Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 04:54 AM EST

PDB ID	:	4U0G
Title	:	Crystal Structure of M. tuberculosis ClpP1P2 bound to ADEP and agonist
Authors	:	Schmitz, K.R.; Carney, D.W.; Sello, J.K.; Sauer, R.T.
Deposited on	:	2014-07-11
Resolution	:	3.20 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 (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 (i)) were used in the production of this report:

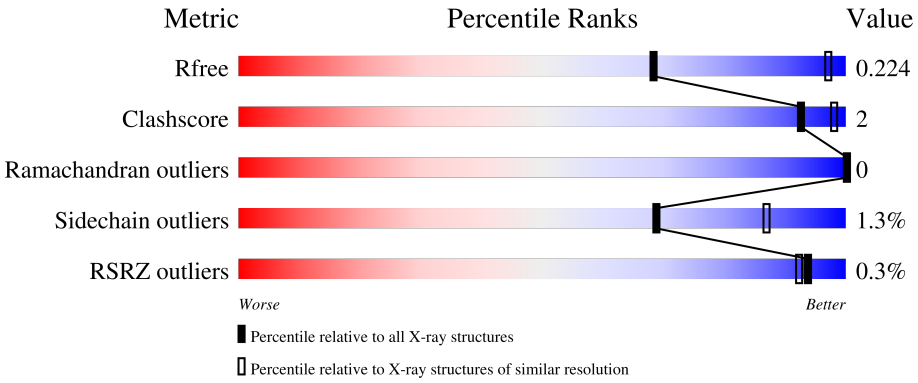
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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% 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	202	92% 6%
1	B	202	90% 7%
1	C	202	92% 5%
1	D	202	89% 8%
1	E	202	92% 5%

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Mol	Chain	Length	Quality of chain
1	F	202	91% 6%
1	G	202	93%
1	O	202	93%
1	P	202	92%
1	Q	202	92%
1	R	202	91% 6%
1	S	202	91% 6%
1	T	202	94%
1	U	202	93%
2	H	194	87% 10%
2	I	194	86% 11%
2	J	194	88% 10%
2	K	194	86% 11%
2	L	194	87% 10%
2	M	194	88% 11%
2	N	194	87% 10%
2	V	194	88% 10%
2	W	194	87% 10%
2	X	194	87% 10%
2	Y	194	87% 10%
2	Z	194	87% 10%
2	a	194	89% 10%
2	b	194	89% 10%
3	c	7	86% 14%
3	d	7	86% 14%

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Mol	Chain	Length	Quality of chain
3	e	7	86% 14%
3	f	7	86% 14%
3	g	7	86% 14%
3	h	7	86% 14%
3	i	7	86% 14%
3	j	7	86% 14%
3	k	7	86% 14%
3	l	7	86% 14%
3	m	7	86% 14%
3	n	7	71% 29%
3	o	7	86% 14%
3	p	7	86% 14%

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
5	SO4	G	302	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 81740 atoms, of which 40656 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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			2997	943	1495	257	294	8			
1	B	197	Total	C	H	N	O	S	0	0	0
			3035	951	1522	258	296	8			
1	C	196	Total	C	H	N	O	S	0	0	0
			2996	942	1498	253	295	8			
1	D	195	Total	C	H	N	O	S	0	0	0
			2961	933	1475	252	293	8			
1	E	197	Total	C	H	N	O	S	0	0	0
			3011	945	1505	257	296	8			
1	F	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	G	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	O	196	Total	C	H	N	O	S	0	0	0
			3000	942	1499	257	294	8			
1	P	194	Total	C	H	N	O	S	0	0	0
			2983	936	1493	254	292	8			
1	Q	195	Total	C	H	N	O	S	0	0	0
			2978	937	1487	255	291	8			
1	R	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	S	196	Total	C	H	N	O	S	0	0	0
			3028	948	1520	257	295	8			
1	T	196	Total	C	H	N	O	S	0	0	0
			3016	945	1511	257	295	8			
1	U	196	Total	C	H	N	O	S	0	0	0
			3013	945	1509	256	295	8			

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	H	174	Total	C	H	N	O	S	Se	0	0	0
			2597	832	1288	219	249	2	7			
2	I	172	Total	C	H	N	O	S	Se	0	0	0
			2572	823	1276	216	248	2	7			
2	J	175	Total	C	H	N	O	S	Se	0	0	0
			2623	839	1300	223	252	2	7			
2	K	172	Total	C	H	N	O	S	Se	0	0	0
			2535	815	1252	213	246	2	7			
2	L	174	Total	C	H	N	O	S	Se	0	0	0
			2608	833	1296	219	251	2	7			
2	M	173	Total	C	H	N	O	S	Se	0	0	0
			2584	827	1283	215	250	2	7			
2	N	174	Total	C	H	N	O	S	Se	0	0	0
			2585	828	1281	218	249	2	7			
2	V	175	Total	C	H	N	O	S	Se	0	0	0
			2603	834	1291	220	249	2	7			
2	W	175	Total	C	H	N	O	S	Se	0	0	0
			2583	829	1278	220	247	2	7			
2	X	175	Total	C	H	N	O	S	Se	0	0	0
			2575	828	1272	216	250	2	7			
2	Y	174	Total	C	H	N	O	S	Se	0	0	0
			2569	826	1269	215	250	2	7			
2	Z	175	Total	C	H	N	O	S	Se	0	0	0
			2611	836	1295	220	251	2	7			
2	a	174	Total	C	H	N	O	S	Se	0	0	0
			2604	833	1293	219	250	2	7			
2	b	175	Total	C	H	N	O	S	Se	0	0	0
			2562	825	1266	216	246	2	7			

- Molecule 3 is a protein called ADEP-2B5Me.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	c	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	i	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	d	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	e	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	f	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	g	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			

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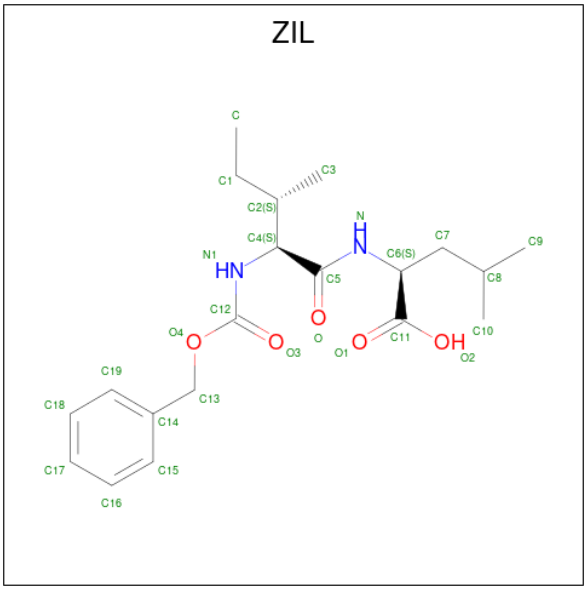
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	h	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	j	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	k	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	l	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	m	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	n	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	o	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			
3	p	7	Total	C	F	H	N	O	0	0	0
			113	41	2	56	6	8			

- Molecule 4 is N-[(benzyloxy)carbonyl]-L-isoleucyl-L-leucine (three-letter code: ZIL) (formula: $C_{20}H_{30}N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	B	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	C	1	Total	C	H	N	O	0	0
			57	20	30	2	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	E	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	F	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	G	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	H	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	I	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	J	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	K	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	L	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	M	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	N	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	O	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	P	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	Q	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	R	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	S	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	T	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	U	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	V	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	W	1	Total	C	H	N	O	0	0
			57	20	30	2	5		
4	X	1	Total	C	H	N	O	0	0
			57	20	30	2	5		

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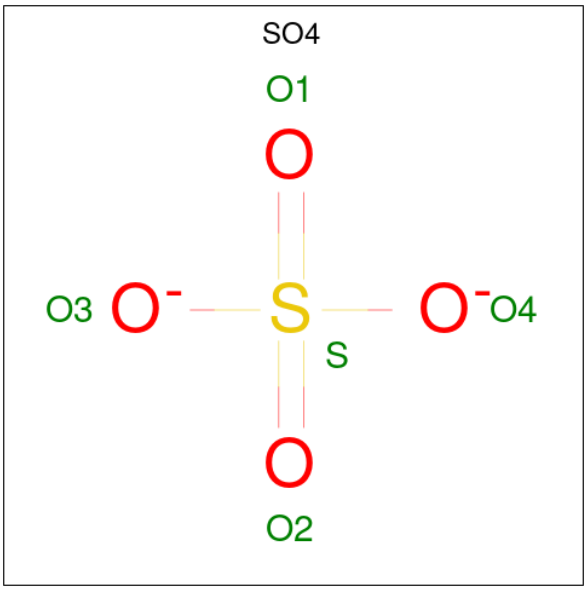
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C H N O 57 20 30 2 5	0	0
4	Z	1	Total C H N O 57 20 30 2 5	0	0
4	a	1	Total C H N O 57 20 30 2 5	0	0
4	b	1	Total C H N O 57 20 30 2 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	M	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0

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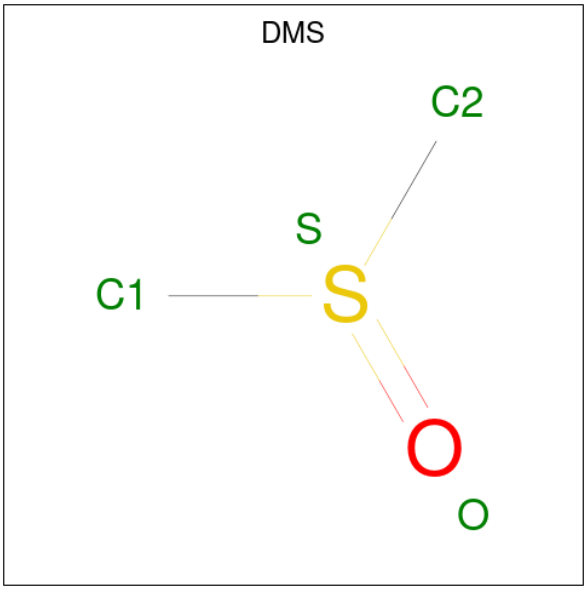
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	U	1	Total O S 5 4 1	0	0
5	W	1	Total O S 5 4 1	0	0
5	p	1	Total O S 5 4 1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O S 10 2 6 1 1	0	0
6	B	1	Total C H O S 10 2 6 1 1	0	0
6	B	1	Total C H O S 10 2 6 1 1	0	0
6	C	1	Total C H O S 10 2 6 1 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	E	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	F	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	O	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	P	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	Q	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	R	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	S	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	T	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	U	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	B	3	Total	O	0	0
			3	3		
7	C	2	Total	O	0	0
			2	2		
7	D	1	Total	O	0	0
			1	1		
7	E	2	Total	O	0	0
			2	2		
7	F	1	Total	O	0	0
			1	1		
7	G	2	Total	O	0	0
			2	2		
7	L	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	O	1	Total O 1 1	0	0
7	P	1	Total O 1 1	0	0
7	Q	1	Total O 1 1	0	0
7	R	1	Total O 1 1	0	0
7	S	2	Total O 2 2	0	0
7	T	4	Total O 4 4	0	0
7	U	2	Total O 2 2	0	0
7	V	1	Total O 1 1	0	0

3 Residue-property plots (i)

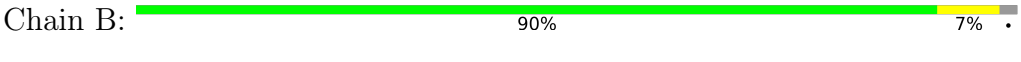
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-dependent Clp protease proteolytic subunit 2

Chain A:

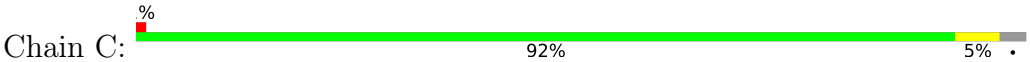
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



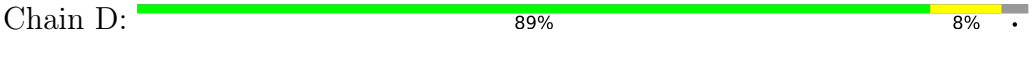
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain C:



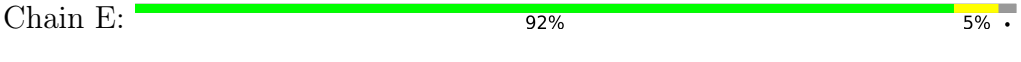
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D:



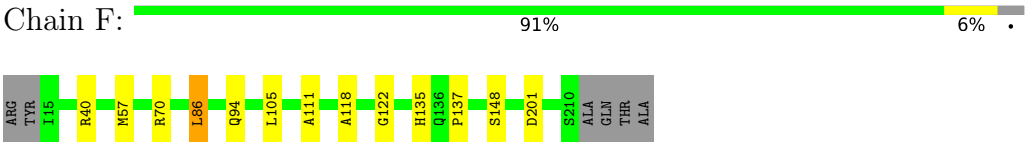
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E:



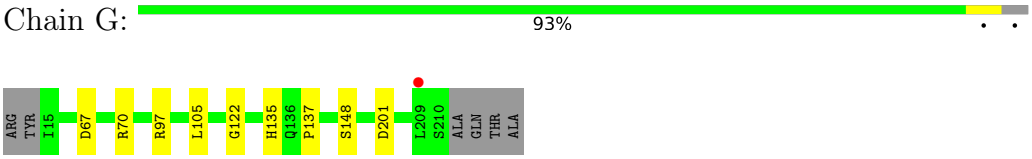
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F:



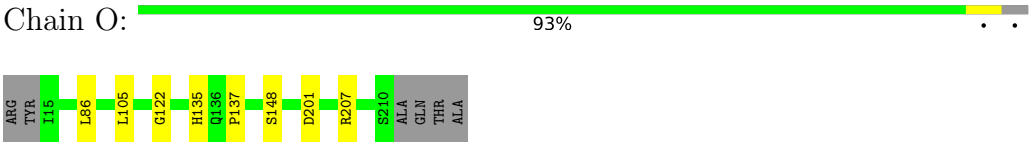
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain G:



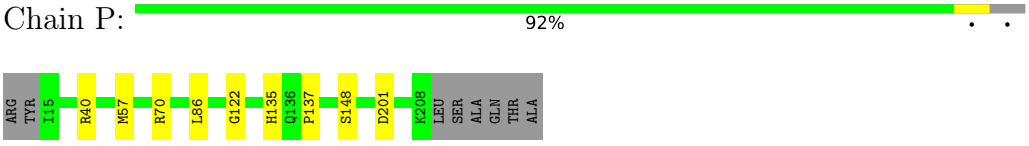
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain O:



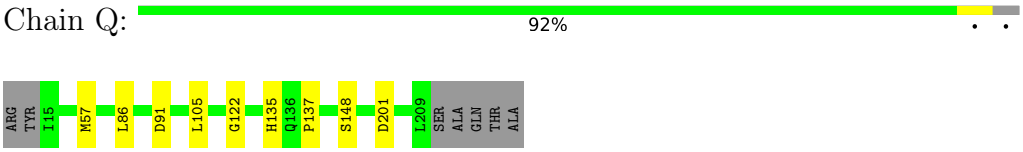
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain P:



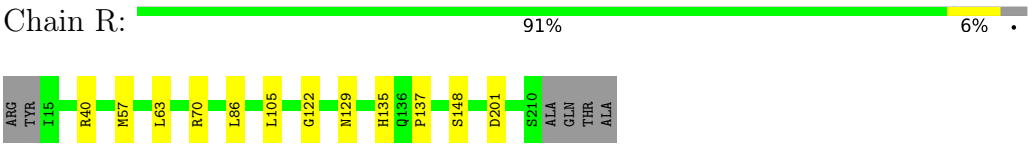
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain Q:



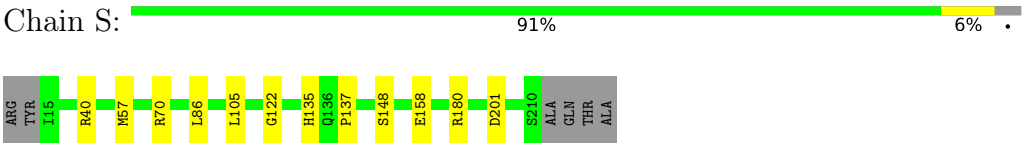
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain R:



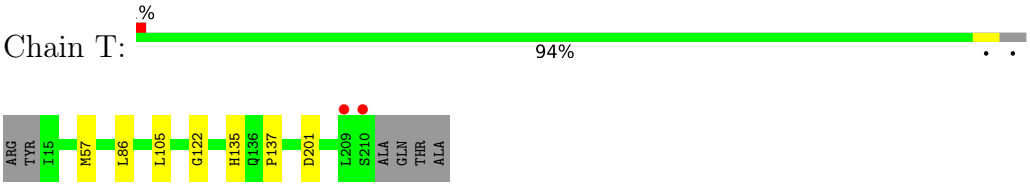
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain S:



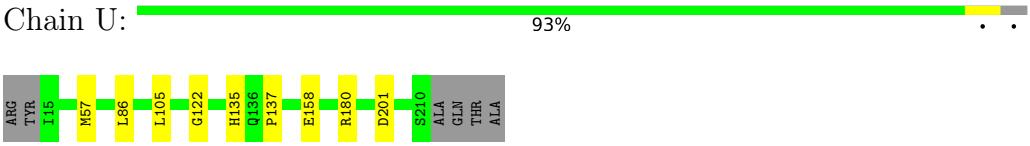
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain T:



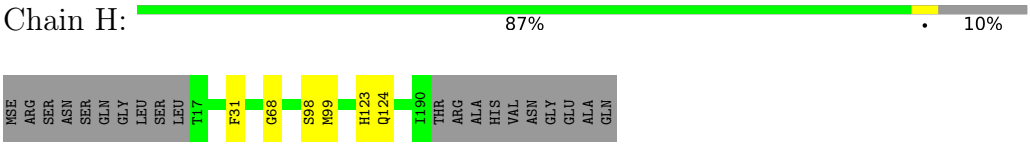
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain U:



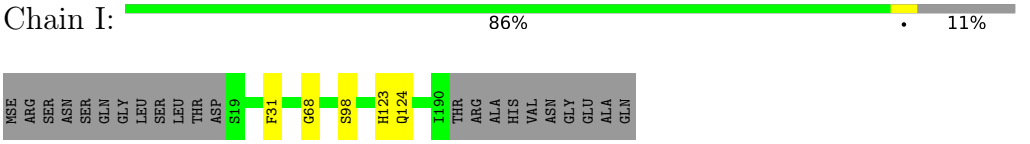
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain H:



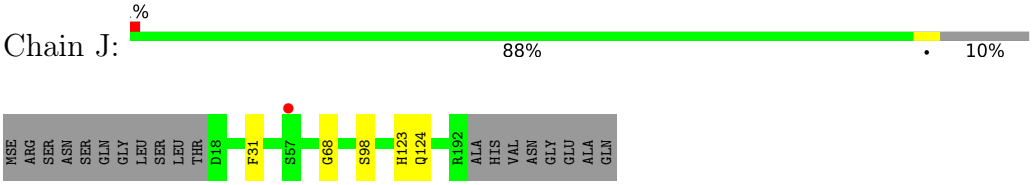
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain I:



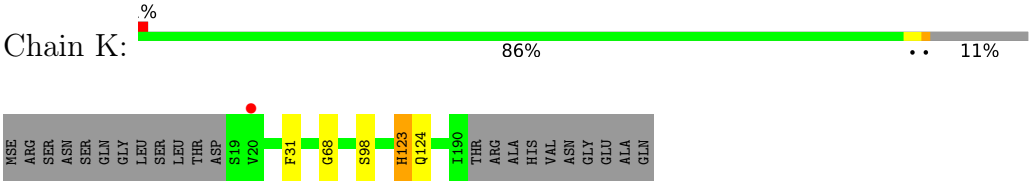
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain J:



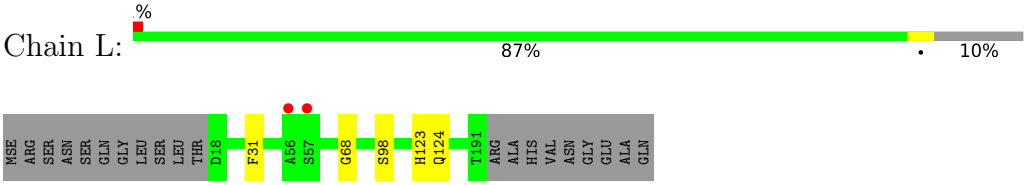
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain K:



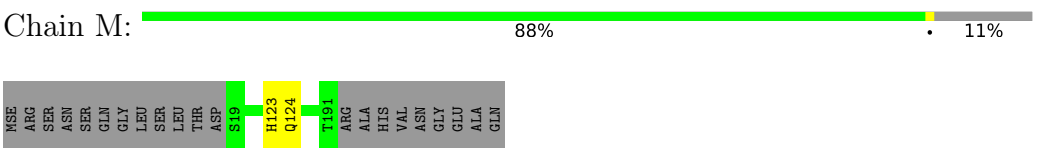
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain L:



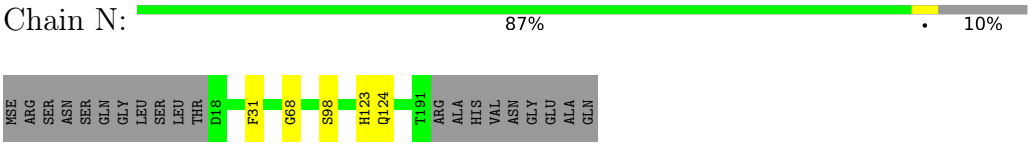
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain M:



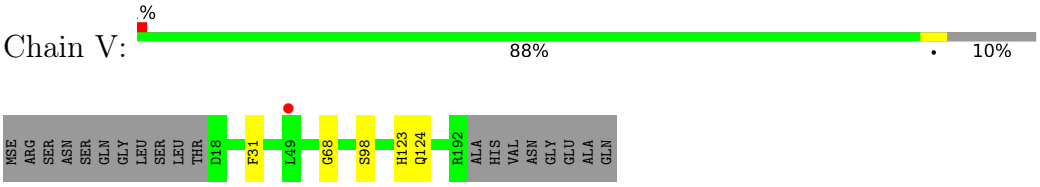
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



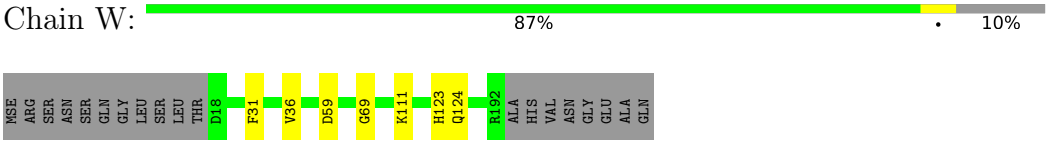
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain V:



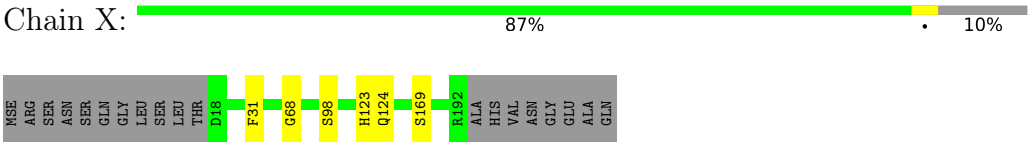
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain W:



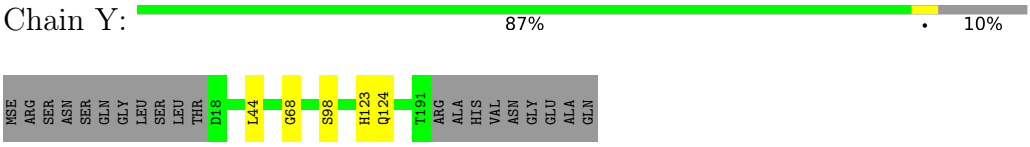
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain X:



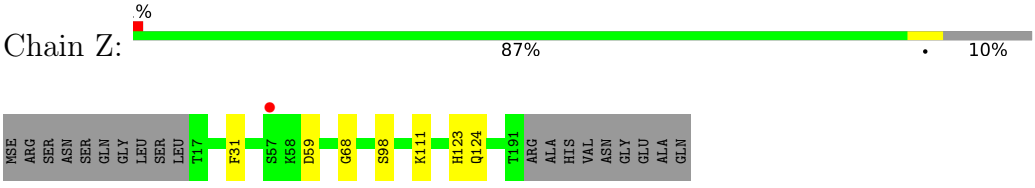
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain Y:



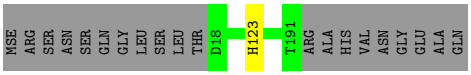
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain Z:



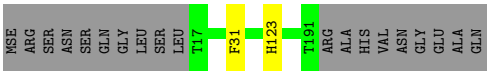
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain a:



• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain b:



• Molecule 3: ADEP-2B5Me

Chain c:

• Molecule 3: ADEP-2B5Me

Chain i:

• Molecule 3: ADEP-2B5Me

Chain d:

• Molecule 3: ADEP-2B5Me

Chain e:

• Molecule 3: ADEP-2B5Me

Chain f:

• Molecule 3: ADEP-2B5Me

Chain g:

• Molecule 3: ADEP-2B5Me

Chain h:

• Molecule 3: ADEP-2B5Me

Chain j:

• Molecule 3: ADEP-2B5Me

Chain k:

• Molecule 3: ADEP-2B5Me

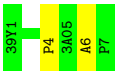
Chain l:

• Molecule 3: ADEP-2B5Me

Chain m:

• Molecule 3: ADEP-2B5Me

Chain n:



• Molecule 3: ADEP-2B5Me

Chain o:

• Molecule 3: ADEP-2B5Me

Chain p:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	154.75Å 187.67Å 294.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.20 49.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.91-3.20) 96.2 (49.91-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.190 , 0.222 0.192 , 0.224	Depositor DCC
R_{free} test set	7092 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	81740	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: SO4, 3A0, DMS, 39Y, WFP, ZIL

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	0.28	0/1523	0.42	0/2062
1	B	0.27	0/1534	0.40	0/2075
1	C	0.26	0/1519	0.40	0/2057
1	D	0.25	0/1507	0.40	0/2041
1	E	0.24	0/1527	0.40	0/2067
1	F	0.25	0/1518	0.40	0/2055
1	G	0.26	0/1518	0.41	0/2055
1	O	0.24	0/1522	0.39	0/2059
1	P	0.24	0/1511	0.40	0/2045
1	Q	0.25	0/1512	0.40	0/2047
1	R	0.27	0/1518	0.42	0/2055
1	S	0.27	0/1529	0.41	0/2068
1	T	0.25	0/1526	0.40	0/2064
1	U	0.26	0/1525	0.41	0/2064
2	H	0.26	0/1324	0.39	0/1780
2	I	0.24	0/1311	0.38	0/1763
2	J	0.24	0/1338	0.38	0/1798
2	K	0.24	0/1298	0.38	0/1747
2	L	0.25	0/1327	0.39	0/1784
2	M	0.25	0/1316	0.38	0/1770
2	N	0.26	0/1319	0.39	0/1775
2	V	0.23	0/1327	0.39	0/1785
2	W	0.24	0/1320	0.40	0/1776
2	X	0.25	0/1318	0.39	0/1775
2	Y	0.26	0/1315	0.38	0/1770
2	Z	0.25	0/1331	0.39	0/1790
2	a	0.25	0/1326	0.39	0/1783
2	b	0.23	0/1311	0.38	0/1767
3	c	0.58	0/26	0.79	0/35
3	d	0.55	0/26	0.82	0/35
3	e	0.56	0/26	0.79	0/35
3	f	0.56	0/26	0.80	0/35

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	g	0.56	0/26	0.81	0/35
3	h	0.56	0/26	0.83	0/35
3	i	0.56	0/26	0.82	0/35
3	j	0.56	0/26	0.82	0/35
3	k	0.56	0/26	0.83	0/35
3	l	0.56	0/26	0.77	0/35
3	m	0.56	0/26	0.79	0/35
3	n	0.56	0/26	0.79	0/35
3	o	0.56	0/26	0.82	0/35
3	p	0.57	0/26	0.77	0/35
All	All	0.26	0/40134	0.40	0/54167

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
3	c	0	1
3	d	0	1
3	e	0	1
3	f	0	1
3	g	0	1
3	h	0	1
3	i	0	1
3	j	0	1
3	k	0	1
3	l	0	1
3	m	0	1
3	n	0	2
3	o	0	1
3	p	0	1
All	All	0	15

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	6	ALA	Mainchain

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Mol	Chain	Res	Type	Group
3	d	6	ALA	Mainchain
3	e	6	ALA	Mainchain
3	f	6	ALA	Mainchain
3	g	6	ALA	Mainchain
3	h	6	ALA	Mainchain
3	i	6	ALA	Mainchain
3	j	6	ALA	Mainchain
3	k	6	ALA	Mainchain
3	l	6	ALA	Mainchain
3	m	6	ALA	Mainchain
3	n	4	PRO	Peptide
3	n	6	ALA	Mainchain
3	o	6	ALA	Mainchain
3	p	6	ALA	Mainchain

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	1502	1495	1499	7	0
1	B	1513	1522	1521	9	0
1	C	1498	1498	1497	8	0
1	D	1486	1475	1474	11	0
1	E	1506	1505	1504	8	0
1	F	1497	1496	1495	9	0
1	G	1497	1496	1495	7	0
1	O	1501	1499	1498	6	0
1	P	1490	1493	1492	6	0
1	Q	1491	1487	1490	6	0
1	R	1497	1496	1493	8	0
1	S	1508	1520	1517	7	0
1	T	1505	1511	1510	4	0
1	U	1504	1509	1506	5	0
2	H	1309	1288	1288	3	0
2	I	1296	1276	1276	2	0
2	J	1323	1300	1309	2	0
2	K	1283	1252	1252	3	0
2	L	1312	1296	1296	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1301	1283	1283	1	0
2	N	1304	1281	1281	2	0
2	V	1312	1291	1291	2	0
2	W	1305	1278	1278	3	0
2	X	1303	1272	1272	3	0
2	Y	1300	1269	1269	2	0
2	Z	1316	1295	1295	3	0
2	a	1311	1293	1293	0	0
2	b	1296	1266	1266	0	0
3	c	57	56	50	0	0
3	d	57	56	50	0	0
3	e	57	56	50	0	0
3	f	57	56	50	0	0
3	g	57	56	50	0	0
3	h	57	56	50	0	0
3	i	57	56	50	0	0
3	j	57	56	50	0	0
3	k	57	56	50	0	0
3	l	57	56	50	0	0
3	m	57	56	50	0	0
3	n	57	56	50	0	0
3	o	57	56	50	0	0
3	p	57	56	50	0	0
4	A	27	30	29	1	0
4	B	27	30	29	1	0
4	C	27	30	29	1	0
4	D	27	30	29	1	0
4	E	27	30	29	1	0
4	F	27	30	29	1	0
4	G	27	30	29	1	0
4	H	27	30	29	1	0
4	I	27	30	29	0	0
4	J	27	30	29	0	0
4	K	27	30	29	1	0
4	L	27	30	29	0	0
4	M	27	30	29	0	0
4	N	27	30	29	0	0
4	O	27	30	29	1	0
4	P	27	30	29	1	0
4	Q	27	30	29	1	0
4	R	27	30	29	1	0
4	S	27	30	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	27	30	29	1	0
4	U	27	30	29	1	0
4	V	27	30	29	0	0
4	W	27	30	29	0	0
4	X	27	30	29	0	0
4	Y	27	30	29	0	0
4	Z	27	30	29	0	0
4	a	27	30	29	0	0
4	b	27	30	29	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
5	C	20	0	0	0	0
5	D	5	0	0	0	0
5	E	20	0	0	0	0
5	F	5	0	0	0	0
5	G	10	0	0	0	0
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	M	5	0	0	0	0
5	O	10	0	0	1	0
5	P	15	0	0	0	0
5	Q	10	0	0	0	0
5	R	15	0	0	0	0
5	S	20	0	0	0	0
5	T	5	0	0	0	0
5	U	5	0	0	0	0
5	W	5	0	0	0	0
5	p	5	0	0	0	0
6	A	4	6	6	0	0
6	B	8	12	12	0	0
6	C	4	6	6	0	0
6	D	4	6	6	0	0
6	E	4	6	6	0	0
6	F	4	6	6	0	0
6	G	4	6	6	0	0
6	O	4	6	6	0	0
6	P	4	6	6	0	0
6	Q	4	6	6	0	0
6	R	4	6	6	0	0
6	S	4	6	6	0	0
6	T	4	6	6	0	0
6	U	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	1	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	L	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	2	0	0	0	0
7	T	4	0	0	0	0
7	U	2	0	0	0	0
7	V	1	0	0	0	0
All	All	41084	40656	40542	101	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 (101) 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:D:122:GLY:N	1:D:201:ASP:OD2	2.30	0.65
1:G:122:GLY:N	1:G:201:ASP:OD2	2.32	0.62
1:S:158:GLU:OE2	1:S:180:ARG:NH2	2.30	0.61
1:A:122:GLY:N	1:A:201:ASP:OD2	2.34	0.61
1:E:122:GLY:N	1:E:201:ASP:OD2	2.34	0.61
1:F:122:GLY:N	1:F:201:ASP:OD2	2.34	0.60
1:F:148:SER:N	2:M:124:GLN:OE1	2.35	0.59
1:U:122:GLY:N	1:U:201:ASP:OD2	2.36	0.59
1:P:122:GLY:N	1:P:201:ASP:OD2	2.36	0.58
1:Q:122:GLY:N	1:Q:201:ASP:OD2	2.36	0.58
1:S:122:GLY:N	1:S:201:ASP:OD2	2.37	0.58
2:H:99:MSE:SE	4:H:301:ZIL:H26	2.54	0.57
1:B:122:GLY:N	1:B:201:ASP:OD2	2.38	0.57
1:U:158:GLU:OE2	1:U:180:ARG:NH2	2.30	0.57
1:O:122:GLY:N	1:O:201:ASP:OD2	2.38	0.56
2:Z:59:ASP:OD2	2:Z:111:LYS:NZ	2.34	0.55
1:R:148:SER:N	2:Y:124:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:122:GLY:N	1:R:201:ASP:OD2	2.40	0.54
1:E:148:SER:N	2:L:124:GLN:OE1	2.40	0.54
1:P:40:ARG:NH2	1:P:70:ARG:O	2.40	0.54
1:G:137:PRO:HB3	4:G:301:ZIL:H7	1.90	0.53
1:C:122:GLY:N	1:C:201:ASP:OD2	2.42	0.53
1:O:207:ARG:NH2	5:O:303:SO4:O3	2.42	0.52
1:Q:137:PRO:HB3	4:Q:301:ZIL:H7	1.91	0.51
1:O:137:PRO:HB3	4:O:301:ZIL:H7	1.92	0.51
1:C:137:PRO:HB3	4:C:301:ZIL:H7	1.92	0.51
1:S:137:PRO:HB3	4:S:301:ZIL:H7	1.93	0.51
1:E:137:PRO:HB3	4:E:301:ZIL:H7	1.92	0.50
1:B:137:PRO:HB3	4:B:301:ZIL:H7	1.93	0.50
1:T:122:GLY:N	1:T:201:ASP:OD2	2.45	0.50
2:W:59:ASP:OD2	2:W:111:LYS:NZ	2.34	0.50
1:A:148:SER:N	2:H:124:GLN:OE1	2.44	0.50
1:D:148:SER:N	2:K:124:GLN:OE1	2.43	0.50
1:B:40:ARG:NH2	1:B:70:ARG:O	2.43	0.50
1:B:148:SER:N	2:I:124:GLN:OE1	2.45	0.50
1:P:137:PRO:HB3	4:P:301:ZIL:H7	1.94	0.49
1:F:137:PRO:HB3	4:F:301:ZIL:H7	1.95	0.49
2:Z:68:GLY:HA3	2:Z:98:SER:HB2	1.95	0.49
1:A:158:GLU:OE2	1:A:180:ARG:NH2	2.38	0.49
2:K:123:HIS:O	4:K:301:ZIL:H29	2.12	0.49
1:P:148:SER:N	2:W:124:GLN:OE1	2.46	0.49
2:N:68:GLY:HA3	2:N:98:SER:HB2	1.95	0.48
1:O:148:SER:N	2:V:124:GLN:OE1	2.46	0.48
2:Y:68:GLY:HA3	2:Y:98:SER:HB2	1.96	0.48
1:U:137:PRO:HB3	4:U:301:ZIL:H7	1.96	0.48
1:D:57:MET:SD	1:E:105:LEU:HD22	2.54	0.48
1:F:57:MET:SD	1:G:105:LEU:HD22	2.54	0.47
1:S:57:MET:SD	1:T:105:LEU:HD22	2.54	0.47
2:V:68:GLY:HA3	2:V:98:SER:HB2	1.96	0.47
1:R:57:MET:SD	1:S:105:LEU:HD22	2.54	0.47
1:Q:148:SER:N	2:X:124:GLN:OE1	2.47	0.47
1:G:148:SER:N	2:N:124:GLN:OE1	2.46	0.47
1:D:137:PRO:HB3	4:D:301:ZIL:H7	1.96	0.47
1:E:57:MET:SD	1:F:105:LEU:HD22	2.55	0.47
1:A:137:PRO:HB3	4:A:301:ZIL:H7	1.96	0.46
1:T:137:PRO:HB3	4:T:301:ZIL:H7	1.96	0.46
1:D:122:GLY:CA	1:D:201:ASP:OD2	2.63	0.46
1:Q:57:MET:SD	1:R:105:LEU:HD22	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:SD	1:B:105:LEU:HD22	2.56	0.46
1:E:40:ARG:NH2	1:E:70:ARG:O	2.49	0.46
1:E:122:GLY:CA	1:E:201:ASP:OD2	2.63	0.46
1:R:40:ARG:NH1	1:R:63:LEU:O	2.47	0.46
1:B:57:MET:SD	1:C:105:LEU:HD22	2.56	0.45
1:T:57:MET:SD	1:U:105:LEU:HD22	2.56	0.45
1:D:40:ARG:NH2	1:D:70:ARG:O	2.48	0.45
1:C:57:MET:SD	1:D:105:LEU:HD22	2.56	0.45
1:R:137:PRO:HB3	4:R:301:ZIL:H7	1.98	0.45
1:A:40:ARG:NH2	1:A:70:ARG:O	2.49	0.45
1:S:148:SER:N	2:Z:124:GLN:OE1	2.50	0.45
2:H:68:GLY:HA3	2:H:98:SER:HB2	1.99	0.44
2:X:68:GLY:HA3	2:X:98:SER:HB2	1.97	0.44
1:P:57:MET:SD	1:Q:105:LEU:HD22	2.57	0.44
1:D:97:ARG:HA	1:E:208:LYS:HA	2.00	0.44
1:O:105:LEU:HD22	1:U:57:MET:SD	2.58	0.44
1:B:96:VAL:O	1:C:208:LYS:NZ	2.47	0.44
2:L:68:GLY:HA3	2:L:98:SER:HB2	2.00	0.43
1:G:122:GLY:CA	1:G:201:ASP:OD2	2.66	0.43
2:I:68:GLY:HA3	2:I:98:SER:HB2	1.99	0.43
1:S:40:ARG:NH2	1:S:70:ARG:O	2.49	0.43
2:K:68:GLY:HA3	2:K:98:SER:HB2	2.00	0.43
1:P:122:GLY:CA	1:P:201:ASP:OD2	2.66	0.43
1:A:208:LYS:HA	1:G:97:ARG:HA	2.01	0.42
2:X:124:GLN:N	2:X:169:SER:O	2.48	0.42
1:C:148:SER:N	2:J:124:GLN:OE1	2.51	0.42
1:R:40:ARG:NH2	1:R:70:ARG:O	2.53	0.42
1:F:40:ARG:NH2	1:F:70:ARG:O	2.49	0.42
1:B:207:ARG:NH2	5:B:302:SO4:O3	2.53	0.42
1:D:158:GLU:OE2	1:D:180:ARG:NH2	2.38	0.42
1:C:40:ARG:NH1	1:C:63:LEU:O	2.49	0.42
1:G:67:ASP:OD2	1:G:70:ARG:HD3	2.20	0.42
1:O:122:GLY:CA	1:O:201:ASP:OD2	2.67	0.41
1:D:81:GLY:N	7:D:401:HOH:O	2.52	0.41
1:F:122:GLY:CA	1:F:201:ASP:OD2	2.68	0.41
2:J:68:GLY:HA3	2:J:98:SER:HB2	2.00	0.41
1:C:122:GLY:CA	1:C:201:ASP:OD2	2.69	0.41
1:F:86:LEU:HD12	1:F:111:ALA:HB1	2.03	0.41
1:Q:91:ASP:OD2	1:R:129:ASN:HB2	2.21	0.40
1:F:94:GLN:NE2	1:F:118:ALA:O	2.54	0.40
2:W:36:VAL:HB	2:W:69:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLN:NE2	1:B:118:ALA:O	2.52	0.40
1:D:40:ARG:NH1	1:D:63:LEU:O	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/202 (96%)	192 (98%)	3 (2%)	0	100	100
1	B	195/202 (96%)	192 (98%)	3 (2%)	0	100	100
1	C	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	D	193/202 (96%)	189 (98%)	4 (2%)	0	100	100
1	E	195/202 (96%)	192 (98%)	3 (2%)	0	100	100
1	F	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	G	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	O	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	P	192/202 (95%)	189 (98%)	3 (2%)	0	100	100
1	Q	193/202 (96%)	190 (98%)	3 (2%)	0	100	100
1	R	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	S	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	T	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
1	U	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
2	H	172/194 (89%)	170 (99%)	2 (1%)	0	100	100
2	I	170/194 (88%)	168 (99%)	2 (1%)	0	100	100
2	J	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
2	K	170/194 (88%)	168 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	172/194 (89%)	170 (99%)	2 (1%)	0	100	100
2	M	171/194 (88%)	169 (99%)	2 (1%)	0	100	100
2	N	172/194 (89%)	170 (99%)	2 (1%)	0	100	100
2	V	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
2	W	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
2	X	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
2	Y	172/194 (89%)	170 (99%)	2 (1%)	0	100	100
2	Z	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
2	a	172/194 (89%)	170 (99%)	2 (1%)	0	100	100
2	b	173/194 (89%)	171 (99%)	2 (1%)	0	100	100
3	c	3/7 (43%)	3 (100%)	0	0	100	100
3	d	3/7 (43%)	3 (100%)	0	0	100	100
3	e	3/7 (43%)	3 (100%)	0	0	100	100
3	f	3/7 (43%)	3 (100%)	0	0	100	100
3	g	3/7 (43%)	3 (100%)	0	0	100	100
3	h	3/7 (43%)	3 (100%)	0	0	100	100
3	i	3/7 (43%)	3 (100%)	0	0	100	100
3	j	3/7 (43%)	3 (100%)	0	0	100	100
3	k	3/7 (43%)	3 (100%)	0	0	100	100
3	l	3/7 (43%)	3 (100%)	0	0	100	100
3	m	3/7 (43%)	3 (100%)	0	0	100	100
3	n	3/7 (43%)	3 (100%)	0	0	100	100
3	o	3/7 (43%)	3 (100%)	0	0	100	100
3	p	3/7 (43%)	3 (100%)	0	0	100	100
All	All	5166/5642 (92%)	5095 (99%)	71 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	160/167 (96%)	158 (99%)	2 (1%)	69	87
1	B	163/167 (98%)	160 (98%)	3 (2%)	59	82
1	C	161/167 (96%)	159 (99%)	2 (1%)	71	88
1	D	158/167 (95%)	155 (98%)	3 (2%)	57	81
1	E	161/167 (96%)	159 (99%)	2 (1%)	71	88
1	F	160/167 (96%)	158 (99%)	2 (1%)	69	87
1	G	160/167 (96%)	159 (99%)	1 (1%)	86	94
1	O	160/167 (96%)	158 (99%)	2 (1%)	69	87
1	P	160/167 (96%)	158 (99%)	2 (1%)	69	87
1	Q	159/167 (95%)	157 (99%)	2 (1%)	69	87
1	R	160/167 (96%)	158 (99%)	2 (1%)	69	87
1	S	163/167 (98%)	161 (99%)	2 (1%)	71	88
1	T	162/167 (97%)	160 (99%)	2 (1%)	71	88
1	U	162/167 (97%)	160 (99%)	2 (1%)	71	88
2	H	130/143 (91%)	128 (98%)	2 (2%)	65	85
2	I	130/143 (91%)	128 (98%)	2 (2%)	65	85
2	J	133/143 (93%)	131 (98%)	2 (2%)	65	85
2	K	127/143 (89%)	125 (98%)	2 (2%)	62	84
2	L	132/143 (92%)	130 (98%)	2 (2%)	65	85
2	M	131/143 (92%)	130 (99%)	1 (1%)	81	93
2	N	130/143 (91%)	128 (98%)	2 (2%)	65	85
2	V	130/143 (91%)	128 (98%)	2 (2%)	65	85
2	W	128/143 (90%)	126 (98%)	2 (2%)	62	84
2	X	129/143 (90%)	127 (98%)	2 (2%)	62	84
2	Y	129/143 (90%)	127 (98%)	2 (2%)	62	84
2	Z	131/143 (92%)	129 (98%)	2 (2%)	65	85
2	a	131/143 (92%)	130 (99%)	1 (1%)	81	93
2	b	127/143 (89%)	125 (98%)	2 (2%)	62	84
3	c	3/3 (100%)	3 (100%)	0	100	100
3	d	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	3/3 (100%)	3 (100%)	0	100	100
3	f	3/3 (100%)	3 (100%)	0	100	100
3	g	3/3 (100%)	3 (100%)	0	100	100
3	h	3/3 (100%)	3 (100%)	0	100	100
3	i	3/3 (100%)	3 (100%)	0	100	100
3	j	3/3 (100%)	3 (100%)	0	100	100
3	k	3/3 (100%)	3 (100%)	0	100	100
3	l	3/3 (100%)	3 (100%)	0	100	100
3	m	3/3 (100%)	3 (100%)	0	100	100
3	n	3/3 (100%)	3 (100%)	0	100	100
3	o	3/3 (100%)	3 (100%)	0	100	100
3	p	3/3 (100%)	3 (100%)	0	100	100
All	All	4109/4382 (94%)	4054 (99%)	55 (1%)	69	87

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	135	HIS
1	B	86	LEU
1	B	134	ILE
1	B	135	HIS
1	C	86	LEU
1	C	135	HIS
1	D	86	LEU
1	D	134	ILE
1	D	135	HIS
1	E	86	LEU
1	E	135	HIS
1	F	86	LEU
1	F	135	HIS
1	G	135	HIS
2	H	31	PHE
2	H	123	HIS
2	I	31	PHE
2	I	123	HIS
2	J	31	PHE
2	J	123	HIS

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Mol	Chain	Res	Type
2	K	31	PHE
2	K	123	HIS
2	L	31	PHE
2	L	123	HIS
2	M	123	HIS
2	N	31	PHE
2	N	123	HIS
1	O	86	LEU
1	O	135	HIS
1	P	86	LEU
1	P	135	HIS
1	Q	86	LEU
1	Q	135	HIS
1	R	86	LEU
1	R	135	HIS
1	S	86	LEU
1	S	135	HIS
1	T	86	LEU
1	T	135	HIS
1	U	86	LEU
1	U	135	HIS
2	V	31	PHE
2	V	123	HIS
2	W	31	PHE
2	W	123	HIS
2	X	31	PHE
2	X	123	HIS
2	Y	44	LEU
2	Y	123	HIS
2	Z	31	PHE
2	Z	123	HIS
2	a	123	HIS
2	b	31	PHE
2	b	123	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	154	ASN
2	J	154	ASN
2	K	154	ASN
2	L	154	ASN

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Mol	Chain	Res	Type
2	M	154	ASN
2	N	154	ASN
2	V	154	ASN
2	W	154	ASN
2	X	154	ASN
2	Y	154	ASN
2	Z	154	ASN
2	a	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	WFP	g	2	3	12,13,14	0.37	0	14,17,19	0.29	0
3	WFP	n	2	3	12,13,14	0.38	0	14,17,19	0.27	0
3	WFP	f	2	3	12,13,14	0.38	0	14,17,19	0.23	0
3	WFP	e	2	3	12,13,14	0.37	0	14,17,19	0.30	0
3	WFP	d	2	3	12,13,14	0.38	0	14,17,19	0.29	0
3	WFP	h	2	3	12,13,14	0.38	0	14,17,19	0.27	0
3	WFP	l	2	3	12,13,14	0.38	0	14,17,19	0.29	0
3	WFP	o	2	3	12,13,14	0.38	0	14,17,19	0.28	0
3	WFP	m	2	3	12,13,14	0.39	0	14,17,19	0.33	0
3	WFP	c	2	3	12,13,14	0.38	0	14,17,19	0.29	0
3	WFP	k	2	3	12,13,14	0.37	0	14,17,19	0.25	0
3	WFP	j	2	3	12,13,14	0.37	0	14,17,19	0.30	0
3	WFP	p	2	3	12,13,14	0.38	0	14,17,19	0.25	0
3	WFP	i	2	3	12,13,14	0.38	0	14,17,19	0.26	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
3	WFP	g	2	3	-	0/5/6/8	0/1/1/1
3	WFP	n	2	3	-	0/5/6/8	0/1/1/1
3	WFP	f	2	3	-	0/5/6/8	0/1/1/1
3	WFP	e	2	3	-	0/5/6/8	0/1/1/1
3	WFP	d	2	3	-	0/5/6/8	0/1/1/1
3	WFP	h	2	3	-	0/5/6/8	0/1/1/1
3	WFP	l	2	3	-	0/5/6/8	0/1/1/1
3	WFP	o	2	3	-	0/5/6/8	0/1/1/1
3	WFP	m	2	3	-	0/5/6/8	0/1/1/1
3	WFP	c	2	3	-	0/5/6/8	0/1/1/1
3	WFP	k	2	3	-	0/5/6/8	0/1/1/1
3	WFP	j	2	3	-	0/5/6/8	0/1/1/1
3	WFP	p	2	3	-	1/5/6/8	0/1/1/1
3	WFP	i	2	3	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	p	2	WFP	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

78 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	$\#\|Z\| > 2$
4	ZIL	R	301	-	27,27,27	0.11	0	35,35,35	0.63	1 (2%)
6	DMS	C	306	-	3,3,3	0.59	0	3,3,3	0.50	0
4	ZIL	M	301	-	27,27,27	0.09	0	35,35,35	0.15	0
5	SO4	E	303	-	4,4,4	0.15	0	6,6,6	0.06	0
6	DMS	O	304	-	3,3,3	0.61	0	3,3,3	0.46	0
6	DMS	G	304	-	3,3,3	0.62	0	3,3,3	0.50	0
4	ZIL	V	301	-	27,27,27	0.10	0	35,35,35	0.17	0
5	SO4	I	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	ZIL	B	301	-	27,27,27	0.11	0	35,35,35	0.65	1 (2%)
5	SO4	T	302	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ZIL	N	301	-	27,27,27	0.11	0	35,35,35	0.23	0
5	SO4	U	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	ZIL	P	301	-	27,27,27	0.12	0	35,35,35	0.63	1 (2%)
5	SO4	R	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	R	304	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	p	101	3	4,4,4	0.20	0	6,6,6	0.10	0
4	ZIL	K	301	-	27,27,27	0.09	0	35,35,35	0.16	0
5	SO4	Q	303	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	P	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	ZIL	L	301	-	27,27,27	0.09	0	35,35,35	0.16	0
5	SO4	R	302	-	4,4,4	0.14	0	6,6,6	0.06	0
6	DMS	S	306	-	3,3,3	0.61	0	3,3,3	0.51	0
4	ZIL	W	301	-	27,27,27	0.11	0	35,35,35	0.17	0
5	SO4	W	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	P	303	-	4,4,4	0.15	0	6,6,6	0.06	0
6	DMS	R	305	-	3,3,3	0.63	0	3,3,3	0.54	0
6	DMS	T	303	-	3,3,3	0.59	0	3,3,3	0.61	0
4	ZIL	T	301	-	27,27,27	0.11	0	35,35,35	0.63	1 (2%)
4	ZIL	a	301	-	27,27,27	0.12	0	35,35,35	0.24	0
5	SO4	P	304	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ZIL	A	301	-	27,27,27	0.12	0	35,35,35	0.63	1 (2%)
6	DMS	E	306	-	3,3,3	0.63	0	3,3,3	0.45	0
6	DMS	D	303	-	3,3,3	0.62	0	3,3,3	0.46	0
4	ZIL	Z	301	-	27,27,27	0.09	0	35,35,35	0.22	0
5	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DMS	P	305	-	3,3,3	0.61	0	3,3,3	0.47	0
4	ZIL	S	301	-	27,27,27	0.12	0	35,35,35	0.63	1 (2%)
6	DMS	U	303	-	3,3,3	0.60	0	3,3,3	0.57	0
4	ZIL	F	301	-	27,27,27	0.11	0	35,35,35	0.64	1 (2%)
4	ZIL	O	301	-	27,27,27	0.12	0	35,35,35	0.65	1 (2%)
4	ZIL	G	301	-	27,27,27	0.13	0	35,35,35	0.64	1 (2%)
6	DMS	B	304	-	3,3,3	0.63	0	3,3,3	0.51	0
4	ZIL	D	301	-	27,27,27	0.12	0	35,35,35	0.63	1 (2%)
4	ZIL	J	301	-	27,27,27	0.10	0	35,35,35	0.14	0
6	DMS	B	303	-	3,3,3	0.60	0	3,3,3	0.48	0
5	SO4	F	302	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	S	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	O	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	303	-	4,4,4	0.14	0	6,6,6	0.06	0
4	ZIL	U	301	-	27,27,27	0.12	0	35,35,35	0.63	1 (2%)
5	SO4	S	305	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ZIL	H	301	-	27,27,27	0.09	0	35,35,35	0.15	0
4	ZIL	I	301	-	27,27,27	0.09	0	35,35,35	0.15	0
6	DMS	Q	304	-	3,3,3	0.62	0	3,3,3	0.55	0
4	ZIL	Y	301	-	27,27,27	0.11	0	35,35,35	0.24	0
5	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	S	304	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	E	304	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	Q	302	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	E	305	-	4,4,4	0.14	0	6,6,6	0.06	0
4	ZIL	C	301	-	27,27,27	0.11	0	35,35,35	0.64	1 (2%)
5	SO4	S	302	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.05	0
6	DMS	A	303	-	3,3,3	0.60	0	3,3,3	0.54	0
6	DMS	F	303	-	3,3,3	0.60	0	3,3,3	0.48	0
5	SO4	O	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	M	302	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	ZIL	E	301	-	27,27,27	0.12	0	35,35,35	0.64	1 (2%)
4	ZIL	b	301	-	27,27,27	0.09	0	35,35,35	0.16	0
4	ZIL	X	301	-	27,27,27	0.10	0	35,35,35	0.19	0
4	ZIL	Q	301	-	27,27,27	0.12	0	35,35,35	0.65	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.07	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
4	ZIL	R	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	Y	301	-	-	7/31/31/31	0/1/1/1
4	ZIL	D	301	-	-	9/31/31/31	0/1/1/1
4	ZIL	J	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	M	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	T	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	V	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	C	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	B	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	a	301	-	-	7/31/31/31	0/1/1/1
4	ZIL	A	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	N	301	-	-	5/31/31/31	0/1/1/1
4	ZIL	P	301	-	-	9/31/31/31	0/1/1/1
4	ZIL	U	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	E	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	H	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	Z	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	K	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	b	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	I	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	X	301	-	-	8/31/31/31	0/1/1/1
4	ZIL	L	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	S	301	-	-	9/31/31/31	0/1/1/1
4	ZIL	W	301	-	-	2/31/31/31	0/1/1/1
4	ZIL	F	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	Q	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	O	301	-	-	10/31/31/31	0/1/1/1
4	ZIL	G	301	-	-	10/31/31/31	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	301	ZIL	C5-C4-N1	2.66	117.61	110.36
4	B	301	ZIL	C5-C4-N1	2.66	117.59	110.36
4	O	301	ZIL	C5-C4-N1	2.65	117.57	110.36
4	T	301	ZIL	C5-C4-N1	2.64	117.56	110.36
4	Q	301	ZIL	C5-C4-N1	2.63	117.52	110.36
4	S	301	ZIL	C5-C4-N1	2.63	117.51	110.36
4	G	301	ZIL	C5-C4-N1	2.60	117.44	110.36
4	P	301	ZIL	C5-C4-N1	2.59	117.42	110.36
4	F	301	ZIL	C5-C4-N1	2.59	117.40	110.36
4	A	301	ZIL	C5-C4-N1	2.56	117.34	110.36
4	E	301	ZIL	C5-C4-N1	2.55	117.31	110.36
4	R	301	ZIL	C5-C4-N1	2.54	117.28	110.36
4	D	301	ZIL	C5-C4-N1	2.43	116.96	110.36
4	U	301	ZIL	C5-C4-N1	2.39	116.88	110.36

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	ZIL	C3-C2-C4-C5
4	A	301	ZIL	C4-C5-N-C6
4	A	301	ZIL	O-C5-N-C6
4	B	301	ZIL	C3-C2-C4-C5
4	B	301	ZIL	C4-C5-N-C6
4	B	301	ZIL	O-C5-N-C6
4	C	301	ZIL	C3-C2-C4-C5
4	C	301	ZIL	C4-C5-N-C6
4	C	301	ZIL	O-C5-N-C6
4	D	301	ZIL	C3-C2-C4-C5
4	D	301	ZIL	C4-C5-N-C6
4	D	301	ZIL	O-C5-N-C6
4	E	301	ZIL	C3-C2-C4-C5
4	E	301	ZIL	C4-C5-N-C6
4	E	301	ZIL	O-C5-N-C6
4	F	301	ZIL	C3-C2-C4-C5
4	F	301	ZIL	C4-C5-N-C6
4	F	301	ZIL	O-C5-N-C6
4	G	301	ZIL	C3-C2-C4-C5
4	G	301	ZIL	C4-C5-N-C6
4	G	301	ZIL	O-C5-N-C6

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Mol	Chain	Res	Type	Atoms
4	O	301	ZIL	C4-C5-N-C6
4	O	301	ZIL	O-C5-N-C6
4	P	301	ZIL	C3-C2-C4-C5
4	P	301	ZIL	C4-C5-N-C6
4	P	301	ZIL	O-C5-N-C6
4	Q	301	ZIL	C3-C2-C4-C5
4	Q	301	ZIL	C4-C5-N-C6
4	Q	301	ZIL	O-C5-N-C6
4	R	301	ZIL	C3-C2-C4-N1
4	R	301	ZIL	C1-C2-C4-C5
4	R	301	ZIL	C3-C2-C4-C5
4	R	301	ZIL	C4-C5-N-C6
4	R	301	ZIL	O-C5-N-C6
4	S	301	ZIL	C3-C2-C4-C5
4	S	301	ZIL	C4-C5-N-C6
4	S	301	ZIL	O-C5-N-C6
4	T	301	ZIL	C3-C2-C4-C5
4	T	301	ZIL	C4-C5-N-C6
4	T	301	ZIL	O-C5-N-C6
4	U	301	ZIL	C3-C2-C4-N1
4	U	301	ZIL	C3-C2-C4-C5
4	U	301	ZIL	C4-C5-N-C6
4	U	301	ZIL	O-C5-N-C6
4	Y	301	ZIL	C11-C6-C7-C8
4	D	301	ZIL	C3-C2-C4-N1
4	F	301	ZIL	C3-C2-C4-N1
4	R	301	ZIL	C1-C2-C4-N1
4	S	301	ZIL	C3-C2-C4-N1
4	U	301	ZIL	C1-C2-C4-N1
4	a	301	ZIL	C-C1-C2-C4
4	A	301	ZIL	C1-C2-C4-C5
4	B	301	ZIL	C1-C2-C4-C5
4	C	301	ZIL	C1-C2-C4-C5
4	D	301	ZIL	C1-C2-C4-C5
4	E	301	ZIL	C1-C2-C4-C5
4	F	301	ZIL	C1-C2-C4-C5
4	O	301	ZIL	C3-C2-C4-C5
4	P	301	ZIL	C1-C2-C4-C5
4	Q	301	ZIL	C1-C2-C4-C5
4	S	301	ZIL	C1-C2-C4-C5
4	T	301	ZIL	C1-C2-C4-C5
4	U	301	ZIL	C1-C2-C4-C5

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Mol	Chain	Res	Type	Atoms
4	Y	301	ZIL	N-C6-C7-C8
4	X	301	ZIL	C6-C7-C8-C10
4	A	301	ZIL	C1-C2-C4-N1
4	D	301	ZIL	C1-C2-C4-N1
4	F	301	ZIL	C1-C2-C4-N1
4	S	301	ZIL	C1-C2-C4-N1
4	X	301	ZIL	C6-C7-C8-C9
4	A	301	ZIL	C3-C2-C4-N1
4	C	301	ZIL	C1-C2-C4-N1
4	C	301	ZIL	C3-C2-C4-N1
4	G	301	ZIL	N1-C4-C5-O
4	a	301	ZIL	C-C1-C2-C3
4	E	301	ZIL	N1-C4-C5-O
4	O	301	ZIL	N1-C4-C5-O
4	N	301	ZIL	C-C1-C2-C4
4	N	301	ZIL	C-C1-C2-C3
4	B	301	ZIL	C1-C2-C4-N1
4	E	301	ZIL	C1-C2-C4-N1
4	P	301	ZIL	C1-C2-C4-N1
4	T	301	ZIL	C1-C2-C4-N1
4	H	301	ZIL	O2-C11-C6-N
4	I	301	ZIL	O1-C11-C6-N
4	M	301	ZIL	O1-C11-C6-N
4	M	301	ZIL	O2-C11-C6-N
4	Z	301	ZIL	O1-C11-C6-N
4	b	301	ZIL	O1-C11-C6-N
4	b	301	ZIL	O2-C11-C6-N
4	B	301	ZIL	C3-C2-C4-N1
4	Q	301	ZIL	C1-C2-C4-N1
4	H	301	ZIL	O1-C11-C6-N
4	I	301	ZIL	O2-C11-C6-N
4	Z	301	ZIL	O2-C11-C6-N
4	F	301	ZIL	N1-C4-C5-O
4	U	301	ZIL	N1-C4-C5-O
4	E	301	ZIL	C3-C2-C4-N1
4	T	301	ZIL	C3-C2-C4-N1
4	G	301	ZIL	C6-C7-C8-C10
4	O	301	ZIL	C6-C7-C8-C10
4	U	301	ZIL	C6-C7-C8-C10
4	C	301	ZIL	C6-C7-C8-C10
4	E	301	ZIL	C6-C7-C8-C10
4	C	301	ZIL	N1-C4-C5-O

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Mol	Chain	Res	Type	Atoms
4	Q	301	ZIL	N1-C4-C5-O
4	G	301	ZIL	C1-C2-C4-C5
4	P	301	ZIL	C3-C2-C4-N1
4	Q	301	ZIL	C3-C2-C4-N1
4	X	301	ZIL	O1-C11-C6-N
4	B	301	ZIL	N1-C4-C5-O
4	D	301	ZIL	C6-C7-C8-C10
4	T	301	ZIL	C6-C7-C8-C10
4	Q	301	ZIL	C6-C7-C8-C10
4	A	301	ZIL	N1-C4-C5-O
4	D	301	ZIL	N1-C4-C5-O
4	S	301	ZIL	N1-C4-C5-O
4	T	301	ZIL	N1-C4-C5-O
4	J	301	ZIL	O1-C11-C6-N
4	J	301	ZIL	O2-C11-C6-N
4	N	301	ZIL	O1-C11-C6-N
4	N	301	ZIL	O2-C11-C6-N
4	W	301	ZIL	O1-C11-C6-N
4	X	301	ZIL	O2-C11-C6-N
4	Y	301	ZIL	C-C1-C2-C4
4	G	301	ZIL	C1-C2-C4-N1
4	a	301	ZIL	C11-C6-C7-C8
4	P	301	ZIL	C6-C7-C8-C10
4	K	301	ZIL	O2-C11-C6-N
4	V	301	ZIL	O1-C11-C6-N
4	V	301	ZIL	O2-C11-C6-N
4	Y	301	ZIL	O1-C11-C6-N
4	Y	301	ZIL	O2-C11-C6-N
4	R	301	ZIL	N1-C4-C5-O
4	P	301	ZIL	N1-C4-C5-O
4	E	301	ZIL	N1-C4-C5-N
4	A	301	ZIL	C6-C7-C8-C10
4	Y	301	ZIL	C-C1-C2-C3
4	K	301	ZIL	O1-C11-C6-N
4	L	301	ZIL	O1-C11-C6-N
4	L	301	ZIL	O2-C11-C6-N
4	W	301	ZIL	O2-C11-C6-N
4	a	301	ZIL	O1-C11-C6-N
4	a	301	ZIL	O2-C11-C6-N
4	S	301	ZIL	C6-C7-C8-C10
4	G	301	ZIL	C3-C2-C4-N1
4	O	301	ZIL	N1-C4-C5-N

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Mol	Chain	Res	Type	Atoms
4	a	301	ZIL	N-C6-C7-C8
4	F	301	ZIL	C6-C7-C8-C10
4	B	301	ZIL	C6-C7-C8-C10
4	O	301	ZIL	C1-C2-C4-C5
4	G	301	ZIL	N1-C4-C5-N
4	F	301	ZIL	N1-C4-C5-N
4	U	301	ZIL	N1-C4-C5-N
4	X	301	ZIL	O2-C11-C6-C7
4	C	301	ZIL	N1-C4-C5-N
4	Q	301	ZIL	N1-C4-C5-N
4	D	301	ZIL	N1-C4-C5-N
4	B	301	ZIL	N1-C4-C5-N
4	X	301	ZIL	O1-C11-C6-C7
4	R	301	ZIL	O4-C12-N1-C4
4	E	301	ZIL	C2-C4-C5-O
4	A	301	ZIL	N1-C4-C5-N
4	S	301	ZIL	N1-C4-C5-N
4	T	301	ZIL	N1-C4-C5-N
4	O	301	ZIL	C2-C4-C5-O
4	Y	301	ZIL	C14-C13-O4-C12
4	a	301	ZIL	C14-C13-O4-C12
4	R	301	ZIL	C6-C7-C8-C10
4	X	301	ZIL	N-C6-C7-C8
4	P	301	ZIL	N1-C4-C5-N
4	R	301	ZIL	N1-C4-C5-N
4	U	301	ZIL	C2-C4-C5-O
4	O	301	ZIL	C1-C2-C4-N1
4	F	301	ZIL	C2-C4-C5-O
4	G	301	ZIL	C2-C4-C5-O
4	B	301	ZIL	C2-C4-C5-O
4	Q	301	ZIL	C2-C4-C5-O
4	N	301	ZIL	C14-C13-O4-C12
4	O	301	ZIL	C3-C2-C4-N1
4	X	301	ZIL	C11-C6-C7-C8
4	T	301	ZIL	O4-C12-N1-C4
4	C	301	ZIL	C2-C4-C5-O
4	A	301	ZIL	C2-C4-C5-O

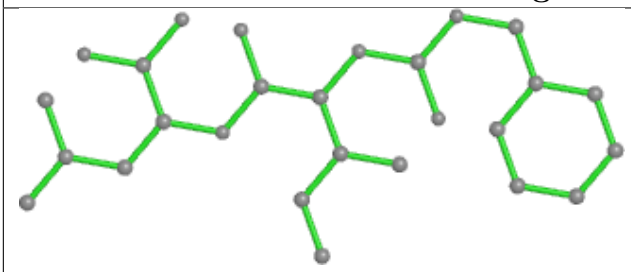
There are no ring outliers.

18 monomers are involved in 18 short contacts:

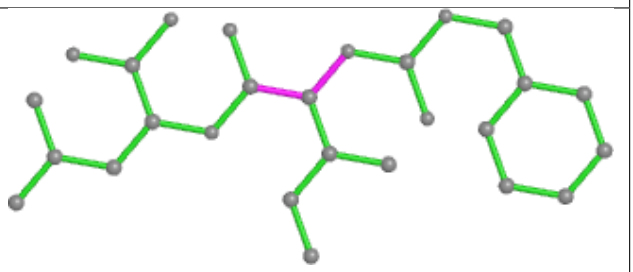
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	301	ZIL	1	0
4	B	301	ZIL	1	0
4	P	301	ZIL	1	0
4	K	301	ZIL	1	0
4	T	301	ZIL	1	0
4	A	301	ZIL	1	0
5	B	302	SO4	1	0
4	S	301	ZIL	1	0
4	F	301	ZIL	1	0
4	O	301	ZIL	1	0
4	G	301	ZIL	1	0
4	D	301	ZIL	1	0
5	O	303	SO4	1	0
4	U	301	ZIL	1	0
4	H	301	ZIL	1	0
4	C	301	ZIL	1	0
4	E	301	ZIL	1	0
4	Q	301	ZIL	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.

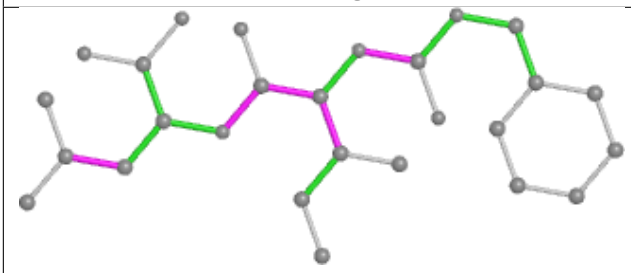
Ligand ZIL R 301



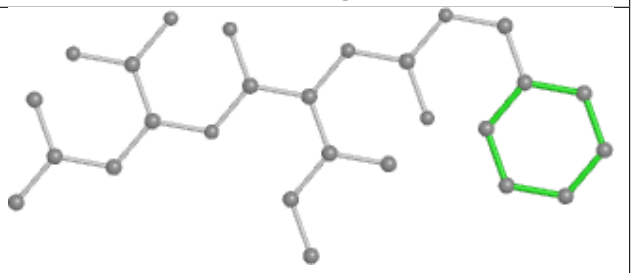
Bond lengths



Bond angles

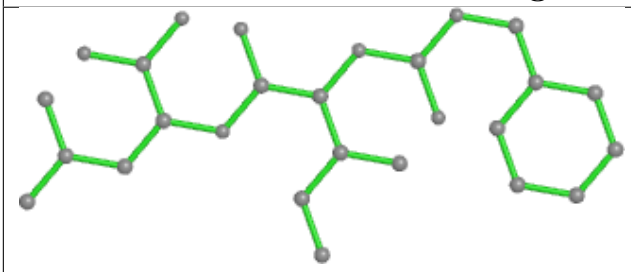


Torsions



Rings

Ligand ZIL M 301



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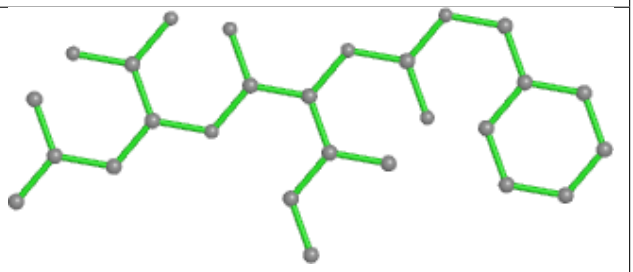

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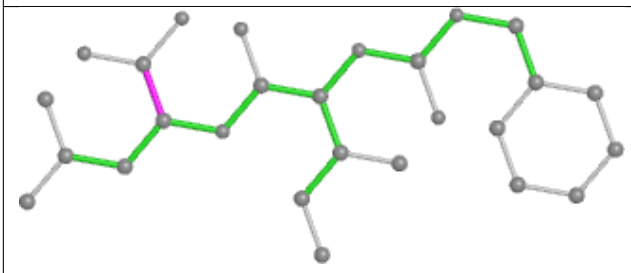

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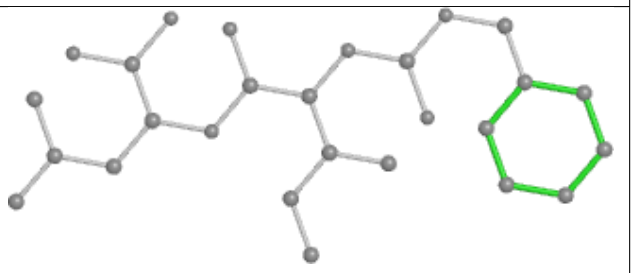
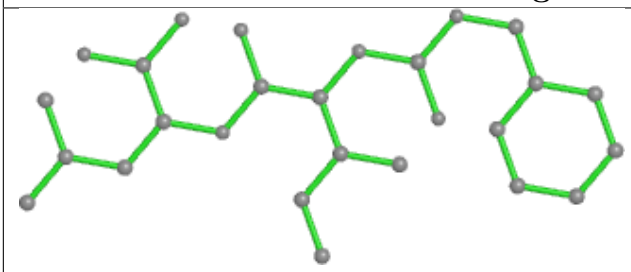


Rings

Ligand ZIL V 301



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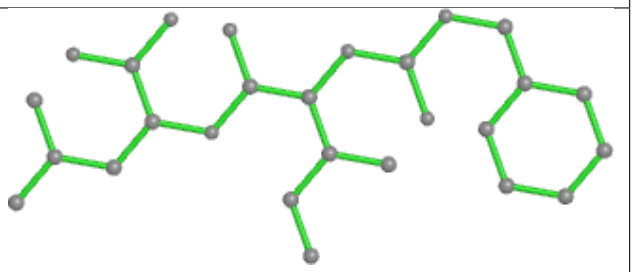
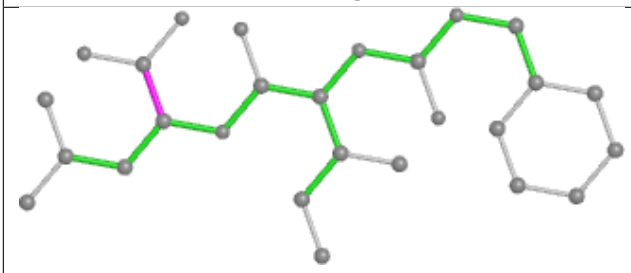
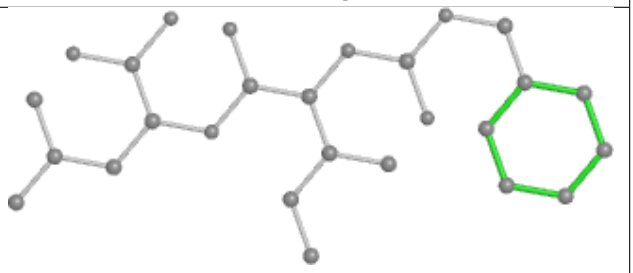


Bond angles

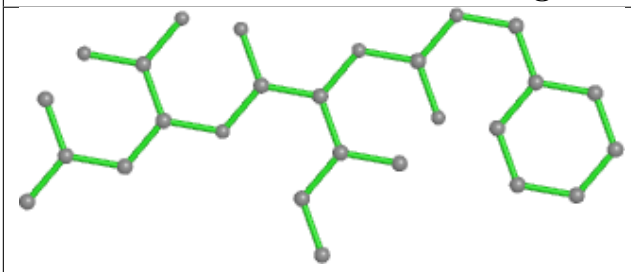


Torsions



Rings

Ligand ZIL B 301



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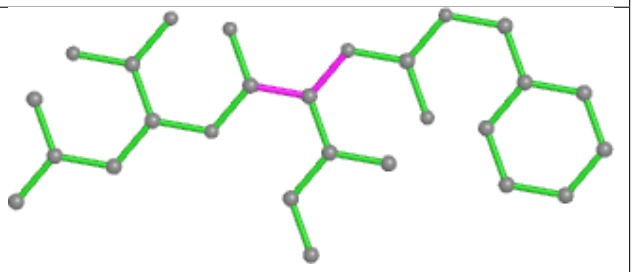
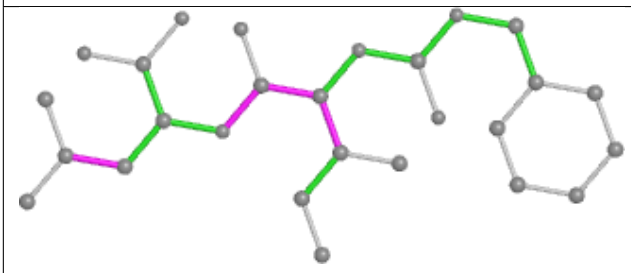


Bond angles



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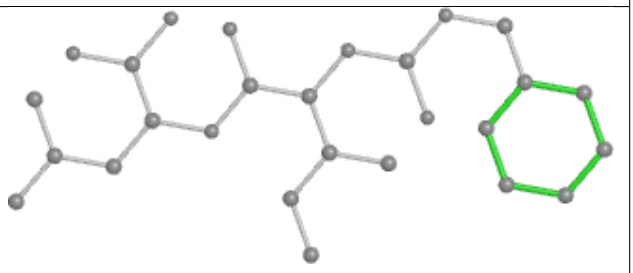
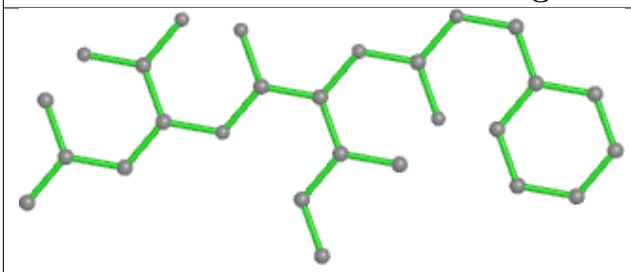


Rings

Ligand ZIL N 301



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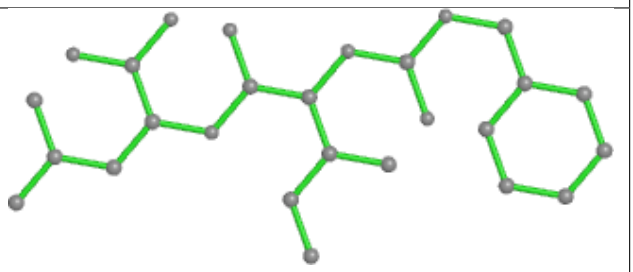

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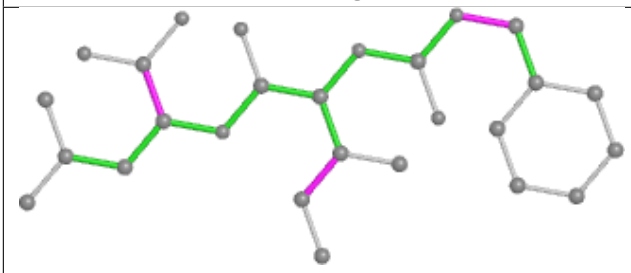

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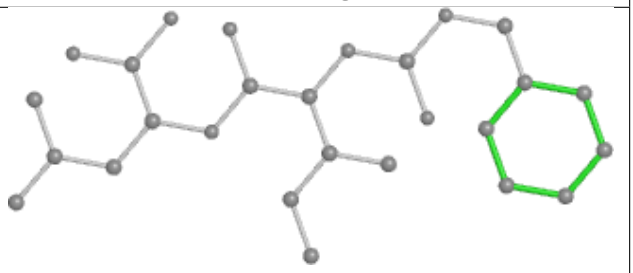

Rings

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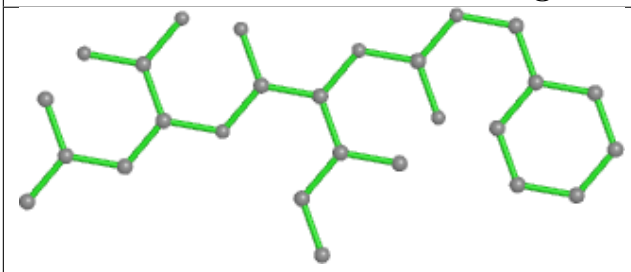

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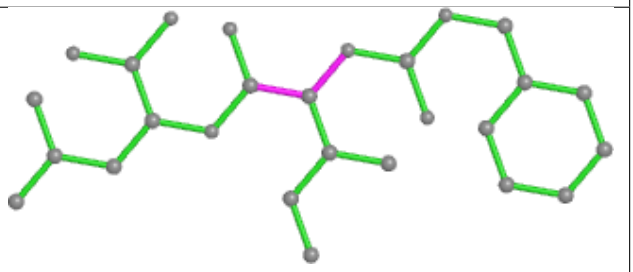

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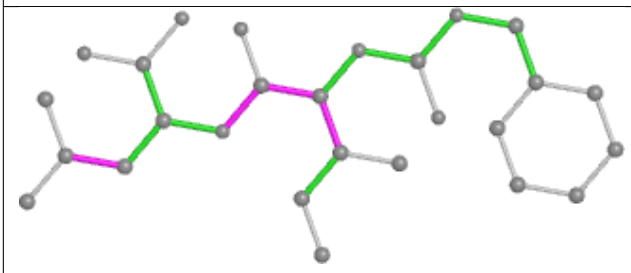

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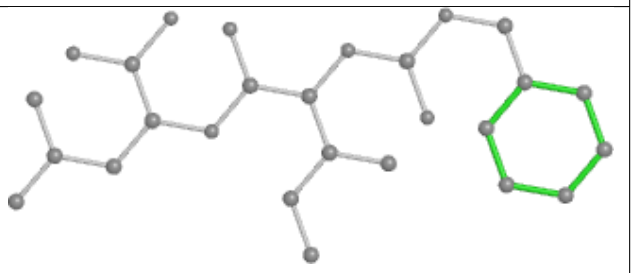

Rings

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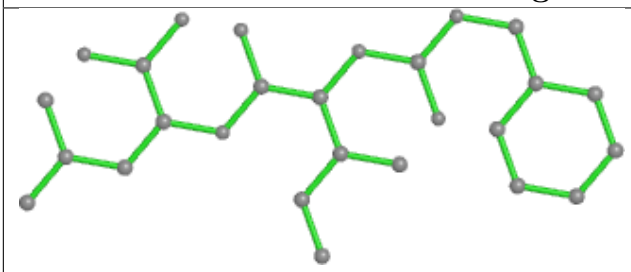

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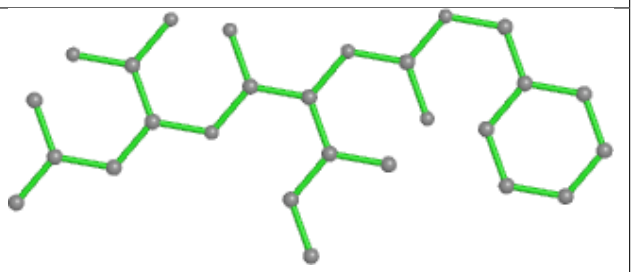

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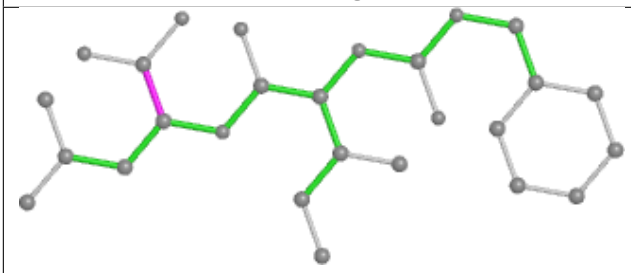

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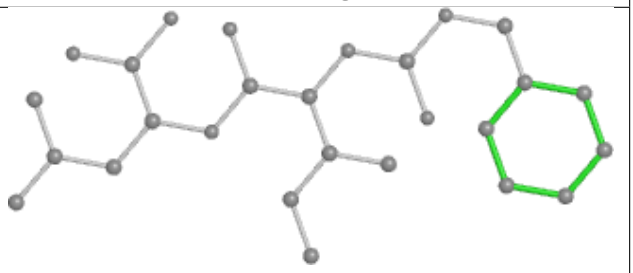

Rings

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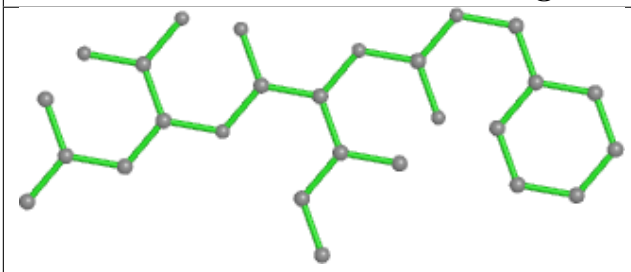

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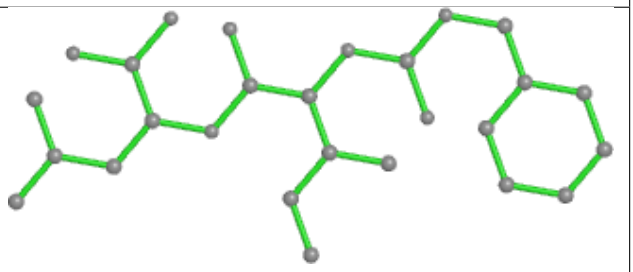

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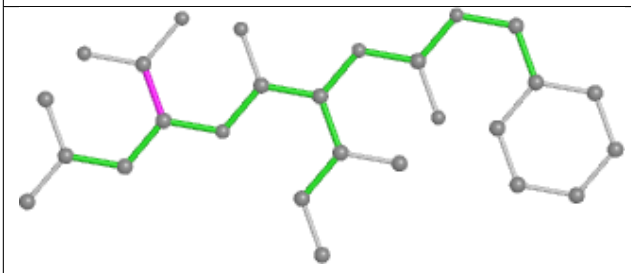

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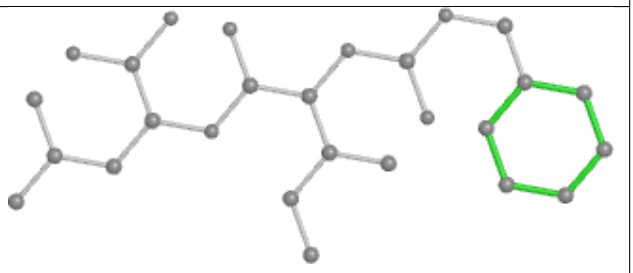
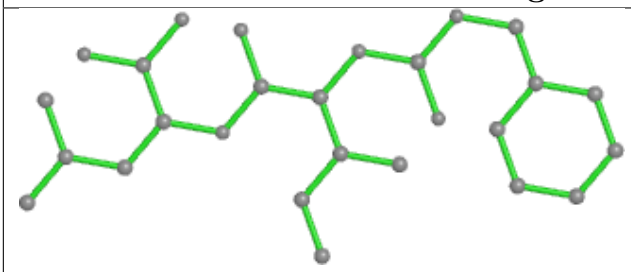


Rings

Ligand ZIL W 301



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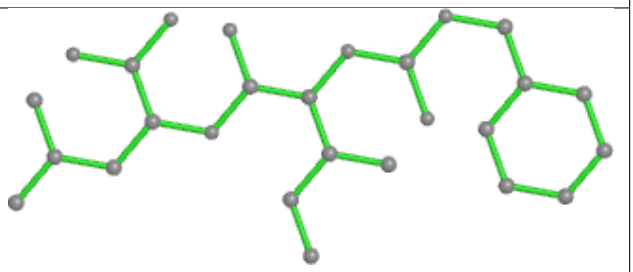
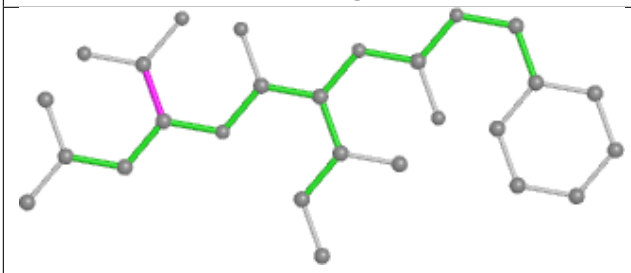


Bond angles



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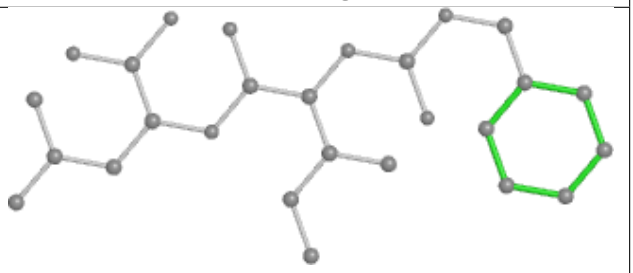
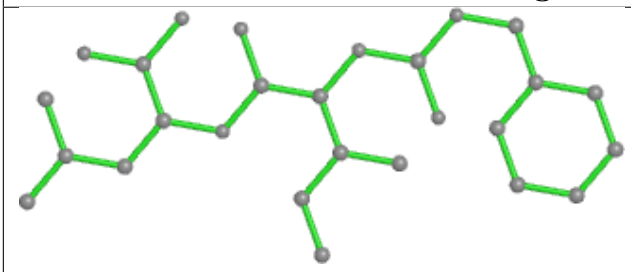


Rings

Ligand ZIL T 301



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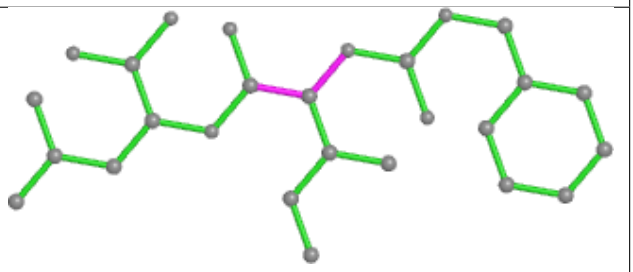

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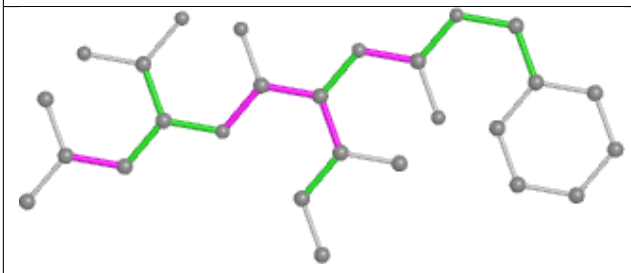

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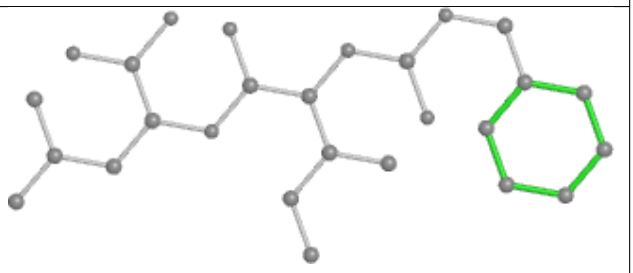
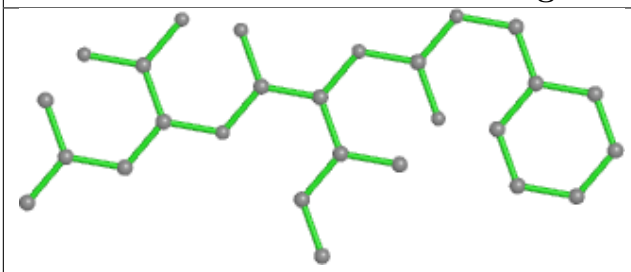


Rings

Ligand ZIL a 301



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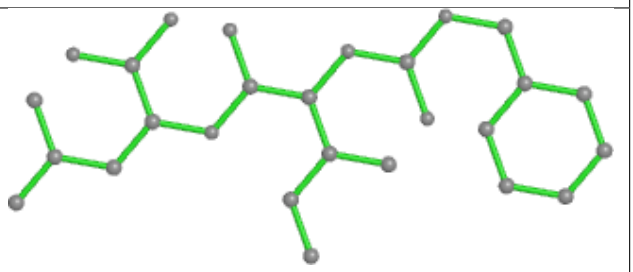

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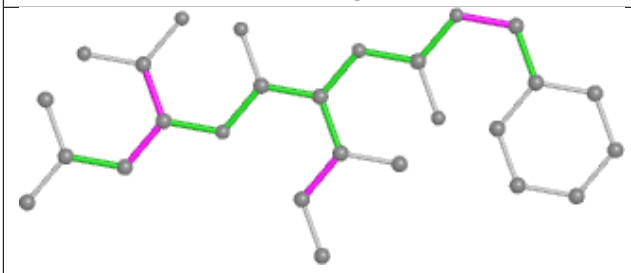

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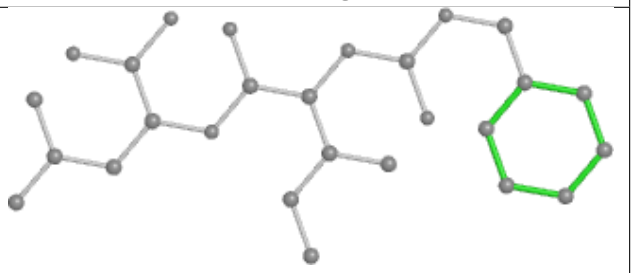
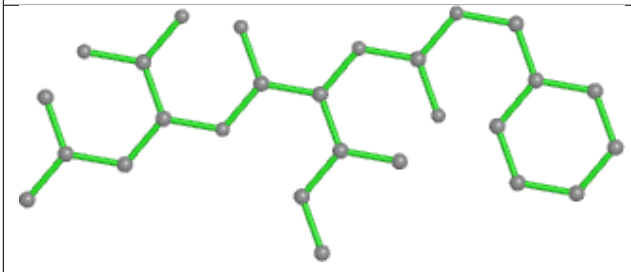


Rings

Ligand ZIL A 301



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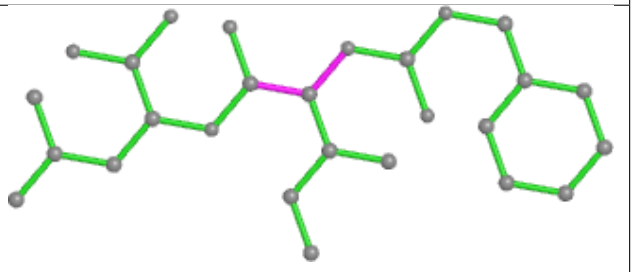
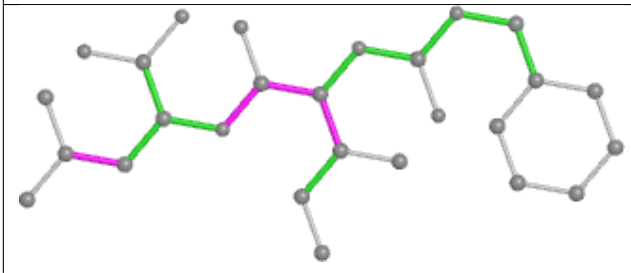


Bond angles



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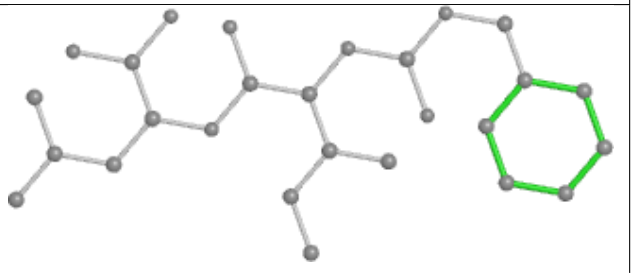
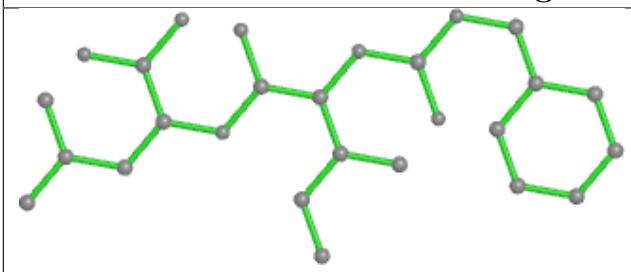
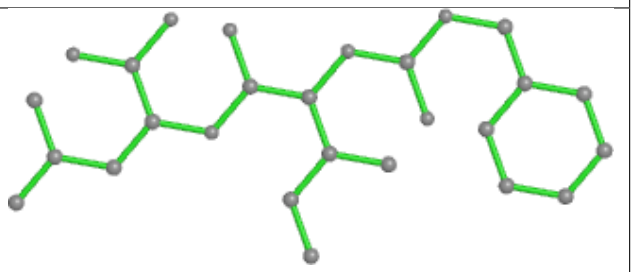


Rings

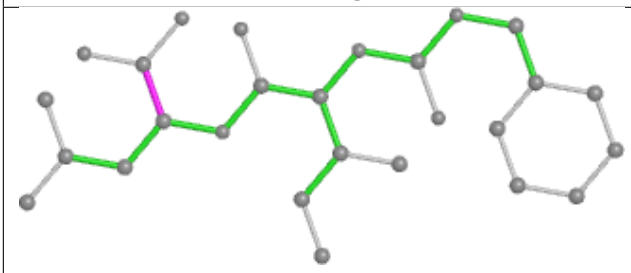
Ligand ZIL Z 301



Bond lengths



Bond angles



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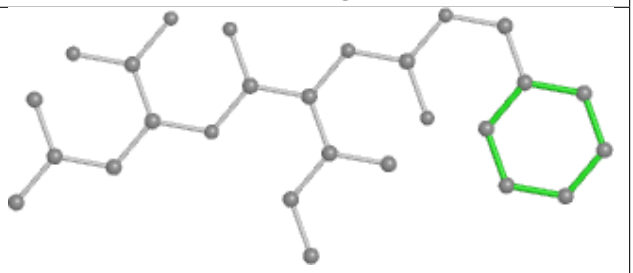
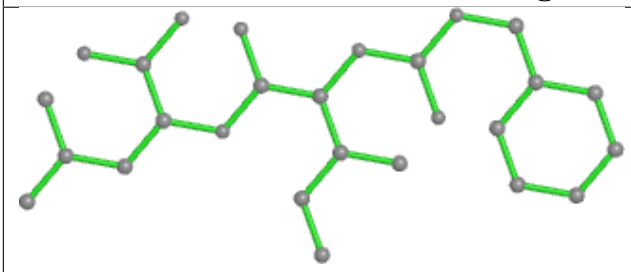


Rings

Ligand ZIL S 301



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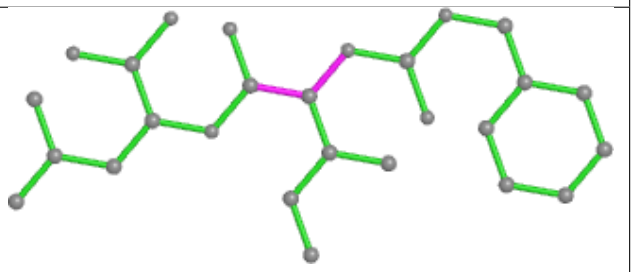

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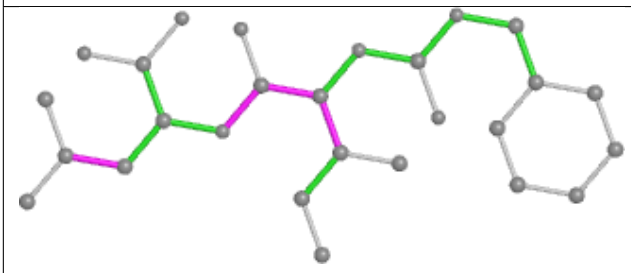

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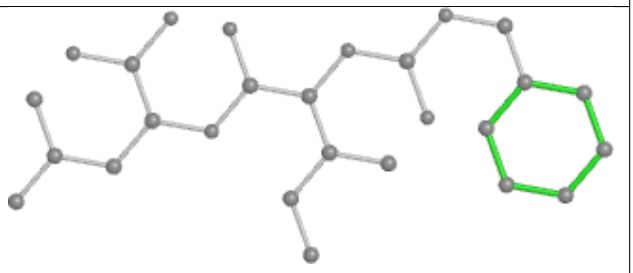

Rings

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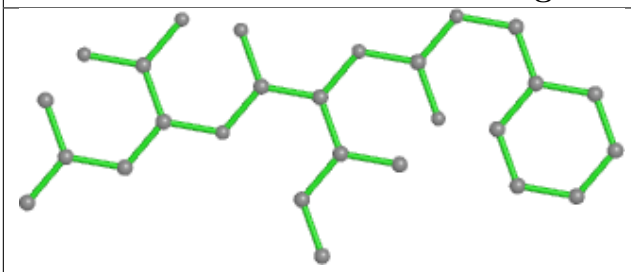

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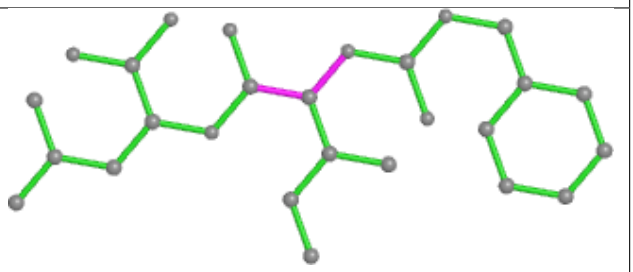

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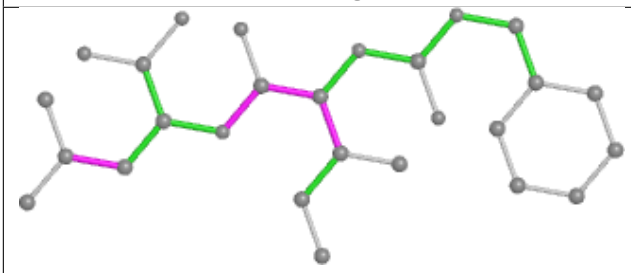

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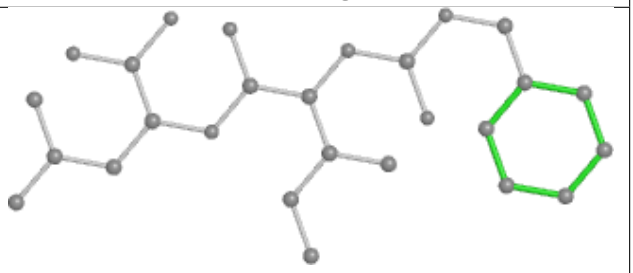

Rings

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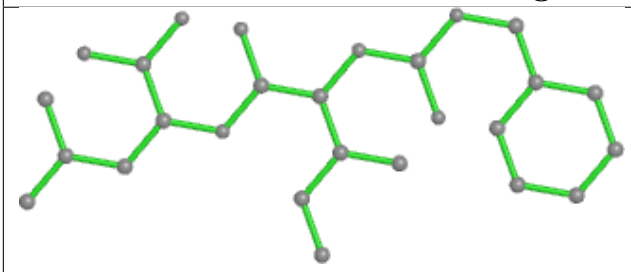

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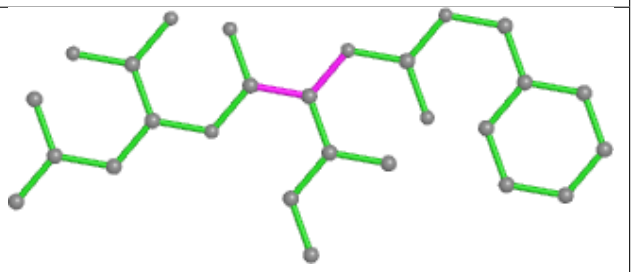

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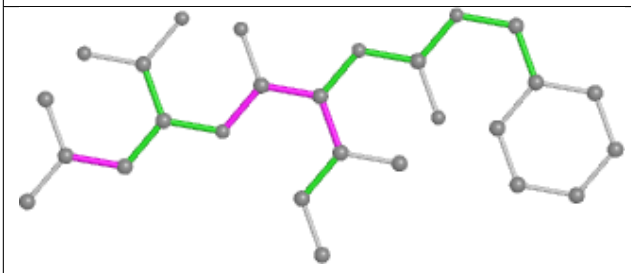

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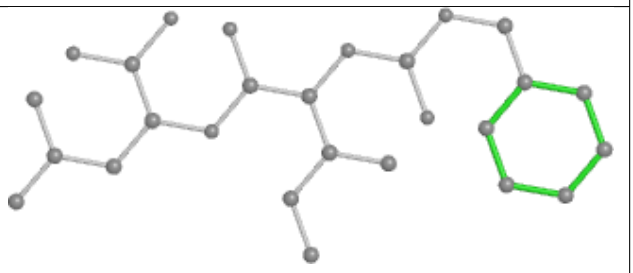

Rings

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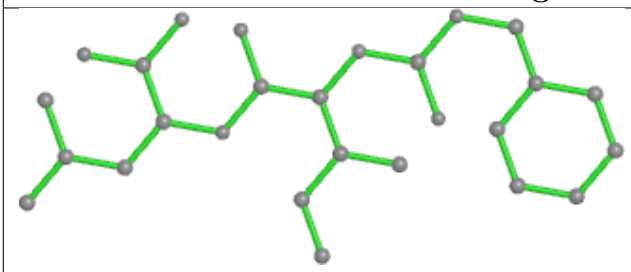

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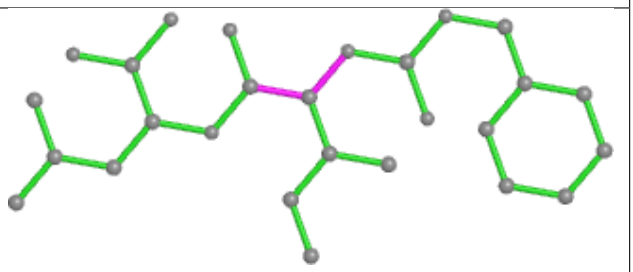

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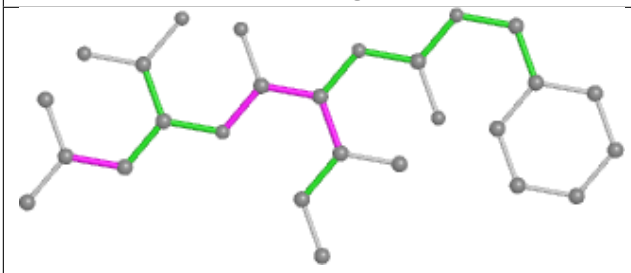

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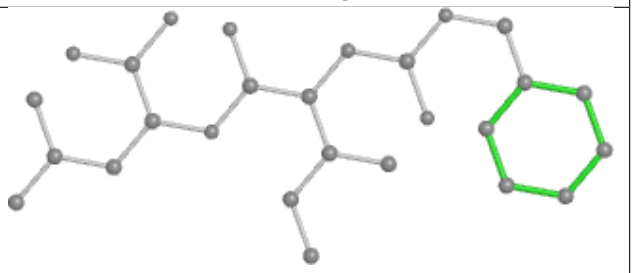

Rings

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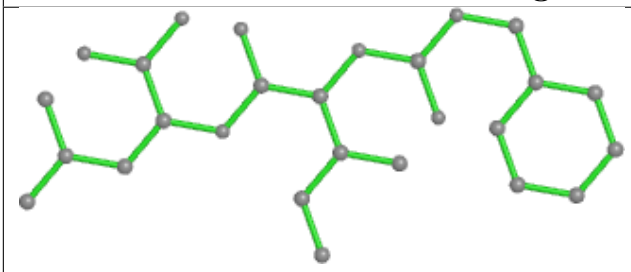

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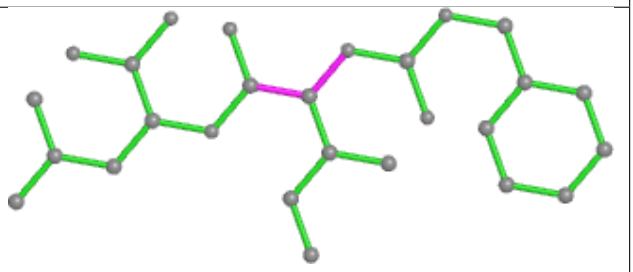

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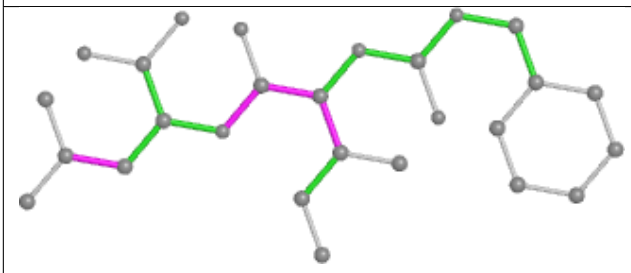

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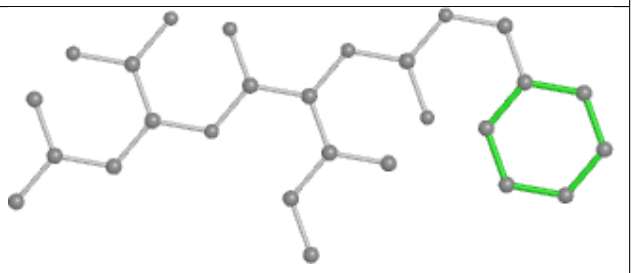

Rings

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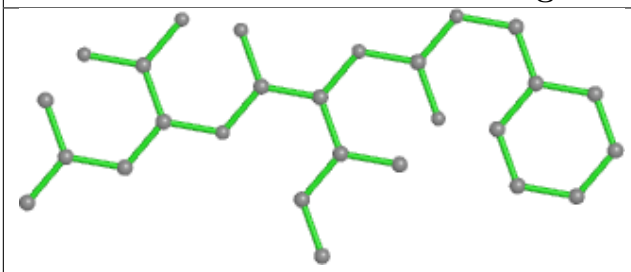

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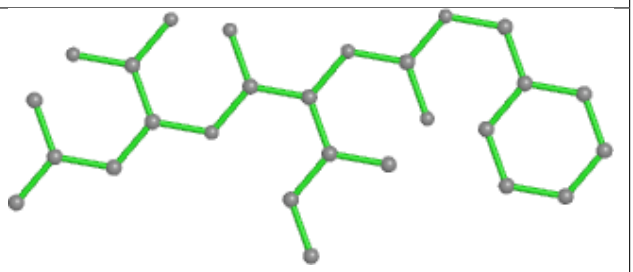

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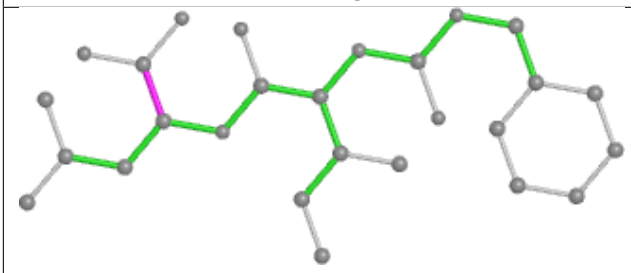

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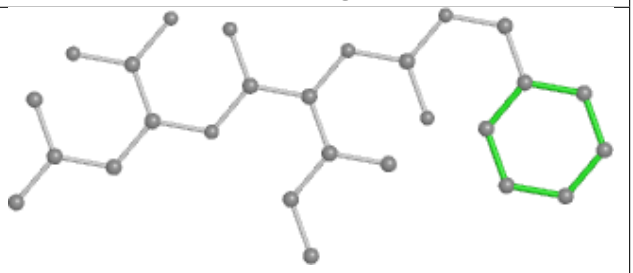

Rings

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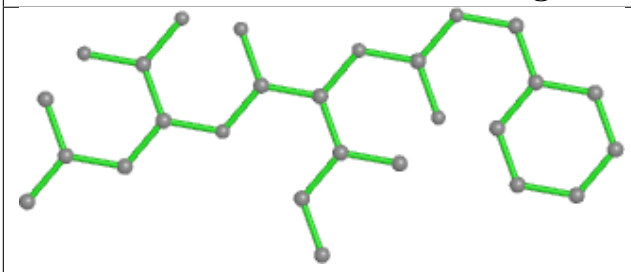

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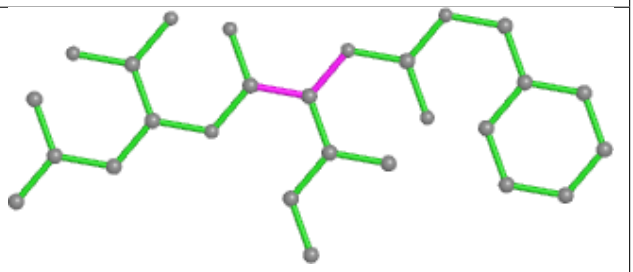

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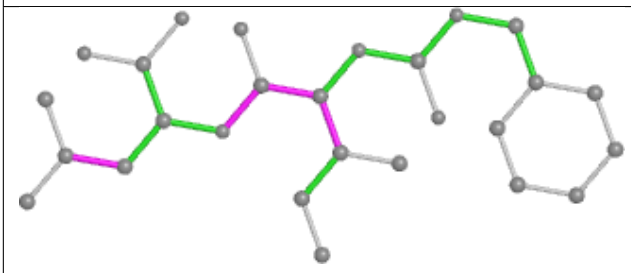

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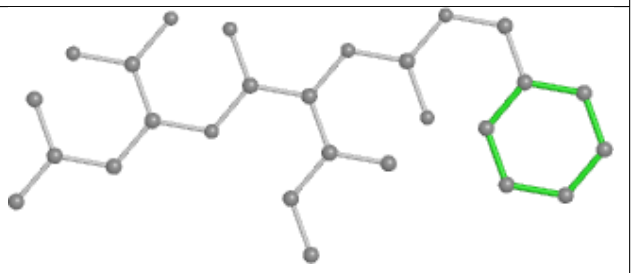

Rings

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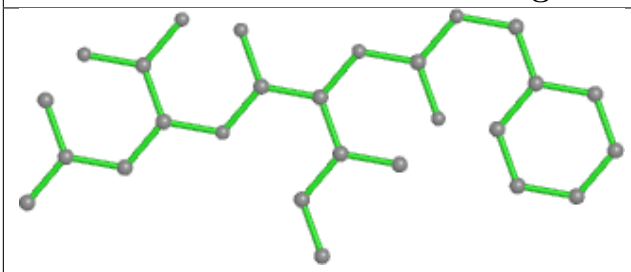

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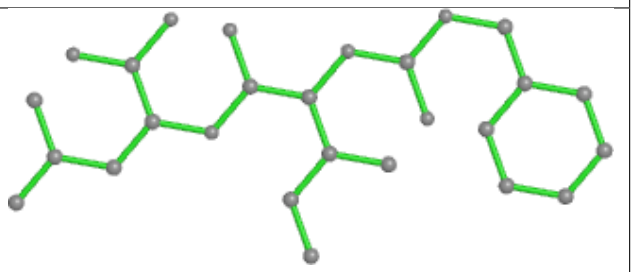

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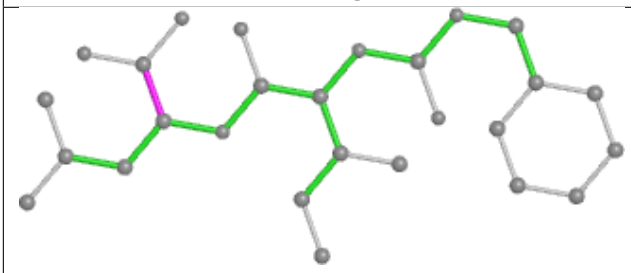

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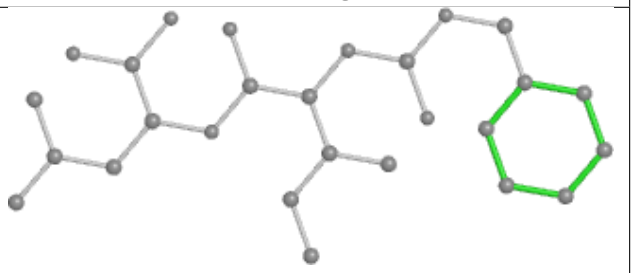

Rings

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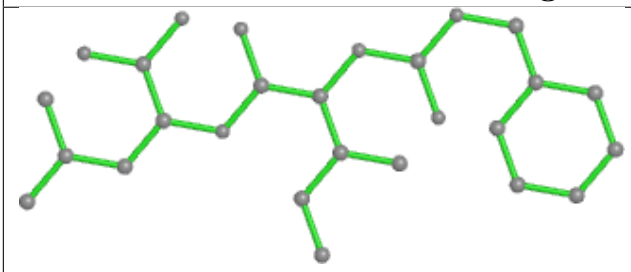

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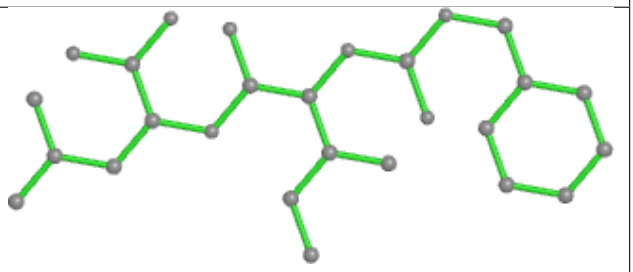

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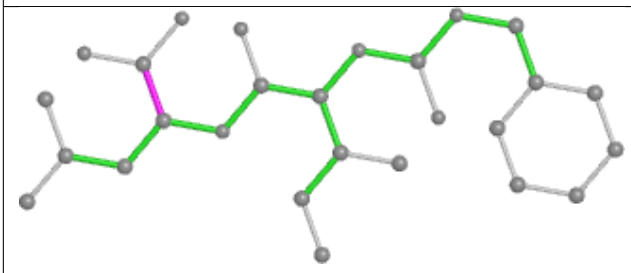

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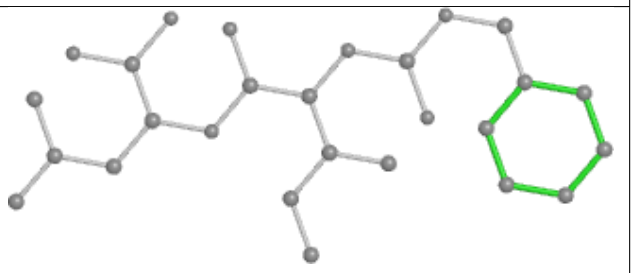

Rings

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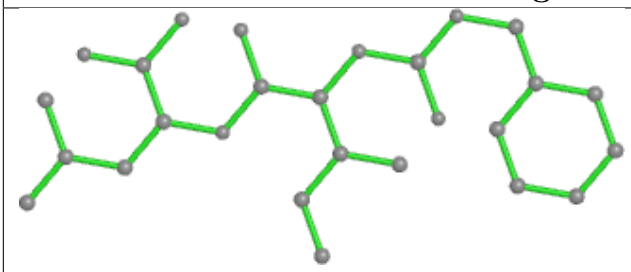

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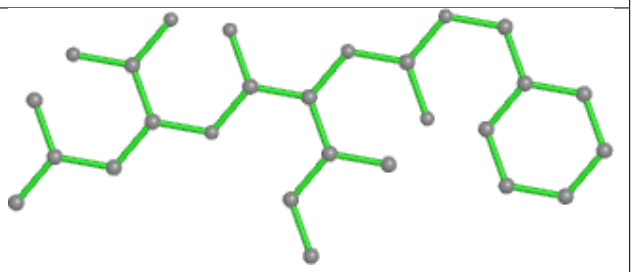

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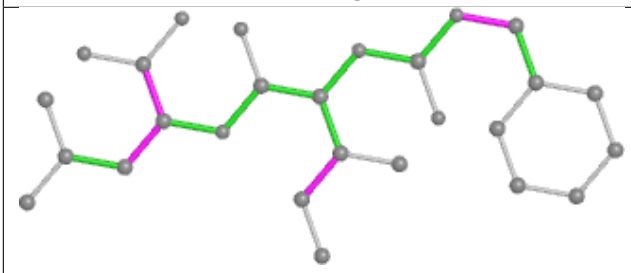

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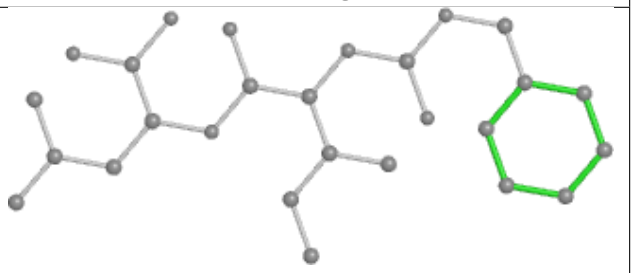

Rings

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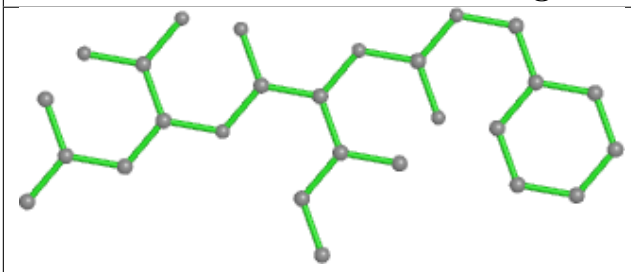

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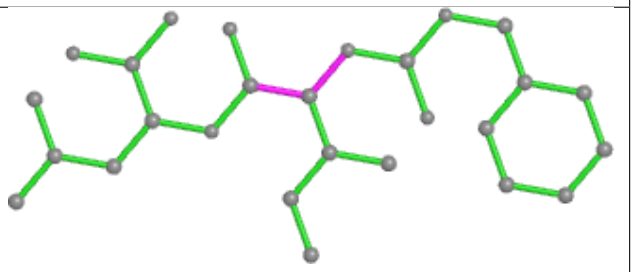

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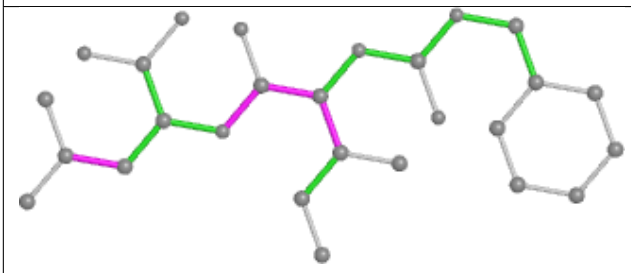

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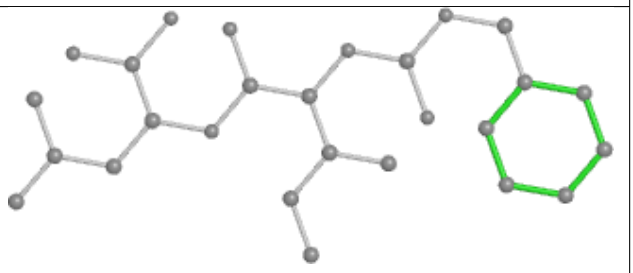

Rings

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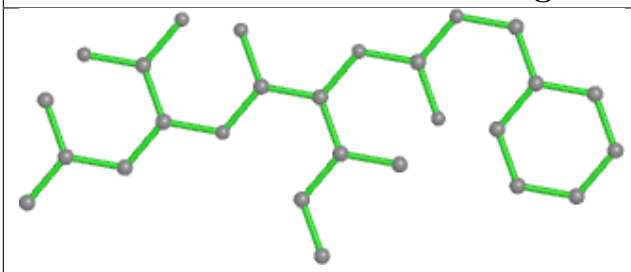

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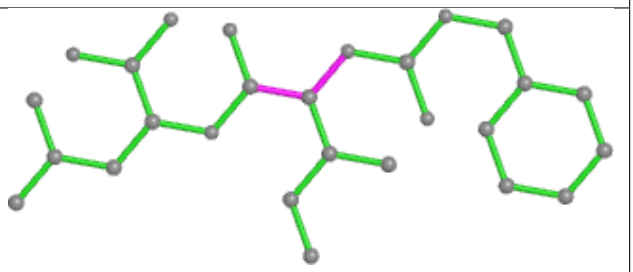

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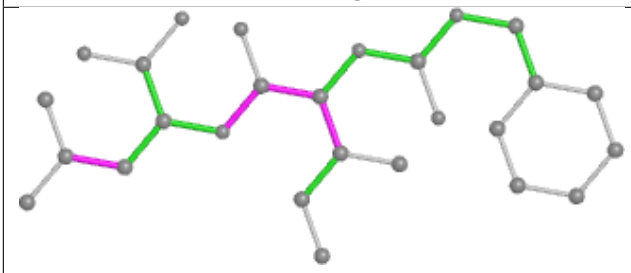

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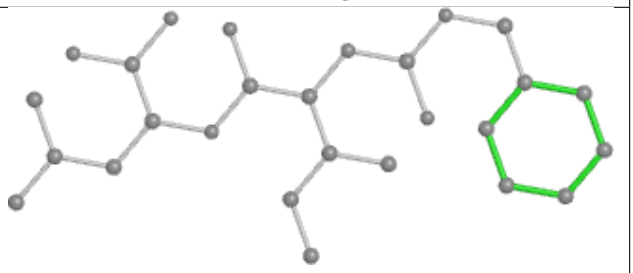
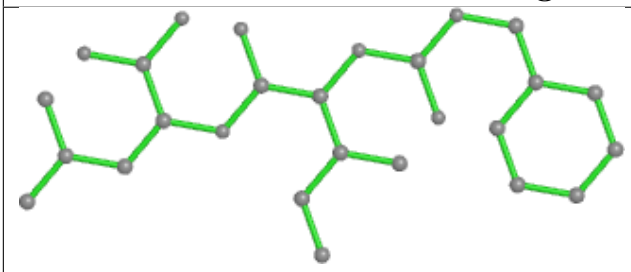


Rings

Ligand ZIL b 301



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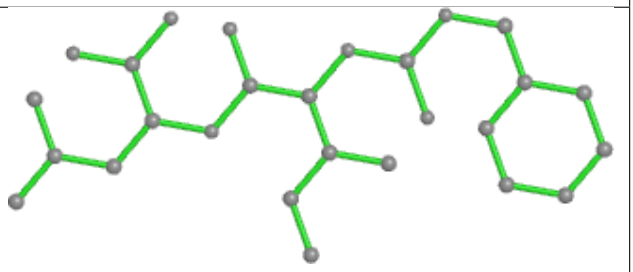

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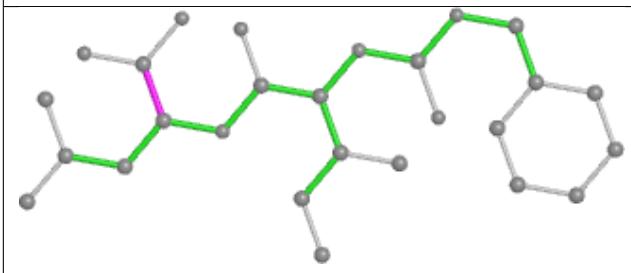

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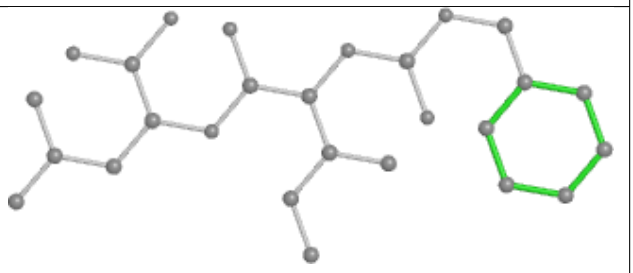
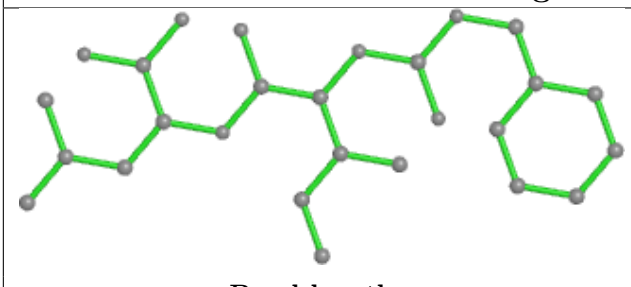


Rings

Ligand ZIL X 301



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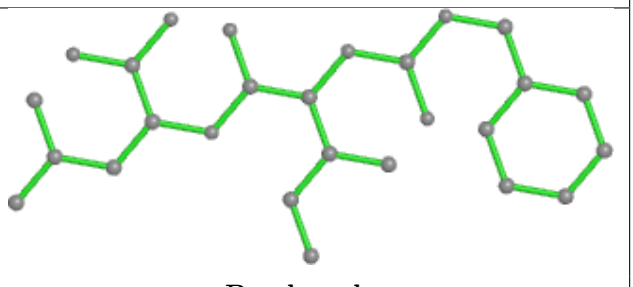

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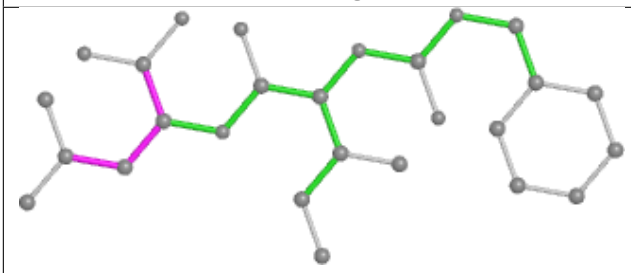

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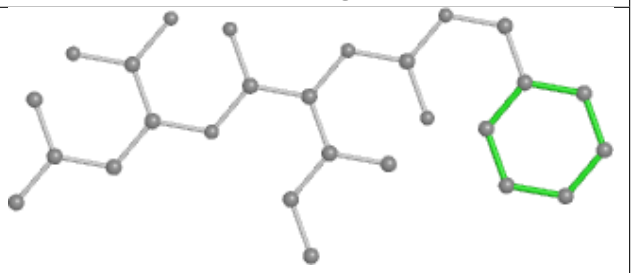

Rings

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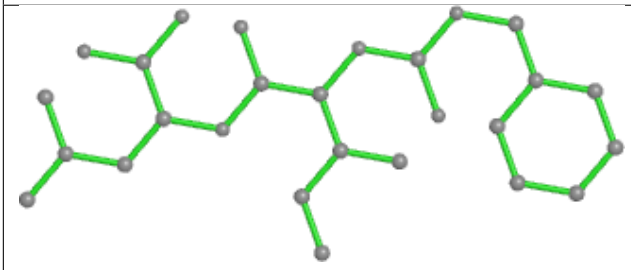

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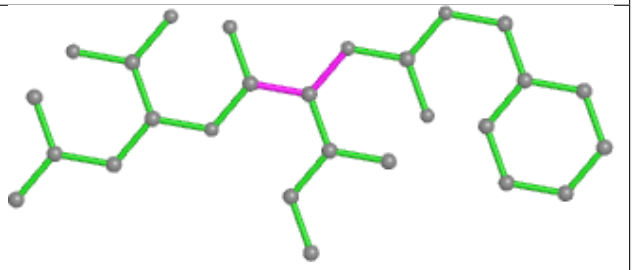
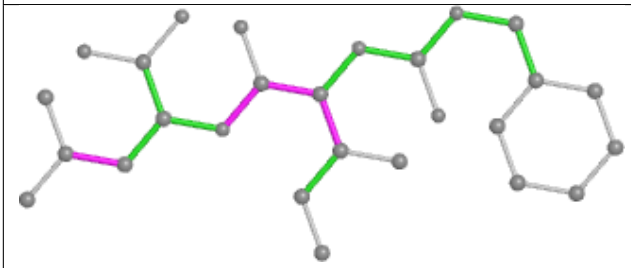
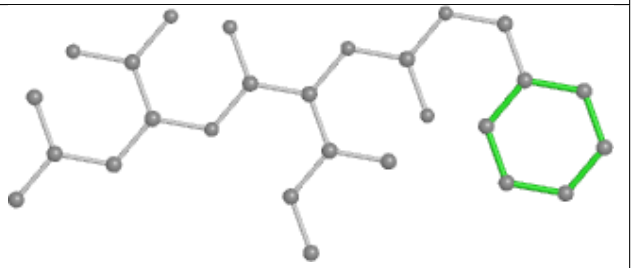


Bond angles



Torsions



Rings

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, 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	197/202 (97%)	-0.26	2 (1%) 82 72	12, 26, 45, 91	0
1	B	197/202 (97%)	-0.21	0 100 100	12, 25, 48, 77	0
1	C	196/202 (97%)	-0.28	2 (1%) 82 72	14, 27, 47, 74	0
1	D	195/202 (96%)	-0.25	0 100 100	12, 28, 45, 64	0
1	E	197/202 (97%)	-0.24	0 100 100	13, 28, 49, 89	0
1	F	196/202 (97%)	-0.25	0 100 100	14, 27, 46, 94	0
1	G	196/202 (97%)	-0.22	1 (0%) 91 86	13, 27, 46, 66	0
1	O	196/202 (97%)	-0.25	0 100 100	15, 28, 49, 61	0
1	P	194/202 (96%)	-0.30	0 100 100	15, 29, 47, 66	0
1	Q	195/202 (96%)	-0.01	0 100 100	15, 28, 46, 66	0
1	R	196/202 (97%)	-0.31	0 100 100	13, 26, 46, 91	0
1	S	196/202 (97%)	-0.23	0 100 100	13, 25, 45, 68	0
1	T	196/202 (97%)	-0.21	2 (1%) 82 72	13, 27, 48, 62	0
1	U	196/202 (97%)	-0.28	0 100 100	13, 27, 46, 74	0
2	H	167/194 (86%)	-0.13	0 100 100	18, 30, 52, 80	0
2	I	165/194 (85%)	-0.21	0 100 100	19, 32, 53, 81	0
2	J	168/194 (86%)	-0.02	1 (0%) 89 83	21, 32, 57, 84	0
2	K	165/194 (85%)	-0.04	1 (0%) 89 83	18, 31, 52, 82	0
2	L	167/194 (86%)	0.05	2 (1%) 79 67	20, 31, 53, 81	0
2	M	166/194 (85%)	-0.20	0 100 100	17, 30, 51, 83	0
2	N	167/194 (86%)	-0.17	0 100 100	19, 30, 50, 78	0
2	V	168/194 (86%)	0.22	1 (0%) 89 83	21, 34, 58, 89	0
2	W	168/194 (86%)	-0.24	0 100 100	22, 34, 56, 95	0
2	X	168/194 (86%)	0.08	0 100 100	21, 33, 55, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	167/194 (86%)	-0.15	0 100 100	19, 30, 51, 84	0
2	Z	168/194 (86%)	-0.12	1 (0%) 89 83	19, 31, 57, 102	0
2	a	167/194 (86%)	-0.14	0 100 100	19, 30, 52, 80	0
2	b	168/194 (86%)	-0.08	0 100 100	21, 32, 53, 101	0
3	c	4/7 (57%)	0.61	0 100 100	34, 34, 47, 53	0
3	d	4/7 (57%)	0.01	0 100 100	40, 41, 56, 57	0
3	e	4/7 (57%)	-0.39	0 100 100	36, 37, 39, 40	0
3	f	4/7 (57%)	0.20	0 100 100	51, 58, 69, 71	0
3	g	4/7 (57%)	0.10	0 100 100	49, 55, 55, 69	0
3	h	4/7 (57%)	-0.00	0 100 100	35, 35, 48, 53	0
3	i	4/7 (57%)	-0.04	0 100 100	40, 40, 54, 58	0
3	j	4/7 (57%)	0.03	0 100 100	52, 52, 58, 60	0
3	k	4/7 (57%)	0.07	0 100 100	41, 45, 49, 55	0
3	l	4/7 (57%)	-0.42	0 100 100	37, 43, 48, 55	0
3	m	4/7 (57%)	-0.07	0 100 100	28, 34, 36, 42	0
3	n	4/7 (57%)	0.54	0 100 100	47, 54, 62, 72	0
3	o	4/7 (57%)	-0.43	0 100 100	38, 45, 51, 56	0
3	p	4/7 (57%)	0.07	0 100 100	50, 53, 56, 72	0
All	All	5138/5642 (91%)	-0.16	13 (0%) 94 92	12, 30, 53, 102	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	SER	3.8
2	Z	57	SER	3.0
1	A	211	ALA	2.9
1	G	209	LEU	2.7
1	C	210	SER	2.5
1	C	209	LEU	2.5
1	T	210	SER	2.4
2	J	57	SER	2.4
2	L	57	SER	2.3
2	L	56	ALA	2.1
1	T	209	LEU	2.1
2	K	20	VAL	2.0
2	V	49	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	WFP	e	2	13/14	0.96	0.21	3,32,41,48	0
3	WFP	j	2	13/14	0.96	0.28	22,43,52,57	0
3	WFP	k	2	13/14	0.96	0.34	24,41,54,55	0
3	WFP	c	2	13/14	0.97	0.26	14,29,36,43	0
3	WFP	f	2	13/14	0.97	0.23	17,34,57,59	0
3	WFP	h	2	13/14	0.97	0.29	21,31,40,42	0
3	WFP	i	2	13/14	0.97	0.24	12,32,50,51	0
3	WFP	d	2	13/14	0.97	0.28	13,32,45,45	0
3	WFP	l	2	13/14	0.97	0.20	26,37,50,52	0
3	WFP	n	2	13/14	0.97	0.32	12,31,52,56	0
3	WFP	p	2	13/14	0.97	0.20	15,35,54,54	0
3	WFP	g	2	13/14	0.98	0.26	18,42,57,66	0
3	WFP	o	2	13/14	0.98	0.21	15,35,45,46	0
3	WFP	m	2	13/14	0.98	0.22	11,29,49,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
5	SO4	p	101	5/5	0.48	0.38	57,76,140,177	0
5	SO4	E	302	5/5	0.74	0.32	80,90,97,128	0
5	SO4	R	303	5/5	0.76	0.36	78,88,109,140	0
5	SO4	S	303	5/5	0.79	0.37	65,67,123,131	0
5	SO4	G	302	5/5	0.79	0.47	86,87,115,148	0
5	SO4	R	302	5/5	0.80	0.28	60,72,127,143	0
5	SO4	W	302	5/5	0.80	0.50	81,92,111,138	0
5	SO4	E	304	5/5	0.80	0.30	60,86,120,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZIL	O	301	27/27	0.81	0.39	12,78,157,190	0
4	ZIL	Q	301	27/27	0.82	0.38	12,79,141,169	0
4	ZIL	G	301	27/27	0.82	0.46	14,77,155,186	0
4	ZIL	P	301	27/27	0.82	0.34	13,75,154,185	0
4	ZIL	D	301	27/27	0.83	0.42	29,70,148,179	0
4	ZIL	S	301	27/27	0.83	0.45	18,78,154,185	0
5	SO4	S	304	5/5	0.83	0.56	63,66,113,125	0
4	ZIL	U	301	27/27	0.83	0.52	30,85,142,163	0
5	SO4	C	303	5/5	0.83	0.28	57,89,103,133	0
5	SO4	C	305	5/5	0.85	0.46	106,110,146,157	0
4	ZIL	E	301	27/27	0.85	0.41	33,70,143,172	0
5	SO4	I	302	5/5	0.85	0.33	80,85,91,221	0
5	SO4	M	302	5/5	0.87	0.31	81,94,113,119	0
5	SO4	Q	303	5/5	0.87	0.31	86,92,113,130	0
4	ZIL	B	301	27/27	0.87	0.41	5,65,144,173	0
4	ZIL	T	301	27/27	0.87	0.43	6,68,140,165	0
4	ZIL	F	301	27/27	0.87	0.36	23,71,129,156	0
4	ZIL	A	301	27/27	0.87	0.38	8,69,121,145	0
5	SO4	C	304	5/5	0.87	0.46	66,72,116,121	0
5	SO4	J	302	5/5	0.87	0.41	67,78,116,117	0
5	SO4	S	302	5/5	0.88	0.29	48,103,121,122	0
5	SO4	P	302	5/5	0.88	0.41	80,82,112,129	0
4	ZIL	C	301	27/27	0.88	0.39	15,75,135,151	0
4	ZIL	R	301	27/27	0.88	0.38	16,67,107,123	0
5	SO4	O	303	5/5	0.88	0.35	90,92,127,139	0
5	SO4	P	304	5/5	0.89	0.31	41,66,87,103	0
5	SO4	P	303	5/5	0.90	0.26	58,62,72,98	0
5	SO4	E	305	5/5	0.91	0.34	78,81,121,123	0
4	ZIL	W	301	27/27	0.92	0.29	22,45,72,75	0
5	SO4	U	302	5/5	0.92	0.14	31,54,75,85	0
5	SO4	B	302	5/5	0.92	0.33	49,81,112,124	0
4	ZIL	L	301	27/27	0.92	0.25	16,43,64,76	0
6	DMS	P	305	4/4	0.92	0.16	19,22,26,140	0
4	ZIL	H	301	27/27	0.93	0.36	16,37,63,82	0
4	ZIL	Z	301	27/27	0.93	0.27	16,40,64,79	0
6	DMS	E	306	4/4	0.93	0.15	13,28,38,122	0
4	ZIL	K	301	27/27	0.93	0.27	19,38,63,64	0
6	DMS	Q	304	4/4	0.93	0.18	21,27,37,103	0
4	ZIL	I	301	27/27	0.94	0.31	15,47,74,81	0
5	SO4	R	304	5/5	0.94	0.15	42,59,70,82	0
4	ZIL	V	301	27/27	0.94	0.42	26,54,86,93	0
4	ZIL	J	301	27/27	0.94	0.34	17,50,72,75	0

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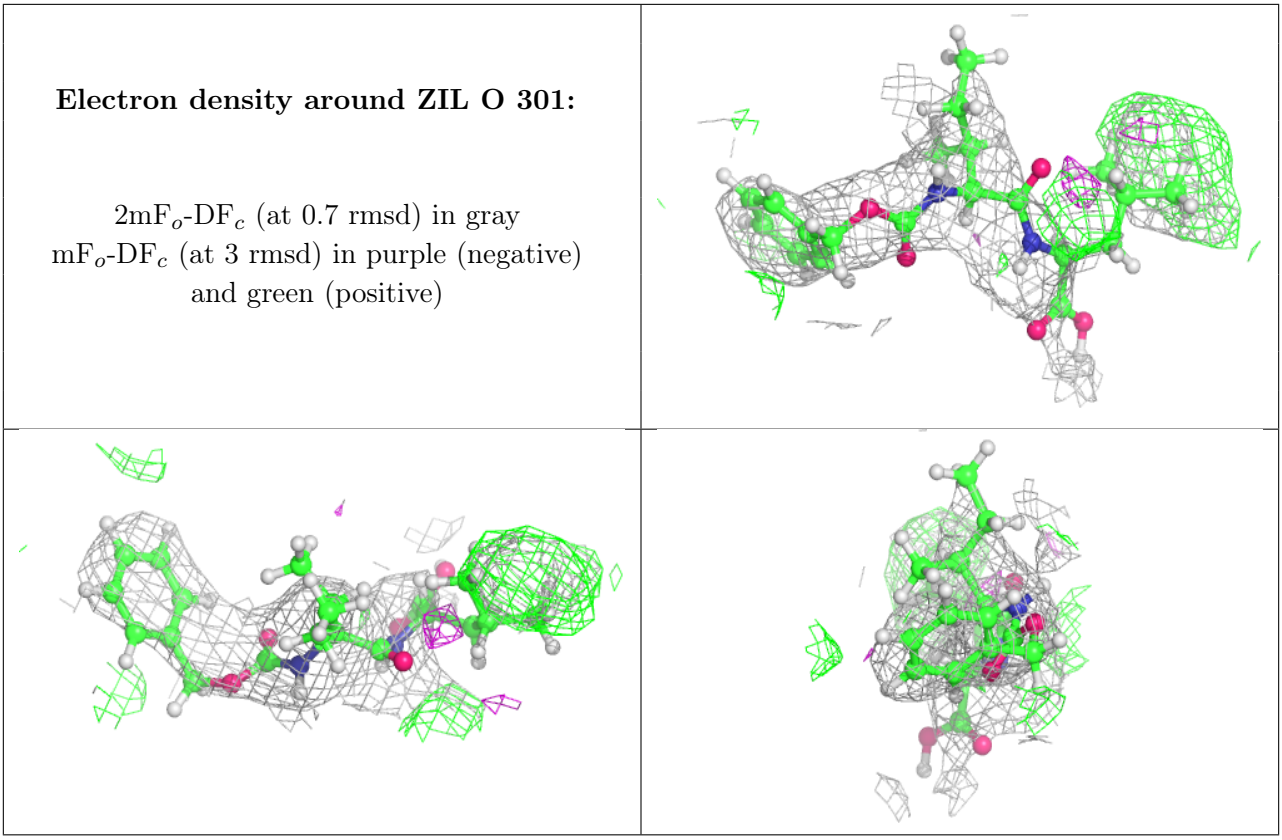
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	O	302	5/5	0.94	0.18	47,67,71,88	0
5	SO4	T	302	5/5	0.94	0.16	23,47,55,80	0
4	ZIL	X	301	27/27	0.94	0.43	24,49,64,77	0
4	ZIL	Y	301	27/27	0.94	0.28	9,36,62,71	0
4	ZIL	M	301	27/27	0.94	0.29	5,33,63,75	0
4	ZIL	a	301	27/27	0.94	0.32	10,34,80,96	0
5	SO4	F	302	5/5	0.94	0.17	42,50,64,92	0
5	SO4	A	302	5/5	0.94	0.23	31,49,71,72	0
4	ZIL	b	301	27/27	0.95	0.33	11,41,73,79	0
6	DMS	G	304	4/4	0.95	0.18	16,32,33,135	0
6	DMS	O	304	4/4	0.95	0.15	10,21,26,128	0
4	ZIL	N	301	27/27	0.95	0.49	9,37,67,71	0
6	DMS	A	303	4/4	0.95	0.17	13,16,34,120	0
6	DMS	R	305	4/4	0.95	0.16	2,17,20,111	0
5	SO4	C	302	5/5	0.96	0.16	47,55,75,90	0
5	SO4	E	303	5/5	0.96	0.24	48,53,86,88	0
5	SO4	Q	302	5/5	0.96	0.20	45,51,73,81	0
6	DMS	B	304	4/4	0.96	0.19	4,16,28,76	0
6	DMS	C	306	4/4	0.96	0.17	5,12,23,115	0
6	DMS	D	303	4/4	0.96	0.16	22,26,33,121	0
6	DMS	U	303	4/4	0.96	0.17	8,12,32,120	0
5	SO4	G	303	5/5	0.97	0.10	38,46,72,97	0
6	DMS	B	303	4/4	0.97	0.17	14,17,34,116	0
5	SO4	S	305	5/5	0.97	0.12	9,31,60,65	0
6	DMS	S	306	4/4	0.97	0.11	18,29,30,120	0
6	DMS	T	303	4/4	0.97	0.17	4,5,12,100	0
5	SO4	D	302	5/5	0.97	0.18	41,52,82,91	0
6	DMS	F	303	4/4	0.98	0.13	16,23,33,98	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.

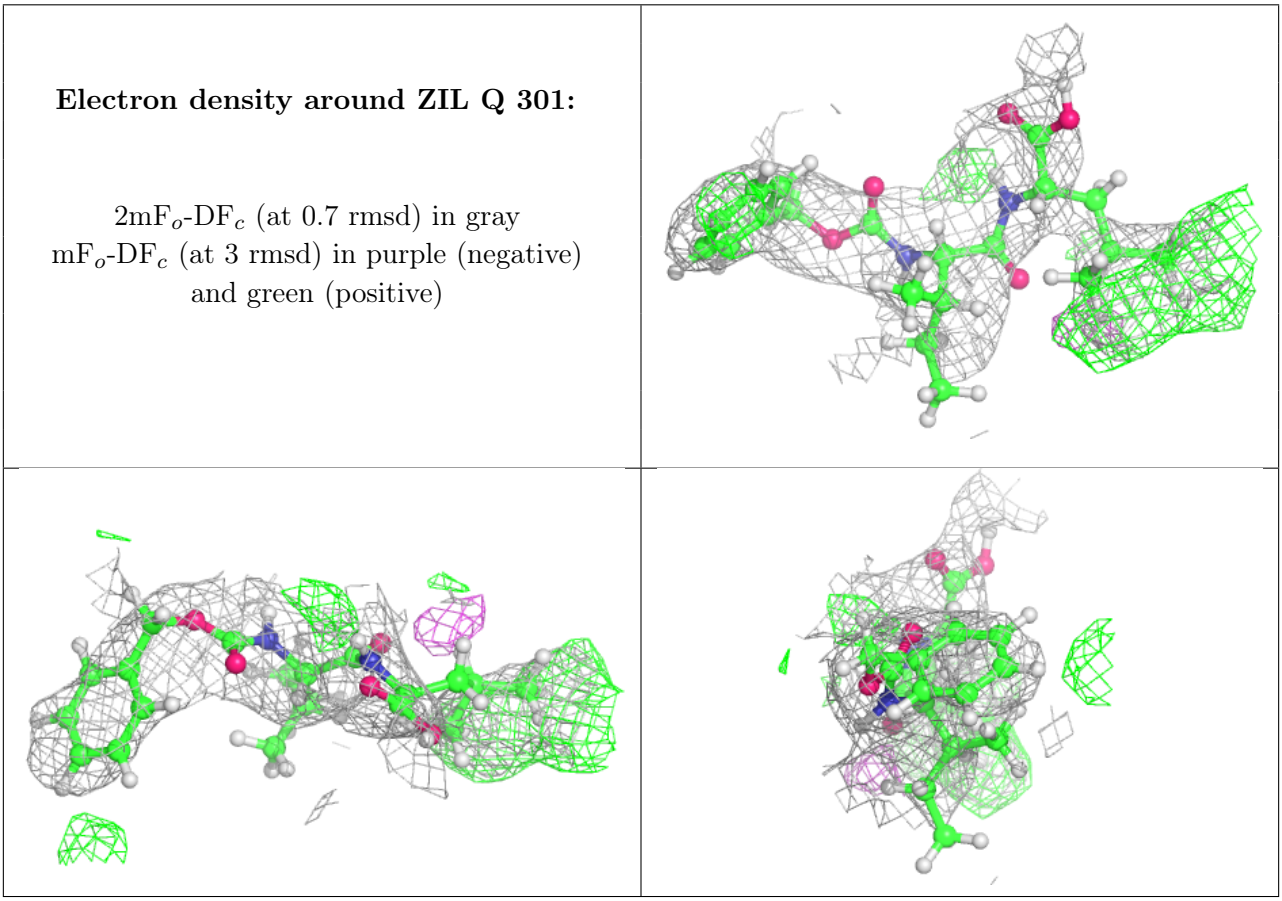
Electron density around ZIL O 301:

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



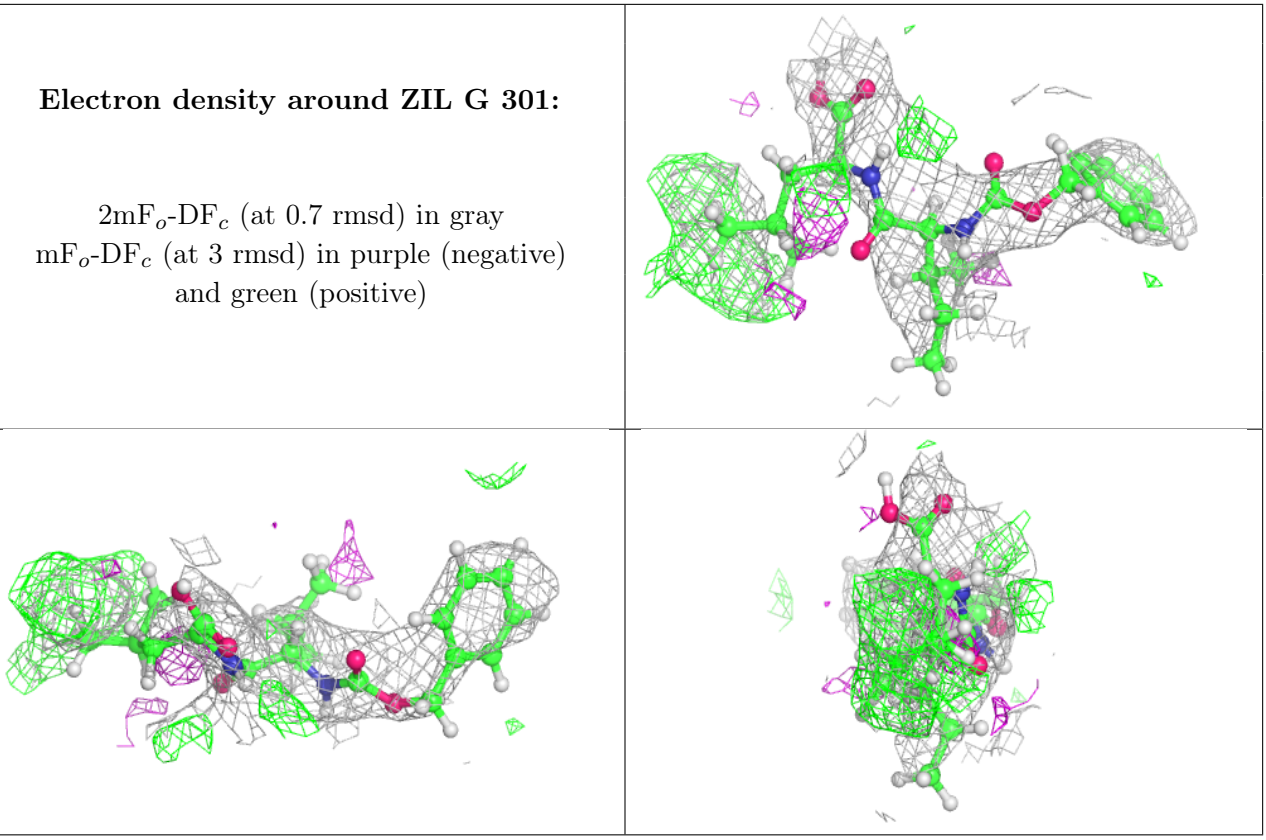
Electron density around ZIL Q 301:

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



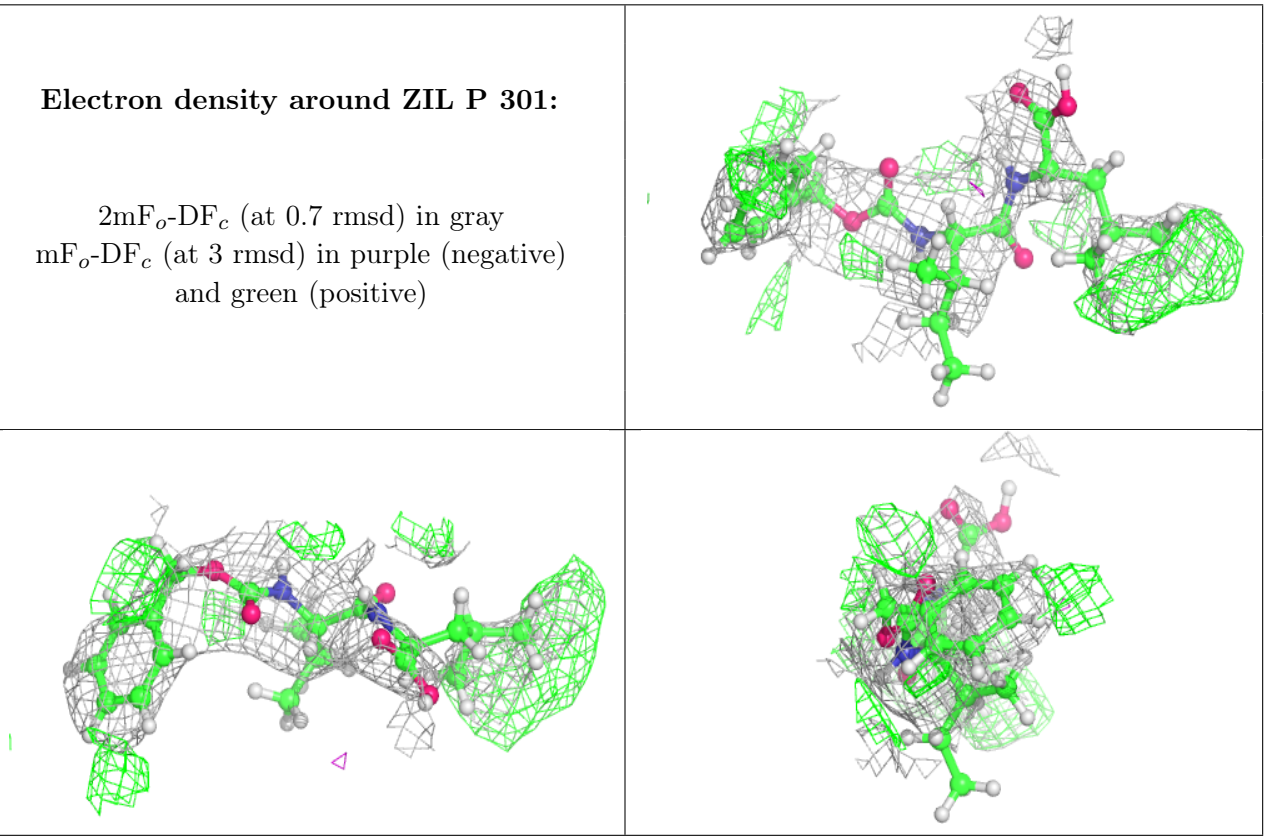
Electron density around ZIL G 301:

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



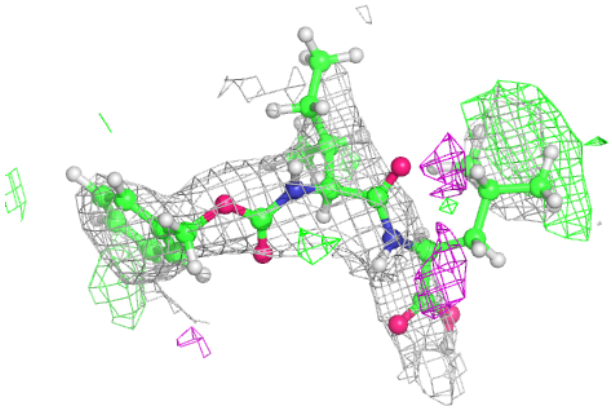
Electron density around ZIL P 301:

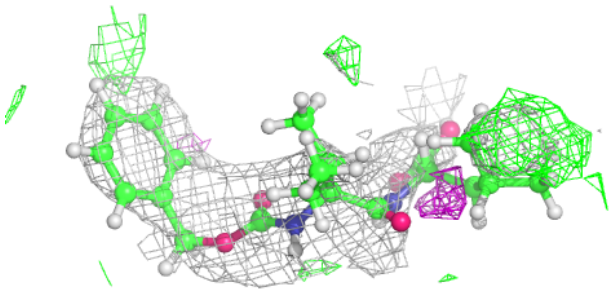
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

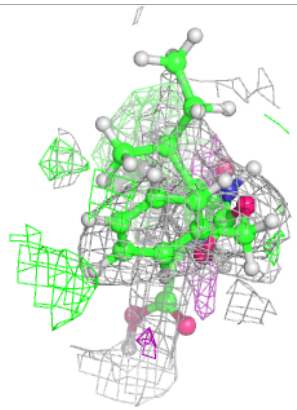


Electron density around ZIL D 301:

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

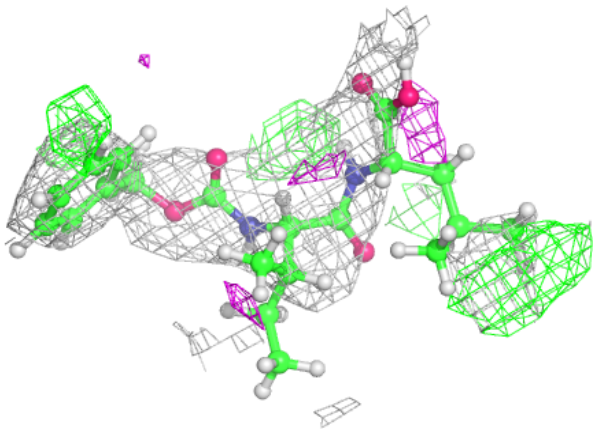


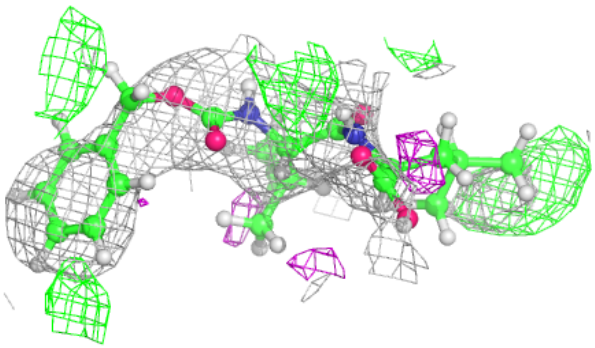


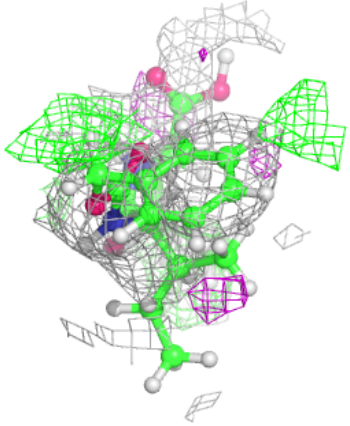


Electron density around ZIL S 301:

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

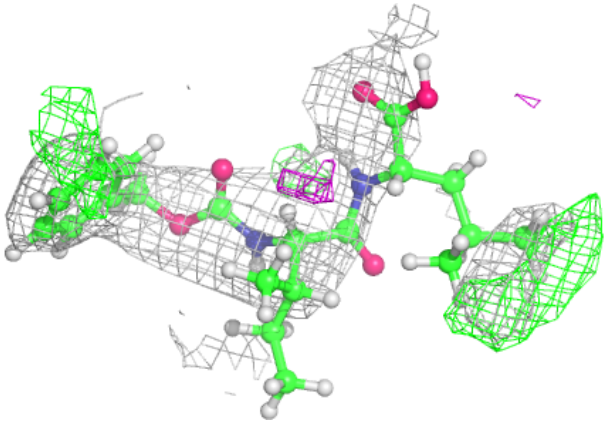


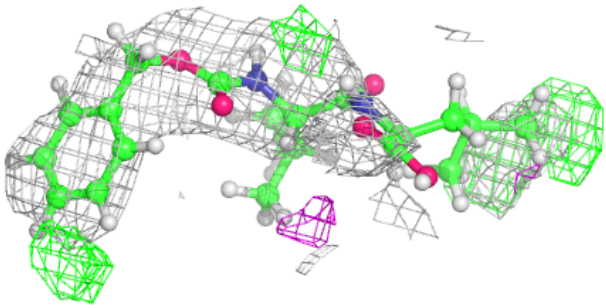


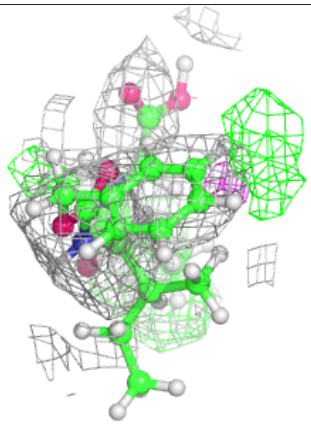


Electron density around ZIL U 301:

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

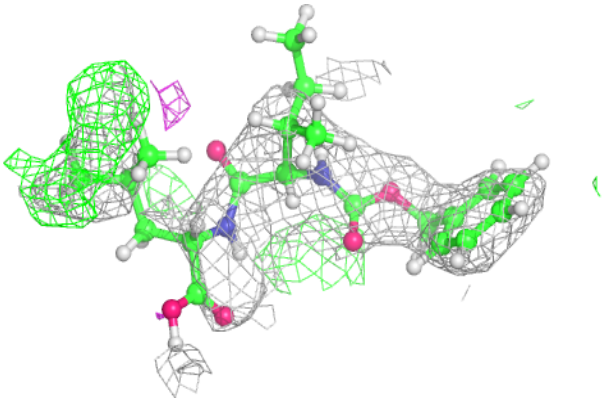


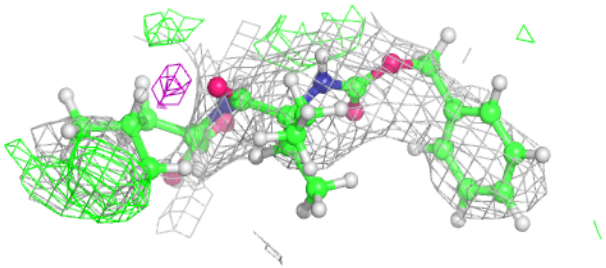


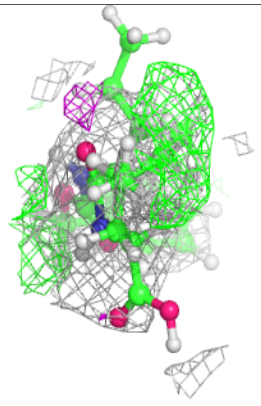


Electron density around ZIL E 301:

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

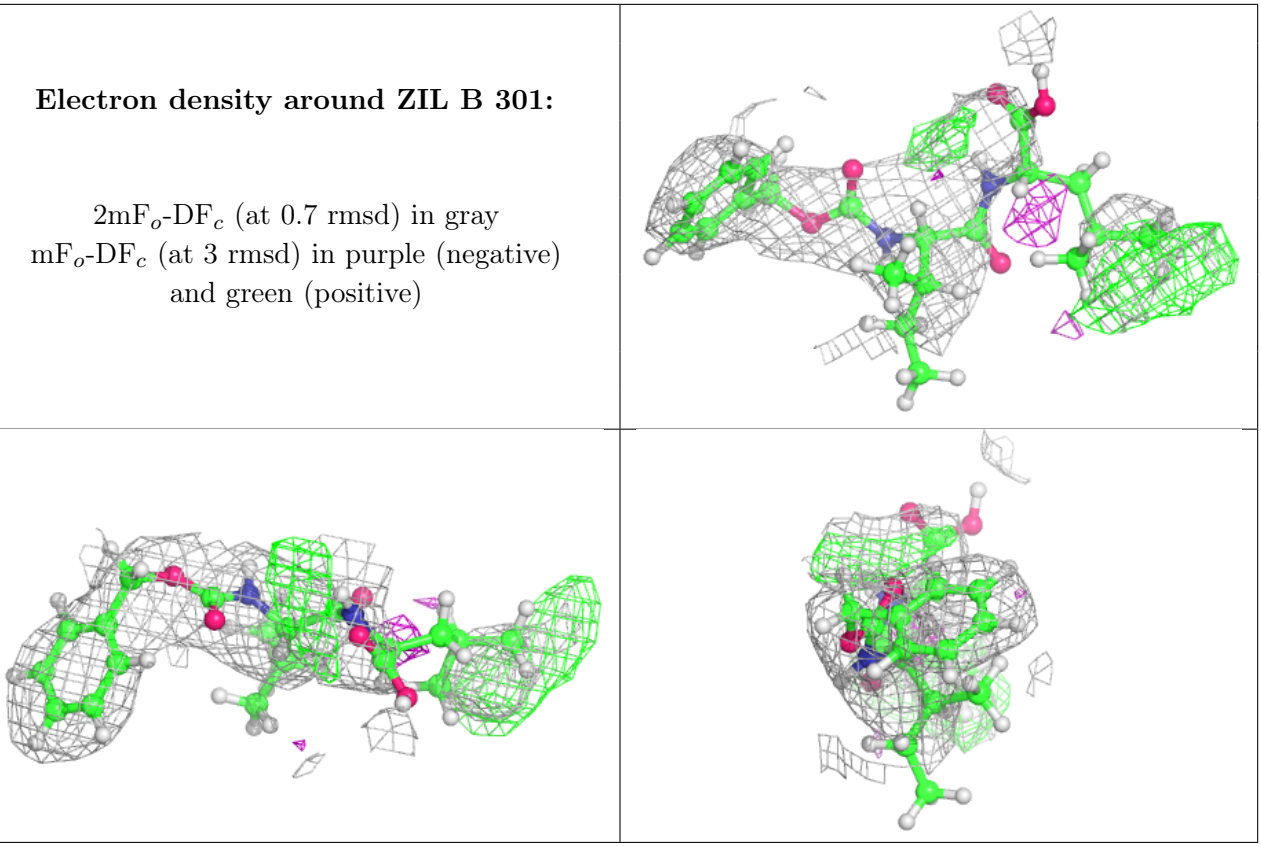






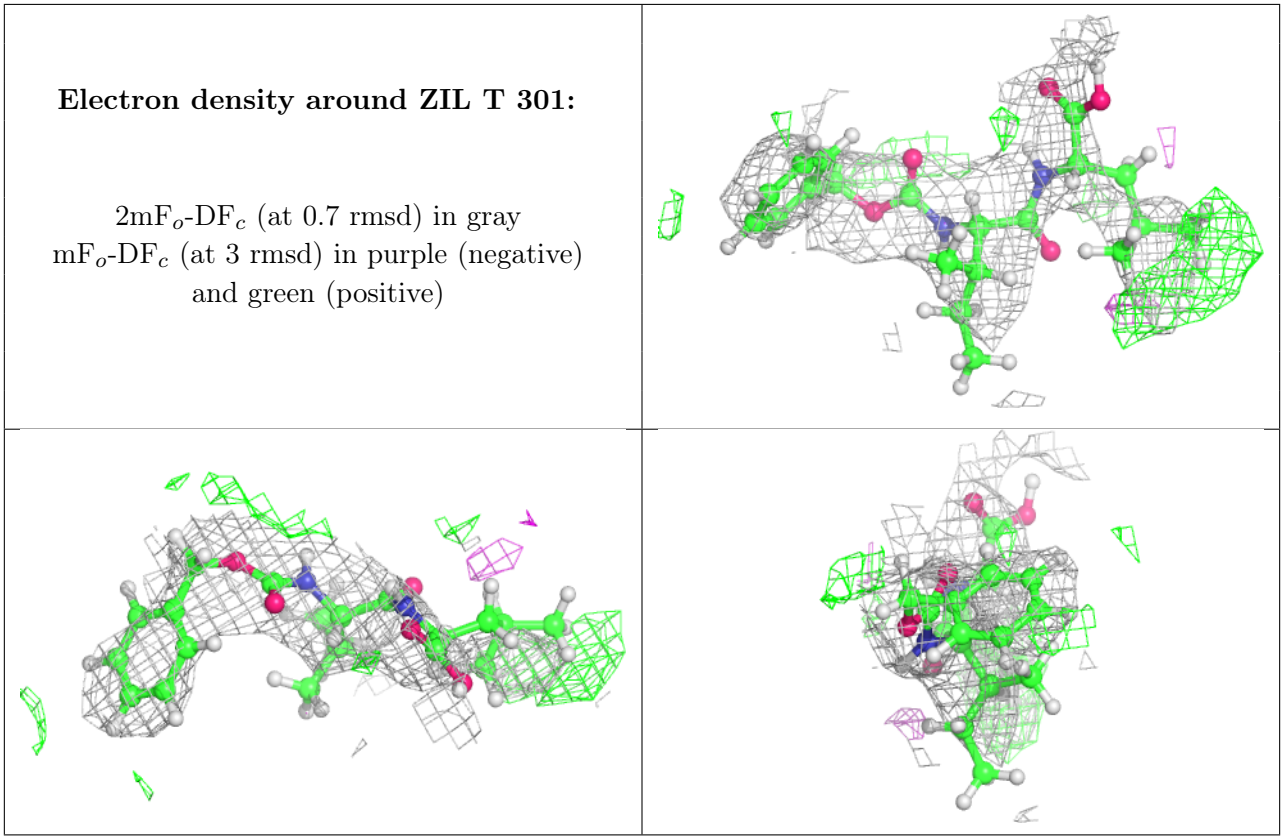
Electron density around ZIL B 301:

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



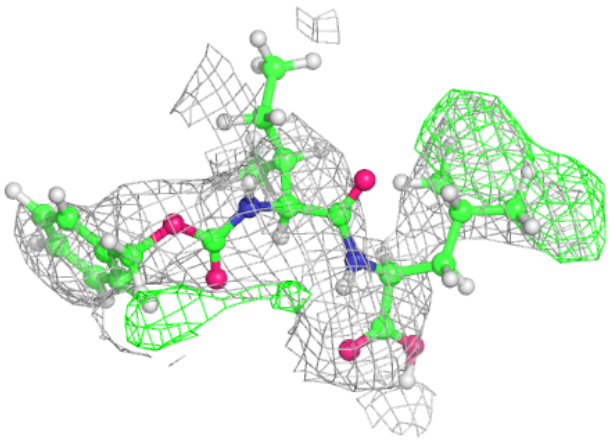
Electron density around ZIL T 301:

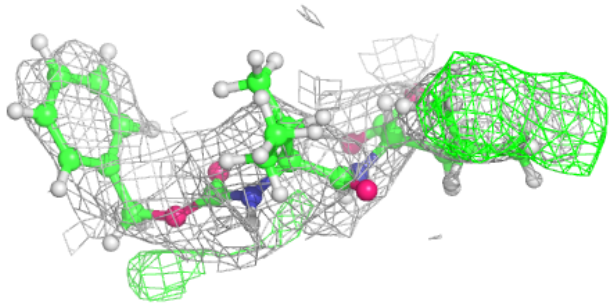
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZIL F 301:

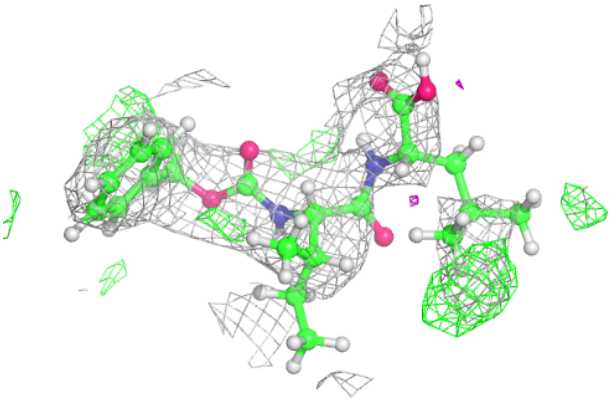
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

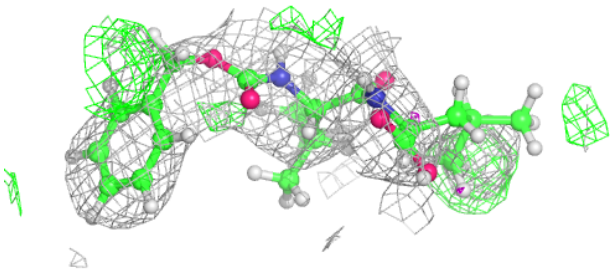


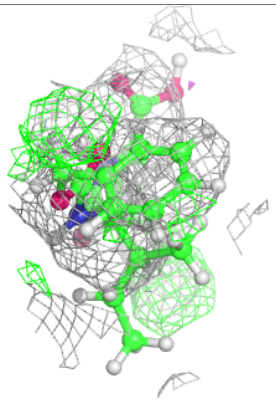


Electron density around ZIL A 301:

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

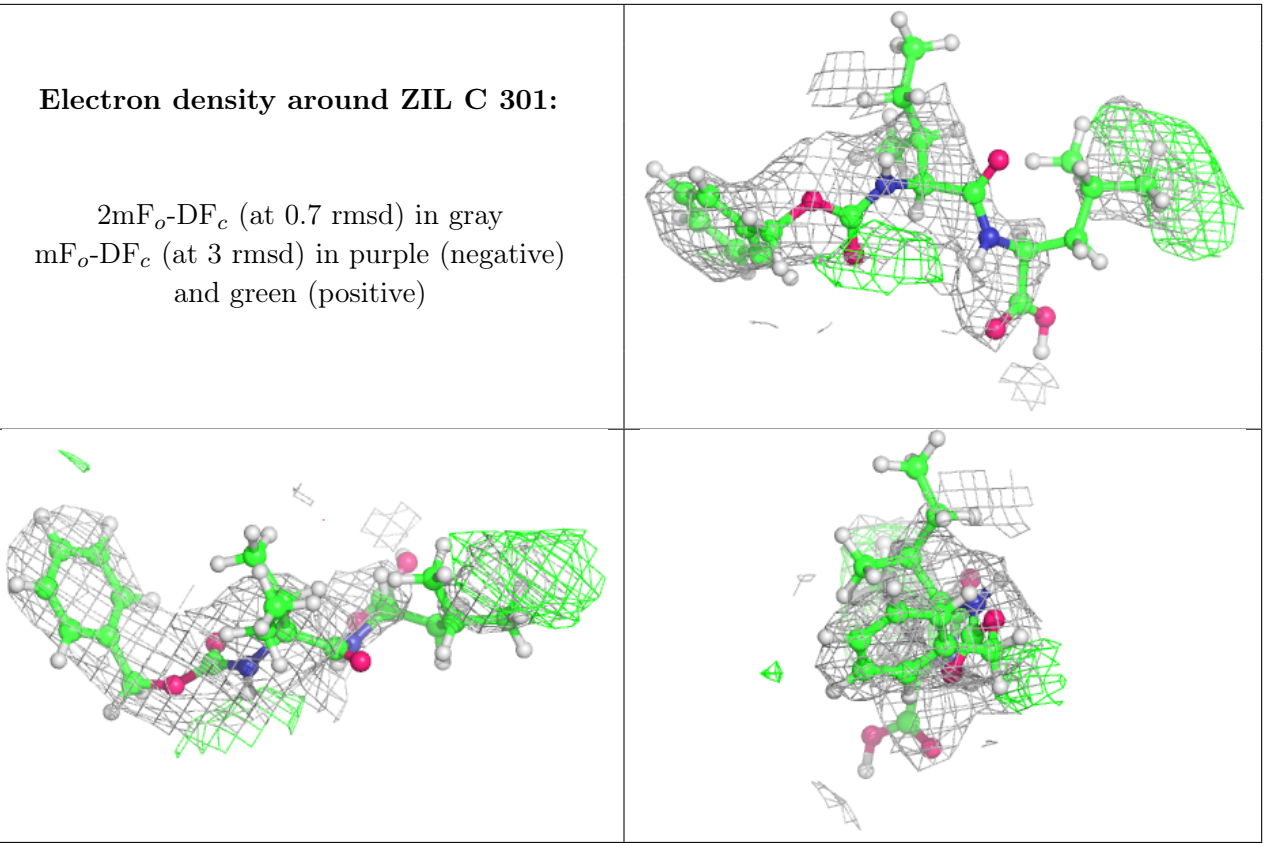






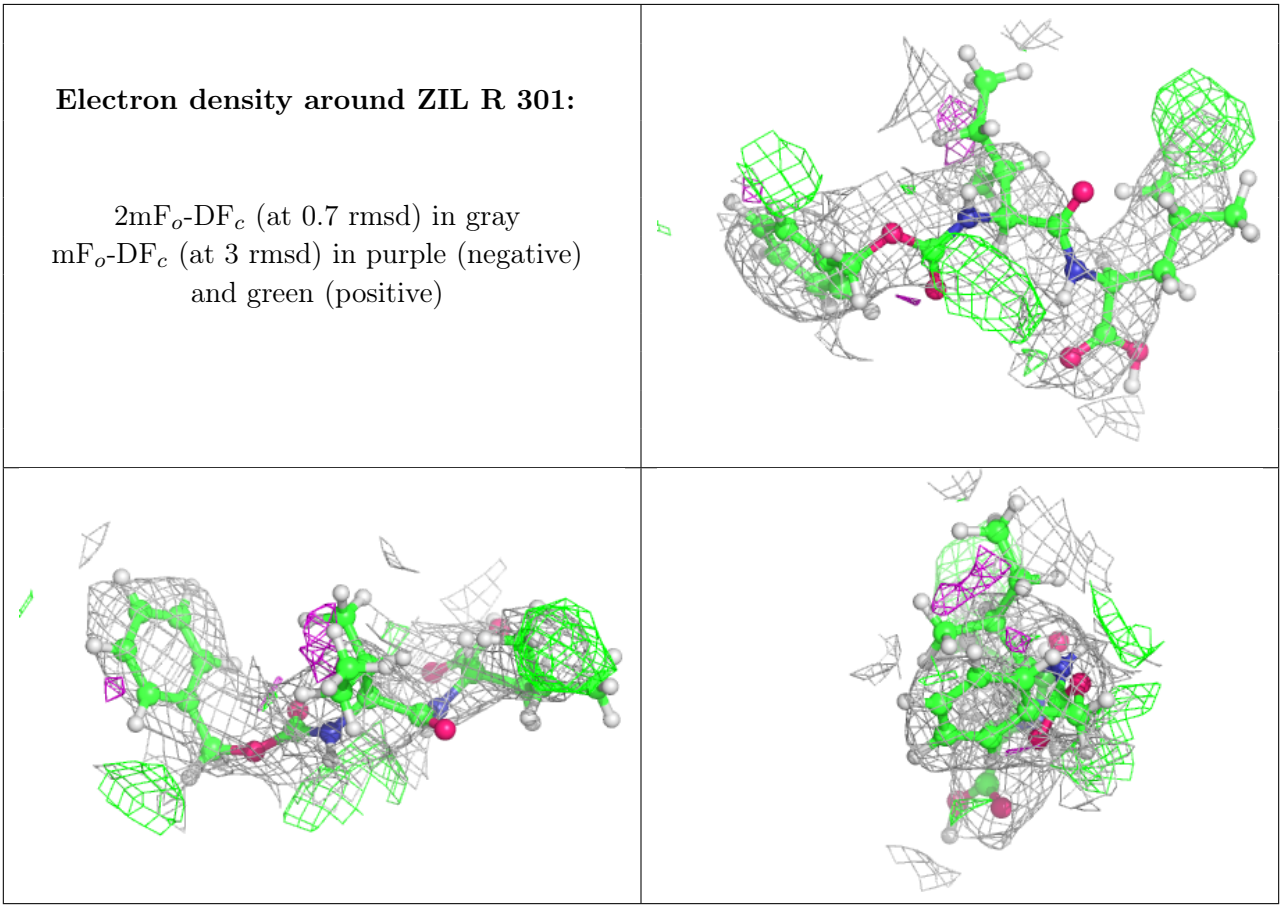
Electron density around ZIL C 301:

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



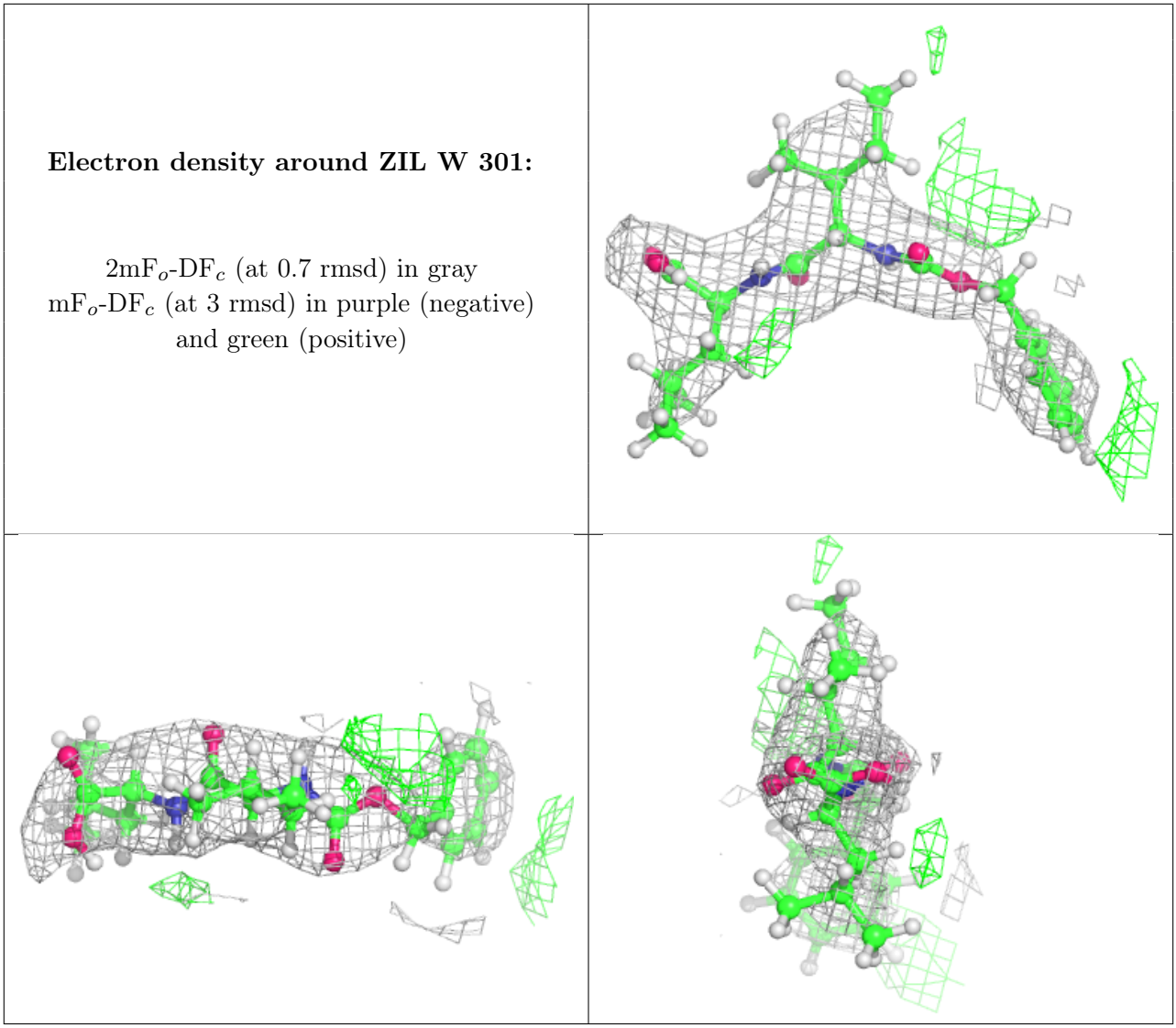
Electron density around ZIL R 301:

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



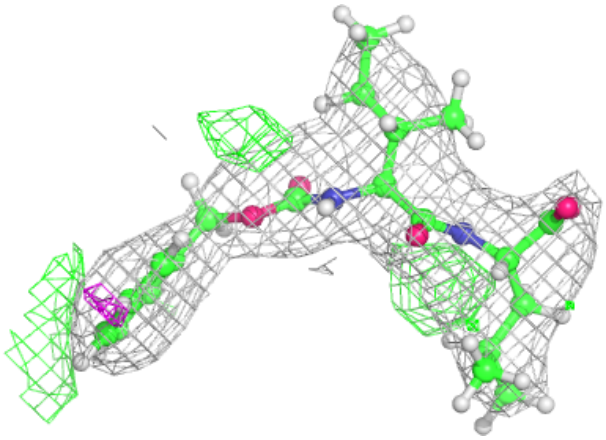
Electron density around ZIL W 301:

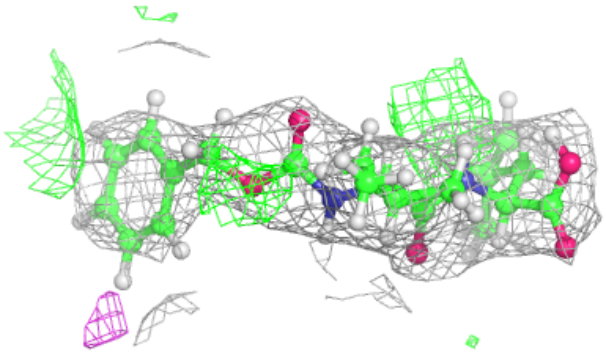
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

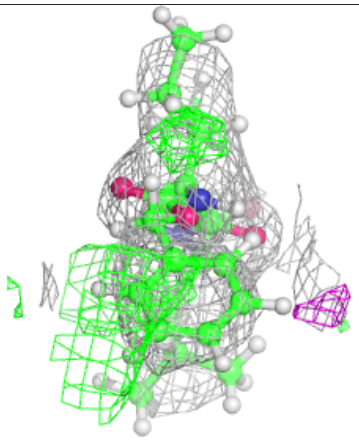


Electron density around ZIL L 301:

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

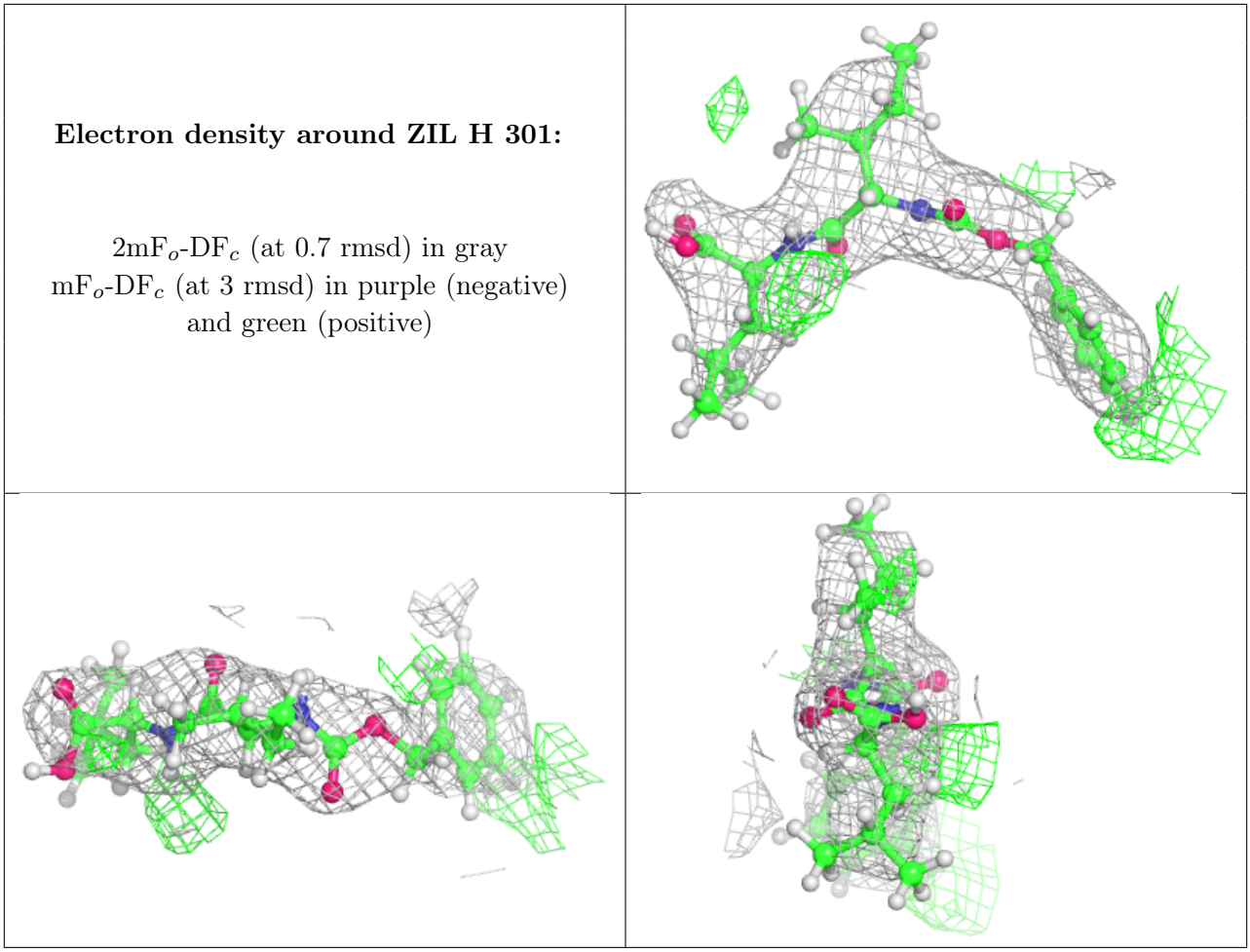






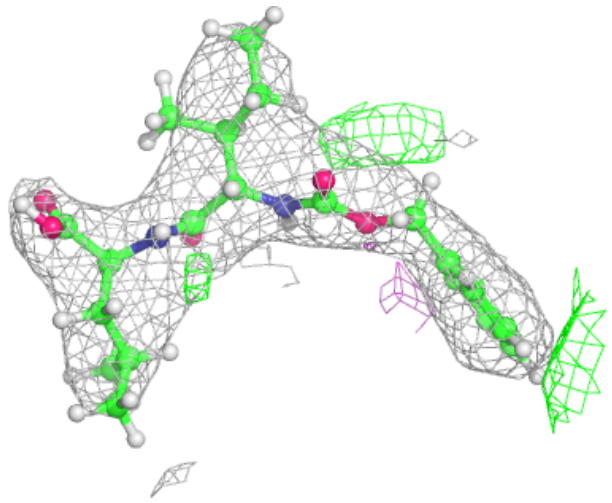
Electron density around ZIL H 301:

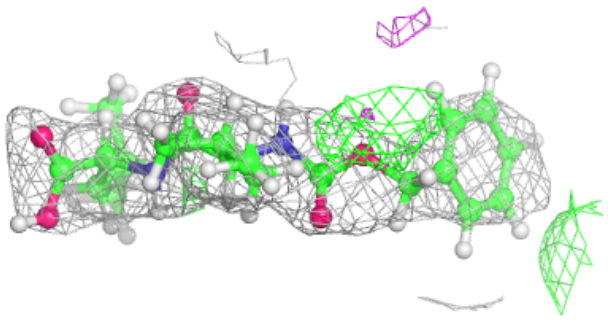
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

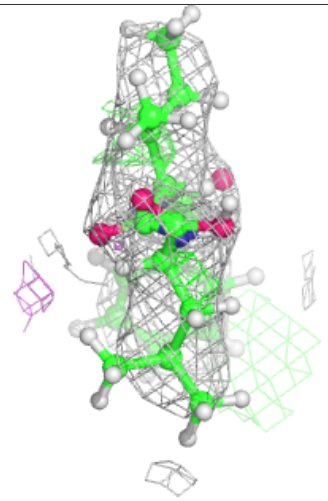


Electron density around ZIL Z 301:

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

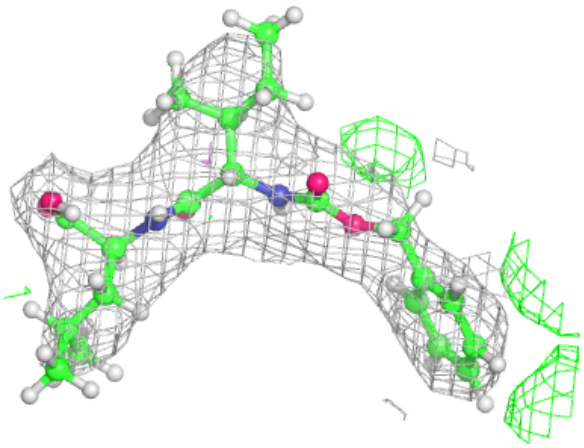


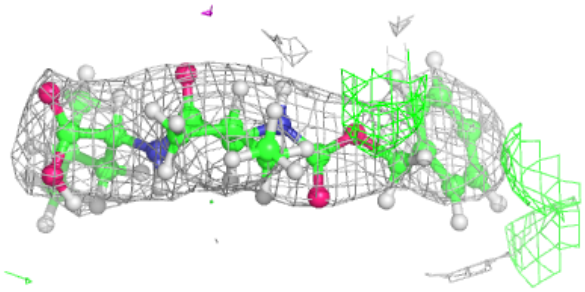


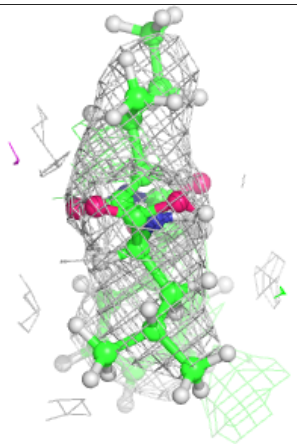


Electron density around ZIL K 301:

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

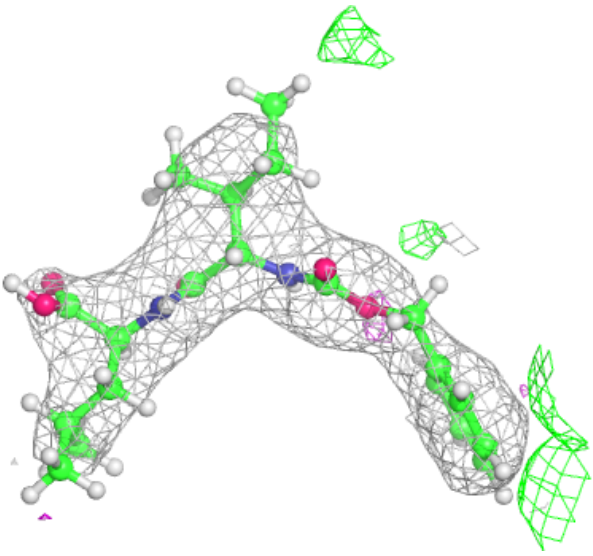


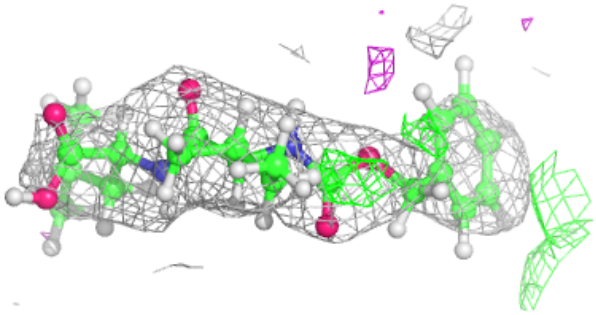


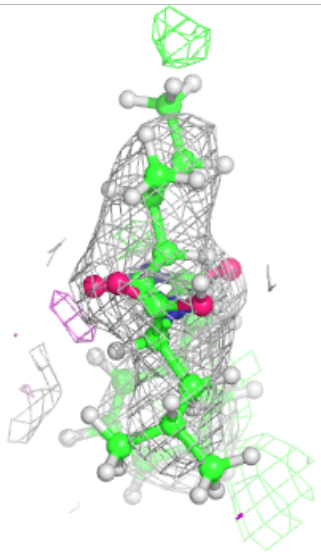


Electron density around ZIL I 301:

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

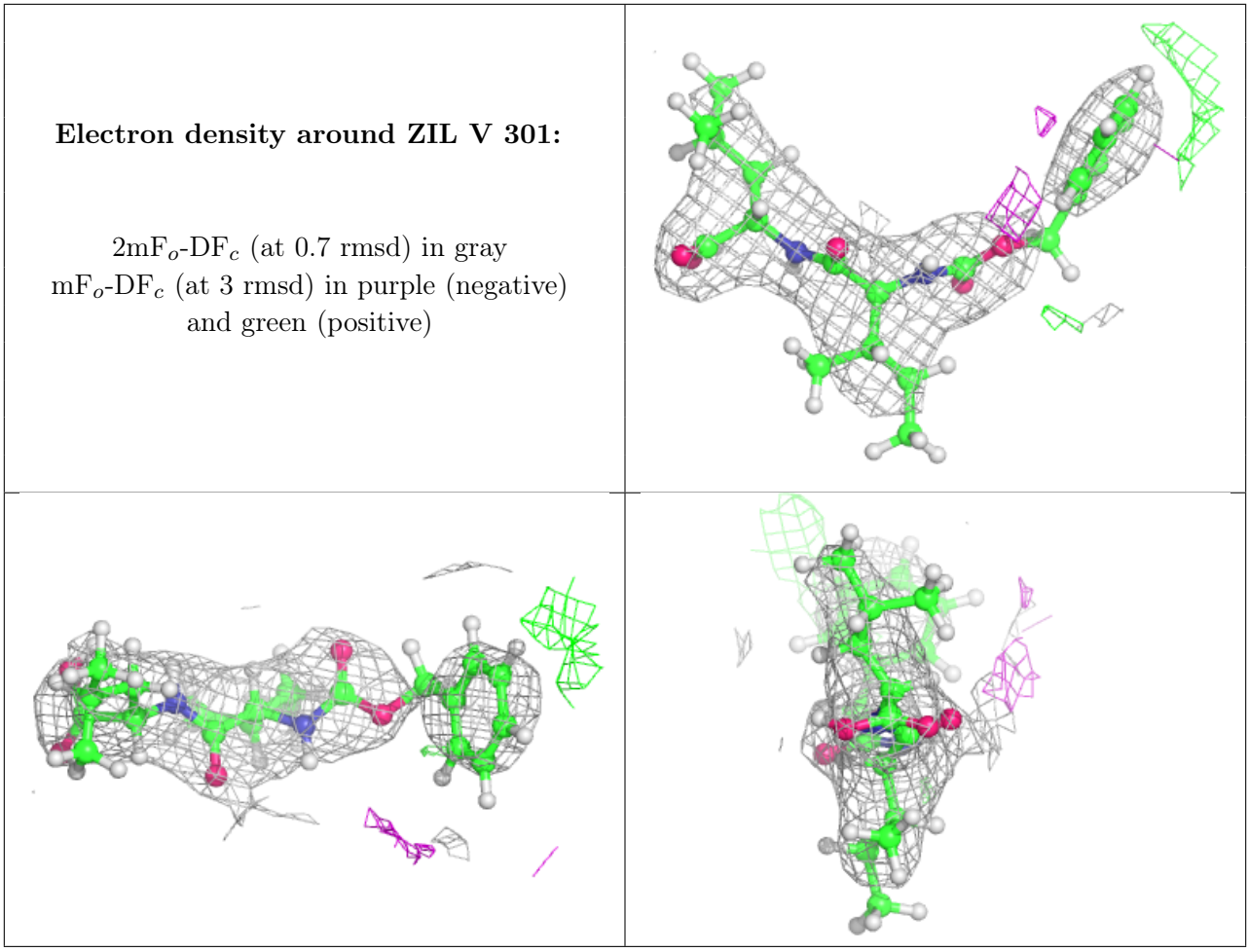






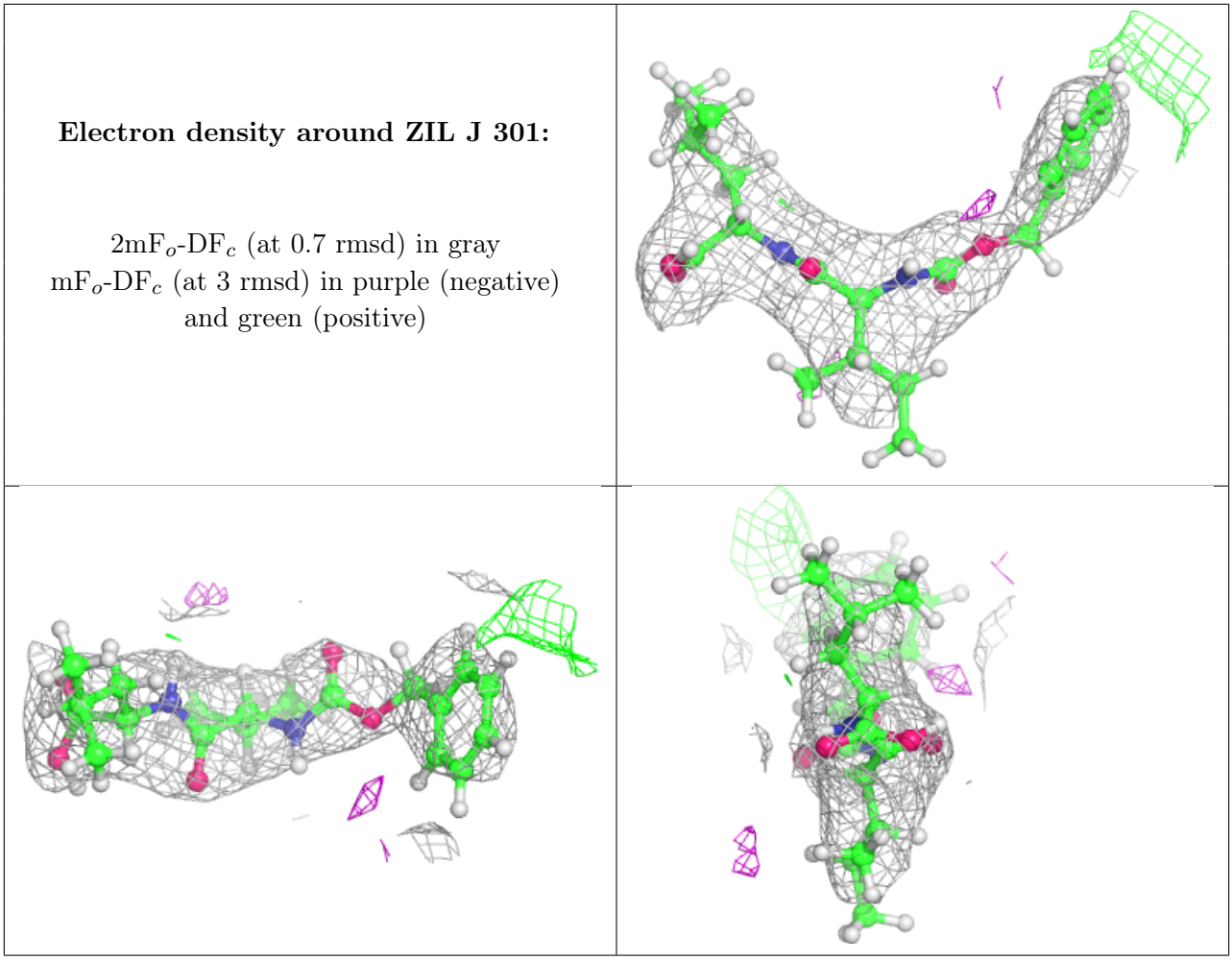
Electron density around ZIL V 301:

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



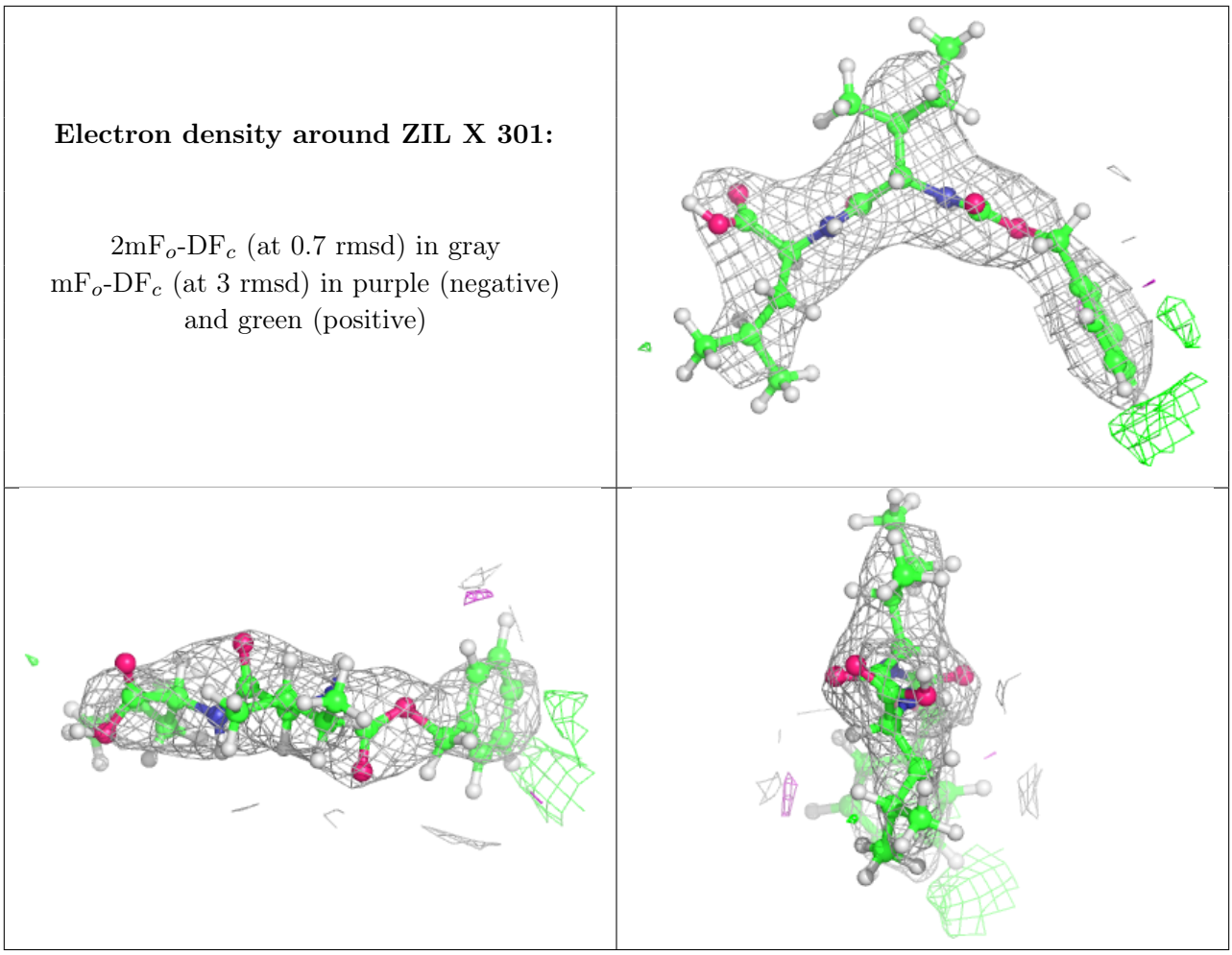
Electron density around ZIL J 301:

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



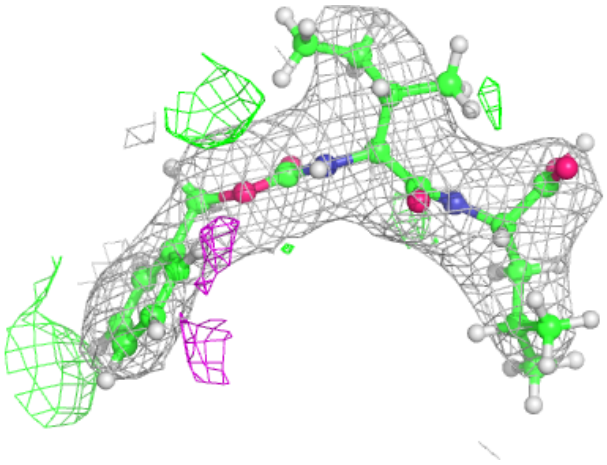
Electron density around ZIL X 301:

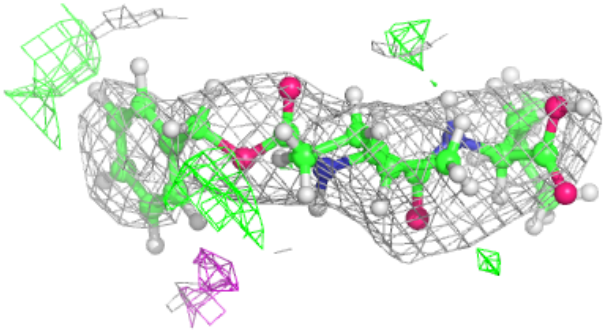
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

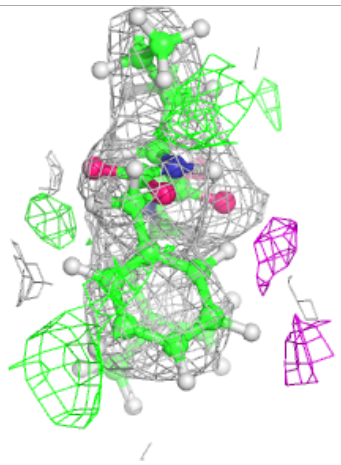


Electron density around ZIL Y 301:

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

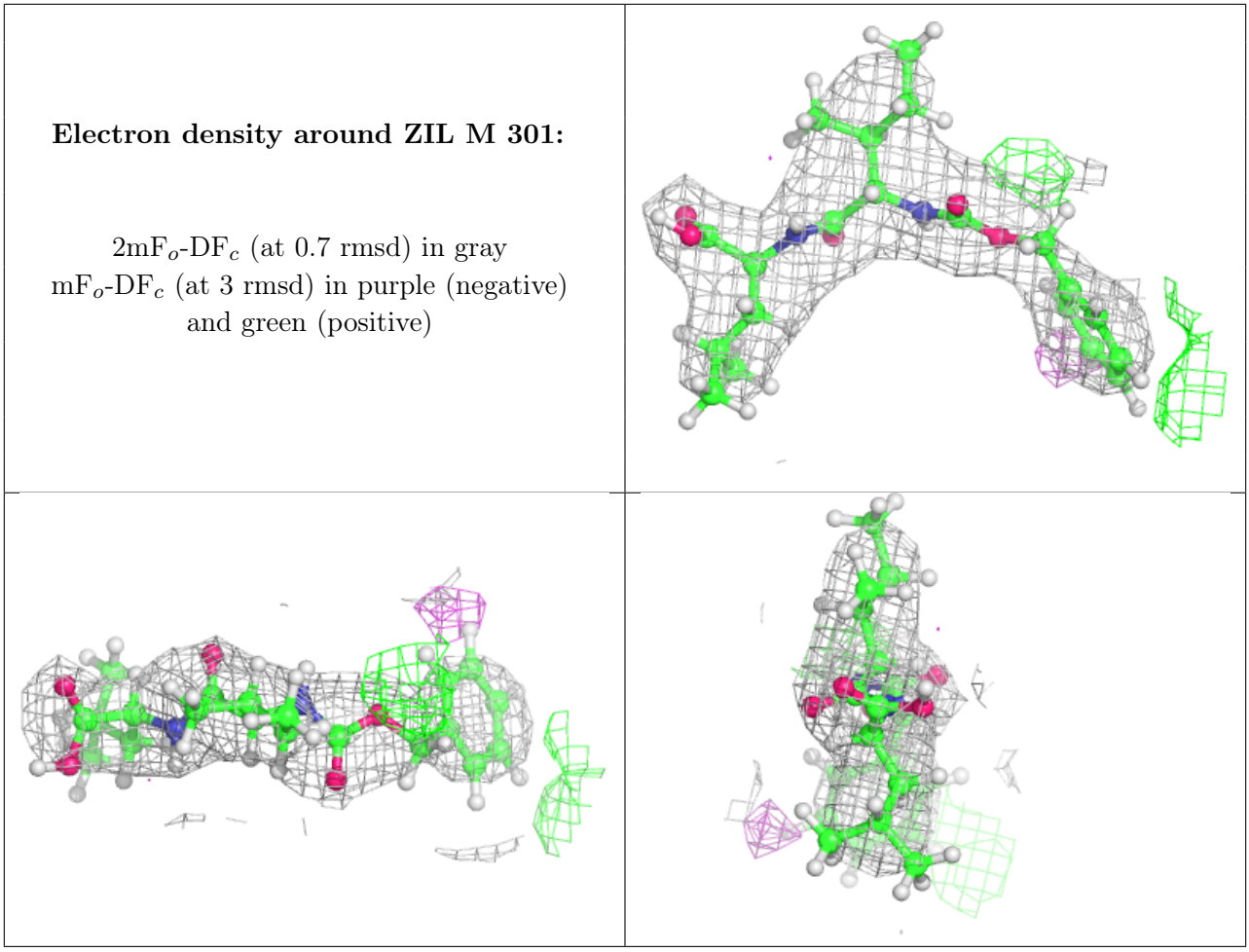






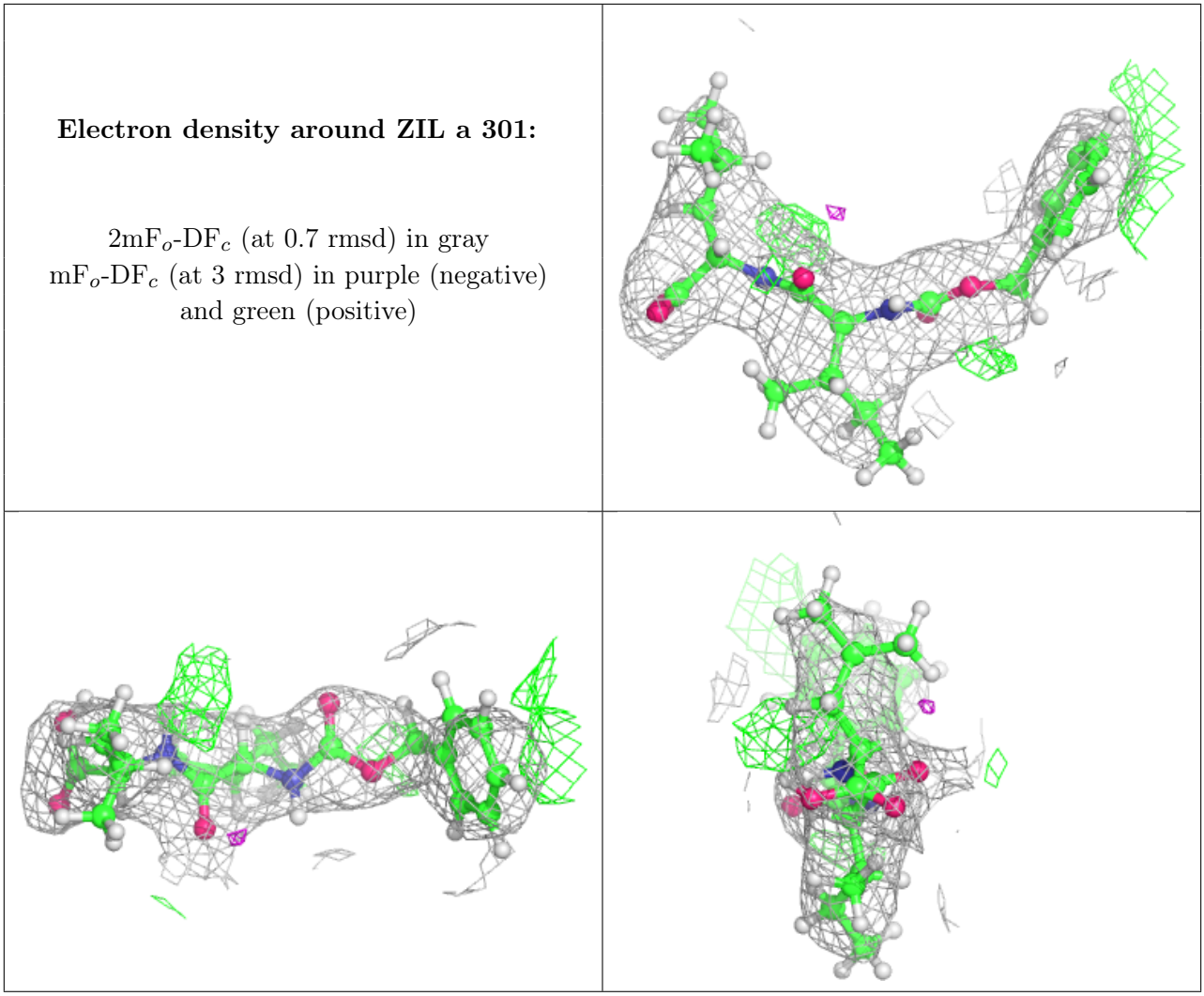
Electron density around ZIL M 301:

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



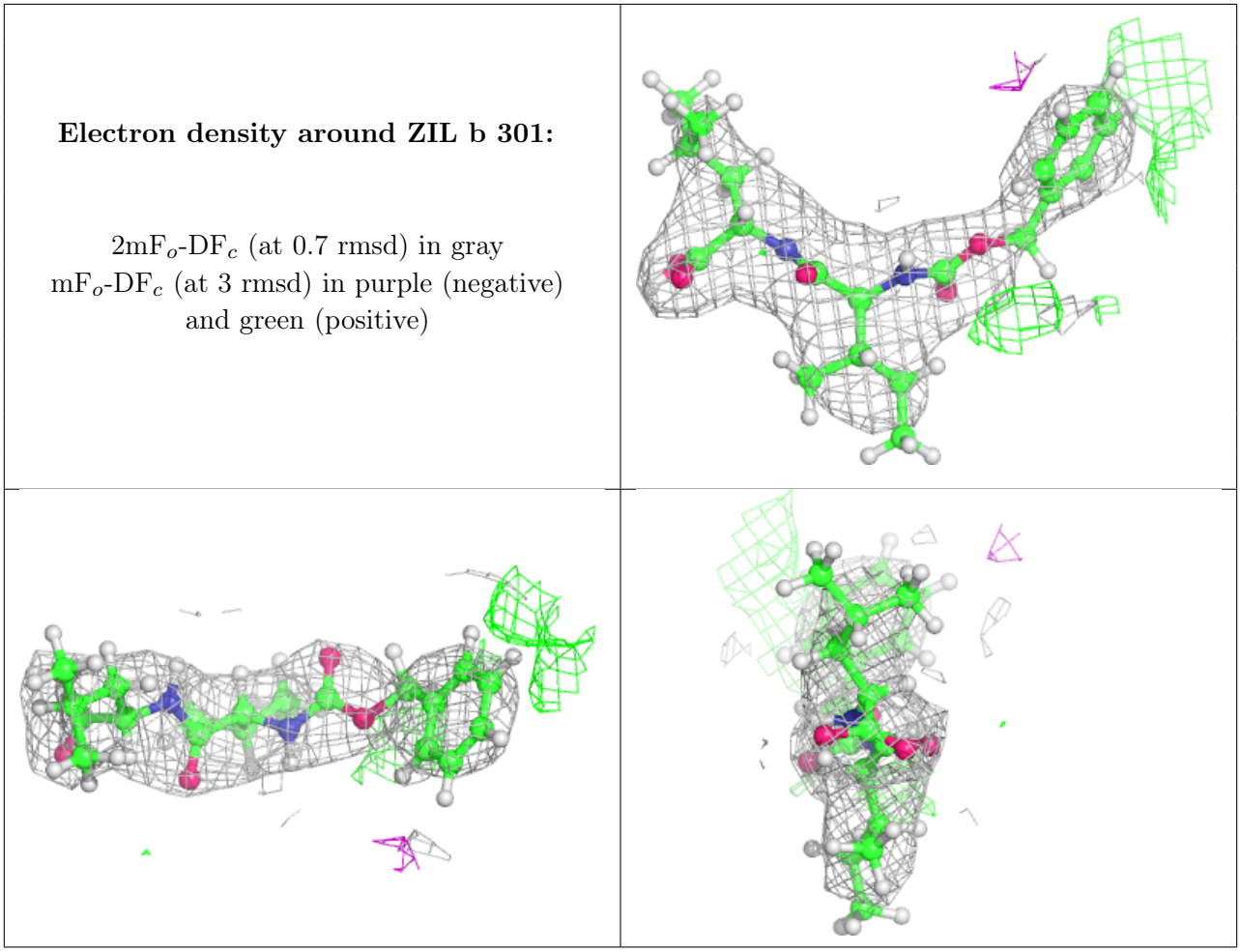
Electron density around ZIL a 301:

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



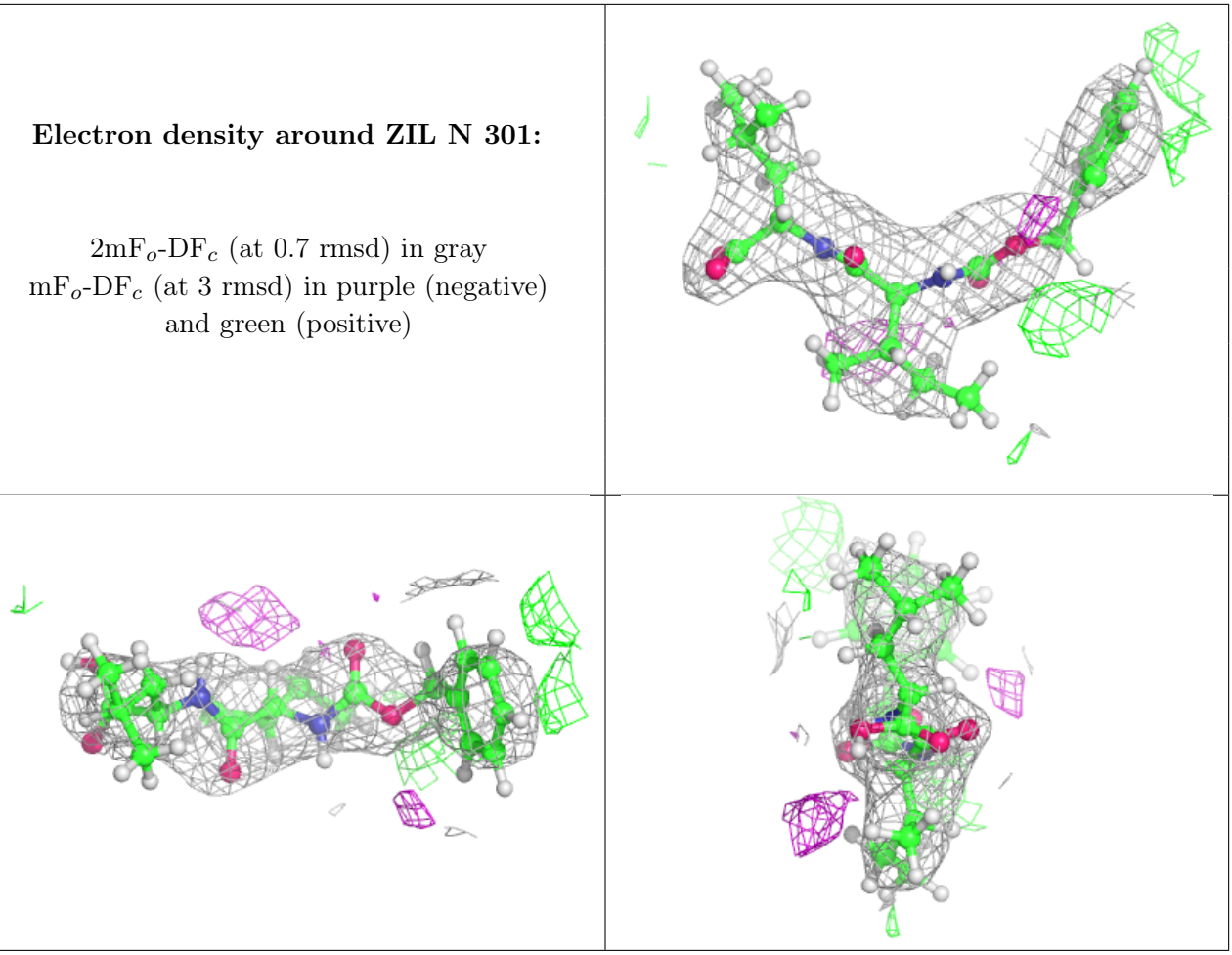
Electron density around ZIL b 301:

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



Electron density around ZIL N 301:

$2mF_o$-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.