wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2024 – 12:16 PM JST

PDB ID	:	9IRP
Title	:	Structure of ClpP from Staphylococcus aureus in complex with ZG297
Authors	:	Wei, B.Y.; Wang, P.Y.; Zhang, T.; Yang, C.-G.
Deposited on	:	2024-07-16
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

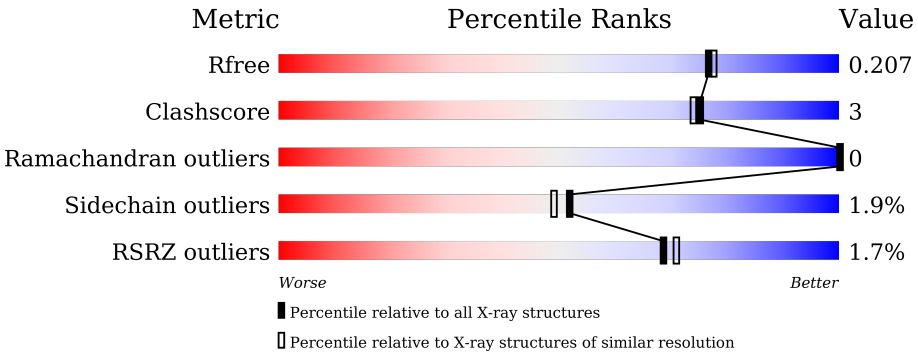
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 <=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	201	89% 6%
1	B	201	3% 91% 5%
1	C	201	2% 90% 7%
1	D	201	4% 88% 6% 6%
1	E	201	88% 6%
1	F	201	89% 8%

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Mol	Chain	Length	Quality of chain
1	G	201	
1	H	201	
1	I	201	
1	J	201	
1	K	201	
1	L	201	
1	M	201	
1	N	201	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22615 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1439	907	245	281	6			
1	B	193	Total	C	N	O	S	0	0	0
			1466	923	255	282	6			
1	C	187	Total	C	N	O	S	0	0	0
			1418	895	242	275	6			
1	D	189	Total	C	N	O	S	0	0	1
			1434	905	243	280	6			
1	E	192	Total	C	N	O	S	0	0	0
			1476	927	253	290	6			
1	F	194	Total	C	N	O	S	0	0	1
			1466	921	250	289	6			
1	G	185	Total	C	N	O	S	0	0	0
			1410	889	238	277	6			
1	H	183	Total	C	N	O	S	0	0	0
			1403	886	238	273	6			
1	I	191	Total	C	N	O	S	0	0	1
			1448	911	246	285	6			
1	J	190	Total	C	N	O	S	0	0	0
			1454	912	247	289	6			
1	K	184	Total	C	N	O	S	0	0	1
			1397	883	238	270	6			
1	L	189	Total	C	N	O	S	0	0	0
			1442	908	248	280	6			
1	M	186	Total	C	N	O	S	0	0	0
			1406	886	241	273	6			
1	N	184	Total	C	N	O	S	0	0	0
			1407	889	238	274	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	HIS	-	expression tag	UNP A0A0D1I3W4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	-	expression tag	UNP A0A0D1I3W4
A	198	HIS	-	expression tag	UNP A0A0D1I3W4
A	199	HIS	-	expression tag	UNP A0A0D1I3W4
A	200	HIS	-	expression tag	UNP A0A0D1I3W4
A	201	HIS	-	expression tag	UNP A0A0D1I3W4
B	196	HIS	-	expression tag	UNP A0A0D1I3W4
B	197	HIS	-	expression tag	UNP A0A0D1I3W4
B	198	HIS	-	expression tag	UNP A0A0D1I3W4
B	199	HIS	-	expression tag	UNP A0A0D1I3W4
B	200	HIS	-	expression tag	UNP A0A0D1I3W4
B	201	HIS	-	expression tag	UNP A0A0D1I3W4
C	196	HIS	-	expression tag	UNP A0A0D1I3W4
C	197	HIS	-	expression tag	UNP A0A0D1I3W4
C	198	HIS	-	expression tag	UNP A0A0D1I3W4
C	199	HIS	-	expression tag	UNP A0A0D1I3W4
C	200	HIS	-	expression tag	UNP A0A0D1I3W4
C	201	HIS	-	expression tag	UNP A0A0D1I3W4
D	196	HIS	-	expression tag	UNP A0A0D1I3W4
D	197	HIS	-	expression tag	UNP A0A0D1I3W4
D	198	HIS	-	expression tag	UNP A0A0D1I3W4
D	199	HIS	-	expression tag	UNP A0A0D1I3W4
D	200	HIS	-	expression tag	UNP A0A0D1I3W4
D	201	HIS	-	expression tag	UNP A0A0D1I3W4
E	196	HIS	-	expression tag	UNP A0A0D1I3W4
E	197	HIS	-	expression tag	UNP A0A0D1I3W4
E	198	HIS	-	expression tag	UNP A0A0D1I3W4
E	199	HIS	-	expression tag	UNP A0A0D1I3W4
E	200	HIS	-	expression tag	UNP A0A0D1I3W4
E	201	HIS	-	expression tag	UNP A0A0D1I3W4
F	196	HIS	-	expression tag	UNP A0A0D1I3W4
F	197	HIS	-	expression tag	UNP A0A0D1I3W4
F	198	HIS	-	expression tag	UNP A0A0D1I3W4
F	199	HIS	-	expression tag	UNP A0A0D1I3W4
F	200	HIS	-	expression tag	UNP A0A0D1I3W4
F	201	HIS	-	expression tag	UNP A0A0D1I3W4
G	196	HIS	-	expression tag	UNP A0A0D1I3W4
G	197	HIS	-	expression tag	UNP A0A0D1I3W4
G	198	HIS	-	expression tag	UNP A0A0D1I3W4
G	199	HIS	-	expression tag	UNP A0A0D1I3W4
G	200	HIS	-	expression tag	UNP A0A0D1I3W4
G	201	HIS	-	expression tag	UNP A0A0D1I3W4
H	196	HIS	-	expression tag	UNP A0A0D1I3W4

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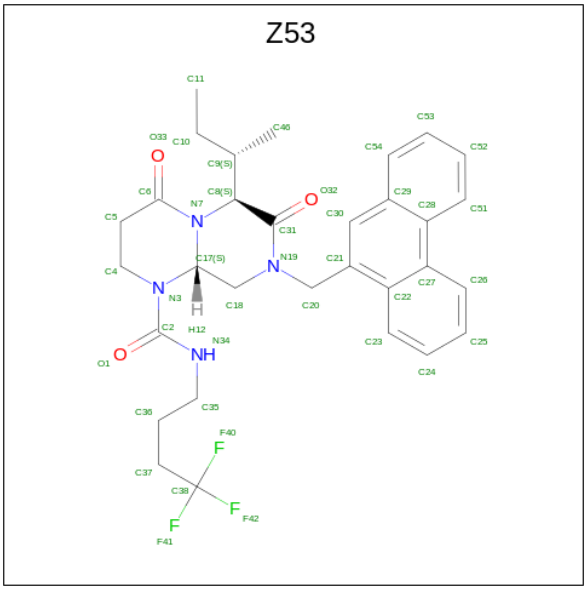
Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	-	expression tag	UNP A0A0D1I3W4
H	198	HIS	-	expression tag	UNP A0A0D1I3W4
H	199	HIS	-	expression tag	UNP A0A0D1I3W4
H	200	HIS	-	expression tag	UNP A0A0D1I3W4
H	201	HIS	-	expression tag	UNP A0A0D1I3W4
I	196	HIS	-	expression tag	UNP A0A0D1I3W4
I	197	HIS	-	expression tag	UNP A0A0D1I3W4
I	198	HIS	-	expression tag	UNP A0A0D1I3W4
I	199	HIS	-	expression tag	UNP A0A0D1I3W4
I	200	HIS	-	expression tag	UNP A0A0D1I3W4
I	201	HIS	-	expression tag	UNP A0A0D1I3W4
J	196	HIS	-	expression tag	UNP A0A0D1I3W4
J	197	HIS	-	expression tag	UNP A0A0D1I3W4
J	198	HIS	-	expression tag	UNP A0A0D1I3W4
J	199	HIS	-	expression tag	UNP A0A0D1I3W4
J	200	HIS	-	expression tag	UNP A0A0D1I3W4
J	201	HIS	-	expression tag	UNP A0A0D1I3W4
K	196	HIS	-	expression tag	UNP A0A0D1I3W4
K	197	HIS	-	expression tag	UNP A0A0D1I3W4
K	198	HIS	-	expression tag	UNP A0A0D1I3W4
K	199	HIS	-	expression tag	UNP A0A0D1I3W4
K	200	HIS	-	expression tag	UNP A0A0D1I3W4
K	201	HIS	-	expression tag	UNP A0A0D1I3W4
L	196	HIS	-	expression tag	UNP A0A0D1I3W4
L	197	HIS	-	expression tag	UNP A0A0D1I3W4
L	198	HIS	-	expression tag	UNP A0A0D1I3W4
L	199	HIS	-	expression tag	UNP A0A0D1I3W4
L	200	HIS	-	expression tag	UNP A0A0D1I3W4
L	201	HIS	-	expression tag	UNP A0A0D1I3W4
M	196	HIS	-	expression tag	UNP A0A0D1I3W4
M	197	HIS	-	expression tag	UNP A0A0D1I3W4
M	198	HIS	-	expression tag	UNP A0A0D1I3W4
M	199	HIS	-	expression tag	UNP A0A0D1I3W4
M	200	HIS	-	expression tag	UNP A0A0D1I3W4
M	201	HIS	-	expression tag	UNP A0A0D1I3W4
N	196	HIS	-	expression tag	UNP A0A0D1I3W4
N	197	HIS	-	expression tag	UNP A0A0D1I3W4
N	198	HIS	-	expression tag	UNP A0A0D1I3W4
N	199	HIS	-	expression tag	UNP A0A0D1I3W4
N	200	HIS	-	expression tag	UNP A0A0D1I3W4
N	201	HIS	-	expression tag	UNP A0A0D1I3W4

- Molecule 2 is (6S,9aS)-6-[(2S)-butan-2-yl]-4,7-bis(oxidanylidene)-8-(phenanthren-9-ylmethyl

)-N-[4,4,4-tris(fluoranyl)butyl]-3,6,9,9a-tetrahydro-2H-pyrazino[1,2-a]pyrimidine-1-carboxamide (three-letter code: Z53) (formula: $C_{31}H_{35}F_3N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	B	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	C	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	D	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	E	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	F	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	G	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	H	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	I	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	J	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	K	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	L	1	Total	C	F	N	O	0	0
			41	31	3	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	F	N	O	0	0
			41	31	3	4	3		
2	N	1	Total	C	F	N	O	0	0
			41	31	3	4	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	127	Total	O	0	0
			127	127		
4	C	117	Total	O	0	0
			117	117		

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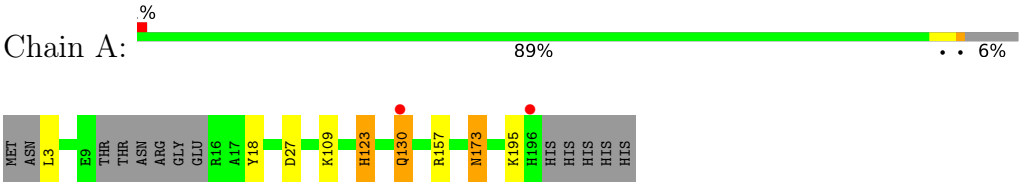
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	146	Total O 146 146	0	0
4	E	169	Total O 169 169	0	0
4	F	170	Total O 170 170	0	0
4	G	157	Total O 157 157	0	0
4	H	111	Total O 111 111	0	0
4	I	149	Total O 149 149	0	0
4	J	159	Total O 159 159	0	0
4	K	147	Total O 147 147	0	0
4	L	156	Total O 156 156	0	0
4	M	110	Total O 110 110	0	0
4	N	82	Total O 82 82	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.

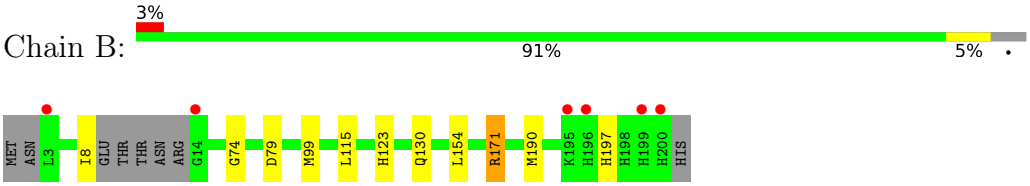
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



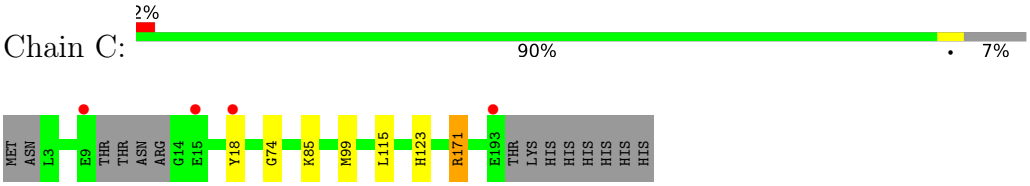
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



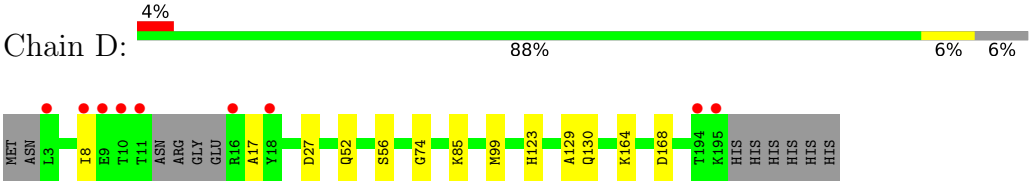
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



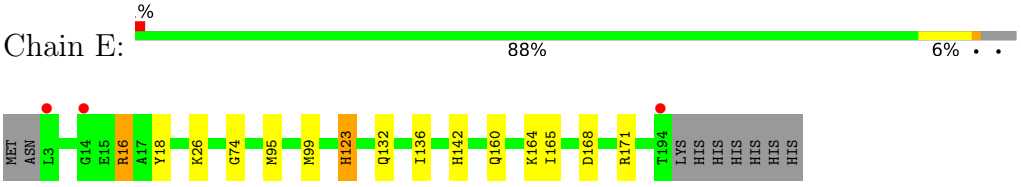
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



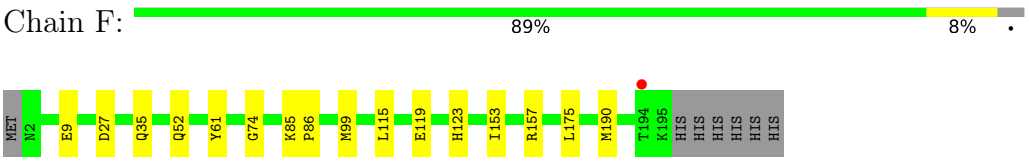
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



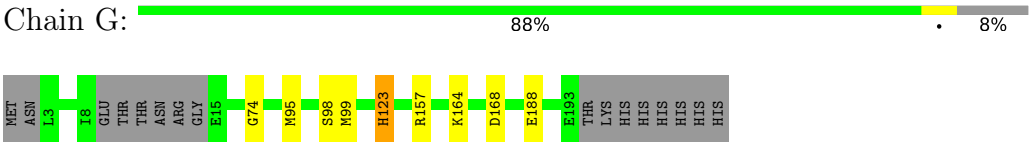
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



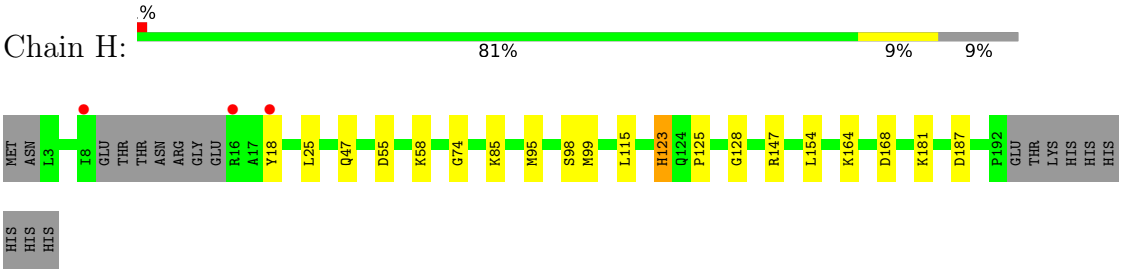
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



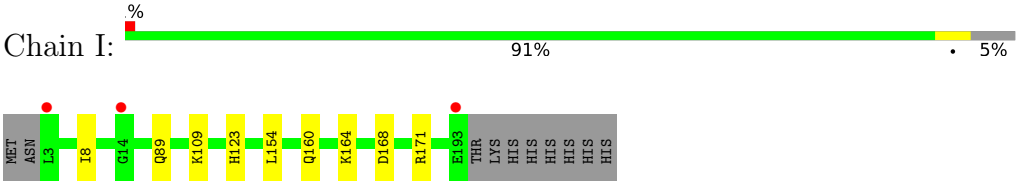
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



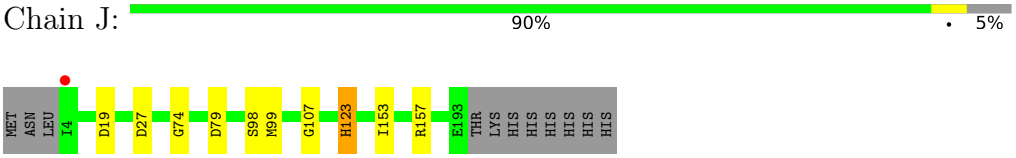
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



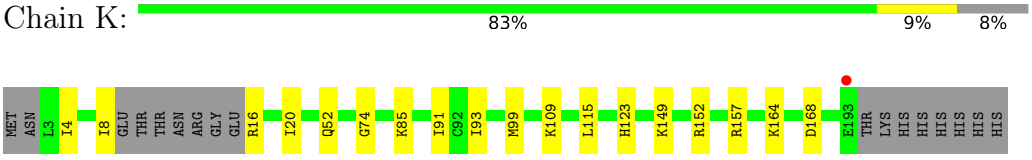
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



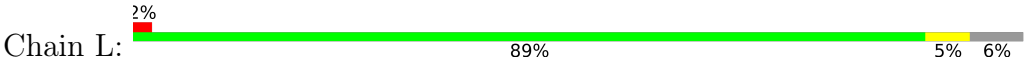
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

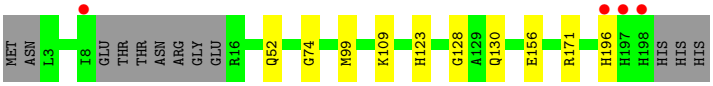
Chain K:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

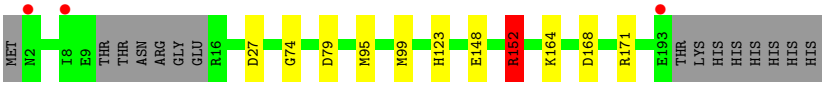
Chain L:





• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.58Å 190.32Å 96.40Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	29.86 – 1.90 29.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.86-1.90) 89.9 (29.86-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.91Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.173 , 0.208 0.173 , 0.207	Depositor DCC
R_{free} test set	12000 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -h-l,k,h 0.013 for l,k,-h-l 0.025 for h,-k,-h-l 0.028 for -h-l,-k,l 0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22615	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, Z53

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	0.41	0/1458	0.60	0/1969
1	B	0.37	0/1488	0.56	0/2013
1	C	0.41	0/1436	0.67	1/1940 (0.1%)
1	D	0.45	0/1452	0.64	0/1961
1	E	0.43	0/1495	0.63	1/2021 (0.0%)
1	F	0.40	0/1485	0.66	1/2009 (0.0%)
1	G	0.46	0/1428	0.62	0/1931
1	H	0.41	0/1421	0.58	0/1919
1	I	0.40	0/1467	0.62	0/1985
1	J	0.44	0/1473	0.65	0/1993
1	K	0.44	0/1415	0.63	0/1912
1	L	0.44	0/1462	0.60	0/1976
1	M	0.41	0/1424	0.62	1/1926 (0.1%)
1	N	0.40	0/1425	0.58	0/1926
All	All	0.42	0/20329	0.62	4/27481 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	175	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	C	85	LYS	CA-CB-CG	5.16	124.76	113.40
1	E	16	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	M	152	ARG	NE-CZ-NH1	-5.13	117.73	120.30

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	1439	0	1441	6	0
1	B	1466	0	1447	9	0
1	C	1418	0	1421	5	0
1	D	1434	0	1440	10	0
1	E	1476	0	1485	16	0
1	F	1466	0	1458	10	0
1	G	1410	0	1404	8	0
1	H	1403	0	1416	15	0
1	I	1448	0	1444	6	0
1	J	1454	0	1447	7	0
1	K	1397	0	1407	14	0
1	L	1442	0	1434	7	1
1	M	1406	0	1398	6	0
1	N	1407	0	1416	9	1
2	A	41	0	0	0	0
2	B	41	0	0	0	0
2	C	41	0	0	0	0
2	D	41	0	0	0	0
2	E	41	0	0	0	0
2	F	41	0	0	0	0
2	G	41	0	0	0	0
2	H	41	0	0	0	0
2	I	41	0	0	0	0
2	J	41	0	0	0	0
2	K	41	0	0	0	0
2	L	41	0	0	0	0
2	M	41	0	0	0	0
2	N	41	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	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	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
4	A	163	0	0	2	0
4	B	127	0	0	0	0
4	C	117	0	0	0	0
4	D	146	0	0	1	0
4	E	169	0	0	1	0
4	F	170	0	0	4	0
4	G	157	0	0	3	0
4	H	111	0	0	2	0
4	I	149	0	0	1	1
4	J	159	0	0	0	1
4	K	147	0	0	1	0
4	L	156	0	0	2	0
4	M	110	0	0	1	0
4	N	82	0	0	1	0
All	All	22615	0	20058	117	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 117 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:H:74:GLY:HA3	1:H:99:MET:CE	2.05	0.86
1:L:74:GLY:HA3	1:L:99:MET:CE	2.08	0.83
1:E:74:GLY:HA3	1:E:99:MET:HE2	1.61	0.82
1:E:74:GLY:HA3	1:E:99:MET:CE	2.10	0.81
1:N:74:GLY:HA3	1:N:99:MET:CE	2.10	0.81

All (2) 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:N:182:GLU:OE1	4:J:500:HOH:O[1_655]	2.10	0.10
1:L:156:GLU:OE1	4:I:530:HOH:O[1_554]	2.17	0.03

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	184/201 (92%)	181 (98%)	3 (2%)	0	100	100
1	B	189/201 (94%)	187 (99%)	2 (1%)	0	100	100
1	C	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
1	D	185/201 (92%)	183 (99%)	2 (1%)	0	100	100
1	E	190/201 (94%)	188 (99%)	2 (1%)	0	100	100
1	F	192/201 (96%)	188 (98%)	4 (2%)	0	100	100
1	G	181/201 (90%)	178 (98%)	3 (2%)	0	100	100
1	H	179/201 (89%)	176 (98%)	3 (2%)	0	100	100
1	I	189/201 (94%)	186 (98%)	3 (2%)	0	100	100
1	J	188/201 (94%)	185 (98%)	3 (2%)	0	100	100
1	K	180/201 (90%)	178 (99%)	2 (1%)	0	100	100
1	L	185/201 (92%)	182 (98%)	3 (2%)	0	100	100
1	M	182/201 (90%)	178 (98%)	4 (2%)	0	100	100
1	N	180/201 (90%)	175 (97%)	5 (3%)	0	100	100
All	All	2587/2814 (92%)	2545 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/169 (90%)	148 (97%)	5 (3%)	33	26
1	B	153/169 (90%)	150 (98%)	3 (2%)	50	47
1	C	149/169 (88%)	147 (99%)	2 (1%)	65	65
1	D	152/169 (90%)	150 (99%)	2 (1%)	65	65
1	E	158/169 (94%)	156 (99%)	2 (1%)	65	65
1	F	154/169 (91%)	152 (99%)	2 (1%)	65	65
1	G	149/169 (88%)	147 (99%)	2 (1%)	65	65
1	H	150/169 (89%)	148 (99%)	2 (1%)	65	65
1	I	153/169 (90%)	151 (99%)	2 (1%)	65	65
1	J	155/169 (92%)	152 (98%)	3 (2%)	52	49
1	K	148/169 (88%)	146 (99%)	2 (1%)	62	62
1	L	152/169 (90%)	149 (98%)	3 (2%)	50	47
1	M	147/169 (87%)	142 (97%)	5 (3%)	32	25
1	N	150/169 (89%)	145 (97%)	5 (3%)	33	26
All	All	2123/2366 (90%)	2083 (98%)	40 (2%)	52	49

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	130	GLN
1	N	26	LYS
1	L	196	HIS
1	M	123	HIS
1	N	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	52	GLN
1	K	89	GLN
1	N	151	ASN
1	B	130	GLN
1	D	130	GLN

5.3.3 RNA

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 26 ligands modelled in this entry, 12 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	Z53	B	301	-	43,45,45	1.16	1 (2%)	57,66,66	1.30	6 (10%)
2	Z53	F	301	-	43,45,45	1.13	1 (2%)	57,66,66	1.37	4 (7%)
2	Z53	H	301	-	43,45,45	1.12	1 (2%)	57,66,66	1.18	4 (7%)
2	Z53	K	301	-	43,45,45	1.15	1 (2%)	57,66,66	1.35	5 (8%)
2	Z53	M	301	-	43,45,45	1.12	1 (2%)	57,66,66	1.40	6 (10%)
2	Z53	D	301	-	43,45,45	1.16	1 (2%)	57,66,66	1.32	4 (7%)
2	Z53	J	301	-	43,45,45	1.16	2 (4%)	57,66,66	1.28	5 (8%)
2	Z53	E	301	-	43,45,45	1.10	1 (2%)	57,66,66	1.29	5 (8%)
2	Z53	N	301	-	43,45,45	1.14	1 (2%)	57,66,66	1.40	7 (12%)
2	Z53	L	301	-	43,45,45	1.14	1 (2%)	57,66,66	1.28	5 (8%)
2	Z53	C	301	-	43,45,45	1.18	1 (2%)	57,66,66	1.29	5 (8%)
2	Z53	I	301	-	43,45,45	1.15	1 (2%)	57,66,66	1.38	4 (7%)
2	Z53	A	301	-	43,45,45	1.15	1 (2%)	57,66,66	1.22	5 (8%)
2	Z53	G	301	-	43,45,45	1.14	1 (2%)	57,66,66	1.35	6 (10%)

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	Z53	B	301	-	-	0/22/55/55	0/5/5/5
2	Z53	F	301	-	-	0/22/55/55	0/5/5/5
2	Z53	H	301	-	-	1/22/55/55	0/5/5/5
2	Z53	K	301	-	-	0/22/55/55	0/5/5/5
2	Z53	M	301	-	-	0/22/55/55	0/5/5/5
2	Z53	D	301	-	-	0/22/55/55	0/5/5/5
2	Z53	J	301	-	-	0/22/55/55	0/5/5/5
2	Z53	E	301	-	-	0/22/55/55	0/5/5/5
2	Z53	N	301	-	-	1/22/55/55	0/5/5/5
2	Z53	L	301	-	-	0/22/55/55	0/5/5/5
2	Z53	C	301	-	-	0/22/55/55	0/5/5/5
2	Z53	I	301	-	-	2/22/55/55	0/5/5/5
2	Z53	A	301	-	-	1/22/55/55	0/5/5/5
2	Z53	G	301	-	-	0/22/55/55	0/5/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	Z53	C37-C36	-5.33	1.33	1.52
2	H	301	Z53	C37-C36	-5.32	1.33	1.52
2	C	301	Z53	C37-C36	-5.32	1.33	1.52
2	A	301	Z53	C37-C36	-5.23	1.33	1.52
2	D	301	Z53	C37-C36	-5.17	1.33	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	Z53	C37-C36-C35	5.10	121.31	112.46
2	D	301	Z53	C37-C36-C35	5.05	121.24	112.46
2	M	301	Z53	C9-C8-N7	-4.84	103.61	111.76
2	N	301	Z53	C37-C36-C35	4.69	120.60	112.46
2	G	301	Z53	C37-C36-C35	4.56	120.38	112.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

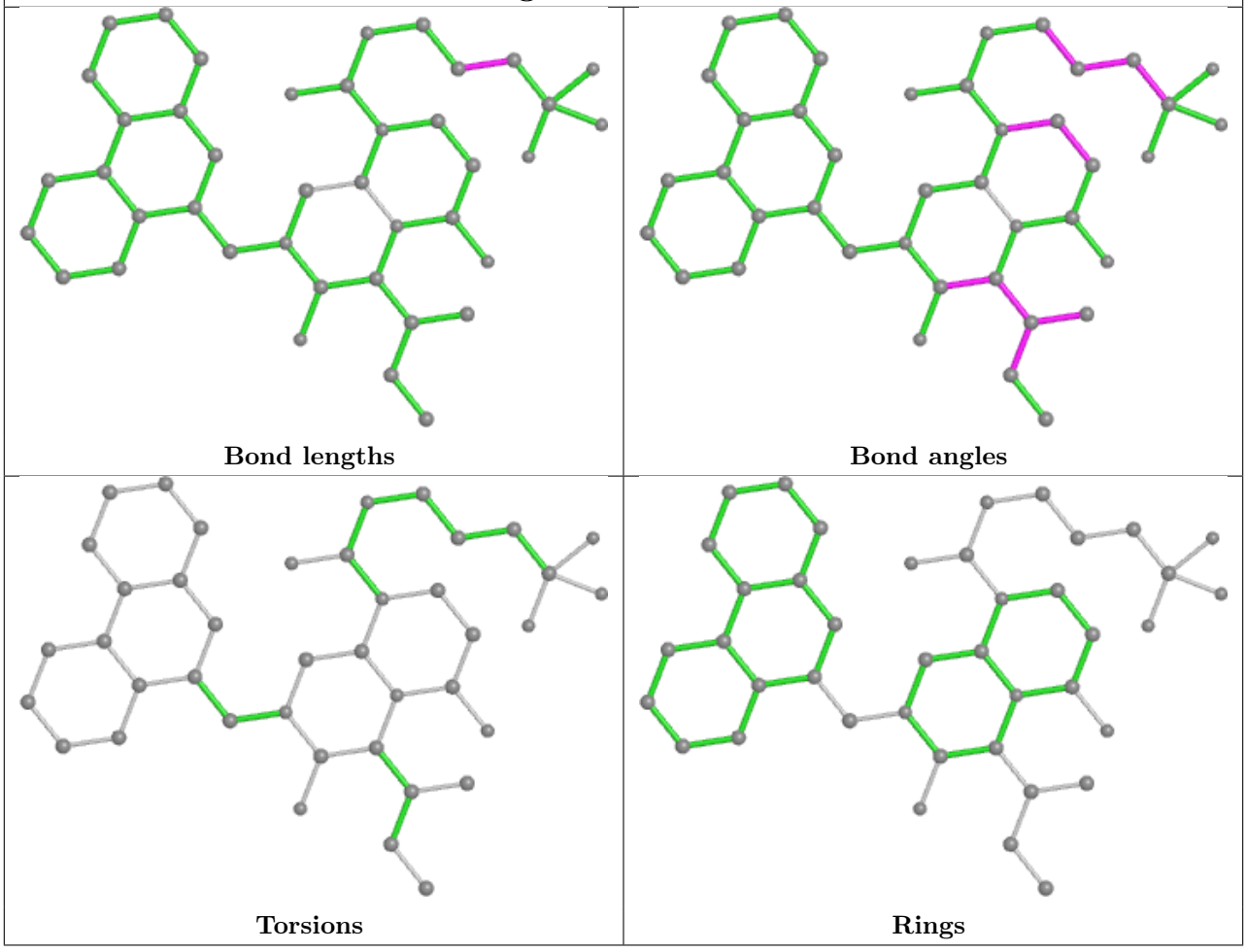
Mol	Chain	Res	Type	Atoms
2	I	301	Z53	C11-C10-C9-C8
2	I	301	Z53	C11-C10-C9-C46
2	H	301	Z53	N34-C35-C36-C37
2	A	301	Z53	C36-C37-C38-F40
2	N	301	Z53	C36-C37-C38-F40

There are no ring outliers.

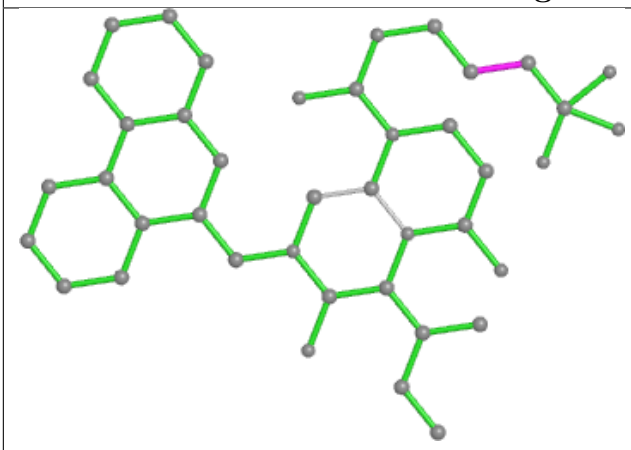
No monomer is involved in short contacts.

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 then 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.

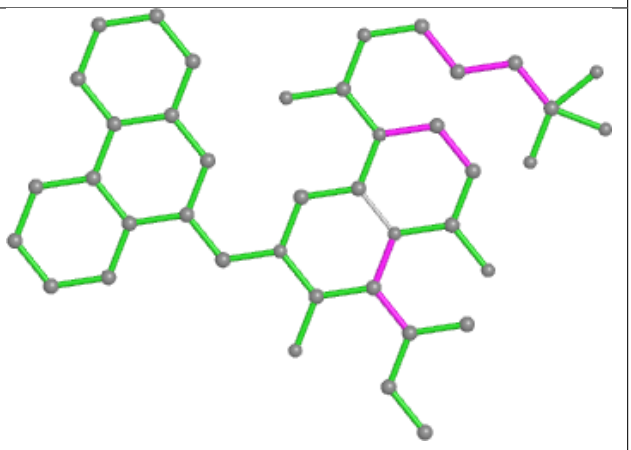
Ligand Z53 B 301



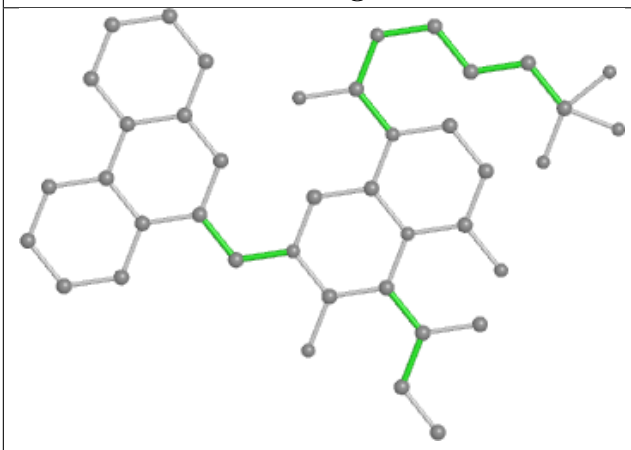
Ligand Z53 F 301



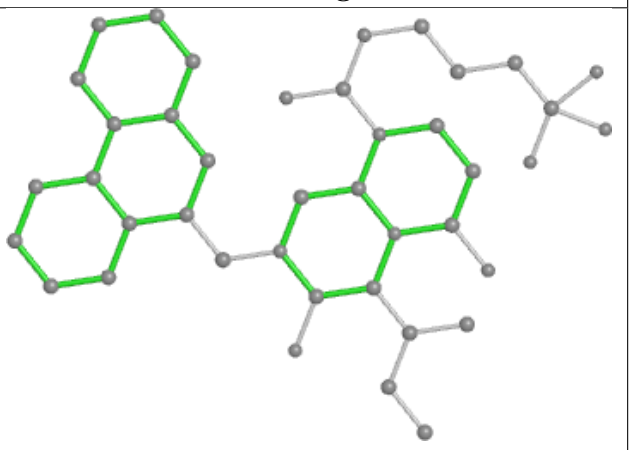
Bond lengths



Bond angles

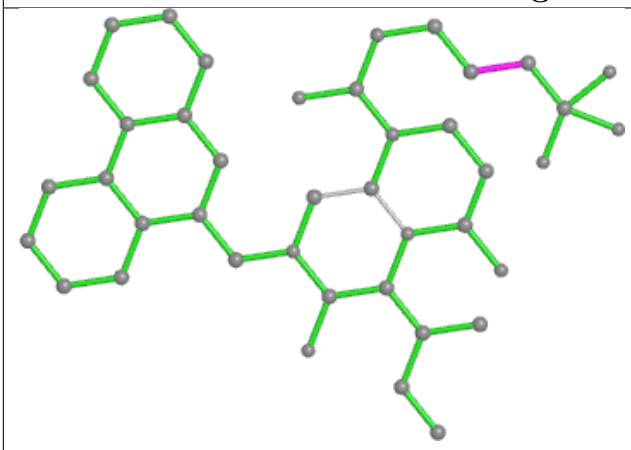


Torsions



Rings

Ligand Z53 H 301



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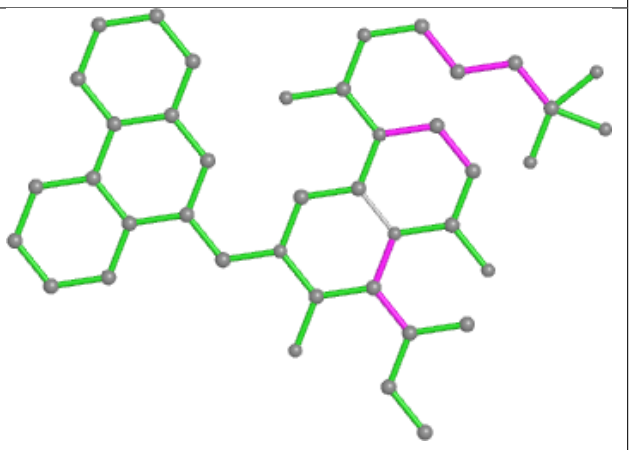
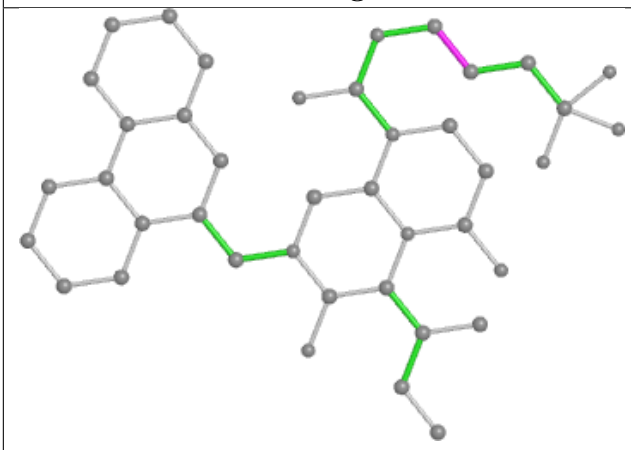


Bond angles



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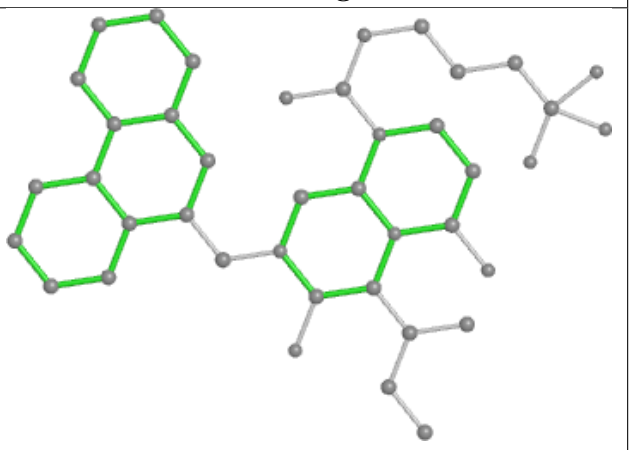
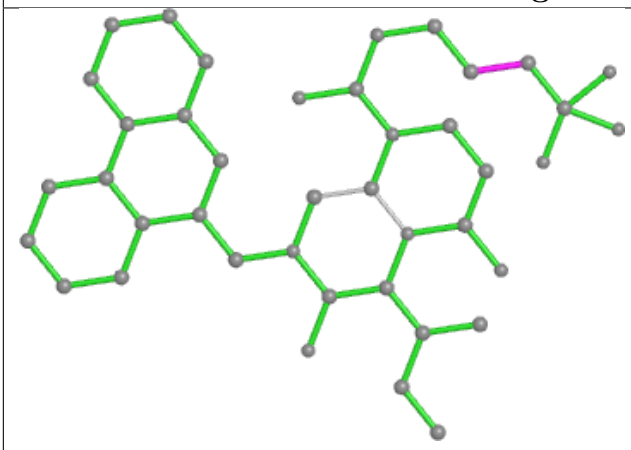
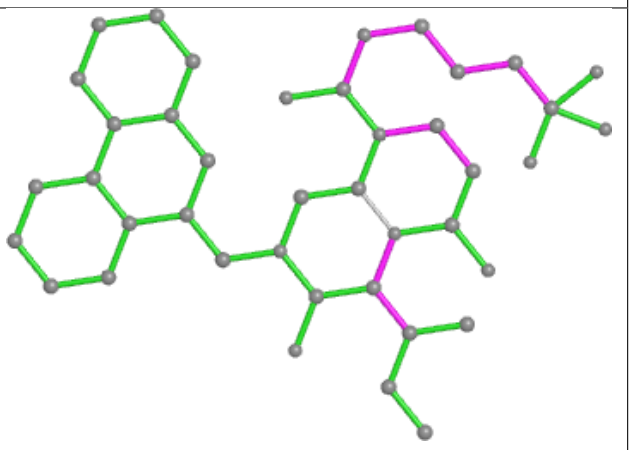


Rings

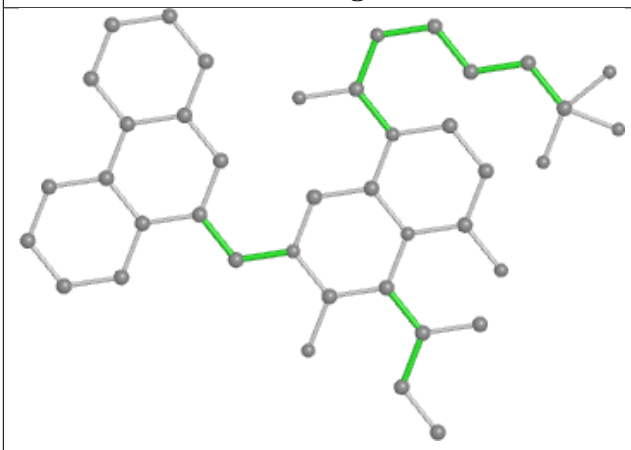
Ligand Z53 K 301



Bond lengths



Bond angles



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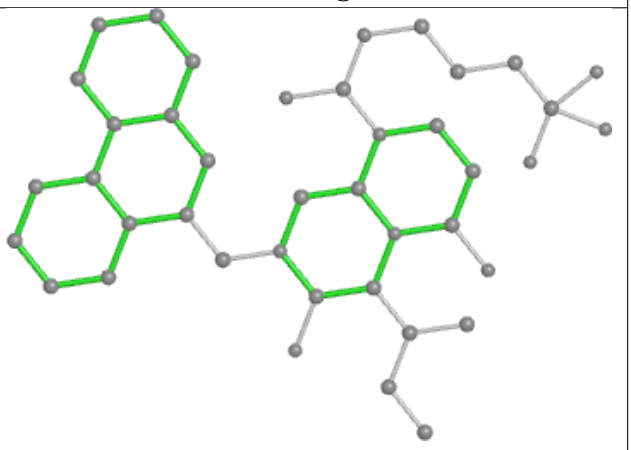
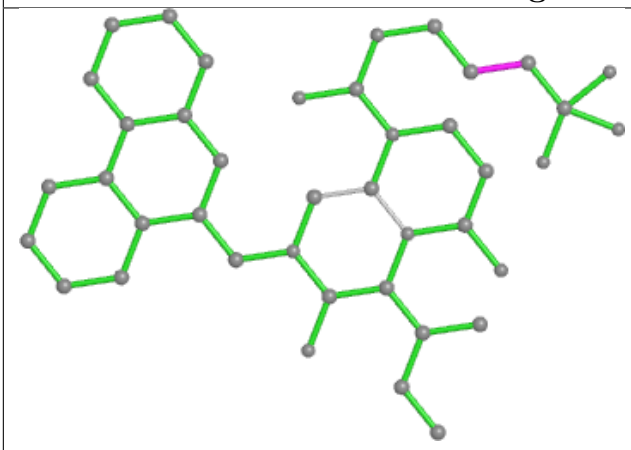
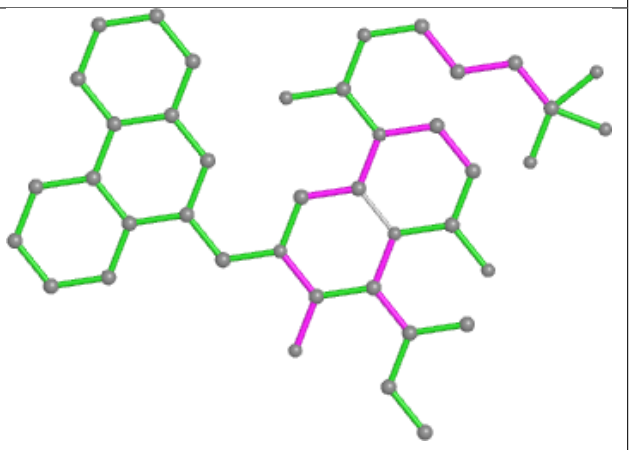


Rings

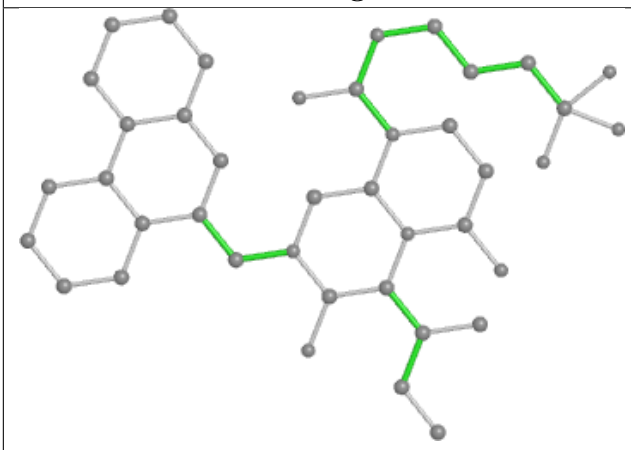
Ligand Z53 M 301



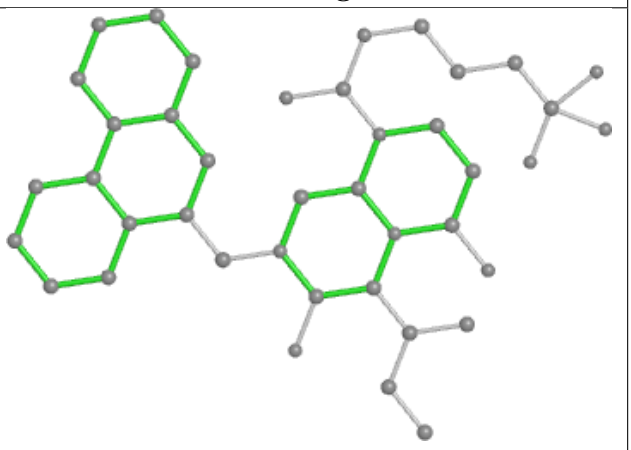
Bond lengths



Bond angles

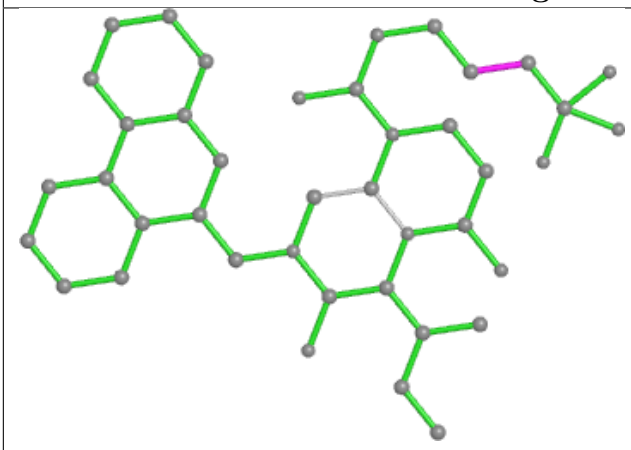


Torsions



Rings

Ligand Z53 D 301



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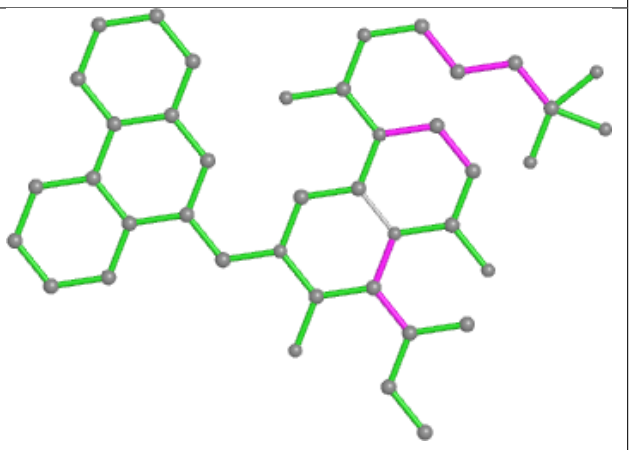
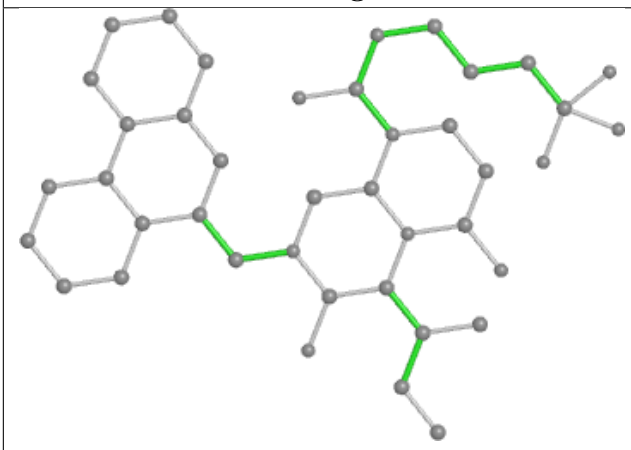


Bond angles



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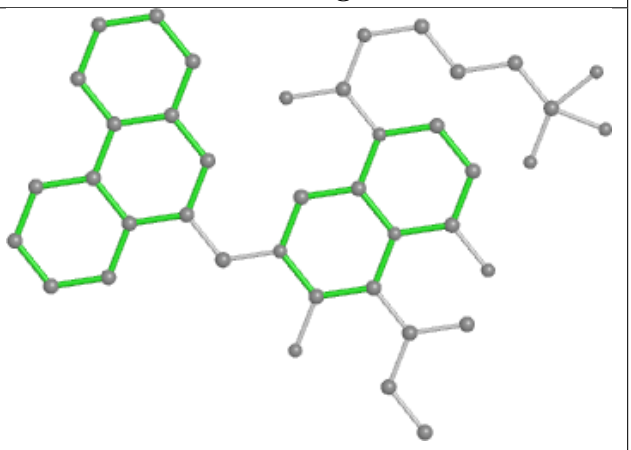
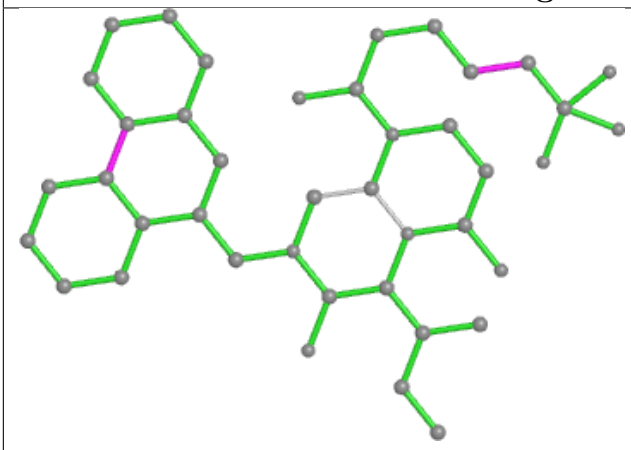


Rings

Ligand Z53 J 301



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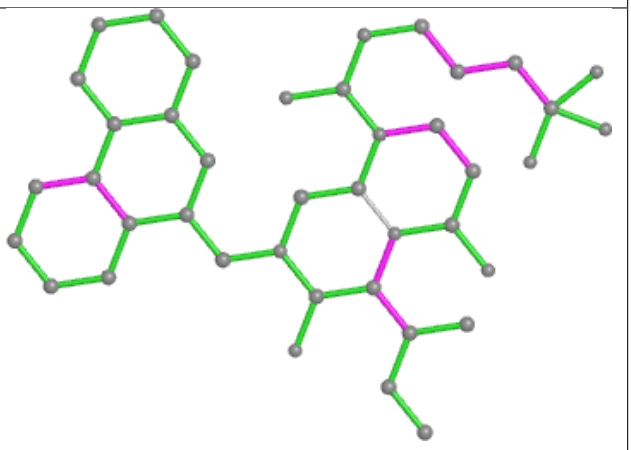

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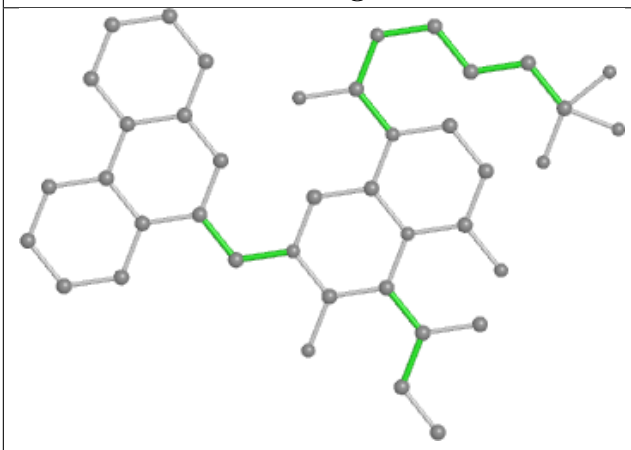
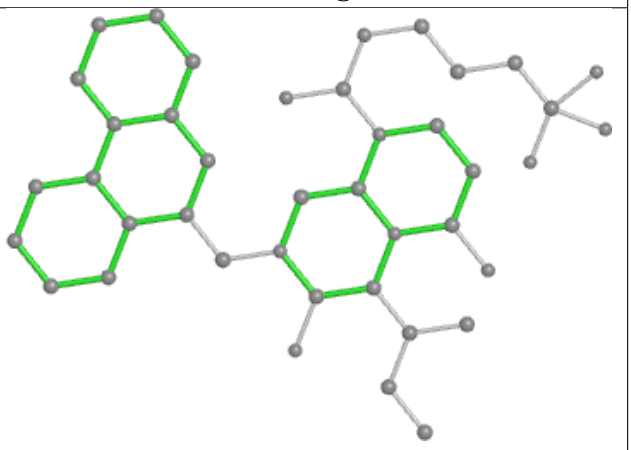
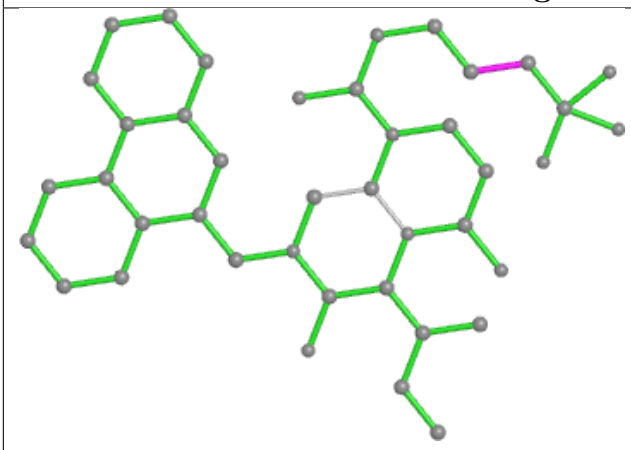


Torsions



Rings

Ligand Z53 E 301



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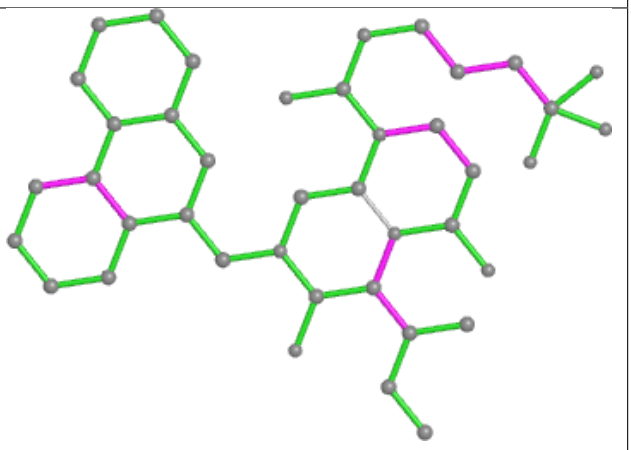

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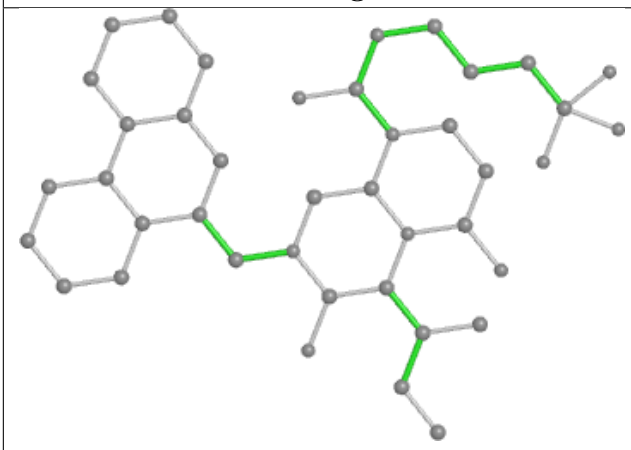

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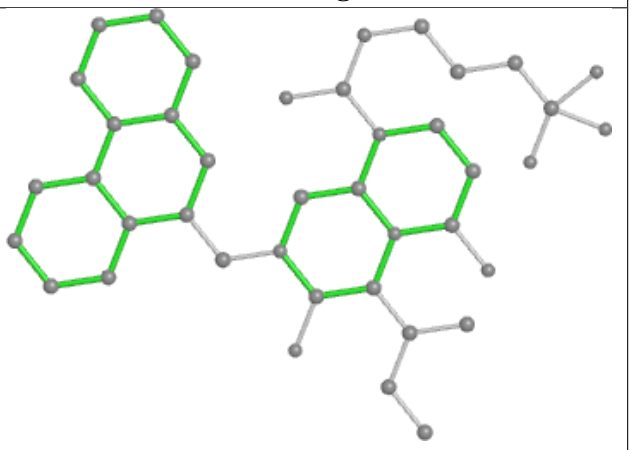
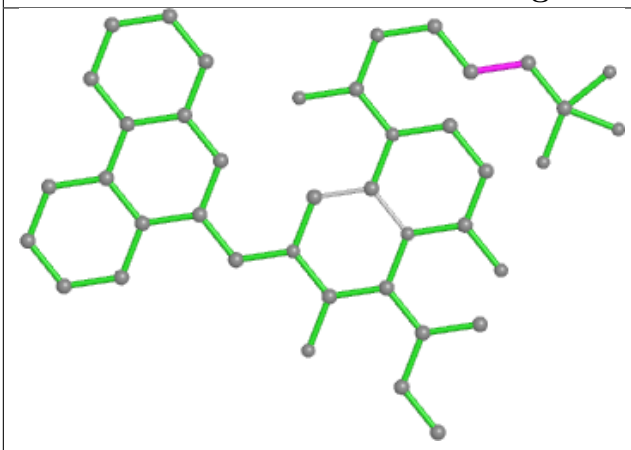


Rings

Ligand Z53 N 301



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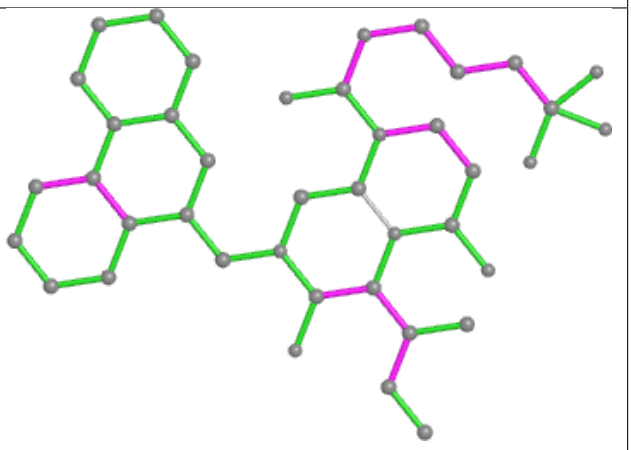

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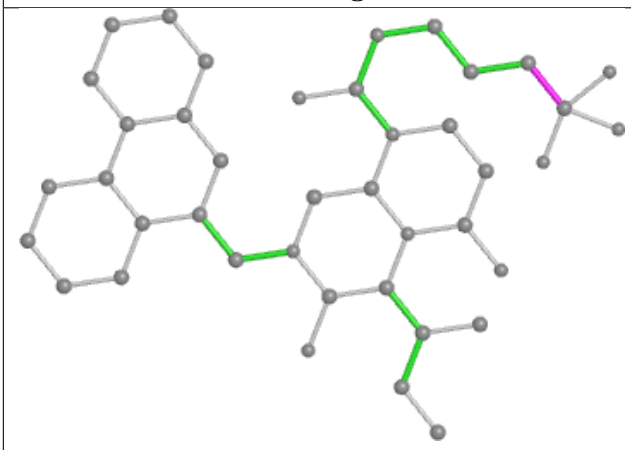

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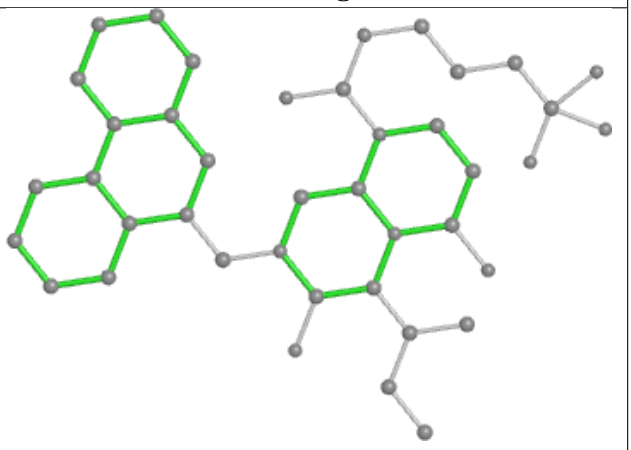
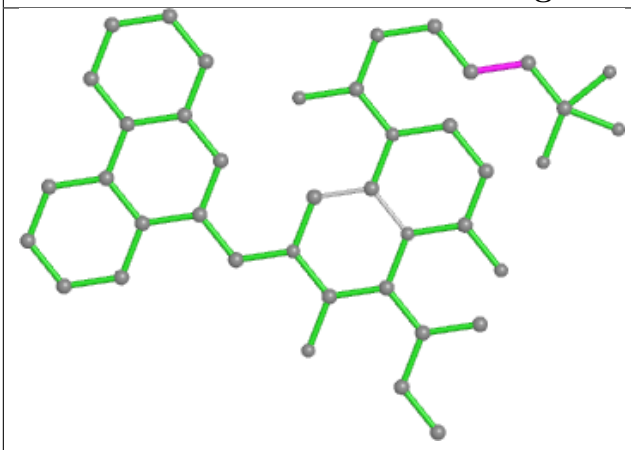


Rings

Ligand Z53 L 301



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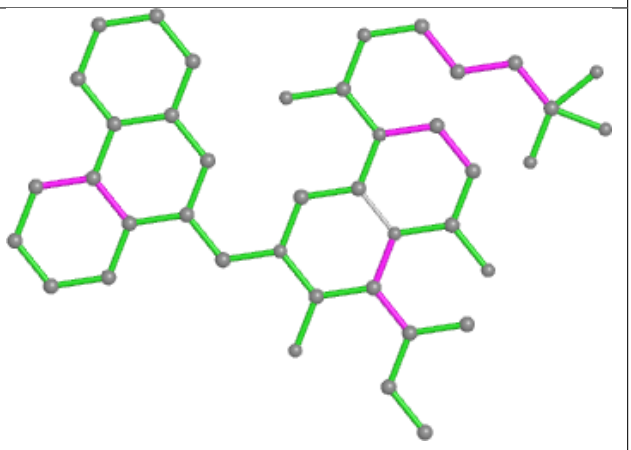

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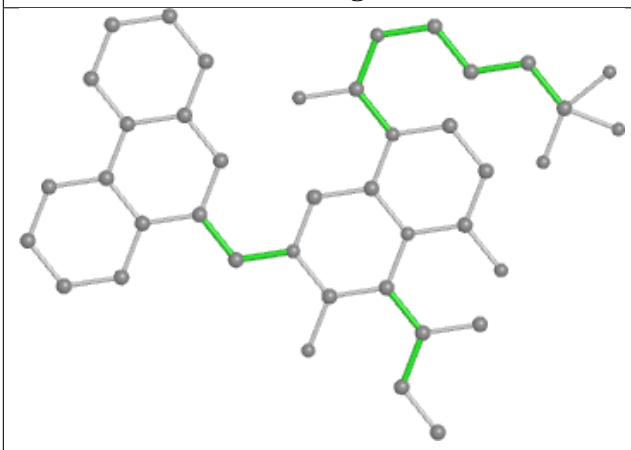

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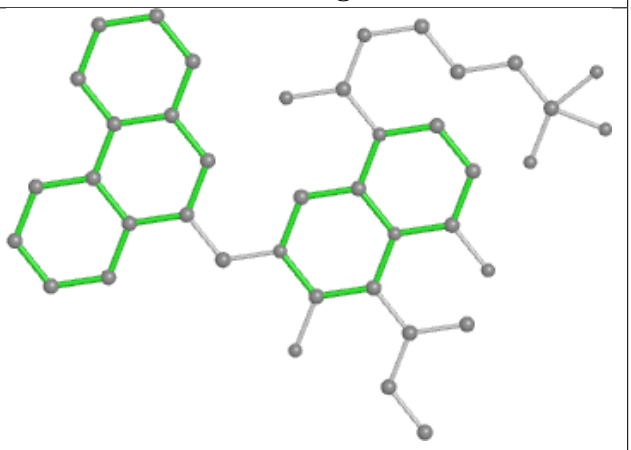
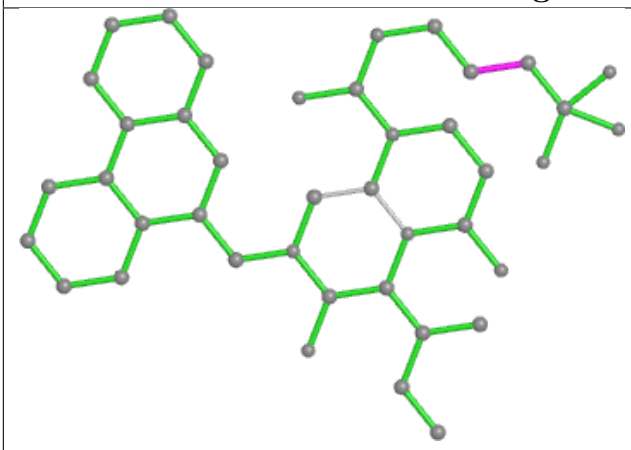


Rings

Ligand Z53 C 301



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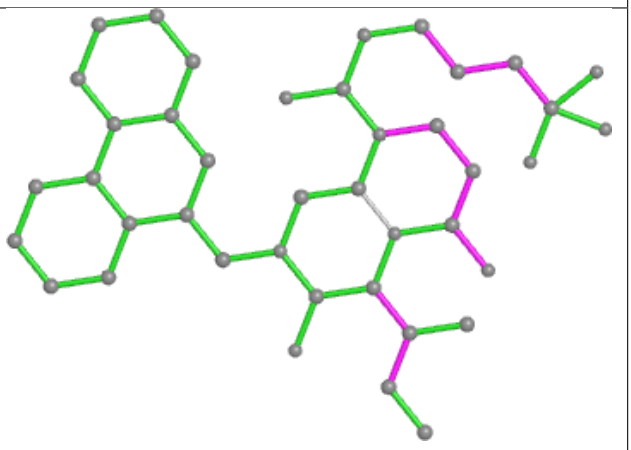

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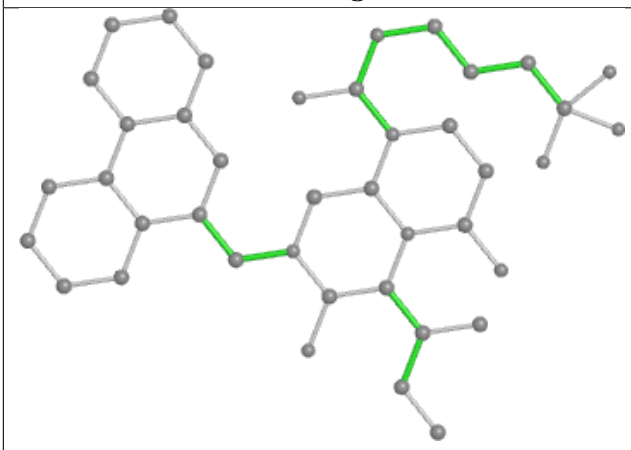

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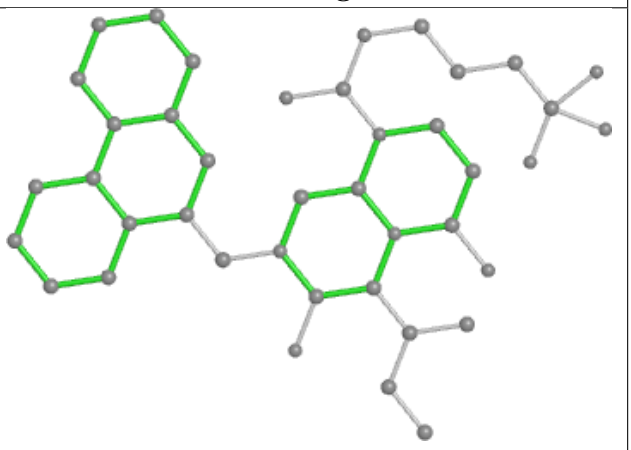
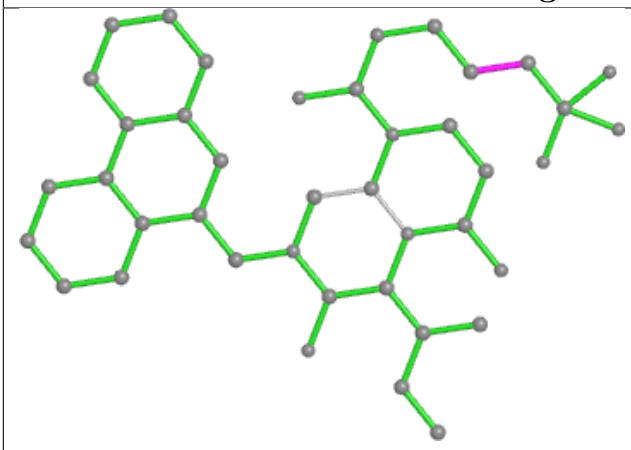


Rings

Ligand Z53 I 301



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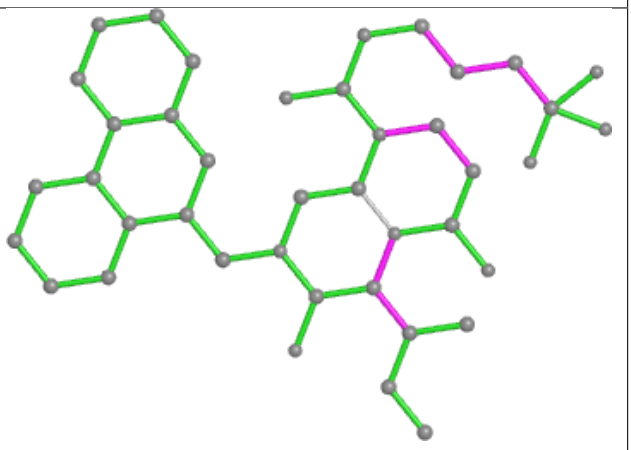

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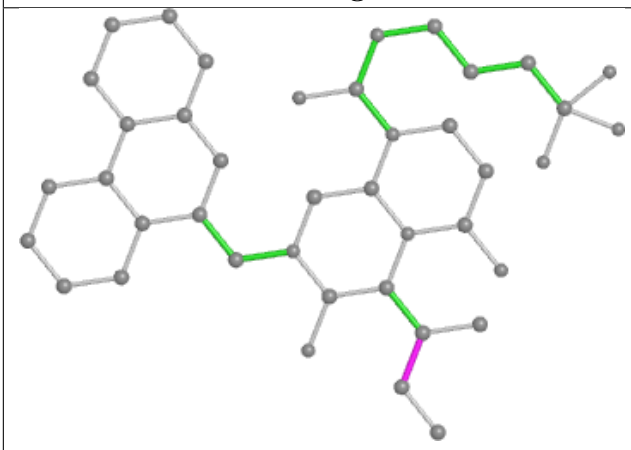

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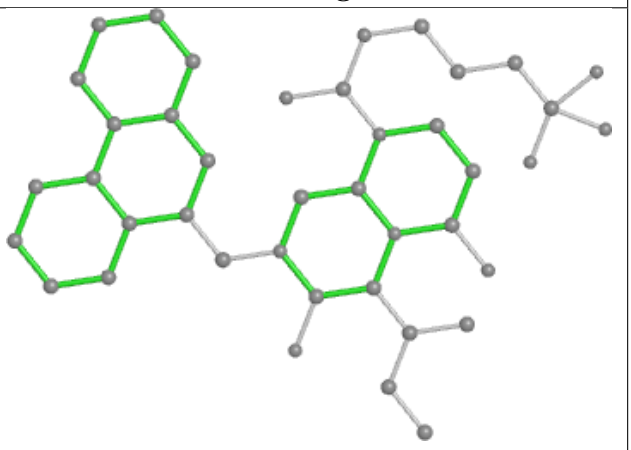
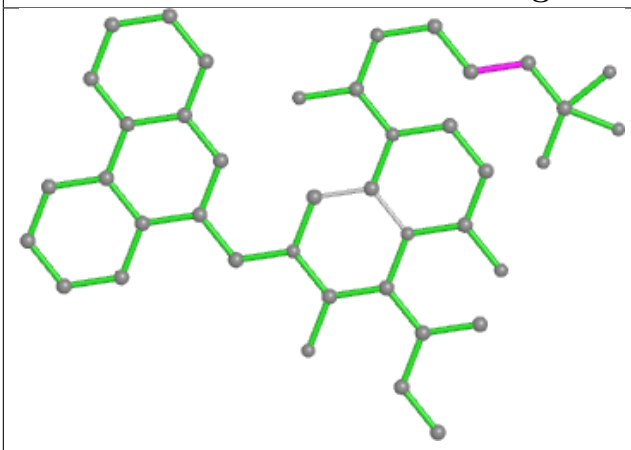
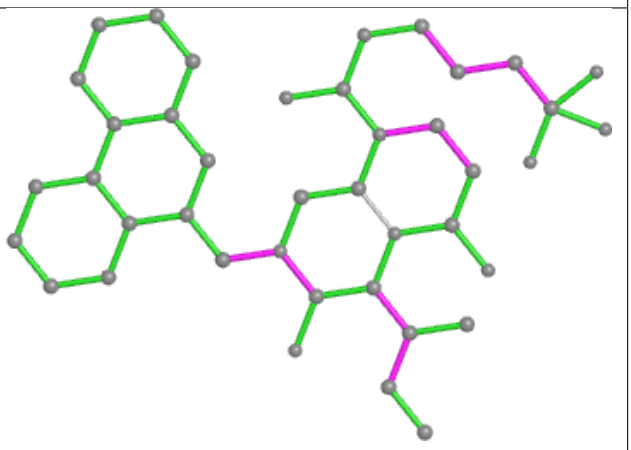


Rings

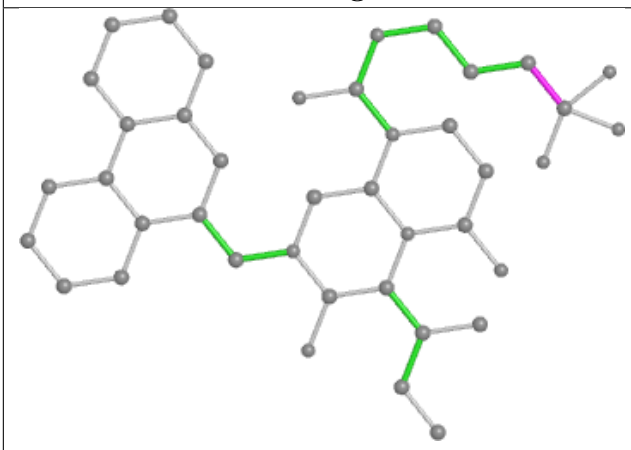
Ligand Z53 A 301



Bond lengths



Bond angles



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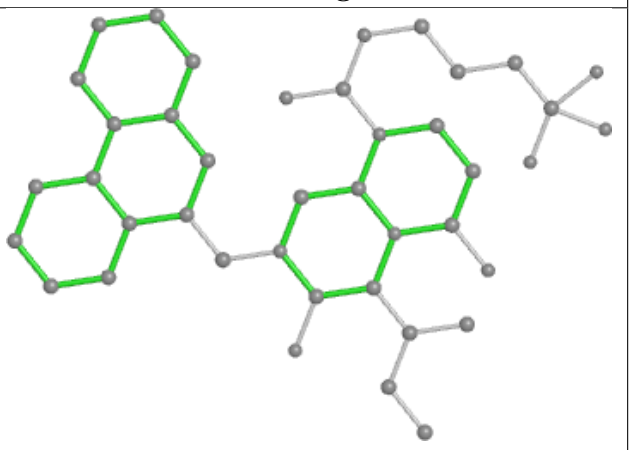
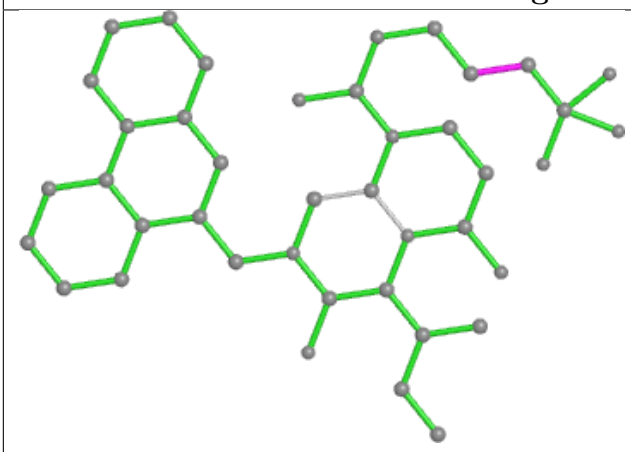


Rings

Ligand Z53 G 301



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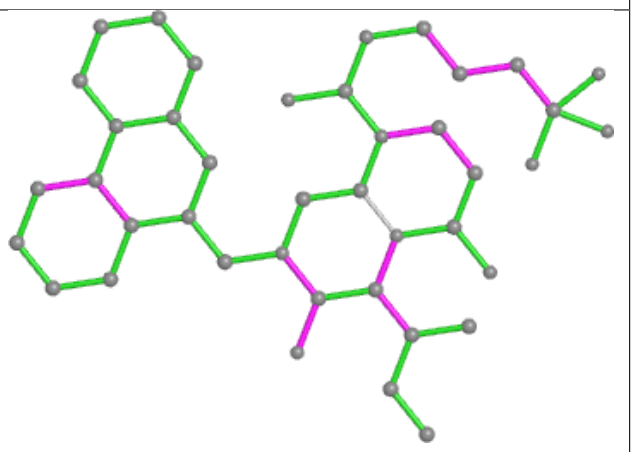

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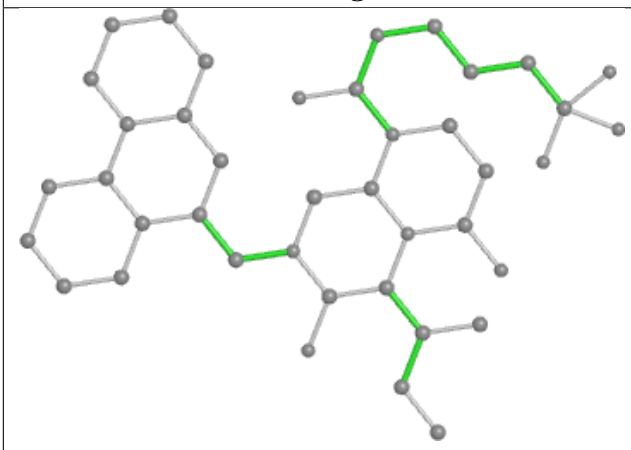
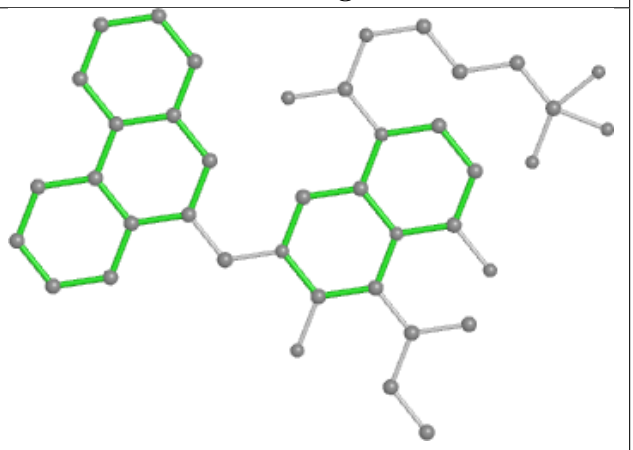


Torsions



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	188/201 (93%)	-0.62	2 (1%)	77	79	10, 17, 29, 58	0
1	B	193/201 (96%)	-0.23	6 (3%)	51	53	15, 24, 44, 55	0
1	C	187/201 (93%)	-0.35	4 (2%)	63	65	13, 23, 40, 56	0
1	D	189/201 (94%)	-0.48	9 (4%)	36	37	10, 18, 41, 65	0
1	E	192/201 (95%)	-0.56	3 (1%)	70	72	9, 15, 38, 56	0
1	F	194/201 (96%)	-0.66	1 (0%)	87	88	9, 15, 29, 60	0
1	G	185/201 (92%)	-0.65	0	100	100	8, 15, 31, 46	0
1	H	183/201 (91%)	-0.15	3 (1%)	70	72	15, 26, 41, 57	0
1	I	191/201 (95%)	-0.45	3 (1%)	70	72	11, 19, 40, 52	0
1	J	190/201 (94%)	-0.53	1 (0%)	87	88	10, 17, 33, 56	0
1	K	184/201 (91%)	-0.57	1 (0%)	87	88	11, 17, 31, 51	0
1	L	189/201 (94%)	-0.54	4 (2%)	63	65	12, 18, 35, 55	0
1	M	186/201 (92%)	-0.15	3 (1%)	70	72	16, 25, 41, 51	0
1	N	184/201 (91%)	-0.05	4 (2%)	62	64	20, 28, 41, 55	0
All	All	2635/2814 (93%)	-0.43	44 (1%)	69	71	8, 20, 38, 65	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	193	GLU	4.3
1	L	196	HIS	4.0
1	K	193	GLU	3.7
1	D	8	ILE	3.5
1	H	18	TYR	3.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

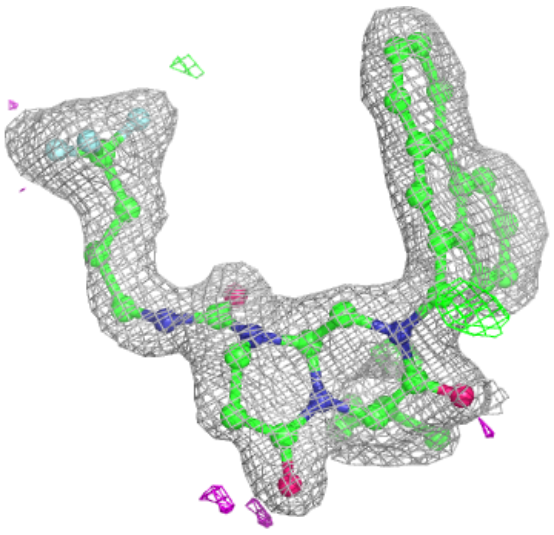
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

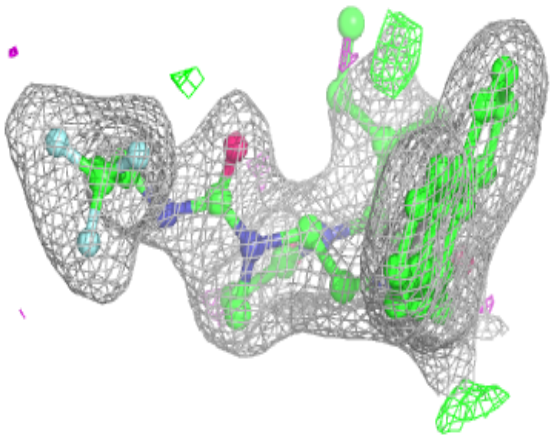
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Z53	N	301	41/41	0.91	0.09	22,31,41,50	0
2	Z53	B	301	41/41	0.93	0.08	18,24,37,42	0
2	Z53	M	301	41/41	0.94	0.07	17,23,30,37	0
2	Z53	H	301	41/41	0.94	0.07	21,29,36,42	0
2	Z53	I	301	41/41	0.95	0.07	16,24,34,43	0
2	Z53	J	301	41/41	0.95	0.06	11,19,29,34	0
2	Z53	D	301	41/41	0.95	0.06	15,20,26,33	0
2	Z53	C	301	41/41	0.95	0.07	16,25,39,43	0
3	MG	G	302	1/1	0.95	0.05	23,23,23,23	0
2	Z53	L	301	41/41	0.96	0.06	12,17,23,27	0
2	Z53	G	301	41/41	0.96	0.06	8,16,28,34	0
2	Z53	E	301	41/41	0.96	0.06	10,15,25,33	0
2	Z53	K	301	41/41	0.96	0.05	12,17,29,33	0
3	MG	H	302	1/1	0.96	0.09	28,28,28,28	0
3	MG	K	302	1/1	0.96	0.11	26,26,26,26	0
2	Z53	A	301	41/41	0.97	0.05	9,15,23,29	0
2	Z53	F	301	41/41	0.97	0.05	8,15,27,31	0
3	MG	I	302	1/1	0.97	0.06	26,26,26,26	0
3	MG	A	302	1/1	0.97	0.07	27,27,27,27	0
3	MG	J	302	1/1	0.98	0.09	25,25,25,25	0
3	MG	E	302	1/1	0.98	0.14	23,23,23,23	0
3	MG	L	302	1/1	0.98	0.05	26,26,26,26	0
3	MG	M	302	1/1	0.98	0.04	34,34,34,34	0
3	MG	C	302	1/1	0.99	0.08	29,29,29,29	0
3	MG	F	302	1/1	0.99	0.07	21,21,21,21	0
3	MG	D	302	1/1	0.99	0.07	22,22,22,22	0

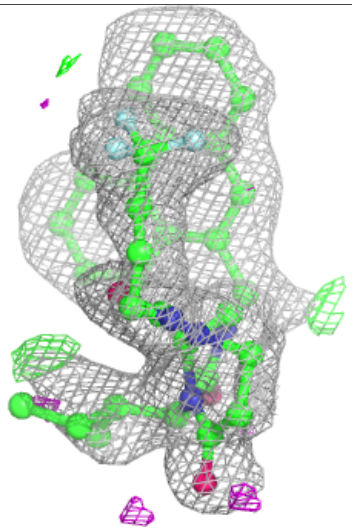
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Z53 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)

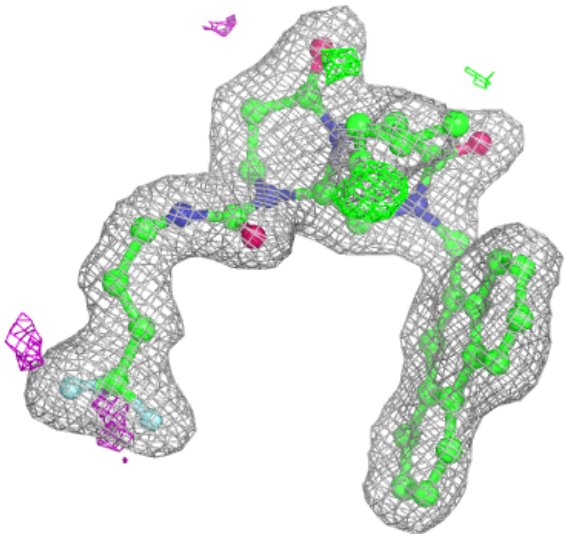


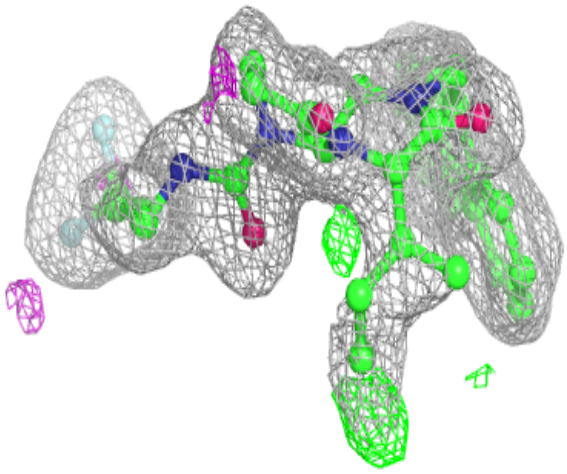


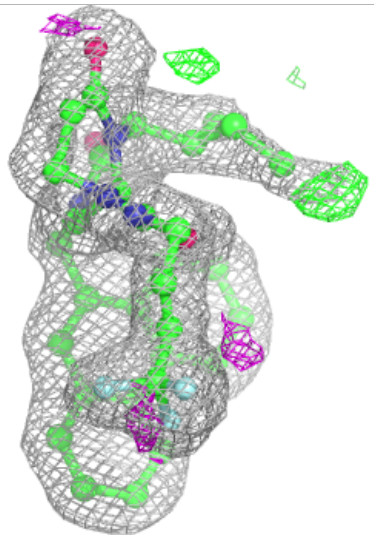


Electron density around Z53 B 301:

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

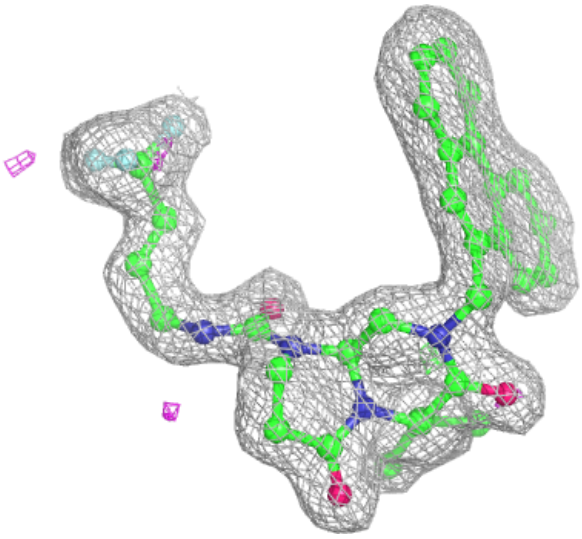


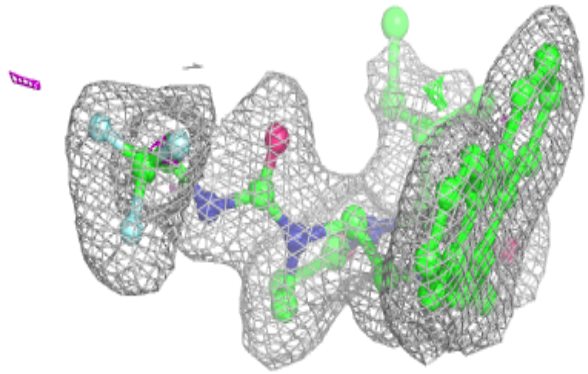


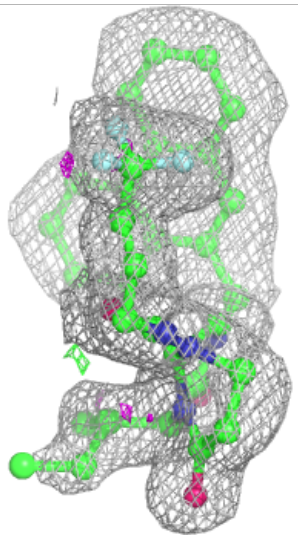


Electron density around Z53 M 301:

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

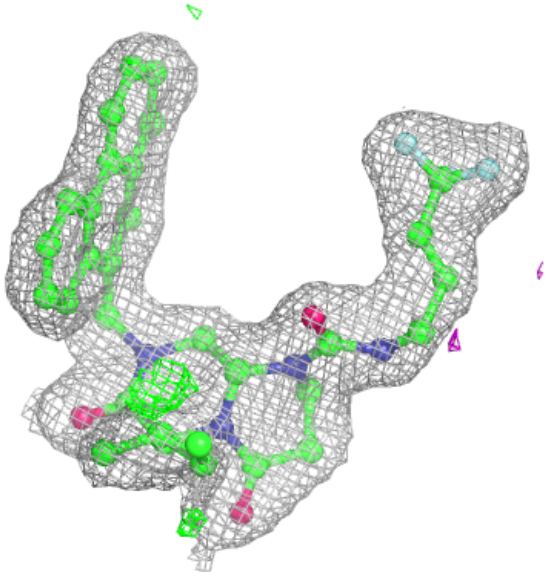


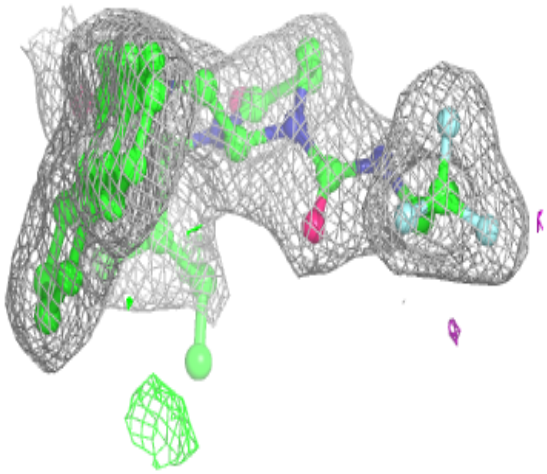


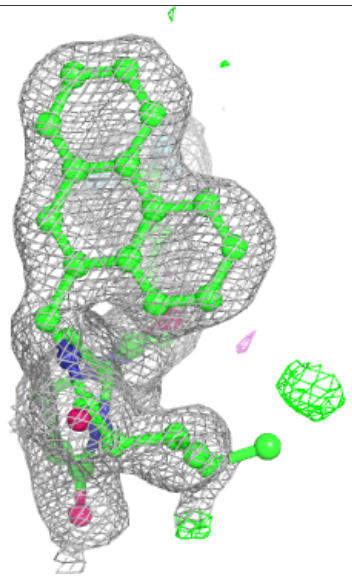


Electron density around Z53 H 301:

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

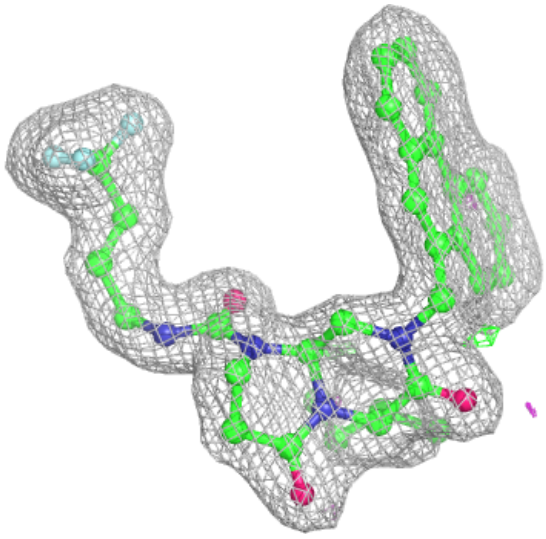


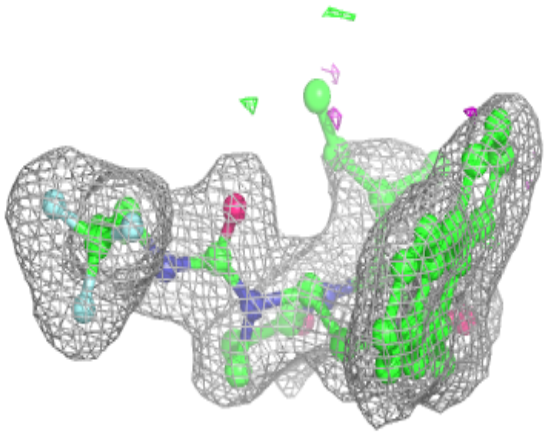


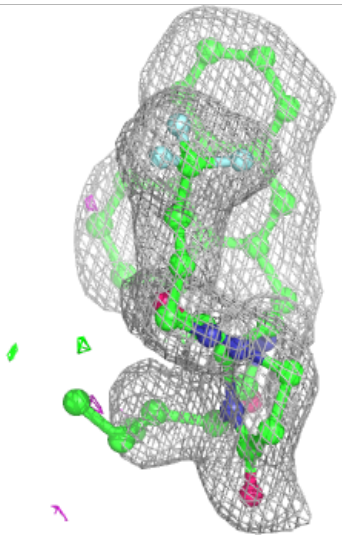


Electron density around Z53 I 301:

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

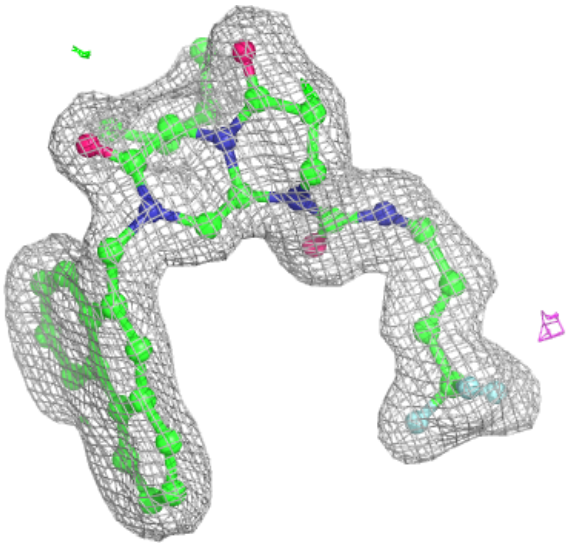


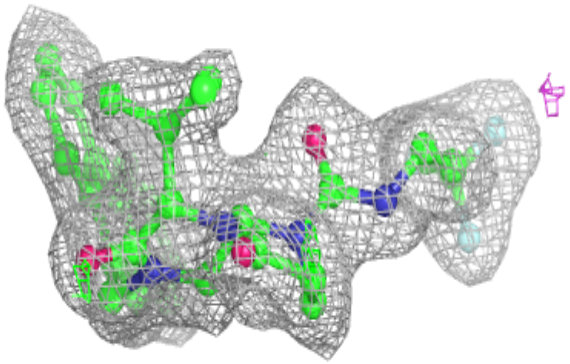


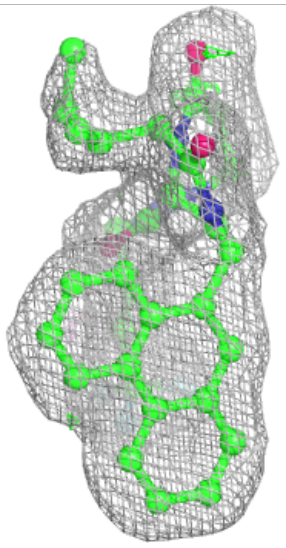


Electron density around Z53 J 301:

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

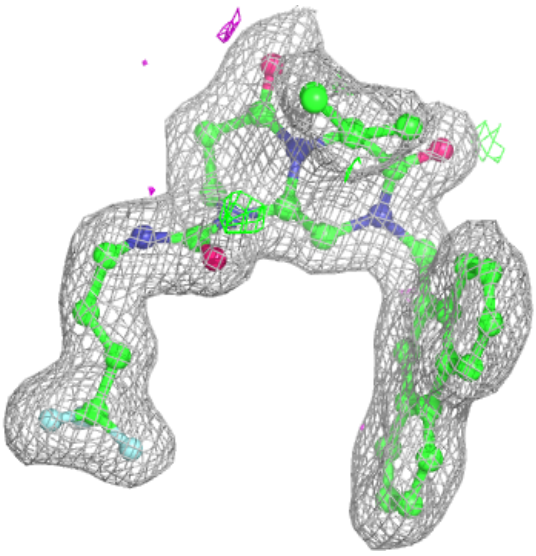


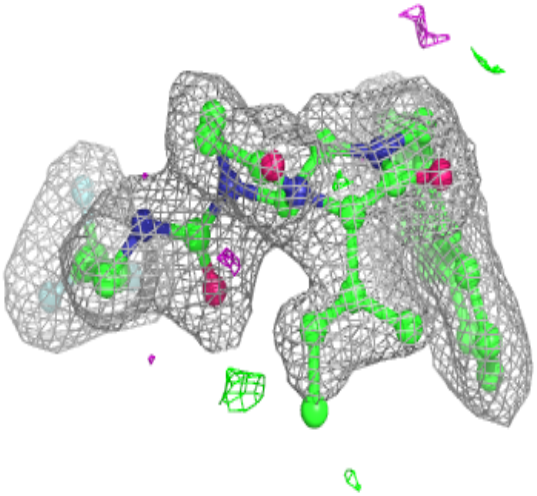


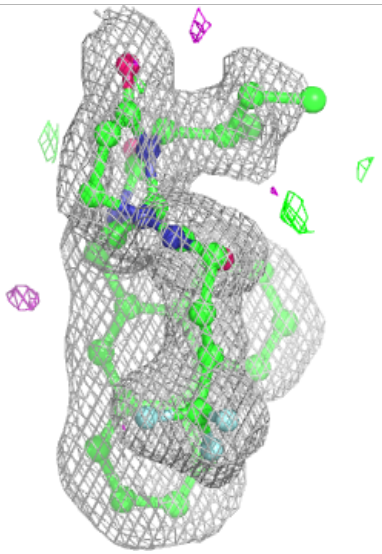


Electron density around Z53 D 301:

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

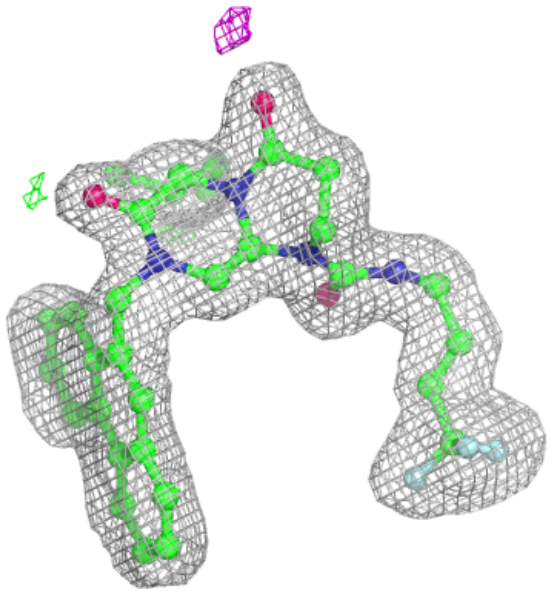


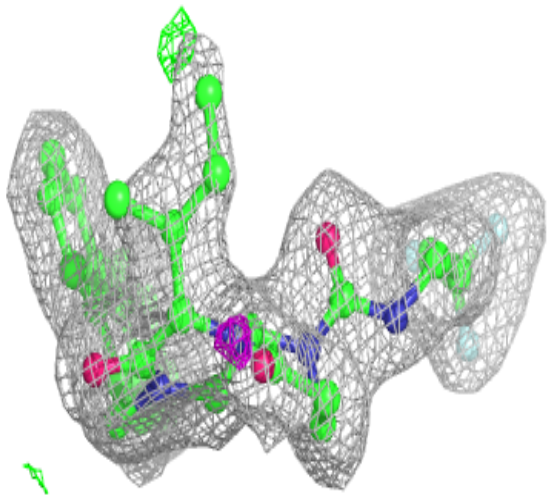


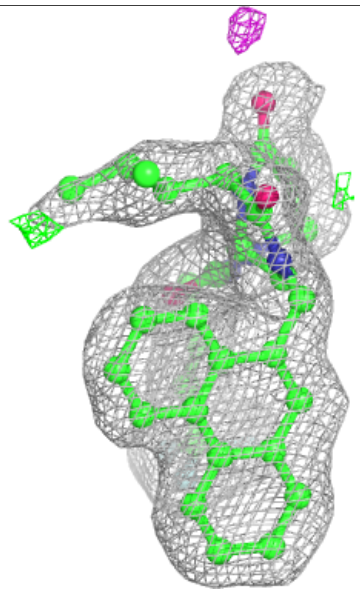


Electron density around Z53 C 301:

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

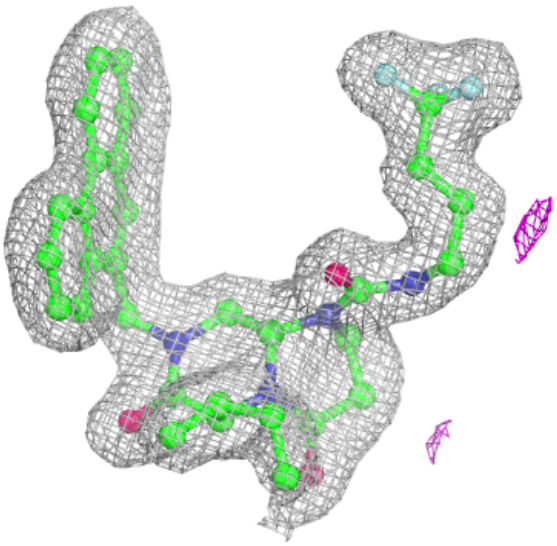


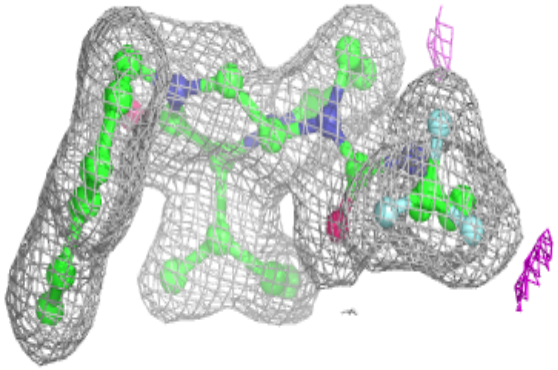


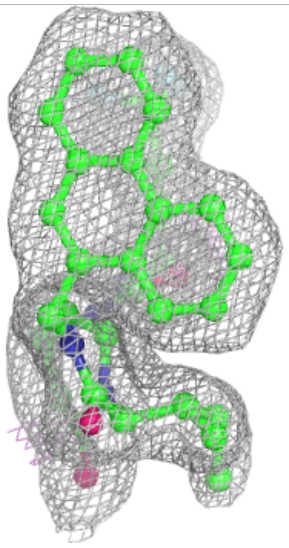


Electron density around Z53 L 301:

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

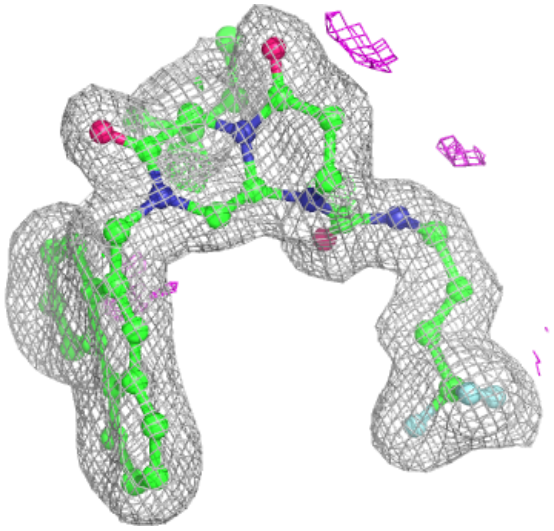


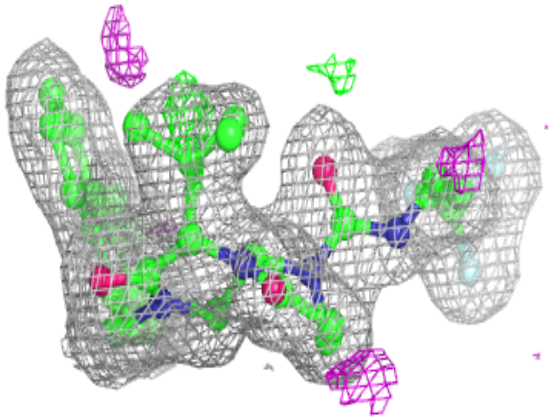


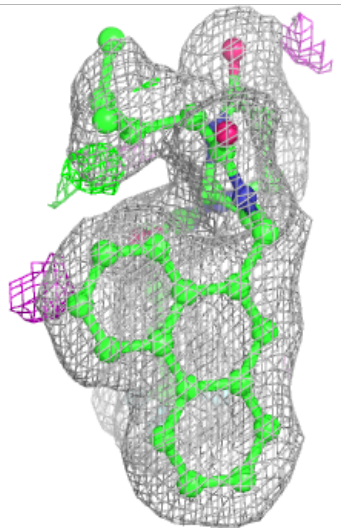


Electron density around Z53 G 301:

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

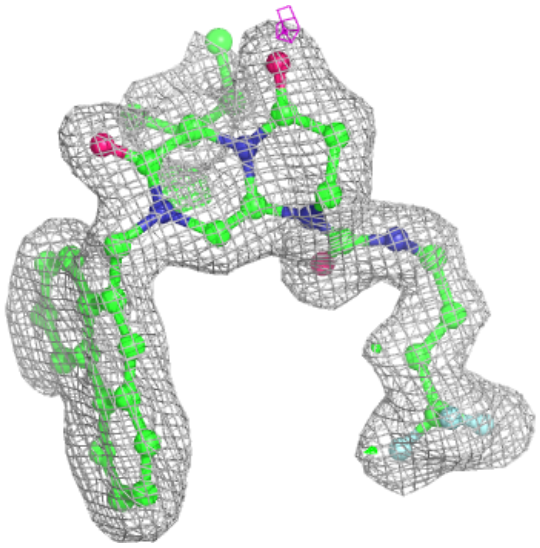


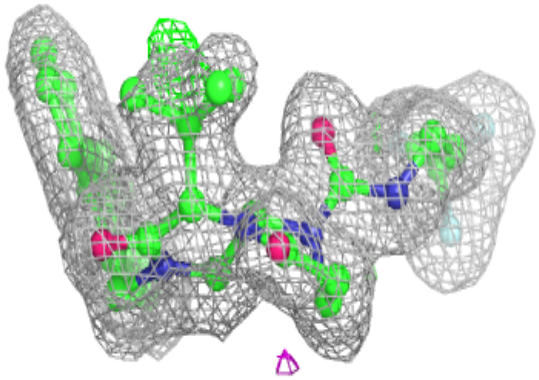


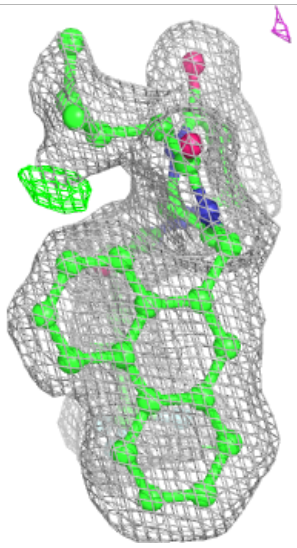


Electron density around Z53 E 301:

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

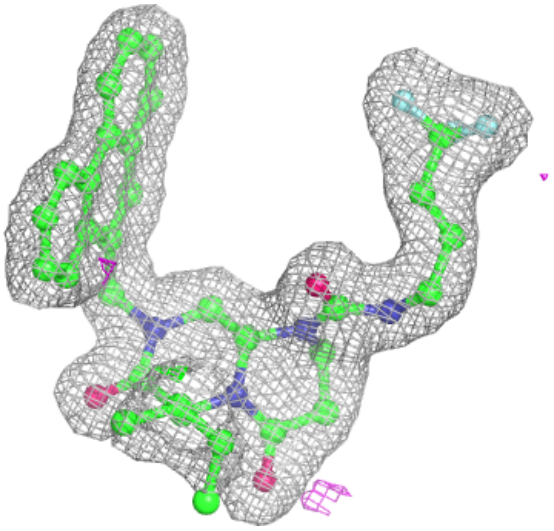


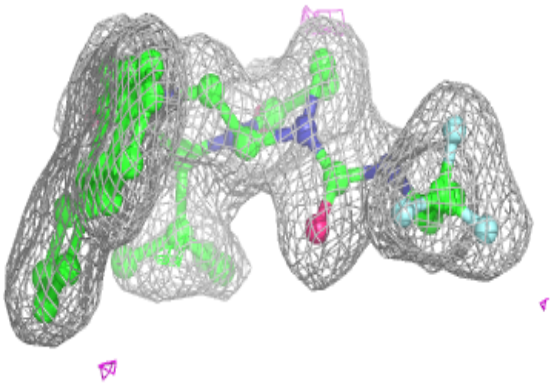


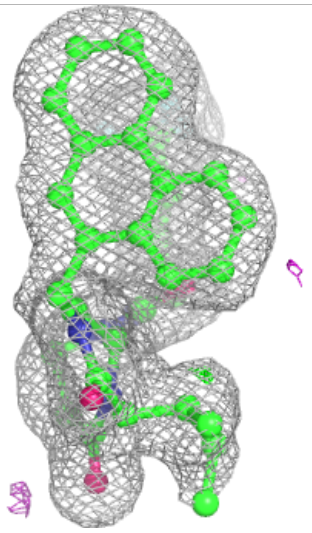


Electron density around Z53 K 301:

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

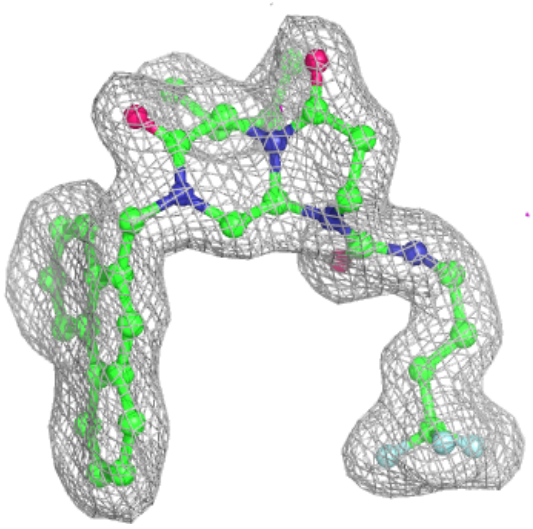


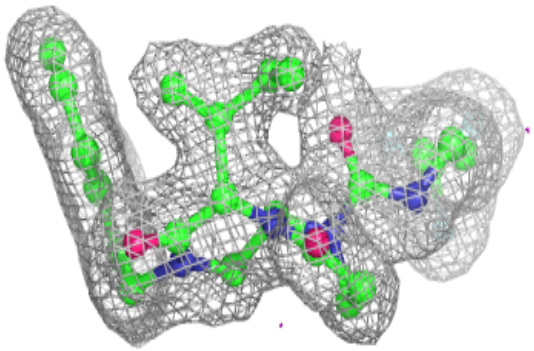


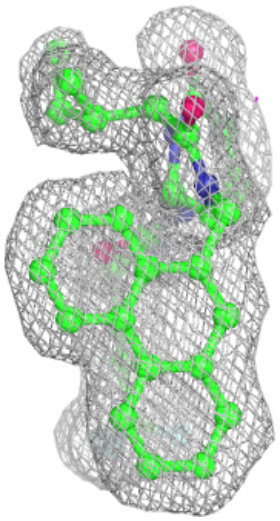


Electron density around Z53 A 301:

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

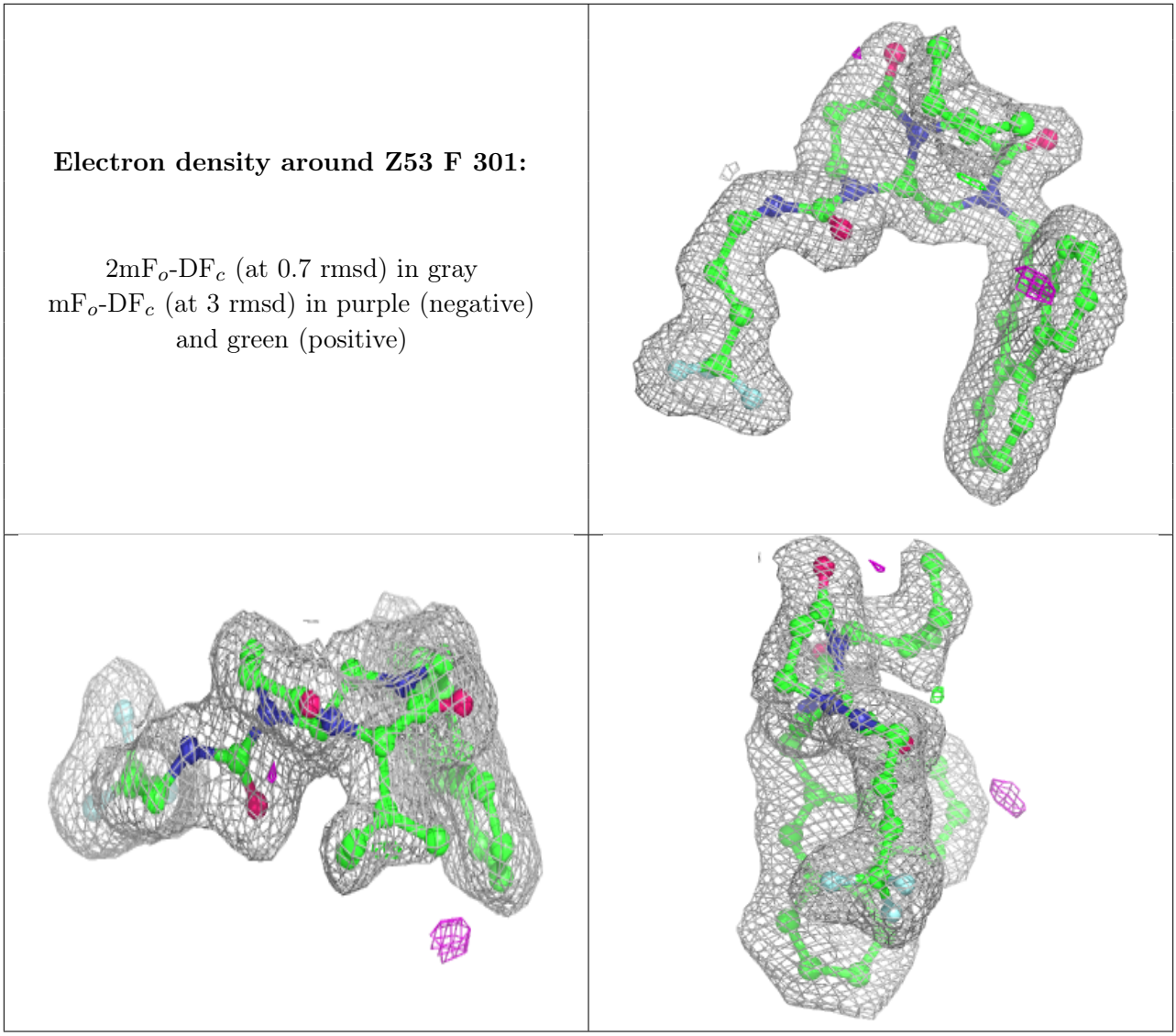






Electron density around Z53 F 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.