



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:15 PM UTC

PDB ID : 5X2Z / pdb_00005x2z
Title : Crystal structure of Pseudomonas putida methionine gamma-lyase C116H mutant with L-methionine intermediates
Authors : Shiba, T.; Sato, D.; Harada, S.
Deposited on : 2017-02-02
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

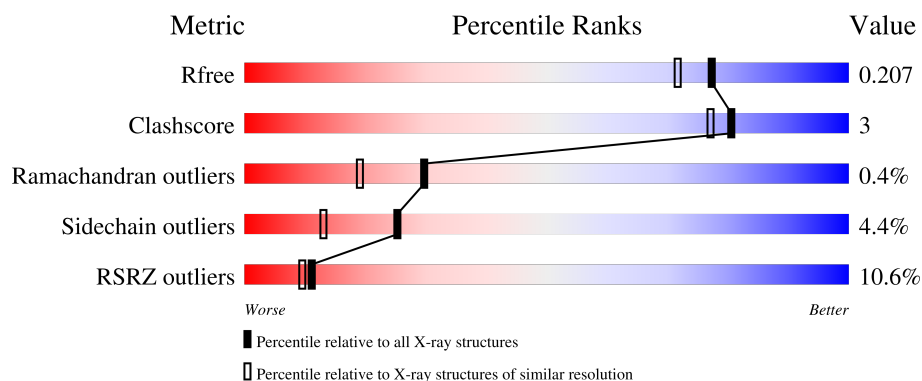
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	13% 91% 7% ..
1	B	398	8% 89% 8% ..
1	C	398	11% 87% 11% ..
1	D	398	11% 92% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12861 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.

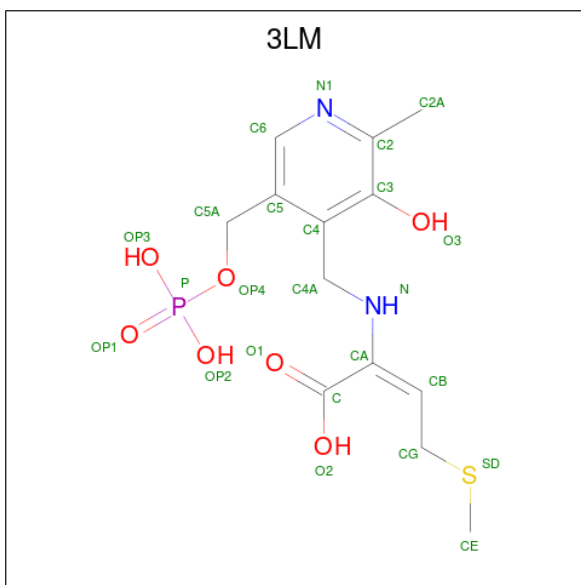
- Molecule 1 is a protein called L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2955	1866	524	549	16			
1	B	392	Total	C	N	O	S	0	1	0
			2959	1868	525	550	16			
1	C	392	Total	C	N	O	S	0	1	0
			2961	1870	525	550	16			
1	D	396	Total	C	N	O	S	0	1	0
			2988	1884	531	557	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	HIS	CYS	engineered mutation	UNP P13254
B	116	HIS	CYS	engineered mutation	UNP P13254
C	116	HIS	CYS	engineered mutation	UNP P13254
D	116	HIS	CYS	engineered mutation	UNP P13254

- Molecule 2 is (2E)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino]-4-(methylsulfanyl)but-2-enoic acid (CCD ID: 3LM) (formula: C₁₃H₁₉N₂O₇PS).



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

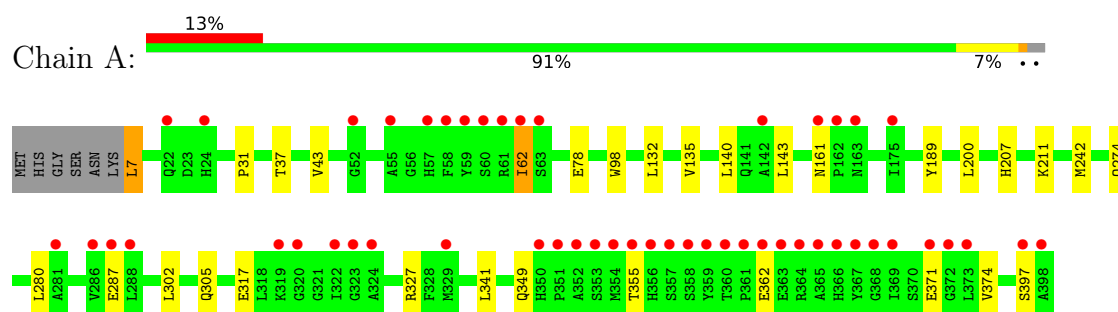
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	248	Total	O	0	0
			248	248		
3	C	229	Total	O	0	0
			229	229		
3	D	247	Total	O	0	0
			247	247		

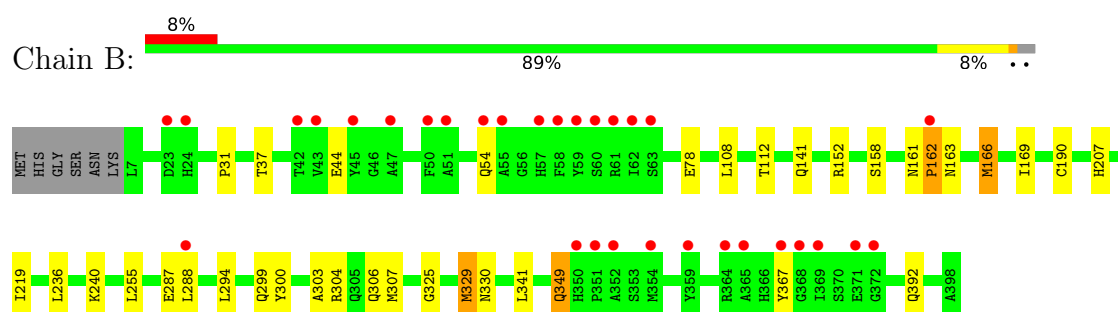
3 Residue-property plots [i](#)

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.

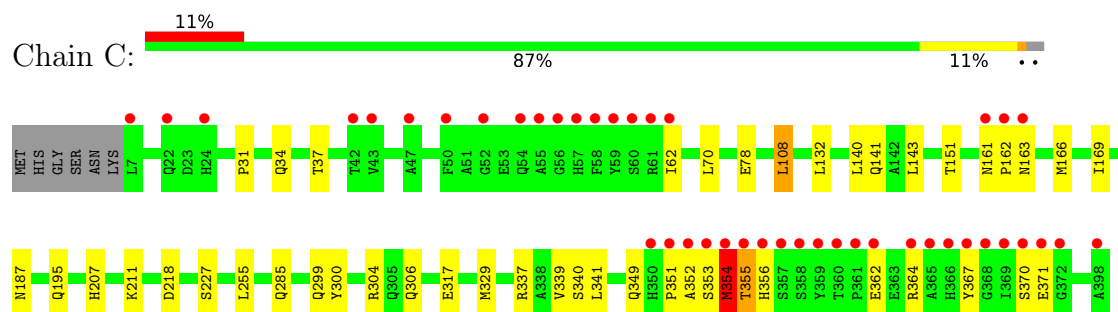
- Molecule 1: L-methionine gamma-lyase



- Molecule 1: L-methionine gamma-lyase

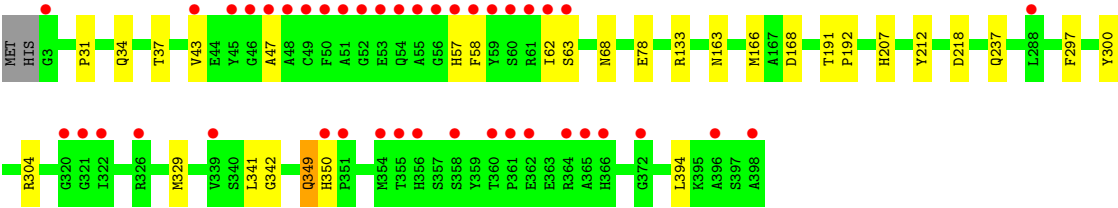


- Molecule 1: L-methionine gamma-lyase



- Molecule 1: L-methionine gamma-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.04Å 153.29Å 80.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-1.80) 93.2 (20.00-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.173 , 0.201 0.182 , 0.207	Depositor DCC
R_{free} test set	8249 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12861	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.73	0/3020	0.87	0/4100
1	B	0.77	0/3024	0.89	1/4106 (0.0%)
1	C	0.76	0/3029	0.91	1/4112 (0.0%)
1	D	0.77	0/3053	0.86	0/4143
All	All	0.76	0/12126	0.88	2/16461 (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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	THR	N-CA-C	5.62	117.73	109.24
1	B	329	MET	CG-SD-CE	-5.44	88.93	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	352	ALA	Peptide
1	D	58	PHE	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	2955	0	2923	14	0
1	B	2959	0	2922	18	0
1	C	2961	0	2931	20	0
1	D	2988	0	2954	15	0
2	A	24	0	15	2	0
2	B	24	0	16	0	0
2	C	24	0	16	1	0
2	D	24	0	15	0	0
3	A	178	0	0	2	0
3	B	248	0	0	0	0
3	C	229	0	0	1	0
3	D	247	0	0	2	0
All	All	12861	0	11792	61	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 3.

All (61) 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:B:112:THR:HG22	1:B:367:TYR:O	1.81	0.81
1:B:166:MET:HE1	1:B:303:ALA:HB2	1.67	0.75
1:C:169:ILE:H	1:C:306:GLN:HE22	1.36	0.73
1:D:329:MET:HE1	1:D:350:HIS:HB2	1.72	0.70
1:B:112:THR:HG21	1:B:163:ASN:HD21	1.56	0.70
1:B:166:MET:H	1:B:299:GLN:HE22	1.43	0.66
1:C:211:LYS:HE2	2:C:401:3LM:H4A	1.79	0.65
1:A:211:LYS:HE2	2:A:401:3LM:H4A	1.79	0.64
1:C:339:VAL:CG1	1:C:355:THR:HG21	2.28	0.62
1:B:300:TYR:CZ	1:B:304:ARG:HD2	2.36	0.61
1:A:43:VAL:H	1:B:330:ASN:HD21	1.51	0.58
1:B:329:MET:HE1	1:B:349:GLN:C	2.29	0.57
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.58	0.56
1:C:166:MET:H	1:C:299:GLN:HE22	1.55	0.55
1:C:351:PRO:O	1:C:354:MET:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.90	0.55
1:C:364:ARG:O	1:C:367:TYR:O	2.26	0.54
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.42	0.54
1:B:190:CYS:SG	1:B:307:MET:HE3	2.48	0.54
1:B:31:PRO:HB2	1:C:31:PRO:HB2	1.89	0.53
1:A:31:PRO:HB2	1:D:31:PRO:HB2	1.90	0.53
1:C:370:SER:OG	1:C:371:GLU:N	2.42	0.52
1:A:327:ARG:NH2	1:A:397:SER:O	2.42	0.52
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.94	0.51
1:A:327:ARG:HB3	1:A:397:SER:HA	1.92	0.51
1:B:325:GLY:O	1:B:329:MET:HG2	2.11	0.50
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.65	0.50
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.47	0.50
1:A:211:LYS:CE	2:A:401:3LM:H4A	2.43	0.49
1:B:329:MET:HE1	1:B:349:GLN:O	2.13	0.48
1:D:78:GLU:OE1	1:D:207:HIS:HE1	1.97	0.47
1:C:161:ASN:CG	3:C:505:HOH:O	2.58	0.47
1:D:63:SER:CB	1:D:68:ASN:HD21	2.28	0.46
1:A:302:LEU:HA	1:A:305:GLN:HE21	1.81	0.46
1:C:34:GLN:HG3	1:D:218:ASP:O	2.16	0.46
1:D:191:THR:HB	1:D:192:PRO:HD2	1.98	0.45
1:D:78:GLU:OE1	1:D:207:HIS:CE1	2.71	0.44
1:A:7:LEU:N	3:A:504:HOH:O	2.51	0.44
1:C:329:MET:HE3	1:C:337:ARG:HG2	1.98	0.44
1:A:161:ASN:HB3	1:A:189:TYR:OH	2.16	0.44
1:C:218:ASP:O	1:D:34:GLN:HG3	2.17	0.44
1:A:207:HIS:HD2	3:A:554:HOH:O	2.00	0.44
1:B:169:ILE:H	1:B:306:GLN:HE22	1.64	0.44
1:B:219:ILE:CD1	1:B:255:LEU:HB2	2.48	0.43
1:B:287:GLU:HG3	1:B:288:LEU:HG	2.01	0.43
1:C:187:ASN:ND2	1:C:195:GLN:HE21	2.17	0.42
1:C:108:LEU:HD22	1:C:151:THR:HG21	2.02	0.42
1:C:161:ASN:HA	1:C:162:PRO:HA	1.85	0.42
1:A:98:TRP:HB3	1:A:242:MET:HE2	2.02	0.42
1:D:212:TYR:CE1	1:D:342:GLY:HA2	2.55	0.41
1:D:349:GLN:HE21	1:D:349:GLN:HB2	1.65	0.41
1:B:161:ASN:HA	1:B:162:PRO:HA	1.87	0.41
1:C:78:GLU:OE2	1:C:207:HIS:NE2	2.49	0.41
1:D:168:ASP:CB	3:D:536:HOH:O	2.68	0.41
1:D:168:ASP:HB3	3:D:536:HOH:O	2.20	0.41
1:D:166:MET:HE3	1:D:297:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD21	1:C:255:LEU:HD23	2.01	0.41
1:C:353:SER:OG	1:D:47:ALA:HB2	2.20	0.41
1:A:135:VAL:HG11	1:A:143:LEU:HA	2.03	0.41
1:B:158:SER:OG	1:B:166:MET:HG3	2.21	0.40
1:C:339:VAL:HG11	1:C:355:THR:HG21	2.02	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	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	36	25
1	B	391/398 (98%)	380 (97%)	10 (3%)	1 (0%)	36	25
1	C	391/398 (98%)	376 (96%)	12 (3%)	3 (1%)	16	6
1	D	395/398 (99%)	378 (96%)	16 (4%)	1 (0%)	36	25
All	All	1567/1592 (98%)	1514 (97%)	47 (3%)	6 (0%)	30	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	354	MET
1	A	62	ILE
1	C	340	SER
1	C	62	ILE
1	D	62	ILE
1	B	162	PRO

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	302/307 (98%)	286 (95%)	16 (5%)	20	9
1	B	302/307 (98%)	289 (96%)	13 (4%)	26	13
1	C	303/307 (99%)	288 (95%)	15 (5%)	22	10
1	D	306/307 (100%)	297 (97%)	9 (3%)	37	25
All	All	1213/1228 (99%)	1160 (96%)	53 (4%)	25	13

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	37	THR
1	A	62	ILE
1	A	132	LEU
1	A	140	LEU
1	A	200	LEU
1	A	274	GLN
1	A	280	LEU
1	A	287	GLU
1	A	317	GLU
1	A	341	LEU
1	A	349	GLN
1	A	355	THR
1	A	362	GLU
1	A	371	GLU
1	A	374	VAL
1	B	37	THR
1	B	44	GLU
1	B	54	GLN
1	B	108	LEU
1	B	141	GLN
1	B	152	ARG
1	B	166	MET
1	B	236	LEU

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Mol	Chain	Res	Type
1	B	240	LYS
1	B	294	LEU
1	B	341	LEU
1	B	349	GLN
1	B	392	GLN
1	C	108	LEU
1	C	132	LEU
1	C	140	LEU
1	C	141	GLN
1	C	143	LEU
1	C	163	ASN
1	C	227	SER
1	C	285	GLN
1	C	317	GLU
1	C	341	LEU
1	C	349	GLN
1	C	354	MET
1	C	355	THR
1	C	356	HIS
1	C	362	GLU
1	D	37	THR
1	D	43	VAL
1	D	57	HIS
1	D	133	ARG
1	D	163	ASN
1	D	237	GLN
1	D	341	LEU
1	D	349	GLN
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	111	ASN
1	A	134	HIS
1	A	207	HIS
1	A	274	GLN
1	A	305	GLN
1	B	22	GLN
1	B	54	GLN
1	B	64	ASN

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Mol	Chain	Res	Type
1	B	111	ASN
1	B	163	ASN
1	B	207	HIS
1	B	274	GLN
1	B	299	GLN
1	B	305	GLN
1	B	306	GLN
1	B	330	ASN
1	B	333	GLN
1	B	392	GLN
1	C	116	HIS
1	C	141	GLN
1	C	161	ASN
1	C	165	HIS
1	C	187	ASN
1	C	195	GLN
1	C	299	GLN
1	C	305	GLN
1	C	306	GLN
1	C	349	GLN
1	C	356	HIS
1	D	17	HIS
1	D	34	GLN
1	D	68	ASN
1	D	163	ASN
1	D	187	ASN
1	D	195	GLN
1	D	207	HIS
1	D	274	GLN
1	D	290	HIS
1	D	330	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](#)

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	$\# Z > 2$
2	3LM	A	401	-	22,24,24	1.52	4 (18%)	29,33,33	1.57	7 (24%)
2	3LM	C	401	-	22,24,24	1.32	2 (9%)	29,33,33	1.68	7 (24%)
2	3LM	B	401	-	22,24,24	1.17	3 (13%)	29,33,33	1.73	7 (24%)
2	3LM	D	401	-	22,24,24	1.37	3 (13%)	29,33,33	1.80	6 (20%)

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	3LM	A	401	-	-	5/18/19/19	0/1/1/1
2	3LM	C	401	-	-	5/18/19/19	0/1/1/1
2	3LM	B	401	-	-	5/18/19/19	0/1/1/1
2	3LM	D	401	-	-	5/18/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	3LM	C6-N1	3.05	1.40	1.34
2	D	401	3LM	C6-N1	2.63	1.39	1.34
2	D	401	3LM	O2-C	-2.53	1.23	1.30
2	D	401	3LM	C5A-C5	2.47	1.57	1.50
2	A	401	3LM	P-OP4	2.32	1.67	1.60
2	C	401	3LM	O2-C	-2.27	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	3LM	C2A-C2	2.24	1.53	1.50
2	B	401	3LM	O2-C	-2.17	1.24	1.30
2	B	401	3LM	C6-N1	2.14	1.38	1.34
2	B	401	3LM	C5A-C5	2.11	1.56	1.50
2	A	401	3LM	C5A-C5	2.09	1.56	1.50
2	A	401	3LM	P-OP2	-2.04	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	3LM	O2-C-CA	4.88	124.79	114.27
2	D	401	3LM	O2-C-CA	4.43	123.81	114.27
2	D	401	3LM	C4A-C4-C3	3.93	125.21	119.98
2	D	401	3LM	C4A-C4-C5	-3.67	115.75	119.75
2	A	401	3LM	C4A-N-CA	3.61	129.81	123.44
2	C	401	3LM	C4A-C4-C3	3.56	124.71	119.98
2	A	401	3LM	OP4-C5A-C5	-3.37	103.03	109.36
2	D	401	3LM	O2-C-O1	-3.29	116.06	123.90
2	C	401	3LM	O2-C-O1	-3.23	116.21	123.90
2	C	401	3LM	C4A-C4-C5	-3.06	116.42	119.75
2	B	401	3LM	C4A-C4-C3	3.03	124.01	119.98
2	B	401	3LM	C4A-C4-C5	-2.94	116.55	119.75
2	B	401	3LM	OP4-C5A-C5	-2.81	104.09	109.36
2	C	401	3LM	C3-C2-N1	-2.79	117.44	120.96
2	A	401	3LM	O2-C-O1	-2.74	117.36	123.90
2	B	401	3LM	O2-C-O1	-2.72	117.42	123.90
2	B	401	3LM	CB-CA-C	2.71	125.76	120.79
2	D	401	3LM	C3-C2-N1	-2.62	117.66	120.96
2	C	401	3LM	O2-C-CA	2.45	119.54	114.27
2	A	401	3LM	C3-C2-N1	-2.44	117.88	120.96
2	C	401	3LM	OP4-C5A-C5	-2.23	105.18	109.36
2	A	401	3LM	CB-CA-C	2.22	124.87	120.79
2	B	401	3LM	C3-C2-N1	-2.20	118.18	120.96
2	A	401	3LM	O2-C-CA	2.19	118.99	114.27
2	C	401	3LM	C4A-N-CA	2.12	127.19	123.44
2	D	401	3LM	C2A-C2-C3	2.12	123.27	120.80
2	A	401	3LM	C4A-C4-C3	2.04	122.69	119.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

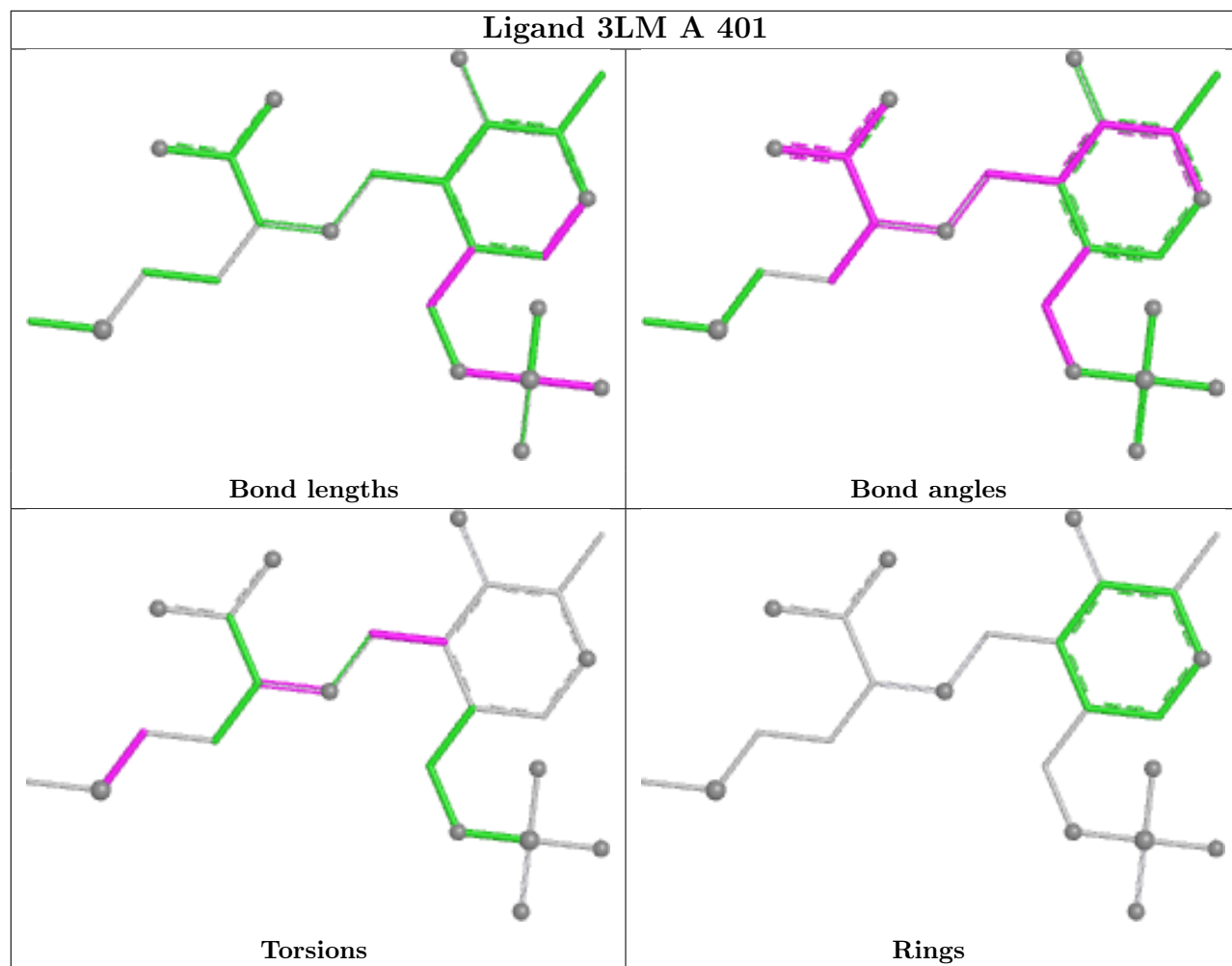
Mol	Chain	Res	Type	Atoms
2	B	401	3LM	C5-C4-C4A-N
2	D	401	3LM	C3-C4-C4A-N
2	D	401	3LM	C5-C4-C4A-N
2	A	401	3LM	C5-C4-C4A-N
2	C	401	3LM	C5-C4-C4A-N
2	C	401	3LM	C3-C4-C4A-N
2	C	401	3LM	CB-CG-SD-CE
2	A	401	3LM	CB-CG-SD-CE
2	A	401	3LM	C3-C4-C4A-N
2	B	401	3LM	CB-CG-SD-CE
2	D	401	3LM	CB-CG-SD-CE
2	A	401	3LM	CB-CA-N-C4A
2	B	401	3LM	CB-CA-N-C4A
2	C	401	3LM	CB-CA-N-C4A
2	D	401	3LM	CB-CA-N-C4A
2	B	401	3LM	C3-C4-C4A-N
2	A	401	3LM	C-CA-N-C4A
2	B	401	3LM	C-CA-N-C4A
2	C	401	3LM	C-CA-N-C4A
2	D	401	3LM	C-CA-N-C4A

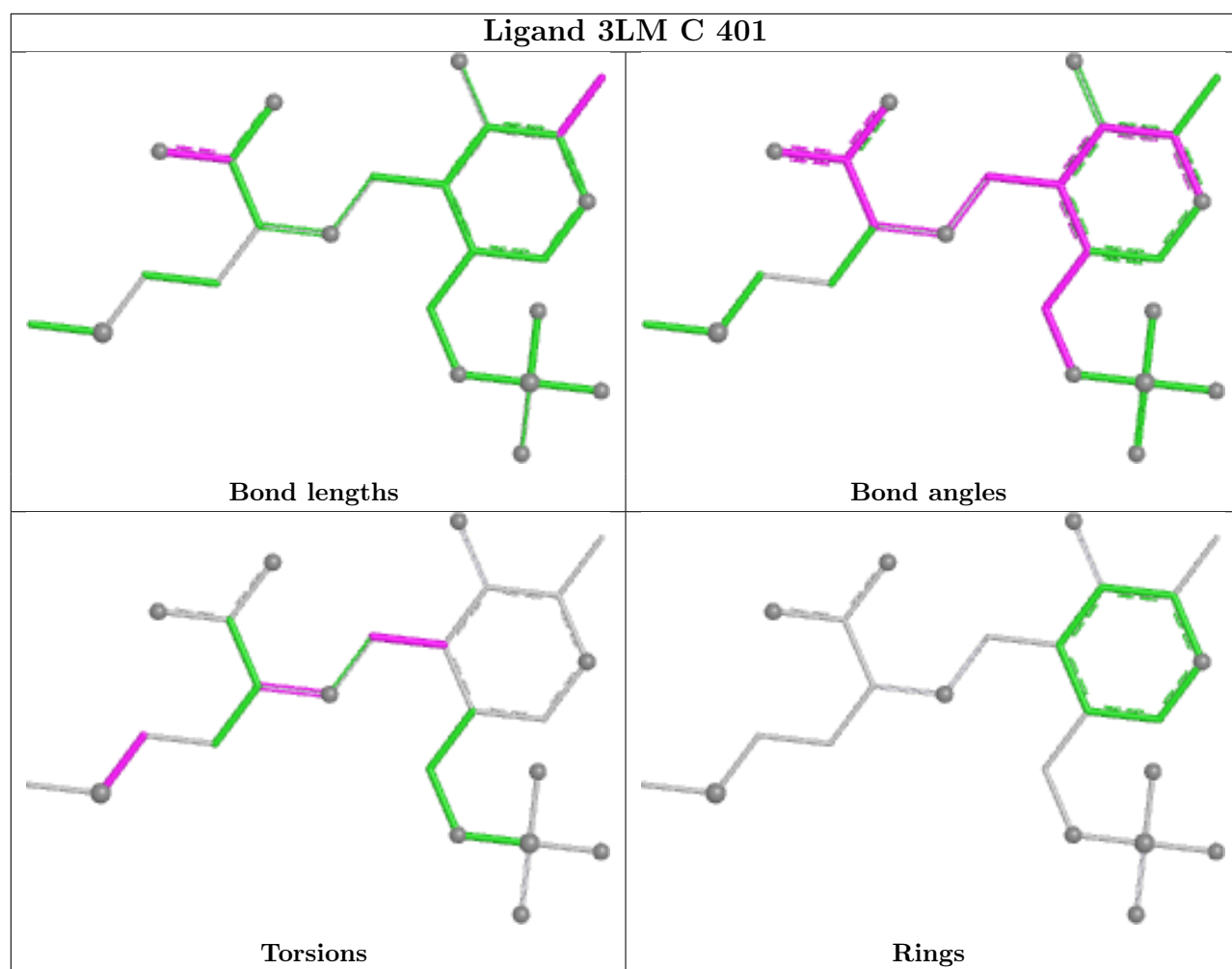
There are no ring outliers.

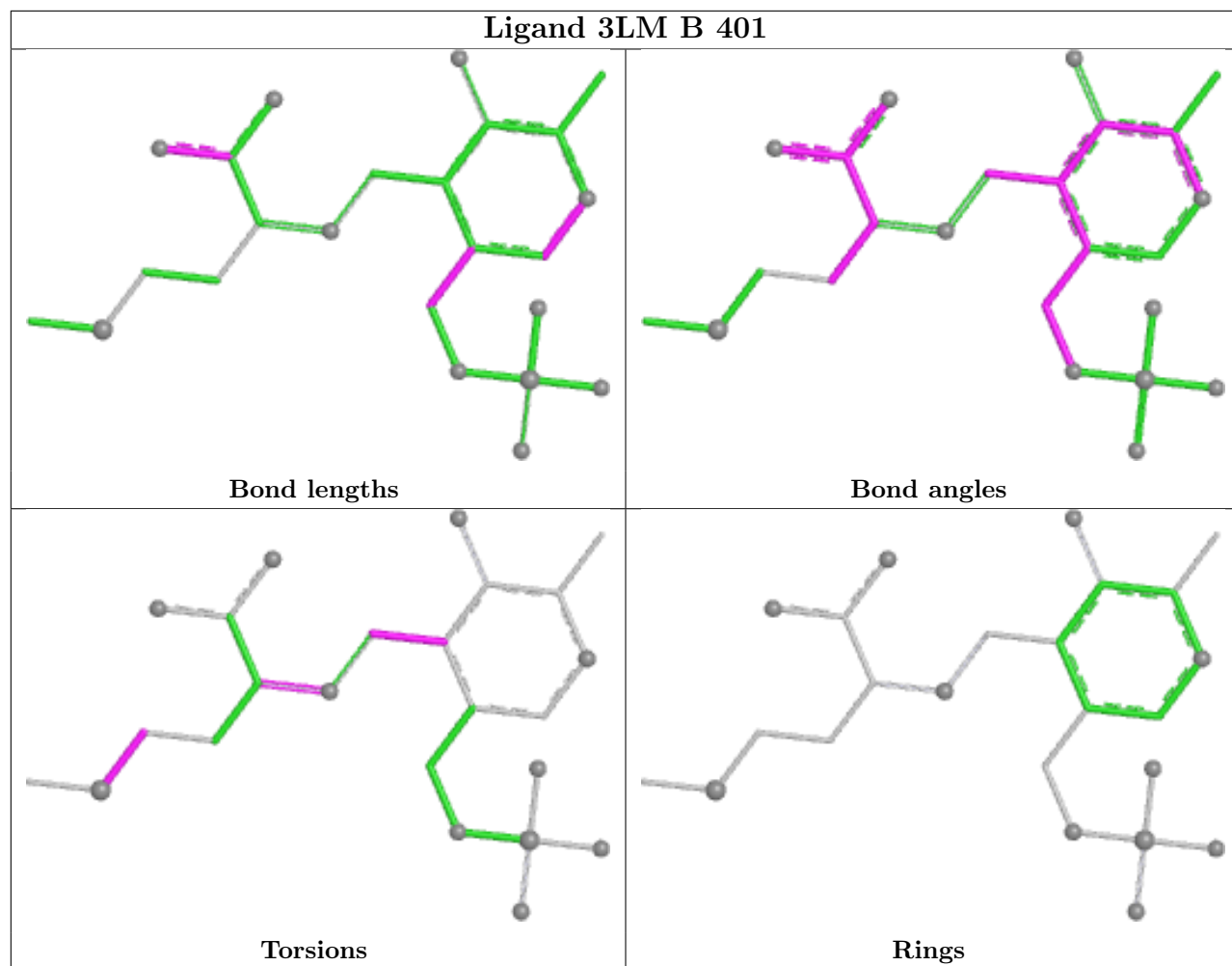
2 monomers are involved in 3 short contacts:

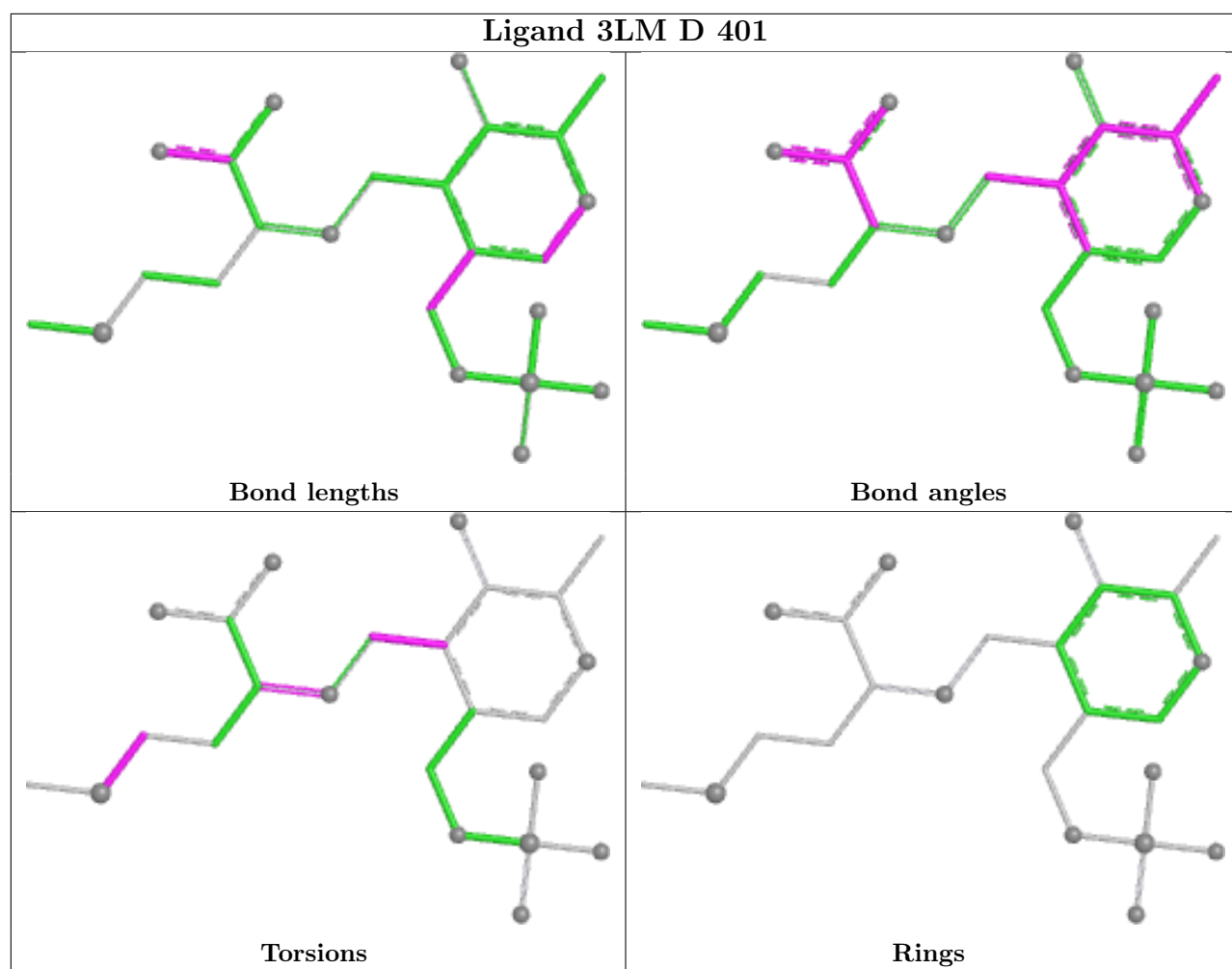
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	3LM	2	0
2	C	401	3LM	1	0

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.









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, 95th 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	392/398 (98%)	0.50	51 (13%) 7 6	12, 27, 71, 91	0
1	B	392/398 (98%)	-0.02	31 (7%) 18 16	7, 19, 56, 94	1 (0%)
1	C	392/398 (98%)	0.15	43 (10%) 10 9	10, 21, 64, 92	1 (0%)
1	D	396/398 (99%)	0.12	42 (10%) 11 9	9, 18, 57, 115	2 (0%)
All	All	1572/1592 (98%)	0.19	167 (10%) 11 9	7, 21, 64, 115	4 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	55	ALA	6.4
1	D	59	TYR	5.9
1	C	355	THR	5.7
1	C	368	GLY	5.7
1	D	62	ILE	5.6
1	D	56	GLY	5.6
1	D	50	PHE	5.6
1	A	62	ILE	5.5
1	A	59	TYR	5.4
1	B	62	ILE	5.3
1	C	367	TYR	5.2
1	D	58	PHE	5.2
1	C	353	SER	5.1
1	C	361	PRO	5.0
1	C	356	HIS	4.9
1	A	288	LEU	4.8
1	C	59	TYR	4.8
1	A	361	PRO	4.8
1	D	57	HIS	4.7
1	D	322	ILE	4.7
1	A	161	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	372	GLY	4.6
1	C	7	LEU	4.5
1	C	58	PHE	4.5
1	C	162	PRO	4.5
1	A	365	ALA	4.4
1	C	354	MET	4.4
1	A	350	HIS	4.4
1	D	51	ALA	4.4
1	D	45	TYR	4.3
1	A	352	ALA	4.3
1	C	55	ALA	4.3
1	A	366	HIS	4.3
1	A	360	THR	4.2
1	A	55	ALA	4.2
1	B	57	HIS	4.2
1	D	60	SER	4.1
1	D	48	ALA	4.1
1	C	352	ALA	4.0
1	D	54	GLN	4.0
1	C	57	HIS	4.0
1	A	354	MET	4.0
1	C	351	PRO	4.0
1	C	360	THR	4.0
1	A	60	SER	4.0
1	A	351	PRO	3.9
1	A	356	HIS	3.9
1	A	322	ILE	3.9
1	B	371	GLU	3.9
1	B	59	TYR	3.9
1	A	358	SER	3.9
1	C	62	ILE	3.9
1	B	60	SER	3.8
1	C	365	ALA	3.8
1	C	369	ILE	3.8
1	A	359	TYR	3.8
1	A	398	ALA	3.8
1	D	47	ALA	3.7
1	D	365	ALA	3.7
1	B	47	ALA	3.6
1	A	357	SER	3.6
1	D	63	SER	3.6
1	D	52	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	355	THR	3.6
1	D	358[A]	SER	3.6
1	A	367	TYR	3.5
1	C	359	TYR	3.5
1	C	43	VAL	3.5
1	C	56	GLY	3.5
1	C	161	ASN	3.5
1	A	57	HIS	3.5
1	A	162	PRO	3.4
1	A	58	PHE	3.4
1	B	58	PHE	3.4
1	C	398	ALA	3.4
1	D	362	GLU	3.4
1	B	50	PHE	3.4
1	C	371	GLU	3.3
1	D	320	GLY	3.3
1	C	54	GLN	3.3
1	A	368	GLY	3.3
1	B	51	ALA	3.3
1	C	22	GLN	3.2
1	B	351	PRO	3.2
1	B	61	ARG	3.2
1	D	361	PRO	3.1
1	C	366	HIS	3.1
1	C	372	GLY	3.1
1	B	352	ALA	3.1
1	B	372	GLY	3.1
1	D	43	VAL	3.0
1	B	54	GLN	3.0
1	A	364	ARG	3.0
1	A	371	GLU	3.0
1	D	46	GLY	2.9
1	D	398	ALA	2.9
1	B	55	ALA	2.8
1	D	49	CYS	2.8
1	D	321	GLY	2.8
1	B	350	HIS	2.8
1	D	354	MET	2.8
1	C	364	ARG	2.8
1	C	358	SER	2.7
1	B	365	ALA	2.7
1	B	43	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLU	2.7
1	B	45	TYR	2.7
1	C	163	ASN	2.7
1	A	319	LYS	2.7
1	A	369	ILE	2.7
1	C	42	THR	2.6
1	D	53	GLU	2.6
1	A	61	ARG	2.6
1	B	162	PRO	2.6
1	B	24	HIS	2.5
1	B	354	MET	2.5
1	D	372	GLY	2.5
1	A	163	ASN	2.5
1	A	353	SER	2.5
1	C	47	ALA	2.5
1	C	61	ARG	2.4
1	C	24	HIS	2.4
1	D	288	LEU	2.4
1	A	281	ALA	2.4
1	D	3	GLY	2.4
1	A	373	LEU	2.4
1	A	324	ALA	2.4
1	D	356	HIS	2.4
1	C	60	SER	2.4
1	B	367	TYR	2.3
1	D	355	THR	2.3
1	A	286	VAL	2.3
1	C	357	SER	2.3
1	D	364	ARG	2.3
1	C	362	GLU	2.3
1	D	360	THR	2.3
1	C	350	HIS	2.3
1	A	175	ILE	2.3
1	A	22	GLN	2.3
1	B	288	LEU	2.3
1	A	24	HIS	2.3
1	C	50	PHE	2.3
1	D	351	PRO	2.3
1	A	63	SER	2.3
1	B	42	THR	2.3
1	A	52	GLY	2.2
1	D	396	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	366	HIS	2.2
1	B	368	GLY	2.2
1	C	370	SER	2.2
1	D	350	HIS	2.2
1	B	23	ASP	2.2
1	B	63	SER	2.2
1	A	323	GLY	2.2
1	B	364	ARG	2.1
1	A	142	ALA	2.1
1	A	320	GLY	2.1
1	B	359	TYR	2.1
1	B	369	ILE	2.1
1	D	61	ARG	2.1
1	D	326	ARG	2.1
1	A	287	GLU	2.1
1	C	52	GLY	2.1
1	D	339	VAL	2.1
1	A	397	SER	2.0
1	A	329	MET	2.0
1	A	363	GLU	2.0

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 oligosaccharides 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, 95th 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	3LM	A	401	24/24	0.92	0.13	19,30,61,72	0
2	3LM	B	401	24/24	0.94	0.10	15,24,47,51	0
2	3LM	C	401	24/24	0.95	0.12	14,21,60,71	0

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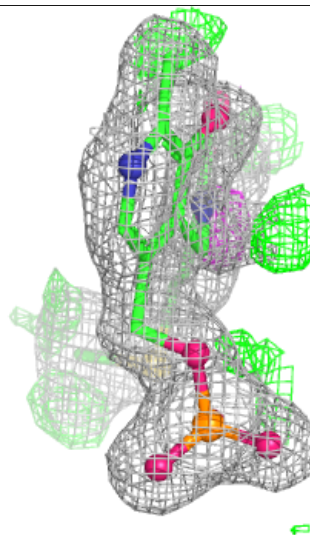
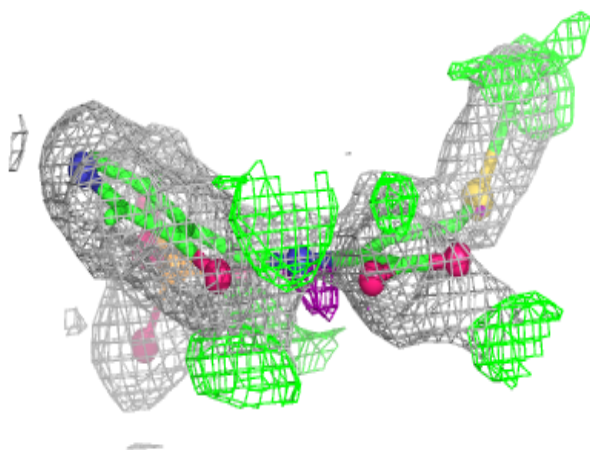
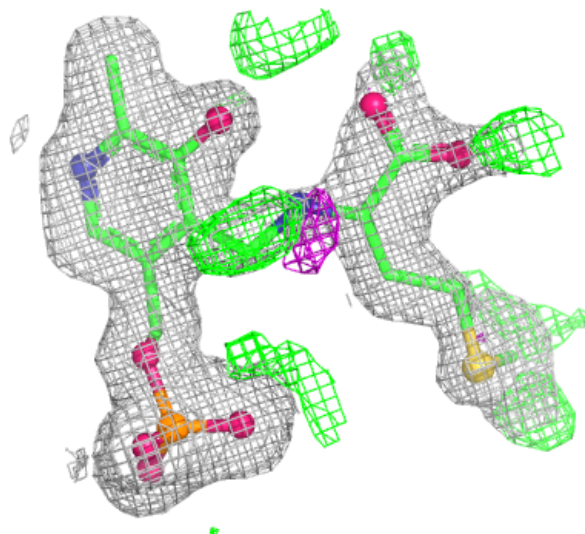
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3LM	D	401	24/24	0.95	0.09	14,20,44,50	0

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.

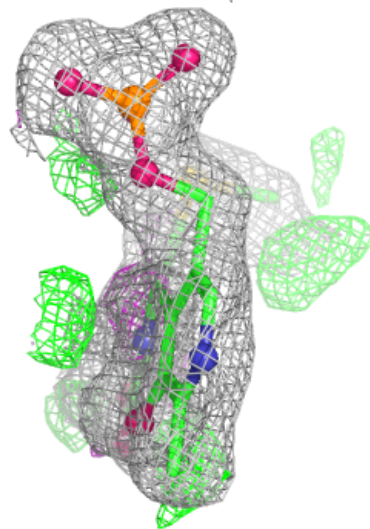
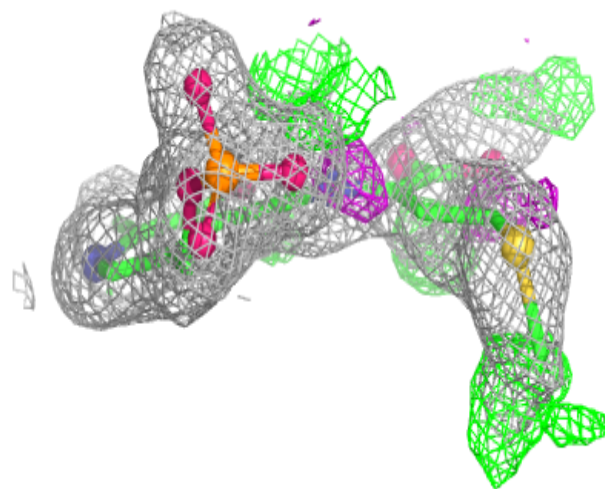
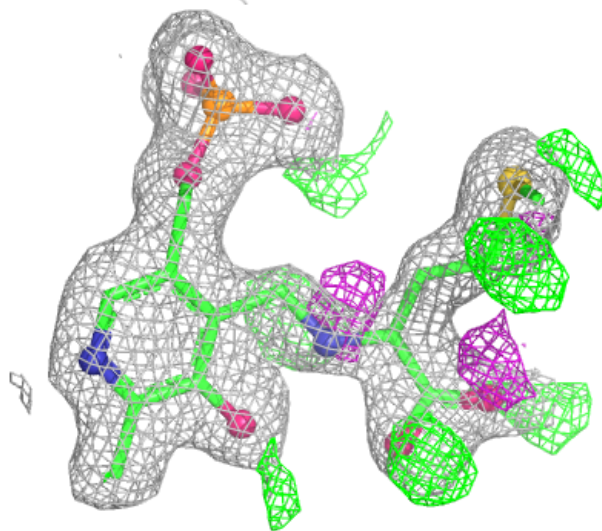
Electron density around 3LM A 401:

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



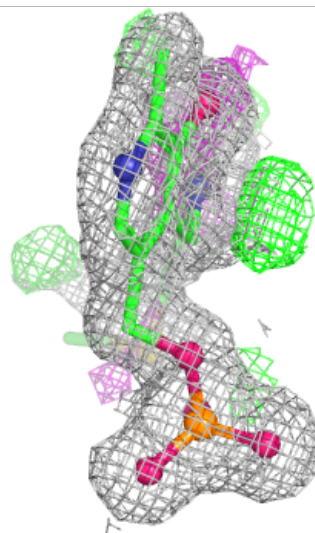
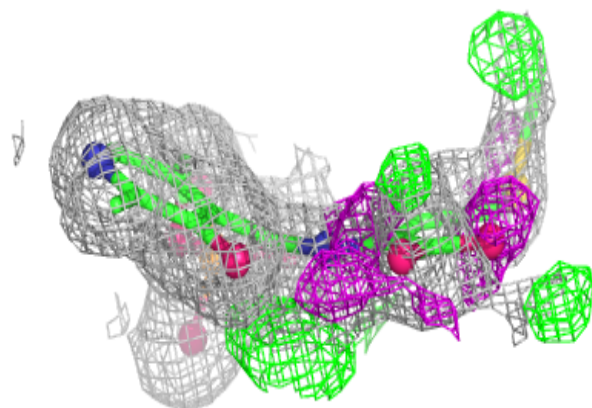
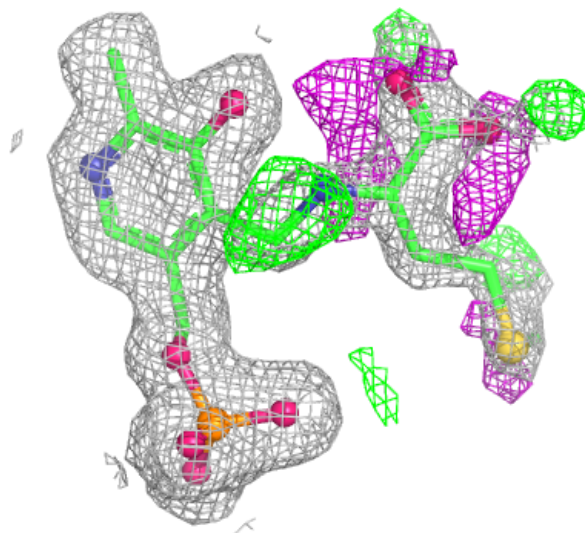
Electron density around 3LM B 401:

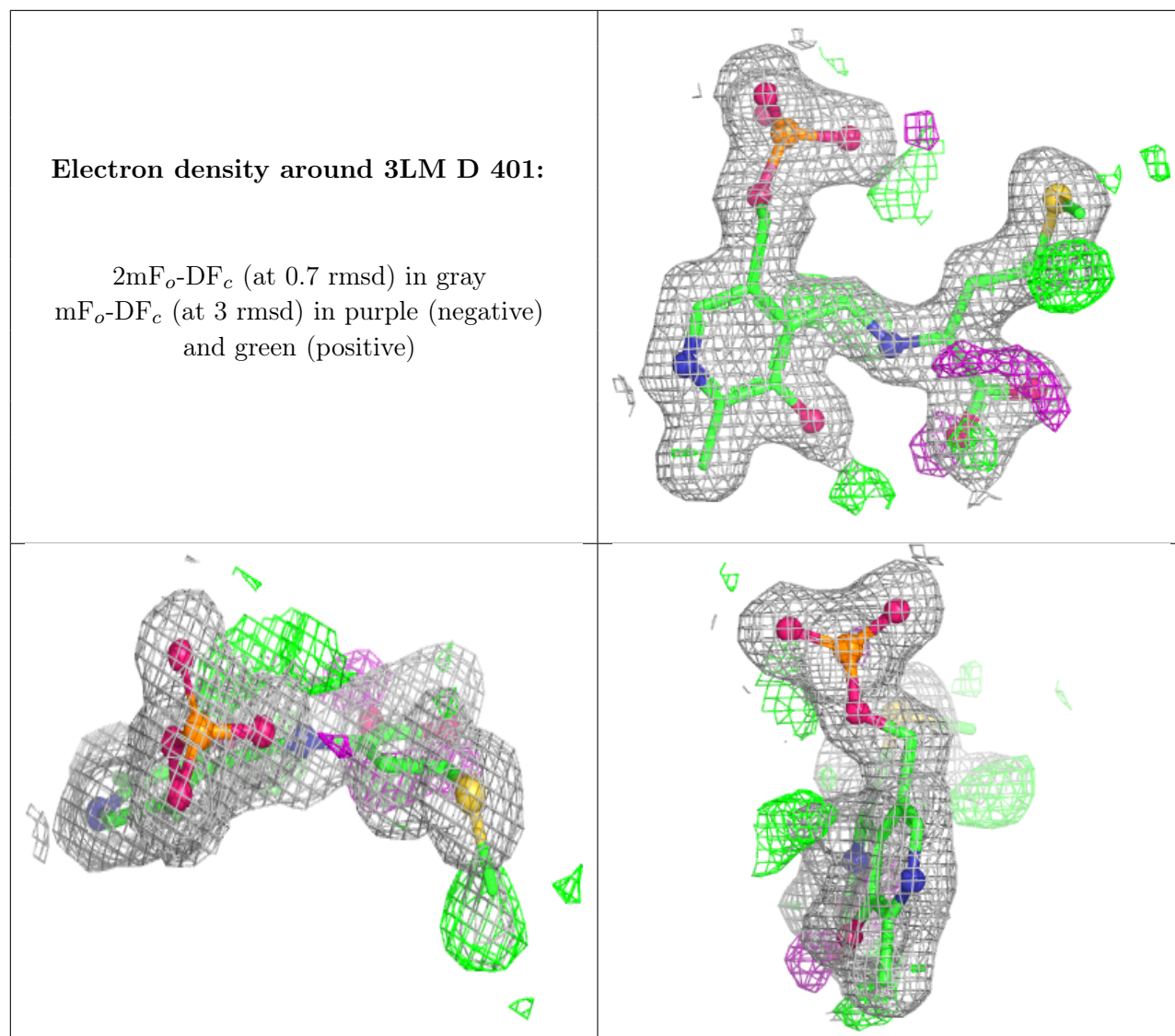
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3LM C 401:

$2mF_o-DF_c$ (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.