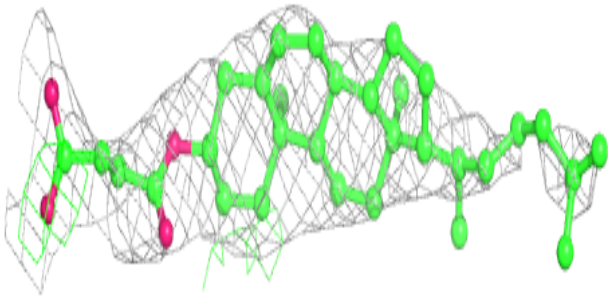




Electron density around Y01 A 507:

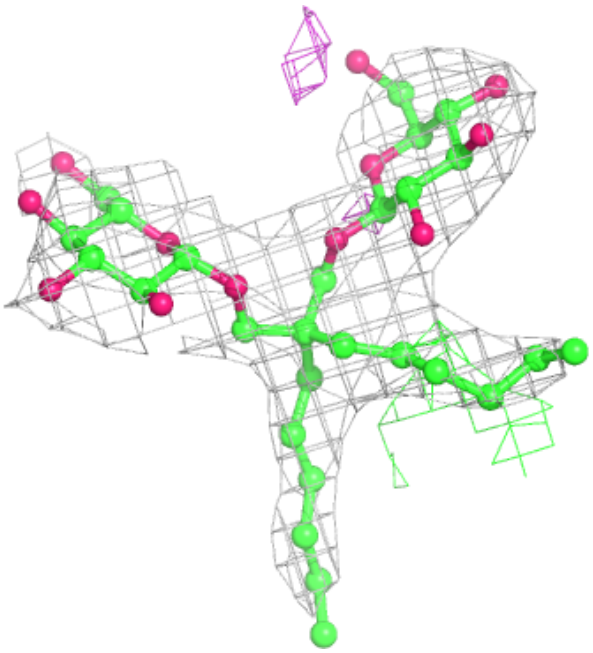
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

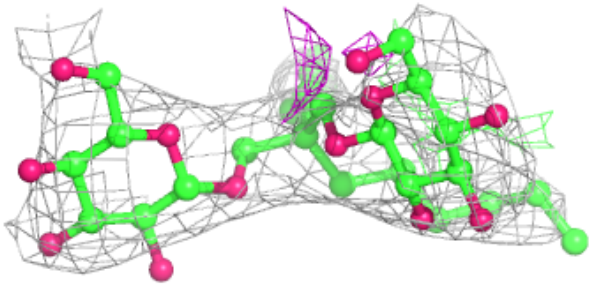


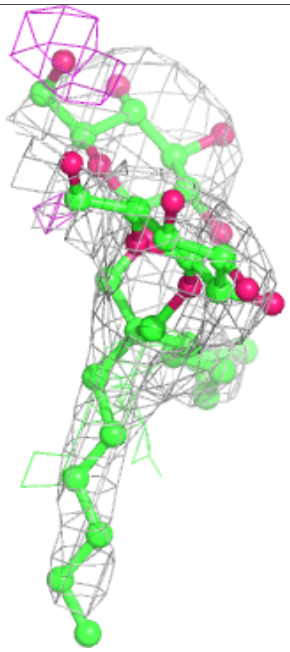


Electron density around 37X A 504:

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

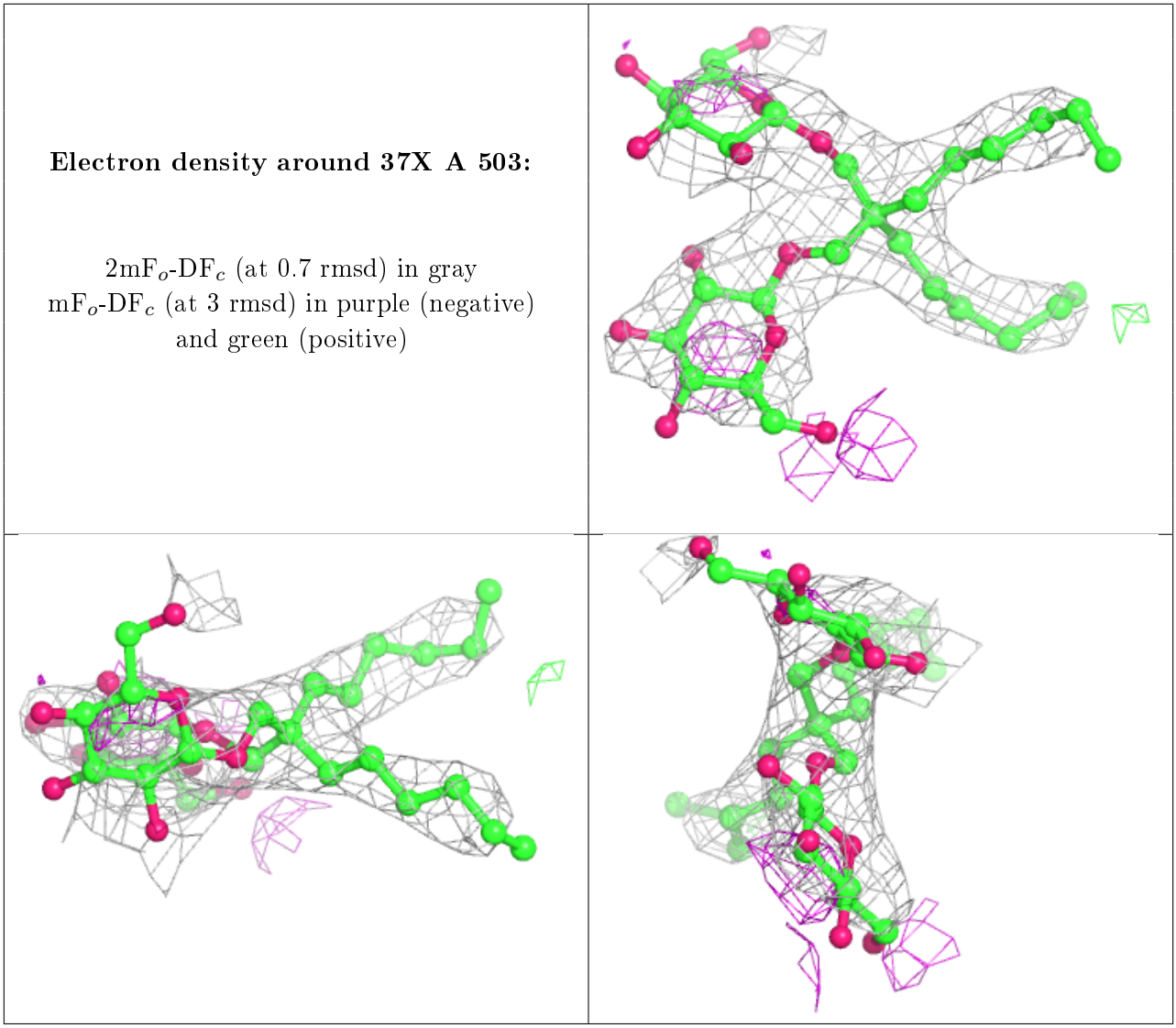






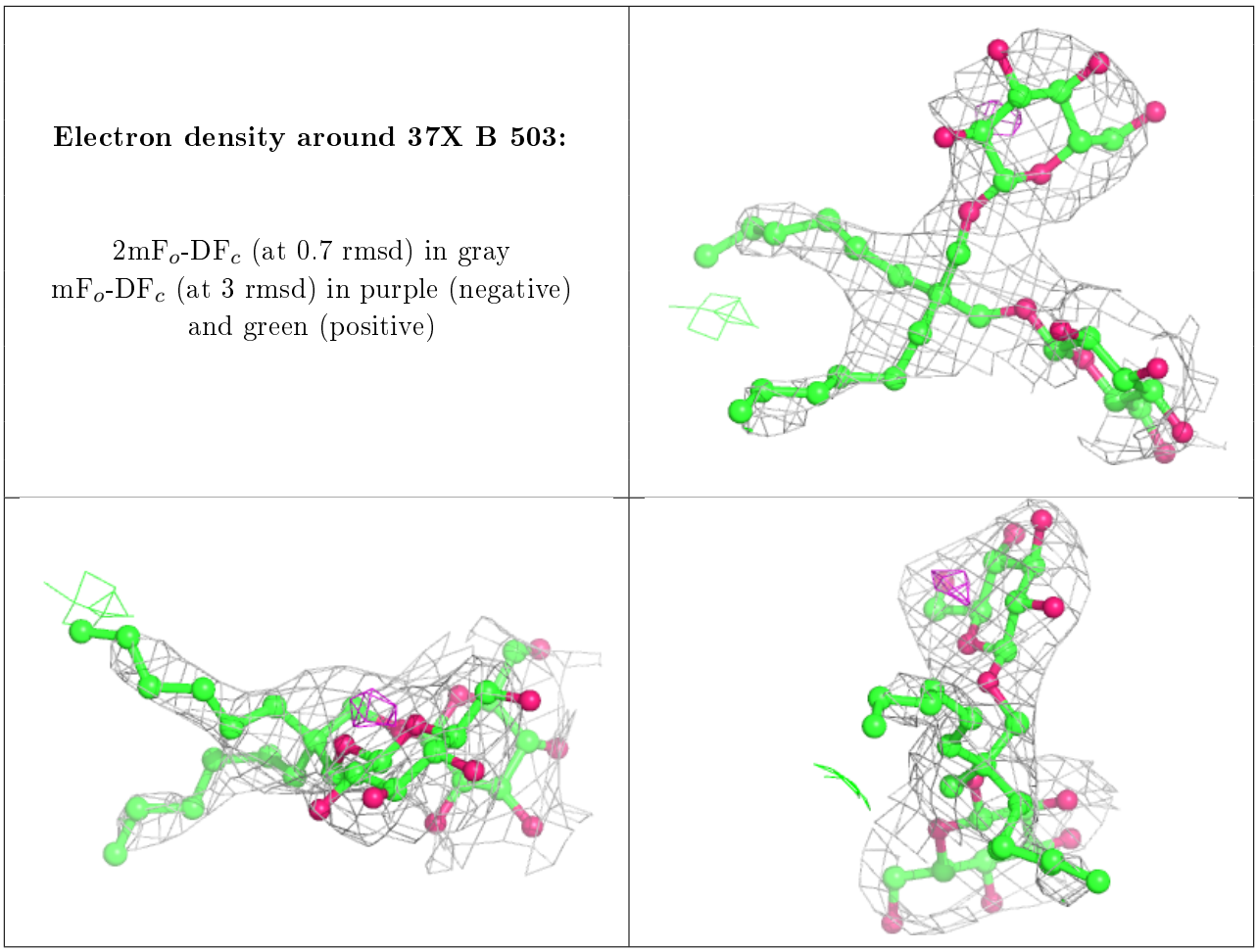
Electron density around 37X A 503:

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



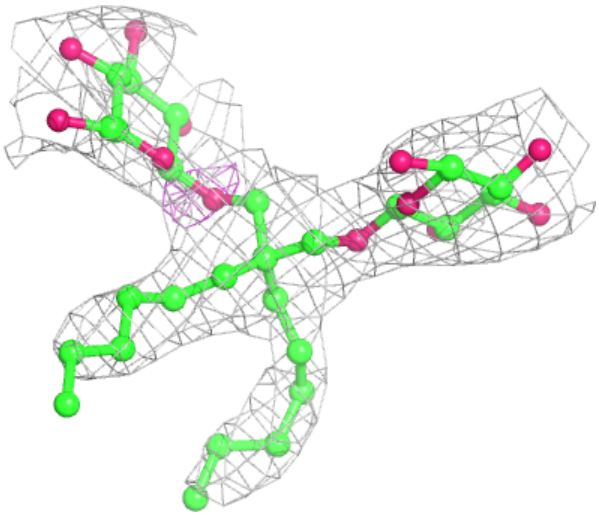
Electron density around 37X B 503:

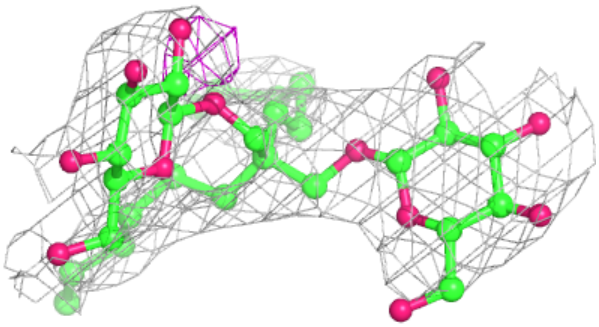
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

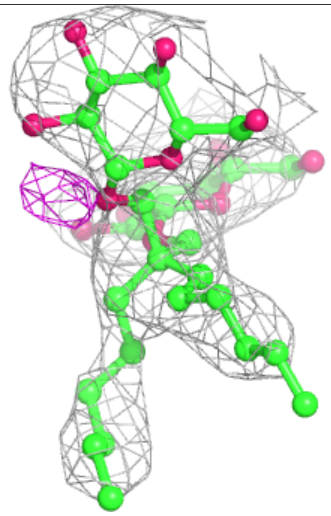


Electron density around 37X A 505:

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

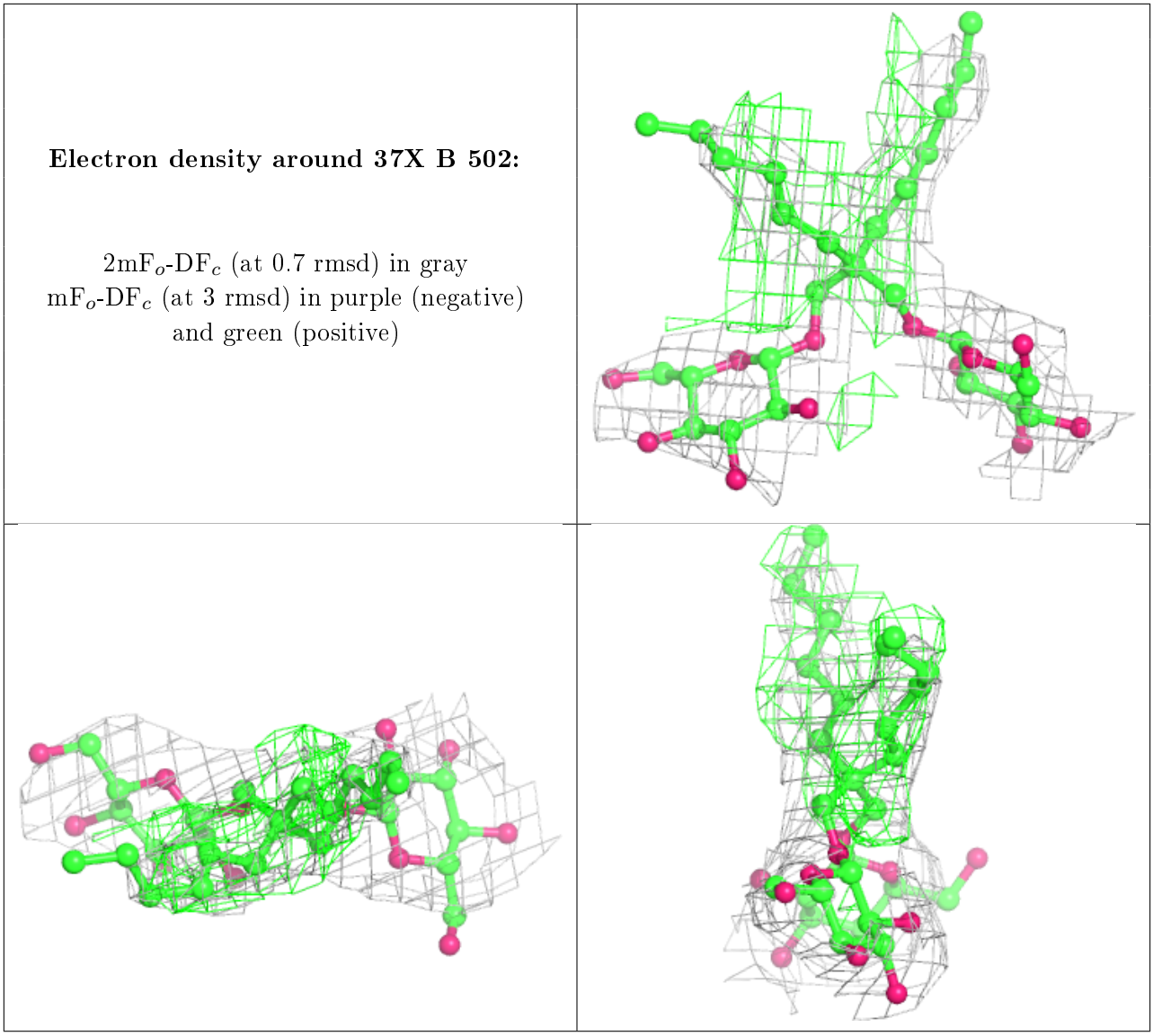






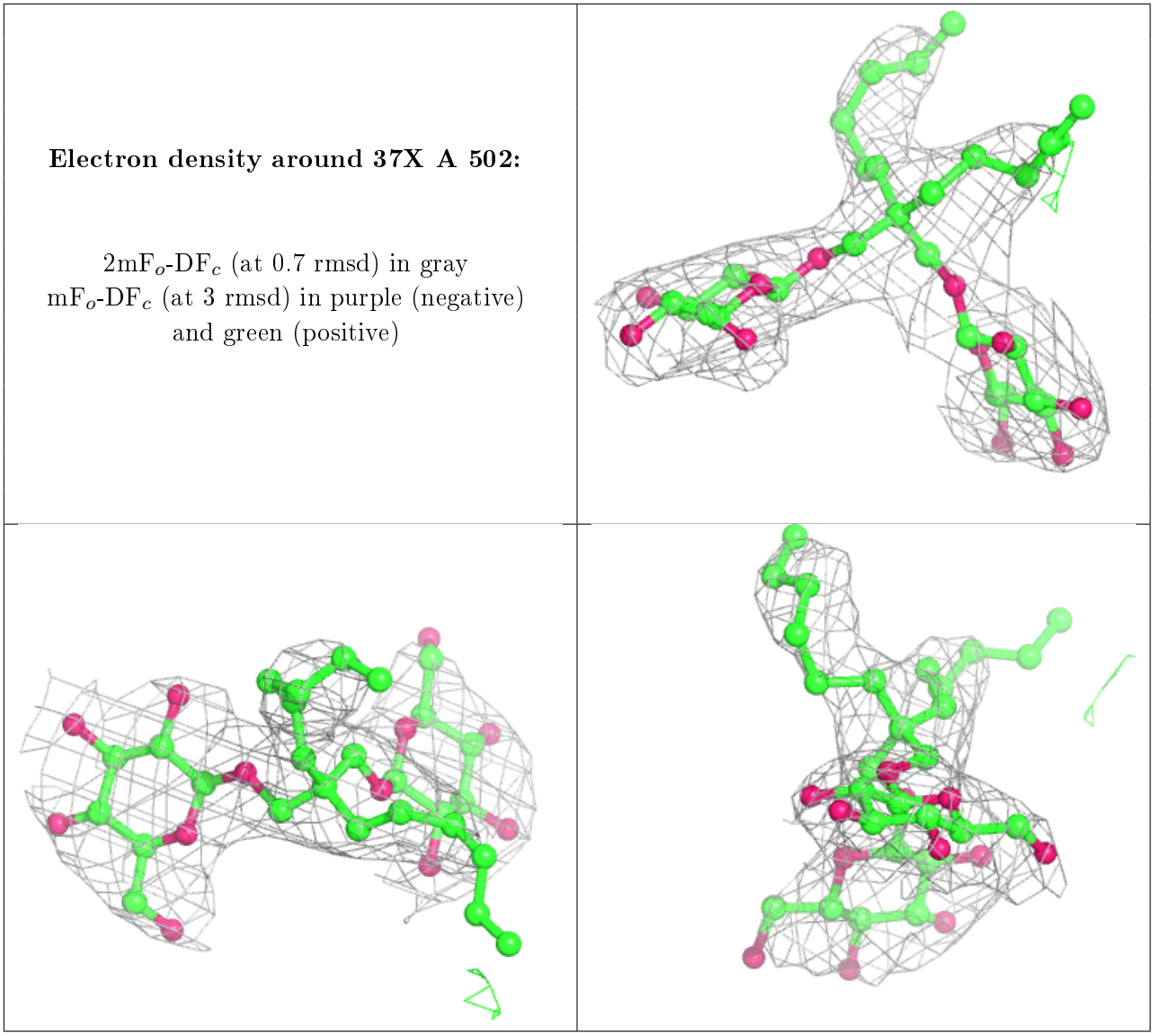
Electron density around 37X B 502:

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



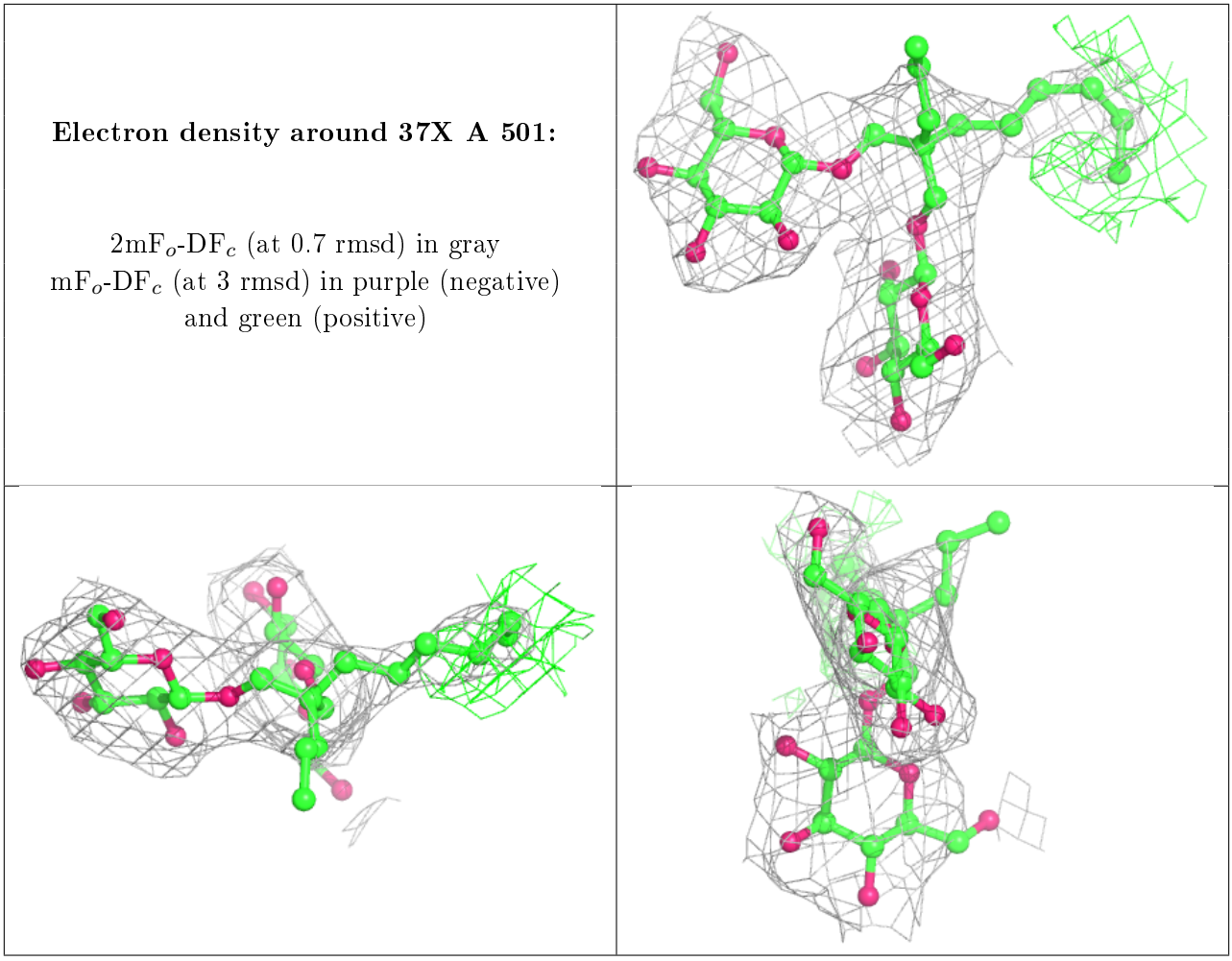
Electron density around 37X A 502:

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



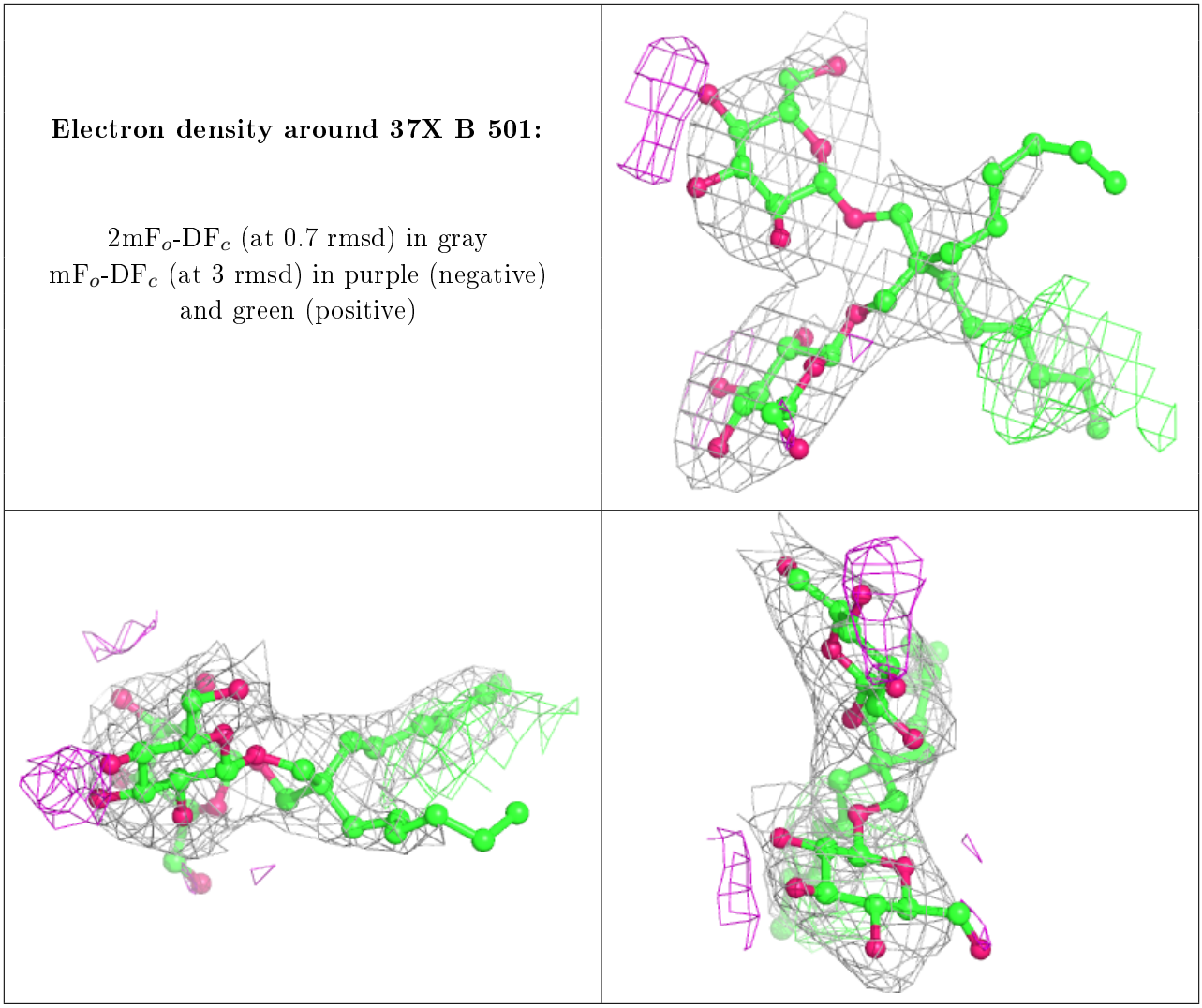
Electron density around 37X A 501:

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



Electron density around 37X B 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

There are no such residues in this entry.