



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 9DQL / pdb_00009dql
Title : human ClpP - Bortezomib - A192E / E196R
Authors : Forrester, T.J.B.; Kimber, M.S.
Deposited on : 2024-09-24
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

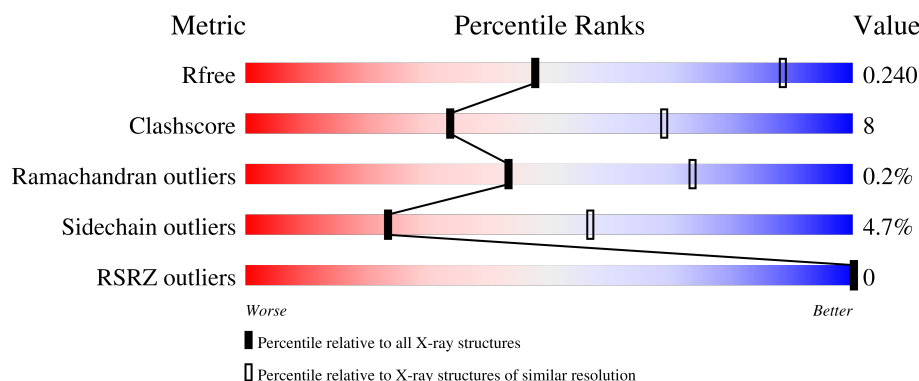
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


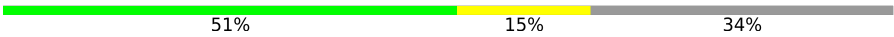



The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	277	
1	B	277	
1	C	277	
1	D	277	
1	E	277	

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Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	
1	J	277	
1	K	277	
1	L	277	
1	M	277	
1	N	277	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20087 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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1404	893	243	255	13			
1	B	183	Total	C	N	O	S	0	0	0
			1419	904	245	257	13			
1	C	182	Total	C	N	O	S	0	0	0
			1412	899	244	256	13			
1	D	180	Total	C	N	O	S	0	0	0
			1397	888	242	254	13			
1	E	181	Total	C	N	O	S	0	0	0
			1404	893	243	255	13			
1	F	181	Total	C	N	O	S	0	1	0
			1413	898	245	257	13			
1	G	180	Total	C	N	O	S	0	0	0
			1398	889	242	254	13			
1	H	185	Total	C	N	O	S	0	0	0
			1435	913	250	259	13			
1	I	178	Total	C	N	O	S	0	0	0
			1382	877	240	252	13			
1	J	179	Total	C	N	O	S	0	0	0
			1386	880	241	252	13			
1	K	178	Total	C	N	O	S	0	0	0
			1383	878	240	252	13			
1	L	180	Total	C	N	O	S	0	0	0
			1397	888	242	254	13			
1	M	184	Total	C	N	O	S	0	0	0
			1428	908	249	258	13			
1	N	183	Total	C	N	O	S	0	1	0
			1428	909	247	259	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLU	ALA	engineered mutation	UNP Q16740
A	196	ARG	GLU	engineered mutation	UNP Q16740
B	192	GLU	ALA	engineered mutation	UNP Q16740
B	196	ARG	GLU	engineered mutation	UNP Q16740
C	192	GLU	ALA	engineered mutation	UNP Q16740
C	196	ARG	GLU	engineered mutation	UNP Q16740
D	192	GLU	ALA	engineered mutation	UNP Q16740
D	196	ARG	GLU	engineered mutation	UNP Q16740
E	192	GLU	ALA	engineered mutation	UNP Q16740
E	196	ARG	GLU	engineered mutation	UNP Q16740
F	192	GLU	ALA	engineered mutation	UNP Q16740
F	196	ARG	GLU	engineered mutation	UNP Q16740
G	192	GLU	ALA	engineered mutation	UNP Q16740
G	196	ARG	GLU	engineered mutation	UNP Q16740
H	192	GLU	ALA	engineered mutation	UNP Q16740
H	196	ARG	GLU	engineered mutation	UNP Q16740
I	192	GLU	ALA	engineered mutation	UNP Q16740
I	196	ARG	GLU	engineered mutation	UNP Q16740
J	192	GLU	ALA	engineered mutation	UNP Q16740
J	196	ARG	GLU	engineered mutation	UNP Q16740
K	192	GLU	ALA	engineered mutation	UNP Q16740
K	196	ARG	GLU	engineered mutation	UNP Q16740
L	192	GLU	ALA	engineered mutation	UNP Q16740
L	196	ARG	GLU	engineered mutation	UNP Q16740
M	192	GLU	ALA	engineered mutation	UNP Q16740
M	196	ARG	GLU	engineered mutation	UNP Q16740
N	192	GLU	ALA	engineered mutation	UNP Q16740
N	196	ARG	GLU	engineered mutation	UNP Q16740

- Molecule 2 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: C₁₉H₂₅BN₄O₄) (labeled as "Ligand of Interest" by depositor).



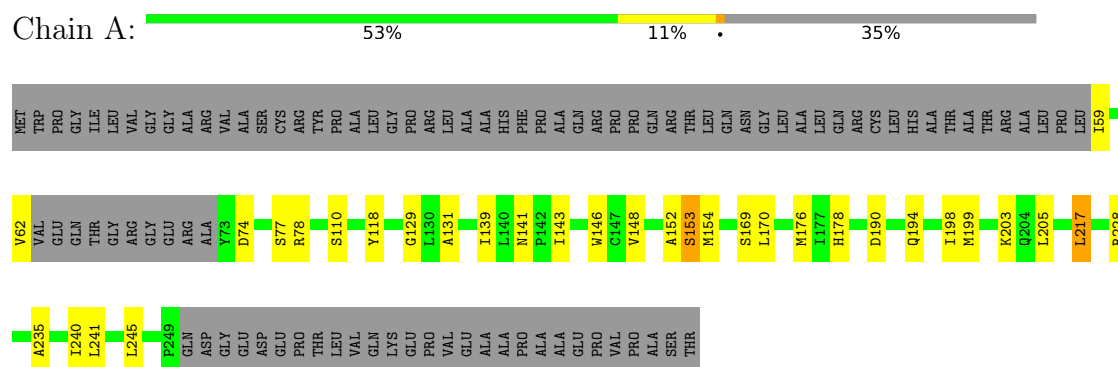
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	C	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	G	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0
3	N	1	Total 1	Cl 1	0	0

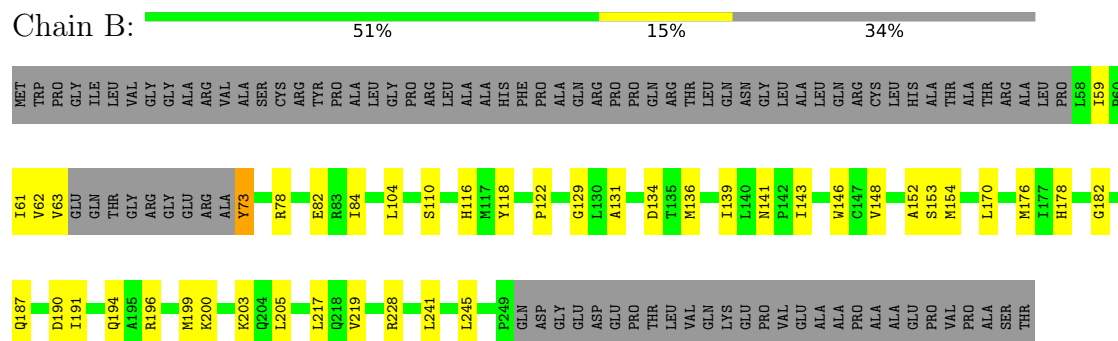
3 Residue-property plots

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.

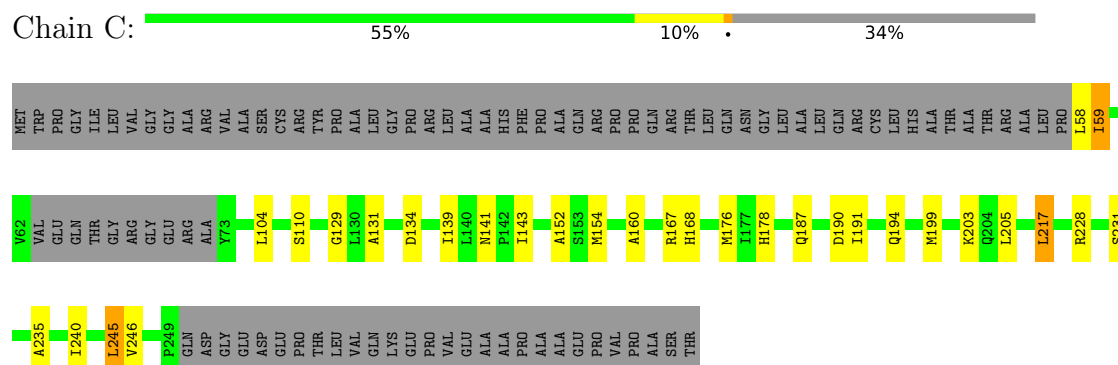
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



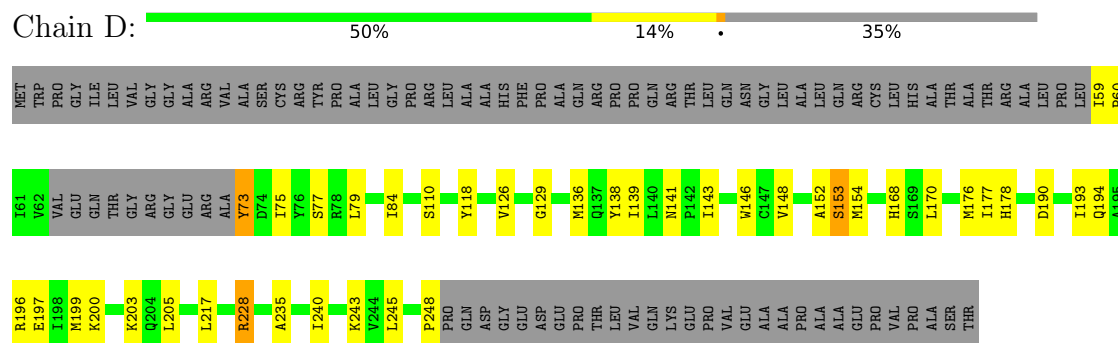
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



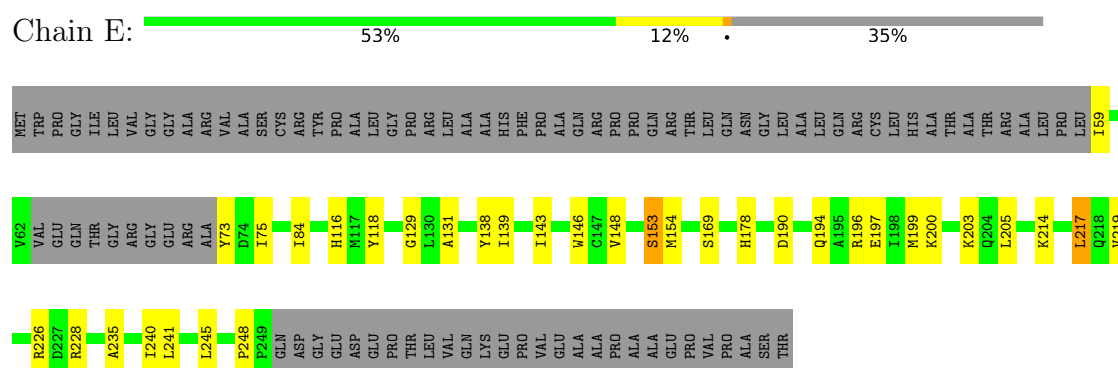
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



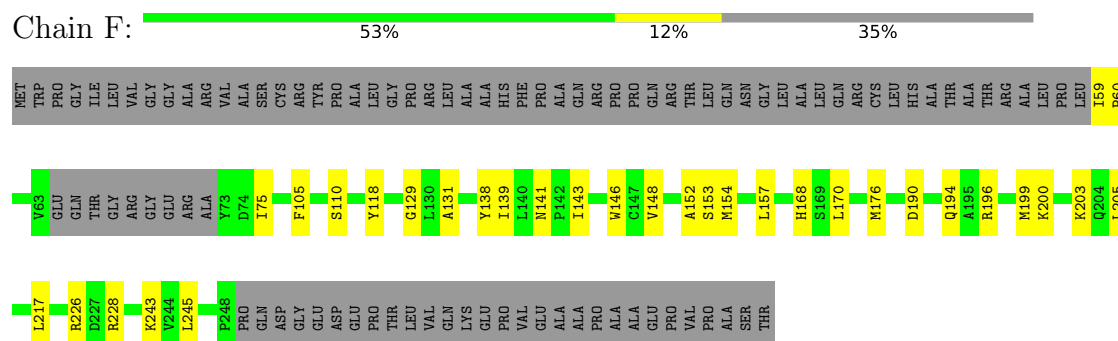
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



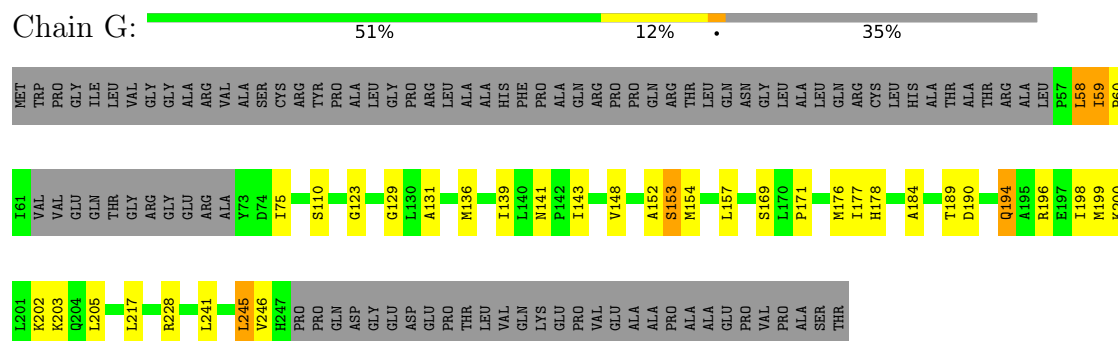
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

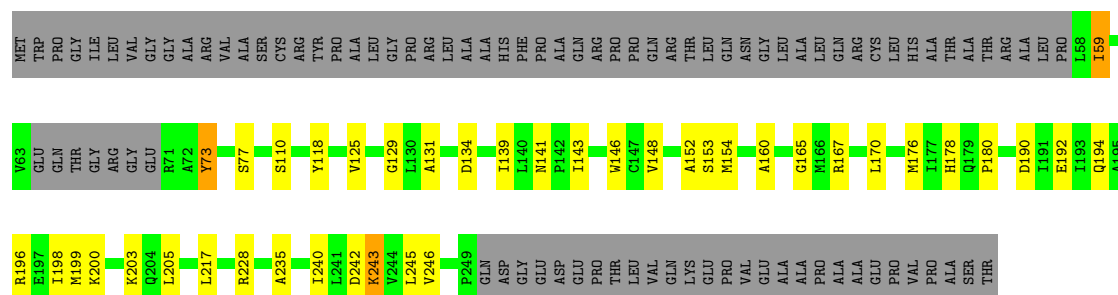


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



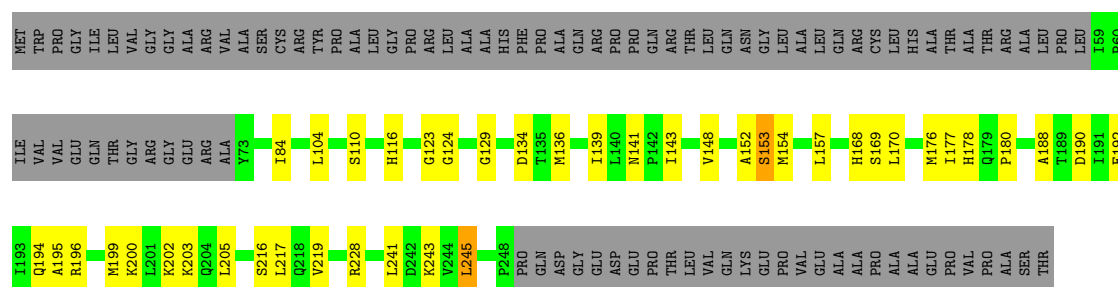
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain H:  52% 14% 33%



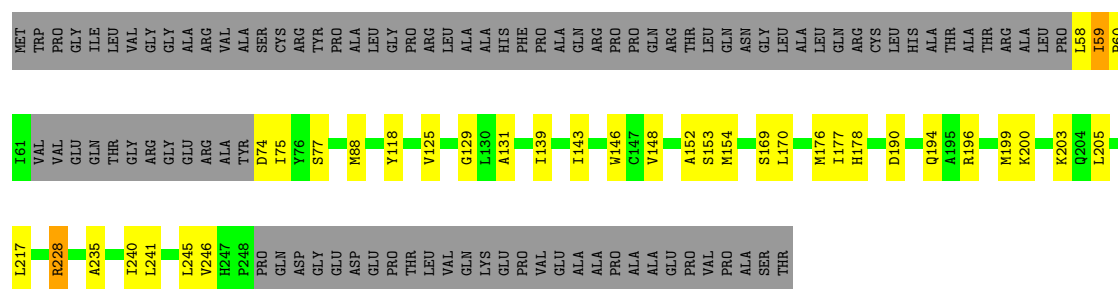
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain I:  49% 14% 36%



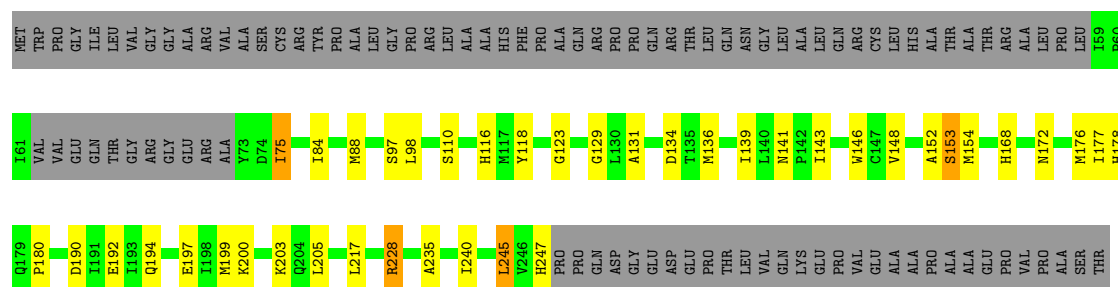
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain J:  51% 13% 35%

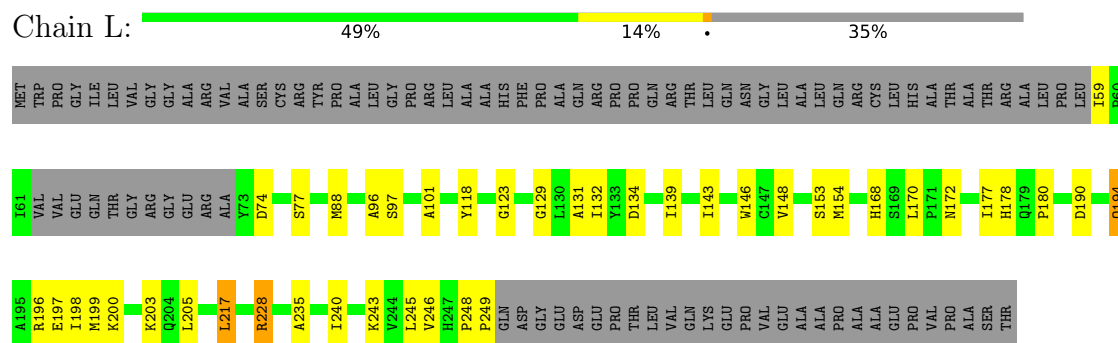


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

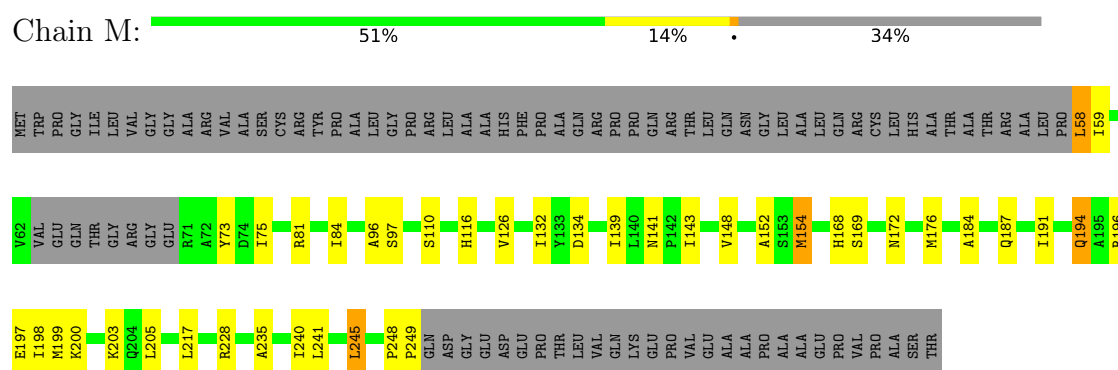
Chain K:  49% 13% 36%



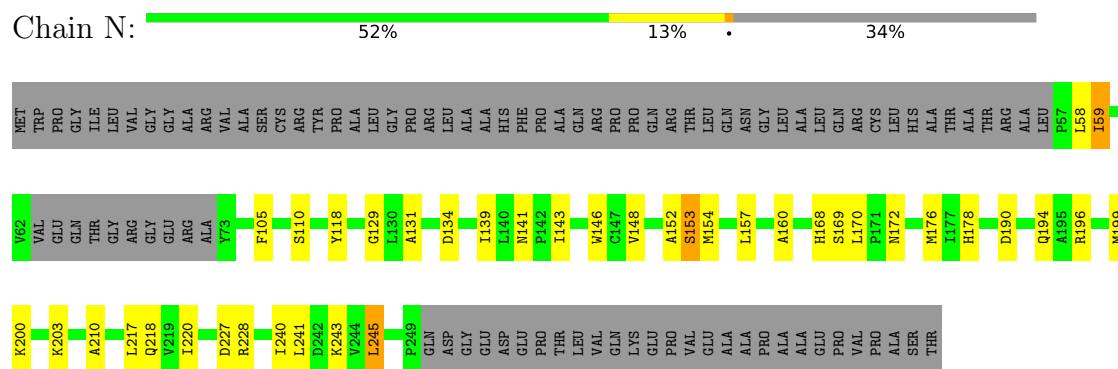
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 93.88Å 133.72Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	44.24 – 3.20 44.24 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.24-3.20) 91.3 (44.24-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.237 (Not available) , 0.240	Depositor DCC
R_{free} test set	1997 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	98.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20087	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BO2

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	0.13	0/1430	0.27	0/1934
1	B	0.13	0/1445	0.29	0/1955
1	C	0.12	0/1438	0.26	0/1945
1	D	0.10	0/1422	0.23	0/1922
1	E	0.12	0/1430	0.24	0/1934
1	F	0.11	0/1438	0.27	0/1944
1	G	0.13	0/1423	0.27	0/1922
1	H	0.13	0/1461	0.28	0/1976
1	I	0.13	0/1407	0.26	0/1901
1	J	0.13	0/1410	0.26	0/1905
1	K	0.10	0/1407	0.23	0/1900
1	L	0.10	0/1423	0.24	0/1924
1	M	0.12	0/1454	0.26	0/1966
1	N	0.14	0/1455	0.27	0/1968
All	All	0.12	0/20043	0.26	0/27096

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1404	0	1442	21	0
1	B	1419	0	1462	24	0
1	C	1412	0	1453	18	0
1	D	1397	0	1435	25	0
1	E	1404	0	1442	22	1
1	F	1413	0	1451	21	0
1	G	1398	0	1438	24	0
1	H	1435	0	1480	25	0
1	I	1382	0	1415	27	1
1	J	1386	0	1428	25	0
1	K	1383	0	1419	26	0
1	L	1397	0	1433	27	0
1	M	1428	0	1471	24	0
1	N	1428	0	1468	30	0
2	A	28	0	25	4	0
2	B	28	0	25	5	0
2	C	28	0	25	4	0
2	D	28	0	25	4	0
2	E	28	0	25	3	0
2	F	28	0	25	2	0
2	G	28	0	25	4	0
2	H	28	0	25	5	0
2	I	28	0	25	5	0
2	J	28	0	25	5	0
2	K	28	0	25	4	0
2	L	28	0	25	5	0
2	M	28	0	24	3	0
2	N	28	0	25	4	0
3	A	2	0	0	1	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
All	All	20087	0	20586	311	1

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 8.

The worst 5 of 311 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:G:205:LEU:HD13	2:G:301:BO2:H243	1.62	0.81
1:N:129:GLY:HA3	1:N:154:MET:HE2	1.68	0.76
1:B:205:LEU:HD13	2:B:301:BO2:H243	1.70	0.73
1:C:205:LEU:HD13	2:C:301:BO2:H243	1.69	0.73
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.69	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:LYS:O	1:I:216:SER:OG[2_344]	2.14	0.06

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	177/277 (64%)	171 (97%)	6 (3%)	0	100	100
1	B	179/277 (65%)	172 (96%)	7 (4%)	0	100	100
1	C	178/277 (64%)	173 (97%)	5 (3%)	0	100	100
1	D	176/277 (64%)	170 (97%)	6 (3%)	0	100	100
1	E	177/277 (64%)	172 (97%)	5 (3%)	0	100	100
1	F	178/277 (64%)	168 (94%)	10 (6%)	0	100	100
1	G	176/277 (64%)	168 (96%)	8 (4%)	0	100	100
1	H	181/277 (65%)	173 (96%)	7 (4%)	1 (1%)	21	56
1	I	174/277 (63%)	168 (97%)	6 (3%)	0	100	100
1	J	175/277 (63%)	165 (94%)	8 (5%)	2 (1%)	11	43
1	K	174/277 (63%)	167 (96%)	7 (4%)	0	100	100
1	L	176/277 (64%)	168 (96%)	7 (4%)	1 (1%)	21	56
1	M	180/277 (65%)	174 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	180/277 (65%)	174 (97%)	6 (3%)	0	100	100
All	All	2481/3878 (64%)	2383 (96%)	94 (4%)	4 (0%)	43	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	59	ILE
1	H	246	VAL
1	J	246	VAL
1	L	246	VAL

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	155/227 (68%)	149 (96%)	6 (4%)	28	62
1	B	157/227 (69%)	146 (93%)	11 (7%)	14	45
1	C	156/227 (69%)	149 (96%)	7 (4%)	24	58
1	D	154/227 (68%)	148 (96%)	6 (4%)	28	62
1	E	155/227 (68%)	148 (96%)	7 (4%)	24	58
1	F	156/227 (69%)	151 (97%)	5 (3%)	34	65
1	G	154/227 (68%)	144 (94%)	10 (6%)	15	47
1	H	158/227 (70%)	149 (94%)	9 (6%)	18	51
1	I	152/227 (67%)	145 (95%)	7 (5%)	24	58
1	J	153/227 (67%)	148 (97%)	5 (3%)	33	65
1	K	152/227 (67%)	145 (95%)	7 (5%)	24	58
1	L	154/227 (68%)	148 (96%)	6 (4%)	28	62
1	M	157/227 (69%)	147 (94%)	10 (6%)	16	48
1	N	158/227 (70%)	152 (96%)	6 (4%)	29	62
All	All	2171/3178 (68%)	2069 (95%)	102 (5%)	23	57

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	217	LEU
1	J	228	ARG
1	N	218	GLN
1	H	243	LYS
1	I	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	120	ASN
1	N	150	GLN
1	I	137	GLN
1	L	236	GLN
1	I	120	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BO2	M	301	-	25,29,29	1.64	3 (12%)	33,38,38	1.27	3 (9%)
2	BO2	A	301	-	25,29,29	1.68	3 (12%)	33,38,38	1.27	4 (12%)
2	BO2	E	301	-	25,29,29	1.66	3 (12%)	33,38,38	1.15	3 (9%)
2	BO2	K	301	-	25,29,29	1.69	3 (12%)	33,38,38	1.33	4 (12%)
2	BO2	J	301	-	25,29,29	1.75	3 (12%)	33,38,38	1.18	4 (12%)
2	BO2	F	301	-	25,29,29	1.69	3 (12%)	33,38,38	1.30	5 (15%)
2	BO2	C	301	-	25,29,29	1.67	3 (12%)	33,38,38	1.23	4 (12%)
2	BO2	D	301	-	25,29,29	1.69	3 (12%)	33,38,38	1.21	3 (9%)
2	BO2	B	301	-	25,29,29	1.67	3 (12%)	33,38,38	1.31	4 (12%)
2	BO2	L	301	-	25,29,29	1.71	3 (12%)	33,38,38	1.20	3 (9%)
2	BO2	G	301	-	25,29,29	1.68	3 (12%)	33,38,38	1.30	3 (9%)
2	BO2	N	301	-	25,29,29	1.76	3 (12%)	33,38,38	1.58	7 (21%)
2	BO2	H	301	-	25,29,29	1.71	3 (12%)	33,38,38	1.14	4 (12%)
2	BO2	I	301	-	25,29,29	1.78	3 (12%)	33,38,38	1.47	6 (18%)

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	BO2	M	301	-	-	2/23/28/28	0/2/2/2
2	BO2	A	301	-	-	2/23/28/28	0/2/2/2
2	BO2	E	301	-	-	4/23/28/28	0/2/2/2
2	BO2	K	301	-	-	4/23/28/28	0/2/2/2
2	BO2	J	301	-	-	0/23/28/28	0/2/2/2
2	BO2	F	301	-	-	2/23/28/28	0/2/2/2
2	BO2	C	301	-	-	2/23/28/28	0/2/2/2
2	BO2	D	301	-	-	3/23/28/28	0/2/2/2
2	BO2	B	301	-	-	3/23/28/28	0/2/2/2
2	BO2	L	301	-	-	3/23/28/28	0/2/2/2
2	BO2	G	301	-	-	7/23/28/28	0/2/2/2
2	BO2	N	301	-	-	5/23/28/28	0/2/2/2
2	BO2	H	301	-	-	2/23/28/28	0/2/2/2
2	BO2	I	301	-	-	7/23/28/28	0/2/2/2

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	BO2	C18-N20	6.25	1.47	1.34
2	N	301	BO2	C18-N20	6.03	1.47	1.34
2	J	301	BO2	C18-N20	5.83	1.46	1.34
2	L	301	BO2	C18-N20	5.64	1.46	1.34
2	H	301	BO2	C18-N20	5.58	1.46	1.34

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	BO2	C21-C22-C23	-4.35	109.76	115.32
2	N	301	BO2	C2-C7-N9	4.00	122.87	115.19
2	N	301	BO2	C21-C22-C23	-3.84	110.42	115.32
2	G	301	BO2	C21-C22-C23	-3.76	110.52	115.32
2	B	301	BO2	C21-C22-C23	-3.53	110.82	115.32

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	BO2	C18-C10-C11-C12
2	C	301	BO2	N9-C10-C11-C12
2	C	301	BO2	C18-C10-C11-C12
2	E	301	BO2	C18-C10-C11-C12
2	G	301	BO2	N9-C10-C11-C12

There are no ring outliers.

14 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301	BO2	3	0
2	A	301	BO2	4	0
2	E	301	BO2	3	0
2	K	301	BO2	4	0
2	J	301	BO2	5	0
2	F	301	BO2	2	0
2	C	301	BO2	4	0
2	D	301	BO2	4	0
2	B	301	BO2	5	0
2	L	301	BO2	5	0
2	G	301	BO2	4	0

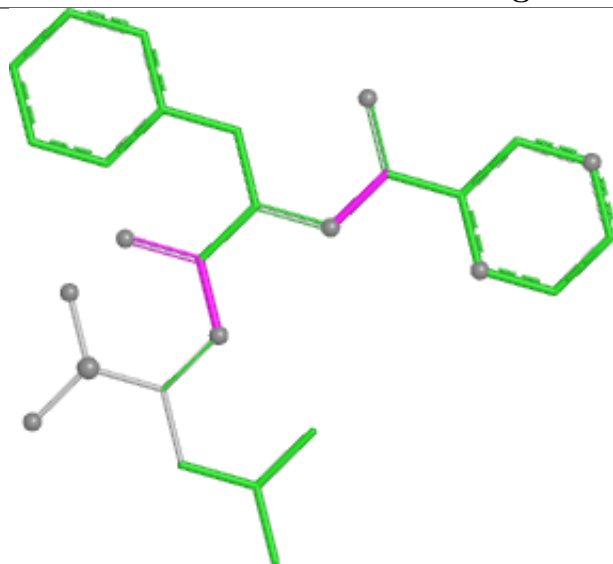
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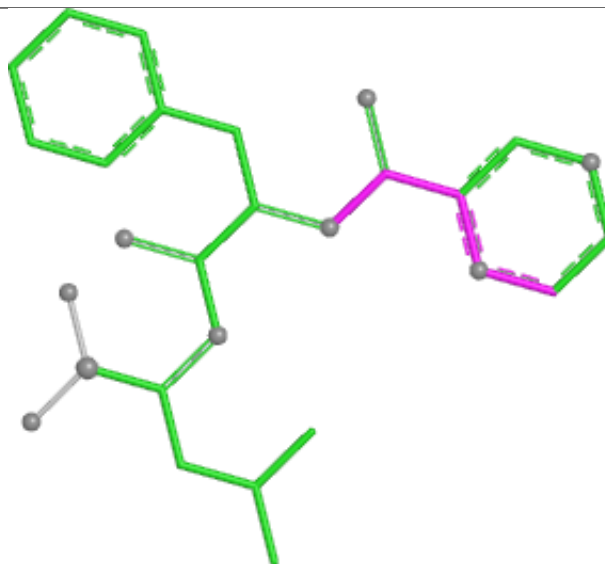
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	301	BO2	4	0
2	H	301	BO2	5	0
2	I	301	BO2	5	0

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.

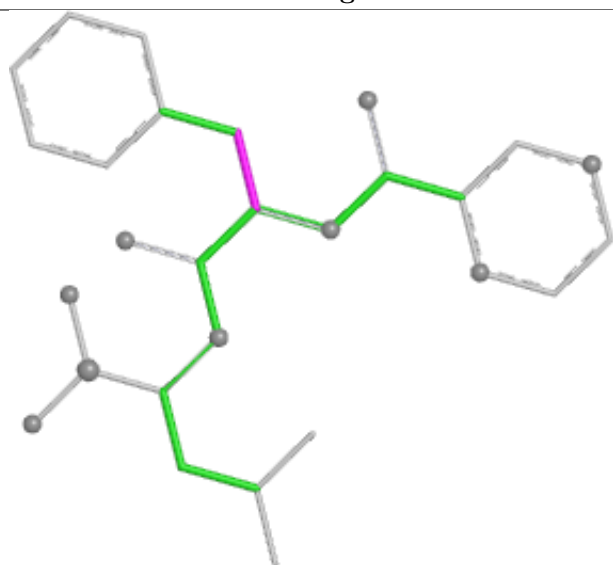
Ligand BO2 M 301



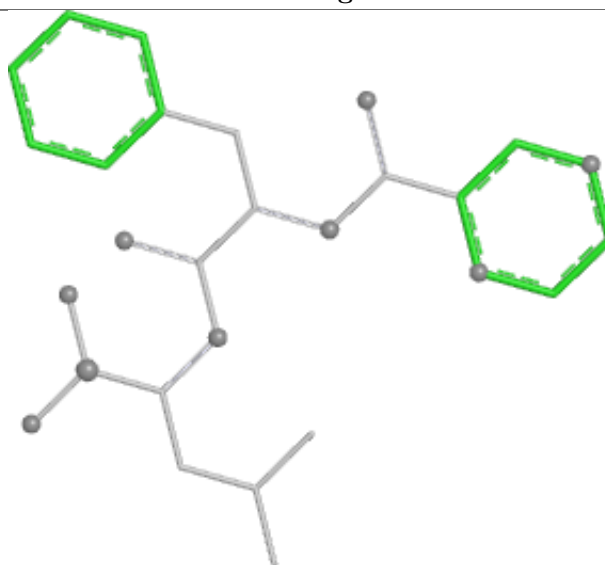
Bond lengths



Bond angles

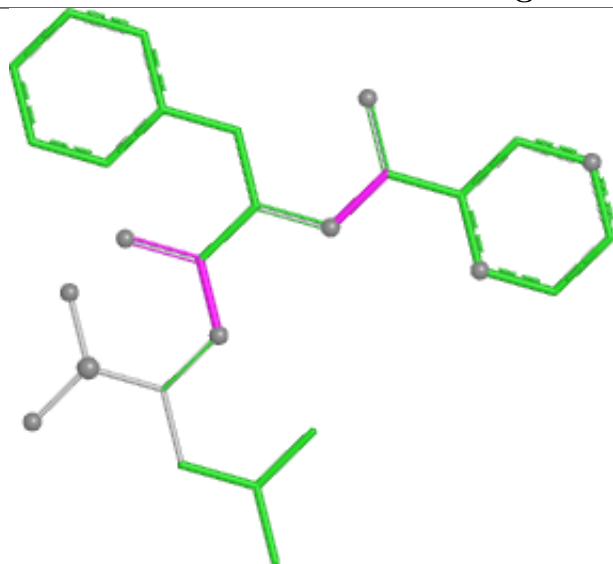


Torsions

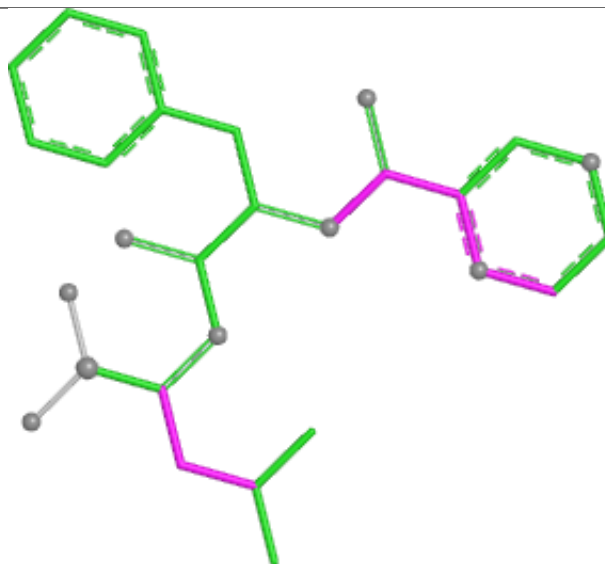


Rings

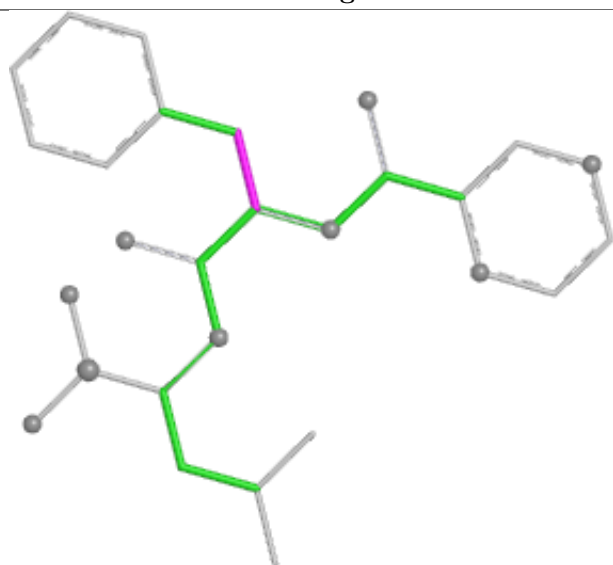
Ligand BO2 A 301



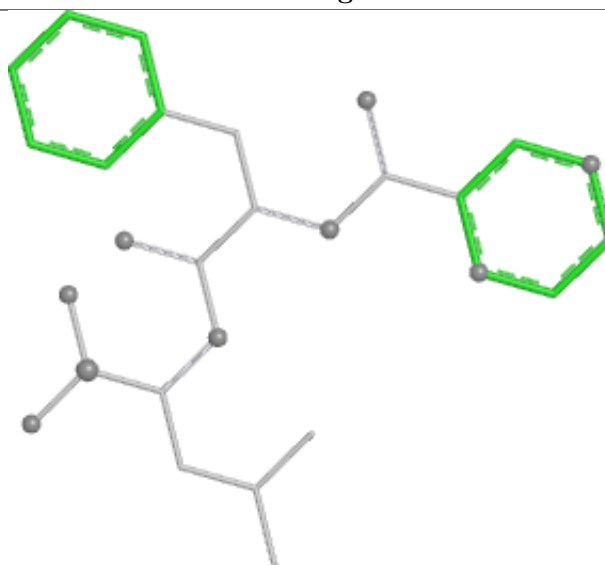
Bond lengths



Bond angles

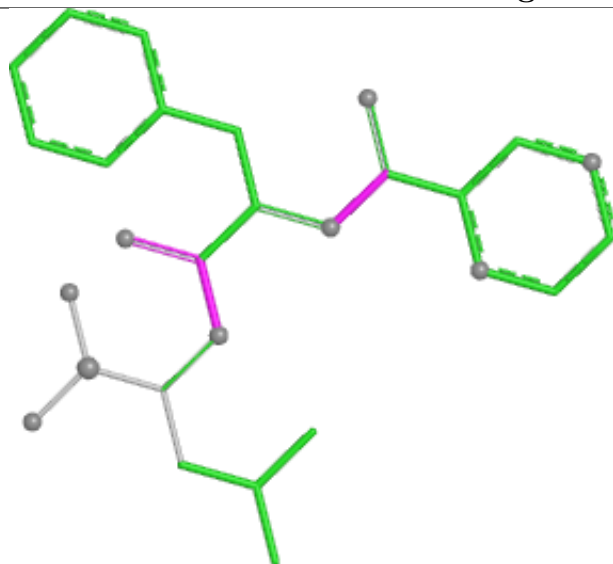


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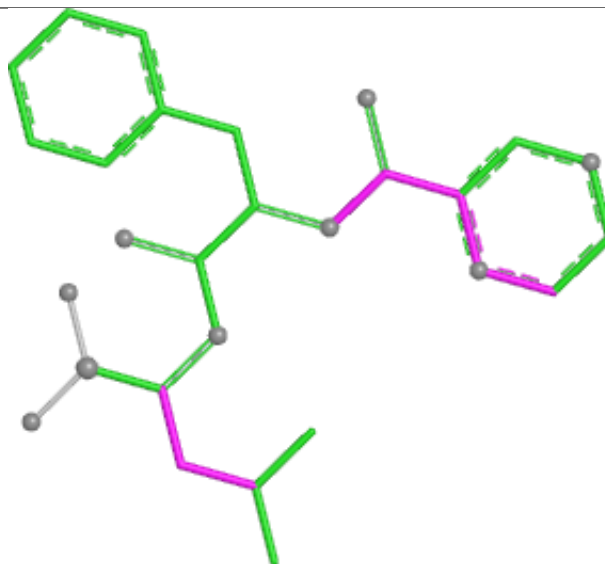


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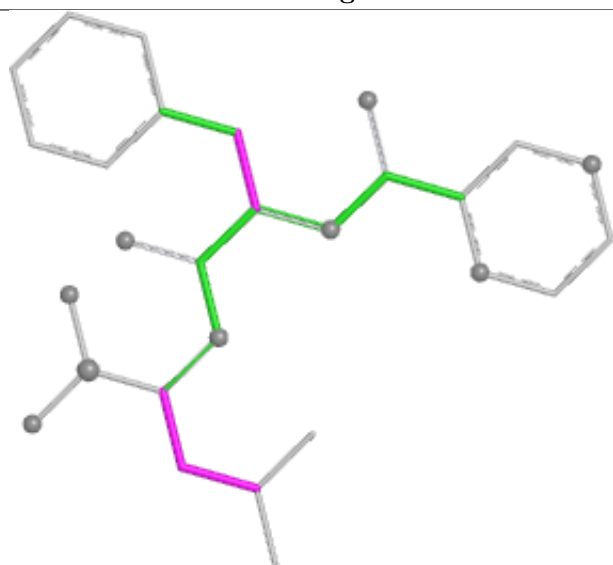
Ligand BO2 E 301



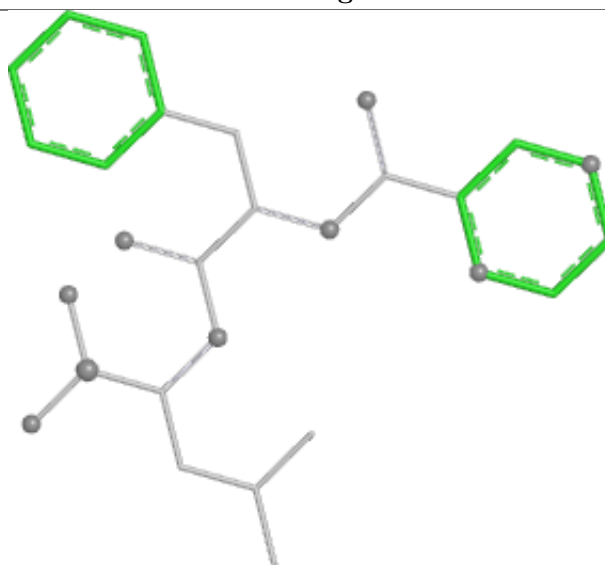
Bond lengths



Bond angles

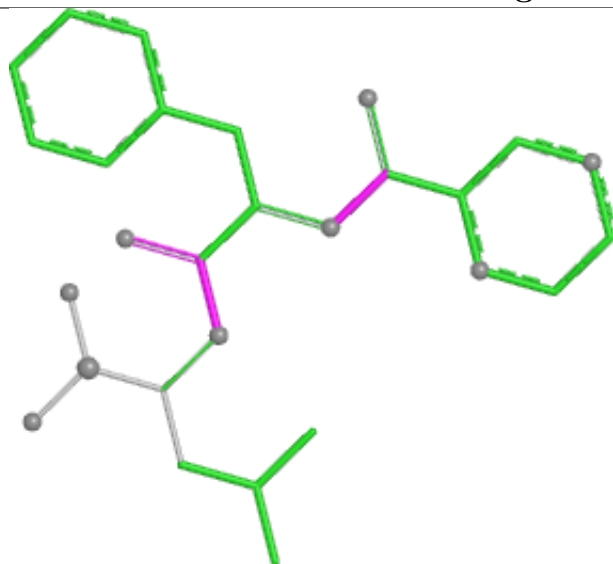


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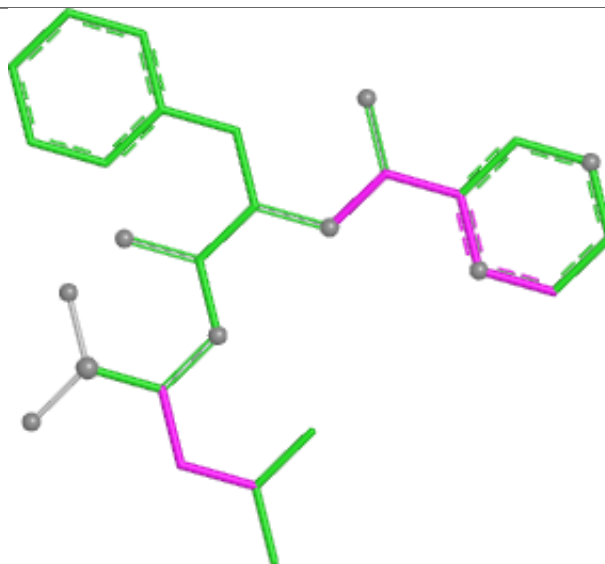


Rings

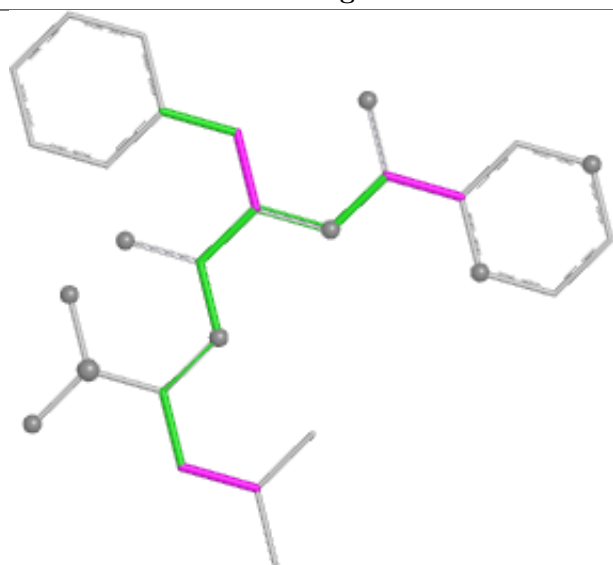
Ligand BO2 K 301



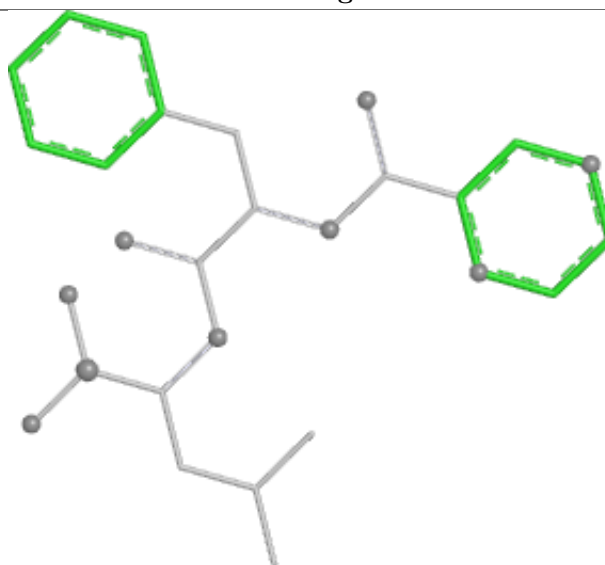
Bond lengths



Bond angles

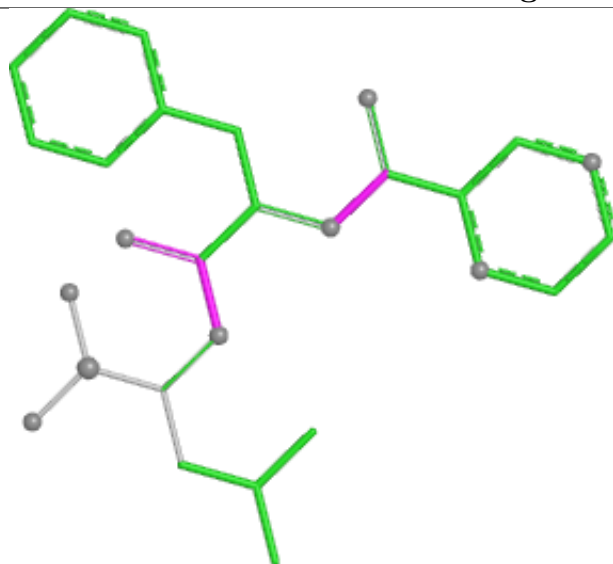


Torsions

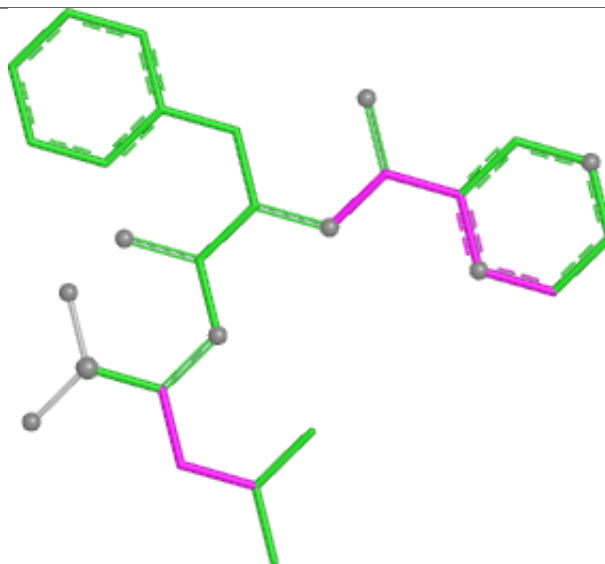


Rings

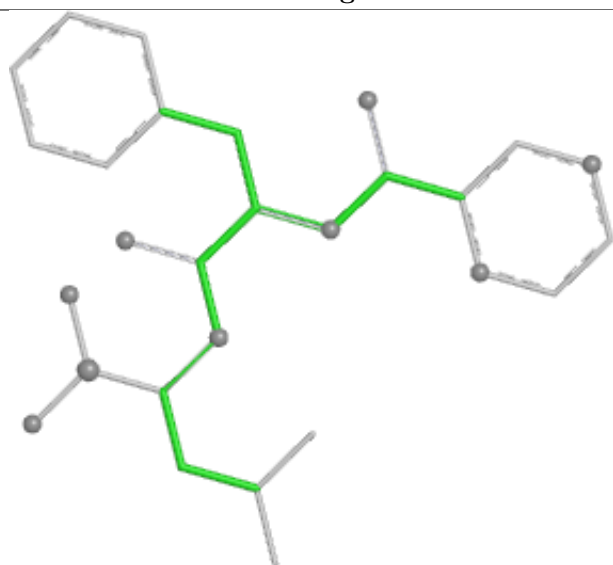
Ligand BO2 J 301



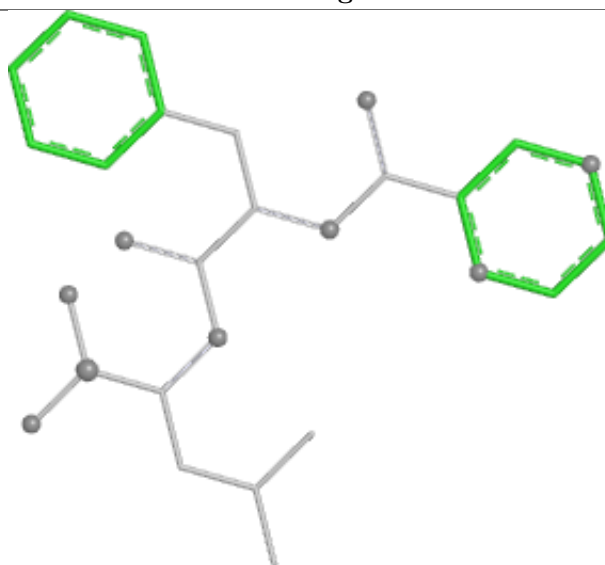
Bond lengths



Bond angles

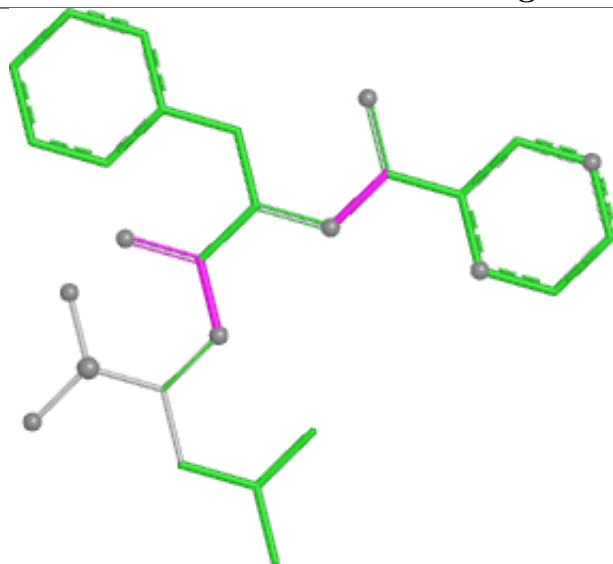


Torsions

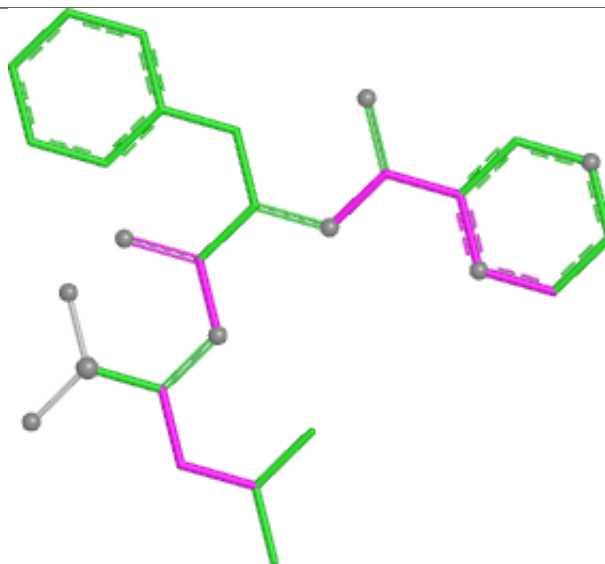


Rings

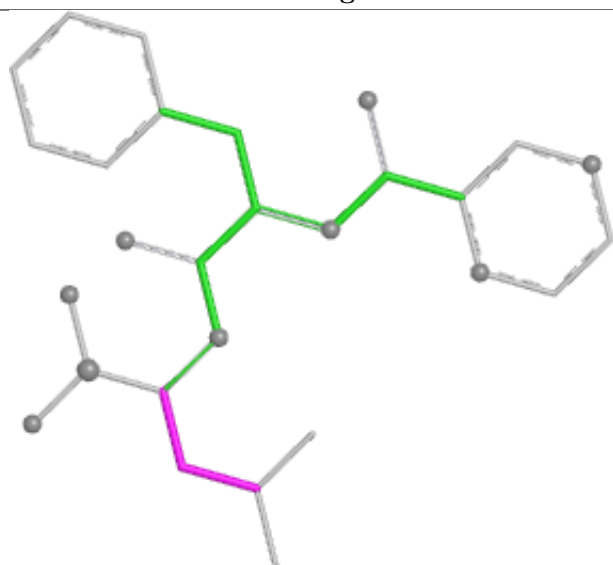
Ligand BO2 F 301



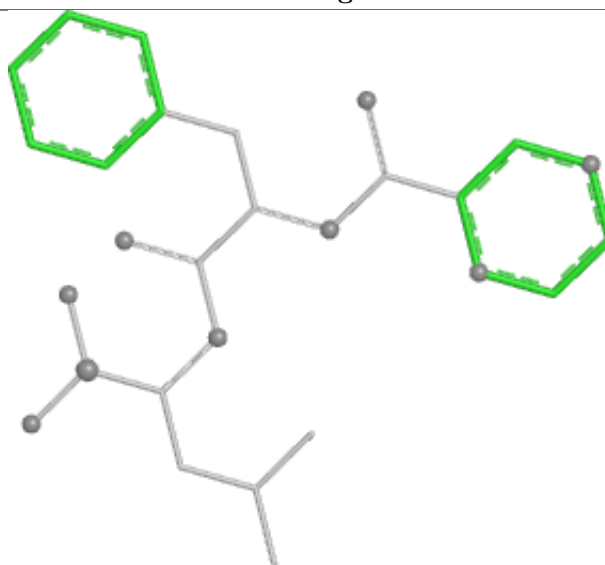
Bond lengths



Bond angles

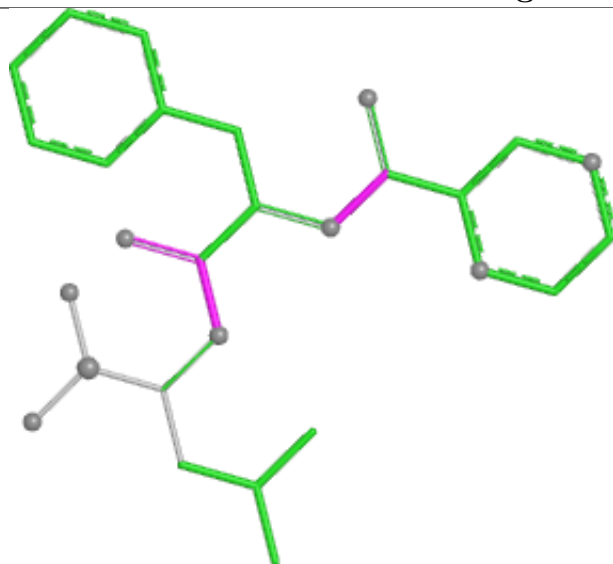


Torsions

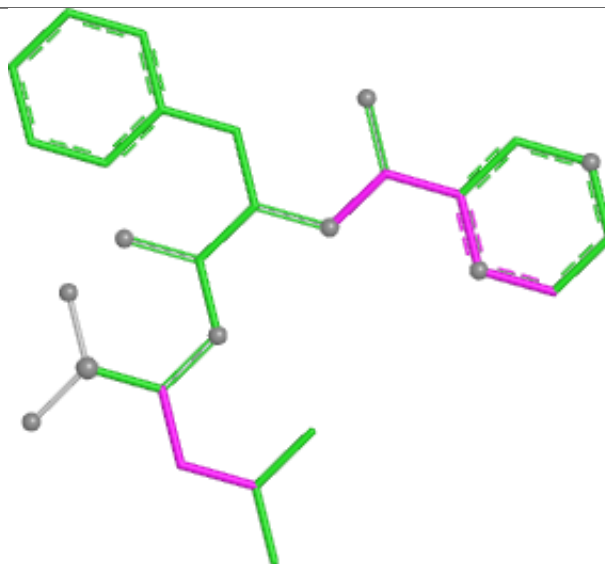


Rings

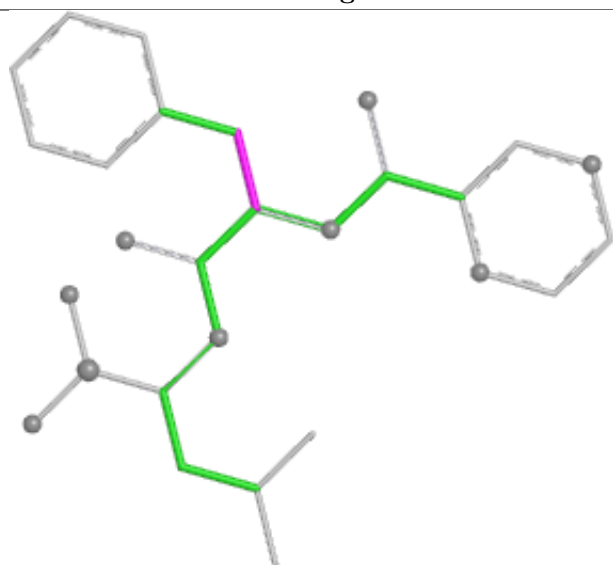
Ligand BO2 C 301



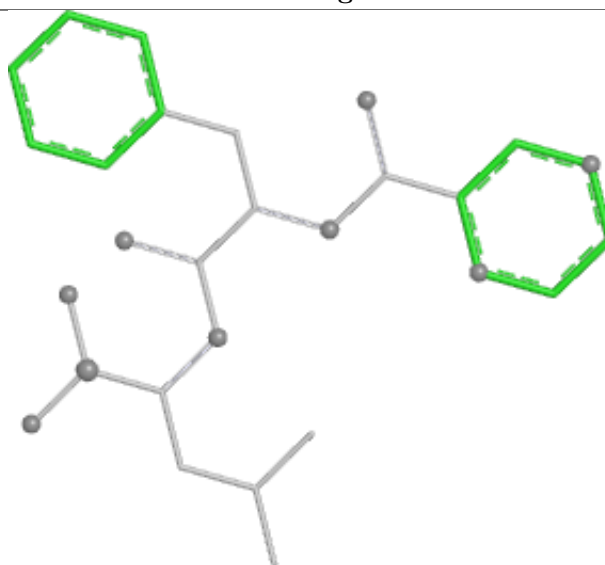
Bond lengths



Bond angles

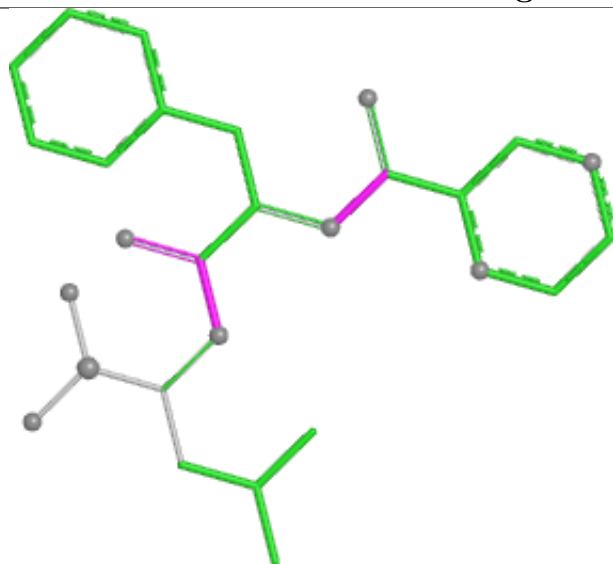


Torsions

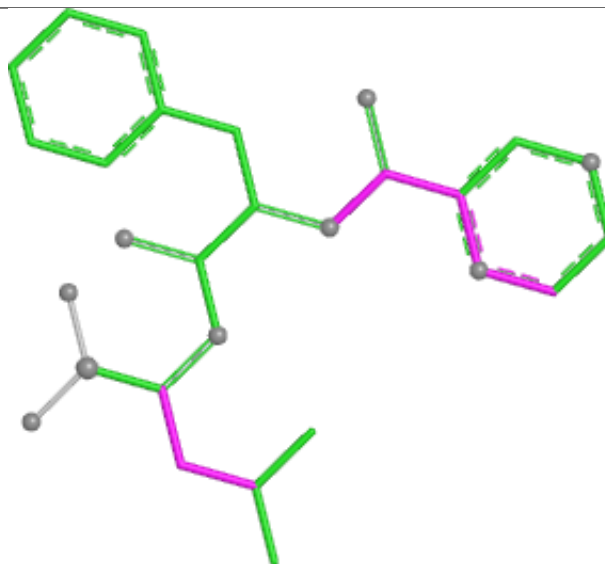


Rings

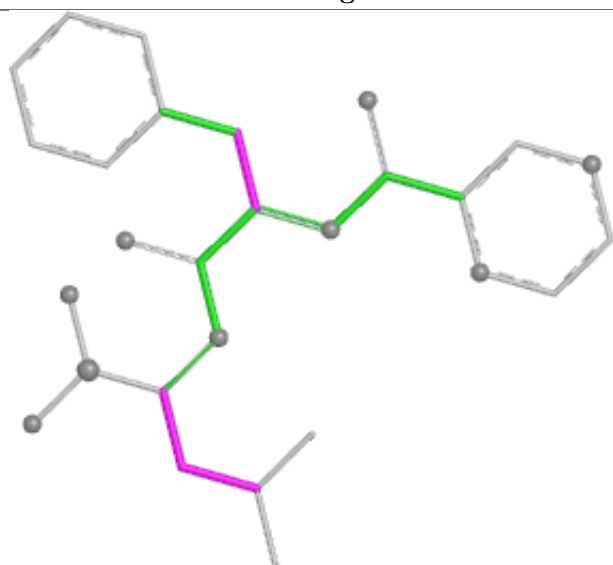
Ligand BO2 D 301



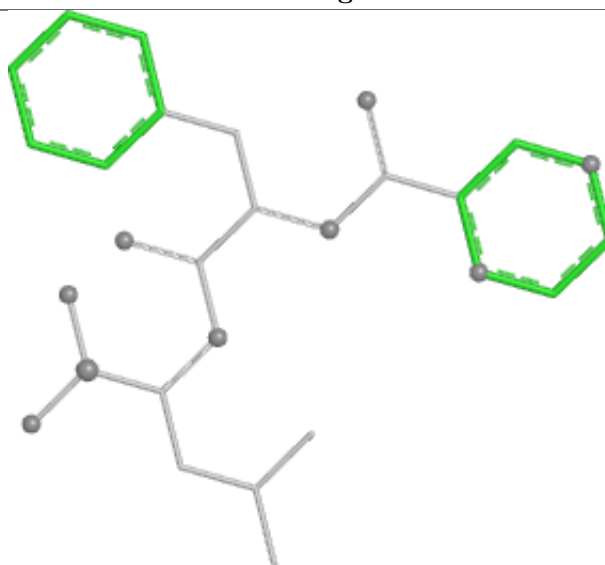
Bond lengths



Bond angles

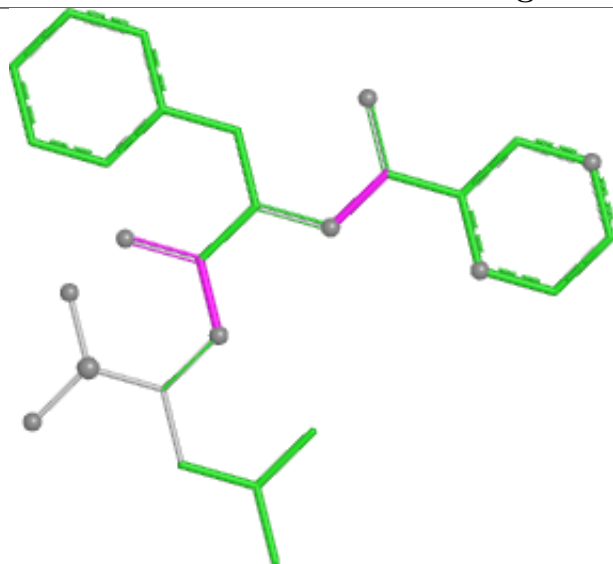


Torsions

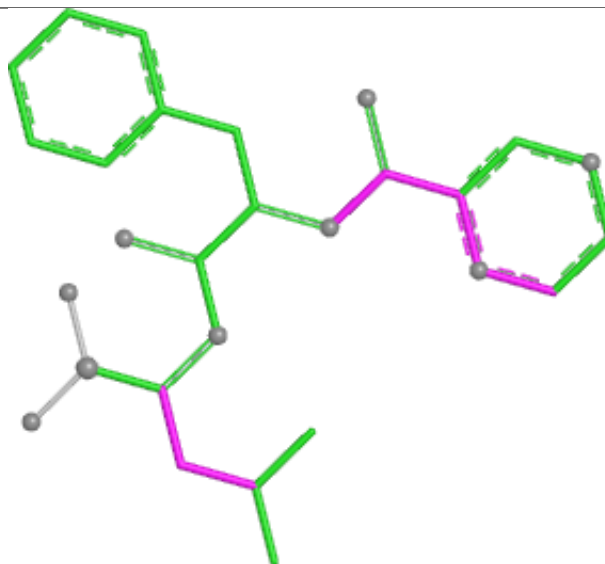


Rings

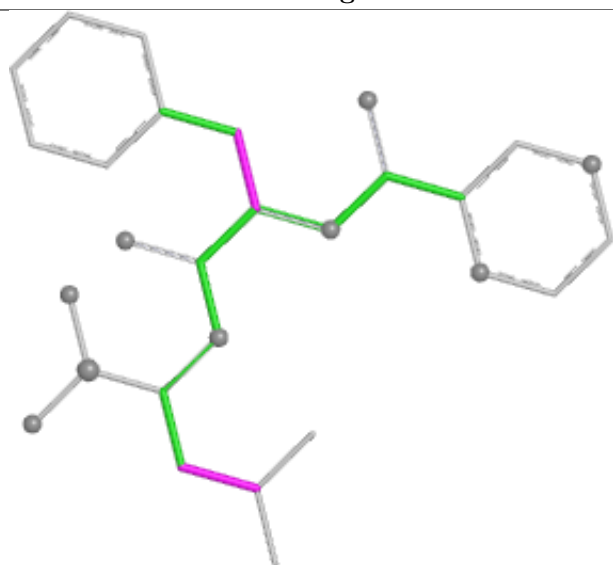
Ligand BO2 B 301



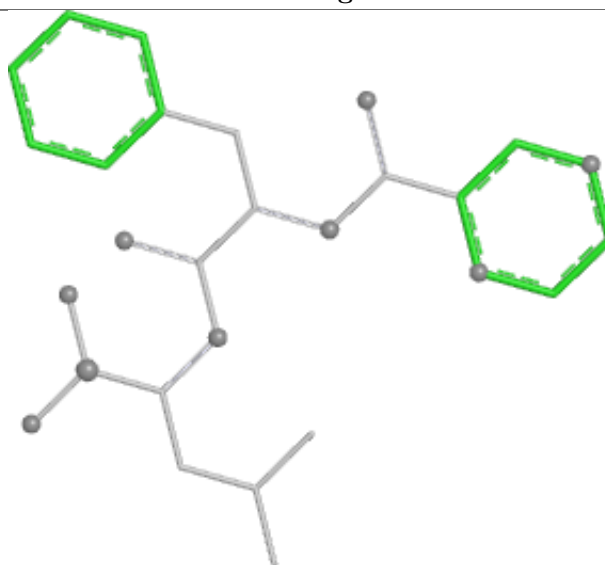
Bond lengths



Bond angles

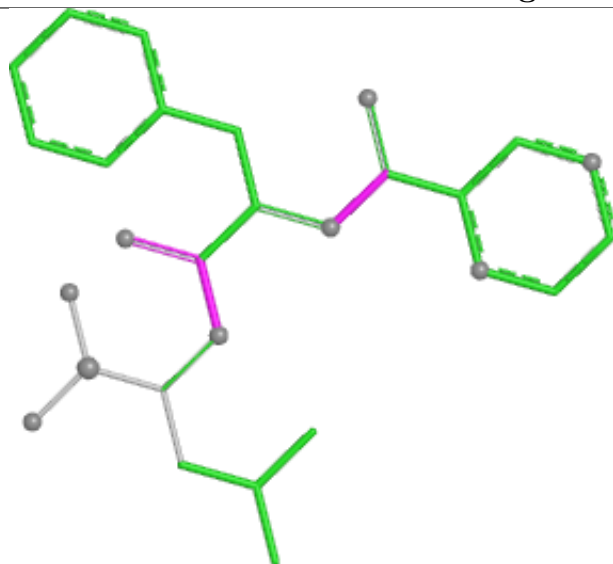


Torsions

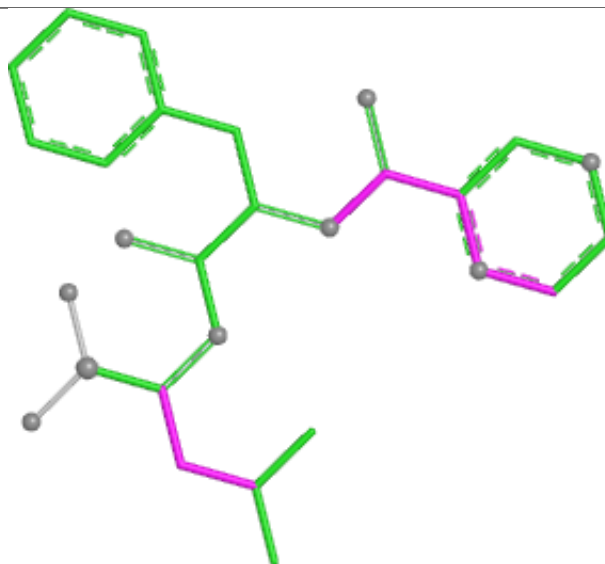


Rings

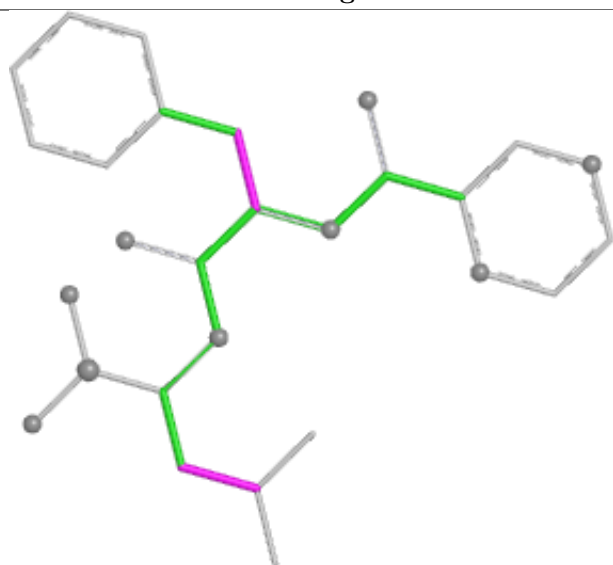
Ligand BO2 L 301



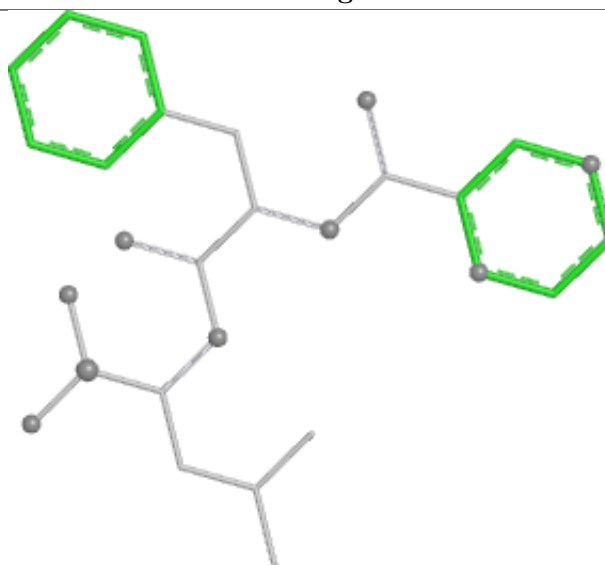
Bond lengths



Bond angles

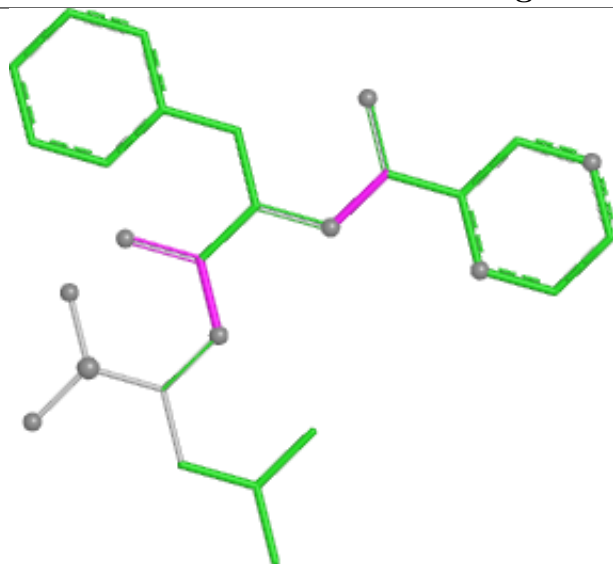


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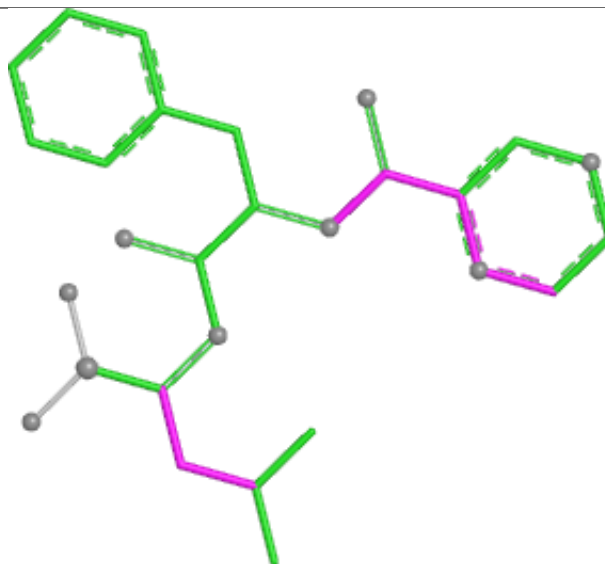


Rings

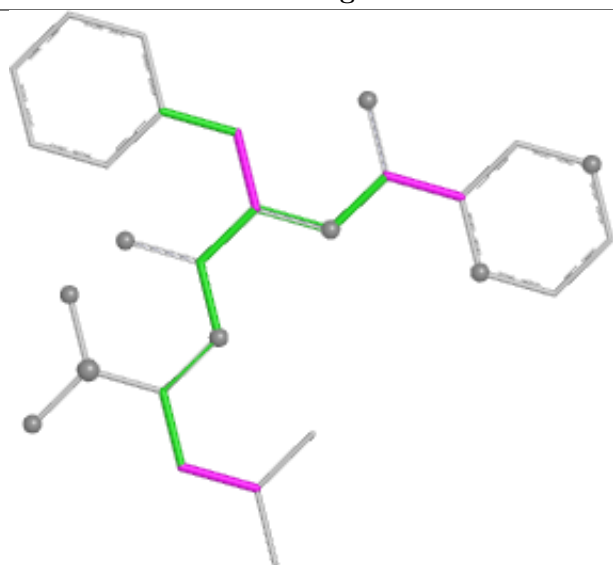
Ligand BO2 G 301



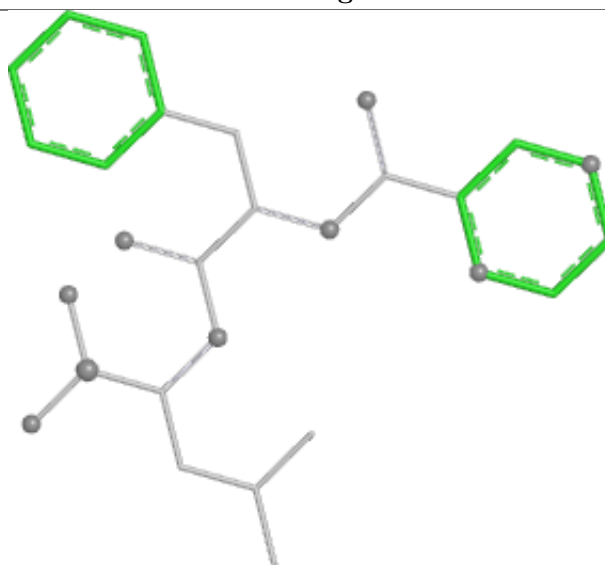
Bond lengths



Bond angles

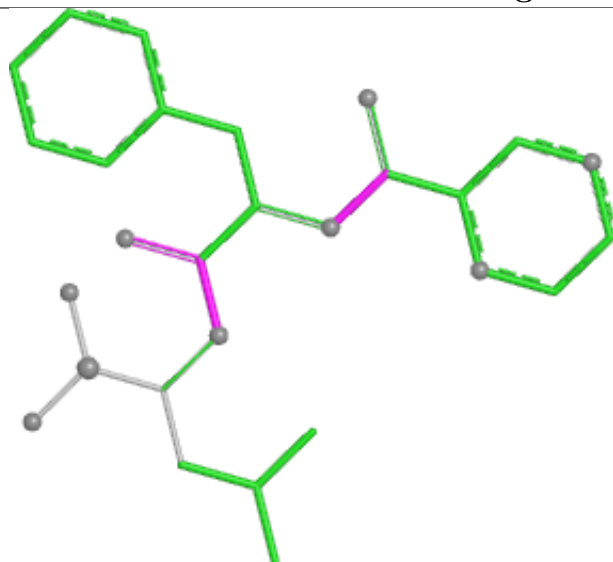


Torsions

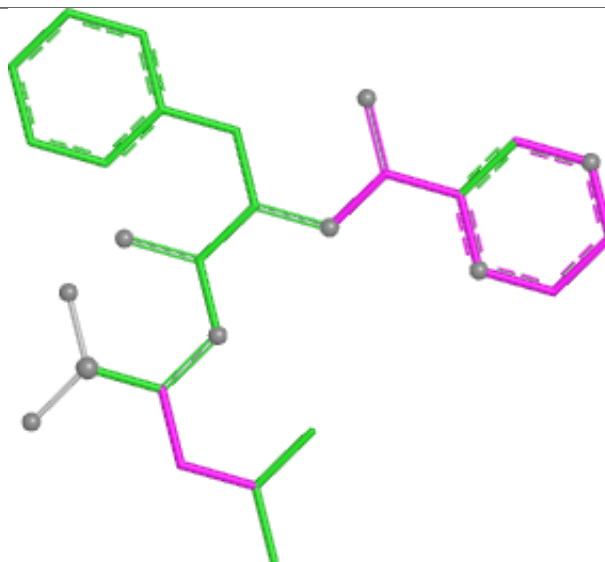


Rings

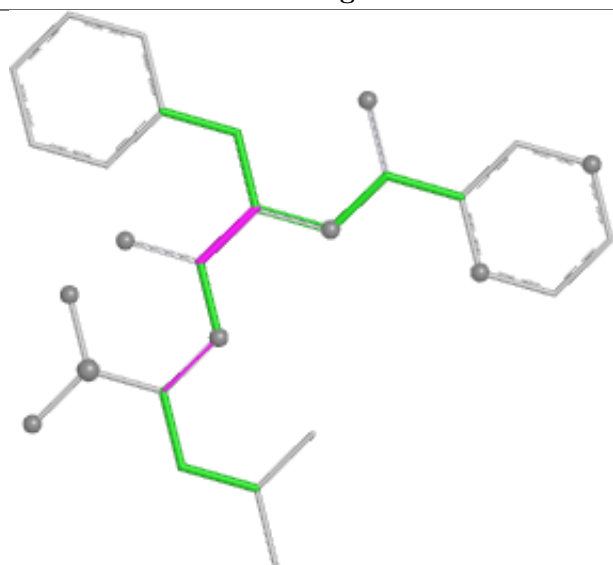
Ligand BO2 N 301



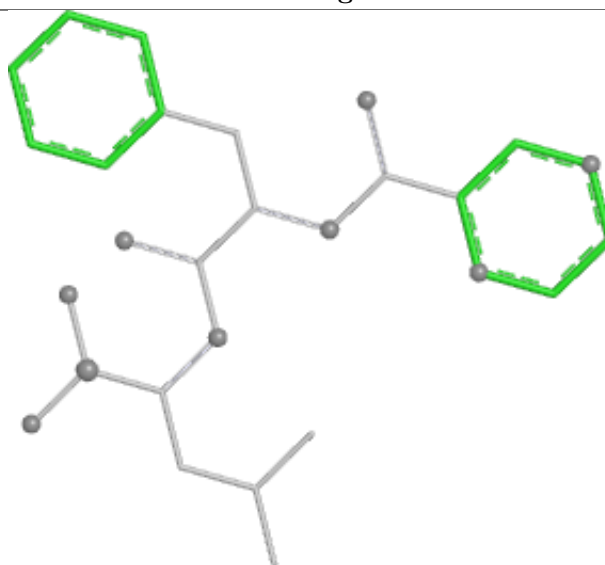
Bond lengths



Bond angles

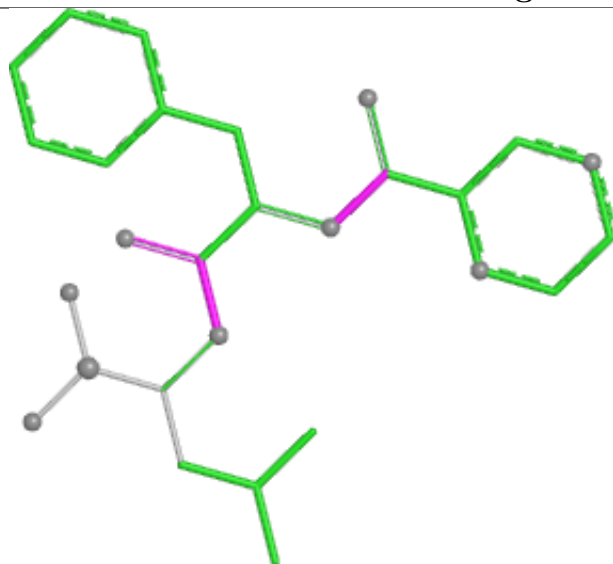


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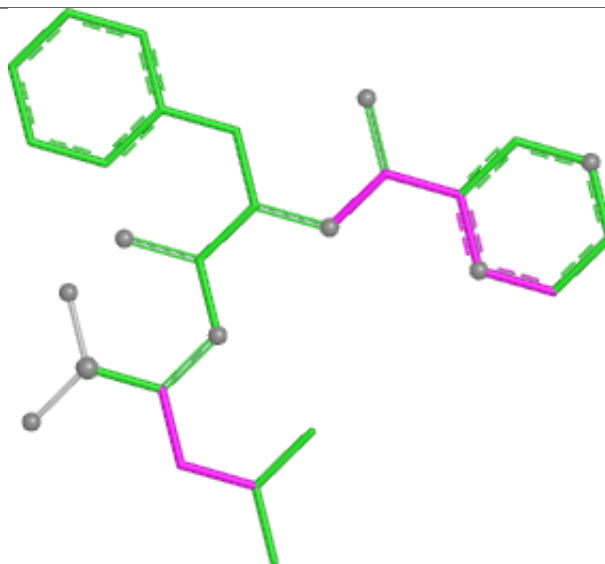


Rings

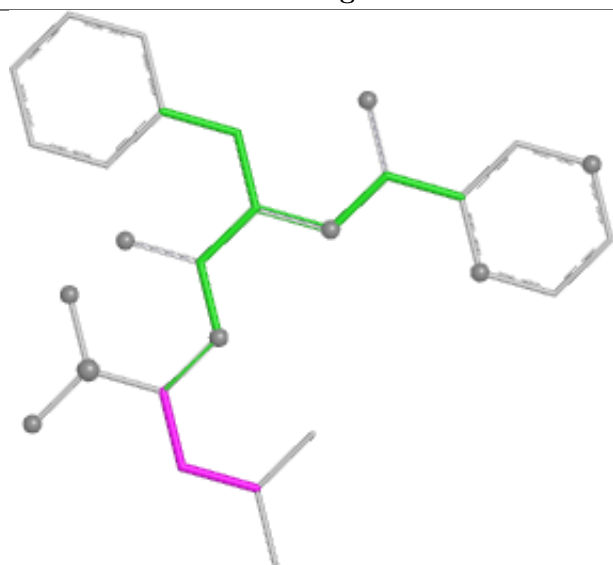
Ligand BO2 H 301



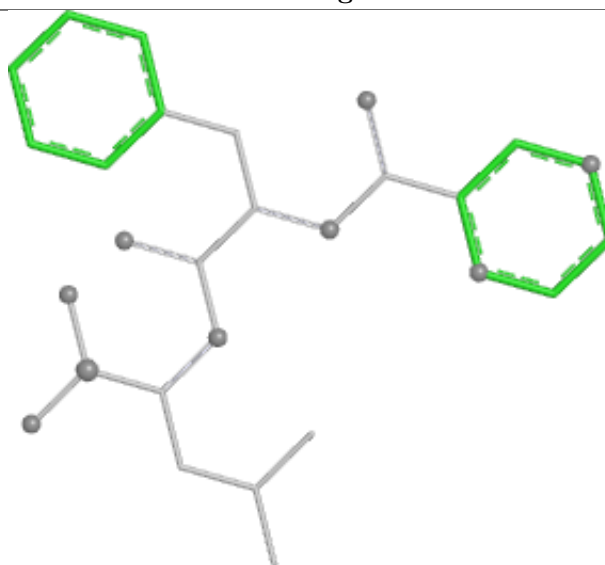
Bond lengths



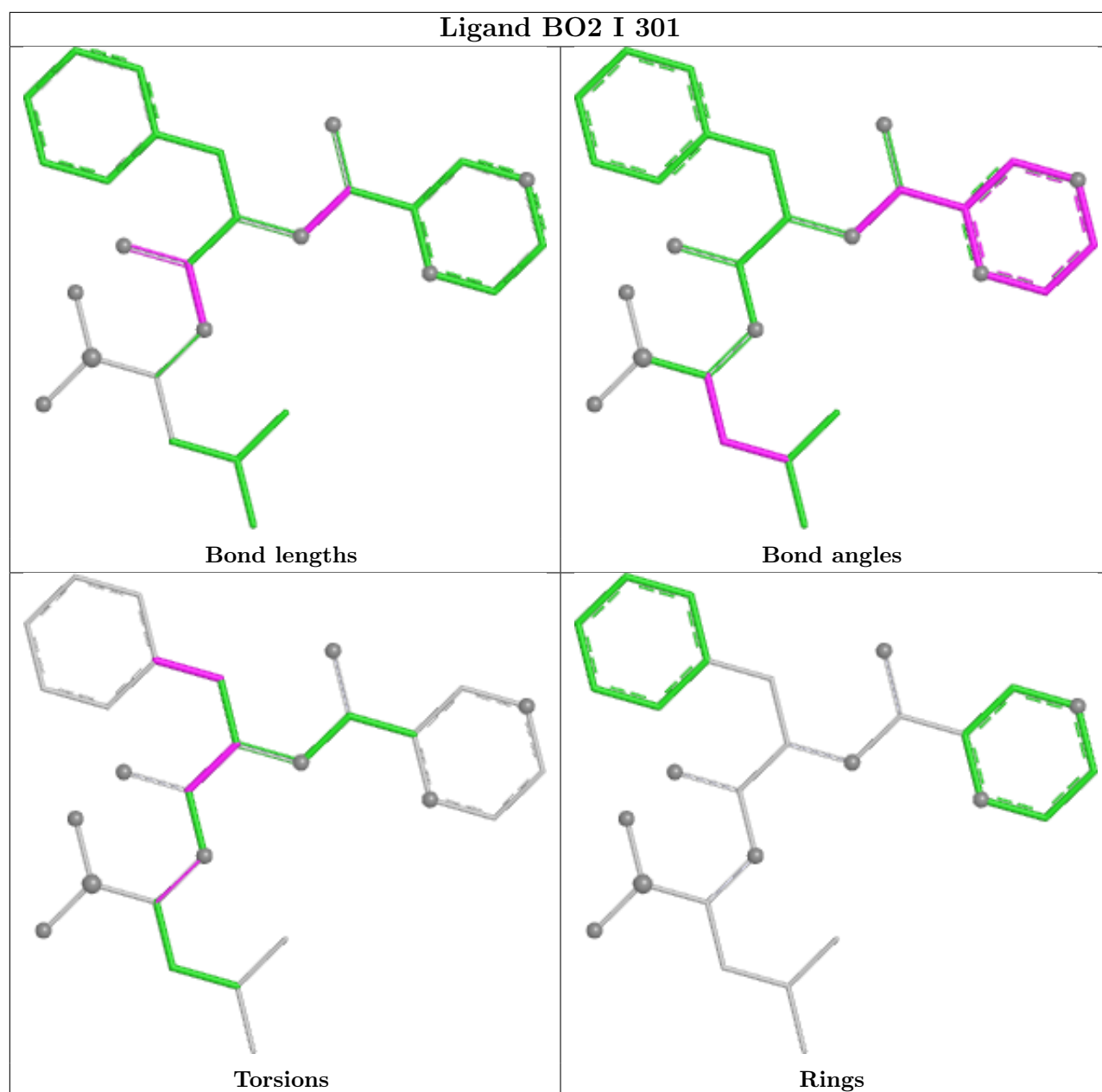
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	181/277 (65%)	-0.84	0 100 100	91, 112, 146, 182	0
1	B	183/277 (66%)	-0.85	0 100 100	86, 108, 140, 169	0
1	C	182/277 (65%)	-0.83	0 100 100	90, 115, 148, 166	0
1	D	180/277 (64%)	-0.79	0 100 100	111, 142, 175, 198	0
1	E	181/277 (65%)	-0.73	0 100 100	113, 146, 180, 208	0
1	F	181/277 (65%)	-0.76	0 100 100	63, 138, 164, 192	1 (0%)
1	G	180/277 (64%)	-0.80	0 100 100	95, 118, 154, 207	0
1	H	185/277 (66%)	-0.83	0 100 100	85, 115, 153, 209	0
1	I	178/277 (64%)	-0.79	0 100 100	107, 139, 171, 213	0
1	J	179/277 (64%)	-0.78	0 100 100	121, 154, 188, 229	0
1	K	178/277 (64%)	-0.76	0 100 100	124, 154, 185, 204	0
1	L	180/277 (64%)	-0.83	0 100 100	106, 137, 172, 198	0
1	M	184/277 (66%)	-0.83	0 100 100	93, 118, 149, 180	0
1	N	183/277 (66%)	-0.84	0 100 100	54, 107, 152, 200	1 (0%)
All	All	2535/3878 (65%)	-0.80	0 100 100	54, 130, 171, 229	2 (0%)

There are no RSRZ outliers to report.

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 ⓘ

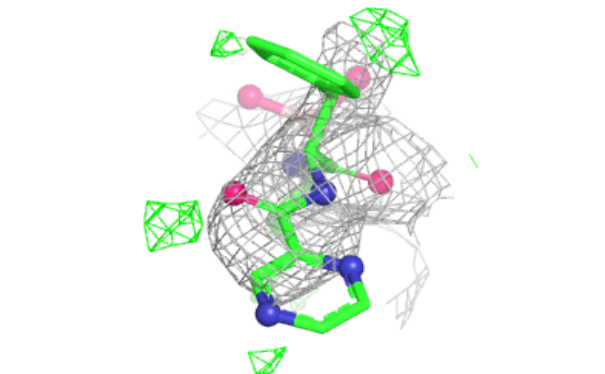
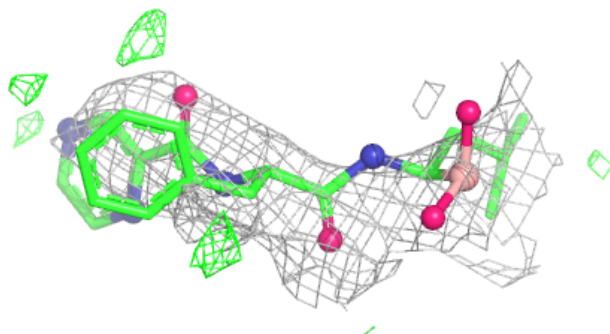
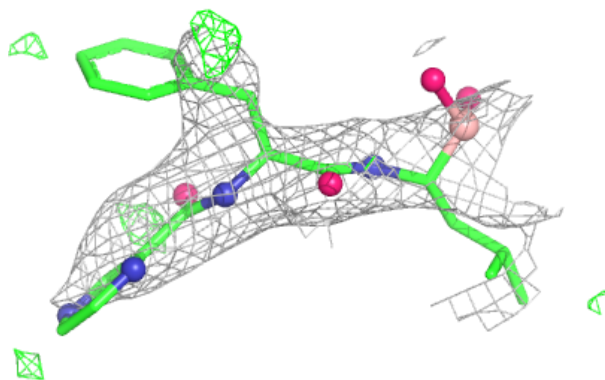
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	G	302	1/1	0.16	0.17	501,501,501,501	0
3	CL	C	302	1/1	0.34	0.16	216,216,216,216	0
3	CL	F	302	1/1	0.42	0.12	358,358,358,358	0
3	CL	I	302	1/1	0.43	0.16	203,203,203,203	0
3	CL	N	302	1/1	0.49	0.15	204,204,204,204	0
3	CL	L	302	1/1	0.65	0.16	222,222,222,222	0
3	CL	H	302	1/1	0.74	0.13	185,185,185,185	0
2	BO2	J	301	28/28	0.85	0.12	120,144,153,157	0
2	BO2	K	301	28/28	0.85	0.12	133,147,167,178	0
2	BO2	D	301	28/28	0.85	0.13	109,129,142,150	28
2	BO2	H	301	28/28	0.86	0.12	96,114,141,151	0
2	BO2	G	301	28/28	0.87	0.11	98,131,150,153	0
2	BO2	L	301	28/28	0.88	0.11	117,137,152,155	0
2	BO2	B	301	28/28	0.89	0.11	92,110,127,128	28
2	BO2	M	301	28/28	0.90	0.11	90,118,131,140	0
2	BO2	C	301	28/28	0.90	0.11	95,113,127,137	28
2	BO2	A	301	28/28	0.90	0.10	90,113,130,143	0
2	BO2	I	301	28/28	0.90	0.09	118,140,152,155	0
2	BO2	N	301	28/28	0.91	0.12	95,115,137,147	28
2	BO2	F	301	28/28	0.92	0.09	113,136,148,153	0
2	BO2	E	301	28/28	0.92	0.11	114,136,152,165	28
3	CL	A	303	1/1	0.95	0.10	149,149,149,149	0
3	CL	A	302	1/1	0.95	0.08	108,108,108,108	0

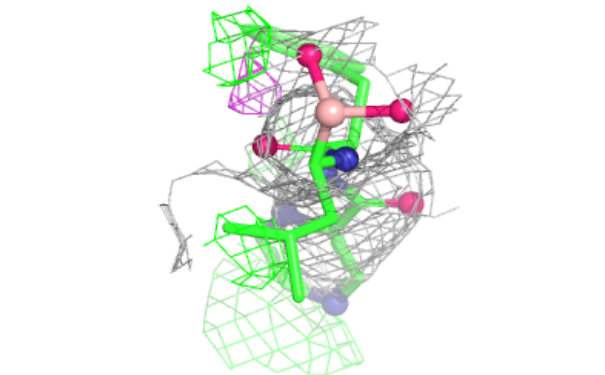
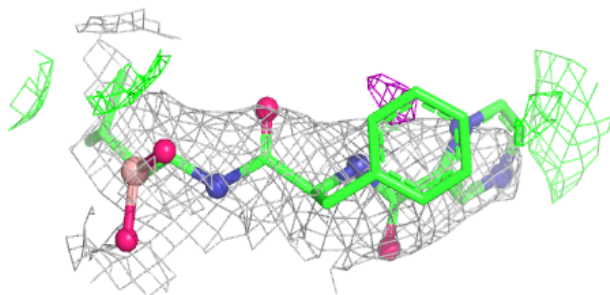
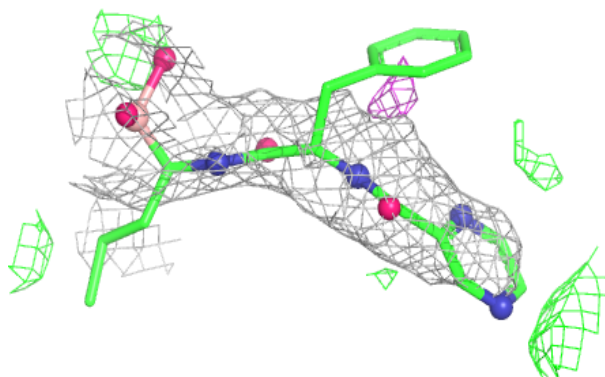
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BO2 J 301:

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

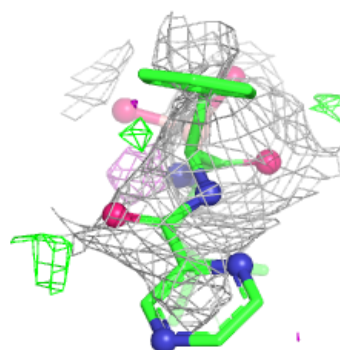
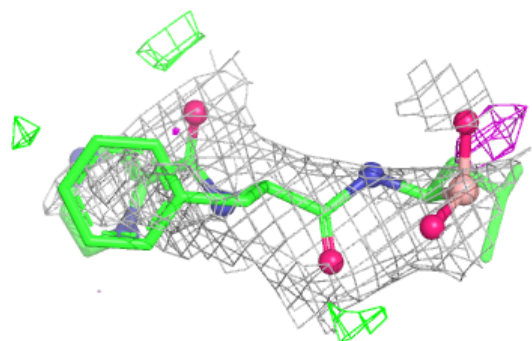
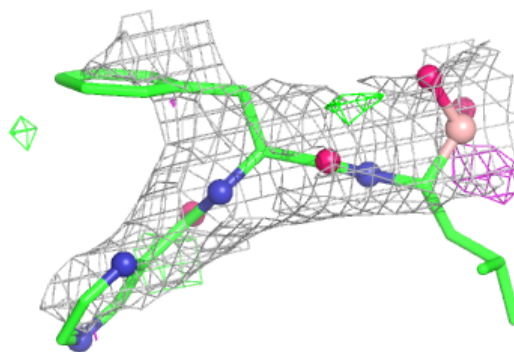
**Electron density around BO2 K 301:**

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

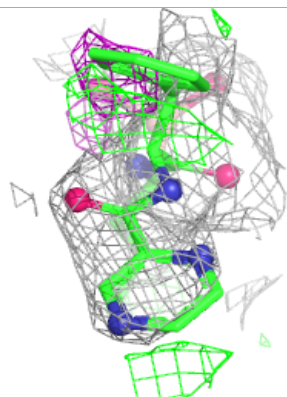
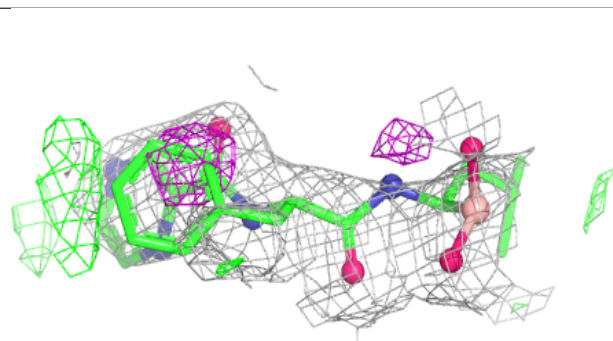
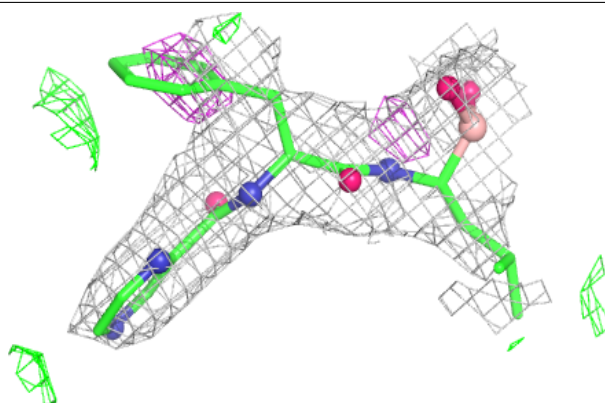


Electron density around BO2 D 301:

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

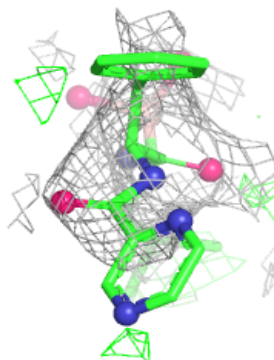
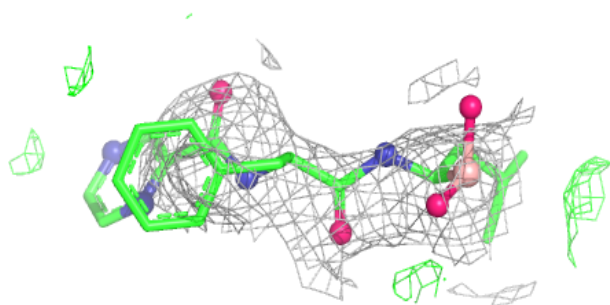
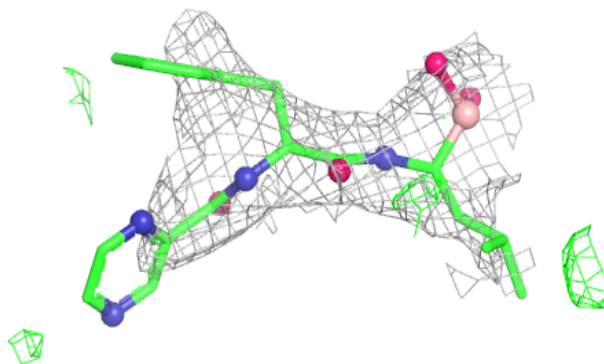
**Electron density around BO2 H 301:**

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

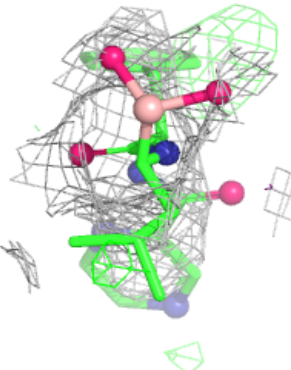
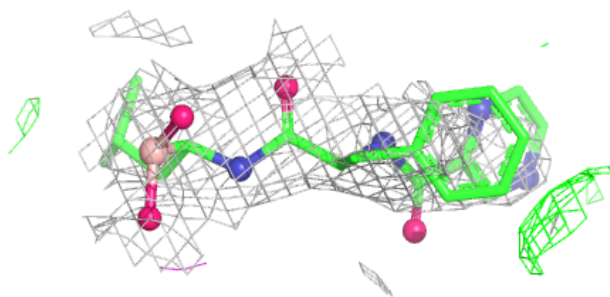
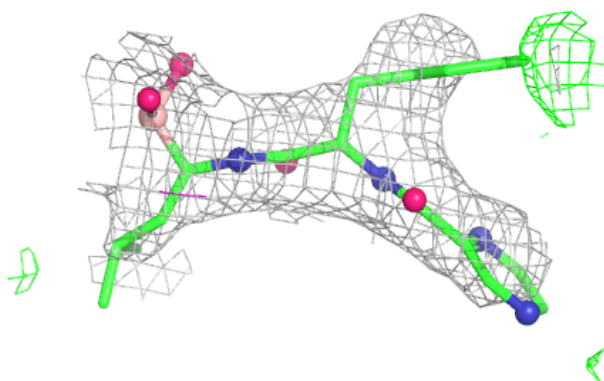


Electron density around BO2 G 301:

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

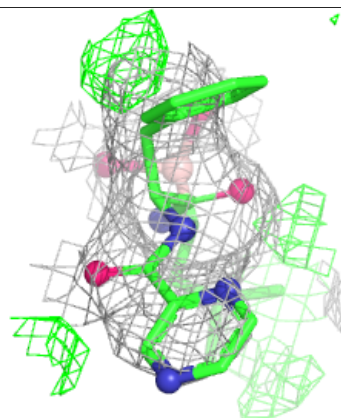
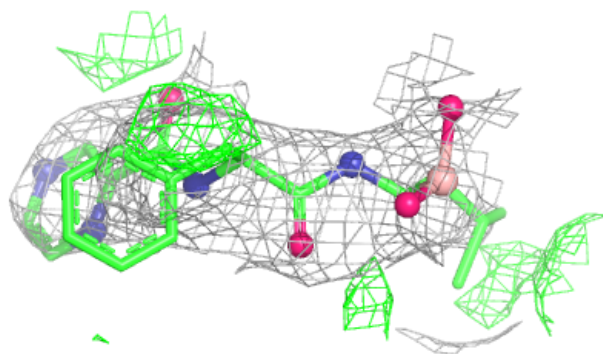
**Electron density around BO2 L 301:**

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



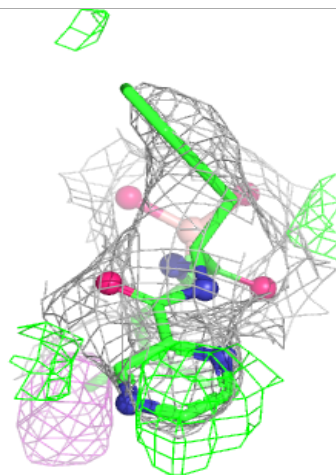
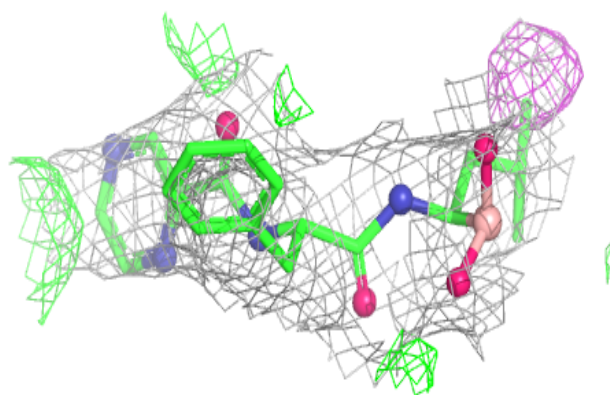
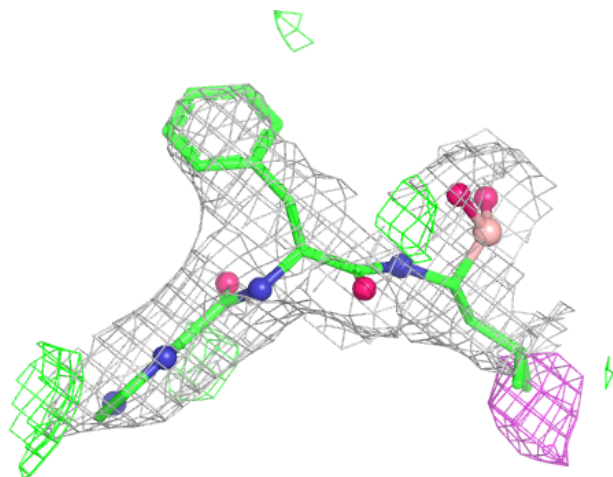
Electron density around BO2 B 301:

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



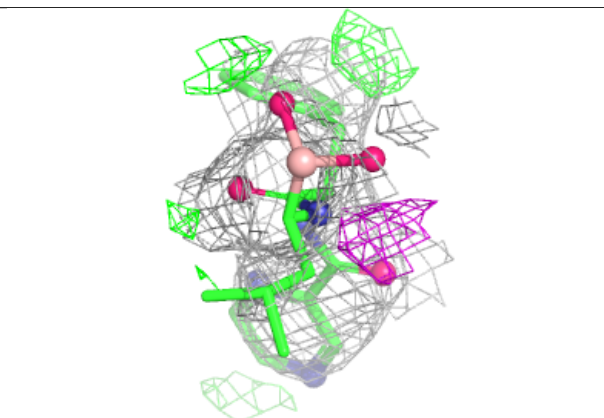
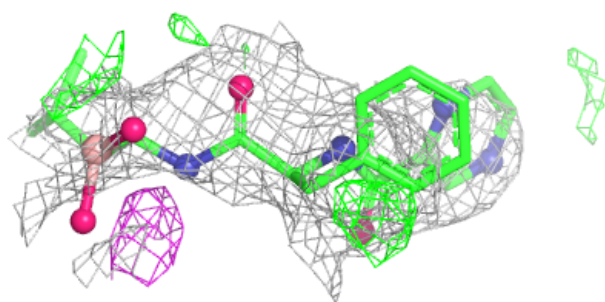
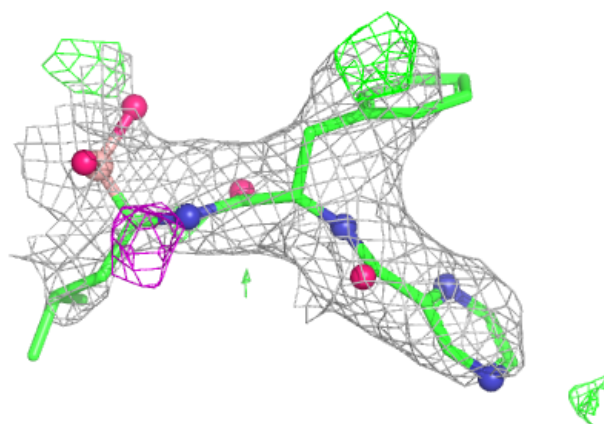
Electron density around BO2 M 301:

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

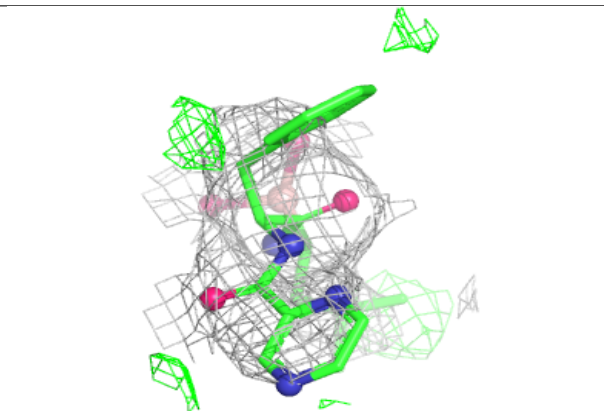
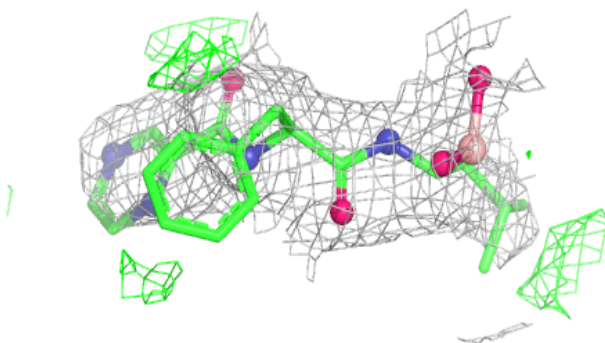
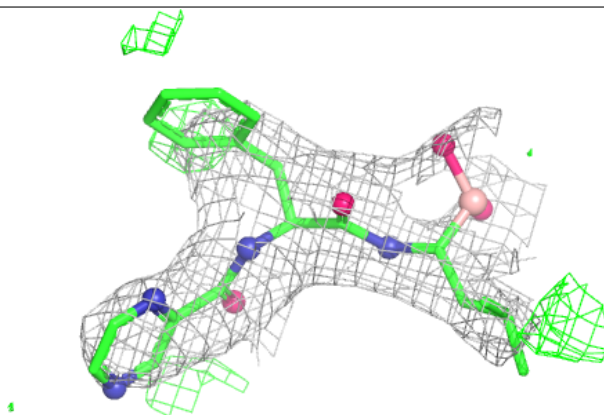


Electron density around BO2 C 301:

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

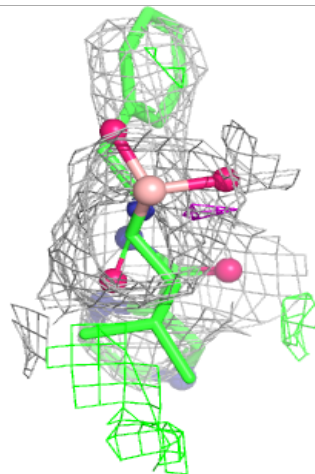
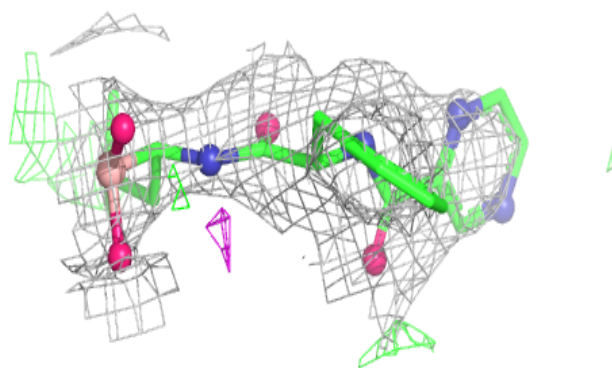
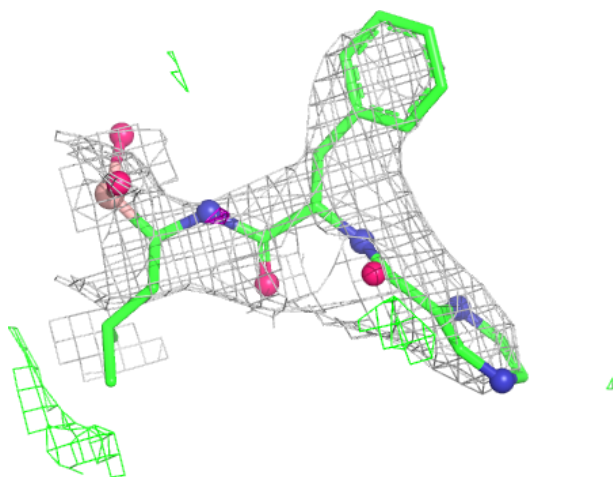
**Electron density around BO2 A 301:**

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



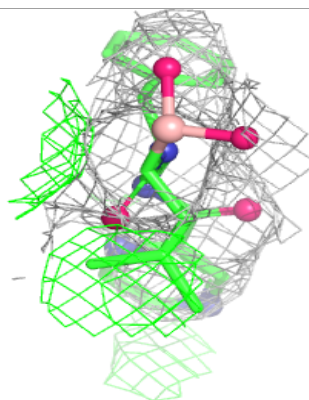
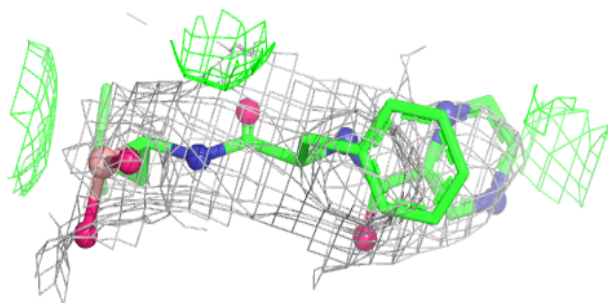
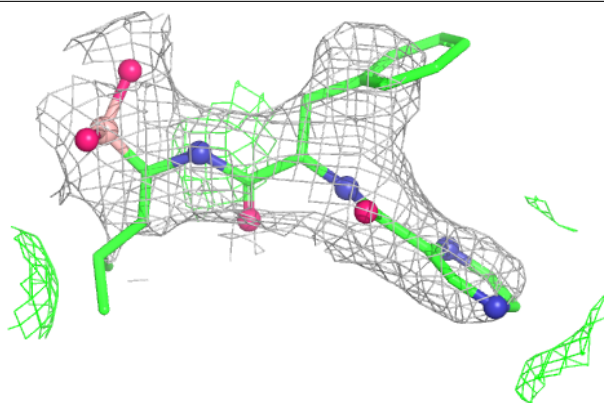
Electron density around BO2 I 301:

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

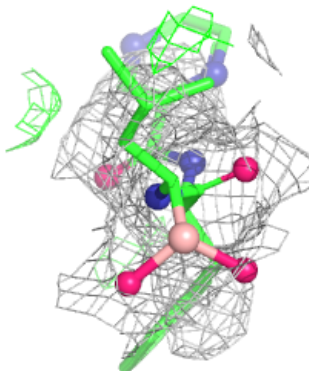
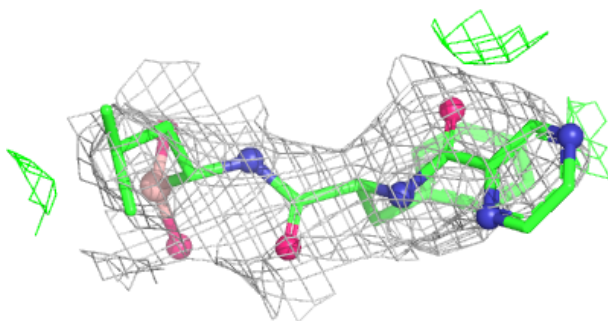
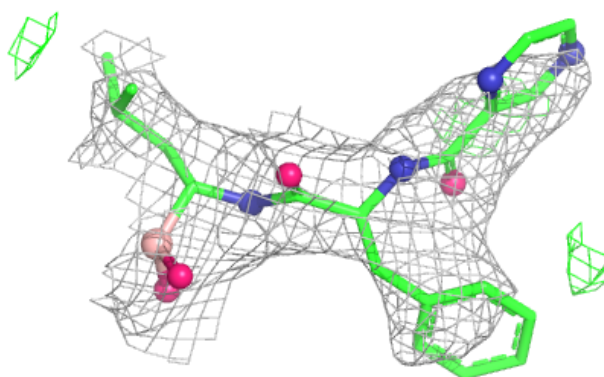


Electron density around BO2 N 301:

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

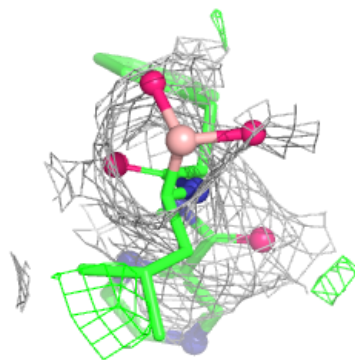
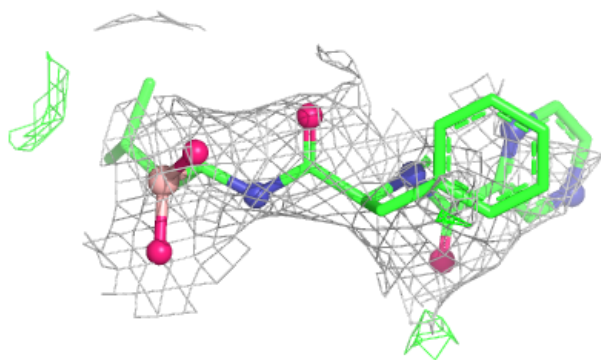
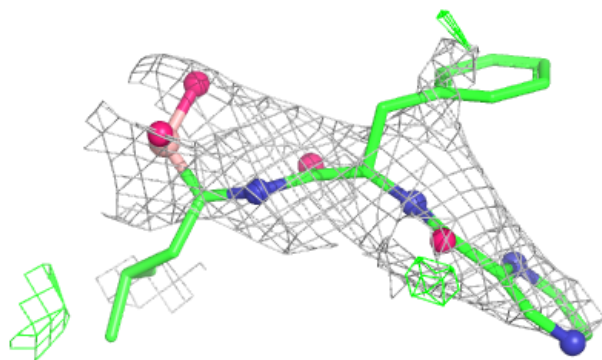
**Electron density around BO2 F 301:**

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



Electron density around BO2 E 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.