wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 09:15 AM EST

PDB ID	:	6XRV
Title	:	X-ray structure of the monoclinic crystal form at 1.43 A resolution of lipase from Thermomyces (Humicola) lanuginosa at 173 K
Authors	:	McPherson, A.
Deposited on	:	2020-07-13
Resolution	:	1.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

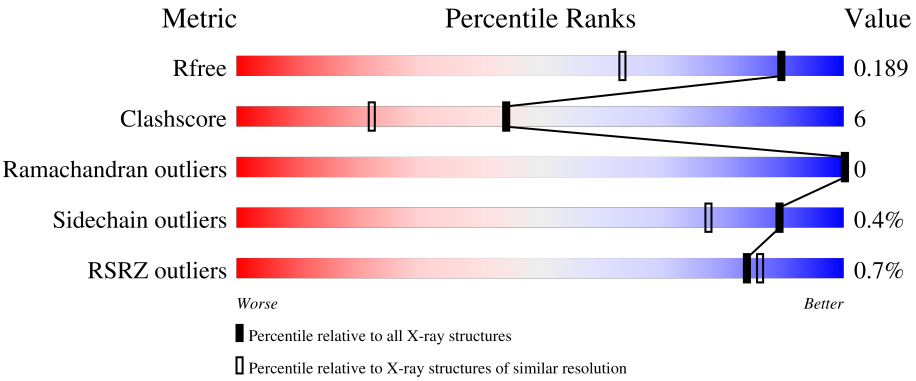
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.43 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}	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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	291	87% 5% 8%
1	B	291	87% 6% 8%
1	C	291	88% 8%
1	D	291	88% 8%
1	E	291	89% 8%

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Mol	Chain	Length	Quality of chain
1	F	291	87% 5% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OCA	A	301	-	-	X	X
2	OCA	B	301	-	-	X	X
2	OCA	C	301	-	-	X	-
2	OCA	D	301	-	-	X	-
2	OCA	E	301	-	-	X	X
2	OCA	F	301	-	-	X	-
4	LTV	A	303	X	-	-	-
4	LTV	F	304	X	-	-	-
5	PO4	D	305	-	-	X	-

2 Entry composition (i)

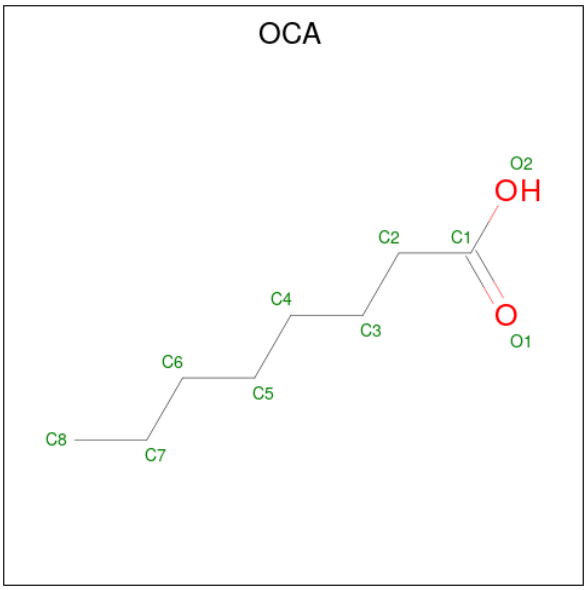
There are 7 unique types of molecules in this entry. The entry contains 26832 atoms, of which 12112 are hydrogens and 0 are deuteriums.

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 Lipase.

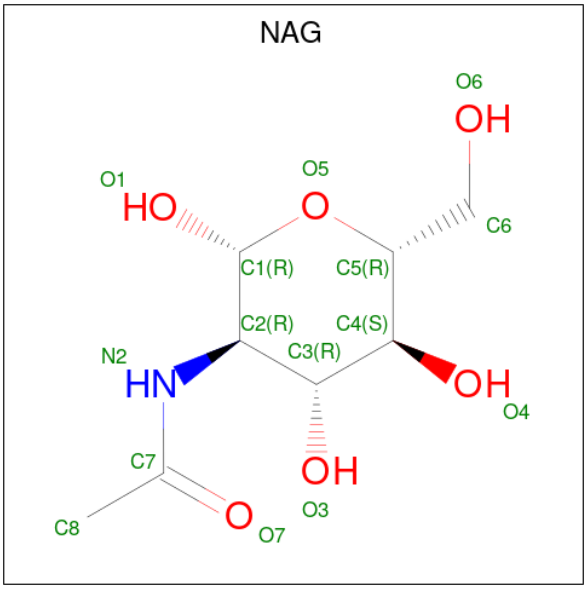
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	H	N	O	S	0	8	0
			4132	1332	2019	364	411	6			
1	B	269	Total	C	H	N	O	S	0	5	0
			4106	1327	2004	364	405	6			
1	C	269	Total	C	H	N	O	S	0	10	0
			4159	1337	2032	371	413	6			
1	E	269	Total	C	H	N	O	S	0	4	0
			4071	1315	1980	361	409	6			
1	D	269	Total	C	H	N	O	S	0	4	0
			4085	1317	1991	364	407	6			
1	F	269	Total	C	H	N	O	S	0	7	0
			4120	1332	2008	365	409	6			

- Molecule 2 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 8 1	0	0
2	B	1	Total C O 9 8 1	0	0
2	C	1	Total C O 9 8 1	0	0
2	E	1	Total C O 9 8 1	0	0
2	D	1	Total C O 9 8 1	0	0
2	F	1	Total C O 9 8 1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 27 8 13 1 5	0	0
3	B	1	Total C H N O 27 8 13 1 5	0	0
3	C	1	Total C H N O 27 8 13 1 5	0	0
3	E	1	Total C H N O 27 8 13 1 5	0	0
3	D	1	Total C H N O 27 8 13 1 5	0	0

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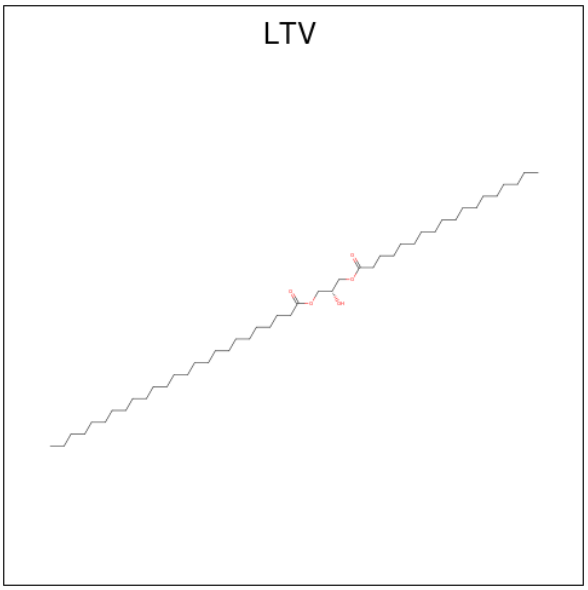
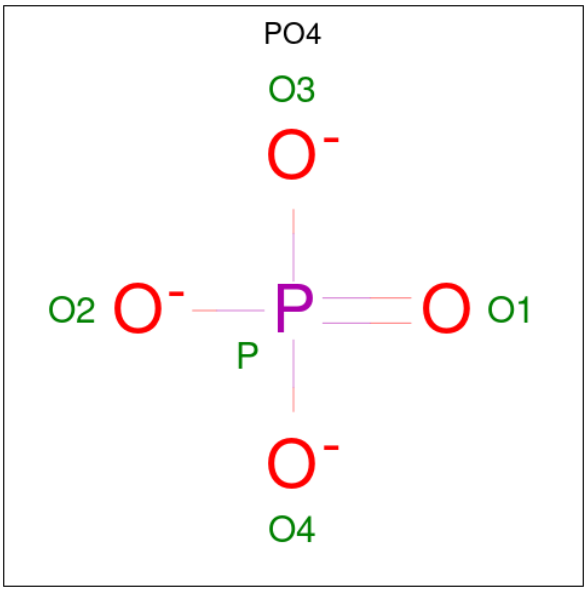
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is 2-hydroxy-3-(octadecanoyloxy)propyl pentacosanoate (three-letter code: LTV) (formula: $C_{46}H_{90}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			36	31	5			
4	B	1	Total	C	O		0	0
			43	38	5			
4	C	1	Total	C	O		0	0
			41	36	5			
4	E	1	Total	C	O		0	0
			51	46	5			
4	D	1	Total	C	O		0	0
			51	46	5			
4	F	1	Total	C	O		0	0
			42	37	5			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Ca 2 2	0	0
6	C	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is water.

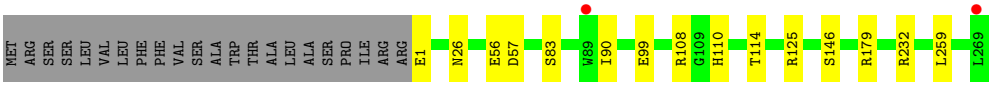
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	305	Total O 308 308	0	3
7	B	308	Total O 311 311	0	4
7	C	256	Total O 256 256	0	1
7	E	202	Total O 202 202	0	0
7	D	244	Total O 246 246	0	2
7	F	303	Total O 305 305	0	3

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.

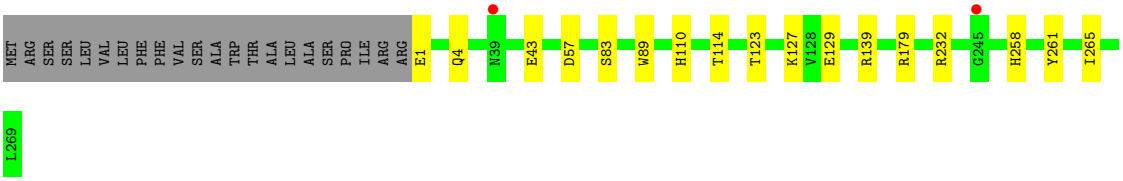
• Molecule 1: Lipase

Chain A:



• Molecule 1: Lipase

Chain B:

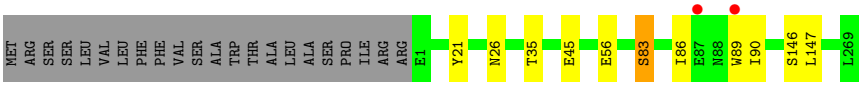


• Molecule 1: Lipase

Chain C:

• Molecule 1: Lipase

Chain E:



• Molecule 1: Lipase

Chain D:

• Molecule 1: Lipase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.93Å 89.94Å 123.42Å 90.00° 94.49° 90.00°	Depositor
Resolution (Å)	77.00 – 1.43 77.00 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (77.00-1.43) 99.7 (77.00-1.43)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.149 , 0.187 0.153 , 0.189	Depositor DCC
R_{free} test set	15469 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	26832	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: OCA, PO4, LTV, CA, NAG

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	0.33	0/2187	0.56	0/2974
1	B	0.32	0/2167	0.56	0/2950
1	C	0.34	0/2211	0.55	0/3005
1	D	0.31	0/2156	0.53	0/2934
1	E	0.30	0/2155	0.51	0/2933
1	F	0.32	0/2188	0.55	0/2978
All	All	0.32	0/13064	0.54	0/17774

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	209[A]	ARG	Sidechain
1	C	209[B]	ARG	Sidechain

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	2113	2019	2014	15	2
1	B	2102	2004	2001	12	1
1	C	2127	2032	2020	18	1
1	D	2094	1991	1992	14	0
1	E	2091	1980	1975	19	0
1	F	2112	2008	1994	21	0
2	A	9	0	15	6	0
2	B	9	0	15	16	0
2	C	9	0	15	26	0
2	D	9	0	15	16	0
2	E	9	0	15	22	0
2	F	9	0	15	15	0
3	A	14	13	13	0	0
3	B	14	13	13	0	0
3	C	14	13	13	0	0
3	D	14	13	13	0	0
3	E	14	13	13	0	0
3	F	14	13	13	0	0
4	A	36	0	0	0	0
4	B	43	0	0	13	0
4	C	41	0	0	16	0
4	D	51	0	0	11	0
4	E	51	0	0	7	0
4	F	42	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	D	10	0	0	2	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	308	0	0	2	0
7	B	311	0	0	4	0
7	C	256	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	246	0	0	4	2
7	E	202	0	0	0	1
7	F	305	0	0	8	1
All	All	14720	12112	12164	149	4

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 6.

The worst 5 of 149 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)
2:B:301:OCA:C7	4:B:306:LTV:C32	1.80	1.60
2:D:301:OCA:H81	4:D:304:LTV:C29	1.35	1.56
2:C:301:OCA:H83	4:C:304:LTV:C31	1.42	1.45
2:D:301:OCA:H81	4:D:304:LTV:C30	1.51	1.41
2:C:301:OCA:C8	4:C:304:LTV:C31	2.01	1.37

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:HZ3	7:E:572:HOH:O[1_455]	1.40	0.20
1:A:179:ARG:HH22	7:D:458:HOH:O[2_647]	1.50	0.10
1:A:179:ARG:NH2	7:D:458:HOH:O[2_647]	2.10	0.10
1:B:43:GLU:OE2	7:F:560:HOH:O[1_655]	2.14	0.06

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	275/291 (94%)	268 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	272/291 (94%)	264 (97%)	8 (3%)	0	100	100
1	C	277/291 (95%)	269 (97%)	8 (3%)	0	100	100
1	D	271/291 (93%)	264 (97%)	7 (3%)	0	100	100
1	E	271/291 (93%)	264 (97%)	7 (3%)	0	100	100
1	F	274/291 (94%)	265 (97%)	9 (3%)	0	100	100
All	All	1640/1746 (94%)	1594 (97%)	46 (3%)	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	228/239 (95%)	228 (100%)	0	100	100
1	B	224/239 (94%)	224 (100%)	0	100	100
1	C	229/239 (96%)	225 (98%)	4 (2%)	56	23
1	D	224/239 (94%)	224 (100%)	0	100	100
1	E	224/239 (94%)	223 (100%)	1 (0%)	89	78
1	F	227/239 (95%)	226 (100%)	1 (0%)	89	78
All	All	1356/1434 (95%)	1350 (100%)	6 (0%)	89	78

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	209[B]	ARG
1	E	83	SER
1	F	146	SER
1	C	146	SER
1	C	83	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 for Mogul analysis.

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	NAG	D	303	1	14,14,15	0.26	0	17,19,21	0.55	0
5	PO4	B	307	-	4,4,4	0.96	0	6,6,6	0.46	0
5	PO4	B	302	-	4,4,4	0.95	0	6,6,6	0.51	0
4	LTV	E	304	-	50,50,50	0.90	2 (4%)	52,52,52	0.95	3 (5%)
5	PO4	A	304	-	4,4,4	0.99	0	6,6,6	0.59	0
2	OCA	C	301	-	7,8,9	0.48	0	6,7,9	1.55	1 (16%)
5	PO4	E	306	-	4,4,4	1.05	0	6,6,6	0.31	0
4	LTV	B	306	-	42,42,50	0.99	2 (4%)	44,44,52	0.99	3 (6%)
2	OCA	B	301	1	7,8,9	0.51	0	6,7,9	0.86	0
4	LTV	A	303	-	35,35,50	1.10	2 (5%)	37,37,52	1.07	2 (5%)
4	LTV	C	304	-	40,40,50	1.00	2 (5%)	42,42,52	0.95	2 (4%)
5	PO4	D	305	-	4,4,4	0.94	0	6,6,6	0.38	0
5	PO4	E	305	-	4,4,4	0.97	0	6,6,6	0.40	0
2	OCA	D	301	1	7,8,9	0.44	0	6,7,9	1.08	0
3	NAG	B	305	1	14,14,15	0.37	0	17,19,21	0.56	0
3	NAG	A	302	1	14,14,15	0.73	1 (7%)	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	303	1	14,14,15	0.30	0	17,19,21	0.48	0
5	PO4	F	305	-	4,4,4	0.91	0	6,6,6	0.40	0
2	OCA	E	301	1	7,8,9	0.45	0	6,7,9	0.75	0
4	LTV	F	304	-	41,41,50	0.99	2 (4%)	43,43,52	0.94	2 (4%)
2	OCA	F	301	1	7,8,9	0.50	0	6,7,9	0.83	0
3	NAG	E	303	1	14,14,15	0.24	0	17,19,21	0.41	0
4	LTV	D	304	-	50,50,50	0.93	2 (4%)	52,52,52	0.90	2 (3%)
5	PO4	A	305	-	4,4,4	0.83	0	6,6,6	0.59	0
5	PO4	D	306	-	4,4,4	0.95	0	6,6,6	0.55	0
3	NAG	F	303	1	14,14,15	0.37	0	17,19,21	0.54	0
2	OCA	A	301	1	7,8,9	0.42	0	6,7,9	1.13	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	LTV	B	306	-	-	22/43/43/51	-
2	OCA	B	301	1	-	4/6/6/7	-
2	OCA	E	301	1	-	3/6/6/7	-
4	LTV	A	303	-	1/1/3/3	22/36/36/51	-
4	LTV	F	304	-	1/1/3/3	21/42/42/51	-
2	OCA	D	301	1	-	5/6/6/7	-
2	OCA	F	301	1	-	4/6/6/7	-
3	NAG	E	303	1	-	1/6/23/26	0/1/1/1
3	NAG	D	303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	305	1	-	0/6/23/26	0/1/1/1
4	LTV	E	304	-	-	22/51/51/51	-
4	LTV	D	304	-	-	21/51/51/51	-
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
2	OCA	C	301	-	-	2/6/6/7	-
3	NAG	C	303	1	-	0/6/23/26	0/1/1/1
4	LTV	C	304	-	-	23/41/41/51	-
3	NAG	F	303	1	-	2/6/23/26	0/1/1/1
2	OCA	A	301	1	-	5/6/6/7	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	LTV	O1-C17	4.42	1.46	1.33
4	B	306	LTV	O3-C21	4.41	1.46	1.33
4	D	304	LTV	O1-C17	4.37	1.46	1.33
4	A	303	LTV	O3-C21	4.35	1.46	1.33
4	D	304	LTV	O3-C21	4.34	1.46	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	303	LTV	O1-C17-C16	3.17	121.51	111.83
4	E	304	LTV	O1-C17-C16	3.04	121.09	111.83
4	B	306	LTV	O3-C21-C22	3.03	121.08	111.83
4	C	304	LTV	O3-C21-C22	2.98	120.91	111.83
4	A	303	LTV	O3-C21-C22	2.93	120.76	111.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	303	LTV	C19
4	F	304	LTV	C19

5 of 157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	OCA	O1-C1-C2-C3
2	C	301	OCA	C1-C2-C3-C4
2	E	301	OCA	C1-C2-C3-C4
4	B	306	LTV	O4-C21-O3-C20
4	B	306	LTV	C22-C21-O3-C20

There are no ring outliers.

11 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	304	LTV	7	0
2	C	301	OCA	26	0
4	B	306	LTV	13	0
2	B	301	OCA	16	0
4	C	304	LTV	16	0
5	D	305	PO4	2	0
2	D	301	OCA	16	0
2	E	301	OCA	22	0

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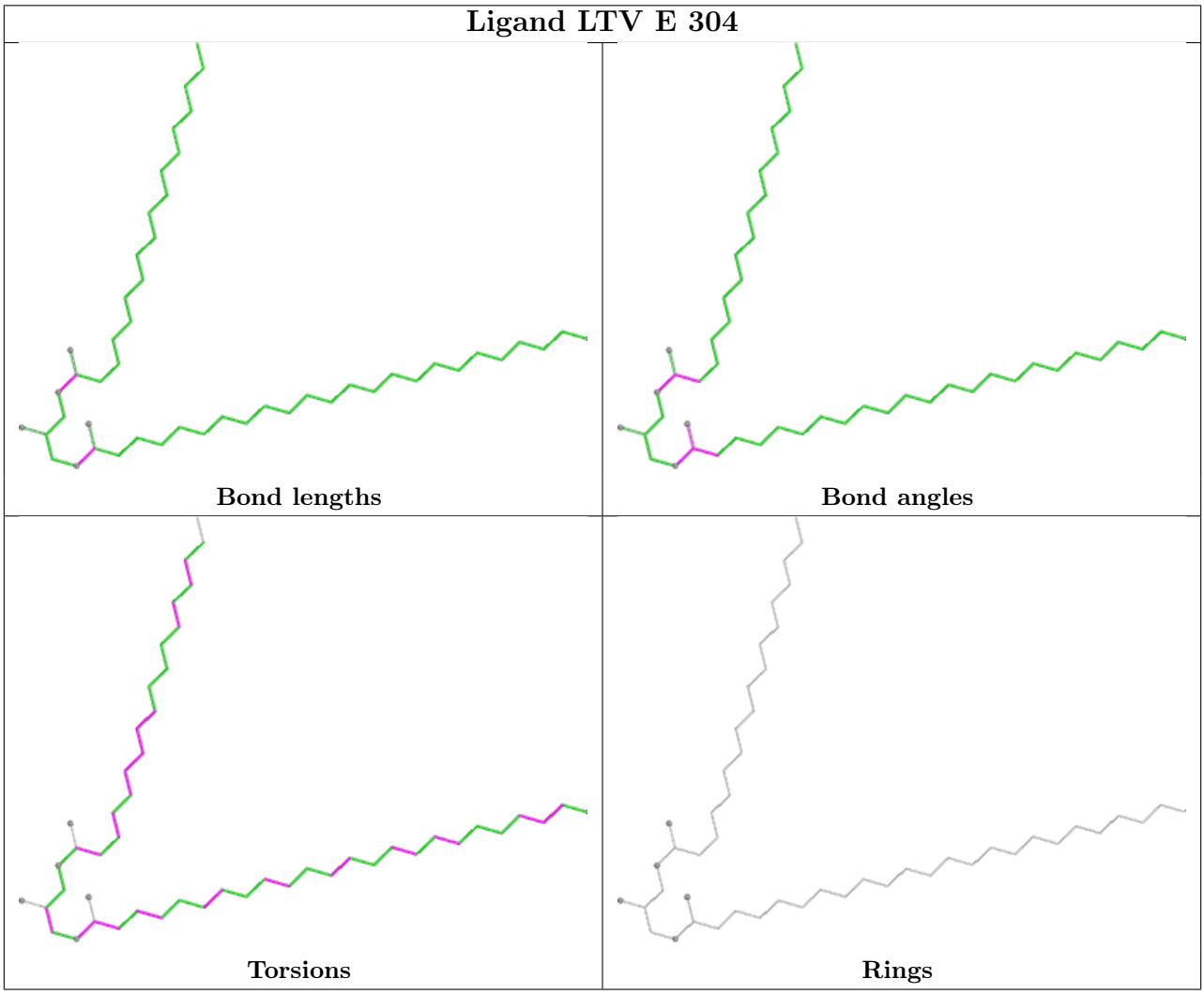
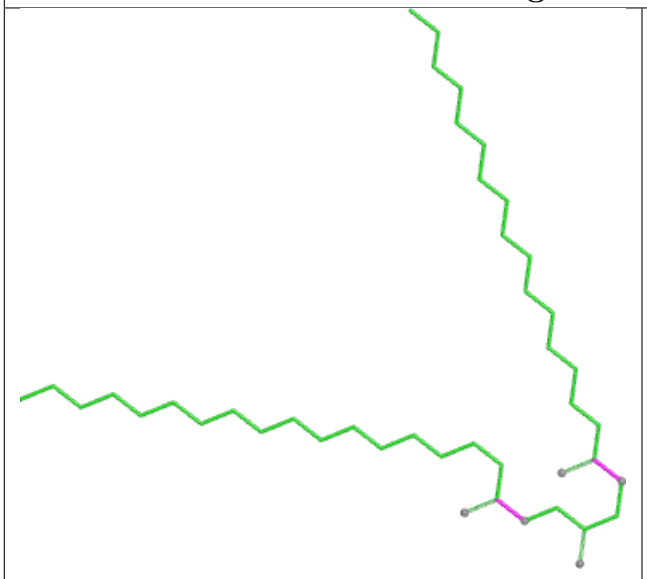
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	OCA	15	0
4	D	304	LTV	11	0
2	A	301	OCA	6	0

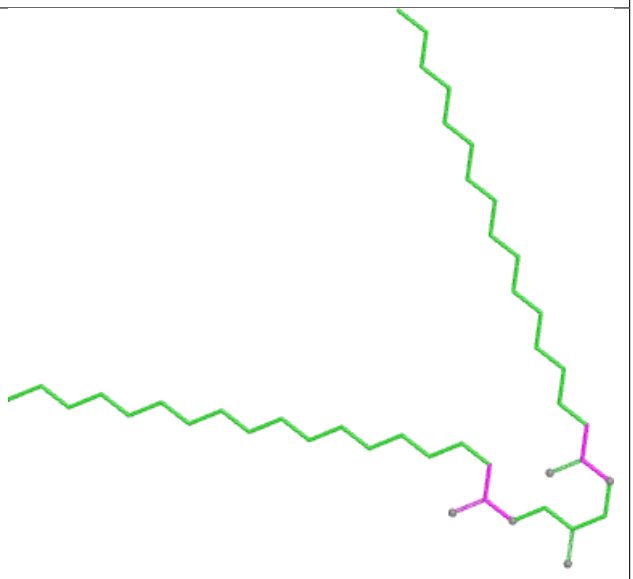
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



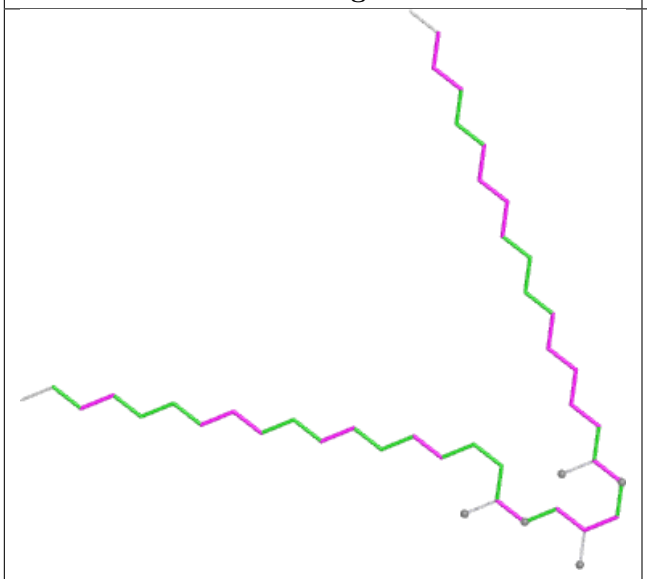
Ligand LTV B 306



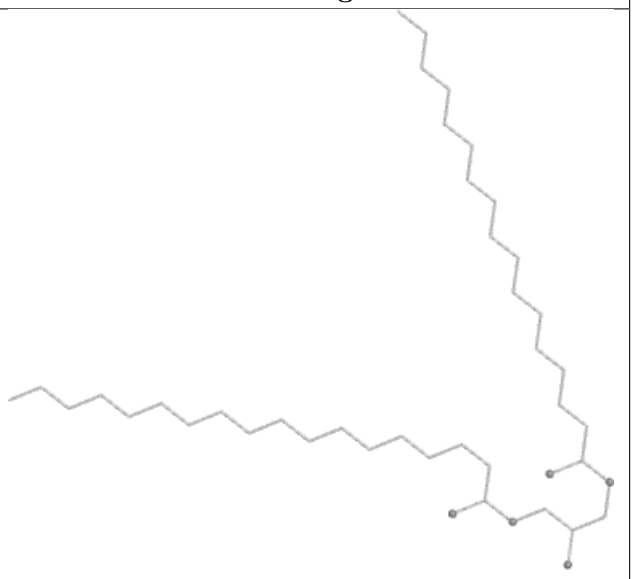
Bond lengths



Bond angles

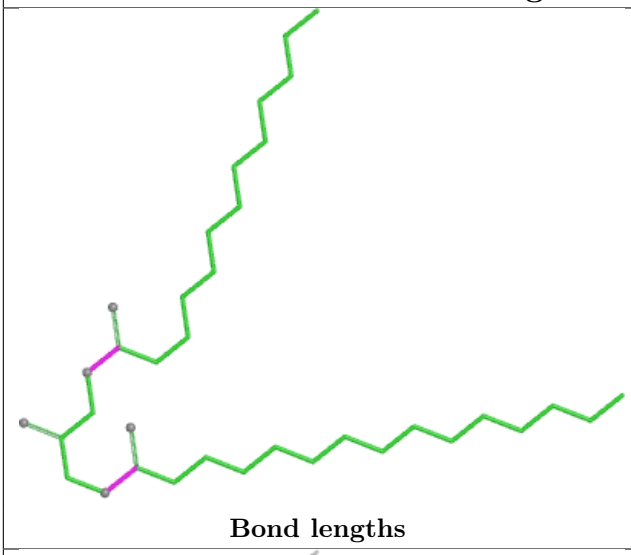


Torsions

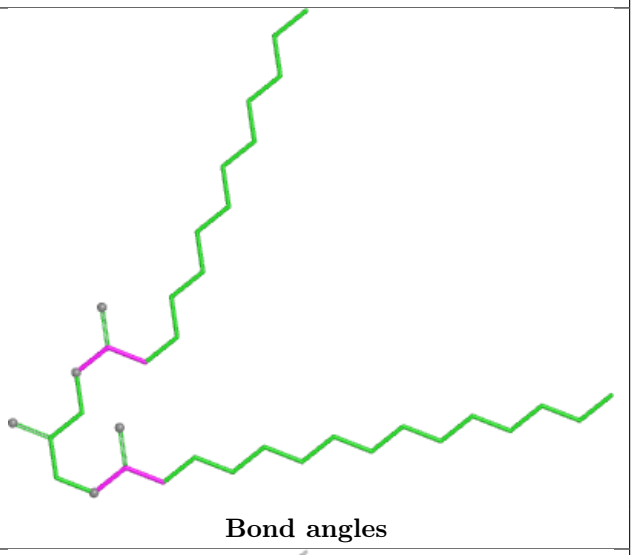


Rings

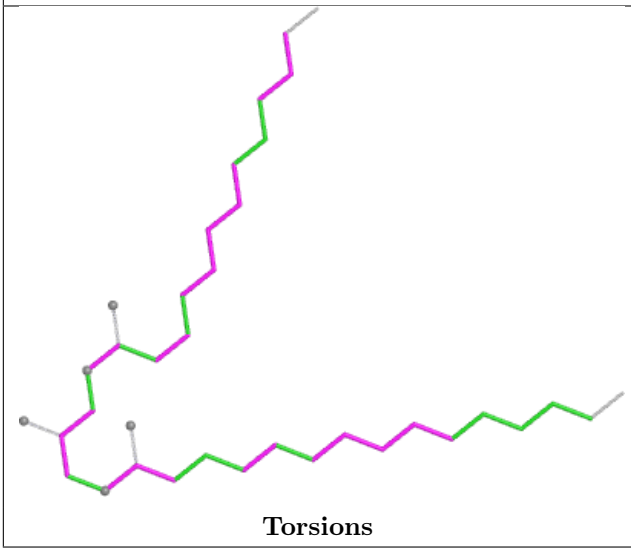
Ligand LTV A 303



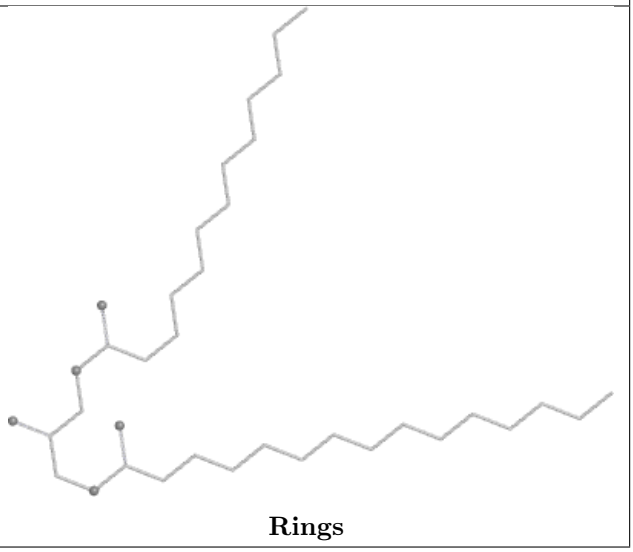
Bond lengths



Bond angles

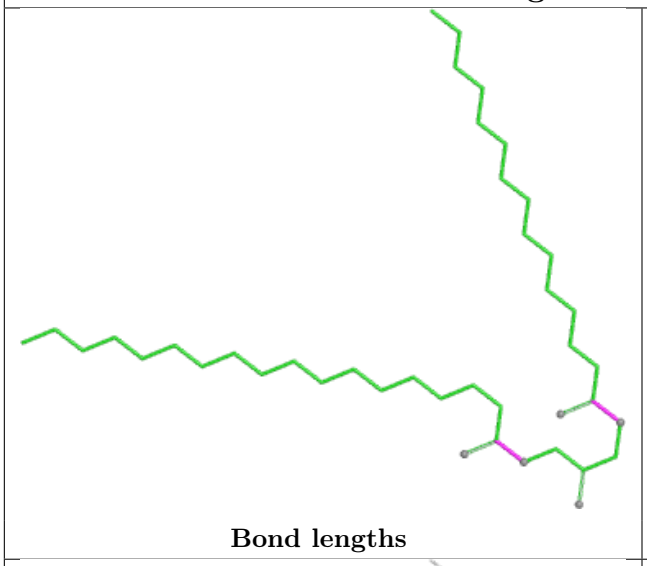


Torsions

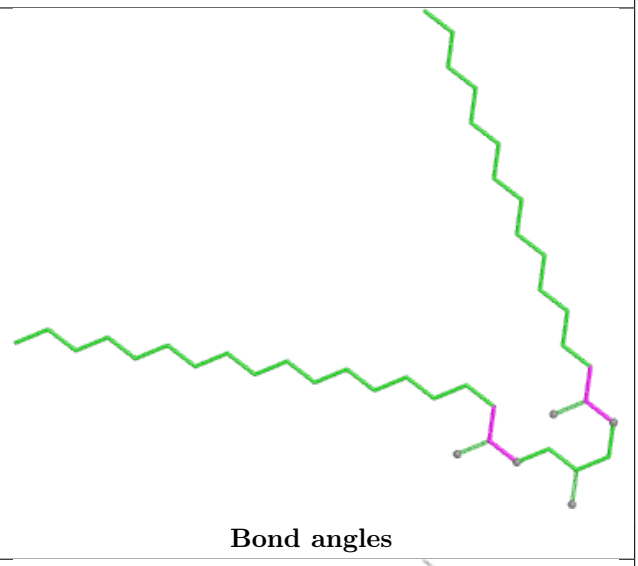


Rings

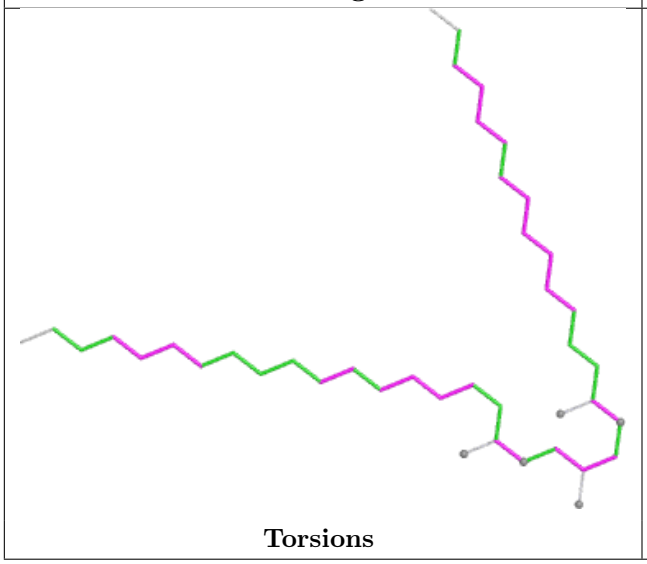
Ligand LTV C 304



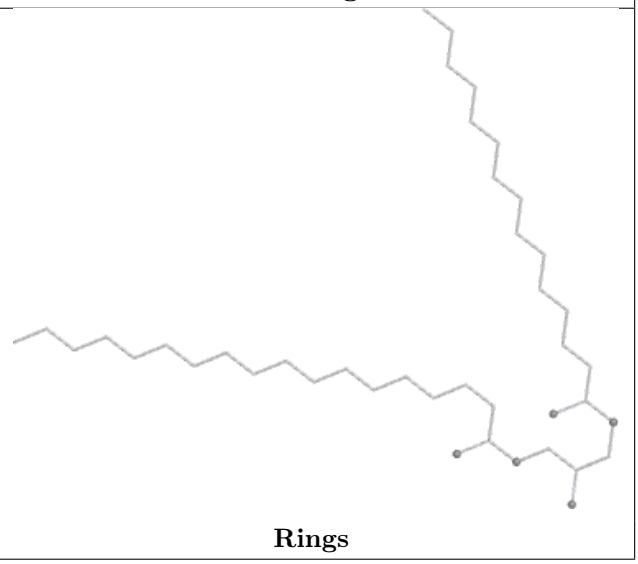
Bond lengths



Bond angles

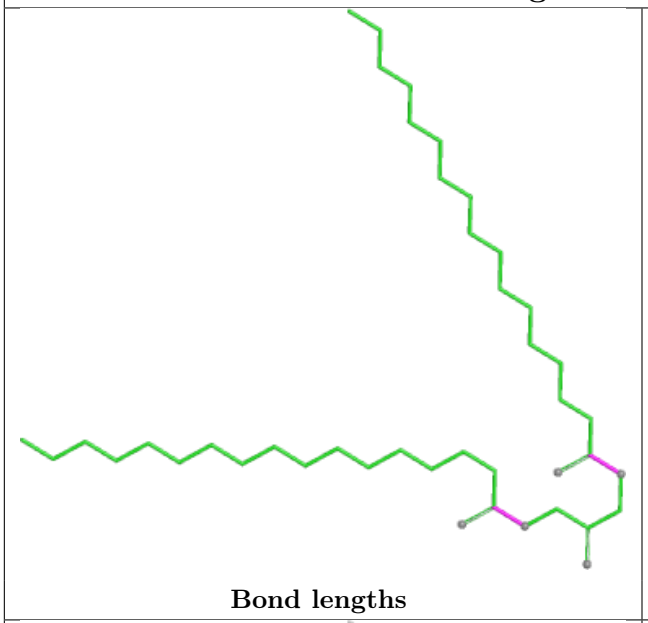


Torsions

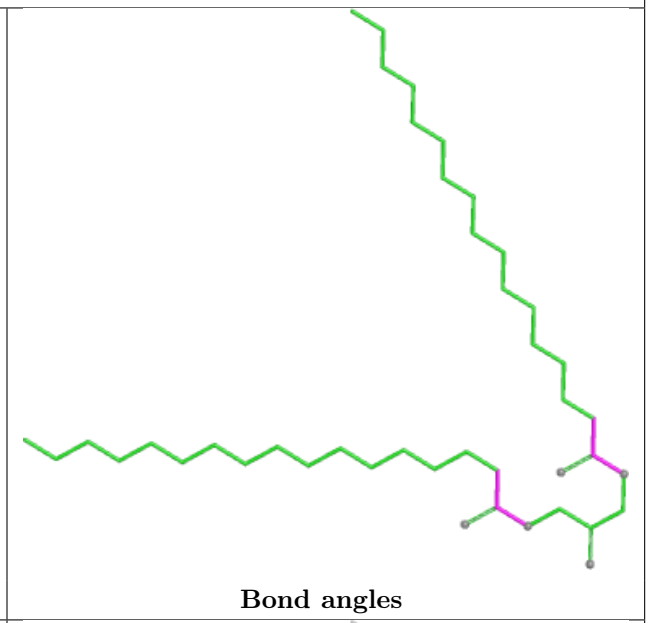


Rings

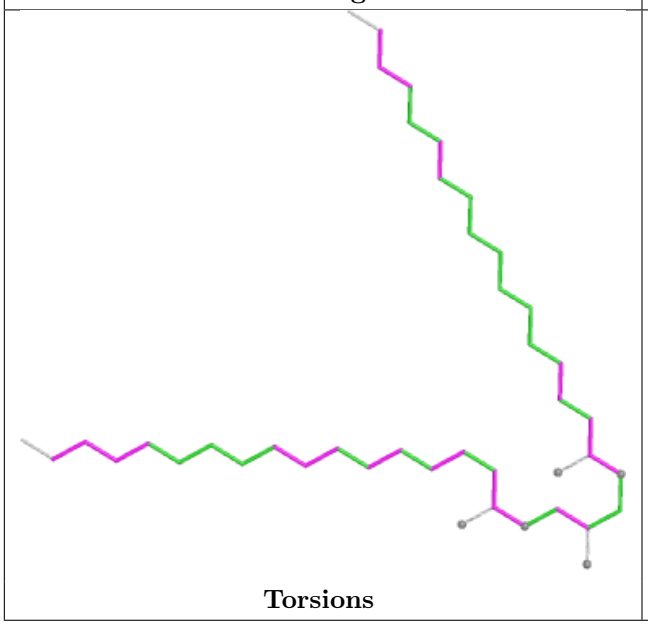
Ligand LTV F 304



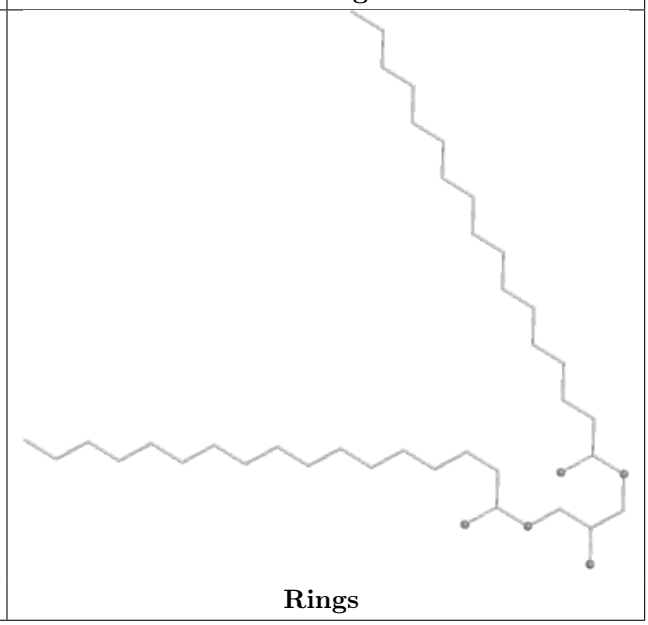
Bond lengths



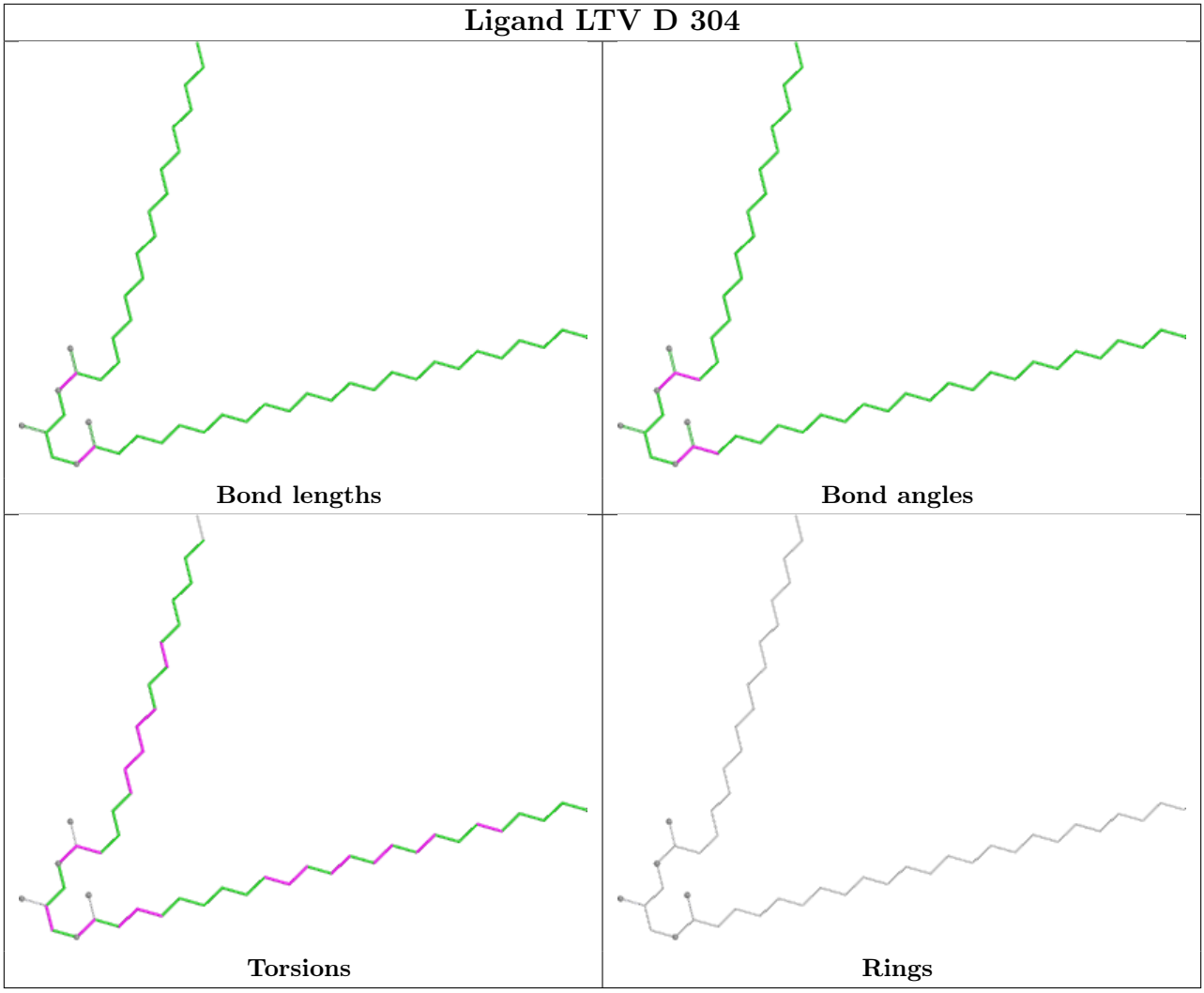
Bond angles



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	269/291 (92%)	-0.39	2 (0%) 84 86	10, 23, 40, 50	8 (2%)
1	B	269/291 (92%)	-0.31	2 (0%) 84 86	12, 25, 41, 51	4 (1%)
1	C	269/291 (92%)	-0.06	4 (1%) 71 74	12, 28, 46, 57	8 (2%)
1	D	269/291 (92%)	-0.31	2 (0%) 84 86	14, 26, 43, 49	5 (1%)
1	E	269/291 (92%)	0.02	2 (0%) 84 86	17, 30, 45, 56	3 (1%)
1	F	269/291 (92%)	-0.42	0 100 100	12, 25, 38, 47	7 (2%)
All	All	1614/1746 (92%)	-0.25	12 (0%) 84 86	10, 26, 43, 57	35 (2%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	89	TRP	4.2
1	C	209[A]	ARG	4.1
1	B	245	GLY	3.7
1	C	99[A]	GLU	3.4
1	E	87[A]	GLU	3.3

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

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

6.3 Carbohydrates

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.

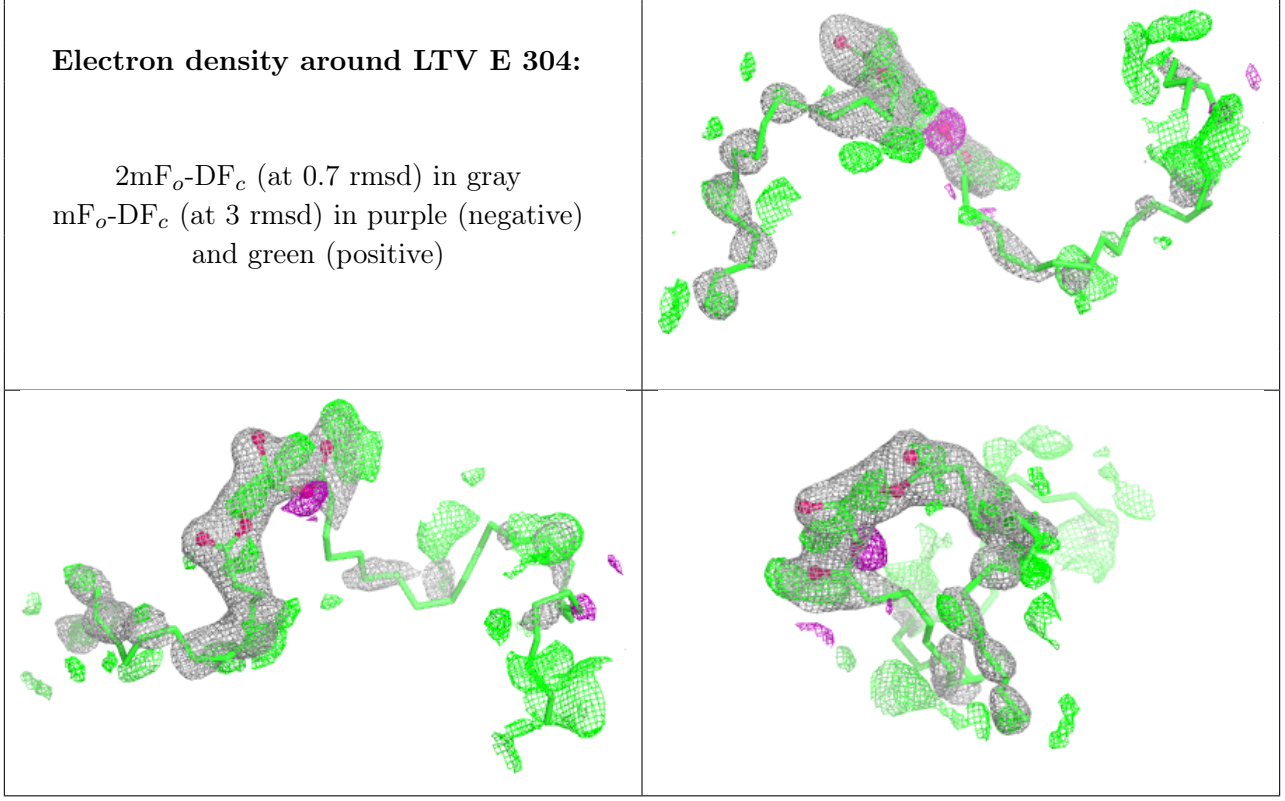
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OCA	A	301	9/10	0.64	0.43	31,38,43,43	9
2	OCA	C	301	9/10	0.66	0.39	37,39,40,41	9
3	NAG	A	302	14/15	0.67	0.14	54,59,71,71	0
2	OCA	E	301	9/10	0.70	0.45	34,38,47,48	9
2	OCA	D	301	9/10	0.72	0.39	38,42,47,47	9
2	OCA	B	301	9/10	0.72	0.52	39,43,53,53	9
2	OCA	F	301	9/10	0.74	0.38	31,39,44,46	9
4	LTV	E	304	51/51	0.75	0.28	53,60,66,66	0
5	PO4	B	307	5/5	0.76	0.17	55,56,56,56	5
4	LTV	F	304	42/51	0.77	0.24	45,53,58,59	0
4	LTV	D	304	51/51	0.77	0.24	52,57,60,60	0
4	LTV	B	306	43/51	0.79	0.23	49,55,62,62	0
3	NAG	C	303	14/15	0.80	0.11	45,53,64,64	0
4	LTV	C	304	41/51	0.80	0.23	52,57,61,61	0
3	NAG	D	303	14/15	0.80	0.11	45,55,66,66	0
5	PO4	D	305	5/5	0.80	0.19	50,54,54,55	5
4	LTV	A	303	36/51	0.81	0.23	50,55,61,61	0
3	NAG	E	303	14/15	0.81	0.12	54,59,71,71	0
3	NAG	F	303	14/15	0.83	0.11	39,45,53,54	0
5	PO4	E	306	5/5	0.85	0.14	39,42,44,45	5
5	PO4	E	305	5/5	0.85	0.12	54,55,55,56	5
5	PO4	A	304	5/5	0.86	0.15	48,50,50,51	5
5	PO4	D	306	5/5	0.88	0.11	45,46,47,47	5
5	PO4	F	305	5/5	0.89	0.12	43,44,44,46	5
5	PO4	A	305	5/5	0.91	0.11	25,29,30,30	5
5	PO4	B	302	5/5	0.91	0.10	37,38,39,41	5
3	NAG	B	305	14/15	0.94	0.07	31,38,46,46	0
6	CA	B	304	1/1	0.96	0.10	56,56,56,56	0
6	CA	C	302	1/1	0.98	0.08	37,37,37,37	1
6	CA	B	303	1/1	0.99	0.02	20,20,20,20	0
6	CA	E	302	1/1	0.99	0.06	50,50,50,50	0
6	CA	F	302	1/1	0.99	0.07	40,40,40,40	1
6	CA	D	302	1/1	1.00	0.04	26,26,26,26	1

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.

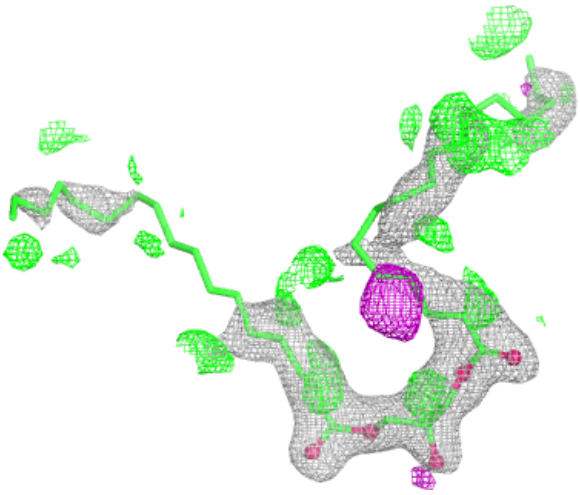
Electron density around LTV E 304:

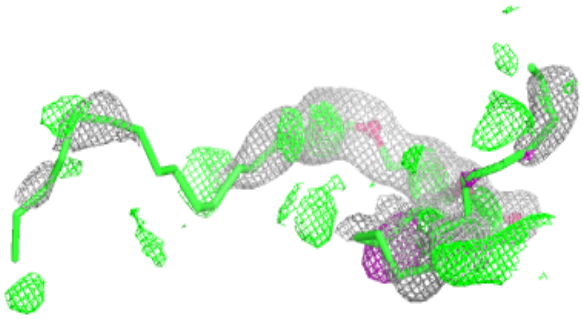
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

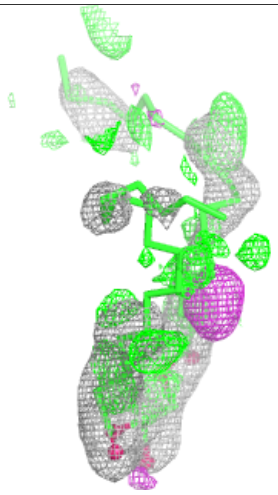


Electron density around LTV F 304:

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

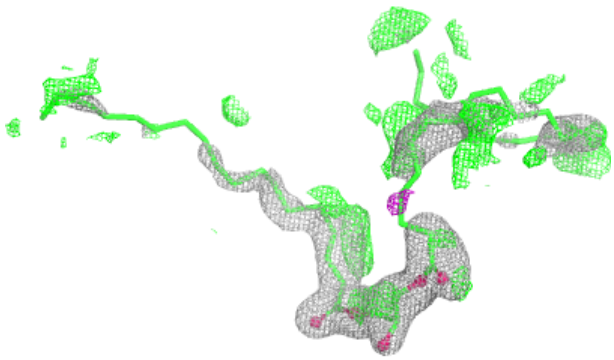


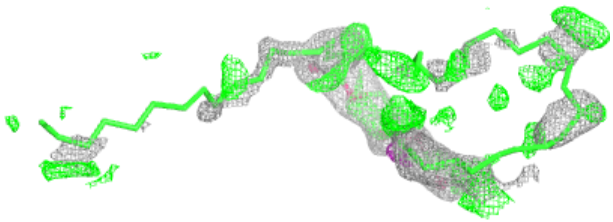


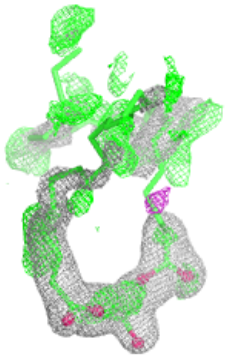


Electron density around LTV D 304:

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

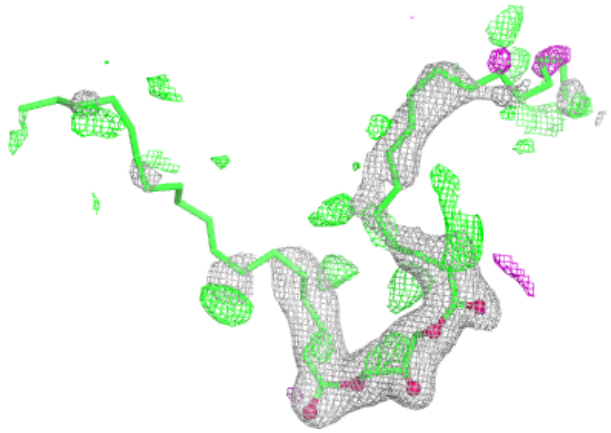


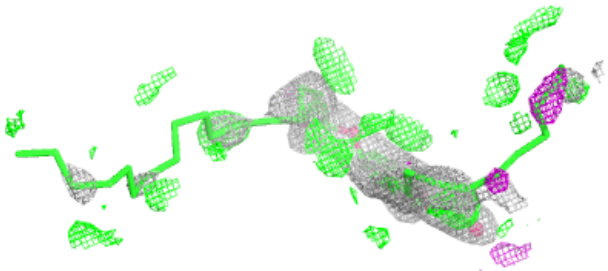


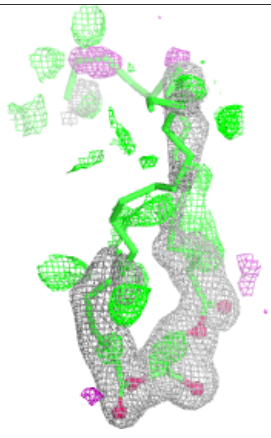


Electron density around LTV B 306:

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

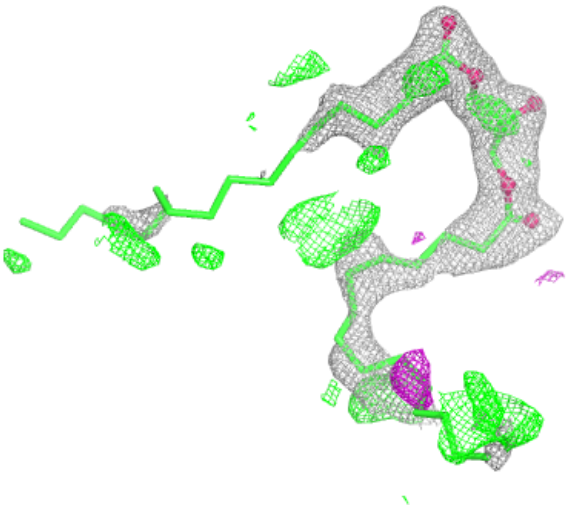


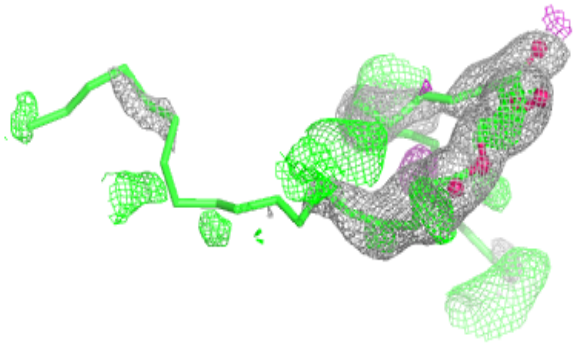


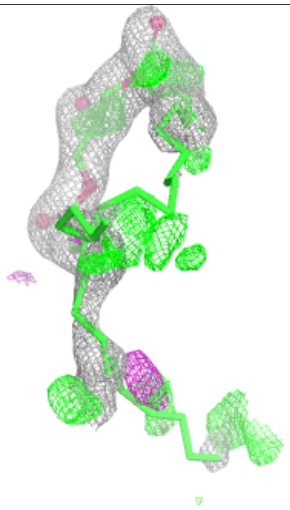


Electron density around LTV C 304:

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

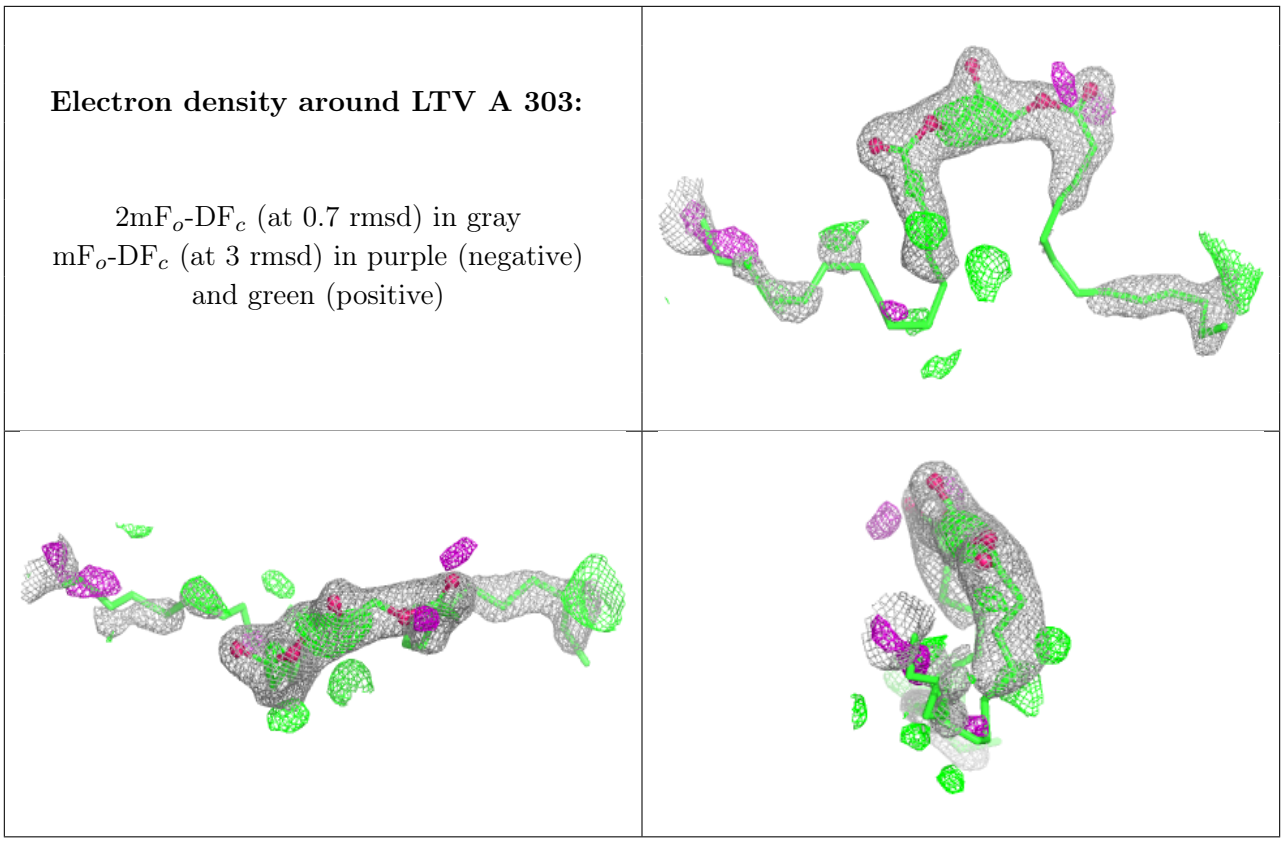






Electron density around LTV A 303:

$2mF_o$-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.