



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 06:07 PM JST

PDB ID : 7F1U  
Title : Crystal structure of Pseudomonas putida methionine gamma-lyase Q349S mutant with L-methionine intermediates  
Authors : Okawa, A.; Handa, H.; Yasuda, E.; Murota, M.; Kudo, D.; Tamura, T.; Shiba, T.; Inagaki, K.  
Deposited on : 2021-06-09  
Resolution : 2.40 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.

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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 : 2.27  
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) : 2.27

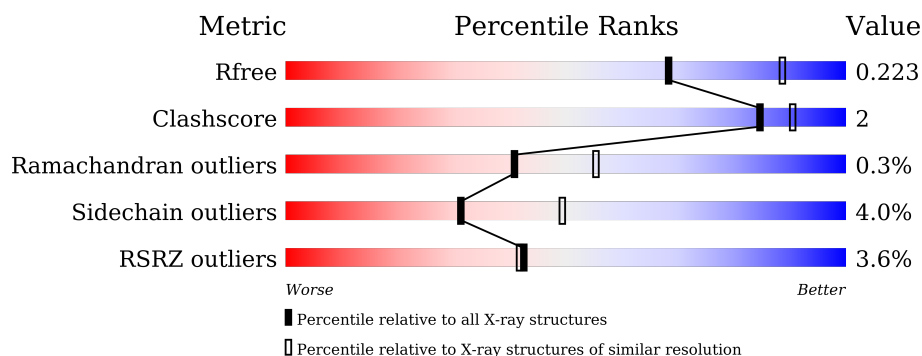
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	398	<div> <div>5%</div> <div>92%</div> <div>6% ..</div> </div>
1	C	398	<div> <div>4%</div> <div>90%</div> <div>7% ..</div> </div>
1	D	398	<div> <div>%</div> <div>89%</div> <div>8% ..</div> </div>
2	B	398	<div> <div>4%</div> <div>92%</div> <div>6% .</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12038 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2975	1876	527	555	17			
1	C	392	Total	C	N	O	S	0	0	0
			2948	1861	521	549	17			
1	D	392	Total	C	N	O	S	0	0	0
			2948	1861	521	549	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	GLN	engineered mutation	UNP P13254
C	349	SER	GLN	engineered mutation	UNP P13254
D	349	SER	GLN	engineered mutation	UNP P13254

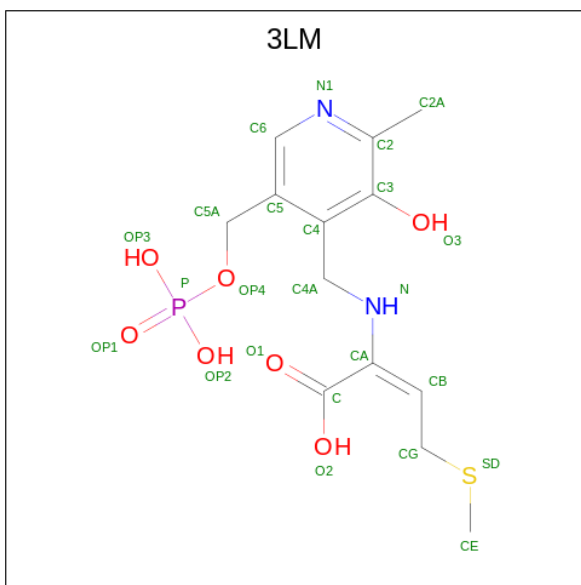
- Molecule 2 is a protein called L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	P S	0	0	0
			2962	1869	522	553	1 17			

There is a discrepancy between the modelled and reference sequences:

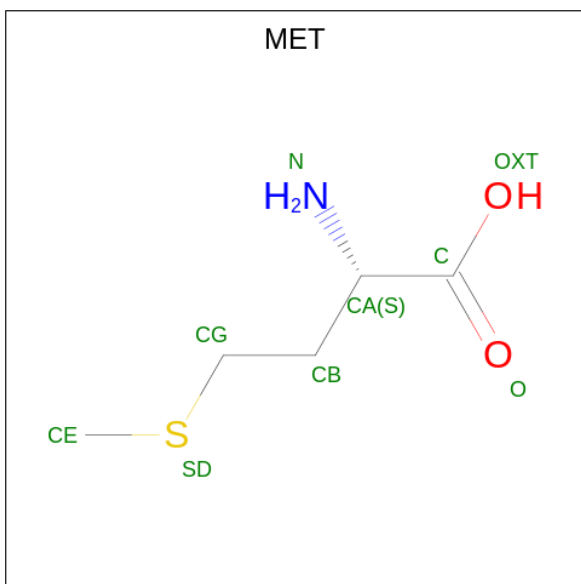
Chain	Residue	Modelled	Actual	Comment	Reference
B	349	SER	GLN	engineered mutation	UNP P13254

- Molecule 3 is (2E)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylamino]-4-(methylsulfanyl)but-2-enoic acid (three-letter code: 3LM) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>2</sub>O<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0
3	C	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0
3	D	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0

- Molecule 4 is METHIONINE (three-letter code: MET) (formula:  $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

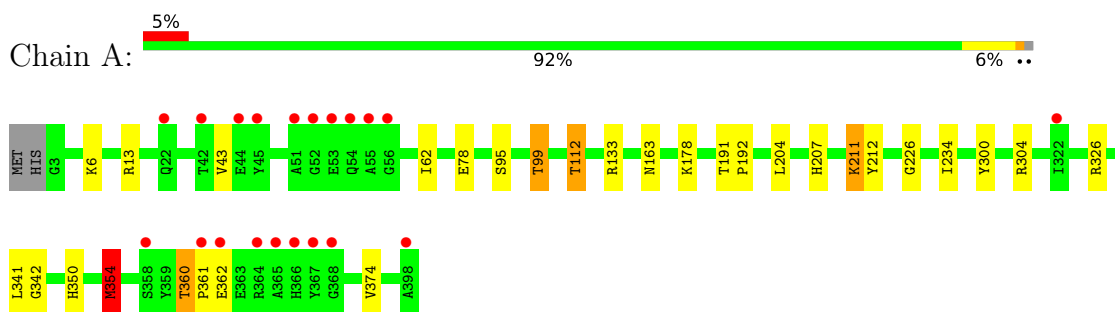
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	29	Total	O	0	0
			29	29		
5	C	21	Total	O	0	0
			21	21		
5	D	36	Total	O	0	0
			36	36		

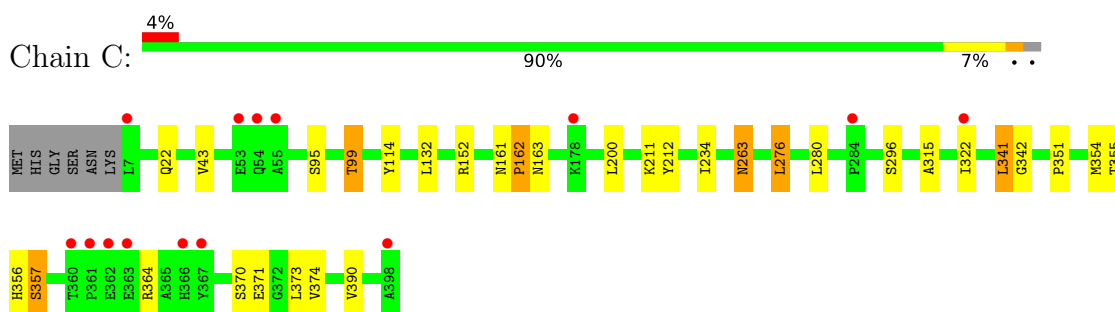
### 3 Residue-property plots [i](#)

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.

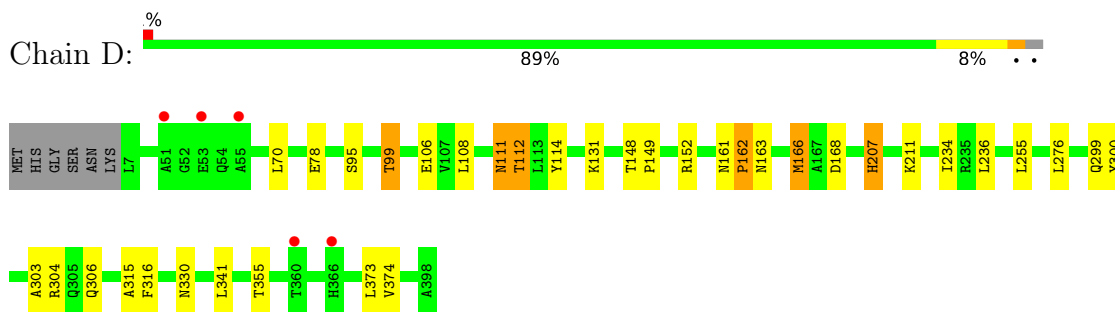
- Molecule 1: L-methionine gamma-lyase



- Molecule 1: L-methionine gamma-lyase

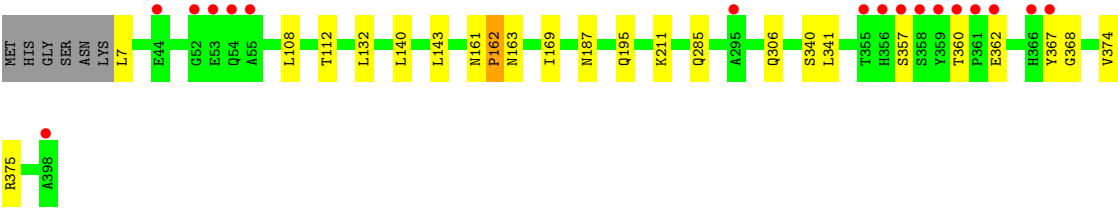


- Molecule 1: L-methionine gamma-lyase



- Molecule 2: L-methionine gamma-lyase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.91Å 152.56Å 80.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.40 19.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.9 (19.93-2.40) 90.1 (19.93-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.45 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.180 , 0.219 0.185 , 0.223	Depositor DCC
$R_{free}$ test set	3464 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3LM, LLP

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	0.50	0/3039	0.73	2/4124 (0.0%)
1	C	0.48	0/3012	0.69	1/4089 (0.0%)
1	D	0.50	0/3012	0.71	1/4089 (0.0%)
2	B	0.50	0/3001	0.72	1/4074 (0.0%)
All	All	0.50	0/12064	0.71	5/16376 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	PRO	CA-N-CD	-5.48	103.83	111.50
1	A	13	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	162	PRO	CA-N-CD	-5.26	104.14	111.50
1	C	162	PRO	CA-N-CD	-5.06	104.42	111.50
1	A	354	MET	CG-SD-CE	5.03	108.24	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	207	HIS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	2942	15	0
1	C	2948	0	2918	17	0
1	D	2948	0	2918	19	0
2	B	2962	0	2918	4	0
3	A	24	0	14	0	0
3	C	24	0	16	4	0
3	D	24	0	16	3	0
4	B	9	0	8	0	0
5	A	38	0	0	0	0
5	B	29	0	0	0	0
5	C	21	0	0	0	0
5	D	36	0	0	0	0
All	All	12038	0	11750	54	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 (54) 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:A:112:THR:HG21	1:A:163:ASN:HD21	1.44	0.82
1:C:355:THR:HG23	1:C:356:HIS:HD2	1.52	0.72
1:C:354:MET:O	1:C:357:SER:OG	2.09	0.70
1:A:99:THR:HG21	1:A:234:ILE:HA	1.79	0.65
1:D:99:THR:HG21	1:D:234:ILE:HA	1.80	0.64
1:C:99:THR:HG21	1:C:234:ILE:HA	1.80	0.63
1:C:211:LYS:NZ	3:C:401:3LM:H4A	2.14	0.61
1:D:355:THR:HG22	3:D:401:3LM:HGA	1.81	0.61
1:C:211:LYS:HZ1	3:C:401:3LM:H4A	1.64	0.61
1:D:112:THR:HG21	1:D:163:ASN:HD21	1.65	0.61
1:A:211:LYS:HG2	1:A:341:LEU:HG	1.82	0.61
1:D:114:TYR:CZ	3:D:401:3LM:H4A1	2.39	0.58
1:A:350:HIS:O	1:A:354:MET:HB2	2.04	0.57
2:B:169:ILE:H	2:B:306:GLN:HE22	1.52	0.56
2:B:112:THR:HG22	2:B:367:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:NZ	3:D:401:3LM:H4A	2.22	0.54
1:D:95:SER:O	1:D:99:THR:CG2	2.56	0.54
1:A:78:GLU:OE1	1:A:207:HIS:HE1	1.94	0.49
1:D:70:LEU:HD21	1:D:255:LEU:HD23	1.94	0.49
1:A:95:SER:O	1:A:99:THR:CG2	2.61	0.48
1:D:148:THR:HB	1:D:149:PRO:HD2	1.96	0.48
1:D:166:MET:H	1:D:299:GLN:HE22	1.60	0.48
1:C:43:VAL:H	1:D:330:ASN:HD21	1.62	0.47
1:C:95:SER:O	1:C:99:THR:CG2	2.63	0.47
1:D:166:MET:HE2	1:D:303:ALA:HB2	1.96	0.47
1:C:351:PRO:HA	1:C:355:THR:HG22	1.96	0.46
1:D:316:PHE:CE1	1:D:374:VAL:HG22	2.50	0.46
1:A:300:TYR:CZ	1:A:304:ARG:HD2	2.51	0.46
1:D:95:SER:O	1:D:99:THR:HG22	2.16	0.46
1:C:161:ASN:HA	1:C:162:PRO:HA	1.52	0.45
1:C:211:LYS:HD2	1:C:341:LEU:HG	1.98	0.45
1:A:78:GLU:OE1	1:A:207:HIS:CE1	2.69	0.45
1:C:212:TYR:CE1	1:C:342:GLY:HA2	2.51	0.45
2:B:161:ASN:HA	2:B:162:PRO:HA	1.66	0.45
1:A:95:SER:O	1:A:99:THR:HG23	2.18	0.44
1:A:204:LEU:HD23	1:A:226:GLY:HA3	2.00	0.44
1:C:263:ASN:H	1:C:263:ASN:HD22	1.66	0.43
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.53	0.43
1:C:370:SER:OG	1:C:371:GLU:N	2.52	0.42
1:C:315:ALA:HB1	1:C:373:LEU:HD11	2.01	0.42
1:D:315:ALA:HB1	1:D:373:LEU:HD11	2.01	0.42
1:A:112:THR:HG21	1:A:163:ASN:ND2	2.24	0.42
1:C:276:LEU:HD21	1:C:390:VAL:HG21	2.02	0.41
1:D:78:GLU:OE2	1:D:207:HIS:CE1	2.73	0.41
1:A:62:ILE:HD12	1:A:62:ILE:N	2.35	0.41
1:D:168:ASP:HA	1:D:306:GLN:HE22	1.86	0.41
1:A:360:THR:OG1	1:A:361:PRO:HD2	2.21	0.41
1:C:114:TYR:OH	3:C:401:3LM:HG	2.20	0.41
1:A:212:TYR:CE1	1:A:342:GLY:HA2	2.56	0.41
1:D:161:ASN:HA	1:D:162:PRO:HA	1.58	0.41
1:A:191:THR:HB	1:A:192:PRO:HD2	2.03	0.40
1:C:114:TYR:CZ	3:C:401:3LM:H4A1	2.56	0.40
1:D:111:ASN:HD22	1:D:111:ASN:HA	1.61	0.40
2:B:187:ASN:ND2	2:B:195:GLN:HE21	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	394/398 (99%)	379 (96%)	15 (4%)	0	100	100
1	C	390/398 (98%)	375 (96%)	15 (4%)	0	100	100
1	D	390/398 (98%)	379 (97%)	11 (3%)	0	100	100
2	B	389/398 (98%)	373 (96%)	12 (3%)	4 (1%)	15	23
All	All	1563/1592 (98%)	1506 (96%)	53 (3%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	362	GLU
2	B	340	SER
2	B	357	SER
2	B	368	GLY

### 5.3.2 Protein sidechains ⓘ

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	305/307 (99%)	293 (96%)	12 (4%)	32	50
1	C	302/307 (98%)	287 (95%)	15 (5%)	24	40
1	D	302/307 (98%)	291 (96%)	11 (4%)	35	54
2	B	300/306 (98%)	289 (96%)	11 (4%)	34	53
All	All	1209/1227 (98%)	1160 (96%)	49 (4%)	31	48

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	43	VAL
1	A	99	THR
1	A	112	THR
1	A	133	ARG
1	A	178	LYS
1	A	211	LYS
1	A	326	ARG
1	A	354	MET
1	A	360	THR
1	A	362	GLU
1	A	374	VAL
2	B	7	LEU
2	B	108	LEU
2	B	132	LEU
2	B	140	LEU
2	B	143	LEU
2	B	163	ASN
2	B	285	GLN
2	B	341	LEU
2	B	360	THR
2	B	374	VAL
2	B	375	ARG
1	C	22	GLN
1	C	99	THR
1	C	132	LEU
1	C	152	ARG
1	C	163	ASN
1	C	200	LEU
1	C	263	ASN
1	C	276	LEU
1	C	280	LEU
1	C	296	SER
1	C	322	ILE
1	C	341	LEU
1	C	357	SER
1	C	364	ARG
1	C	374	VAL
1	D	99	THR
1	D	106	GLU
1	D	108	LEU
1	D	111	ASN

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Mol	Chain	Res	Type
1	D	112	THR
1	D	131	LYS
1	D	152	ARG
1	D	166	MET
1	D	236	LEU
1	D	276	LEU
1	D	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	187	ASN
1	A	195	GLN
1	A	207	HIS
1	A	237	GLN
1	A	274	GLN
1	A	309	GLN
1	A	330	ASN
1	A	356	HIS
2	B	22	GLN
2	B	34	GLN
2	B	57	HIS
2	B	187	ASN
2	B	250	HIS
2	B	285	GLN
2	B	299	GLN
2	B	306	GLN
2	B	309	GLN
1	C	22	GLN
1	C	68	ASN
1	C	111	ASN
1	C	134	HIS
1	C	163	ASN
1	C	263	ASN
1	C	356	HIS
1	D	64	ASN
1	D	111	ASN
1	D	207	HIS
1	D	228	GLN
1	D	274	GLN
1	D	299	GLN

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Mol	Chain	Res	Type
1	D	306	GLN
1	D	309	GLN
1	D	330	ASN
1	D	356	HIS
1	D	391	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LLP	B	211	2	23,24,25	2.75	5 (21%)	25,32,34	1.54	6 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLP	B	211	2	-	4/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	LLP	C3-C2	6.88	1.47	1.40
2	B	211	LLP	C4-C5	6.66	1.50	1.42
2	B	211	LLP	C4'-NZ	6.41	1.48	1.27
2	B	211	LLP	C4-C3	4.85	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	LLP	C4-C4'	3.33	1.53	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	LLP	OP4-P-OP1	-2.87	98.41	106.47
2	B	211	LLP	C6-N1-C2	2.79	124.33	119.17
2	B	211	LLP	C3-C4-C5	-2.34	116.47	118.26
2	B	211	LLP	C4-C3-C2	-2.21	118.82	120.19
2	B	211	LLP	C4-C4'-NZ	-2.06	114.84	124.31
2	B	211	LLP	C5-C4-C4'	2.01	124.86	121.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	211	LLP	O-C-CA-CB
2	B	211	LLP	C4-C4'-NZ-CE
2	B	211	LLP	CD-CE-NZ-C4'
2	B	211	LLP	C3-C4-C4'-NZ

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](#)

4 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
3	3LM	C	401	-	20,24,24	2.89	8 (40%)	23,33,33	2.11	9 (39%)
3	3LM	A	401	-	20,24,24	2.84	8 (40%)	23,33,33	2.05	10 (43%)
4	MET	B	401	-	4,8,8	0.64	0	2,9,9	0.42	0
3	3LM	D	401	-	20,24,24	2.97	8 (40%)	23,33,33	2.05	8 (34%)

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	3LM	C	401	-	-	7/13/19/19	0/1/1/1
3	3LM	A	401	-	-	6/13/19/19	0/1/1/1
4	MET	B	401	-	-	1/4/8/8	-
3	3LM	D	401	-	-	6/13/19/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	3LM	C4A-C4	-7.84	1.41	1.51
3	A	401	3LM	C4A-C4	-7.40	1.42	1.51
3	C	401	3LM	C4A-C4	-6.58	1.43	1.51
3	D	401	3LM	C2A-C2	-6.08	1.40	1.50
3	C	401	3LM	C2A-C2	-5.82	1.40	1.50
3	C	401	3LM	C4A-N	-5.64	1.35	1.46
3	A	401	3LM	C2A-C2	-5.36	1.41	1.50
3	D	401	3LM	C4A-N	-5.32	1.35	1.46
3	A	401	3LM	C4A-N	-5.15	1.36	1.46
3	C	401	3LM	C2-N1	4.08	1.41	1.33
3	D	401	3LM	C2-N1	3.56	1.40	1.33
3	C	401	3LM	C5A-C5	-3.14	1.42	1.50
3	A	401	3LM	C5A-C5	-2.91	1.43	1.50
3	A	401	3LM	CA-N	2.72	1.37	1.34
3	A	401	3LM	C2-N1	2.55	1.38	1.33
3	C	401	3LM	C3-C4	2.51	1.43	1.40
3	A	401	3LM	C-CA	2.26	1.55	1.52
3	D	401	3LM	C5A-C5	-2.25	1.44	1.50
3	C	401	3LM	C5-C4	2.16	1.43	1.40
3	A	401	3LM	C5-C4	2.16	1.43	1.40
3	C	401	3LM	P-OP2	-2.12	1.46	1.54
3	D	401	3LM	CA-N	2.12	1.36	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	3LM	C3-C2	-2.08	1.38	1.40
3	D	401	3LM	P-OP2	-2.03	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	3LM	C4-C4A-N	4.44	120.31	111.22
3	A	401	3LM	OP3-P-OP4	-3.92	96.30	106.73
3	D	401	3LM	OP2-P-OP4	-3.92	96.30	106.73
3	C	401	3LM	C4-C4A-N	3.49	118.35	111.22
3	C	401	3LM	OP4-P-OP1	-3.30	97.21	106.47
3	A	401	3LM	OP4-P-OP1	-3.27	97.31	106.47
3	C	401	3LM	OP3-P-OP4	-3.23	98.14	106.73
3	C	401	3LM	C4A-C4-C5	3.21	123.28	119.71
3	A	401	3LM	OP3-P-OP2	3.14	119.64	107.64
3	D	401	3LM	C3-C2-N1	-3.10	116.77	120.77
3	C	401	3LM	OP2-P-OP4	-3.06	98.59	106.73
3	A	401	3LM	C3-C4-C5	-3.04	115.81	118.72
3	A	401	3LM	C4-C4A-N	2.92	117.20	111.22
3	C	401	3LM	OP3-P-OP2	2.89	118.68	107.64
3	D	401	3LM	OP3-P-OP2	2.77	118.21	107.64
3	D	401	3LM	OP3-P-OP4	-2.74	99.44	106.73
3	D	401	3LM	OP4-P-OP1	-2.71	98.88	106.47
3	C	401	3LM	C3-C4-C5	-2.64	116.18	118.72
3	A	401	3LM	OP2-P-OP4	-2.52	100.02	106.73
3	A	401	3LM	C4A-C4-C5	2.49	122.48	119.71
3	C	401	3LM	C3-C2-N1	-2.37	117.71	120.77
3	A	401	3LM	C5A-C5-C6	-2.35	115.51	119.37
3	C	401	3LM	CB-CA-N	2.23	128.64	122.98
3	D	401	3LM	C4A-C4-C5	2.08	122.03	119.71
3	D	401	3LM	OP2-P-OP1	2.03	118.62	110.68
3	A	401	3LM	C3-C2-N1	-2.02	118.16	120.77
3	A	401	3LM	C2A-C2-C3	2.01	123.37	120.89

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	3LM	C-CA-N-C4A
3	A	401	3LM	CB-CA-N-C4A
3	A	401	3LM	N-CA-CB-CG
3	C	401	3LM	C5-C4-C4A-N

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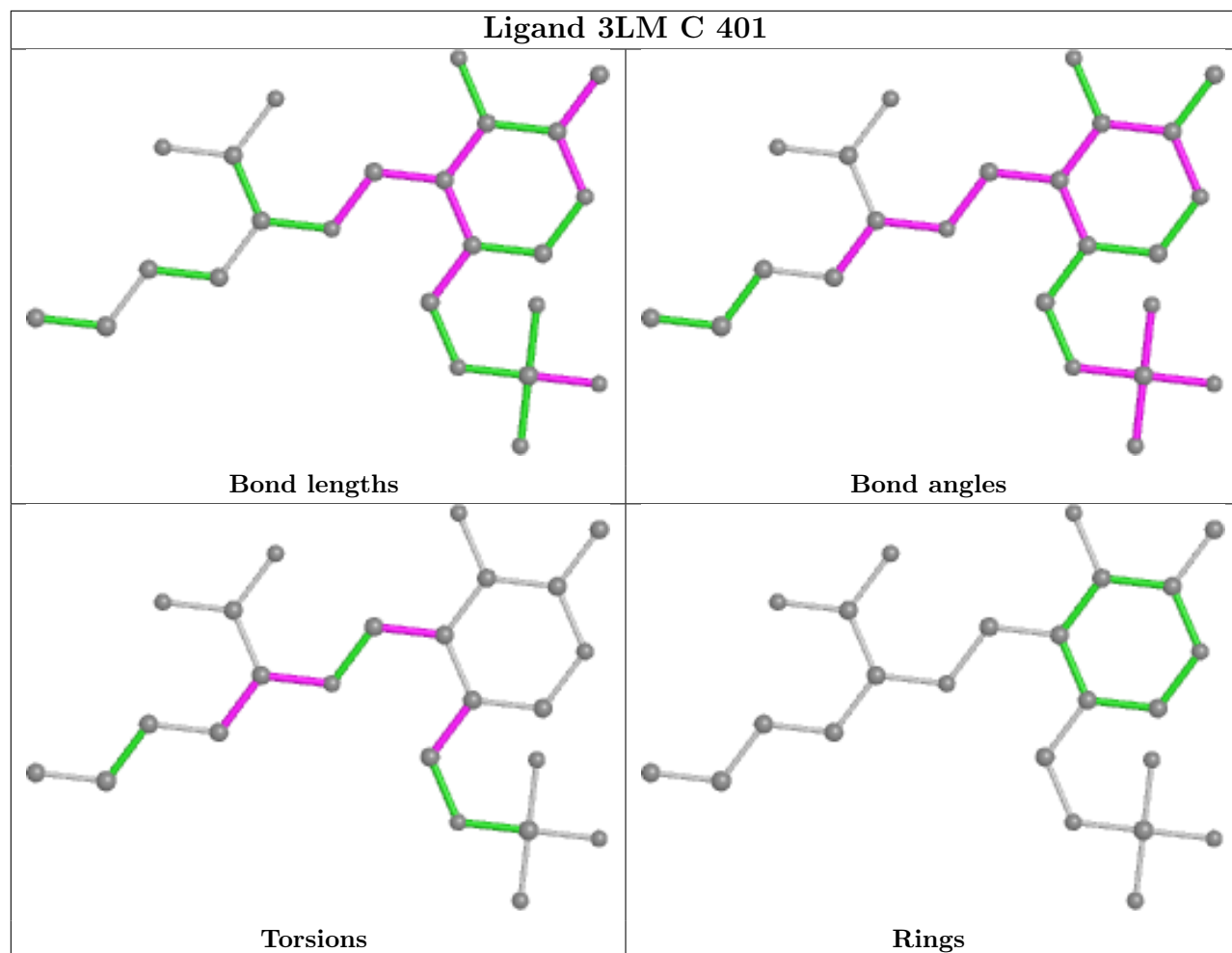
Mol	Chain	Res	Type	Atoms
3	C	401	3LM	N-CA-CB-CG
3	D	401	3LM	C5-C4-C4A-N
3	D	401	3LM	N-CA-CB-CG
3	A	401	3LM	C5-C4-C4A-N
3	A	401	3LM	CB-CG-SD-CE
3	D	401	3LM	CB-CG-SD-CE
3	C	401	3LM	C-CA-N-C4A
3	D	401	3LM	C-CA-N-C4A
3	A	401	3LM	C3-C4-C4A-N
3	C	401	3LM	C3-C4-C4A-N
3	C	401	3LM	C4-C5-C5A-OP4
3	C	401	3LM	CB-CA-N-C4A
3	D	401	3LM	CB-CA-N-C4A
3	D	401	3LM	C3-C4-C4A-N
3	C	401	3LM	C6-C5-C5A-OP4
4	B	401	MET	N-CA-CB-CG

There are no ring outliers.

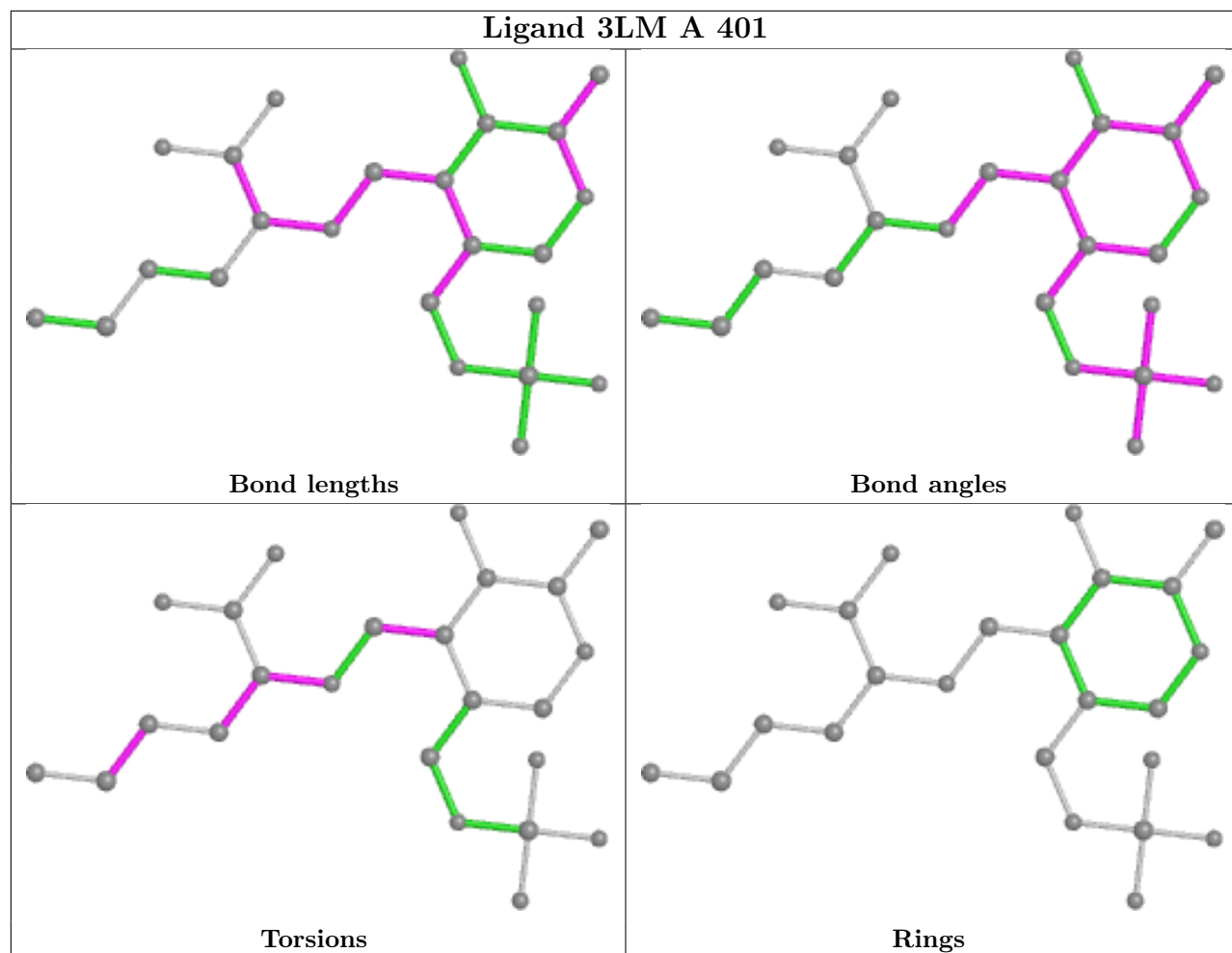
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	3LM	4	0
3	D	401	3LM	3	0

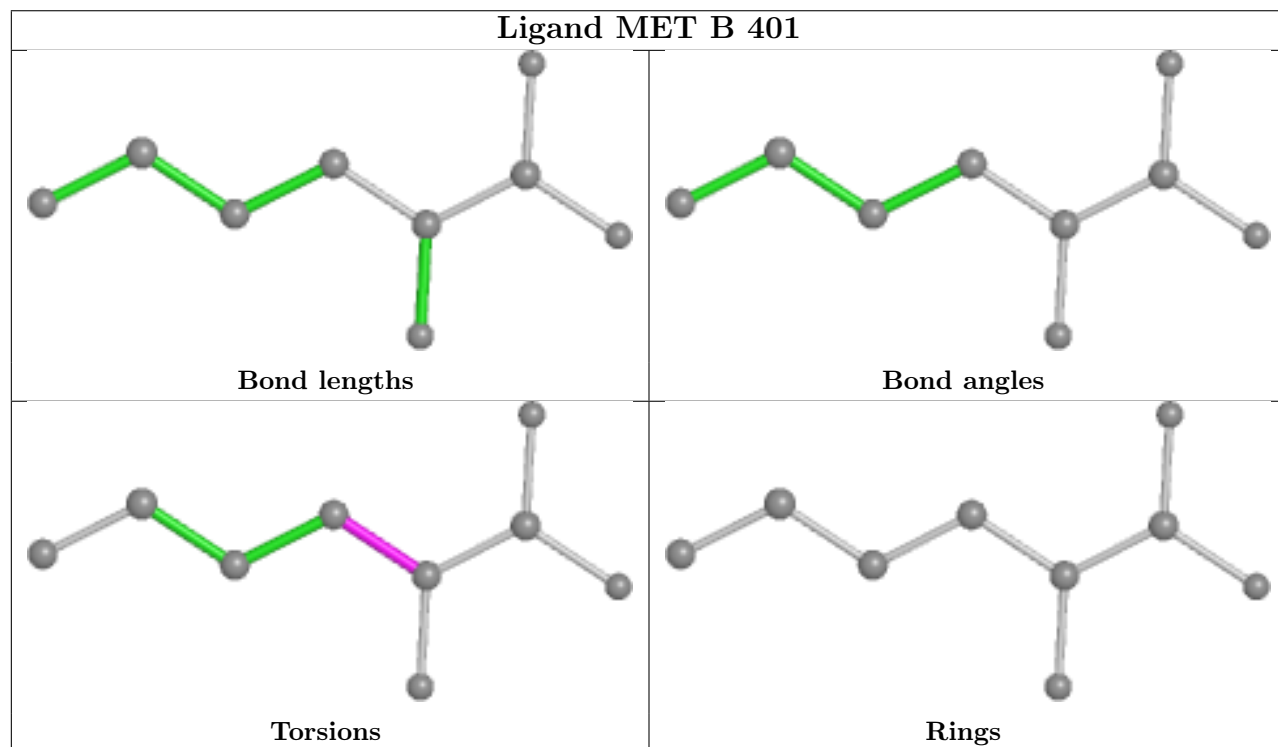
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

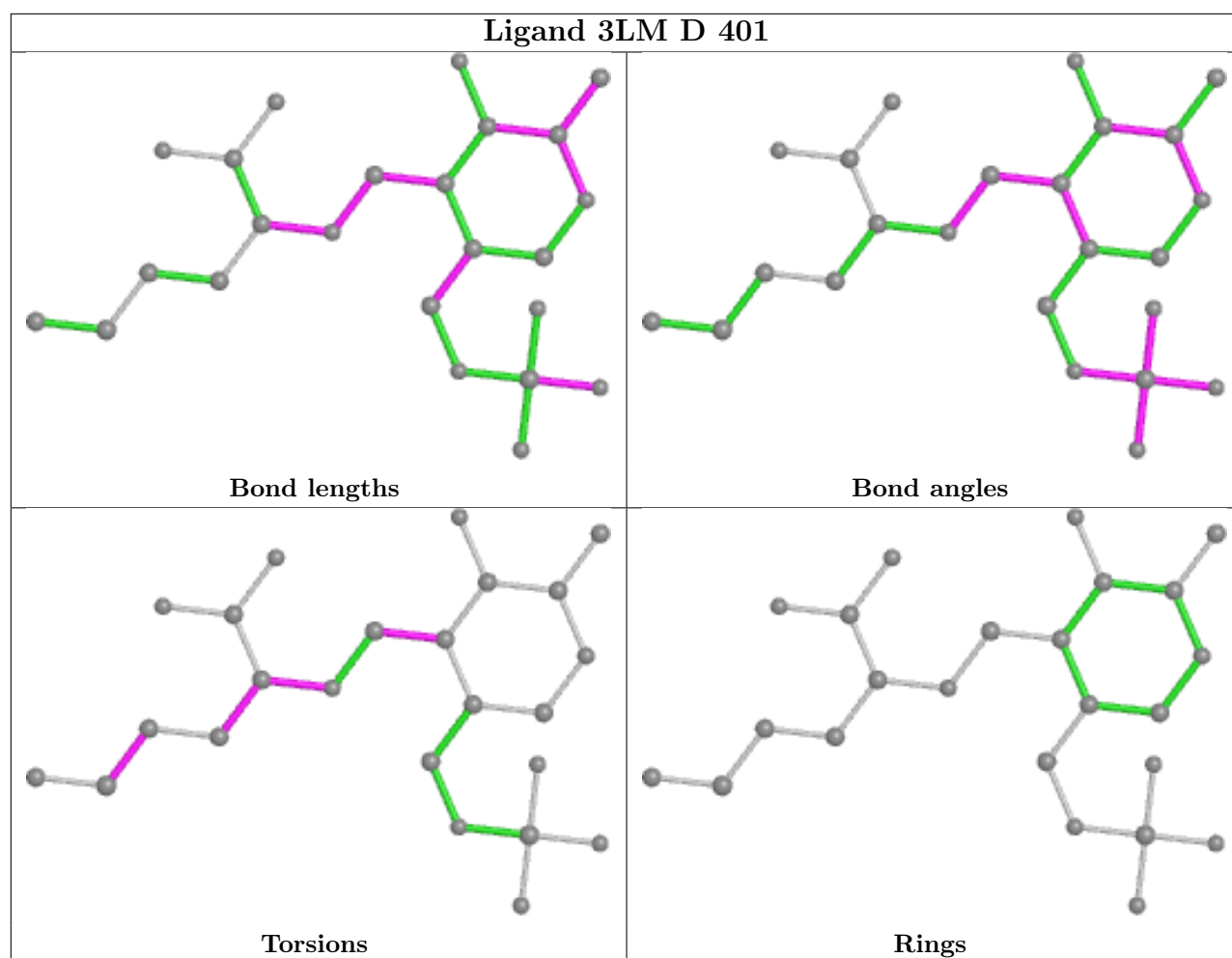


## Ligand 3LM A 401



## Ligand MET B 401





## 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	396/398 (99%)	-0.30	20 (5%)	28 26	20, 35, 76, 115	0
1	C	392/398 (98%)	-0.27	14 (3%)	42 42	27, 43, 83, 114	0
1	D	392/398 (98%)	-0.52	5 (1%)	77 75	24, 35, 65, 88	0
2	B	391/398 (98%)	-0.30	17 (4%)	35 33	23, 37, 83, 129	0
All	All	1571/1592 (98%)	-0.35	56 (3%)	42 42	20, 37, 78, 129	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	362	GLU	10.7
1	A	52	GLY	6.1
1	C	55	ALA	5.9
2	B	360	THR	5.0
1	A	55	ALA	5.0
2	B	367	TYR	4.8
2	B	55	ALA	4.6
1	A	362	GLU	4.2
1	A	51	ALA	4.1
1	C	360	THR	3.9
1	A	398	ALA	3.9
2	B	357	SER	3.7
1	C	361	PRO	3.7
1	C	367	TYR	3.6
1	A	53	GLU	3.5
2	B	359	TYR	3.4
1	A	54	GLN	3.3
1	A	366	HIS	3.3
2	B	358	SER	3.3
2	B	53	GLU	3.2
1	A	358	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	361	PRO	3.1
1	C	284	PRO	3.0
1	C	398	ALA	3.0
1	C	366	HIS	3.0
1	A	45	TYR	2.9
1	D	366	HIS	2.9
1	C	53	GLU	2.9
2	B	355	THR	2.8
1	C	322	ILE	2.8
1	A	322	ILE	2.7
1	D	51	ALA	2.7
1	D	55	ALA	2.7
1	A	56	GLY	2.6
2	B	52	GLY	2.6
1	C	54	GLN	2.6
1	C	362	GLU	2.5
1	C	178	LYS	2.5
2	B	54	GLN	2.4
1	C	7	LEU	2.4
2	B	295	ALA	2.4
1	D	53	GLU	2.4
1	C	363	GLU	2.4
1	A	44	GLU	2.3
2	B	356	HIS	2.3
1	A	364	ARG	2.2
1	D	360	THR	2.2
2	B	361	PRO	2.2
2	B	366	HIS	2.2
1	A	367	TYR	2.1
1	A	368	GLY	2.1
1	A	42	THR	2.1
1	A	365	ALA	2.1
1	A	22	GLN	2.1
2	B	44	GLU	2.1
2	B	398	ALA	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
2	LLP	B	211	24/25	0.97	0.10	26,35,44,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

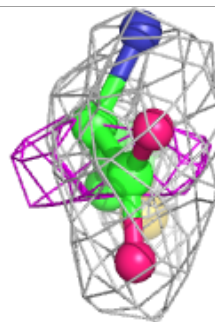
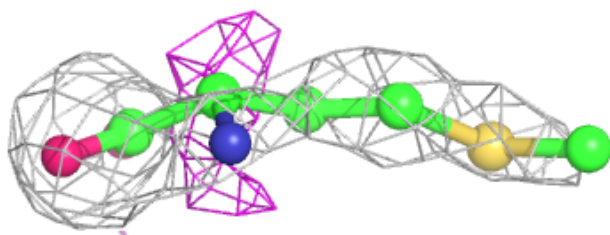
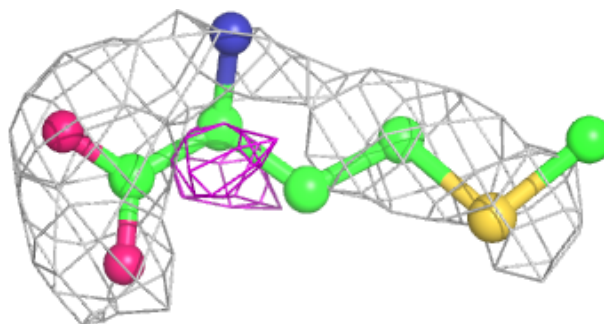
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MET	B	401	9/9	0.76	0.37	72,85,105,106	0
3	3LM	C	401	24/24	0.95	0.14	31,48,71,84	0
3	3LM	D	401	24/24	0.96	0.13	29,42,70,77	0
3	3LM	A	401	24/24	0.96	0.12	25,34,64,85	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.

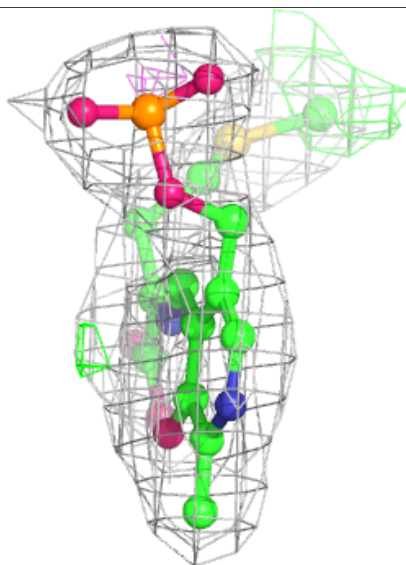
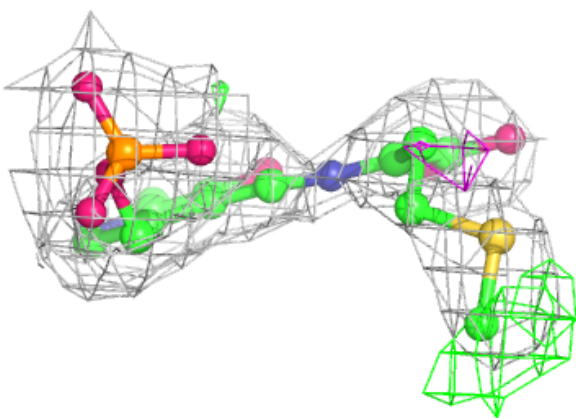
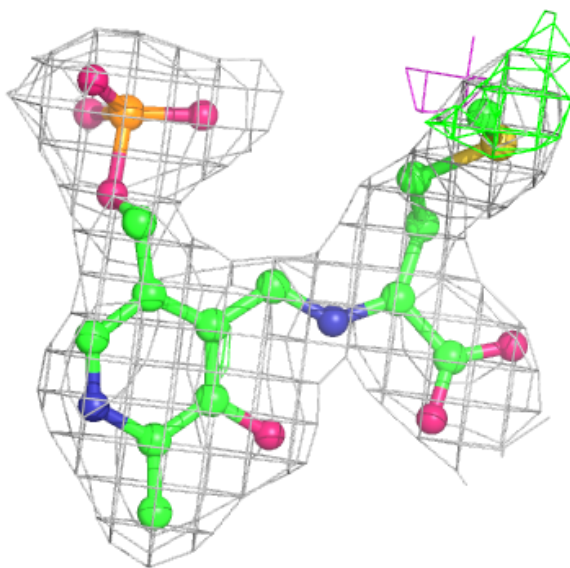
**Electron density around MET B 401:**

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



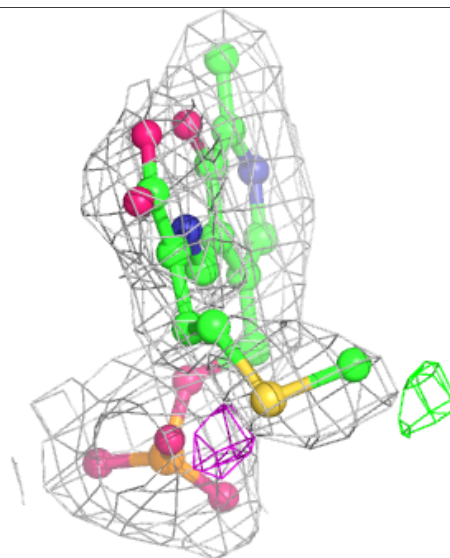
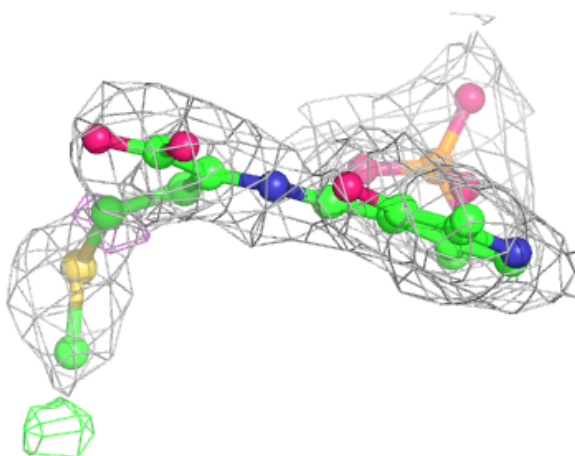
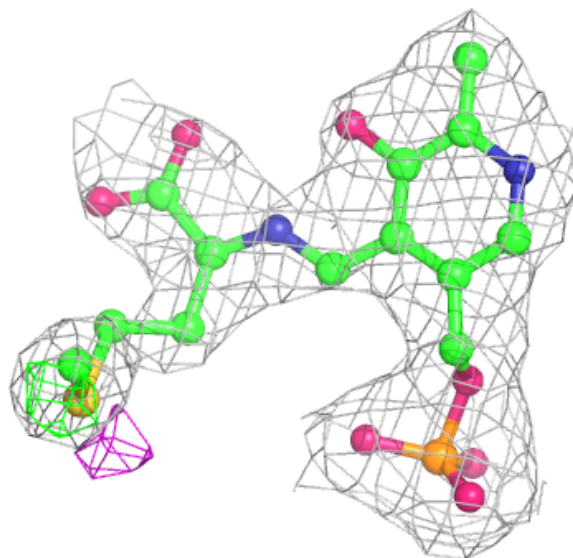
**Electron density around 3LM C 401:**

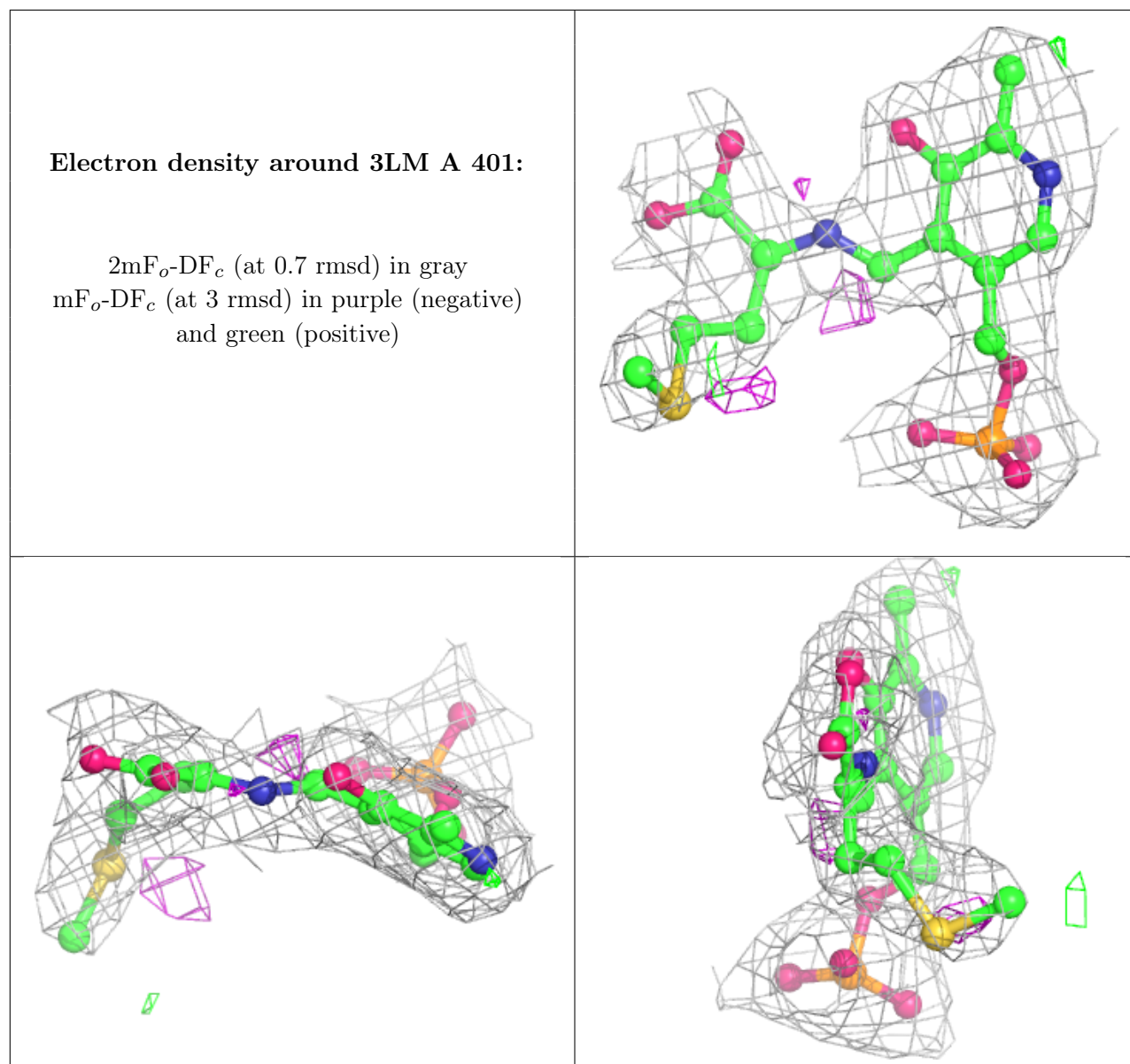
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 3LM D 401:**

$2mF_o-DF_c$  (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.