



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 01:11 PM JST

PDB ID : 5B6F  
Title : Crystal structure of the Fab fragment of an anti-Leukotriene C4 monoclonal antibody complexed with LTC4  
Authors : Sugahara, M.; Ago, H.; Saino, H.; Miyano, M.  
Deposited on : 2016-05-27  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

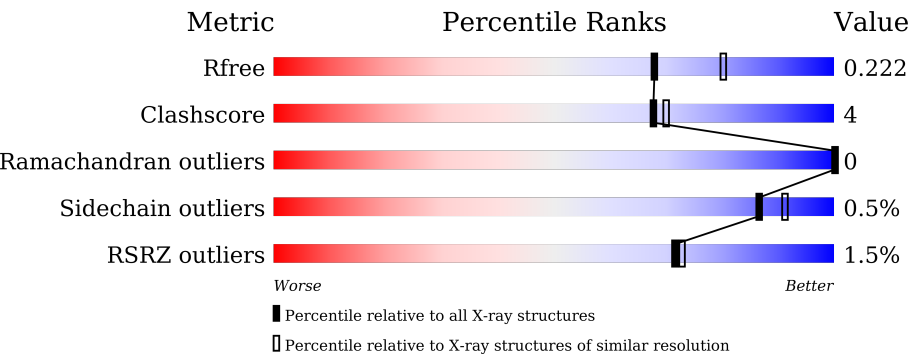
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	<div><div>2%</div><div><div></div><div>79%</div><div>11%</div><div>9%</div></div></div>
1	C	238	<div><div>3%</div><div><div></div><div>83%</div><div>8%</div><div>9%</div></div></div>
1	E	238	<div><div>%</div><div><div></div><div>86%</div><div>5%</div><div>9%</div></div></div>
1	G	238	<div><div></div><div><div></div><div>83%</div><div>8%</div><div>9%</div></div></div>
2	B	237	<div><div></div><div><div></div><div>86%</div><div>•</div><div>11%</div></div></div>
2	D	237	<div><div>%</div><div><div></div><div>79%</div><div>10%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	237	<div><div>%</div><div><div></div><div>82%</div><div>7%</div><div>11%</div></div></div>
2	H	237	<div><div>3%</div><div><div></div><div>79%</div><div>9%</div><div>11%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

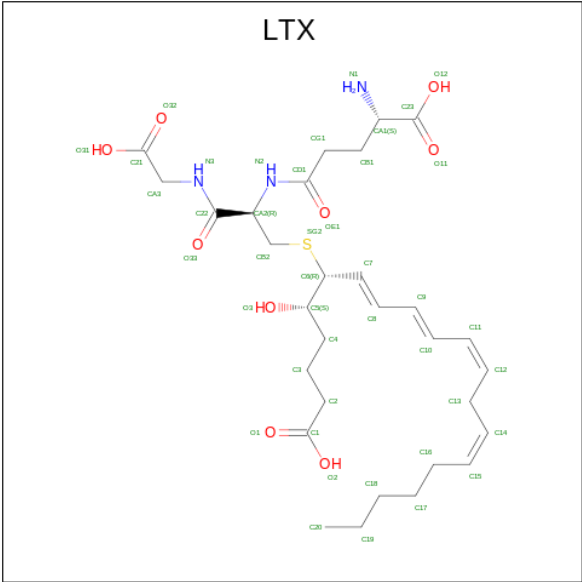
- Molecule 1 is a protein called anti-leukotriene C4 monoclonal antibody immunoglobulin kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1677	1052	284	335	6			
1	C	217	Total	C	N	O	S	0	2	0
			1697	1062	288	339	8			
1	E	216	Total	C	N	O	S	0	0	0
			1677	1052	284	335	6			
1	G	217	Total	C	N	O	S	0	0	0
			1685	1056	286	337	6			

- Molecule 2 is a protein called anti-leukotriene C4 monoclonal antibody immunoglobulin gamma1 heavy chain.

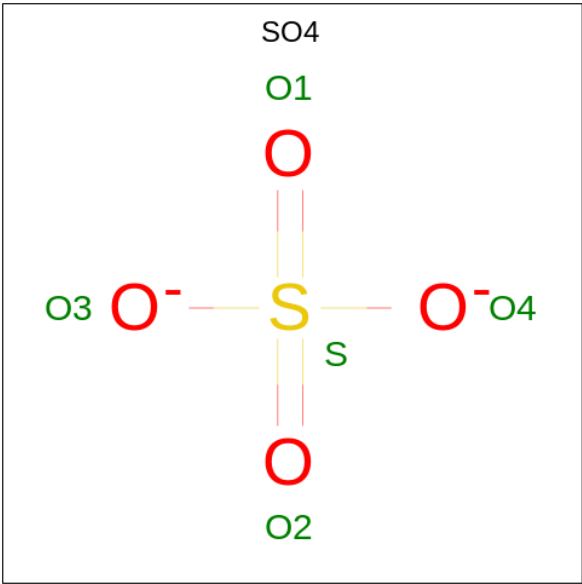
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	4	0
			1641	1043	270	317	11			
2	D	211	Total	C	N	O	S	0	2	0
			1631	1038	269	314	10			
2	F	212	Total	C	N	O	S	0	1	0
			1630	1038	268	315	9			
2	H	210	Total	C	N	O	S	0	0	0
			1609	1027	262	312	8			

- Molecule 3 is (5 {S},6 {R},7 {E},9 {E},11 {Z},14 {Z})-6-[(2 {R})-2-[(4 {S})-4-azanyl-5-oxidanyl-5-oxidanylidene-pentanoyl]amino]-3-(2-hydroxy-2-oxoethylamino)-3-oxidanylidene-propyl]sulfanyl-5-oxidanyl-icosa-7,9,11,14-tetraenoic acid (three-letter code: LTX) (formula: C<sub>30</sub>H<sub>47</sub>N<sub>3</sub>O<sub>9</sub>S).



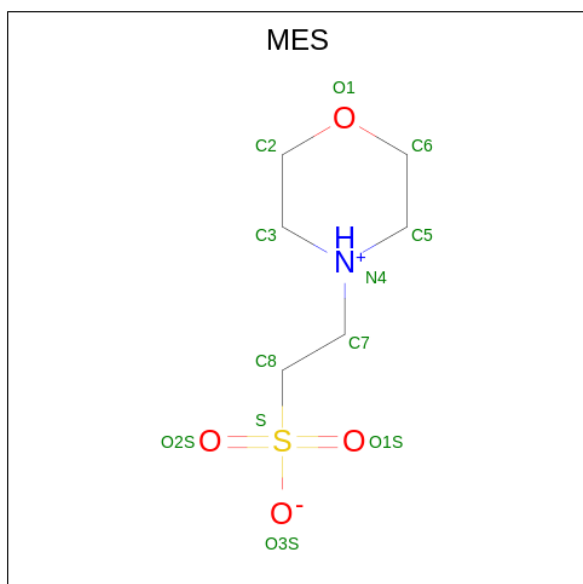
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			43	30	3	9	1		
3	C	1	Total	C	N	O	S	0	0
			43	30	3	9	1		
3	E	1	Total	C	N	O	S	0	0
			43	30	3	9	1		
3	G	1	Total	C	N	O	S	0	0
			43	30	3	9	1		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	D	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	F	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	H	1	Total 12	C 6	N 1	O 4	S 1	0	0

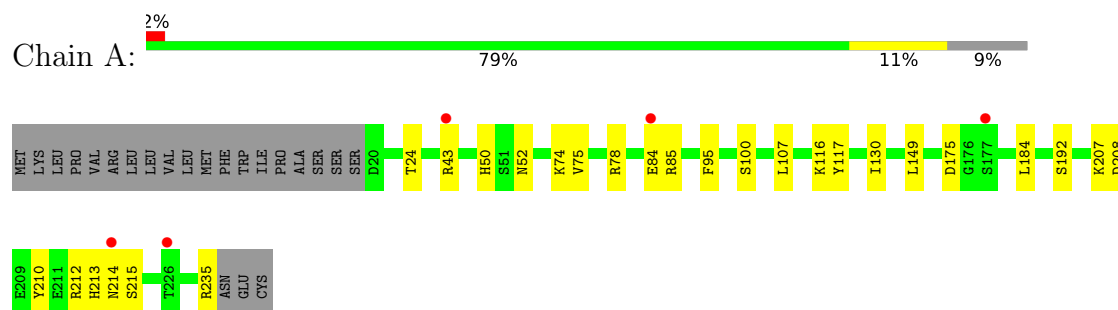
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total 171	O 171	0	0
6	B	193	Total 193	O 193	0	0
6	C	154	Total 154	O 154	0	0
6	D	135	Total 135	O 135	0	0
6	E	120	Total 120	O 120	0	0
6	F	195	Total 195	O 195	0	0
6	G	199	Total 199	O 199	0	0
6	H	92	Total 92	O 92	0	0

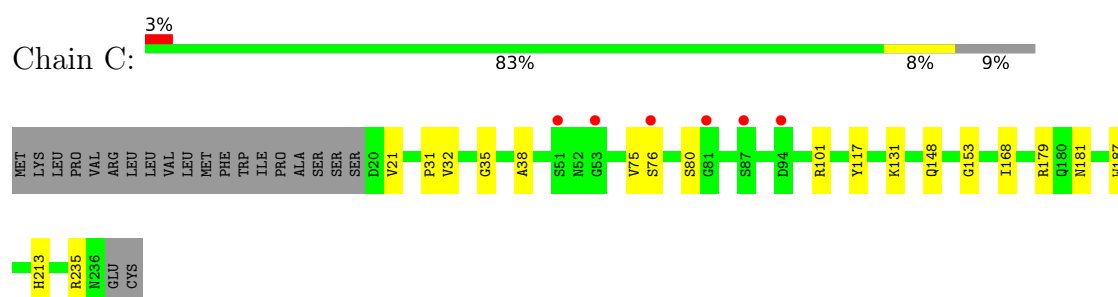
### 3 Residue-property plots [i](#)

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.

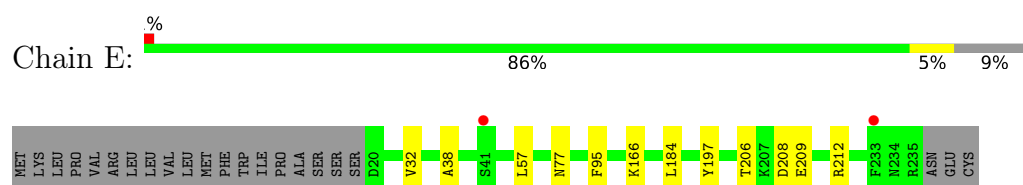
- Molecule 1: anti-leukotriene C4 monoclonal antibody immunoglobulin kappa light chain



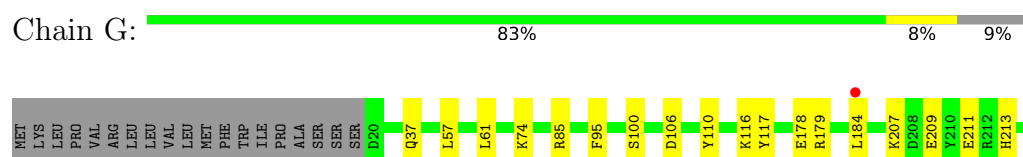
- Molecule 1: anti-leukotriene C4 monoclonal antibody immunoglobulin kappa light chain



- Molecule 1: anti-leukotriene C4 monoclonal antibody immunoglobulin kappa light chain




- Molecule 1: anti-leukotriene C4 monoclonal antibody immunoglobulin kappa light chain




- Molecule 2: anti-leukotriene C4 monoclonal antibody immunoglobulin gamma1 heavy chain



Chain B:  86% 11%




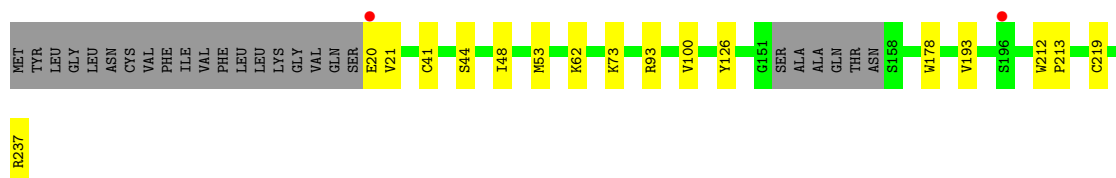
- Molecule 2: anti-leukotriene C4 monoclonal antibody immunoglobulin gamma1 heavy chain

Chain D:  79% 10% 11%




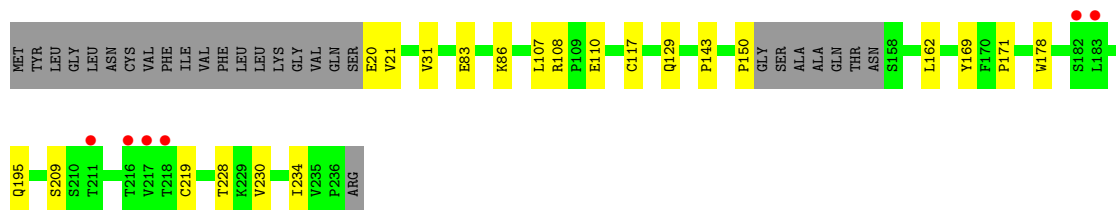
- Molecule 2: anti-leukotriene C4 monoclonal antibody immunoglobulin gamma1 heavy chain

Chain F:  82% 7% 11%



- Molecule 2: anti-leukotriene C4 monoclonal antibody immunoglobulin gamma1 heavy chain

Chain H:  79% 9% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.60Å 173.98Å 75.46Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	37.73 – 2.10 37.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	73.8 (37.73-2.10) 90.8 (37.73-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, CNS, REFMAC	Depositor
R, $R_{free}$	0.195 , 0.222 0.196 , 0.222	Depositor DCC
$R_{free}$ test set	5042 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,k,-h 0.027 for h,-k,-l 0.090 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LTX, MES

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	0.30	0/1716	0.48	0/2327
1	C	0.30	0/1736	0.49	0/2354
1	E	0.29	0/1716	0.47	0/2327
1	G	0.31	0/1724	0.49	0/2338
2	B	0.31	0/1686	0.48	0/2305
2	D	0.31	0/1676	0.47	0/2292
2	F	0.32	0/1675	0.49	0/2290
2	H	0.30	0/1654	0.47	0/2263
All	All	0.30	0/13583	0.48	0/18496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1677	0	1625	19	0
1	C	1697	0	1637	11	0
1	E	1677	0	1625	8	0
1	G	1685	0	1631	13	0
2	B	1641	0	1595	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1631	0	1592	13	0
2	F	1630	0	1592	14	0
2	H	1609	0	1573	14	0
3	A	43	0	0	1	0
3	C	43	0	0	0	0
3	E	43	0	0	1	0
3	G	43	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	B	12	0	13	0	0
5	D	12	0	13	2	0
5	F	12	0	13	4	0
5	H	12	0	13	2	0
6	A	171	0	0	1	0
6	B	193	0	0	2	0
6	C	154	0	0	0	0
6	D	135	0	0	2	0
6	E	120	0	0	0	0
6	F	195	0	0	2	0
6	G	199	0	0	2	0
6	H	92	0	0	2	0
All	All	14756	0	12922	93	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 4.

All (93) 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:D:207:VAL:HB	2:D:211:THR:HG21	1.72	0.71
1:E:32:VAL:HG21	1:E:38:ALA:HB2	1.75	0.69
2:D:231:ASP:OD2	6:D:601:HOH:O	2.10	0.68
1:A:24:THR:HB	1:A:43:ARG:HG3	1.75	0.68
2:D:21:VAL:O	5:D:502:MES:H52	1.96	0.66
1:C:31:PRO:HB2	1:C:131:LYS:HE3	1.80	0.64
2:D:157:ASN:O	2:D:209:SER:OG	2.12	0.62
1:G:74:LYS:NZ	3:G:302:LTX:O32	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ARG:NH1	1:C:181:ASN:O	2.32	0.62
1:C:32:VAL:HG21	1:C:38:ALA:HB2	1.81	0.62
1:A:175:ASP:OD2	1:A:213:HIS:ND1	2.23	0.61
1:G:85:ARG:NH1	1:G:106:ASP:OD2	2.26	0.60
2:D:208:PRO:O	2:D:211:THR:HG22	2.03	0.59
2:F:126:TYR:CZ	5:F:501:MES:H31	2.39	0.56
1:G:37:GLN:NE2	1:G:100:SER:OG	2.38	0.56
1:A:107:LEU:HB3	1:A:130:ILE:CD1	2.36	0.56
1:G:213:HIS:O	1:G:235:ARG:HD3	2.06	0.55
1:G:234:ASN:ND2	6:G:406:HOH:O	2.35	0.55
2:H:228:THR:HG22	2:H:230:VAL:HG23	1.88	0.55
1:E:77:ASN:ND2	3:E:301:LTX:O11	2.40	0.55
2:F:126:TYR:CE1	5:F:501:MES:H31	2.42	0.55
1:A:74:LYS:NZ	3:A:301:LTX:O32	2.22	0.55
2:F:20:GLU:HG3	2:F:21:VAL:N	2.22	0.55
2:F:237:ARG:NH2	6:F:605:HOH:O	2.39	0.55
2:B:48:ILE:O	2:B:93:ARG:NH2	2.41	0.54
2:B:237:ARG:NH2	6:B:604:HOH:O	2.40	0.54
1:E:208:ASP:O	1:E:212:ARG:HG3	2.08	0.54
2:F:20:GLU:HG2	5:F:501:MES:H61	1.90	0.54
2:H:21:VAL:O	5:H:502:MES:H52	2.07	0.54
1:G:184:LEU:HD21	2:H:195:GLN:OE1	2.09	0.53
2:H:143:PRO:HB3	2:H:169:TYR:HB3	1.90	0.53
1:C:168:ILE:HG22	1:C:187:TRP:CH2	2.44	0.53
2:H:162:LEU:HD22	2:H:234:ILE:HG21	1.89	0.53
1:E:166:LYS:HD2	1:E:197:TYR:CE2	2.44	0.52
2:F:21:VAL:O	5:F:501:MES:H52	2.09	0.52
2:D:50:ASN:OD1	6:D:602:HOH:O	2.18	0.52
1:E:57:LEU:HG	1:E:95:PHE:CD1	2.45	0.51
2:D:31:VAL:HG11	2:D:107:LEU:HD13	1.93	0.51
1:G:179:ARG:NH2	1:G:209:GLU:OE2	2.34	0.50
1:C:213:HIS:O	1:C:235:ARG:HD3	2.11	0.50
1:G:178:GLU:OE2	6:G:401:HOH:O	2.19	0.50
2:H:178:TRP:CZ3	2:H:219:CYS:HB3	2.47	0.50
1:A:107:LEU:HD21	1:A:192:SER:HA	1.93	0.50
2:D:48:ILE:O	2:D:93:ARG:NH2	2.45	0.50
2:H:83:GLU:HA	2:H:86:LYS:HG3	1.94	0.50
1:A:85:ARG:HB2	1:A:100:SER:O	2.12	0.49
2:H:20:GLU:N	6:H:609:HOH:O	2.45	0.49
2:D:126:TYR:CE1	5:D:502:MES:H31	2.48	0.49
2:D:183:LEU:HD13	2:D:205:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:ARG:NE	2:H:110:GLU:OE1	2.44	0.49
1:G:57:LEU:HG	1:G:95:PHE:CG	2.48	0.48
1:G:179:ARG:HH22	1:G:209:GLU:CD	2.17	0.47
2:B:194:LEU:HB2	2:B:199:TYR:CE1	2.50	0.47
1:E:184:LEU:HD23	1:E:184:LEU:HA	1.80	0.47
1:C:168:ILE:HG22	1:C:187:TRP:HH2	1.80	0.47
1:G:207:LYS:O	1:G:211:GLU:HG3	2.15	0.47
1:A:175:ASP:OD1	1:A:215:SER:HB3	2.16	0.46
1:C:187:TRP:NE1	2:F:73:LYS:HE2	2.30	0.46
1:A:78:ARG:NH1	1:A:84:GLU:HG2	2.30	0.46
1:A:214:ASN:HA	1:A:235:ARG:HB3	1.97	0.46
2:F:62:LYS:HD2	6:F:719:HOH:O	2.15	0.46
2:H:129:GLN:NE2	5:H:502:MES:O1S	2.47	0.45
1:A:149:LEU:O	1:A:207:LYS:HD2	2.16	0.45
2:F:21:VAL:HA	2:F:44:SER:O	2.17	0.45
1:A:75:VAL:HG22	1:A:95:PHE:CE2	2.52	0.45
2:F:48:ILE:O	2:F:93:ARG:NH2	2.50	0.45
1:G:116:LYS:HD3	1:G:117:TYR:CE2	2.51	0.45
1:A:208:ASP:O	1:A:212:ARG:HG3	2.16	0.45
1:E:206:THR:OG1	1:E:209:GLU:HG3	2.17	0.44
1:C:35:GLY:O	1:C:101:ARG:HA	2.18	0.44
2:D:212:TRP:CG	2:D:213:PRO:HA	2.53	0.43
1:E:184:LEU:HD22	2:F:193:VAL:HG11	2.00	0.43
2:F:53:MET:HG3	2:F:100:VAL:HG11	2.00	0.43
2:H:150:PRO:HD3	2:H:162:LEU:HD23	2.01	0.43
1:A:50:HIS:HB3	1:A:52:ASN:OD1	2.17	0.43
1:C:148:GLN:HG2	1:C:153:GLY:O	2.18	0.42
2:F:178:TRP:CZ3	2:F:219:CYS:HB3	2.55	0.42
2:H:171:PRO:HB2	6:H:608:HOH:O	2.18	0.42
1:A:85:ARG:NH2	6:A:401:HOH:O	2.18	0.42
1:A:116:LYS:HD3	1:A:117:TYR:CE2	2.54	0.42
2:B:167:LYS:NZ	6:B:617:HOH:O	2.53	0.41
1:A:184:LEU:HD22	2:B:193:VAL:HG11	2.03	0.41
2:F:212:TRP:CG	2:F:213:PRO:HA	2.55	0.41
1:A:78:ARG:CZ	1:A:84:GLU:HG2	2.51	0.41
1:A:213:HIS:O	1:A:235:ARG:NE	2.44	0.41
1:G:61:LEU:HD13	1:G:110:TYR:CZ	2.56	0.41
1:C:75:VAL:HG12	1:C:76:SER:OG	2.21	0.41
2:H:31:VAL:HG11	2:H:107:LEU:HD13	2.02	0.41
2:D:210:SER:O	2:D:214:SER:OG	2.29	0.40
1:C:21:VAL:HG21	1:C:117:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE2	1:A:235:ARG:HD3	2.56	0.40
2:D:223:HIS:HB3	2:D:228:THR:HB	2.04	0.40
2:H:178:TRP:CH2	2:H:219:CYS:HB3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/238 (90%)	211 (99%)	3 (1%)	0	100	100
1	C	217/238 (91%)	214 (99%)	3 (1%)	0	100	100
1	E	214/238 (90%)	213 (100%)	1 (0%)	0	100	100
1	G	215/238 (90%)	212 (99%)	3 (1%)	0	100	100
2	B	211/237 (89%)	207 (98%)	4 (2%)	0	100	100
2	D	209/237 (88%)	206 (99%)	3 (1%)	0	100	100
2	F	209/237 (88%)	205 (98%)	4 (2%)	0	100	100
2	H	206/237 (87%)	202 (98%)	4 (2%)	0	100	100
All	All	1695/1900 (89%)	1670 (98%)	25 (2%)	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	194/215 (90%)	194 (100%)	0	100	100
1	C	197/215 (92%)	196 (100%)	1 (0%)	86	91
1	E	194/215 (90%)	194 (100%)	0	100	100
1	G	195/215 (91%)	195 (100%)	0	100	100
2	B	189/207 (91%)	188 (100%)	1 (0%)	86	91
2	D	188/207 (91%)	183 (97%)	5 (3%)	40	44
2	F	187/207 (90%)	186 (100%)	1 (0%)	86	91
2	H	185/207 (89%)	183 (99%)	2 (1%)	70	77
All	All	1529/1688 (91%)	1519 (99%)	10 (1%)	86	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	220	ASN
1	C	80	SER
2	D	41	CYS
2	D	117[A]	CYS
2	D	117[B]	CYS
2	D	219[A]	CYS
2	D	219[B]	CYS
2	F	41	CYS
2	H	117	CYS
2	H	209	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	37	GLN
2	H	76	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	SO4	G	301	-	4,4,4	0.17	0	6,6,6	0.06	0
3	LTX	E	301	-	38,42,42	0.70	0	42,50,50	0.98	2 (4%)
4	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.16	0
5	MES	H	502	-	12,12,12	0.65	0	14,16,16	1.09	1 (7%)
3	LTX	A	301	-	38,42,42	0.76	0	42,50,50	1.04	2 (4%)
5	MES	D	502	-	12,12,12	0.76	0	14,16,16	1.22	1 (7%)
4	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.11	0
5	MES	B	502	-	12,12,12	0.59	0	14,16,16	1.00	1 (7%)
5	MES	F	501	-	12,12,12	0.66	0	14,16,16	1.08	1 (7%)
4	SO4	C	302	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	H	501	-	4,4,4	0.16	0	6,6,6	0.11	0
3	LTX	C	301	-	38,42,42	0.76	0	42,50,50	1.00	2 (4%)
3	LTX	G	302	-	38,42,42	0.76	0	42,50,50	1.20	2 (4%)

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	LTX	E	301	-	-	11/51/51/51	-
5	MES	H	502	-	-	0/6/14/14	0/1/1/1
3	LTX	A	301	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	D	502	-	-	0/6/14/14	0/1/1/1
5	MES	B	502	-	-	1/6/14/14	0/1/1/1
5	MES	F	501	-	-	0/6/14/14	0/1/1/1
3	LTX	C	301	-	-	14/51/51/51	-
3	LTX	G	302	-	-	10/51/51/51	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	LTX	C11-C10-C9	-4.16	115.56	124.81
3	C	301	LTX	C11-C10-C9	-3.46	117.11	124.81
3	A	301	LTX	C11-C10-C9	-3.21	117.67	124.81
3	E	301	LTX	C11-C10-C9	-2.89	118.38	124.81
3	C	301	LTX	C3-C2-C1	-2.39	108.44	114.47
5	B	502	MES	O2S-S-C8	2.28	109.66	106.92
5	H	502	MES	O2S-S-C8	2.25	109.62	106.92
3	E	301	LTX	O2-C1-C2	2.18	121.02	114.03
3	A	301	LTX	O2-C1-C2	2.14	120.90	114.03
5	D	502	MES	O1S-S-C8	2.13	109.48	106.92
3	G	302	LTX	C3-C2-C1	-2.04	109.34	114.47
5	F	501	MES	O3S-S-C8	2.03	109.05	105.77

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	LTX	SG2-C6-C7-C8
3	A	301	LTX	O11-C23-CA1-N1
3	C	301	LTX	C3-C4-C5-O3
3	C	301	LTX	CA1-CB1-CG1-CD1
3	C	301	LTX	O11-C23-CA1-N1
3	E	301	LTX	O32-C21-CA3-N3
3	E	301	LTX	O31-C21-CA3-N3
3	E	301	LTX	C23-CA1-CB1-CG1
3	A	301	LTX	CG1-CD1-N2-CA2
3	C	301	LTX	CG1-CD1-N2-CA2
3	E	301	LTX	CG1-CD1-N2-CA2
3	G	302	LTX	CG1-CD1-N2-CA2
3	A	301	LTX	O12-C23-CA1-N1
3	A	301	LTX	OE1-CD1-N2-CA2

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Mol	Chain	Res	Type	Atoms
3	C	301	LTX	OE1-CD1-N2-CA2
3	E	301	LTX	OE1-CD1-N2-CA2
3	G	302	LTX	OE1-CD1-N2-CA2
3	A	301	LTX	CA1-CB1-CG1-CD1
3	G	302	LTX	CA1-CB1-CG1-CD1
3	C	301	LTX	O12-C23-CA1-N1
3	E	301	LTX	CA1-CB1-CG1-CD1
3	A	301	LTX	C16-C17-C18-C19
3	C	301	LTX	C15-C16-C17-C18
3	E	301	LTX	C16-C17-C18-C19
3	A	301	LTX	C5-C6-C7-C8
3	G	302	LTX	C1-C2-C3-C4
3	E	301	LTX	O11-C23-CA1-CB1
3	G	302	LTX	C17-C18-C19-C20
3	E	301	LTX	O12-C23-CA1-CB1
3	G	302	LTX	O12-C23-CA1-N1
3	G	302	LTX	O11-C23-CA1-N1
3	A	301	LTX	N1-CA1-CB1-CG1
3	C	301	LTX	C17-C18-C19-C20
3	A	301	LTX	O11-C23-CA1-CB1
3	C	301	LTX	C3-C4-C5-C6
3	G	302	LTX	O1-C1-C2-C3
3	C	301	LTX	CA2-CB2-SG2-C6
3	A	301	LTX	C14-C15-C16-C17
3	A	301	LTX	C2-C3-C4-C5
3	G	302	LTX	O2-C1-C2-C3
3	C	301	LTX	O1-C1-C2-C3
3	G	302	LTX	C14-C15-C16-C17
3	C	301	LTX	C4-C5-C6-SG2
3	E	301	LTX	C14-C15-C16-C17
3	C	301	LTX	C4-C5-C6-C7
3	A	301	LTX	O12-C23-CA1-CB1
3	C	301	LTX	O2-C1-C2-C3
5	B	502	MES	C7-C8-S-O1S
3	E	301	LTX	C21-CA3-N3-C22

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	LTX	1	0
5	H	502	MES	2	0

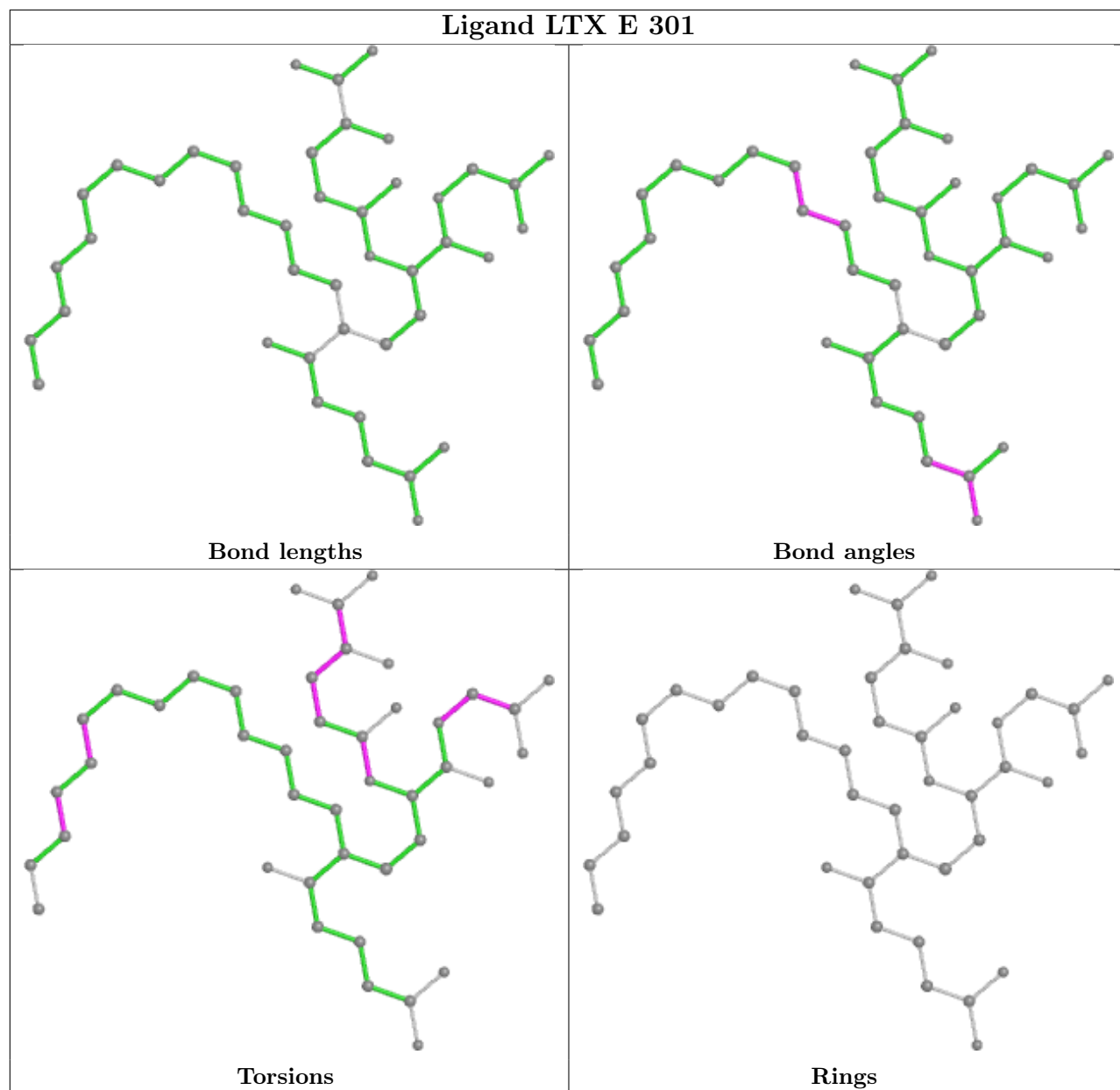
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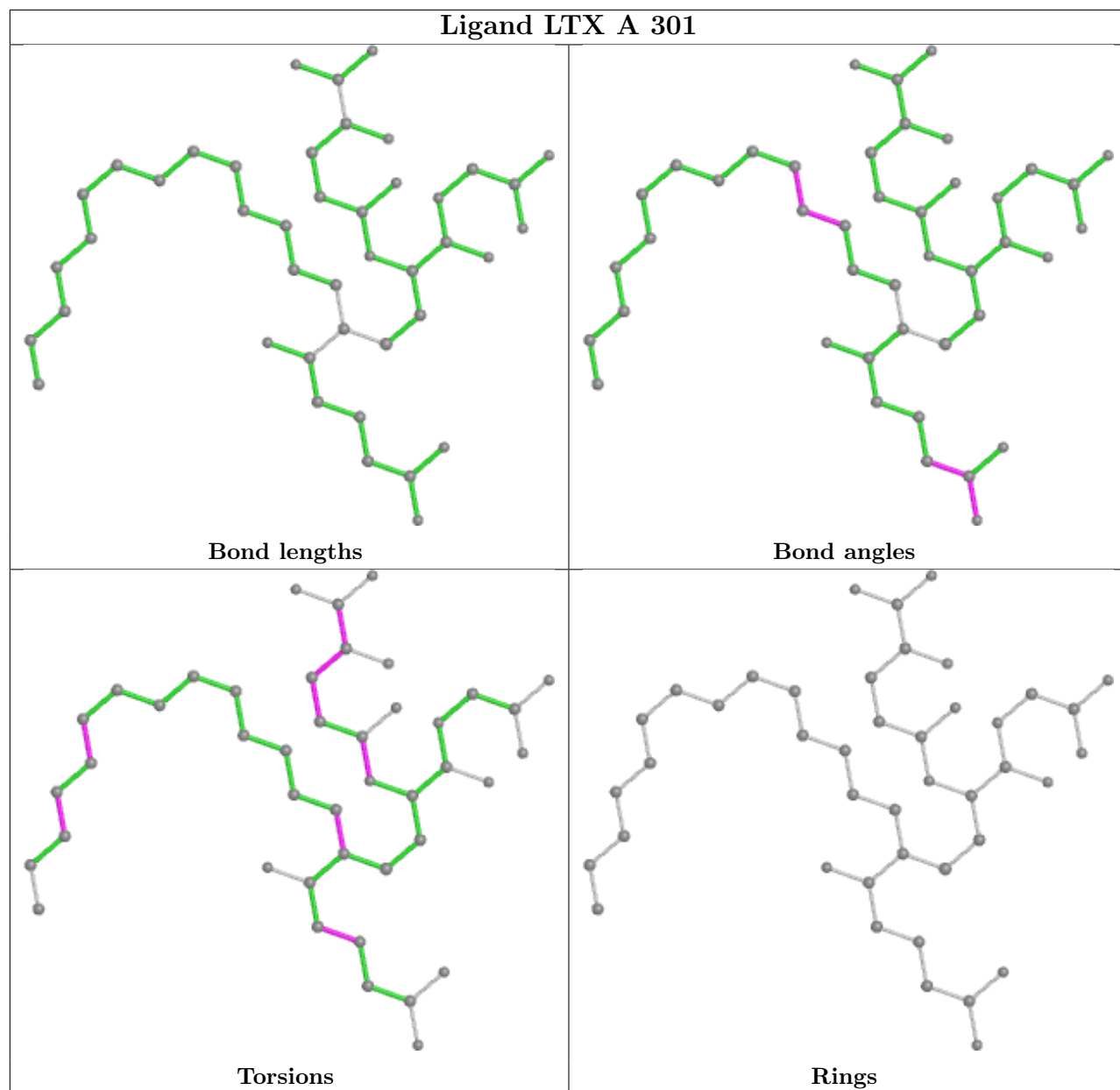
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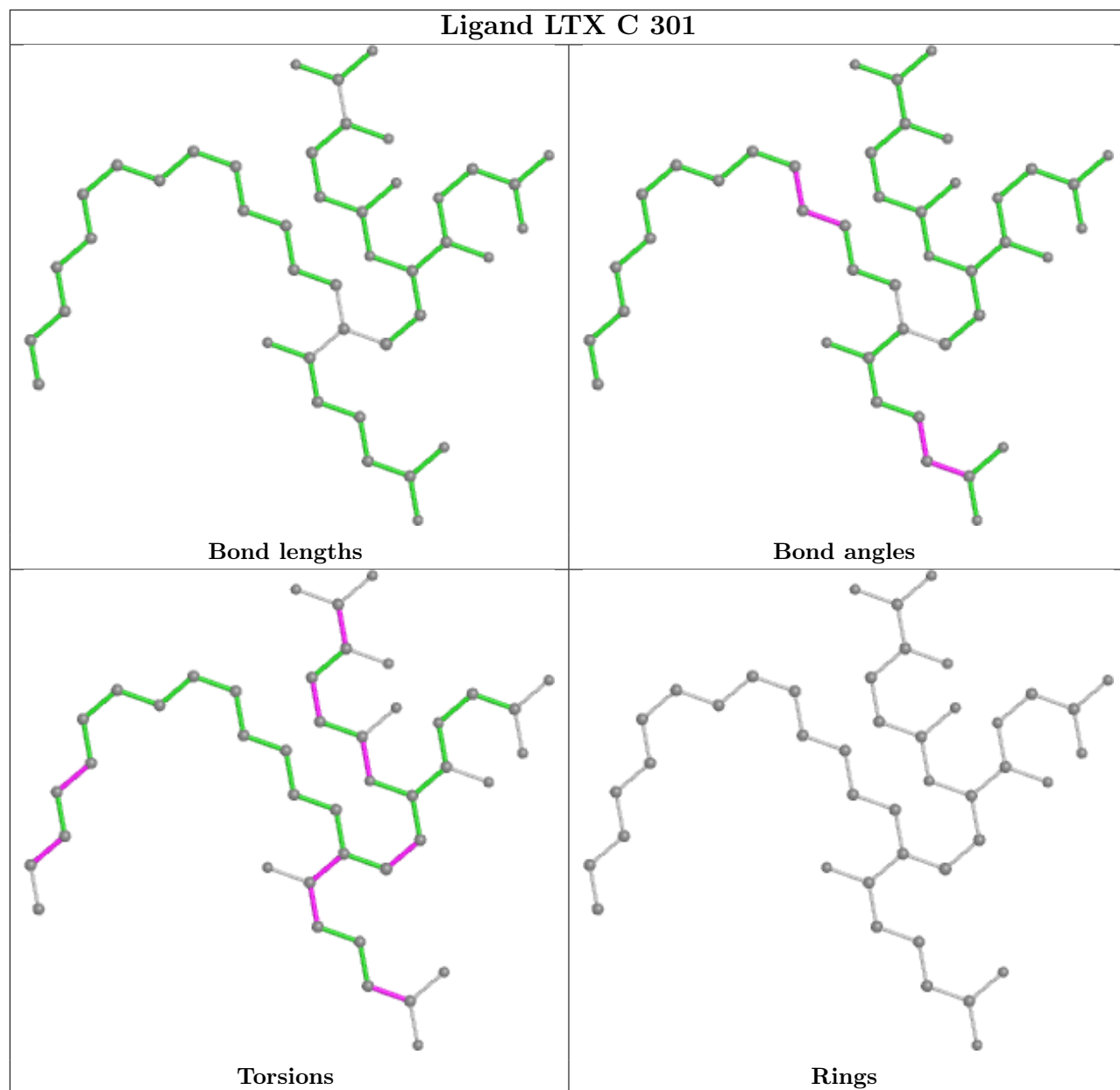
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	LTX	1	0
5	D	502	MES	2	0
5	F	501	MES	4	0
3	G	302	LTX	1	0

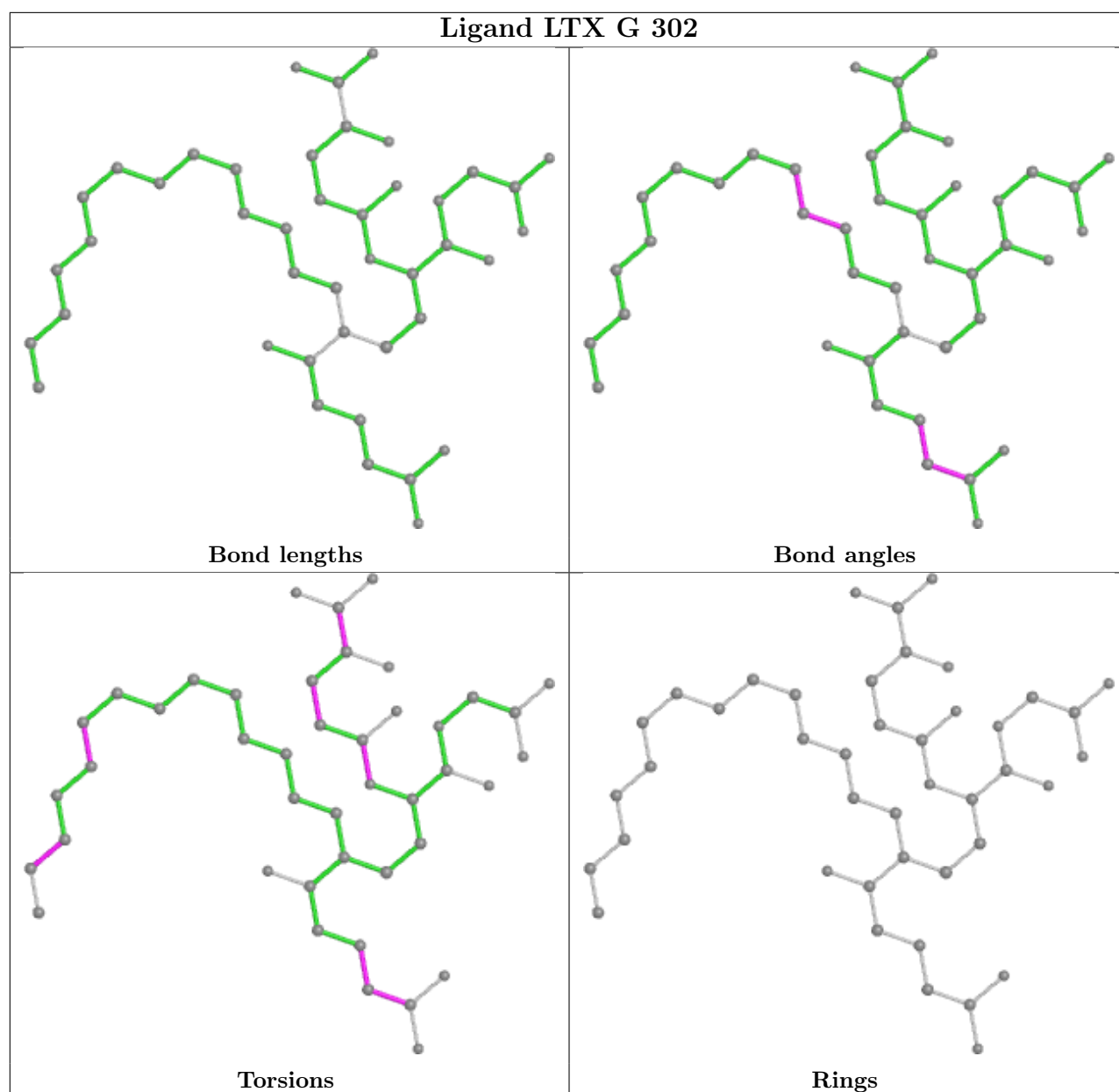
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand LTX E 301









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	216/238 (90%)	0.12	5 (2%) 61 63	16, 30, 45, 48	0
1	C	217/238 (91%)	0.09	6 (2%) 55 57	9, 27, 43, 48	2 (0%)
1	E	216/238 (90%)	0.15	2 (0%) 81 82	19, 33, 44, 50	0
1	G	217/238 (91%)	-0.16	1 (0%) 87 88	14, 26, 37, 44	0
2	B	211/237 (89%)	-0.34	0 100 100	9, 22, 35, 44	4 (1%)
2	D	211/237 (89%)	-0.05	3 (1%) 73 74	9, 26, 44, 52	2 (0%)
2	F	212/237 (89%)	-0.20	2 (0%) 81 82	11, 24, 36, 48	1 (0%)
2	H	210/237 (88%)	0.32	6 (2%) 54 55	16, 29, 47, 53	0
All	All	1710/1900 (90%)	-0.01	25 (1%) 71 73	9, 27, 44, 53	9 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	182	SER	3.8
1	A	43	ARG	3.5
2	H	183	LEU	3.2
2	F	196	SER	3.1
1	C	94	ASP	2.9
2	H	211	THR	2.8
1	A	214	ASN	2.7
2	D	211	THR	2.6
1	C	81	GLY	2.5
2	H	216	THR	2.5
1	A	84	GLU	2.4
1	C	76	SER	2.4
1	C	87	SER	2.4
2	F	20	GLU	2.3
1	A	226	THR	2.3
2	D	182	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	218	THR	2.3
2	D	21	VAL	2.2
1	G	184	LEU	2.2
2	H	217	VAL	2.2
1	A	177	SER	2.1
1	E	233	PHE	2.1
1	E	41	SER	2.1
1	C	53	GLY	2.1
1	C	51	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

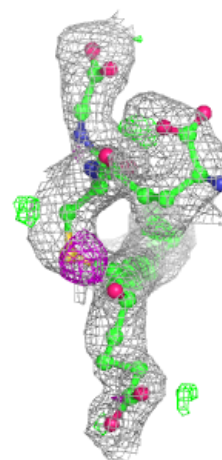
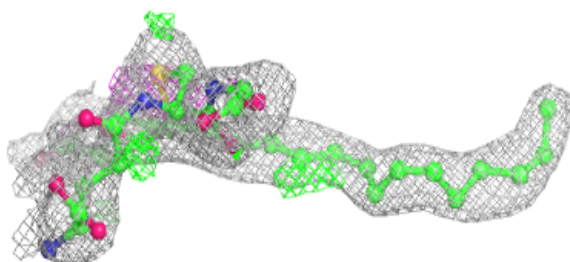
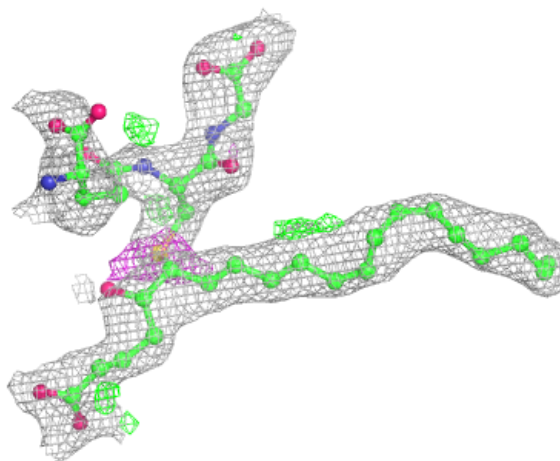
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	E	302	5/5	0.80	0.20	43,45,51,71	0
3	LTX	C	301	43/43	0.81	0.13	22,36,59,71	0
3	LTX	A	301	43/43	0.83	0.13	20,36,61,73	0
3	LTX	G	302	43/43	0.84	0.12	25,33,58,70	0
4	SO4	H	501	5/5	0.86	0.14	38,42,51,58	0
3	LTX	E	301	43/43	0.87	0.11	23,35,62,70	0
4	SO4	C	302	5/5	0.90	0.11	45,46,53,65	0
4	SO4	B	501	5/5	0.91	0.20	34,36,46,54	0
5	MES	H	502	12/12	0.92	0.10	33,36,43,44	0
4	SO4	D	501	5/5	0.93	0.15	32,34,42,43	0
5	MES	F	501	12/12	0.94	0.09	28,34,38,38	0
5	MES	D	502	12/12	0.94	0.08	25,34,39,41	0
4	SO4	G	301	5/5	0.95	0.11	35,36,42,48	0
5	MES	B	502	12/12	0.97	0.07	26,29,32,37	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.

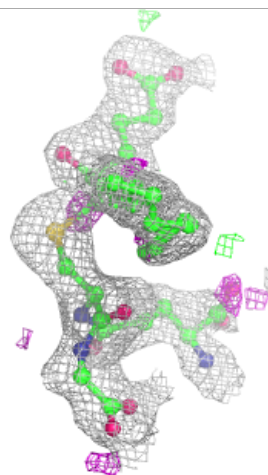
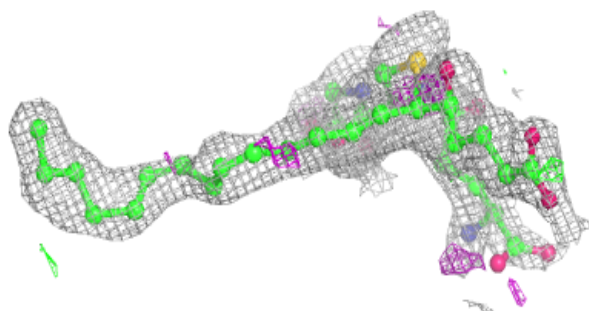
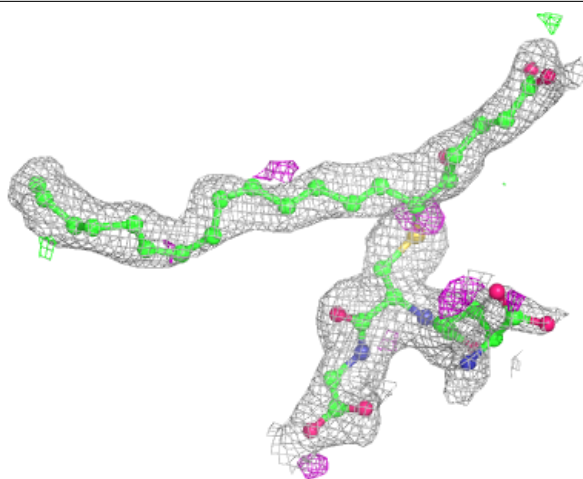
**Electron density around LTX C 301:**

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



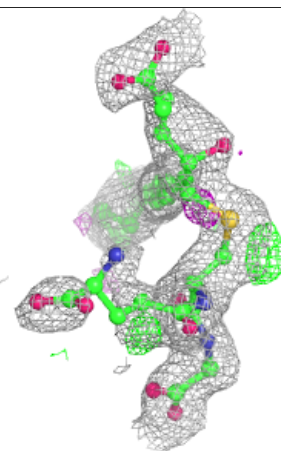
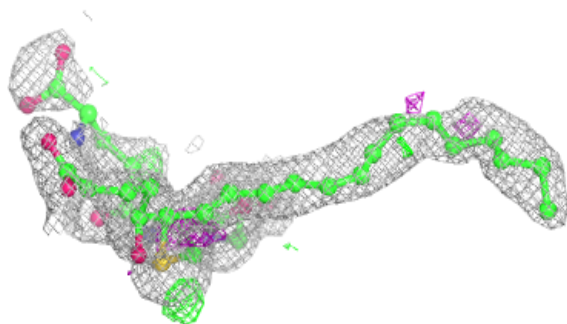
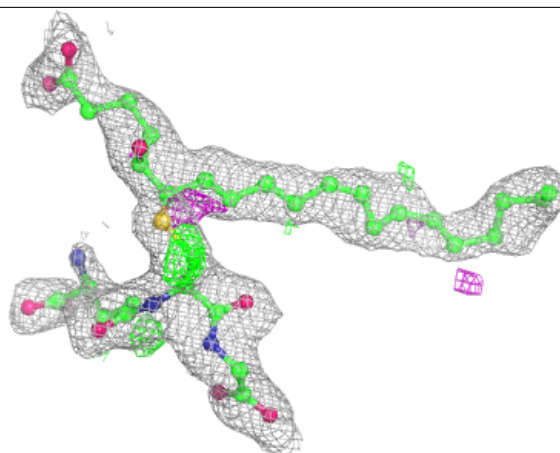
**Electron density around LTX A 301:**

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



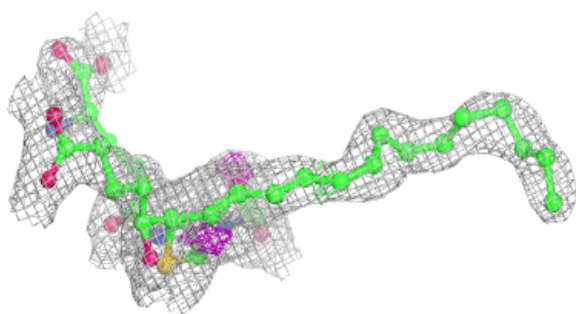
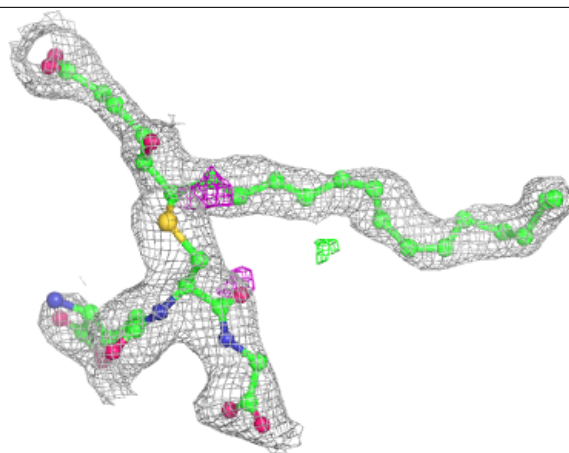
**Electron density around LTX G 302:**

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



**Electron density around LTX 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.