



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:00 PM UTC

PDB ID : 8CTA / pdb\_00008cta  
Title : Minimal 2:2 Ternary Complex between BI-224436 bound HIV-1 Integrase Catalytic Core Domain Dimer and Carboxy Terminal Domains  
Authors : Gupta, K.; Van Duyne, G.D.; Eilers, G.; Bushman, F.D.  
Deposited on : 2022-05-13  
Resolution : 2.93 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

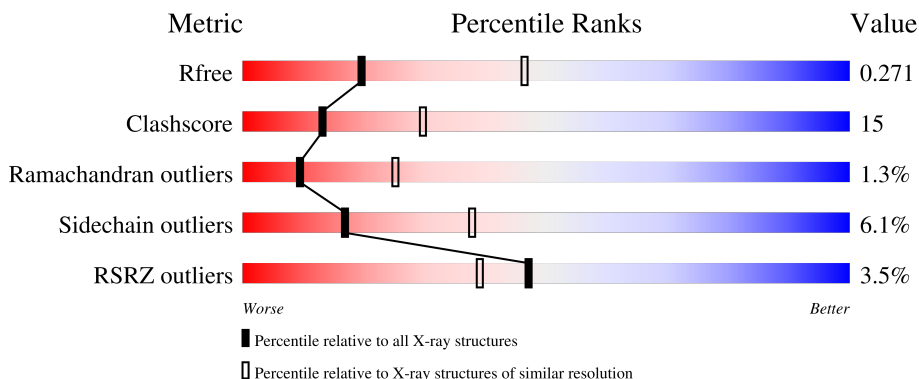
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	161	 6% 60% 19% 5% 16%
1	B	161	 2% 65% 17% 14%
1	E	161	 3% 60% 23% 12%
1	F	161	 66% 17% 14%
1	I	161	 2% 72% 14% 10%

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Mol	Chain	Length	Quality of chain
1	J	161	
1	M	161	
1	N	161	
2	C	53	
2	D	53	
2	G	53	
2	H	53	
2	K	53	
2	L	53	
2	O	53	
2	P	53	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	F	501	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12460 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 Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	136	1056	676	184	192	4	0	0	0
1	B	138	1081	690	186	200	5	0	0	0
1	E	141	1091	698	189	200	4	0	0	0
1	F	138	1084	693	187	200	4	0	0	0
1	I	145	1123	718	194	207	4	0	0	0
1	J	135	1056	675	183	194	4	0	0	0
1	M	151	1163	740	203	215	5	0	0	0
1	N	137	1075	686	186	198	5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	expression tag	UNP Q72498
A	185	LYS	PHE	engineered mutation	UNP Q72498
B	50	GLY	-	expression tag	UNP Q72498
B	185	LYS	PHE	engineered mutation	UNP Q72498
E	50	GLY	-	expression tag	UNP Q72498
E	185	LYS	PHE	engineered mutation	UNP Q72498
F	50	GLY	-	expression tag	UNP Q72498
F	185	LYS	PHE	engineered mutation	UNP Q72498
I	50	GLY	-	expression tag	UNP Q72498
I	185	LYS	PHE	engineered mutation	UNP Q72498
J	50	GLY	-	expression tag	UNP Q72498
J	185	LYS	PHE	engineered mutation	UNP Q72498
M	50	GLY	-	expression tag	UNP Q72498

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Chain	Residue	Modelled	Actual	Comment	Reference
M	185	LYS	PHE	engineered mutation	UNP Q72498
N	50	GLY	-	expression tag	UNP Q72498
N	185	LYS	PHE	engineered mutation	UNP Q72498

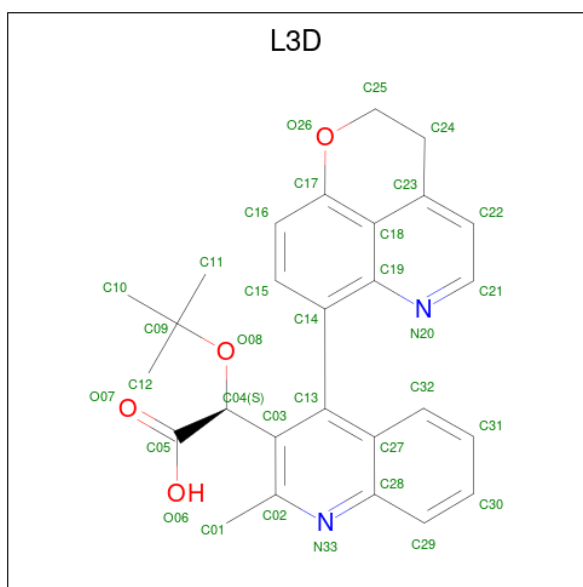
- Molecule 2 is a protein called Integrase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	46	Total	C	N	O	0	0	0
			389	253	73	63			
2	D	50	Total	C	N	O	0	0	0
			420	270	79	71			
2	G	49	Total	C	N	O	0	0	0
			410	265	76	69			
2	H	50	Total	C	N	O	0	0	0
			420	270	79	71			
2	K	46	Total	C	N	O	0	0	0
			385	252	70	63			
2	L	51	Total	C	N	O	0	0	0
			429	275	81	73			
2	O	48	Total	C	N	O	0	0	0
			404	262	75	67			
2	P	52	Total	C	N	O	0	0	0
			437	281	82	74			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	219	GLY	-	expression tag	UNP Q72498
D	219	GLY	-	expression tag	UNP Q72498
G	219	GLY	-	expression tag	UNP Q72498
H	219	GLY	-	expression tag	UNP Q72498
K	219	GLY	-	expression tag	UNP Q72498
L	219	GLY	-	expression tag	UNP Q72498
O	219	GLY	-	expression tag	UNP Q72498
P	219	GLY	-	expression tag	UNP Q72498

- Molecule 3 is (2S)-tert-butoxy[4-(2,3-dihydropyrano[4,3,2-de]quinolin-7-yl)-2-methylquinolin-3-yl]acetic acid (CCD ID: L3D) (formula: C<sub>27</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	27	2	4	0	0
3	B	1	33	27	2	4	0	0
3	E	1	33	27	2	4	0	0
3	F	1	33	27	2	4	0	0
3	I	1	33	27	2	4	0	0
3	J	1	33	27	2	4	0	0
3	M	1	33	27	2	4	0	0
3	N	1	33	27	2	4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	M	1	Total C O 4 2 2	0	0
4	N	1	Total C O 4 2 2	0	0
4	N	1	Total C O 4 2 2	0	0
4	O	1	Total C O 4 2 2	0	0
4	P	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	2	Total O 2 2	0	0
5	D	3	Total O 3 3	0	0
5	E	5	Total O 5 5	0	0
5	F	5	Total O 5 5	0	0
5	H	5	Total O 5 5	0	0

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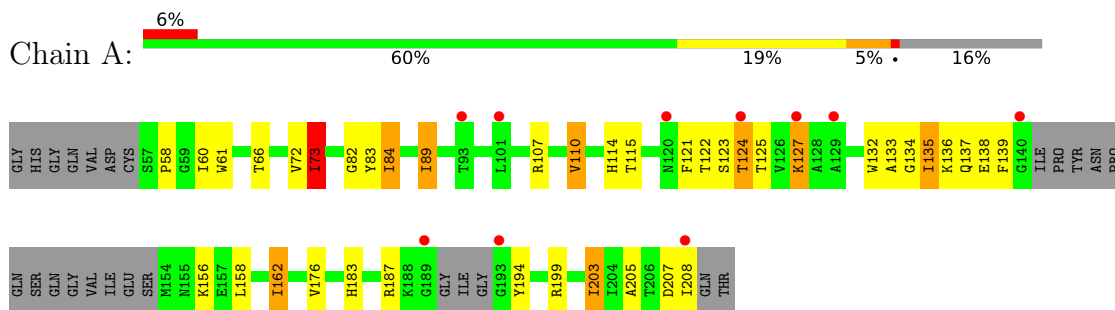
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	I	9	Total O 9 9	0	0
5	J	8	Total O 8 8	0	0
5	L	7	Total O 7 7	0	0
5	M	6	Total O 6 6	0	0
5	N	11	Total O 11 11	0	0
5	O	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0

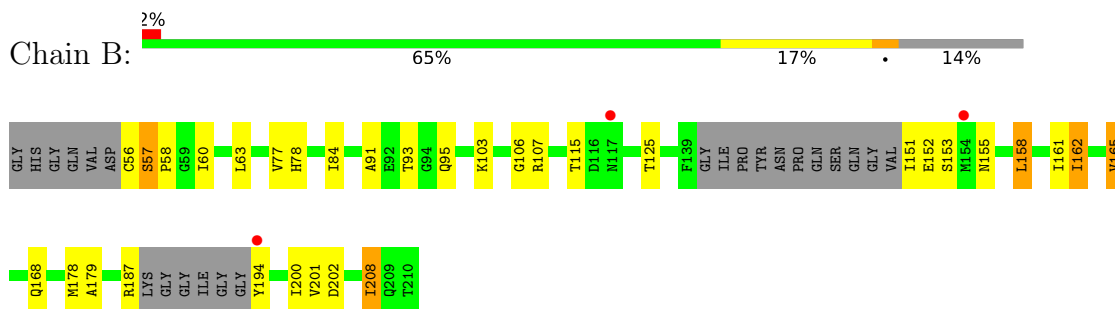
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

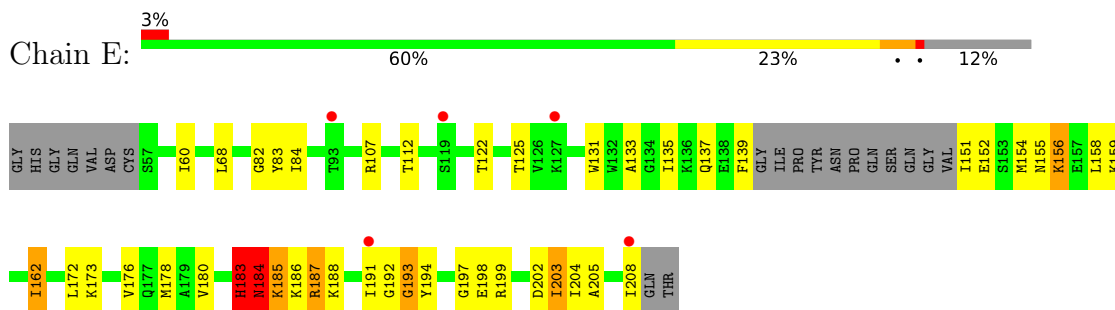
- Molecule 1: Integrase



- Molecule 1: Integrase

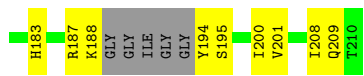
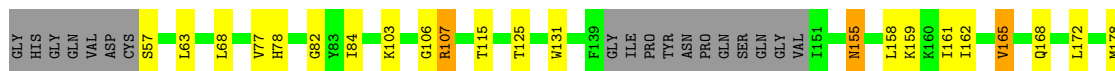


- Molecule 1: Integrase

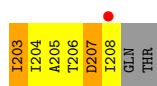
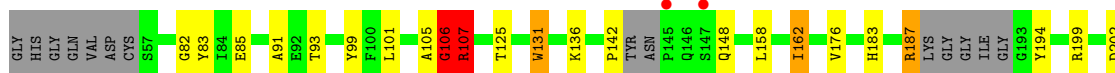


- Molecule 1: Integrase

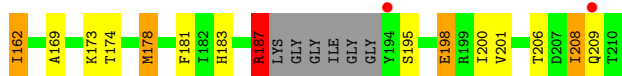
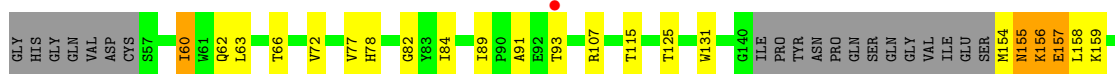




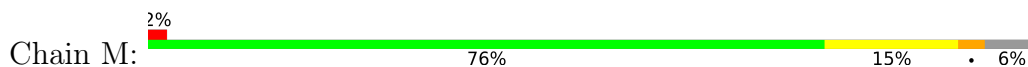
• Molecule 1: Integrase



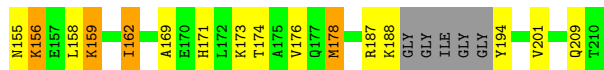
• Molecule 1: Integrase



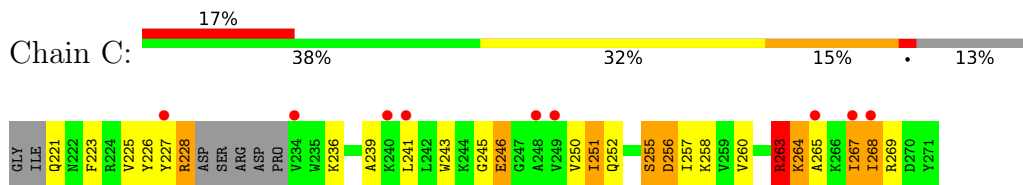
• Molecule 1: Integrase



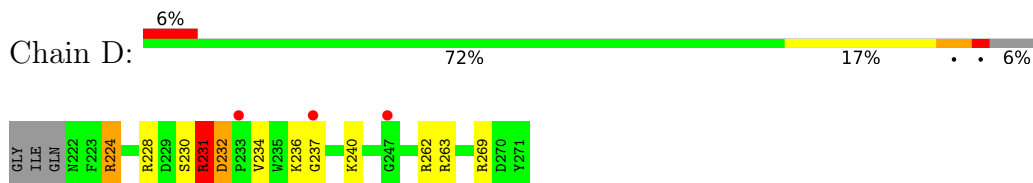
• Molecule 1: Integrase



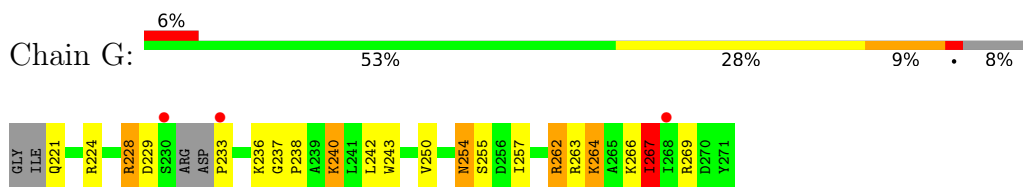
- Molecule 2: Integrase



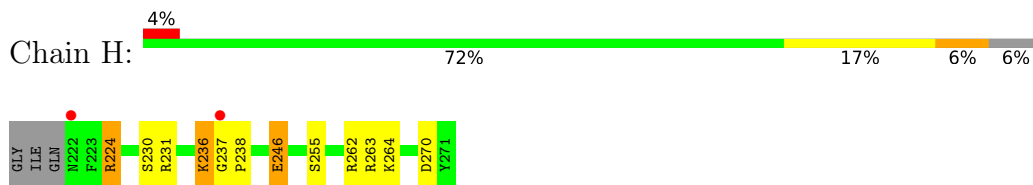
- Molecule 2: Integrase



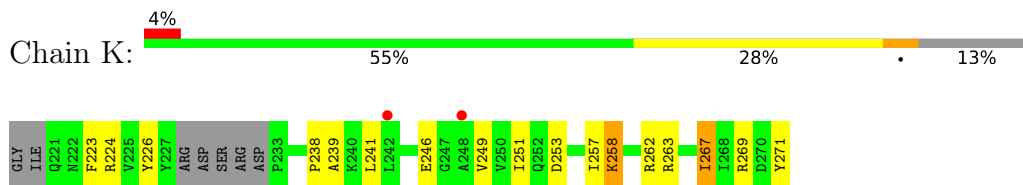
- Molecule 2: Integrase



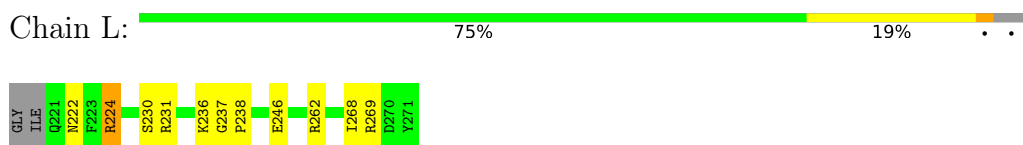
- Molecule 2: Integrase



- Molecule 2: Integrase



- Molecule 2: Integrase

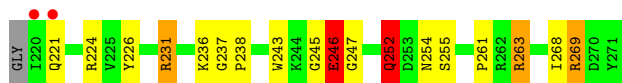


- Molecule 2: Integrase





● Molecule 2: Integrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.51Å 116.51Å 112.80Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	19.85 – 2.93 19.85 – 2.93	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.85-2.93) 90.3 (19.85-2.93)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.93Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.216 , 0.261 0.223 , 0.271	Depositor DCC
$R_{free}$ test set	4441 reflections (9.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5211e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: L3D, EDO

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	0.85	4/1076 (0.4%)	1.05	2/1453 (0.1%)
1	B	0.73	1/1101 (0.1%)	0.96	0/1488
1	E	0.73	2/1112 (0.2%)	1.06	5/1503 (0.3%)
1	F	0.67	0/1104	0.97	1/1491 (0.1%)
1	I	0.68	0/1145	1.01	3/1549 (0.2%)
1	J	0.77	2/1076 (0.2%)	1.02	0/1454
1	M	0.69	0/1185	1.01	1/1602 (0.1%)
1	N	0.72	1/1095 (0.1%)	0.99	2/1479 (0.1%)
2	C	0.69	0/397	1.13	3/531 (0.6%)
2	D	0.62	0/430	1.02	1/578 (0.2%)
2	G	0.74	1/419 (0.2%)	1.02	2/561 (0.4%)
2	H	0.61	0/430	1.01	1/578 (0.2%)
2	K	0.65	0/394	0.88	0/528
2	L	0.65	0/439	0.98	1/590 (0.2%)
2	O	0.62	0/413	0.87	0/553
2	P	0.63	0/447	1.01	1/601 (0.2%)
All	All	0.71	11/12263 (0.1%)	1.00	23/16539 (0.1%)

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	A	0	2
1	E	0	1
1	F	0	1
1	I	0	1
1	J	0	2
1	M	0	2
2	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4
2	G	0	3
2	H	0	4
2	K	0	3
2	L	0	3
2	O	0	1
2	P	0	4
All	All	0	33

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	178	MET	SD-CE	-11.47	1.50	1.79
1	N	178	MET	SD-CE	-10.88	1.52	1.79
1	B	162	ILE	CG1-CD1	-10.57	1.10	1.51
1	A	73	ILE	CG1-CD1	-8.56	1.18	1.51
1	A	60	ILE	CG1-CD1	-8.47	1.18	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	ASN	N-CA-C	-9.54	90.48	110.80
2	P	252	GLN	N-CA-C	7.96	124.17	113.97
1	A	133	ALA	N-CA-C	-7.96	98.00	109.31
1	I	107	ARG	N-CA-C	7.68	127.16	110.80
2	C	263	ARG	CA-C-N	-7.14	113.34	123.20

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	187	ARG	Sidechain
2	C	228	ARG	Sidechain
2	C	263	ARG	Sidechain
2	D	224	ARG	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1056	0	1067	38	0
1	B	1081	0	1087	32	0
1	E	1091	0	1104	38	0
1	F	1084	0	1095	35	0
1	I	1123	0	1132	26	0
1	J	1056	0	1063	45	0
1	M	1163	0	1169	31	0
1	N	1075	0	1082	38	0
2	C	389	0	406	34	0
2	D	420	0	432	6	0
2	G	410	0	423	16	0
2	H	420	0	432	10	0
2	K	385	0	401	20	0
2	L	429	0	440	7	0
2	O	404	0	418	19	0
2	P	437	0	451	15	0
3	A	33	0	0	0	0
3	B	33	0	0	1	0
3	E	33	0	0	0	0
3	F	33	0	0	0	0
3	I	33	0	0	0	0
3	J	33	0	0	4	0
3	M	33	0	0	0	0
3	N	33	0	0	4	0
4	A	4	0	6	3	0
4	B	8	0	12	0	0
4	D	8	0	12	2	0
4	E	12	0	18	3	0
4	F	20	0	30	7	0
4	G	4	0	6	0	0
4	H	4	0	6	2	0
4	I	4	0	6	0	0
4	J	4	0	6	0	0
4	K	8	0	12	2	0
4	L	12	0	18	1	0
4	M	4	0	6	0	0
4	N	8	0	12	2	0
4	O	4	0	6	1	0
4	P	4	0	6	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	3	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
5	H	5	0	0	1	0
5	I	9	0	0	0	0
5	J	8	0	0	0	0
5	L	7	0	0	0	0
5	M	6	0	0	1	0
5	N	11	0	0	4	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	12460	0	12364	369	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 15.

The worst 5 of 369 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:G:267:ILE:CD1	2:G:267:ILE:CG1	1.77	1.59
2:C:241:LEU:HA	2:C:251:ILE:HD11	1.29	1.11
1:J:155:ASN:HA	1:J:157:GLU:CD	1.81	1.03
1:M:107:ARG:HD3	1:N:107:ARG:HD3	1.40	1.03
1:A:107:ARG:HD3	1:B:107:ARG:HD3	1.43	0.99

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	130/161 (81%)	126 (97%)	3 (2%)	1 (1%)	<b>16</b> <b>36</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	132/161 (82%)	128 (97%)	4 (3%)	0	100	100
1	E	137/161 (85%)	127 (93%)	6 (4%)	4 (3%)	3	9
1	F	132/161 (82%)	127 (96%)	5 (4%)	0	100	100
1	I	139/161 (86%)	134 (96%)	3 (2%)	2 (1%)	9	24
1	J	129/161 (80%)	123 (95%)	4 (3%)	2 (2%)	7	21
1	M	145/161 (90%)	142 (98%)	2 (1%)	1 (1%)	18	40
1	N	131/161 (81%)	127 (97%)	4 (3%)	0	100	100
2	C	42/53 (79%)	32 (76%)	7 (17%)	3 (7%)	1	1
2	D	48/53 (91%)	42 (88%)	3 (6%)	3 (6%)	1	2
2	G	45/53 (85%)	42 (93%)	3 (7%)	0	100	100
2	H	48/53 (91%)	44 (92%)	4 (8%)	0	100	100
2	K	42/53 (79%)	40 (95%)	1 (2%)	1 (2%)	4	13
2	L	49/53 (92%)	45 (92%)	4 (8%)	0	100	100
2	O	44/53 (83%)	38 (86%)	5 (11%)	1 (2%)	5	14
2	P	50/53 (94%)	45 (90%)	4 (8%)	1 (2%)	6	17
All	All	1443/1712 (84%)	1362 (94%)	62 (4%)	19 (1%)	9	25

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
2	D	232	ASP
1	E	185	LYS
1	E	188	LYS
1	I	107	ARG

### 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	110/130 (85%)	100 (91%)	10 (9%)	9	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	115/130 (88%)	109 (95%)	6 (5%)	21	44
1	E	114/130 (88%)	105 (92%)	9 (8%)	11	27
1	F	115/130 (88%)	110 (96%)	5 (4%)	26	51
1	I	119/130 (92%)	113 (95%)	6 (5%)	22	46
1	J	111/130 (85%)	103 (93%)	8 (7%)	13	31
1	M	123/130 (95%)	118 (96%)	5 (4%)	27	52
1	N	114/130 (88%)	108 (95%)	6 (5%)	20	43
2	C	40/46 (87%)	36 (90%)	4 (10%)	7	19
2	D	44/46 (96%)	43 (98%)	1 (2%)	44	68
2	G	43/46 (94%)	37 (86%)	6 (14%)	3	9
2	H	44/46 (96%)	43 (98%)	1 (2%)	44	68
2	K	40/46 (87%)	37 (92%)	3 (8%)	12	29
2	L	45/46 (98%)	43 (96%)	2 (4%)	25	50
2	O	42/46 (91%)	40 (95%)	2 (5%)	23	47
2	P	46/46 (100%)	43 (94%)	3 (6%)	15	35
All	All	1265/1408 (90%)	1188 (94%)	77 (6%)	17	38

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	258	LYS
1	N	162	ILE
2	L	230	SER
1	M	162	ILE
2	P	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	148	GLN
1	M	155	ASN
2	P	252	GLN
1	E	183	HIS
1	E	114	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

35 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	EDO	I	302	-	3,3,3	0.13	0	2,2,2	0.17	0
4	EDO	L	502	-	3,3,3	0.13	0	2,2,2	0.12	0
3	L3D	F	502	-	34,37,37	0.79	1 (2%)	44,56,56	1.01	3 (6%)
4	EDO	B	303	-	3,3,3	0.13	0	2,2,2	0.10	0
4	EDO	K	501	-	3,3,3	0.10	0	2,2,2	0.27	0
4	EDO	F	501	-	3,3,3	0.33	0	2,2,2	0.76	0
4	EDO	H	301	-	3,3,3	0.21	0	2,2,2	0.41	0
3	L3D	M	301	-	34,37,37	0.82	1 (2%)	44,56,56	1.07	3 (6%)
4	EDO	D	301	-	3,3,3	0.12	0	2,2,2	0.44	0
4	EDO	F	506	-	3,3,3	0.22	0	2,2,2	0.34	0
4	EDO	M	302	-	3,3,3	0.17	0	2,2,2	0.27	0
3	L3D	I	301	-	34,37,37	0.94	3 (8%)	44,56,56	1.07	2 (4%)
4	EDO	F	504	-	3,3,3	0.23	0	2,2,2	0.64	0
4	EDO	J	302	-	3,3,3	0.14	0	2,2,2	0.20	0
3	L3D	E	301	-	34,37,37	0.88	3 (8%)	44,56,56	1.02	3 (6%)
4	EDO	L	503	-	3,3,3	0.18	0	2,2,2	0.25	0
4	EDO	F	503	-	3,3,3	0.23	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	O	301	-	3,3,3	0.10	0	2,2,2	0.11	0
4	EDO	D	302	-	3,3,3	0.16	0	2,2,2	0.16	0
4	EDO	K	502	-	3,3,3	0.10	0	2,2,2	0.11	0
3	L3D	A	301	-	34,37,37	0.89	2 (5%)	44,56,56	1.15	3 (6%)
4	EDO	E	302	-	3,3,3	0.04	0	2,2,2	0.25	0
4	EDO	N	303	-	3,3,3	0.33	0	2,2,2	0.50	0
4	EDO	G	301	-	3,3,3	0.10	0	2,2,2	0.22	0
4	EDO	L	501	-	3,3,3	0.12	0	2,2,2	0.16	0
4	EDO	N	302	-	3,3,3	0.31	0	2,2,2	0.38	0
4	EDO	E	303	-	3,3,3	0.11	0	2,2,2	0.19	0
3	L3D	N	301	-	34,37,37	1.05	3 (8%)	44,56,56	0.98	2 (4%)
4	EDO	E	304	-	3,3,3	0.16	0	2,2,2	0.52	0
4	EDO	A	302	-	3,3,3	0.39	0	2,2,2	0.59	0
3	L3D	J	301	-	34,37,37	1.15	3 (8%)	44,56,56	1.01	3 (6%)
3	L3D	B	301	-	34,37,37	0.79	1 (2%)	44,56,56	1.08	4 (9%)
4	EDO	P	301	-	3,3,3	0.12	0	2,2,2	0.09	0
4	EDO	F	505	-	3,3,3	0.11	0	2,2,2	0.12	0
4	EDO	B	302	-	3,3,3	0.29	0	2,2,2	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	I	302	-	-	0/1/1/1	-
4	EDO	L	502	-	-	1/1/1/1	-
3	L3D	F	502	-	-	2/17/23/23	0/4/5/5
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	K	501	-	-	1/1/1/1	-
4	EDO	F	501	-	-	1/1/1/1	-
4	EDO	H	301	-	-	0/1/1/1	-
3	L3D	M	301	-	-	4/17/23/23	0/4/5/5
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	F	506	-	-	1/1/1/1	-
4	EDO	M	302	-	-	0/1/1/1	-
3	L3D	I	301	-	-	4/17/23/23	0/4/5/5
4	EDO	F	504	-	-	1/1/1/1	-
4	EDO	J	302	-	-	1/1/1/1	-
3	L3D	E	301	-	-	4/17/23/23	0/4/5/5
4	EDO	L	503	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	503	-	-	1/1/1/1	-
4	EDO	O	301	-	-	0/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	K	502	-	-	1/1/1/1	-
3	L3D	A	301	-	-	4/17/23/23	0/4/5/5
4	EDO	E	302	-	-	0/1/1/1	-
4	EDO	N	303	-	-	0/1/1/1	-
4	EDO	G	301	-	-	1/1/1/1	-
4	EDO	L	501	-	-	1/1/1/1	-
4	EDO	N	302	-	-	1/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
3	L3D	N	301	-	-	4/17/23/23	0/4/5/5
4	EDO	E	304	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
3	L3D	J	301	-	-	3/17/23/23	0/4/5/5
3	L3D	B	301	-	-	5/17/23/23	0/4/5/5
4	EDO	P	301	-	-	1/1/1/1	-
4	EDO	F	505	-	-	0/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	L3D	C14-C19	-4.69	1.35	1.43
3	N	301	L3D	C14-C19	-3.90	1.36	1.43
3	I	301	L3D	C14-C19	-3.13	1.38	1.43
3	E	301	L3D	C14-C19	-2.69	1.38	1.43
3	A	301	L3D	O06-C05	-2.58	1.22	1.30

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	L3D	O26-C17-C18	4.26	122.52	118.54
3	I	301	L3D	O26-C17-C18	3.81	122.10	118.54
3	M	301	L3D	O26-C17-C18	3.77	122.06	118.54
3	E	301	L3D	O26-C17-C18	3.58	121.89	118.54
3	B	301	L3D	O26-C17-C18	3.49	121.81	118.54

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

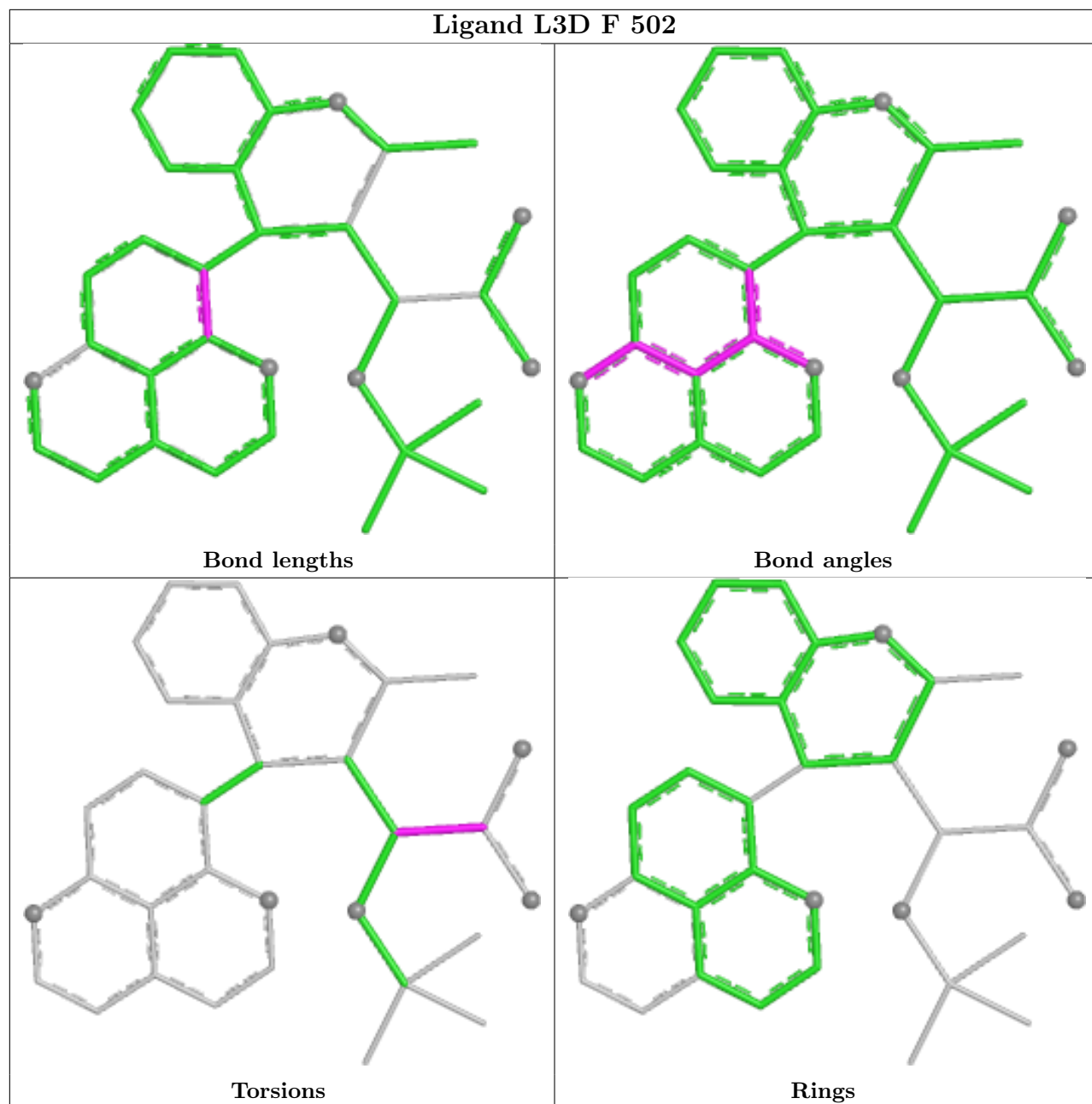
Mol	Chain	Res	Type	Atoms
3	I	301	L3D	C03-C04-O08-C09
3	I	301	L3D	C05-C04-O08-C09
3	J	301	L3D	C03-C04-C05-O06
3	M	301	L3D	C03-C04-C05-O06
3	N	301	L3D	C03-C04-C05-O06

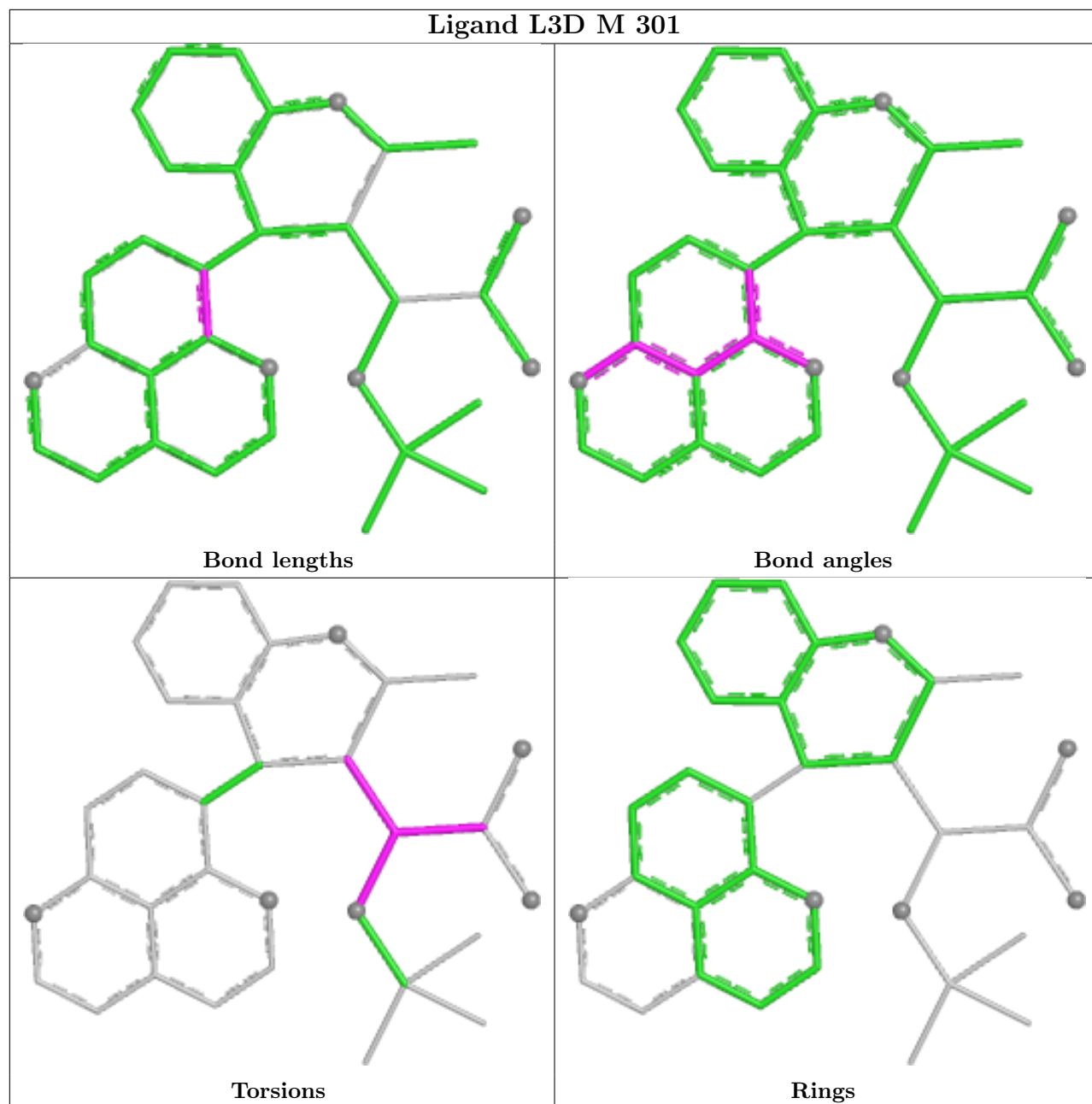
There are no ring outliers.

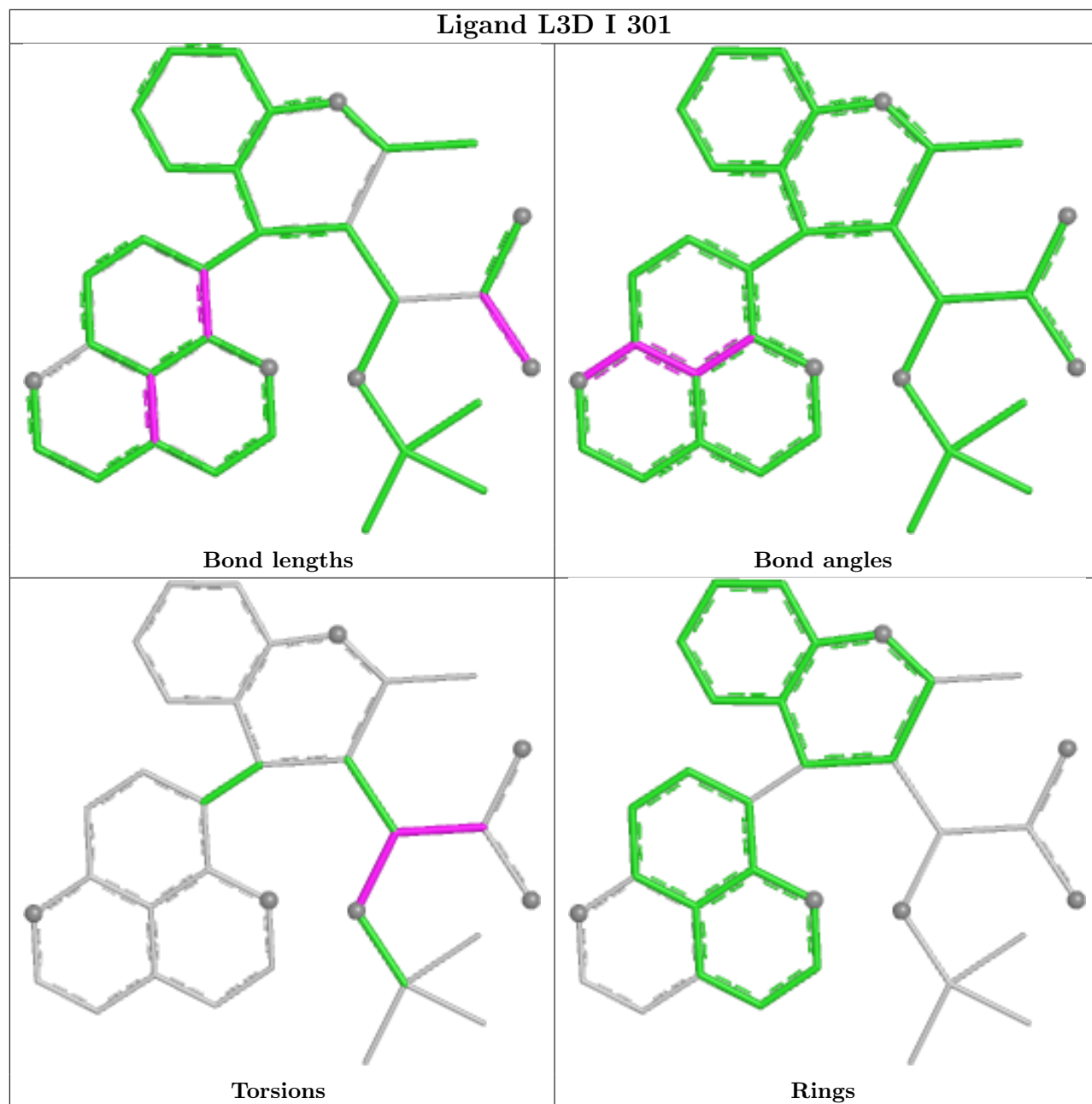
16 monomers are involved in 35 short contacts:

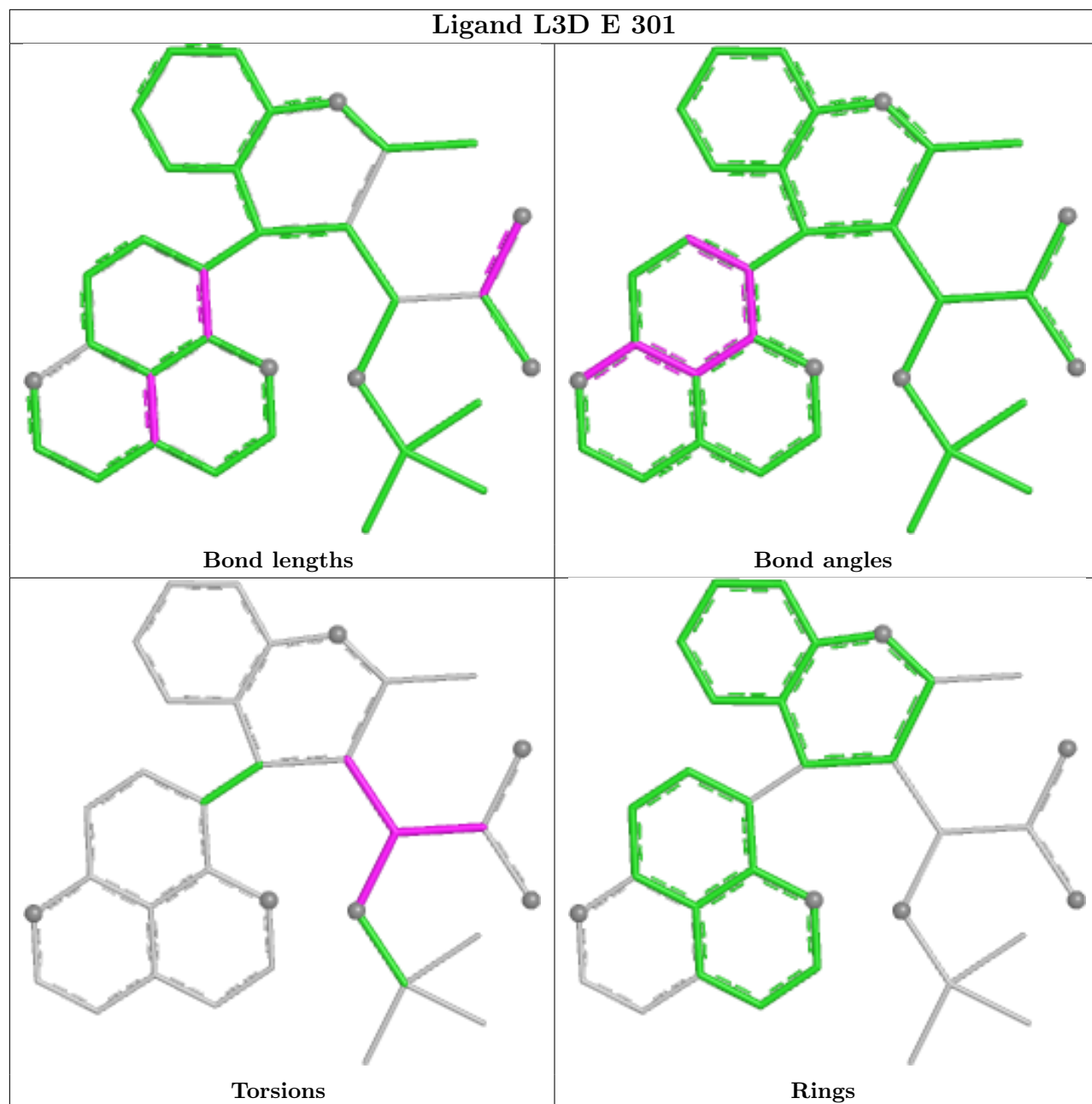
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	501	EDO	2	0
4	F	501	EDO	4	0
4	H	301	EDO	2	0
4	D	301	EDO	2	0
4	F	506	EDO	2	0
4	F	504	EDO	1	0
4	O	301	EDO	1	0
4	E	302	EDO	1	0
4	N	303	EDO	2	0
4	L	501	EDO	1	0
3	N	301	L3D	4	0
4	E	304	EDO	2	0
4	A	302	EDO	3	0
3	J	301	L3D	4	0
3	B	301	L3D	1	0
4	P	301	EDO	3	0

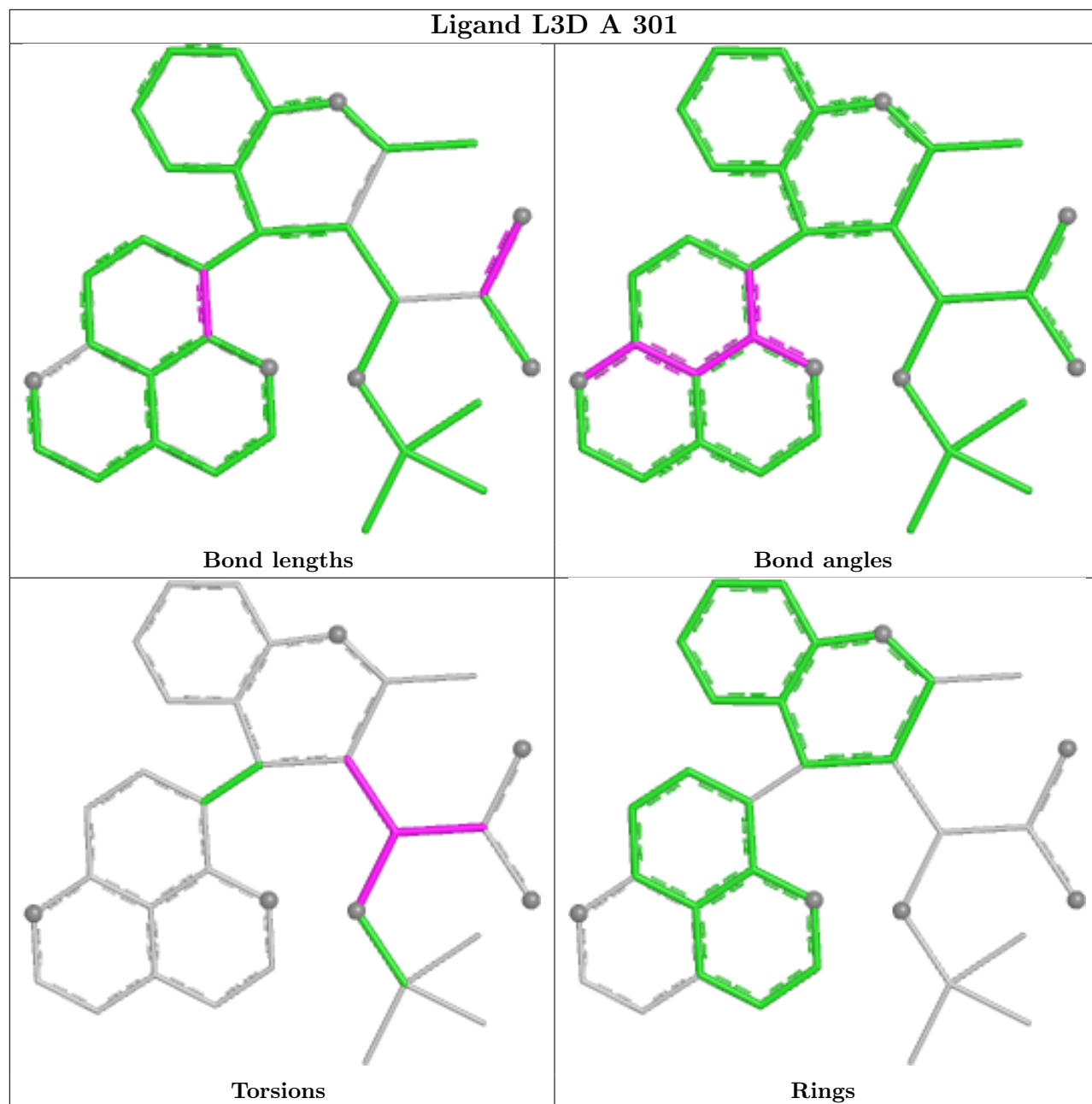
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

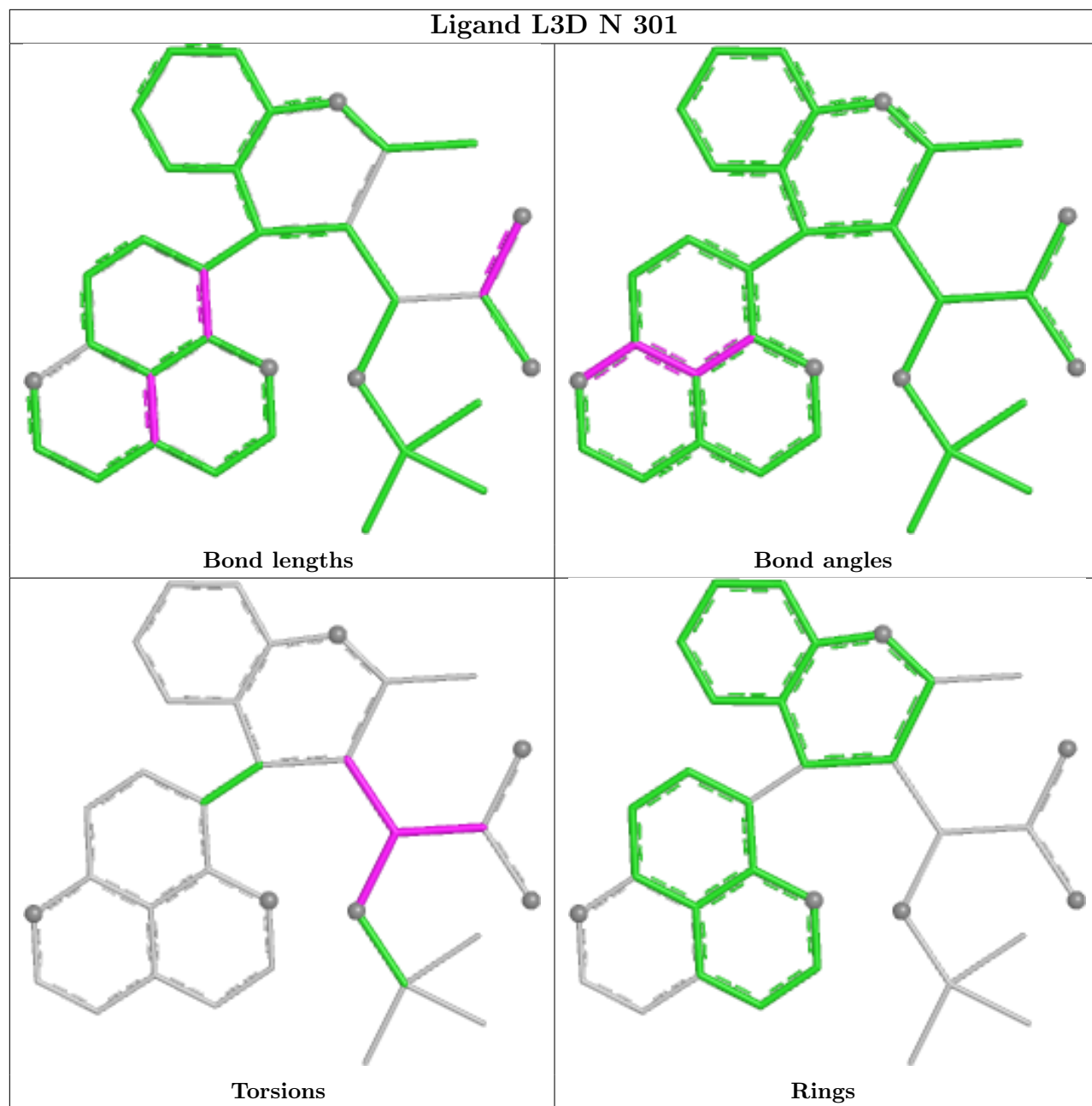


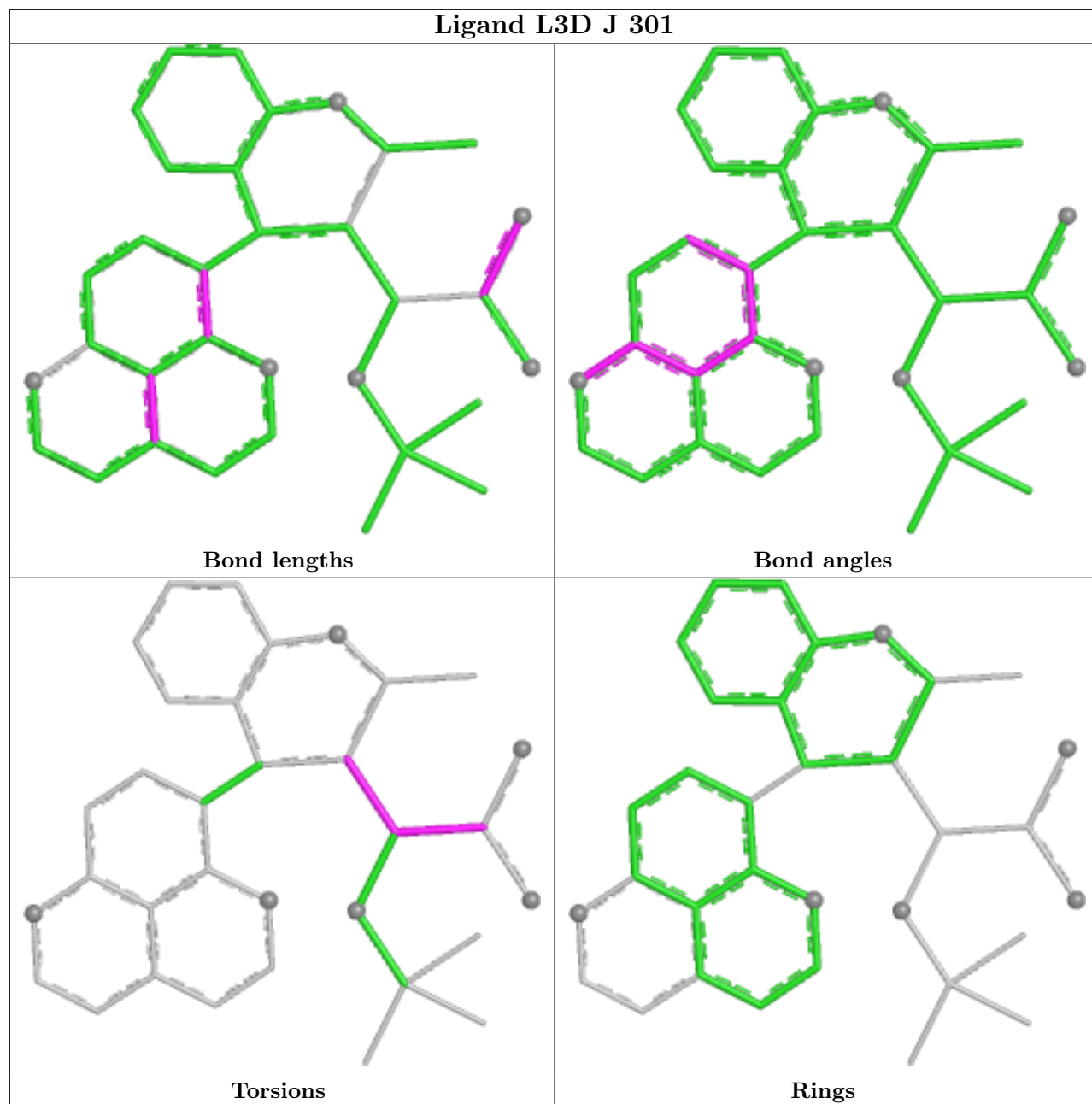


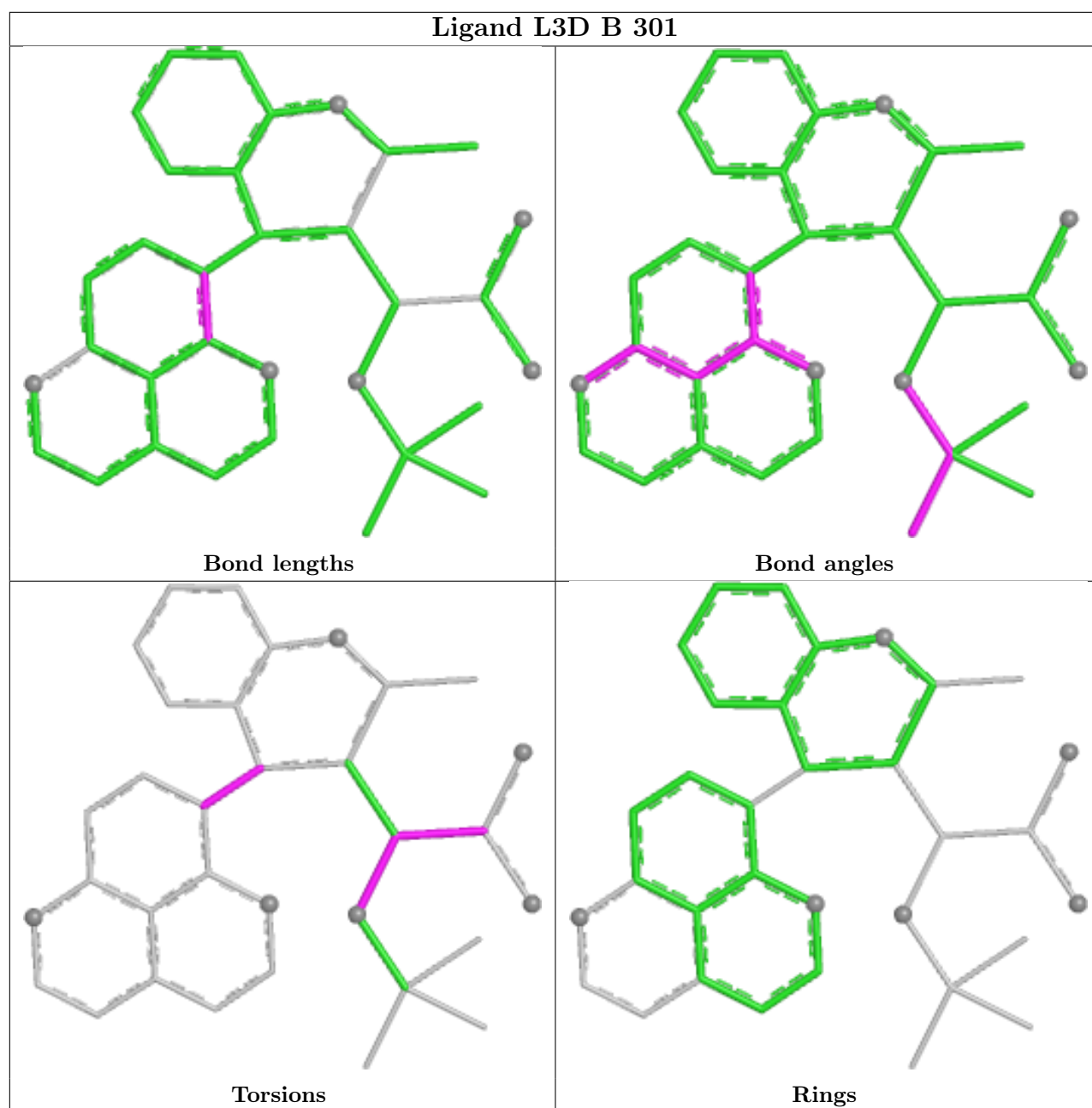












## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	136/161 (84%)	0.63	10 (7%) 20 18	46, 89, 128, 168	0
1	B	138/161 (85%)	0.21	3 (2%) 62 53	39, 77, 121, 134	0
1	E	141/161 (87%)	0.21	5 (3%) 47 39	36, 69, 114, 141	0
1	F	138/161 (85%)	-0.02	0 100 100	31, 63, 105, 138	0
1	I	145/161 (90%)	0.04	3 (2%) 63 54	26, 62, 102, 125	0
1	J	135/161 (83%)	0.11	3 (2%) 62 53	32, 69, 110, 158	0
1	M	151/161 (93%)	0.04	4 (2%) 57 48	25, 58, 104, 127	0
1	N	137/161 (85%)	0.13	3 (2%) 62 53	32, 66, 105, 152	0
2	C	46/53 (86%)	1.03	9 (19%) 3 3	108, 132, 150, 153	0
2	D	50/53 (94%)	0.38	3 (6%) 27 23	37, 63, 117, 153	0
2	G	49/53 (92%)	0.75	3 (6%) 27 22	93, 107, 131, 136	0
2	H	50/53 (94%)	0.33	2 (4%) 42 34	39, 70, 131, 139	0
2	K	46/53 (86%)	0.55	2 (4%) 40 31	90, 103, 126, 141	0
2	L	51/53 (96%)	-0.01	0 100 100	39, 57, 105, 135	0
2	O	48/53 (90%)	0.57	1 (2%) 63 54	70, 96, 117, 131	0
2	P	52/53 (98%)	0.34	2 (3%) 44 36	40, 62, 119, 153	0
All	All	1513/1712 (88%)	0.25	53 (3%) 47 39	25, 71, 127, 168	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	249	VAL	4.3
1	A	129	ALA	4.2
1	E	119	SER	3.9
1	A	208	ILE	3.7
1	N	154	MET	3.6

## 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, 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.

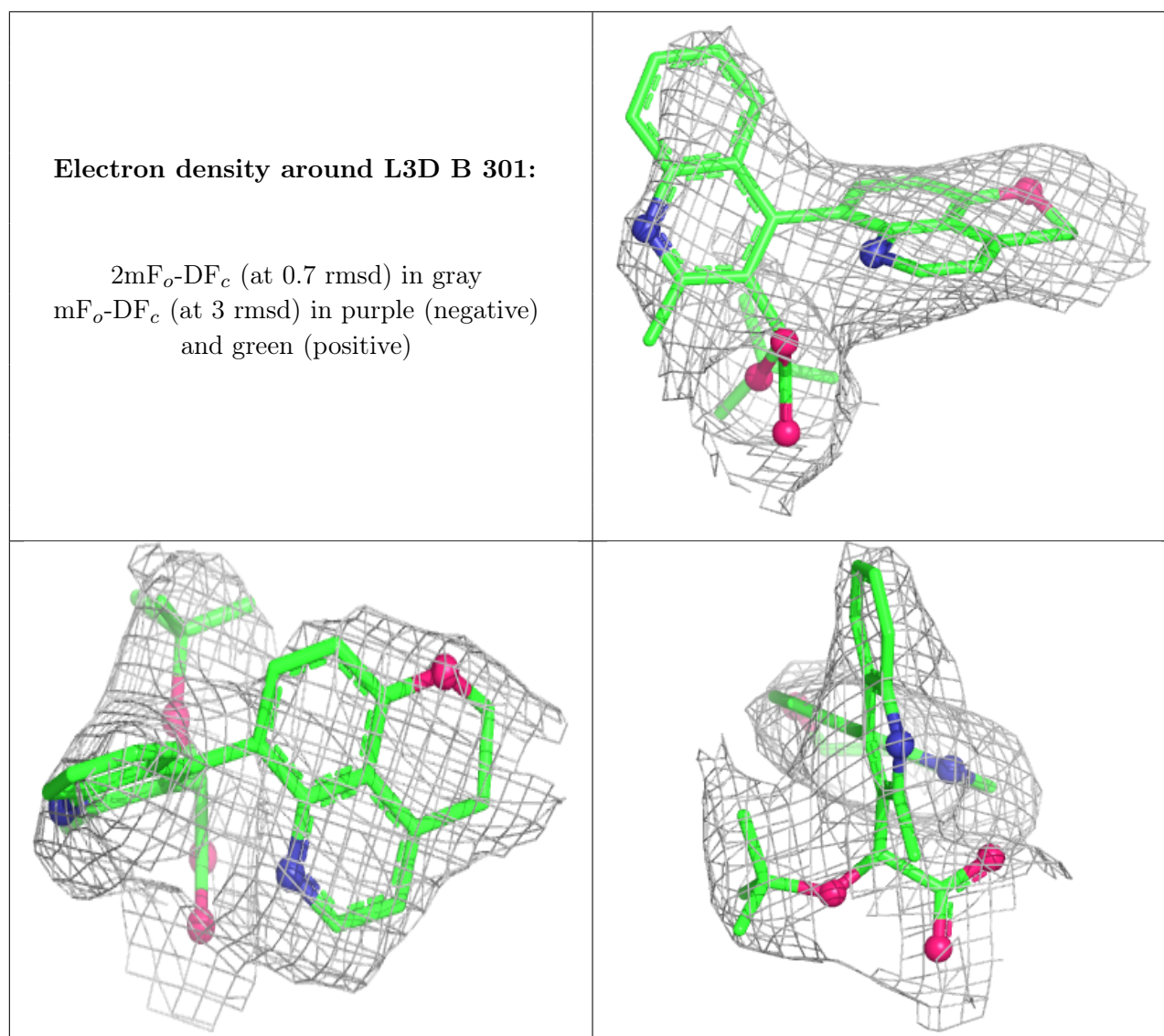
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	303	4/4	0.70	0.13	69,75,75,80	0
4	EDO	M	302	4/4	0.73	0.16	71,87,92,98	0
4	EDO	I	302	4/4	0.74	0.17	96,97,108,115	0
4	EDO	L	503	4/4	0.78	0.14	69,76,78,94	0
4	EDO	E	302	4/4	0.79	0.14	84,99,108,118	0
4	EDO	F	505	4/4	0.80	0.13	66,67,70,75	0
4	EDO	B	302	4/4	0.82	0.18	52,63,78,86	0
4	EDO	K	501	4/4	0.82	0.12	64,85,85,87	0
4	EDO	E	303	4/4	0.86	0.24	83,91,97,105	0
4	EDO	K	502	4/4	0.86	0.16	79,106,116,132	0
4	EDO	F	503	4/4	0.87	0.12	51,53,66,71	0
4	EDO	N	302	4/4	0.87	0.15	57,59,63,66	0
4	EDO	O	301	4/4	0.88	0.20	112,119,124,133	0
4	EDO	F	506	4/4	0.89	0.11	58,81,84,100	0
4	EDO	N	303	4/4	0.89	0.20	75,84,85,99	0
4	EDO	L	502	4/4	0.89	0.10	52,66,70,76	0
3	L3D	B	301	33/33	0.90	0.10	56,84,104,117	0
4	EDO	H	301	4/4	0.90	0.15	56,62,70,77	0
4	EDO	D	301	4/4	0.90	0.16	69,76,91,92	0
4	EDO	J	302	4/4	0.90	0.18	70,72,75,82	0
3	L3D	N	301	33/33	0.91	0.14	43,56,76,80	0
4	EDO	D	302	4/4	0.91	0.11	71,72,75,81	0
4	EDO	A	302	4/4	0.91	0.15	45,83,87,89	0
4	EDO	F	504	4/4	0.92	0.19	55,72,74,114	0
4	EDO	F	501	4/4	0.92	0.17	45,72,78,85	0
4	EDO	L	501	4/4	0.92	0.21	56,73,82,85	0
4	EDO	P	301	4/4	0.92	0.19	69,95,96,97	0

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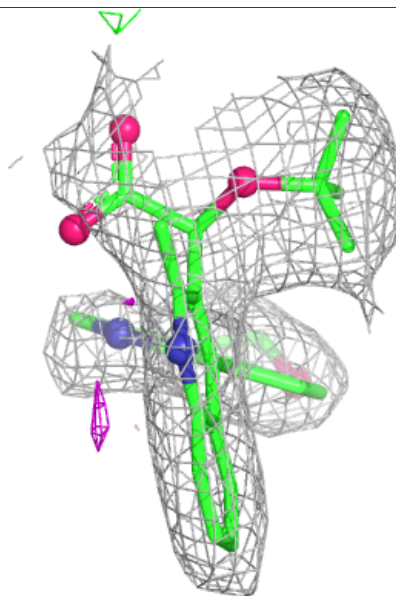
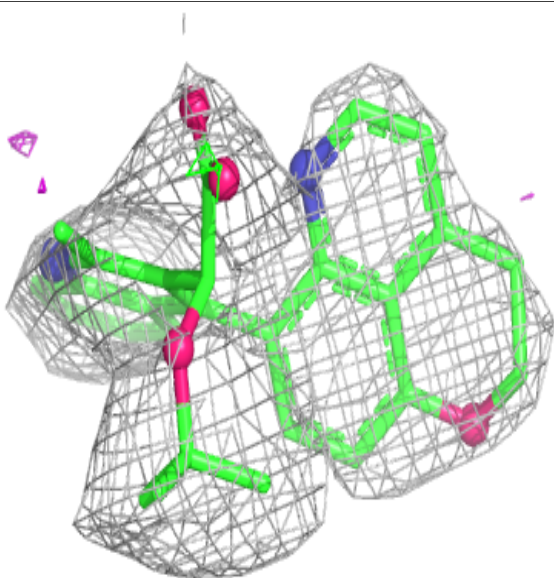
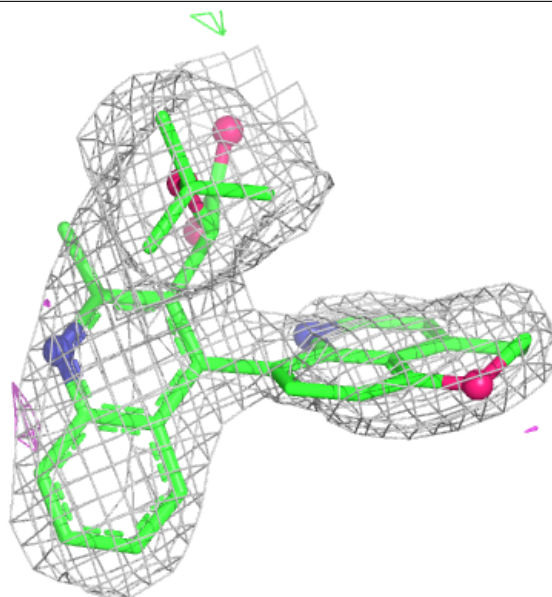
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	L3D	F	502	33/33	0.93	0.10	48,65,85,86	0
3	L3D	J	301	33/33	0.93	0.12	38,56,67,75	0
4	EDO	E	304	4/4	0.94	0.38	58,70,73,81	0
3	L3D	I	301	33/33	0.96	0.08	23,37,48,48	0
4	EDO	G	301	4/4	0.96	0.41	141,145,153,164	0
3	L3D	E	301	33/33	0.96	0.08	24,36,44,49	0
3	L3D	M	301	33/33	0.96	0.07	30,37,49,50	0
3	L3D	A	301	33/33	0.96	0.09	29,41,54,59	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.



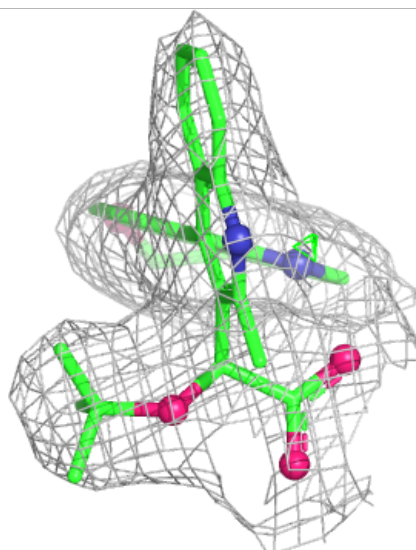
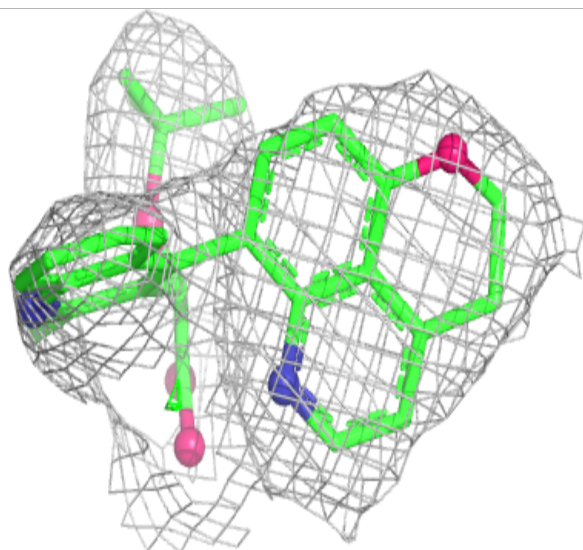
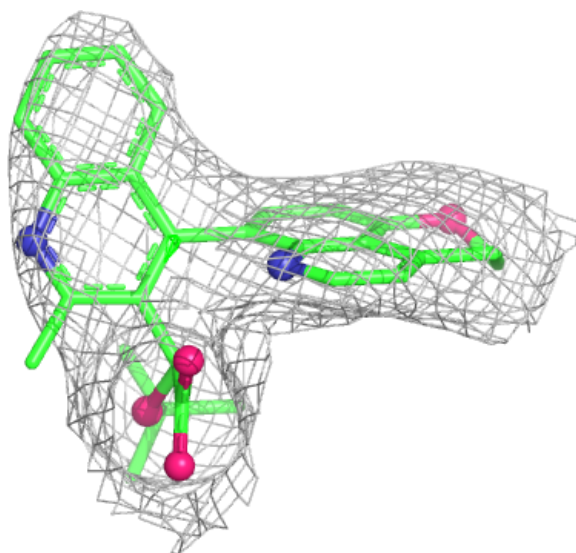
**Electron density around L3D N 301:**

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



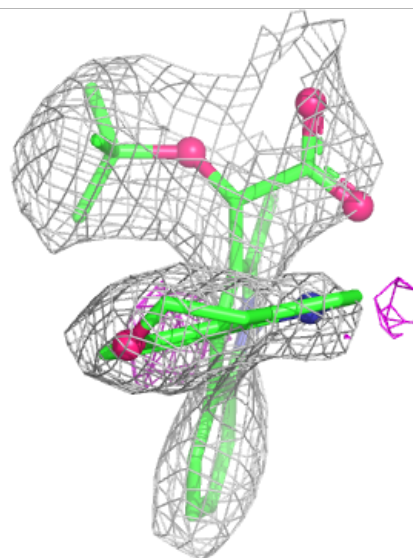
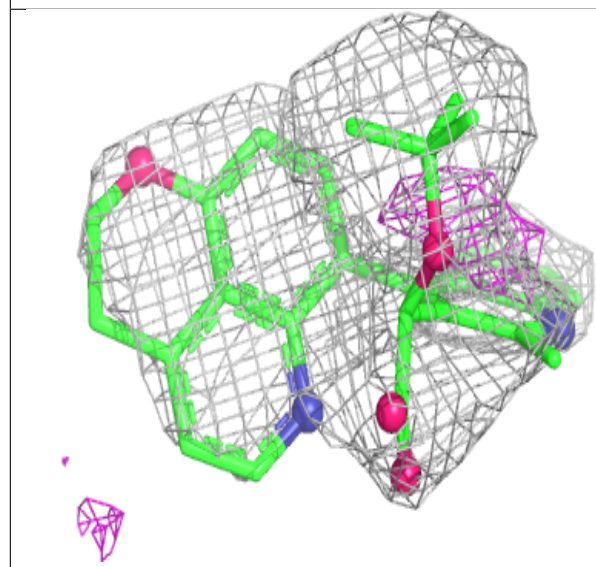
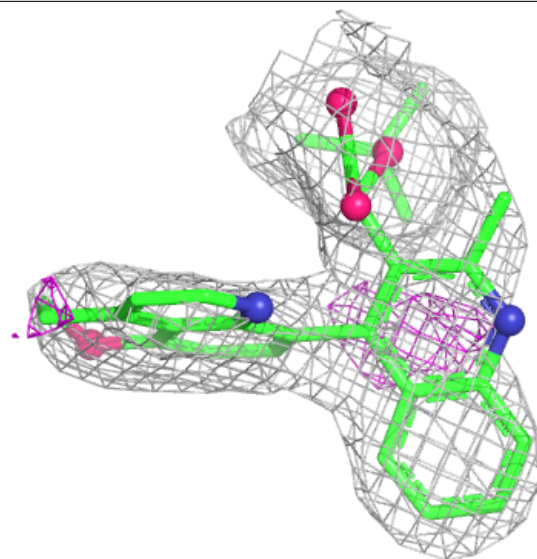
**Electron density around L3D F 502:**

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



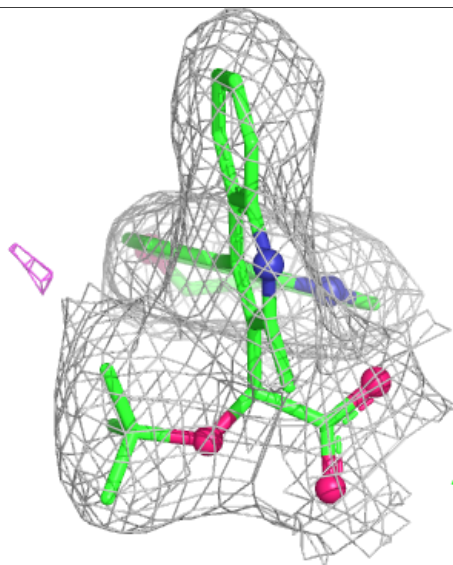
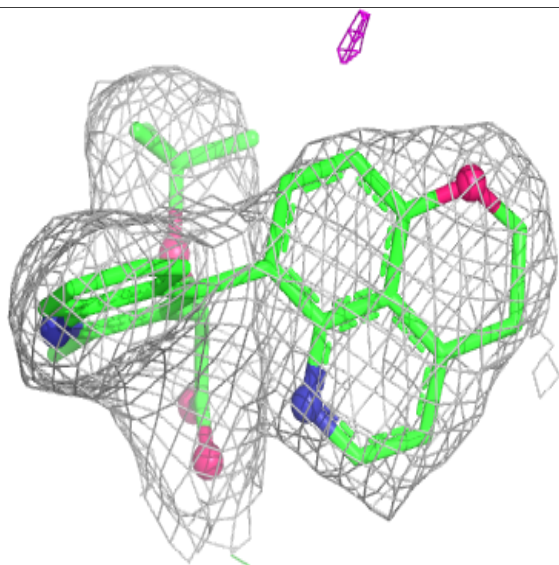
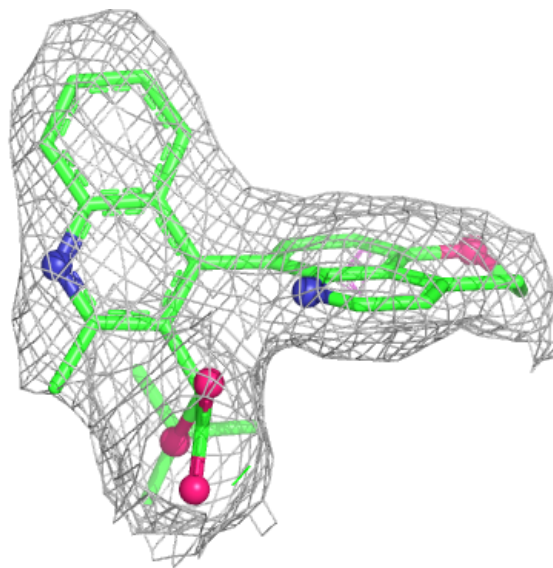
**Electron density around L3D J 301:**

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



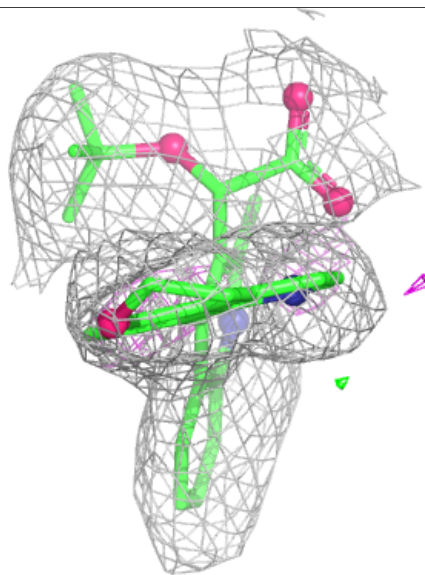
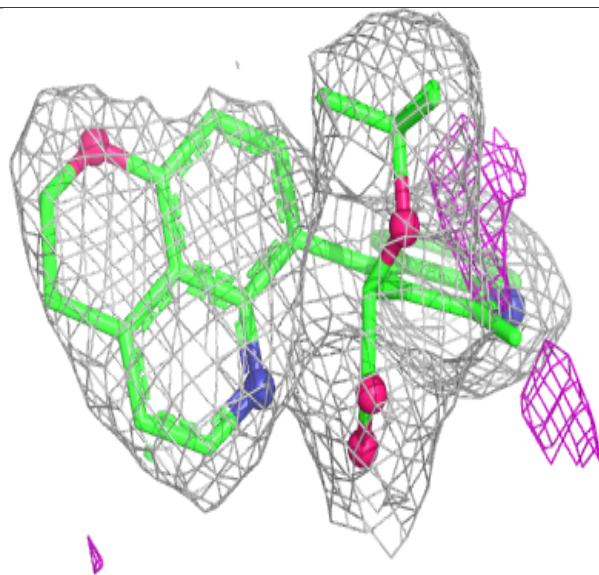
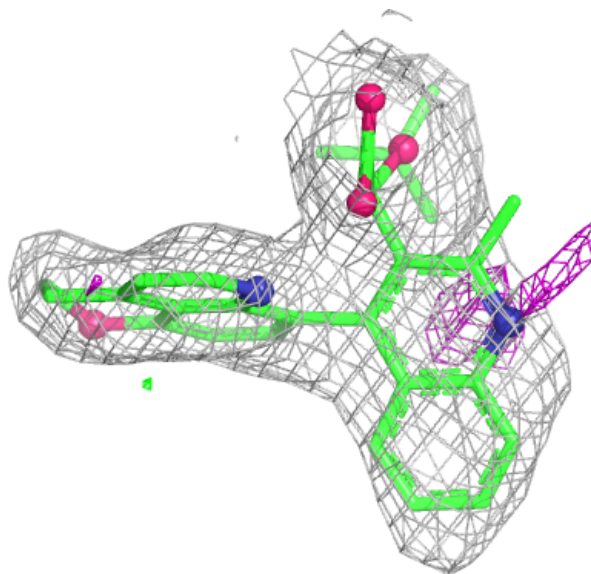
**Electron density around L3D I 301:**

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



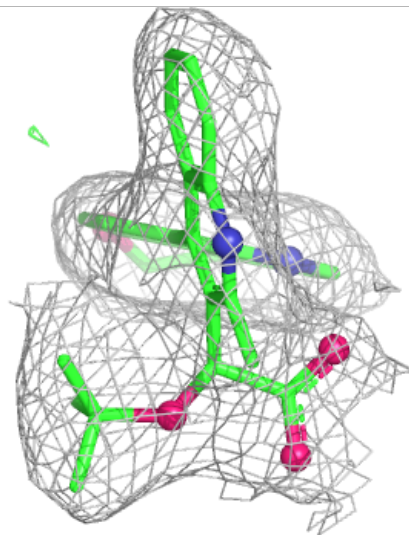
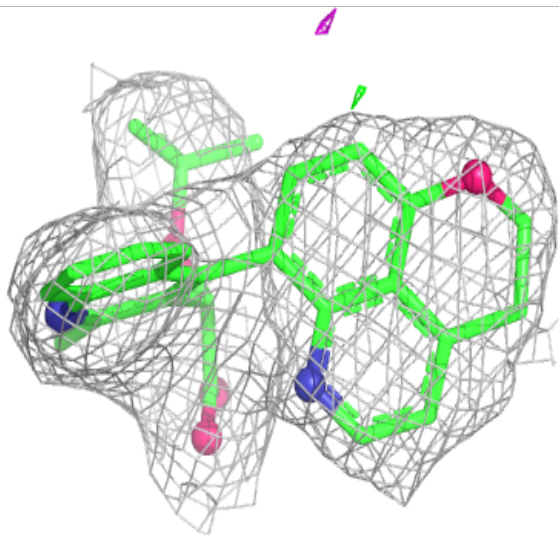
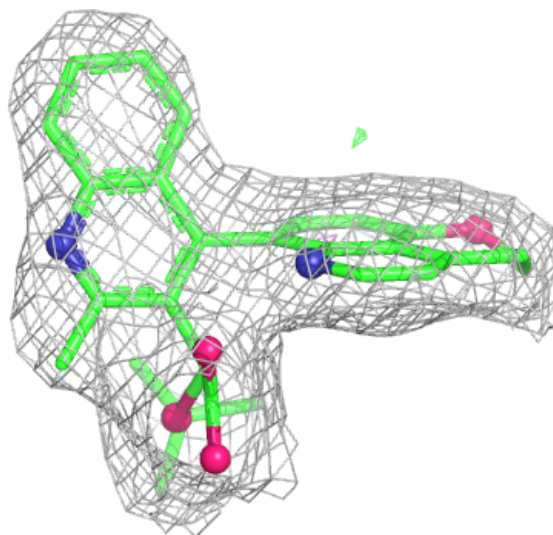
**Electron density around L3D E 301:**

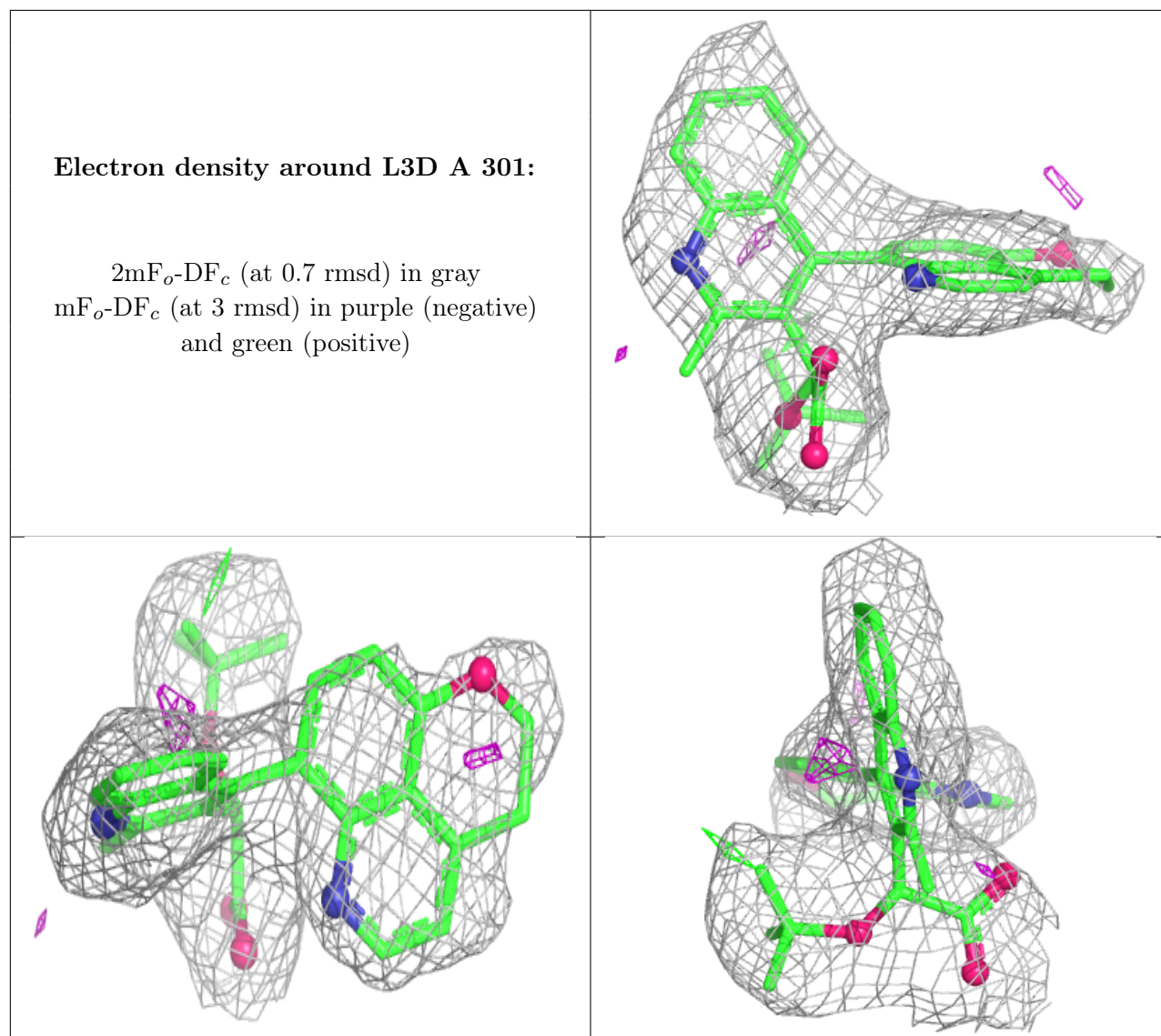
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around L3D M 301:**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.