wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2024 – 12:17 PM EDT

PDB ID	:	8SZN
Title	:	Crystal structure of Neisseria meningitidis ClpP protease in complex with phosphine oxide compound ACP6-12
Authors	:	Mabanglo, M.F.; Houry, W.A.
Deposited on	:	2023-05-30
Resolution	:	2.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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:

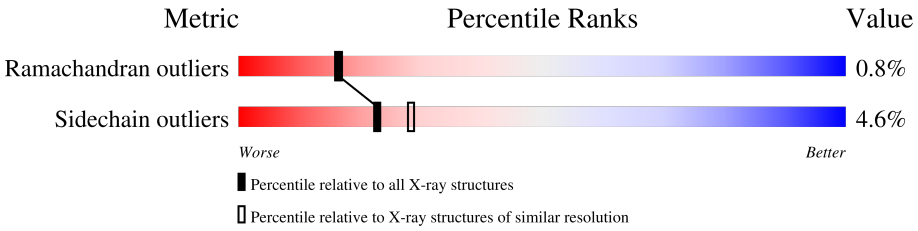
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.33 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))
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	204	89% · 8%
1	B	204	86% 5% 9%
1	C	204	88% · 9%
1	D	204	81% · 15%
1	E	204	78% 7% 14%
1	F	204	83% · 15%
1	G	204	84% 5% 11%
1	H	204	82% 6% 11%
1	I	204	86% 5% 9%

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Mol	Chain	Length	Quality of chain
1	J	204	
1	K	204	
1	L	204	
1	M	204	
1	N	204	
1	V	204	
1	W	204	
1	X	204	
1	Y	204	
1	Z	204	
1	a	204	
1	b	204	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31127 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	193	Total	C	N	O	S	0	0	0
			1504	947	259	290	8			
1	W	190	Total	C	N	O	S	0	0	0
			1478	927	256	287	8			
1	X	194	Total	C	N	O	S	0	0	0
			1508	949	260	291	8			
1	Y	181	Total	C	N	O	S	0	0	0
			1420	893	246	273	8			
1	Z	176	Total	C	N	O	S	0	0	0
			1373	864	235	266	8			
1	a	193	Total	C	N	O	S	0	0	0
			1504	947	259	290	8			
1	b	191	Total	C	N	O	S	0	0	0
			1490	938	257	287	8			
1	A	188	Total	C	N	O	S	0	0	0
			1475	930	254	283	8			
1	B	186	Total	C	N	O	S	0	0	0
			1448	915	248	277	8			
1	C	185	Total	C	N	O	S	0	0	0
			1441	911	244	278	8			
1	D	174	Total	C	N	O	S	0	0	0
			1363	859	233	263	8			
1	E	175	Total	C	N	O	S	0	0	0
			1367	861	234	264	8			
1	F	174	Total	C	N	O	S	0	0	0
			1362	858	233	263	8			
1	G	182	Total	C	N	O	S	0	0	0
			1414	892	241	273	8			
1	H	181	Total	C	N	O	S	0	0	0
			1417	899	240	270	8			
1	I	185	Total	C	N	O	S	0	0	0
			1440	911	244	277	8			

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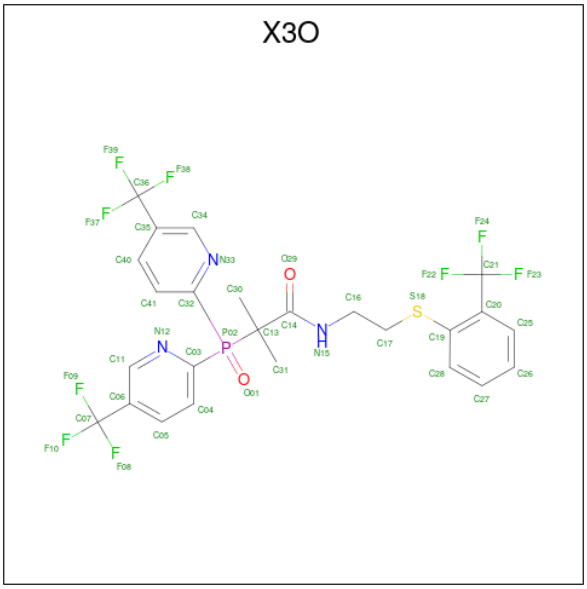
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	187	Total	C	N	O	S	0	0	0
			1457	922	247	280	8			
1	K	181	Total	C	N	O	S	0	0	0
			1418	899	240	271	8			
1	L	183	Total	C	N	O	S	0	0	0
			1429	905	240	276	8			
1	M	186	Total	C	N	O	S	0	0	0
			1456	920	249	279	8			
1	N	183	Total	C	N	O	S	0	0	0
			1430	906	242	274	8			

- Molecule 2 is 2-{bis[5-(trifluoromethyl)pyridin-2-yl]phosphoryl}-2-methyl-N-(2-{[2-(trifluoromethyl)phenyl]sulfanyl}ethyl)propanamide (three-letter code: X3O) (formula: $C_{25}H_{21}F_9N_3O_2PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	V	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	W	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	X	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	Z	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	a	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	b	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	H	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	J	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	L	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	M	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		
2	N	1	Total	C	F	N	O	P	S	0	0
			41	25	9	3	2	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	41	Total	O	0	0
			41	41		
3	W	19	Total	O	0	0
			19	19		
3	X	35	Total	O	0	0
			35	35		
3	Y	25	Total	O	0	0
			25	25		
3	Z	26	Total	O	0	0
			26	26		
3	a	32	Total	O	0	0
			32	32		
3	b	38	Total	O	0	0
			38	38		
3	A	44	Total	O	0	0
			44	44		
3	B	35	Total	O	0	0
			35	35		
3	C	16	Total	O	0	0
			16	16		
3	D	19	Total	O	0	0
			19	19		
3	E	14	Total	O	0	0
			14	14		
3	F	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	30	Total O 30 30	0	0
3	H	14	Total O 14 14	0	0
3	I	9	Total O 9 9	0	0
3	J	10	Total O 10 10	0	0
3	K	13	Total O 13 13	0	0
3	L	7	Total O 7 7	0	0
3	M	14	Total O 14 14	0	0
3	N	21	Total O 21 21	0	0

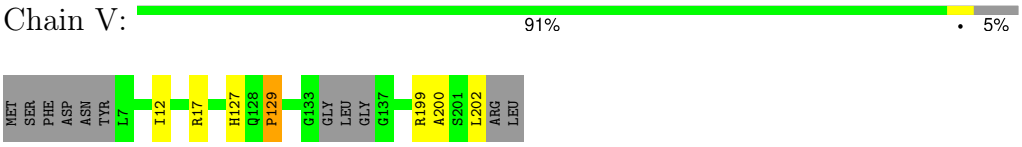
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

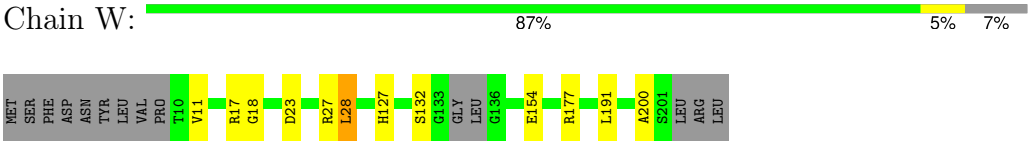
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



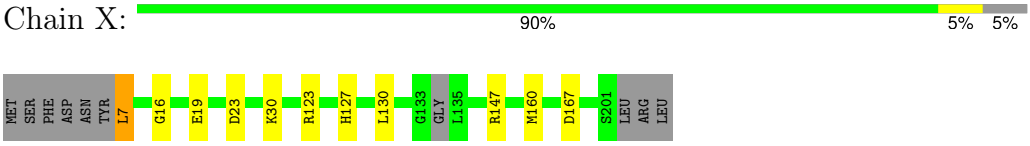
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



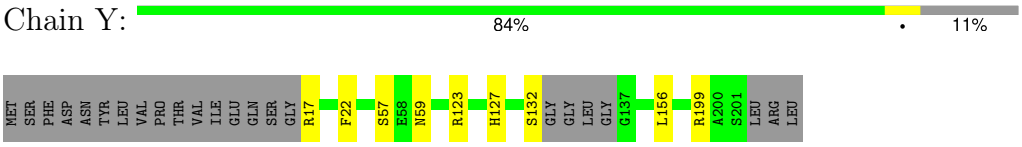
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



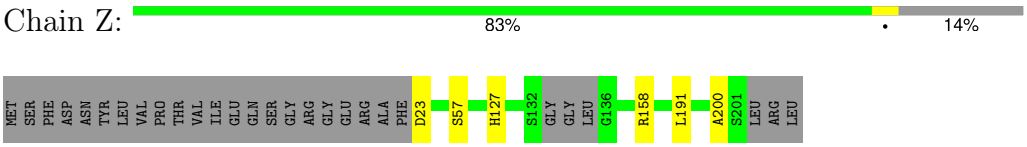
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



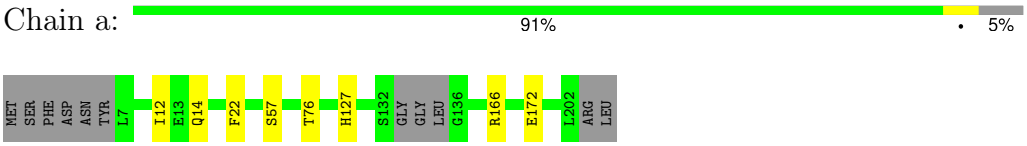
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



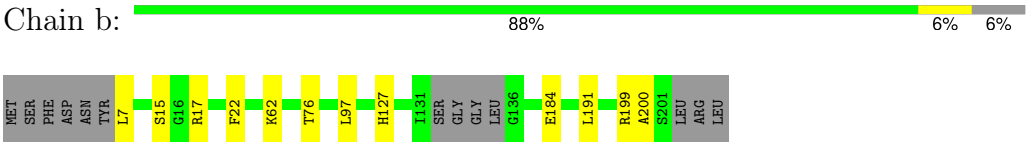
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



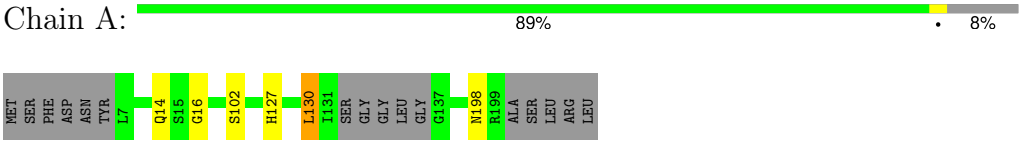
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:



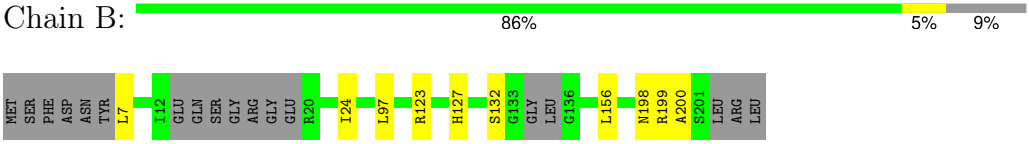
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



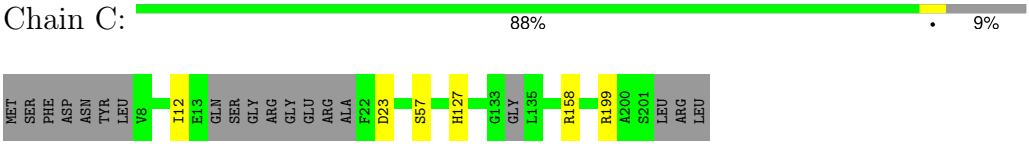
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



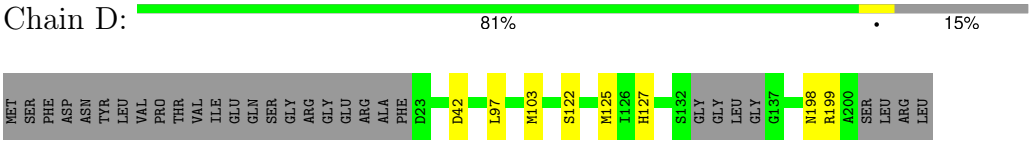
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



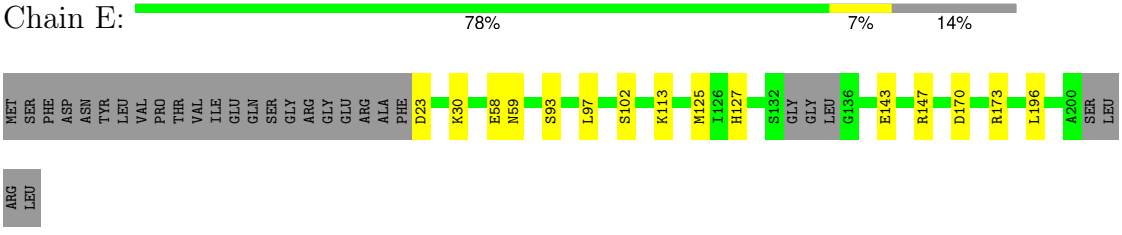
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



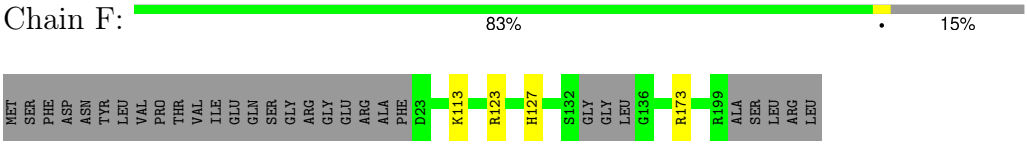
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



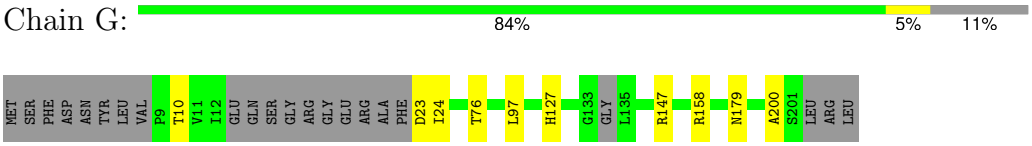
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



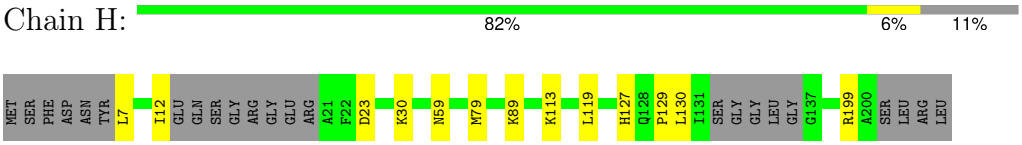
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



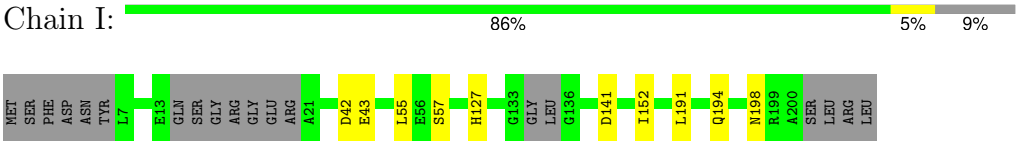
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



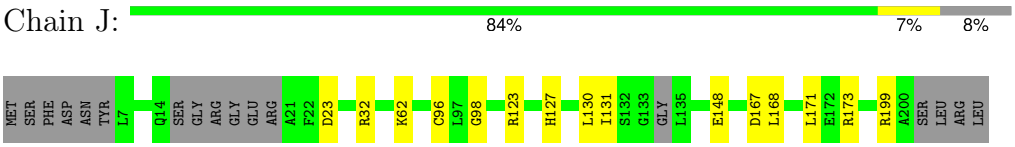
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



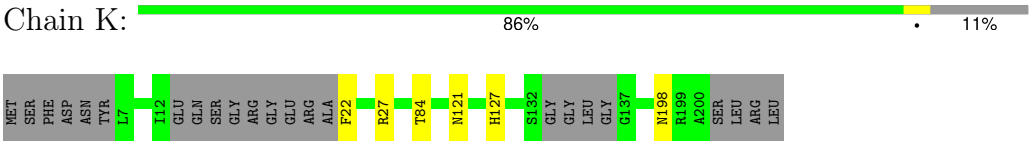
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



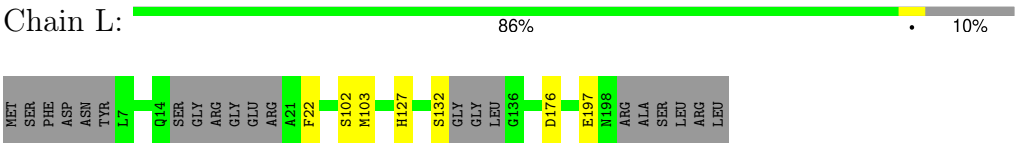
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



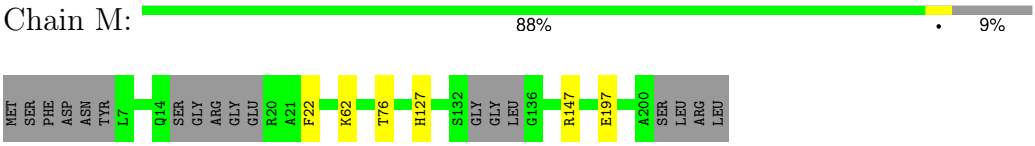
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



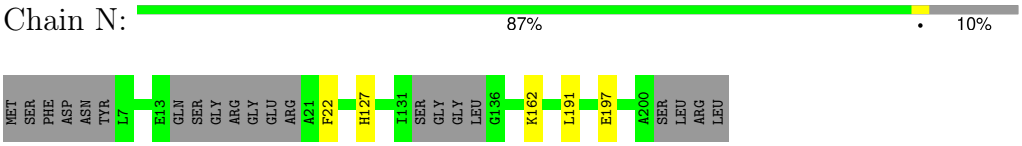
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	152.80Å 357.78Å 180.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.33	Depositor
% Data completeness (in resolution range)	98.8 (48.85-2.33)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.29 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.222 , 0.282	Depositor
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.021	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31127	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: X3O

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	0.53	0/1496	0.68	0/2013
1	B	0.48	0/1468	0.66	0/1975
1	C	0.41	0/1461	0.63	0/1966
1	D	0.36	0/1382	0.61	0/1859
1	E	0.40	0/1386	0.62	0/1864
1	F	0.41	0/1381	0.63	0/1857
1	G	0.49	0/1433	0.68	1/1927 (0.1%)
1	H	0.44	0/1437	0.63	0/1935
1	I	0.36	0/1460	0.60	0/1965
1	J	0.38	0/1477	0.60	0/1988
1	K	0.34	0/1438	0.58	0/1936
1	L	0.37	0/1449	0.57	0/1951
1	M	0.43	0/1476	0.62	0/1986
1	N	0.47	1/1450 (0.1%)	0.63	0/1952
1	V	0.49	0/1525	0.71	0/2052
1	W	0.48	0/1498	0.71	1/2013 (0.0%)
1	X	0.46	0/1529	0.69	1/2057 (0.0%)
1	Y	0.47	0/1440	0.68	0/1935
1	Z	0.47	0/1392	0.67	0/1872
1	a	0.50	0/1525	0.68	0/2052
1	b	0.49	0/1511	0.73	2/2033 (0.1%)
All	All	0.44	1/30614 (0.0%)	0.65	5/41188 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	197	GLU	CB-CG	5.43	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	97	LEU	CA-CB-CG	6.91	131.20	115.30
1	b	191	LEU	CA-CB-CG	6.66	130.62	115.30
1	b	97	LEU	CA-CB-CG	6.12	129.36	115.30
1	W	28	LEU	CA-CB-CG	5.27	127.42	115.30
1	X	7	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	129	PRO	Peptide
1	H	199	ARG	Sidechain
1	J	199	ARG	Sidechain
1	W	177	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	184/204 (90%)	174 (95%)	7 (4%)	3 (2%)	8 6
1	B	180/204 (88%)	173 (96%)	4 (2%)	3 (2%)	7 5
1	C	179/204 (88%)	172 (96%)	7 (4%)	0	100 100
1	D	170/204 (83%)	158 (93%)	10 (6%)	2 (1%)	11 9
1	E	171/204 (84%)	163 (95%)	8 (5%)	0	100 100
1	F	170/204 (83%)	160 (94%)	10 (6%)	0	100 100
1	G	176/204 (86%)	169 (96%)	6 (3%)	1 (1%)	22 23
1	H	175/204 (86%)	163 (93%)	10 (6%)	2 (1%)	12 10
1	I	179/204 (88%)	163 (91%)	15 (8%)	1 (1%)	22 23
1	J	181/204 (89%)	165 (91%)	14 (8%)	2 (1%)	12 10
1	K	175/204 (86%)	157 (90%)	18 (10%)	0	100 100
1	L	177/204 (87%)	164 (93%)	12 (7%)	1 (1%)	22 23
1	M	180/204 (88%)	172 (96%)	8 (4%)	0	100 100
1	N	177/204 (87%)	169 (96%)	8 (4%)	0	100 100
1	V	189/204 (93%)	179 (95%)	7 (4%)	3 (2%)	8 6
1	W	186/204 (91%)	177 (95%)	5 (3%)	4 (2%)	5 3
1	X	190/204 (93%)	180 (95%)	9 (5%)	1 (0%)	25 27
1	Y	177/204 (87%)	169 (96%)	7 (4%)	1 (1%)	22 23
1	Z	172/204 (84%)	165 (96%)	6 (4%)	1 (1%)	22 23
1	a	189/204 (93%)	177 (94%)	12 (6%)	0	100 100
1	b	187/204 (92%)	177 (95%)	6 (3%)	4 (2%)	5 3
All	All	3764/4284 (88%)	3546 (94%)	189 (5%)	29 (1%)	16 16

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	200	ALA
1	W	11	VAL
1	W	200	ALA
1	Z	200	ALA
1	b	15	SER

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	161/173 (93%)	157 (98%)	4 (2%)	42	53
1	B	158/173 (91%)	151 (96%)	7 (4%)	24	30
1	C	158/173 (91%)	152 (96%)	6 (4%)	28	36
1	D	149/173 (86%)	143 (96%)	6 (4%)	27	34
1	E	149/173 (86%)	134 (90%)	15 (10%)	6	5
1	F	149/173 (86%)	145 (97%)	4 (3%)	40	50
1	G	155/173 (90%)	147 (95%)	8 (5%)	19	24
1	H	155/173 (90%)	146 (94%)	9 (6%)	17	19
1	I	157/173 (91%)	148 (94%)	9 (6%)	17	20
1	J	159/173 (92%)	147 (92%)	12 (8%)	11	11
1	K	156/173 (90%)	150 (96%)	6 (4%)	28	36
1	L	157/173 (91%)	151 (96%)	6 (4%)	28	36
1	M	159/173 (92%)	153 (96%)	6 (4%)	28	36
1	N	156/173 (90%)	152 (97%)	4 (3%)	41	51
1	V	164/173 (95%)	159 (97%)	5 (3%)	36	45
1	W	160/173 (92%)	153 (96%)	7 (4%)	24	30
1	X	164/173 (95%)	154 (94%)	10 (6%)	15	17
1	Y	154/173 (89%)	146 (95%)	8 (5%)	19	24
1	Z	150/173 (87%)	145 (97%)	5 (3%)	33	41
1	a	164/173 (95%)	156 (95%)	8 (5%)	21	26
1	b	162/173 (94%)	156 (96%)	6 (4%)	29	37
All	All	3296/3633 (91%)	3145 (95%)	151 (5%)	23	28

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	194	GLN
1	M	76	THR

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Mol	Chain	Res	Type
1	J	96	CYS
1	K	27	ARG
1	N	191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	46	ASN
1	I	46	ASN
1	G	179	ASN
1	I	157	ASN
1	B	138	GLN

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)

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	X3O	V	301	-	39,43,43	1.47	4 (10%)	53,67,67	1.62	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	X3O	N	301	-	39,43,43	1.51	5 (12%)	53,67,67	1.77	13 (24%)
2	X3O	Z	301	-	39,43,43	1.49	5 (12%)	53,67,67	1.74	14 (26%)
2	X3O	a	301	-	39,43,43	1.46	5 (12%)	53,67,67	1.65	12 (22%)
2	X3O	H	301	-	39,43,43	1.29	3 (7%)	53,67,67	1.59	13 (24%)
2	X3O	M	301	-	39,43,43	1.48	5 (12%)	53,67,67	1.44	12 (22%)
2	X3O	b	301	-	39,43,43	1.43	5 (12%)	53,67,67	1.94	15 (28%)
2	X3O	W	301	-	39,43,43	1.41	4 (10%)	53,67,67	1.70	11 (20%)
2	X3O	X	301	-	39,43,43	1.45	5 (12%)	53,67,67	1.63	11 (20%)
2	X3O	J	301	-	39,43,43	1.52	6 (15%)	53,67,67	1.78	14 (26%)
2	X3O	L	301	-	39,43,43	1.48	4 (10%)	53,67,67	1.57	10 (18%)

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	X3O	V	301	-	-	2/47/52/52	0/3/3/3
2	X3O	N	301	-	-	8/47/52/52	0/3/3/3
2	X3O	Z	301	-	-	9/47/52/52	0/3/3/3
2	X3O	a	301	-	-	9/47/52/52	0/3/3/3
2	X3O	H	301	-	-	9/47/52/52	0/3/3/3
2	X3O	M	301	-	-	7/47/52/52	0/3/3/3
2	X3O	b	301	-	-	7/47/52/52	0/3/3/3
2	X3O	W	301	-	-	5/47/52/52	0/3/3/3
2	X3O	X	301	-	-	4/47/52/52	0/3/3/3
2	X3O	J	301	-	-	13/47/52/52	0/3/3/3
2	X3O	L	301	-	-	5/47/52/52	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	X3O	C14-N15	5.43	1.46	1.33
2	a	301	X3O	C14-N15	5.40	1.46	1.33
2	J	301	X3O	C14-N15	5.29	1.46	1.33
2	Z	301	X3O	C14-N15	5.19	1.46	1.33
2	M	301	X3O	C14-N15	5.17	1.46	1.33

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	301	X3O	C17-S18-C19	6.26	116.07	103.05
2	b	301	X3O	C35-C34-N33	-5.16	118.54	123.38
2	N	301	X3O	C35-C34-N33	-4.85	118.83	123.38
2	X	301	X3O	C13-C14-N15	4.78	122.55	116.95
2	a	301	X3O	C35-C34-N33	-4.57	119.09	123.38

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

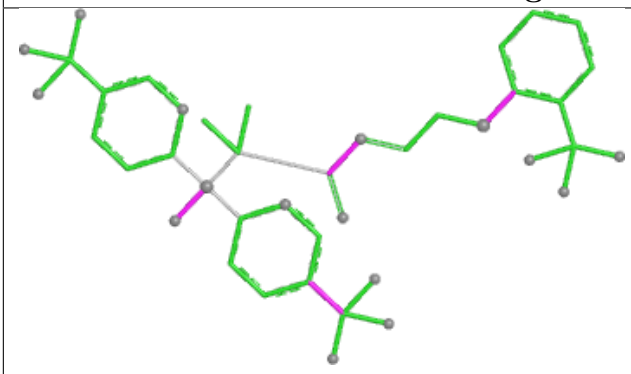
Mol	Chain	Res	Type	Atoms
2	W	301	X3O	N15-C16-C17-S18
2	W	301	X3O	N12-C03-P02-C13
2	X	301	X3O	N15-C16-C17-S18
2	X	301	X3O	C16-C17-S18-C19
2	Z	301	X3O	C19-C20-C21-F22

There are no ring outliers.

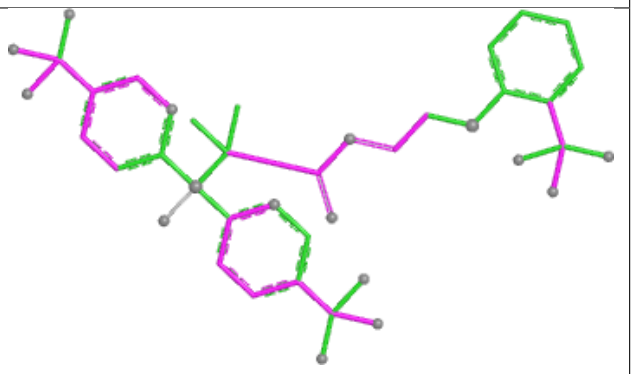
No monomer is involved in short contacts.

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.

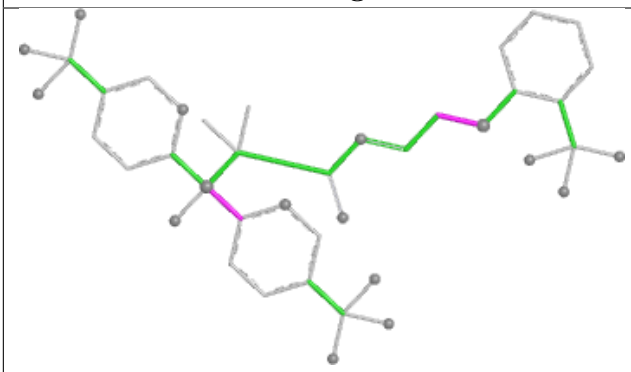
Ligand X3O V 301



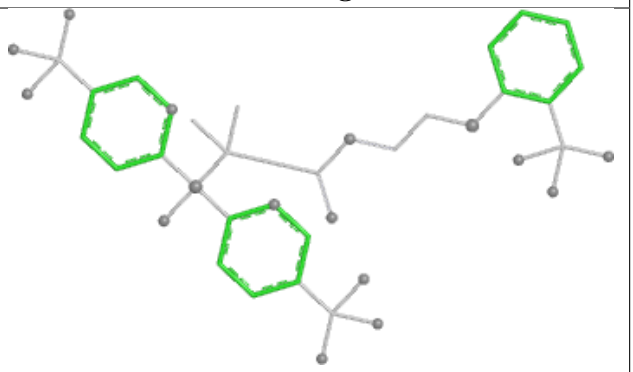
Bond lengths



Bond angles

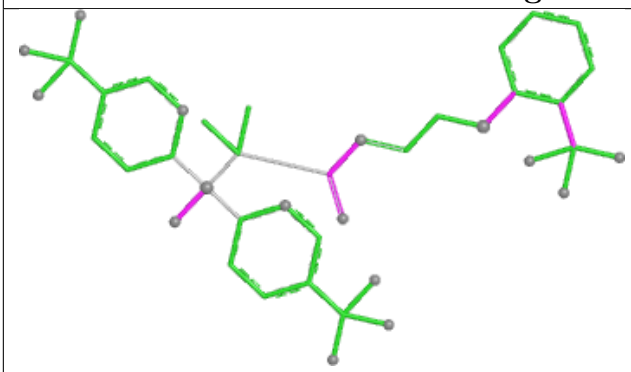


Torsions



Rings

Ligand X3O N 301



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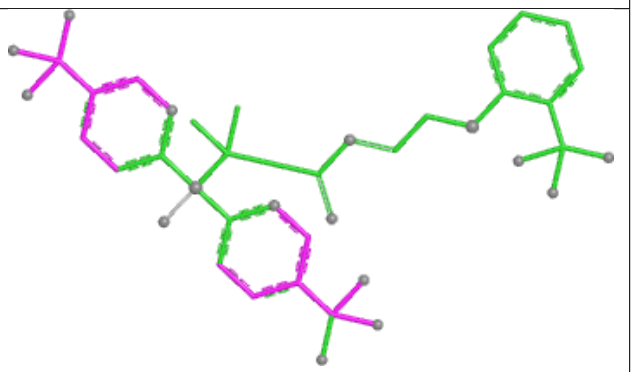

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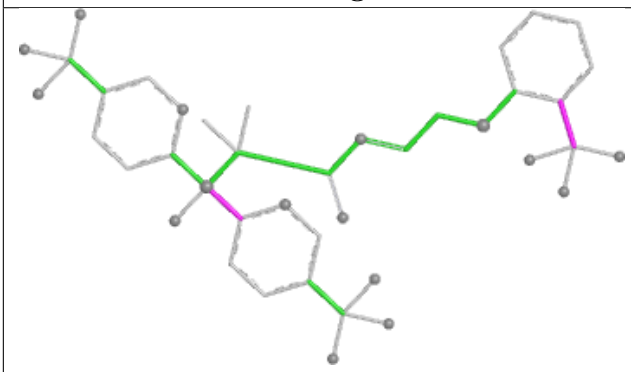

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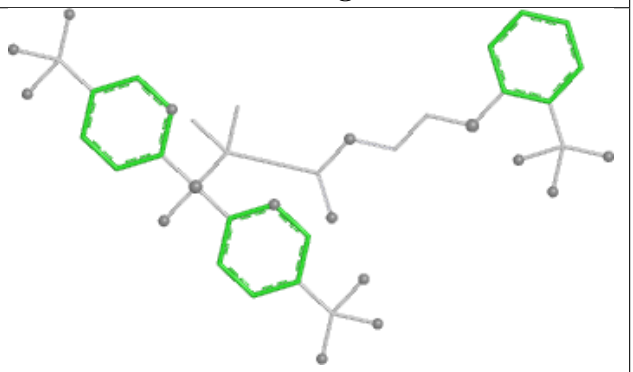
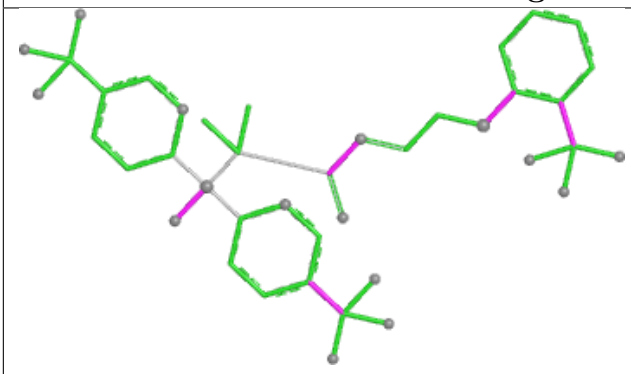


Rings

Ligand X3O Z 301



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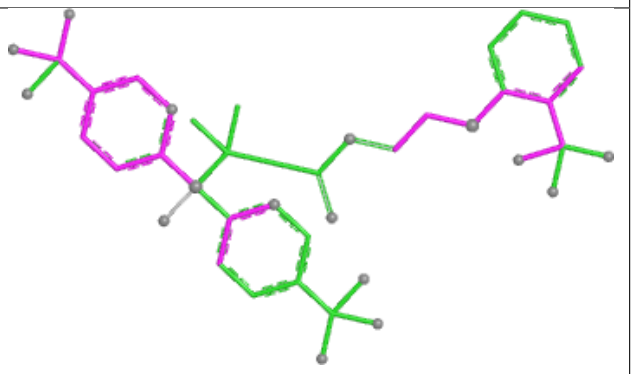

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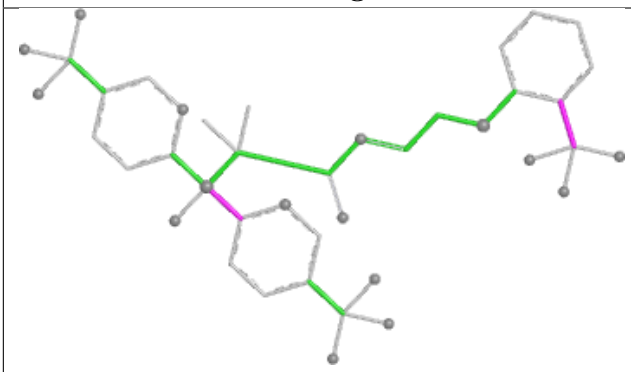

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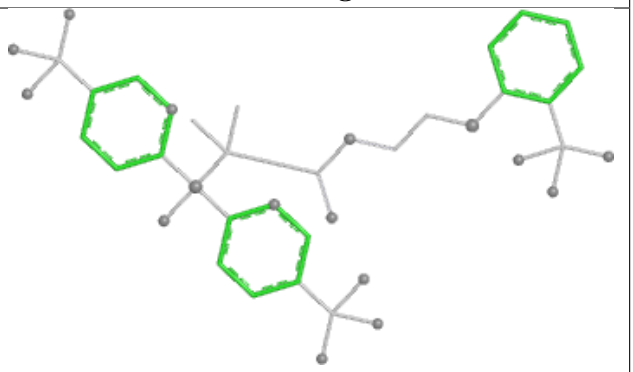
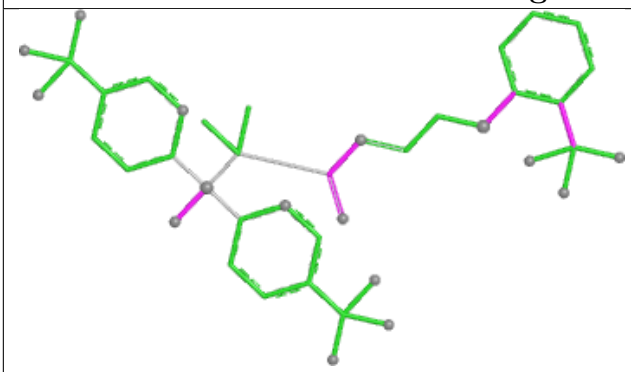


Rings

Ligand X3O a 301



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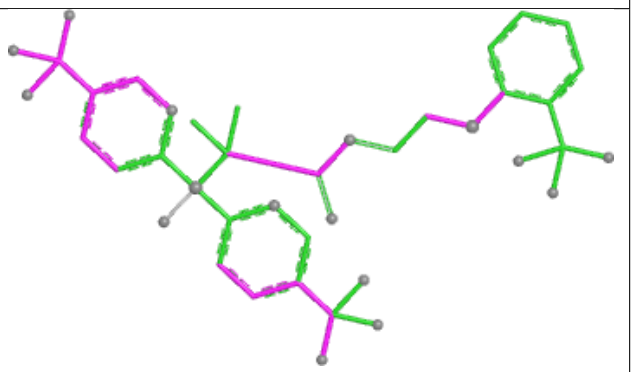

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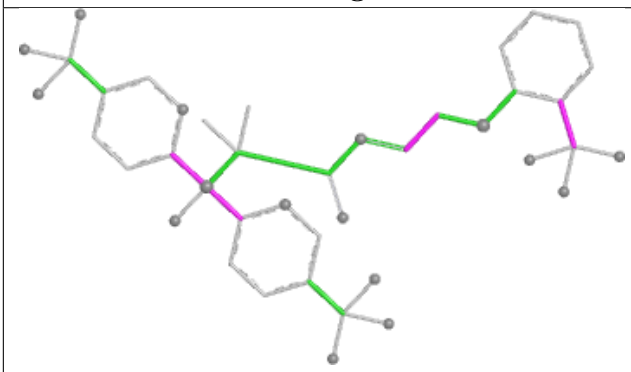

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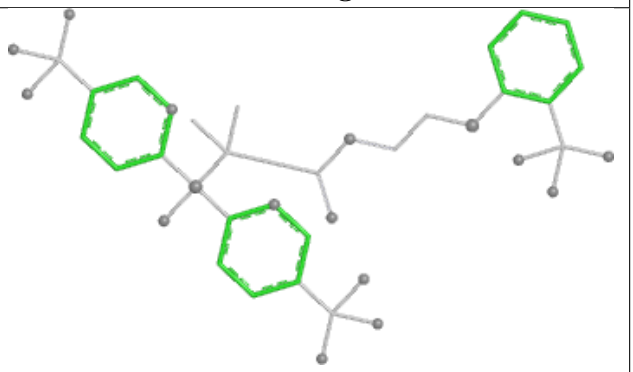
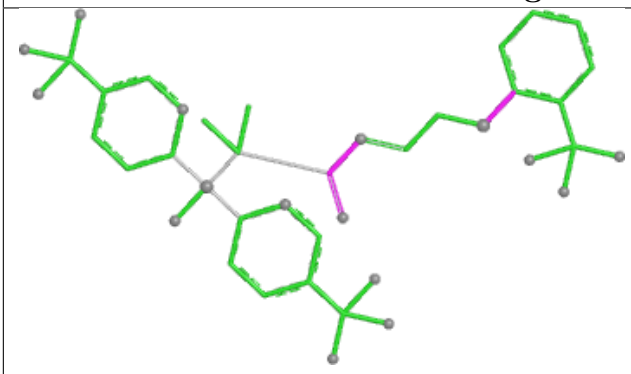


Rings

Ligand X3O H 301



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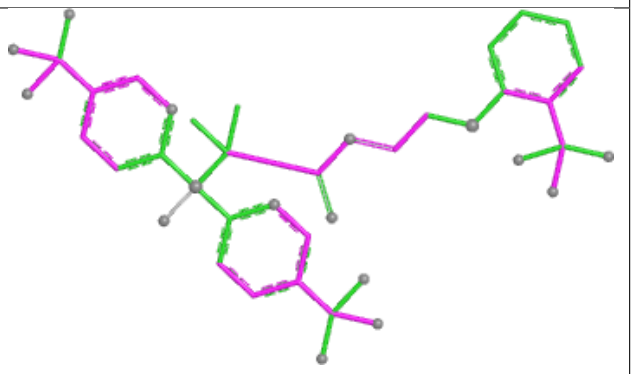

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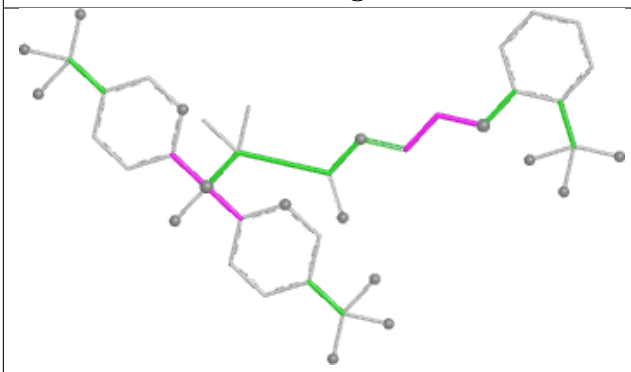

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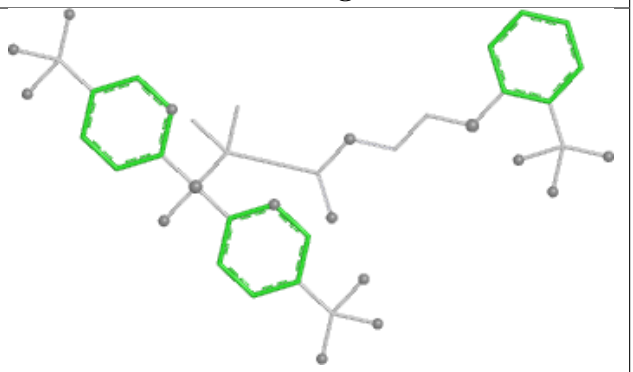
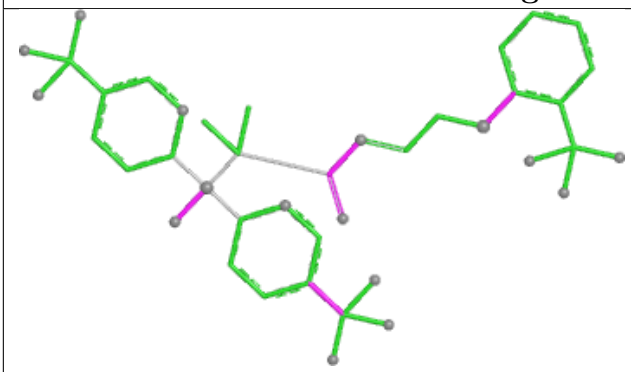


Rings

Ligand X3O M 301



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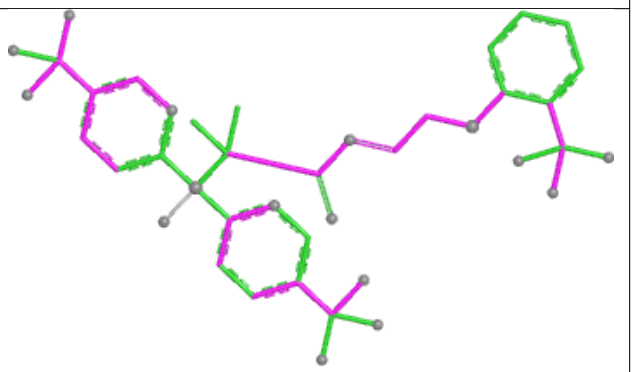

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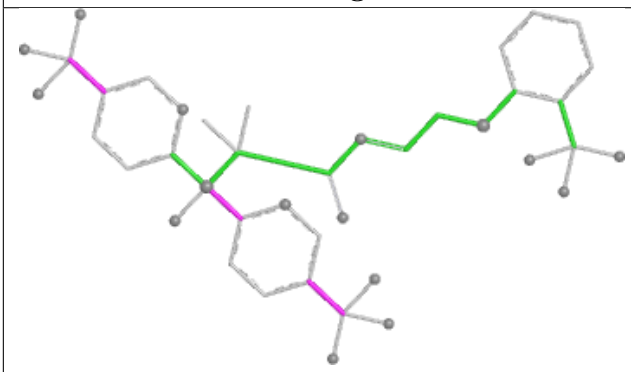

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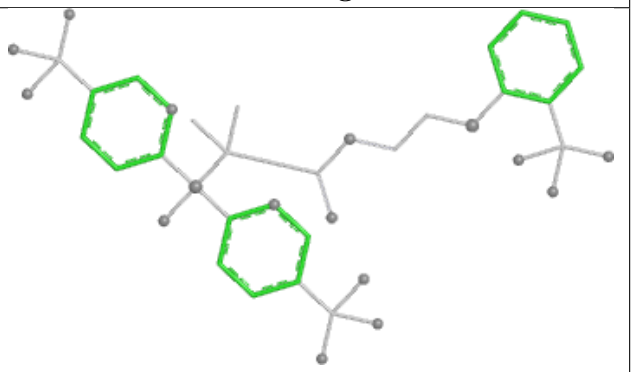
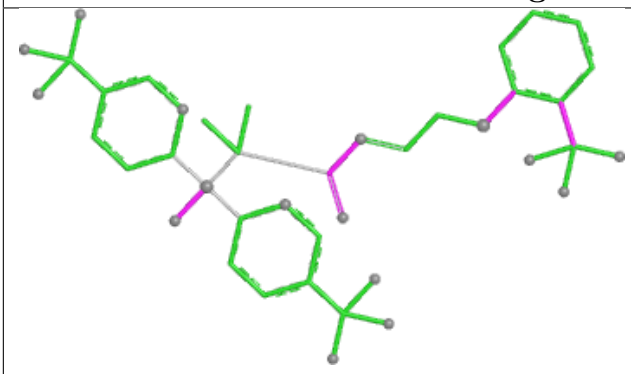
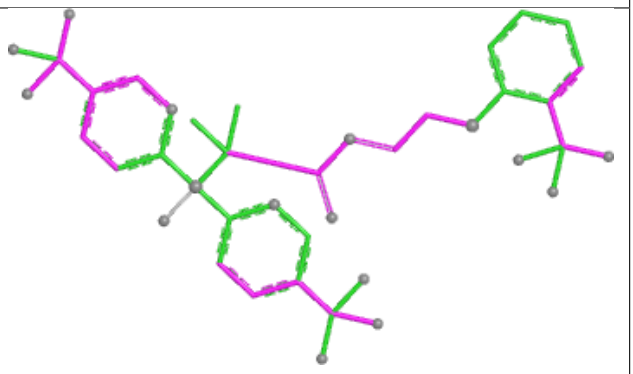


Rings

Ligand X3O b 301



Bond lengths



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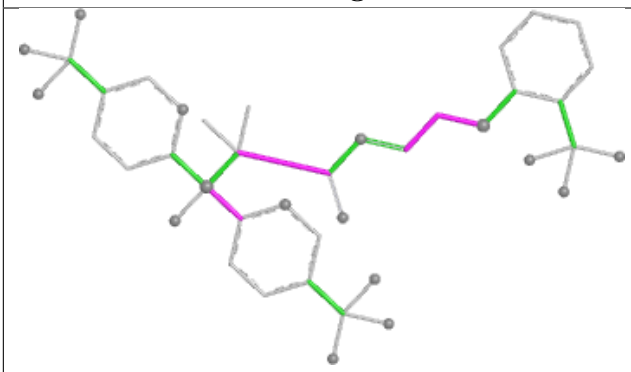

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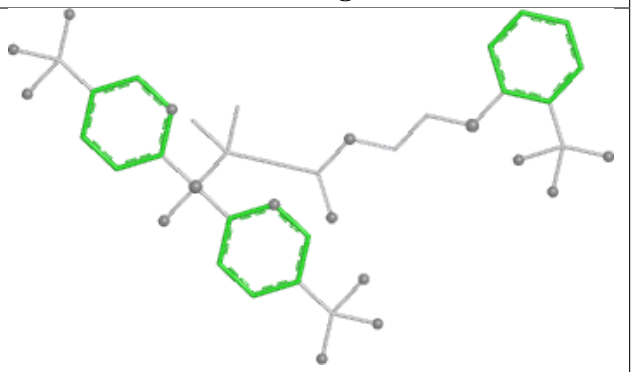
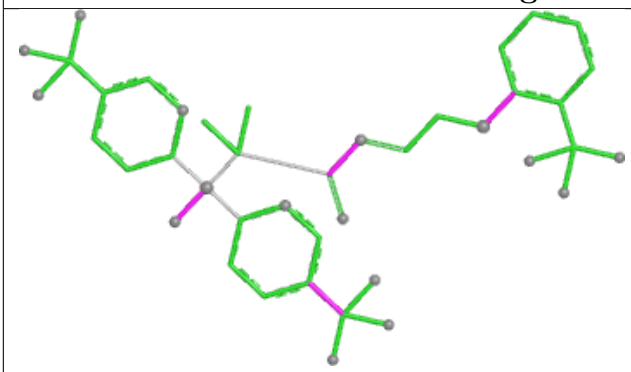
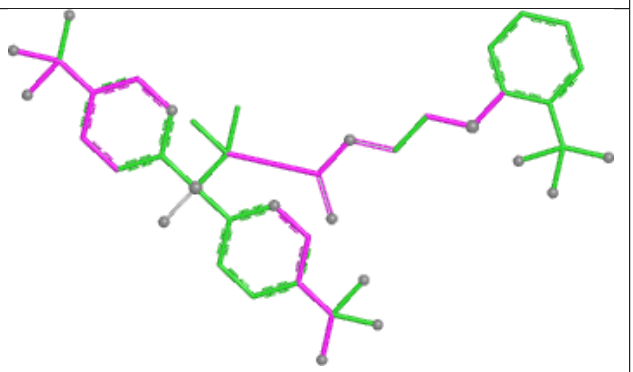


Rings

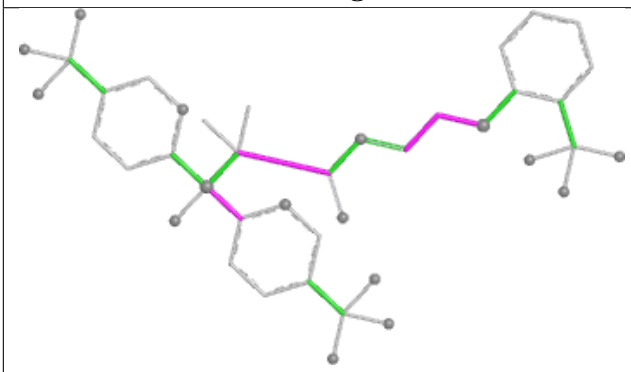
Ligand X3O W 301



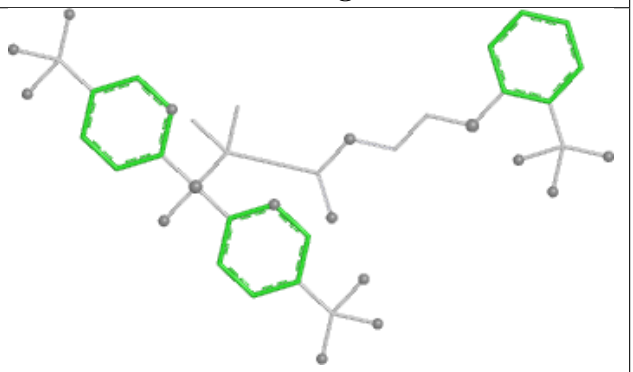
Bond lengths



Bond angles

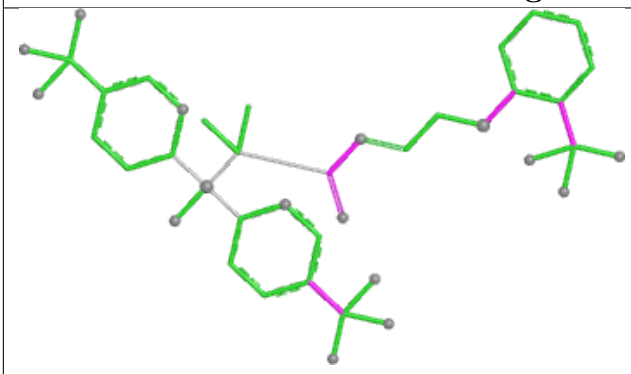


Torsions

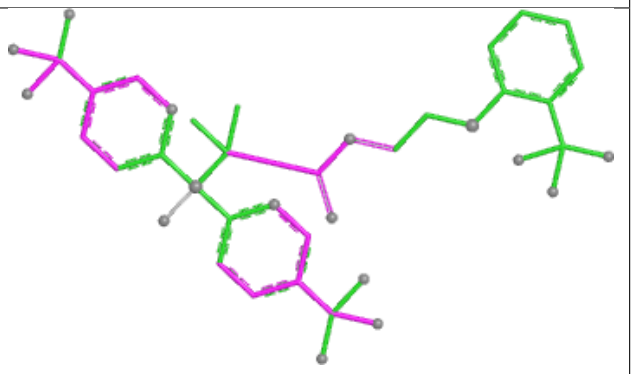


Rings

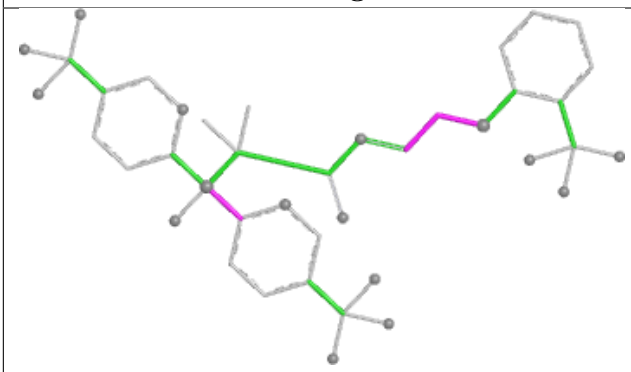
Ligand X3O X 301



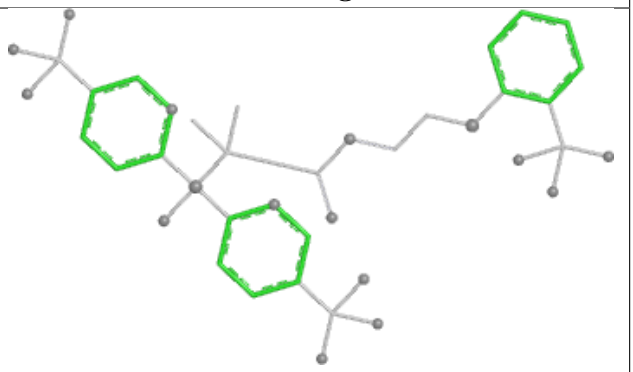
Bond lengths



Bond angles

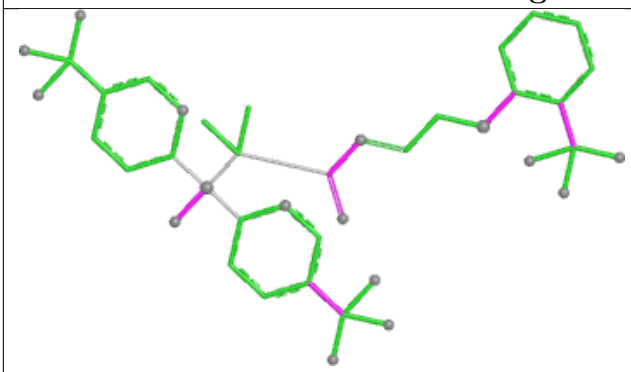


Torsions

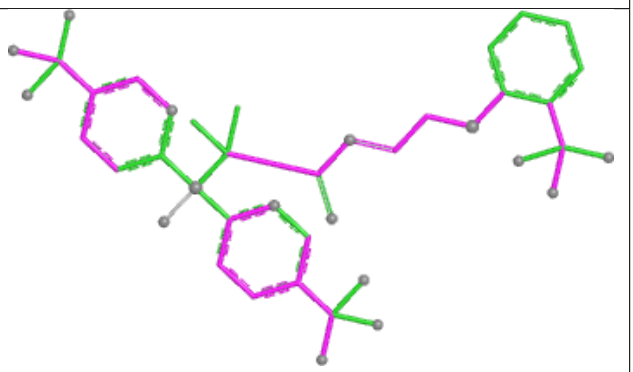


Rings

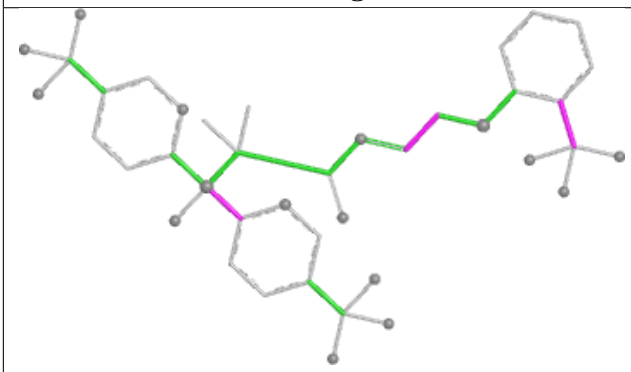
Ligand X3O J 301



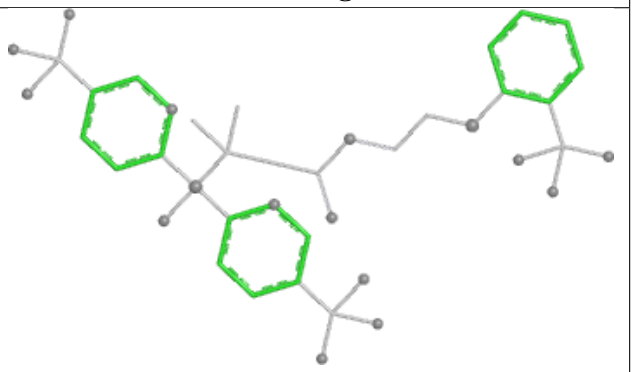
Bond lengths



Bond angles

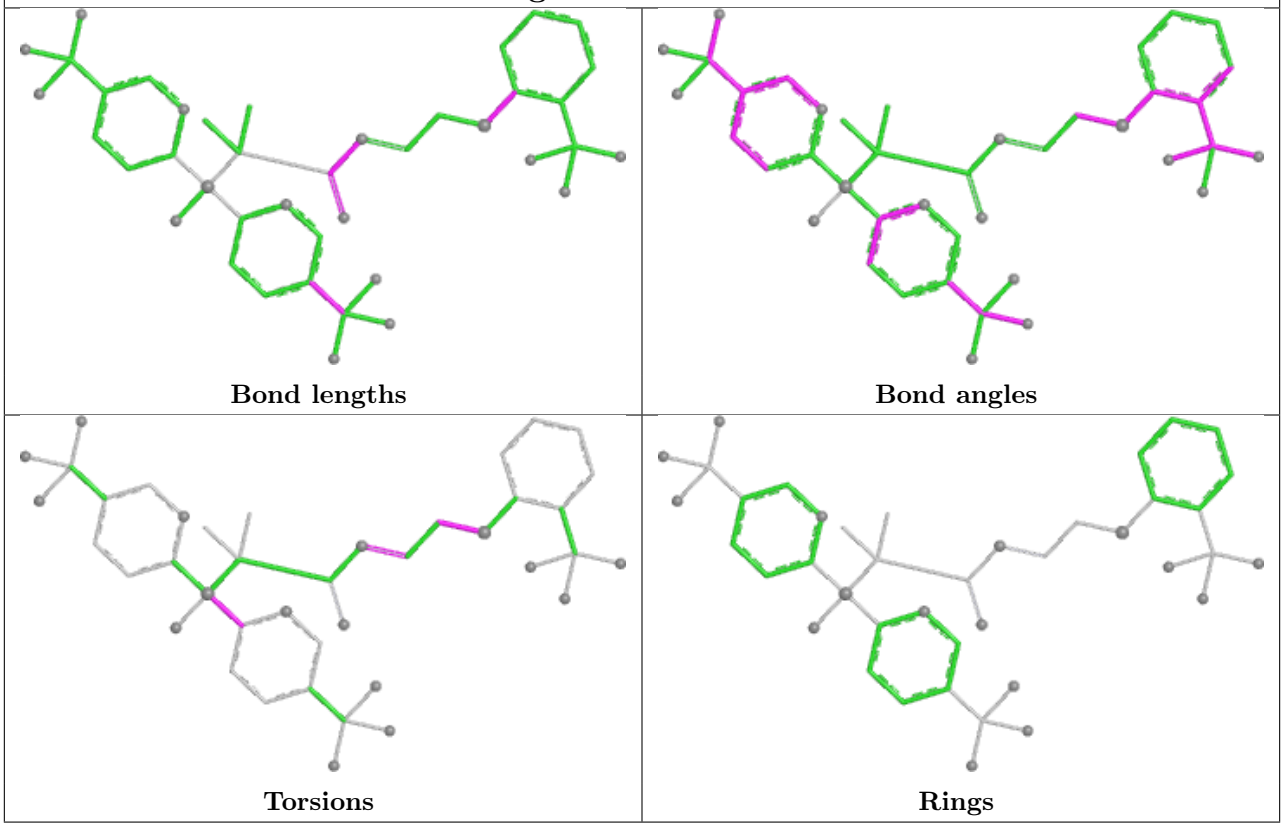


Torsions



Rings

Ligand X3O L 301



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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.