Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2025 – 01:18 PM JST

PDB ID	:	9K2K
Title	:	Structure of ClpP from Staphylococcus aureus in complex with ZY7
Authors	:	Li, J.H.; Wu, W.; Zhang, T.; Yang, C.-G.
Deposited on	:	2024-10-17
Resolution	:	2.74 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

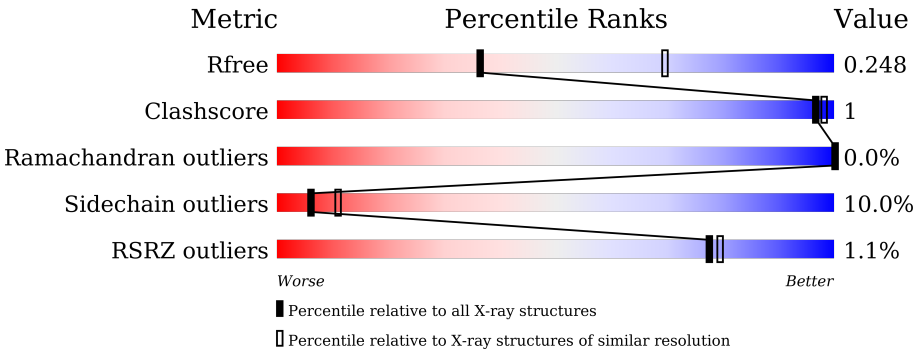
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.74 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	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	84% 7% 8%
1	B	201	83% 10% 7%
1	C	201	82% 10% 7%
1	D	201	84% 10% 6%
1	E	201	84% 9% • 5%
1	F	201	85% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	G	201	87% 8% 5%
1	H	201	% 83% 8% 8%
1	I	201	82% 8% 9%
1	J	201	% 85% 9% 6%
1	K	201	3% 86% 9% 5%
1	L	201	2% 85% 9% 5%
1	M	201	% 87% 7% 6%
1	N	201	84% 7% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20630 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	184	Total	C	N	O	S	0	0	0
			1408	889	239	274	6			
1	B	186	Total	C	N	O	S	0	0	0
			1424	898	241	279	6			
1	C	186	Total	C	N	O	S	0	0	0
			1424	898	241	279	6			
1	D	188	Total	C	N	O	S	0	0	0
			1440	907	243	284	6			
1	E	190	Total	C	N	O	S	0	0	0
			1464	919	252	287	6			
1	F	190	Total	C	N	O	S	0	0	0
			1454	914	249	285	6			
1	G	191	Total	C	N	O	S	0	0	0
			1450	913	246	285	6			
1	H	184	Total	C	N	O	S	0	0	0
			1415	894	239	276	6			
1	I	183	Total	C	N	O	S	0	0	0
			1407	888	238	275	6			
1	J	189	Total	C	N	O	S	0	0	0
			1450	912	245	287	6			
1	K	191	Total	C	N	O	S	0	0	0
			1466	921	249	290	6			
1	L	190	Total	C	N	O	S	0	0	0
			1452	913	246	287	6			
1	M	189	Total	C	N	O	S	0	0	0
			1449	911	248	284	6			
1	N	183	Total	C	N	O	S	0	0	0
			1409	888	240	275	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	HIS	-	expression tag	UNP A7WZR9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	-	expression tag	UNP A7WZR9
A	198	HIS	-	expression tag	UNP A7WZR9
A	199	HIS	-	expression tag	UNP A7WZR9
A	200	HIS	-	expression tag	UNP A7WZR9
A	201	HIS	-	expression tag	UNP A7WZR9
B	196	HIS	-	expression tag	UNP A7WZR9
B	197	HIS	-	expression tag	UNP A7WZR9
B	198	HIS	-	expression tag	UNP A7WZR9
B	199	HIS	-	expression tag	UNP A7WZR9
B	200	HIS	-	expression tag	UNP A7WZR9
B	201	HIS	-	expression tag	UNP A7WZR9
C	196	HIS	-	expression tag	UNP A7WZR9
C	197	HIS	-	expression tag	UNP A7WZR9
C	198	HIS	-	expression tag	UNP A7WZR9
C	199	HIS	-	expression tag	UNP A7WZR9
C	200	HIS	-	expression tag	UNP A7WZR9
C	201	HIS	-	expression tag	UNP A7WZR9
D	196	HIS	-	expression tag	UNP A7WZR9
D	197	HIS	-	expression tag	UNP A7WZR9
D	198	HIS	-	expression tag	UNP A7WZR9
D	199	HIS	-	expression tag	UNP A7WZR9
D	200	HIS	-	expression tag	UNP A7WZR9
D	201	HIS	-	expression tag	UNP A7WZR9
E	196	HIS	-	expression tag	UNP A7WZR9
E	197	HIS	-	expression tag	UNP A7WZR9
E	198	HIS	-	expression tag	UNP A7WZR9
E	199	HIS	-	expression tag	UNP A7WZR9
E	200	HIS	-	expression tag	UNP A7WZR9
E	201	HIS	-	expression tag	UNP A7WZR9
F	196	HIS	-	expression tag	UNP A7WZR9
F	197	HIS	-	expression tag	UNP A7WZR9
F	198	HIS	-	expression tag	UNP A7WZR9
F	199	HIS	-	expression tag	UNP A7WZR9
F	200	HIS	-	expression tag	UNP A7WZR9
F	201	HIS	-	expression tag	UNP A7WZR9
G	196	HIS	-	expression tag	UNP A7WZR9
G	197	HIS	-	expression tag	UNP A7WZR9
G	198	HIS	-	expression tag	UNP A7WZR9
G	199	HIS	-	expression tag	UNP A7WZR9
G	200	HIS	-	expression tag	UNP A7WZR9
G	201	HIS	-	expression tag	UNP A7WZR9
H	196	HIS	-	expression tag	UNP A7WZR9

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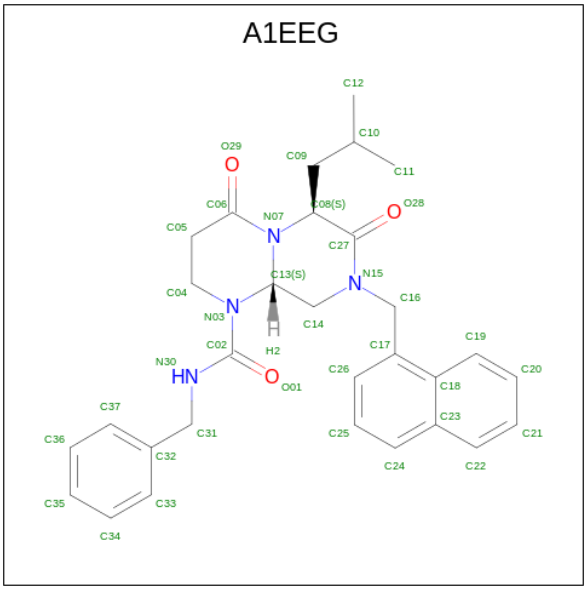
Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	-	expression tag	UNP A7WZR9
H	198	HIS	-	expression tag	UNP A7WZR9
H	199	HIS	-	expression tag	UNP A7WZR9
H	200	HIS	-	expression tag	UNP A7WZR9
H	201	HIS	-	expression tag	UNP A7WZR9
I	196	HIS	-	expression tag	UNP A7WZR9
I	197	HIS	-	expression tag	UNP A7WZR9
I	198	HIS	-	expression tag	UNP A7WZR9
I	199	HIS	-	expression tag	UNP A7WZR9
I	200	HIS	-	expression tag	UNP A7WZR9
I	201	HIS	-	expression tag	UNP A7WZR9
J	196	HIS	-	expression tag	UNP A7WZR9
J	197	HIS	-	expression tag	UNP A7WZR9
J	198	HIS	-	expression tag	UNP A7WZR9
J	199	HIS	-	expression tag	UNP A7WZR9
J	200	HIS	-	expression tag	UNP A7WZR9
J	201	HIS	-	expression tag	UNP A7WZR9
K	196	HIS	-	expression tag	UNP A7WZR9
K	197	HIS	-	expression tag	UNP A7WZR9
K	198	HIS	-	expression tag	UNP A7WZR9
K	199	HIS	-	expression tag	UNP A7WZR9
K	200	HIS	-	expression tag	UNP A7WZR9
K	201	HIS	-	expression tag	UNP A7WZR9
L	196	HIS	-	expression tag	UNP A7WZR9
L	197	HIS	-	expression tag	UNP A7WZR9
L	198	HIS	-	expression tag	UNP A7WZR9
L	199	HIS	-	expression tag	UNP A7WZR9
L	200	HIS	-	expression tag	UNP A7WZR9
L	201	HIS	-	expression tag	UNP A7WZR9
M	196	HIS	-	expression tag	UNP A7WZR9
M	197	HIS	-	expression tag	UNP A7WZR9
M	198	HIS	-	expression tag	UNP A7WZR9
M	199	HIS	-	expression tag	UNP A7WZR9
M	200	HIS	-	expression tag	UNP A7WZR9
M	201	HIS	-	expression tag	UNP A7WZR9
N	196	HIS	-	expression tag	UNP A7WZR9
N	197	HIS	-	expression tag	UNP A7WZR9
N	198	HIS	-	expression tag	UNP A7WZR9
N	199	HIS	-	expression tag	UNP A7WZR9
N	200	HIS	-	expression tag	UNP A7WZR9
N	201	HIS	-	expression tag	UNP A7WZR9

- Molecule 2 is (6 {S},9 {a} {S})-6-(2-methylpropyl)-8-(naphthalen-1-ylmethyl)-4,7-bis(oxi

danylidene)- {N}-(phenylmethyl)-3,6,9,9 {a}-tetrahydro-2 {H}-pyrazino[1,2-a]pyrimidine -1-carboxamide (three-letter code: A1EEG) (formula: $C_{30}H_{34}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	30	4	3		
2	B	1	Total	C	N	O	0	0
			37	30	4	3		
2	C	1	Total	C	N	O	0	0
			37	30	4	3		
2	D	1	Total	C	N	O	0	0
			37	30	4	3		
2	E	1	Total	C	N	O	0	0
			37	30	4	3		
2	F	1	Total	C	N	O	0	0
			37	30	4	3		
2	G	1	Total	C	N	O	0	0
			37	30	4	3		
2	H	1	Total	C	N	O	0	0
			37	30	4	3		
2	I	1	Total	C	N	O	0	0
			37	30	4	3		
2	J	1	Total	C	N	O	0	0
			37	30	4	3		
2	K	1	Total	C	N	O	0	0
			37	30	4	3		
2	L	1	Total	C	N	O	0	0
			37	30	4	3		

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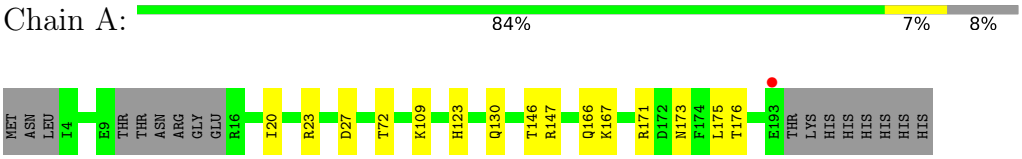
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	N	O	0	0
			37	30	4	3		
2	N	1	Total	C	N	O	0	0
			37	30	4	3		

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.

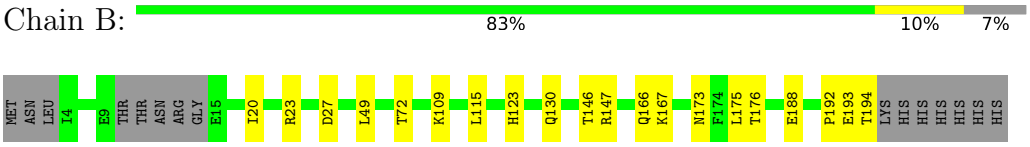
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



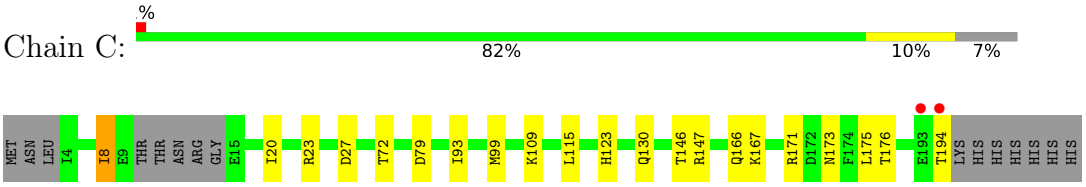
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



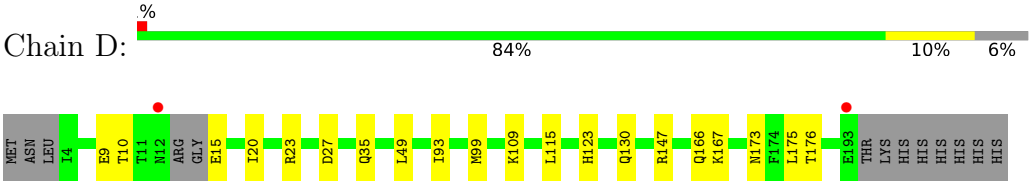
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



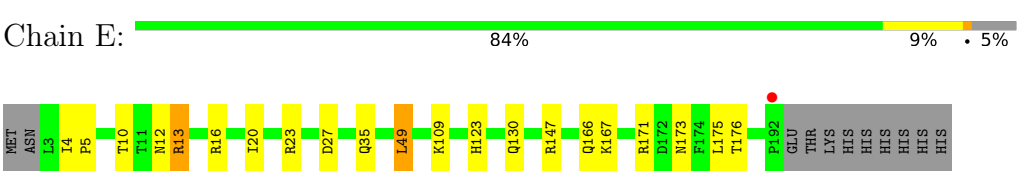
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



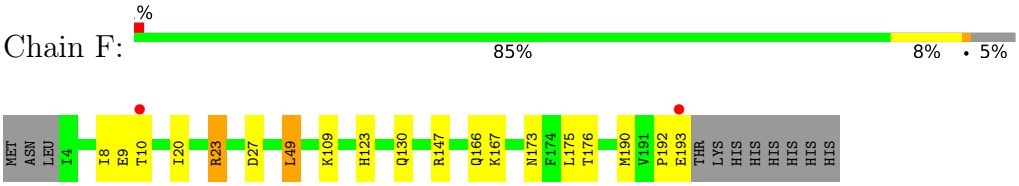
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



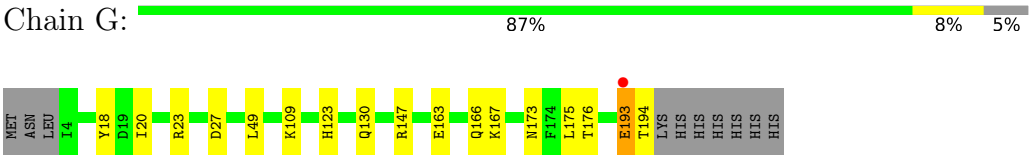
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



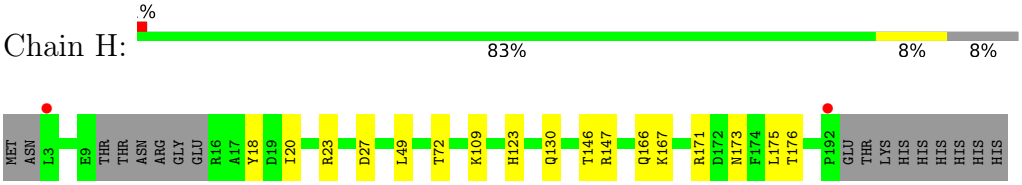
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



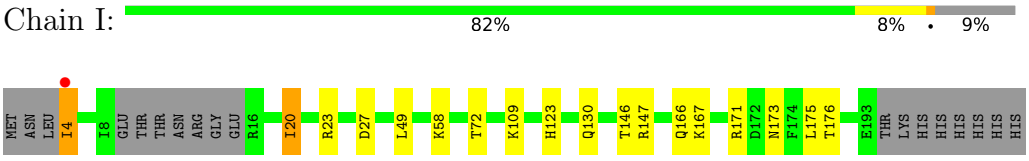
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



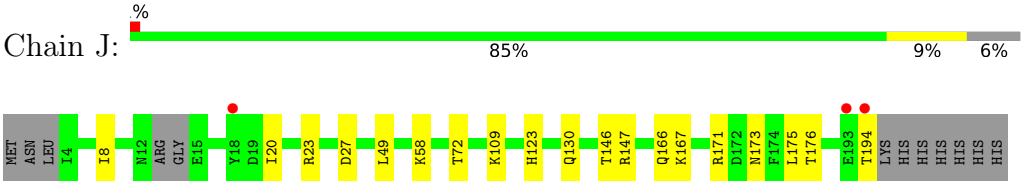
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



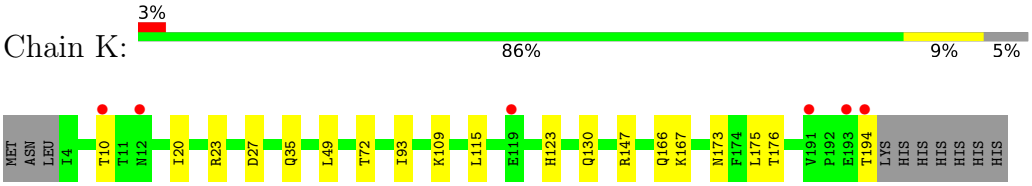
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



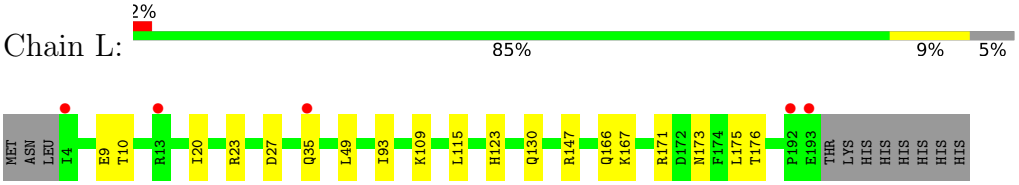
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



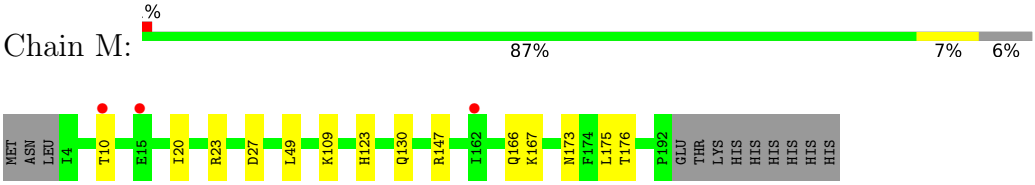
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



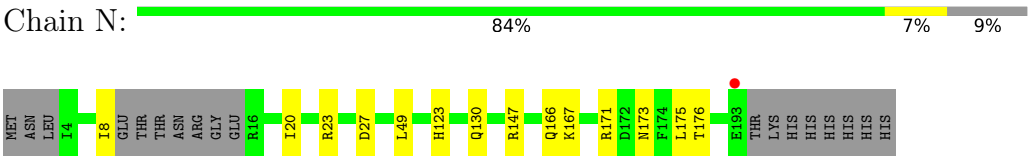
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.37Å 174.51Å 194.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.88 – 2.74 129.88 – 2.74	Depositor EDS
% Data completeness (in resolution range)	75.8 (129.88-2.74) 75.8 (129.88-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.226 , 0.249 0.226 , 0.248	Depositor DCC
R_{free} test set	4466 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 0.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: A1EEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/1426	0.75	0/1926
1	B	0.48	0/1442	0.75	0/1948
1	C	0.53	0/1442	0.75	0/1948
1	D	0.50	0/1458	0.76	0/1970
1	E	0.54	0/1483	0.78	0/2003
1	F	0.48	0/1473	0.75	0/1991
1	G	0.53	0/1469	0.77	0/1987
1	H	0.47	0/1433	0.74	0/1935
1	I	0.49	0/1425	0.73	0/1924
1	J	0.50	0/1468	0.75	0/1984
1	K	0.49	0/1485	0.75	0/2007
1	L	0.51	0/1471	0.76	0/1989
1	M	0.48	0/1468	0.72	0/1984
1	N	0.51	0/1427	0.75	0/1927
All	All	0.50	0/20370	0.75	0/27523

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	L	0	1
1	N	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	ARG	Sidechain
1	C	171	ARG	Sidechain
1	E	171	ARG	Sidechain
1	H	171	ARG	Sidechain
1	I	171	ARG	Sidechain
1	J	171	ARG	Sidechain
1	L	171	ARG	Sidechain
1	N	171	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1408	0	1418	0	0
1	B	1424	0	1431	3	0
1	C	1424	0	1431	3	0
1	D	1440	0	1444	4	0
1	E	1464	0	1476	4	0
1	F	1454	0	1461	4	0
1	G	1450	0	1448	2	0
1	H	1415	0	1431	2	0
1	I	1407	0	1420	2	0
1	J	1450	0	1455	1	0
1	K	1466	0	1472	1	0
1	L	1452	0	1454	1	0
1	M	1449	0	1459	0	0
1	N	1409	0	1420	1	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
2	C	37	0	0	0	0
2	D	37	0	0	1	0
2	E	37	0	0	2	0
2	F	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	37	0	0	0	0
2	H	37	0	0	2	0
2	I	37	0	0	1	0
2	J	37	0	0	0	0
2	K	37	0	0	0	0
2	L	37	0	0	3	0
2	M	37	0	0	2	0
2	N	37	0	0	4	0
All	All	20630	0	20220	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:301:A1EEG:C08	2:N:301:A1EEG:C27	1.88	1.51
2:L:301:A1EEG:C08	2:L:301:A1EEG:C27	1.87	1.49
2:M:301:A1EEG:C08	2:M:301:A1EEG:C27	1.89	1.48
2:L:301:A1EEG:C27	2:L:301:A1EEG:N07	2.51	0.68
1:C:93:ILE:HG12	1:C:115:LEU:HD13	1.79	0.65
1:K:93:ILE:HG12	1:K:115:LEU:HD13	1.79	0.64
1:L:93:ILE:HG12	1:L:115:LEU:HD13	1.79	0.64
1:I:4:ILE:HD12	1:I:20:ILE:HG22	1.80	0.63
1:D:93:ILE:HG12	1:D:115:LEU:HD13	1.80	0.62
2:N:301:A1EEG:C27	2:N:301:A1EEG:N07	2.49	0.61
2:L:301:A1EEG:C27	2:L:301:A1EEG:C09	2.81	0.56
1:G:193:GLU:O	1:G:194:THR:C	2.45	0.55
1:B:192:PRO:HB2	1:B:193:GLU:O	2.06	0.55
2:I:301:A1EEG:C24	1:J:49:LEU:HD22	2.37	0.55
2:H:301:A1EEG:C24	1:I:49:LEU:HD22	2.37	0.54
1:F:192:PRO:O	1:F:193:GLU:C	2.47	0.53
2:E:301:A1EEG:C13	2:E:301:A1EEG:C10	2.86	0.53
1:F:8:ILE:HD12	1:G:18:TYR:CE1	2.44	0.52
2:N:301:A1EEG:C27	2:N:301:A1EEG:C09	2.80	0.52
2:D:301:A1EEG:O01	1:E:49:LEU:HD21	2.10	0.52
1:E:13:ARG:HB2	1:E:13:ARG:NH1	2.26	0.50
1:D:9:GLU:OE2	1:D:9:GLU:HA	2.12	0.49
1:D:10:THR:HA	1:D:15:GLU:HG2	1.95	0.48
1:D:15:GLU:OE1	1:E:16:ARG:NH1	2.42	0.48
2:M:301:A1EEG:C27	2:M:301:A1EEG:N07	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:A1EEG:C12	2:B:301:A1EEG:C27	2.93	0.46
1:C:8:ILE:O	1:C:8:ILE:HG13	2.11	0.45
2:E:301:A1EEG:O01	1:F:49:LEU:HD21	2.18	0.44
2:A:301:A1EEG:C24	1:B:49:LEU:HD22	2.48	0.43
1:H:49:LEU:HD22	2:N:301:A1EEG:C24	2.49	0.43
2:H:301:A1EEG:N07	2:H:301:A1EEG:C11	2.81	0.42
1:F:9:GLU:OE1	1:F:23:ARG:NH1	2.49	0.41
1:B:115:LEU:HD13	1:C:79:ASP:HB3	2.04	0.40
1:H:18:TYR:CE1	1:N:8:ILE:HD12	2.56	0.40
1:E:4:ILE:HA	1:E:5:PRO:HD3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/201 (90%)	178 (99%)	2 (1%)	0	100	100
1	B	182/201 (90%)	179 (98%)	3 (2%)	0	100	100
1	C	182/201 (90%)	179 (98%)	3 (2%)	0	100	100
1	D	184/201 (92%)	180 (98%)	4 (2%)	0	100	100
1	E	188/201 (94%)	185 (98%)	3 (2%)	0	100	100
1	F	188/201 (94%)	183 (97%)	5 (3%)	0	100	100
1	G	189/201 (94%)	183 (97%)	5 (3%)	1 (0%)	25	41
1	H	180/201 (90%)	176 (98%)	4 (2%)	0	100	100
1	I	179/201 (89%)	177 (99%)	2 (1%)	0	100	100
1	J	185/201 (92%)	181 (98%)	4 (2%)	0	100	100
1	K	189/201 (94%)	185 (98%)	4 (2%)	0	100	100
1	L	188/201 (94%)	185 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	187/201 (93%)	183 (98%)	4 (2%)	0	100	100
1	N	179/201 (89%)	177 (99%)	2 (1%)	0	100	100
All	All	2580/2814 (92%)	2531 (98%)	48 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	193	GLU

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	150/169 (89%)	136 (91%)	14 (9%)	7	13
1	B	152/169 (90%)	136 (90%)	16 (10%)	5	10
1	C	152/169 (90%)	135 (89%)	17 (11%)	5	8
1	D	154/169 (91%)	139 (90%)	15 (10%)	6	12
1	E	157/169 (93%)	140 (89%)	17 (11%)	5	9
1	F	155/169 (92%)	140 (90%)	15 (10%)	6	12
1	G	153/169 (90%)	139 (91%)	14 (9%)	7	14
1	H	152/169 (90%)	138 (91%)	14 (9%)	7	14
1	I	151/169 (89%)	135 (89%)	16 (11%)	5	9
1	J	156/169 (92%)	139 (89%)	17 (11%)	5	9
1	K	157/169 (93%)	140 (89%)	17 (11%)	5	9
1	L	155/169 (92%)	139 (90%)	16 (10%)	6	10
1	M	155/169 (92%)	141 (91%)	14 (9%)	8	15
1	N	151/169 (89%)	139 (92%)	12 (8%)	10	19
All	All	2150/2366 (91%)	1936 (90%)	214 (10%)	6	11

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	23	ARG
1	A	27	ASP
1	A	72	THR
1	A	109	LYS
1	A	123	HIS
1	A	130	GLN
1	A	146	THR
1	A	147	ARG
1	A	166	GLN
1	A	167	LYS
1	A	173	ASN
1	A	175	LEU
1	A	176	THR
1	B	20	ILE
1	B	23	ARG
1	B	27	ASP
1	B	72	THR
1	B	109	LYS
1	B	123	HIS
1	B	130	GLN
1	B	146	THR
1	B	147	ARG
1	B	166	GLN
1	B	167	LYS
1	B	173	ASN
1	B	175	LEU
1	B	176	THR
1	B	188	GLU
1	B	194	THR
1	C	8	ILE
1	C	20	ILE
1	C	23	ARG
1	C	27	ASP
1	C	72	THR
1	C	99	MET
1	C	109	LYS
1	C	123	HIS
1	C	130	GLN
1	C	146	THR
1	C	147	ARG
1	C	166	GLN
1	C	167	LYS

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Mol	Chain	Res	Type
1	C	173	ASN
1	C	175	LEU
1	C	176	THR
1	C	194	THR
1	D	20	ILE
1	D	23	ARG
1	D	27	ASP
1	D	35	GLN
1	D	49	LEU
1	D	99	MET
1	D	109	LYS
1	D	123	HIS
1	D	130	GLN
1	D	147	ARG
1	D	166	GLN
1	D	167	LYS
1	D	173	ASN
1	D	175	LEU
1	D	176	THR
1	E	10	THR
1	E	12	ASN
1	E	13	ARG
1	E	20	ILE
1	E	23	ARG
1	E	27	ASP
1	E	35	GLN
1	E	49	LEU
1	E	109	LYS
1	E	123	HIS
1	E	130	GLN
1	E	147	ARG
1	E	166	GLN
1	E	167	LYS
1	E	173	ASN
1	E	175	LEU
1	E	176	THR
1	F	10	THR
1	F	20	ILE
1	F	23	ARG
1	F	27	ASP
1	F	49	LEU
1	F	109	LYS

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Mol	Chain	Res	Type
1	F	123	HIS
1	F	130	GLN
1	F	147	ARG
1	F	166	GLN
1	F	167	LYS
1	F	173	ASN
1	F	175	LEU
1	F	176	THR
1	F	190	MET
1	G	20	ILE
1	G	23	ARG
1	G	27	ASP
1	G	49	LEU
1	G	109	LYS
1	G	123	HIS
1	G	130	GLN
1	G	147	ARG
1	G	163	GLU
1	G	166	GLN
1	G	167	LYS
1	G	173	ASN
1	G	175	LEU
1	G	176	THR
1	H	20	ILE
1	H	23	ARG
1	H	27	ASP
1	H	72	THR
1	H	109	LYS
1	H	123	HIS
1	H	130	GLN
1	H	146	THR
1	H	147	ARG
1	H	166	GLN
1	H	167	LYS
1	H	173	ASN
1	H	175	LEU
1	H	176	THR
1	I	4	ILE
1	I	20	ILE
1	I	23	ARG
1	I	27	ASP
1	I	58	LYS

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Mol	Chain	Res	Type
1	I	72	THR
1	I	109	LYS
1	I	123	HIS
1	I	130	GLN
1	I	146	THR
1	I	147	ARG
1	I	166	GLN
1	I	167	LYS
1	I	173	ASN
1	I	175	LEU
1	I	176	THR
1	J	8	ILE
1	J	20	ILE
1	J	23	ARG
1	J	27	ASP
1	J	58	LYS
1	J	72	THR
1	J	109	LYS
1	J	123	HIS
1	J	130	GLN
1	J	146	THR
1	J	147	ARG
1	J	166	GLN
1	J	167	LYS
1	J	173	ASN
1	J	175	LEU
1	J	176	THR
1	J	194	THR
1	K	10	THR
1	K	20	ILE
1	K	23	ARG
1	K	27	ASP
1	K	35	GLN
1	K	49	LEU
1	K	72	THR
1	K	109	LYS
1	K	123	HIS
1	K	130	GLN
1	K	147	ARG
1	K	166	GLN
1	K	167	LYS
1	K	173	ASN

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Mol	Chain	Res	Type
1	K	175	LEU
1	K	176	THR
1	K	194	THR
1	L	9	GLU
1	L	10	THR
1	L	20	ILE
1	L	23	ARG
1	L	27	ASP
1	L	35	GLN
1	L	49	LEU
1	L	109	LYS
1	L	123	HIS
1	L	130	GLN
1	L	147	ARG
1	L	166	GLN
1	L	167	LYS
1	L	173	ASN
1	L	175	LEU
1	L	176	THR
1	M	10	THR
1	M	20	ILE
1	M	23	ARG
1	M	27	ASP
1	M	49	LEU
1	M	109	LYS
1	M	123	HIS
1	M	130	GLN
1	M	147	ARG
1	M	166	GLN
1	M	167	LYS
1	M	173	ASN
1	M	175	LEU
1	M	176	THR
1	N	20	ILE
1	N	23	ARG
1	N	27	ASP
1	N	49	LEU
1	N	123	HIS
1	N	130	GLN
1	N	147	ARG
1	N	166	GLN
1	N	167	LYS

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Mol	Chain	Res	Type
1	N	173	ASN
1	N	175	LEU
1	N	176	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	89	GLN
1	A	123	HIS
1	A	160	GLN
1	A	173	ASN
1	B	82	GLN
1	B	89	GLN
1	B	123	HIS
1	B	160	GLN
1	B	173	ASN
1	C	82	GLN
1	C	89	GLN
1	C	123	HIS
1	C	160	GLN
1	C	173	ASN
1	D	82	GLN
1	D	89	GLN
1	D	123	HIS
1	D	160	GLN
1	D	173	ASN
1	E	82	GLN
1	E	89	GLN
1	E	123	HIS
1	E	160	GLN
1	E	173	ASN
1	F	82	GLN
1	F	89	GLN
1	F	123	HIS
1	F	160	GLN
1	F	173	ASN
1	G	82	GLN
1	G	89	GLN
1	G	123	HIS
1	G	160	GLN
1	G	173	ASN

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Mol	Chain	Res	Type
1	H	82	GLN
1	H	89	GLN
1	H	123	HIS
1	H	160	GLN
1	H	173	ASN
1	I	82	GLN
1	I	89	GLN
1	I	123	HIS
1	I	160	GLN
1	I	173	ASN
1	J	82	GLN
1	J	89	GLN
1	J	123	HIS
1	J	160	GLN
1	J	173	ASN
1	K	82	GLN
1	K	89	GLN
1	K	123	HIS
1	K	160	GLN
1	K	173	ASN
1	L	82	GLN
1	L	89	GLN
1	L	123	HIS
1	L	160	GLN
1	L	173	ASN
1	M	82	GLN
1	M	89	GLN
1	M	123	HIS
1	M	160	GLN
1	M	173	ASN
1	N	82	GLN
1	N	89	GLN
1	N	123	HIS
1	N	160	GLN
1	N	173	ASN

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)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1EEG	B	301	-	39,41,41	2.68	10 (25%)	48,58,58	1.46	7 (14%)
2	A1EEG	H	301	-	39,41,41	2.86	9 (23%)	48,58,58	1.39	5 (10%)
2	A1EEG	K	301	-	39,41,41	2.88	10 (25%)	48,58,58	1.39	6 (12%)
2	A1EEG	I	301	-	39,41,41	2.69	12 (30%)	48,58,58	1.35	7 (14%)
2	A1EEG	L	301	-	39,41,41	5.30	13 (33%)	48,58,58	1.57	4 (8%)
2	A1EEG	A	301	-	39,41,41	2.56	12 (30%)	48,58,58	1.37	9 (18%)
2	A1EEG	M	301	-	39,41,41	5.51	13 (33%)	48,58,58	1.26	4 (8%)
2	A1EEG	D	301	-	39,41,41	2.54	11 (28%)	48,58,58	1.43	10 (20%)
2	A1EEG	G	301	-	39,41,41	2.73	12 (30%)	48,58,58	1.44	5 (10%)
2	A1EEG	J	301	-	39,41,41	2.79	12 (30%)	48,58,58	1.24	5 (10%)
2	A1EEG	C	301	-	39,41,41	2.73	11 (28%)	48,58,58	1.23	8 (16%)
2	A1EEG	N	301	-	39,41,41	5.59	13 (33%)	48,58,58	1.32	8 (16%)
2	A1EEG	F	301	-	39,41,41	2.66	11 (28%)	48,58,58	1.41	6 (12%)
2	A1EEG	E	301	-	39,41,41	2.85	8 (20%)	48,58,58	1.59	8 (16%)

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	A1EEG	B	301	-	-	3/17/50/50	0/5/5/5
2	A1EEG	H	301	-	-	1/17/50/50	0/5/5/5
2	A1EEG	K	301	-	-	2/17/50/50	0/5/5/5
2	A1EEG	I	301	-	-	4/17/50/50	0/5/5/5
2	A1EEG	L	301	-	-	4/17/50/50	0/5/5/5
2	A1EEG	A	301	-	-	0/17/50/50	0/5/5/5
2	A1EEG	M	301	-	-	5/17/50/50	0/5/5/5
2	A1EEG	D	301	-	-	0/17/50/50	0/5/5/5
2	A1EEG	G	301	-	-	4/17/50/50	0/5/5/5
2	A1EEG	J	301	-	-	2/17/50/50	0/5/5/5
2	A1EEG	C	301	-	-	4/17/50/50	0/5/5/5
2	A1EEG	N	301	-	-	2/17/50/50	0/5/5/5
2	A1EEG	F	301	-	-	2/17/50/50	0/5/5/5
2	A1EEG	E	301	-	-	2/17/50/50	0/5/5/5

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	A1EEG	C08-N07	-20.19	1.14	1.47
2	M	301	A1EEG	C08-N07	-19.26	1.16	1.47
2	M	301	A1EEG	C08-C27	19.08	1.89	1.51
2	N	301	A1EEG	C06-N07	18.83	1.51	1.35
2	N	301	A1EEG	C08-C27	18.65	1.88	1.51
2	L	301	A1EEG	C08-N07	-18.62	1.17	1.47
2	L	301	A1EEG	C08-C27	18.35	1.87	1.51
2	M	301	A1EEG	C06-N07	18.09	1.51	1.35
2	L	301	A1EEG	C06-N07	17.05	1.50	1.35
2	K	301	A1EEG	C06-N07	13.52	1.47	1.35
2	H	301	A1EEG	C06-N07	13.21	1.46	1.35
2	E	301	A1EEG	C06-N07	13.08	1.46	1.35
2	G	301	A1EEG	C06-N07	11.77	1.45	1.35
2	J	301	A1EEG	C06-N07	11.61	1.45	1.35
2	C	301	A1EEG	C06-N07	11.54	1.45	1.35
2	I	301	A1EEG	C06-N07	10.99	1.44	1.35
2	F	301	A1EEG	C06-N07	10.86	1.44	1.35
2	A	301	A1EEG	C06-N07	10.61	1.44	1.35
2	B	301	A1EEG	C06-N07	10.05	1.44	1.35
2	D	301	A1EEG	C06-N07	9.32	1.43	1.35
2	I	301	A1EEG	C14-N15	-8.31	1.37	1.46
2	B	301	A1EEG	C14-N15	-8.30	1.37	1.46
2	C	301	A1EEG	C14-N15	-8.28	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	A1EEG	C14-N15	-8.27	1.37	1.46
2	J	301	A1EEG	C14-N15	-8.19	1.37	1.46
2	K	301	A1EEG	C14-N15	-8.17	1.37	1.46
2	F	301	A1EEG	C14-N15	-8.13	1.37	1.46
2	D	301	A1EEG	C14-N15	-8.05	1.37	1.46
2	G	301	A1EEG	C14-N15	-7.85	1.37	1.46
2	H	301	A1EEG	C14-N15	-7.83	1.37	1.46
2	A	301	A1EEG	C14-N15	-7.38	1.38	1.46
2	B	301	A1EEG	C08-N07	-5.37	1.38	1.47
2	L	301	A1EEG	C13-N03	5.14	1.52	1.46
2	D	301	A1EEG	C08-N07	-5.07	1.39	1.47
2	M	301	A1EEG	C14-N15	-4.73	1.41	1.46
2	F	301	A1EEG	C08-N07	-4.46	1.40	1.47
2	C	301	A1EEG	C18-C23	-4.27	1.35	1.43
2	N	301	A1EEG	C14-N15	-4.26	1.41	1.46
2	J	301	A1EEG	C08-N07	-4.22	1.40	1.47
2	N	301	A1EEG	C27-N15	3.98	1.44	1.35
2	J	301	A1EEG	C18-C23	-3.97	1.35	1.43
2	B	301	A1EEG	C18-C23	-3.93	1.35	1.43
2	A	301	A1EEG	C08-N07	-3.85	1.41	1.47
2	I	301	A1EEG	C08-N07	-3.80	1.41	1.47
2	E	301	A1EEG	C18-C23	-3.78	1.36	1.43
2	G	301	A1EEG	C18-C23	-3.77	1.36	1.43
2	H	301	A1EEG	C08-N07	-3.77	1.41	1.47
2	I	301	A1EEG	C18-C23	-3.50	1.36	1.43
2	L	301	A1EEG	C02-N03	3.39	1.48	1.37
2	G	301	A1EEG	C08-N07	-3.35	1.42	1.47
2	M	301	A1EEG	C02-N03	3.34	1.48	1.37
2	A	301	A1EEG	C18-C23	-3.34	1.36	1.43
2	M	301	A1EEG	C27-N15	3.32	1.42	1.35
2	M	301	A1EEG	C09-C08	3.24	1.60	1.53
2	D	301	A1EEG	C18-C23	-3.23	1.37	1.43
2	H	301	A1EEG	C18-C23	-3.20	1.37	1.43
2	C	301	A1EEG	C08-N07	-3.17	1.42	1.47
2	E	301	A1EEG	C04-N03	-3.08	1.41	1.47
2	I	301	A1EEG	C19-C18	-3.07	1.36	1.42
2	K	301	A1EEG	C18-C23	-3.05	1.37	1.43
2	L	301	A1EEG	O29-C06	-2.94	1.16	1.23
2	M	301	A1EEG	C02-N30	2.92	1.47	1.34
2	N	301	A1EEG	C02-N03	2.91	1.47	1.37
2	F	301	A1EEG	C04-N03	-2.88	1.41	1.47
2	F	301	A1EEG	C18-C23	-2.87	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	A1EEG	C02-N30	2.85	1.47	1.34
2	N	301	A1EEG	C09-C08	2.85	1.59	1.53
2	G	301	A1EEG	C19-C18	-2.82	1.36	1.42
2	J	301	A1EEG	C17-C18	-2.80	1.36	1.42
2	E	301	A1EEG	C08-N07	-2.78	1.42	1.47
2	L	301	A1EEG	O28-C27	-2.76	1.17	1.22
2	L	301	A1EEG	C27-N15	2.72	1.41	1.35
2	N	301	A1EEG	C02-N30	2.71	1.46	1.34
2	F	301	A1EEG	O01-C02	-2.70	1.18	1.23
2	N	301	A1EEG	O01-C02	-2.69	1.18	1.23
2	B	301	A1EEG	C04-N03	-2.69	1.42	1.47
2	C	301	A1EEG	C19-C18	-2.67	1.36	1.42
2	L	301	A1EEG	C09-C08	2.67	1.59	1.53
2	K	301	A1EEG	C08-N07	-2.66	1.43	1.47
2	J	301	A1EEG	C19-C18	-2.65	1.36	1.42
2	M	301	A1EEG	O28-C27	-2.63	1.17	1.22
2	B	301	A1EEG	O01-C02	-2.61	1.18	1.23
2	J	301	A1EEG	C24-C23	-2.60	1.35	1.41
2	K	301	A1EEG	C04-N03	-2.58	1.42	1.47
2	L	301	A1EEG	C14-N15	-2.58	1.43	1.46
2	N	301	A1EEG	C18-C23	-2.57	1.38	1.43
2	D	301	A1EEG	C04-N03	-2.52	1.42	1.47
2	L	301	A1EEG	C18-C23	-2.50	1.38	1.43
2	C	301	A1EEG	C02-N03	2.49	1.45	1.37
2	K	301	A1EEG	C19-C18	-2.49	1.37	1.42
2	H	301	A1EEG	C19-C18	-2.47	1.37	1.42
2	A	301	A1EEG	C19-C18	-2.45	1.37	1.42
2	H	301	A1EEG	C04-N03	-2.45	1.42	1.47
2	G	301	A1EEG	C24-C23	-2.45	1.36	1.41
2	A	301	A1EEG	O01-C02	-2.43	1.18	1.23
2	B	301	A1EEG	C27-N15	2.43	1.40	1.35
2	N	301	A1EEG	O28-C27	-2.42	1.18	1.22
2	K	301	A1EEG	C04-C05	-2.42	1.45	1.52
2	A	301	A1EEG	C04-N03	-2.41	1.42	1.47
2	F	301	A1EEG	C19-C18	-2.41	1.37	1.42
2	I	301	A1EEG	C22-C23	-2.41	1.36	1.41
2	F	301	A1EEG	C22-C23	-2.41	1.36	1.41
2	G	301	A1EEG	C04-N03	-2.40	1.42	1.47
2	I	301	A1EEG	C24-C23	-2.39	1.36	1.41
2	G	301	A1EEG	O01-C02	-2.38	1.18	1.23
2	C	301	A1EEG	O01-C02	-2.37	1.18	1.23
2	E	301	A1EEG	C17-C18	-2.37	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1EEG	C27-N15	2.37	1.40	1.35
2	J	301	A1EEG	O29-C06	-2.36	1.17	1.23
2	G	301	A1EEG	C17-C18	-2.36	1.37	1.42
2	L	301	A1EEG	O01-C02	-2.34	1.18	1.23
2	D	301	A1EEG	O28-C27	-2.34	1.18	1.22
2	C	301	A1EEG	C27-N15	2.33	1.40	1.35
2	A	301	A1EEG	C27-N15	2.33	1.40	1.35
2	H	301	A1EEG	C04-C05	-2.33	1.46	1.52
2	B	301	A1EEG	C17-C18	-2.31	1.37	1.42
2	G	301	A1EEG	C04-C05	-2.31	1.46	1.52
2	I	301	A1EEG	C17-C18	-2.29	1.37	1.42
2	D	301	A1EEG	O01-C02	-2.28	1.18	1.23
2	M	301	A1EEG	O29-C06	-2.28	1.17	1.23
2	G	301	A1EEG	C22-C23	-2.27	1.36	1.41
2	I	301	A1EEG	O01-C02	-2.26	1.18	1.23
2	A	301	A1EEG	C17-C18	-2.25	1.37	1.42
2	N	301	A1EEG	C16-N15	2.25	1.50	1.46
2	F	301	A1EEG	C02-N03	2.24	1.45	1.37
2	E	301	A1EEG	C19-C18	-2.24	1.37	1.42
2	D	301	A1EEG	C13-N03	-2.24	1.44	1.46
2	B	301	A1EEG	C19-C18	-2.23	1.37	1.42
2	C	301	A1EEG	C22-C23	-2.22	1.36	1.41
2	D	301	A1EEG	C19-C18	-2.22	1.37	1.42
2	K	301	A1EEG	C17-C18	-2.22	1.37	1.42
2	F	301	A1EEG	C24-C23	-2.20	1.36	1.41
2	K	301	A1EEG	O01-C02	-2.17	1.19	1.23
2	H	301	A1EEG	C17-C18	-2.16	1.37	1.42
2	H	301	A1EEG	C24-C23	-2.16	1.36	1.41
2	K	301	A1EEG	C24-C23	-2.15	1.36	1.41
2	M	301	A1EEG	C18-C23	-2.15	1.39	1.43
2	J	301	A1EEG	O01-C02	-2.15	1.19	1.23
2	A	301	A1EEG	C24-C23	-2.14	1.36	1.41
2	F	301	A1EEG	C04-C05	-2.13	1.46	1.52
2	G	301	A1EEG	C02-N03	2.12	1.44	1.37
2	J	301	A1EEG	C04-N03	-2.11	1.43	1.47
2	A	301	A1EEG	C02-N03	2.11	1.44	1.37
2	B	301	A1EEG	C24-C23	-2.09	1.36	1.41
2	M	301	A1EEG	C26-C17	2.07	1.41	1.37
2	I	301	A1EEG	C02-N03	2.07	1.44	1.37
2	J	301	A1EEG	C22-C23	-2.06	1.37	1.41
2	A	301	A1EEG	O28-C27	-2.06	1.18	1.22
2	M	301	A1EEG	C16-N15	2.05	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	A1EEG	C16-C17	2.05	1.57	1.52
2	I	301	A1EEG	C04-N03	-2.04	1.43	1.47
2	J	301	A1EEG	C04-C05	-2.04	1.46	1.52
2	E	301	A1EEG	C24-C23	-2.03	1.37	1.41
2	D	301	A1EEG	C22-C23	-2.02	1.37	1.41
2	D	301	A1EEG	O29-C06	-2.01	1.18	1.23
2	C	301	A1EEG	C24-C23	-2.01	1.37	1.41
2	C	301	A1EEG	O29-C06	-2.01	1.18	1.23

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	301	A1EEG	C13-C14-N15	7.65	120.77	111.02
2	E	301	A1EEG	C13-C14-N15	5.57	118.12	111.02
2	K	301	A1EEG	C13-C14-N15	5.18	117.62	111.02
2	G	301	A1EEG	C13-C14-N15	4.86	117.21	111.02
2	H	301	A1EEG	C13-C14-N15	4.72	117.03	111.02
2	B	301	A1EEG	C16-N15-C14	4.27	122.86	115.69
2	F	301	A1EEG	C13-C14-N15	4.03	116.16	111.02
2	J	301	A1EEG	C16-N15-C14	4.03	122.45	115.69
2	D	301	A1EEG	C31-N30-C02	-3.94	117.30	120.84
2	L	301	A1EEG	C16-N15-C14	3.79	122.05	115.69
2	E	301	A1EEG	C05-C04-N03	-3.71	99.39	111.61
2	F	301	A1EEG	C16-N15-C14	3.50	121.57	115.69
2	H	301	A1EEG	C16-N15-C14	3.47	121.51	115.69
2	G	301	A1EEG	C27-C08-N07	-3.33	105.67	112.29
2	I	301	A1EEG	C16-N15-C14	3.32	121.27	115.69
2	N	301	A1EEG	C16-N15-C27	3.28	122.79	119.73
2	A	301	A1EEG	C16-N15-C14	3.27	121.18	115.69
2	B	301	A1EEG	O29-C06-N07	-3.26	118.12	122.28
2	E	301	A1EEG	C17-C16-N15	-3.24	107.86	113.45
2	K	301	A1EEG	C16-N15-C14	3.18	121.02	115.69
2	M	301	A1EEG	C13-C14-N15	3.16	115.04	111.02
2	J	301	A1EEG	C13-C14-N15	3.11	114.98	111.02
2	C	301	A1EEG	C05-C04-N03	-3.10	101.41	111.61
2	H	301	A1EEG	C31-N30-C02	-3.06	118.08	120.84
2	A	301	A1EEG	O29-C06-N07	-3.06	118.38	122.28
2	F	301	A1EEG	C05-C04-N03	-3.02	101.68	111.61
2	D	301	A1EEG	C16-N15-C14	2.96	120.66	115.69
2	I	301	A1EEG	C32-C31-N30	-2.94	106.74	113.05
2	E	301	A1EEG	C32-C31-N30	2.91	119.29	113.05
2	G	301	A1EEG	C16-N15-C14	2.87	120.50	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	A1EEG	C16-N15-C27	-2.80	117.13	119.73
2	M	301	A1EEG	C16-N15-C27	2.80	122.33	119.73
2	N	301	A1EEG	O28-C27-N15	2.78	125.77	122.49
2	H	301	A1EEG	C17-C16-N15	-2.74	108.73	113.45
2	D	301	A1EEG	O29-C06-N07	-2.73	118.80	122.28
2	K	301	A1EEG	C32-C31-N30	2.71	118.86	113.05
2	G	301	A1EEG	C17-C16-N15	-2.71	108.78	113.45
2	I	301	A1EEG	O29-C06-N07	-2.68	118.86	122.28
2	N	301	A1EEG	C17-C16-N15	-2.65	108.89	113.45
2	C	301	A1EEG	C27-C08-N07	-2.60	107.12	112.29
2	D	301	A1EEG	C05-C04-N03	-2.58	103.10	111.61
2	I	301	A1EEG	C31-N30-C02	-2.55	118.54	120.84
2	E	301	A1EEG	C16-N15-C14	2.55	119.97	115.69
2	M	301	A1EEG	C10-C09-C08	2.52	120.78	115.19
2	H	301	A1EEG	C05-C04-N03	-2.51	103.34	111.61
2	B	301	A1EEG	C10-C09-C08	-2.51	109.62	115.19
2	B	301	A1EEG	C05-C04-N03	-2.49	103.41	111.61
2	B	301	A1EEG	C37-C32-C33	2.49	122.08	118.17
2	E	301	A1EEG	C27-C08-N07	-2.48	107.35	112.29
2	N	301	A1EEG	C24-C23-C22	-2.48	117.40	123.19
2	A	301	A1EEG	C27-C08-N07	-2.46	107.40	112.29
2	E	301	A1EEG	O28-C27-N15	-2.44	119.61	122.49
2	A	301	A1EEG	C17-C16-N15	-2.43	109.26	113.45
2	N	301	A1EEG	C05-C04-N03	-2.39	103.73	111.61
2	D	301	A1EEG	C32-C31-N30	2.39	118.17	113.05
2	J	301	A1EEG	C05-C04-N03	-2.39	103.75	111.61
2	C	301	A1EEG	O01-C02-N30	-2.37	117.19	123.53
2	L	301	A1EEG	C24-C23-C22	-2.37	117.65	123.19
2	N	301	A1EEG	C13-C14-N15	2.37	114.04	111.02
2	C	301	A1EEG	C13-C14-N15	2.37	114.04	111.02
2	J	301	A1EEG	C16-N15-C27	-2.36	117.53	119.73
2	D	301	A1EEG	C27-C08-N07	-2.36	107.59	112.29
2	D	301	A1EEG	C17-C16-N15	-2.27	109.54	113.45
2	F	301	A1EEG	O29-C06-N07	-2.26	119.39	122.28
2	F	301	A1EEG	C24-C23-C22	-2.25	117.92	123.19
2	D	301	A1EEG	C13-C14-N15	2.25	113.89	111.02
2	A	301	A1EEG	C37-C32-C33	2.24	121.69	118.17
2	A	301	A1EEG	O01-C02-N30	-2.21	117.62	123.53
2	K	301	A1EEG	C27-C08-N07	-2.18	107.94	112.29
2	B	301	A1EEG	O29-C06-C05	2.18	126.36	121.32
2	C	301	A1EEG	O29-C06-N07	-2.17	119.51	122.28
2	N	301	A1EEG	O28-C27-C08	-2.16	115.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	A1EEG	C24-C23-C22	-2.16	118.14	123.19
2	J	301	A1EEG	C10-C09-C08	-2.16	110.40	115.19
2	F	301	A1EEG	C16-C17-C18	2.12	123.63	119.93
2	C	301	A1EEG	O28-C27-N15	-2.11	120.00	122.49
2	L	301	A1EEG	C05-C04-N03	-2.10	104.69	111.61
2	E	301	A1EEG	C14-C13-N03	-2.10	109.00	112.59
2	D	301	A1EEG	C08-C27-N15	2.09	121.55	116.85
2	I	301	A1EEG	O28-C27-N15	-2.08	120.03	122.49
2	A	301	A1EEG	C16-N15-C27	-2.07	117.80	119.73
2	G	301	A1EEG	C05-C04-N03	-2.04	104.89	111.61
2	K	301	A1EEG	C16-C17-C18	2.03	123.48	119.93
2	C	301	A1EEG	C14-C13-N03	-2.03	109.12	112.59
2	A	301	A1EEG	C08-C27-N15	2.03	121.42	116.85
2	K	301	A1EEG	C05-C04-N03	-2.03	104.93	111.61
2	N	301	A1EEG	C16-C17-C18	2.03	123.48	119.93
2	I	301	A1EEG	C16-N15-C27	-2.02	117.85	119.73
2	M	301	A1EEG	C16-N15-C14	2.01	119.06	115.69
2	A	301	A1EEG	C10-C09-C08	-2.00	110.74	115.19
2	C	301	A1EEG	C08-C27-N15	2.00	121.36	116.85
2	D	301	A1EEG	C37-C32-C33	2.00	121.31	118.17

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	A1EEG	C27-C08-C09-C10
2	C	301	A1EEG	N07-C08-C09-C10
2	E	301	A1EEG	N07-C08-C09-C10
2	F	301	A1EEG	N07-C08-C09-C10
2	F	301	A1EEG	C27-C08-C09-C10
2	I	301	A1EEG	N07-C08-C09-C10
2	I	301	A1EEG	C27-C08-C09-C10
2	J	301	A1EEG	C27-C08-C09-C10
2	M	301	A1EEG	N07-C08-C09-C10
2	M	301	A1EEG	C27-C08-C09-C10
2	C	301	A1EEG	C08-C09-C10-C11
2	I	301	A1EEG	C08-C09-C10-C12
2	C	301	A1EEG	C08-C09-C10-C12
2	G	301	A1EEG	C08-C09-C10-C12
2	I	301	A1EEG	C08-C09-C10-C11
2	M	301	A1EEG	C08-C09-C10-C12
2	G	301	A1EEG	C08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
2	L	301	A1EEG	C17-C16-N15-C14
2	M	301	A1EEG	C08-C09-C10-C11
2	M	301	A1EEG	C17-C16-N15-C14
2	H	301	A1EEG	C08-C09-C10-C11
2	G	301	A1EEG	C17-C16-N15-C14
2	C	301	A1EEG	C27-C08-C09-C10
2	E	301	A1EEG	C27-C08-C09-C10
2	L	301	A1EEG	C27-C08-C09-C10
2	N	301	A1EEG	C27-C08-C09-C10
2	B	301	A1EEG	N07-C08-C09-C10
2	G	301	A1EEG	N07-C08-C09-C10
2	J	301	A1EEG	N07-C08-C09-C10
2	L	301	A1EEG	N07-C08-C09-C10
2	N	301	A1EEG	N07-C08-C09-C10
2	L	301	A1EEG	C17-C16-N15-C27
2	K	301	A1EEG	N07-C08-C09-C10
2	K	301	A1EEG	C08-C09-C10-C11
2	B	301	A1EEG	C08-C09-C10-C12

There are no ring outliers.

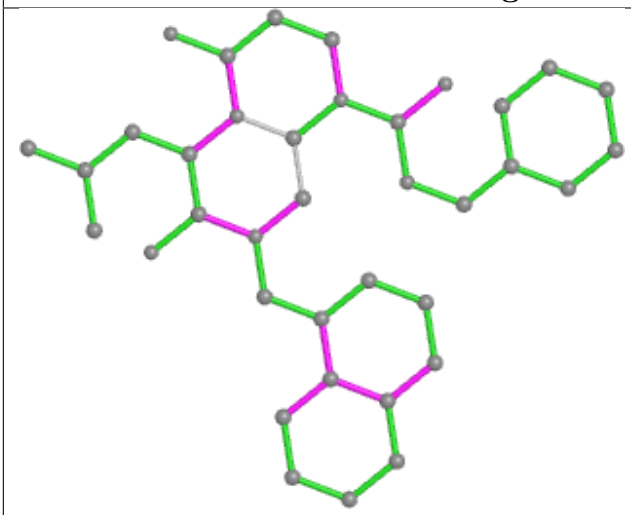
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	A1EEG	1	0
2	H	301	A1EEG	2	0
2	I	301	A1EEG	1	0
2	L	301	A1EEG	3	0
2	A	301	A1EEG	1	0
2	M	301	A1EEG	2	0
2	D	301	A1EEG	1	0
2	N	301	A1EEG	4	0
2	E	301	A1EEG	2	0

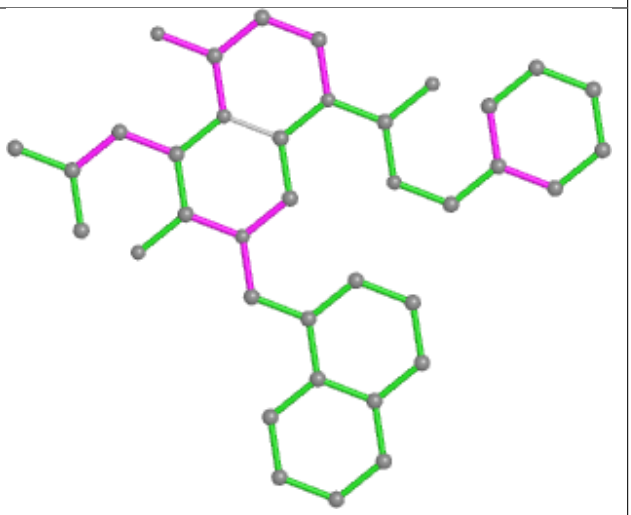
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

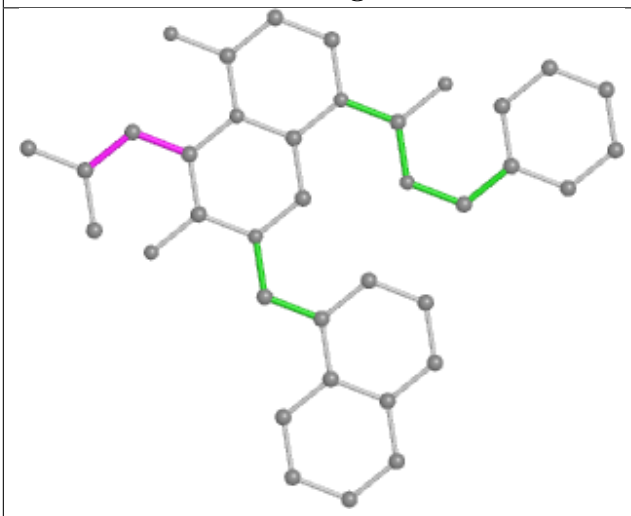
Ligand A1EEG B 301



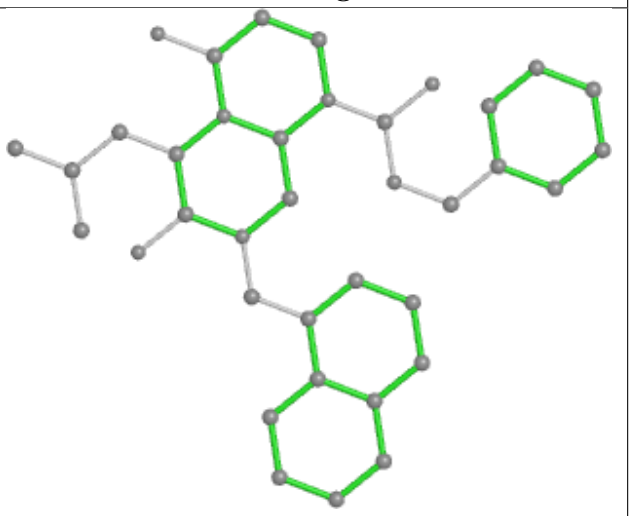
Bond lengths



Bond angles

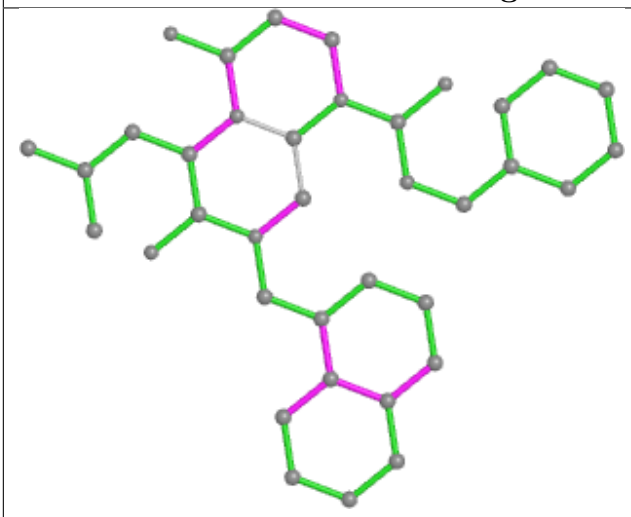


Torsions



Rings

Ligand A1EEG H 301



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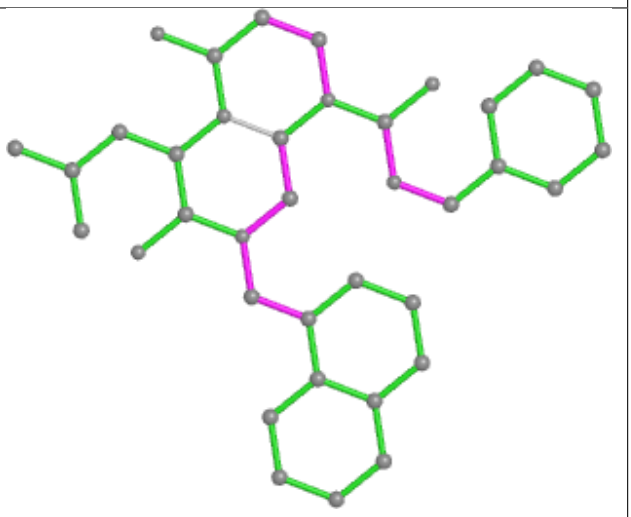

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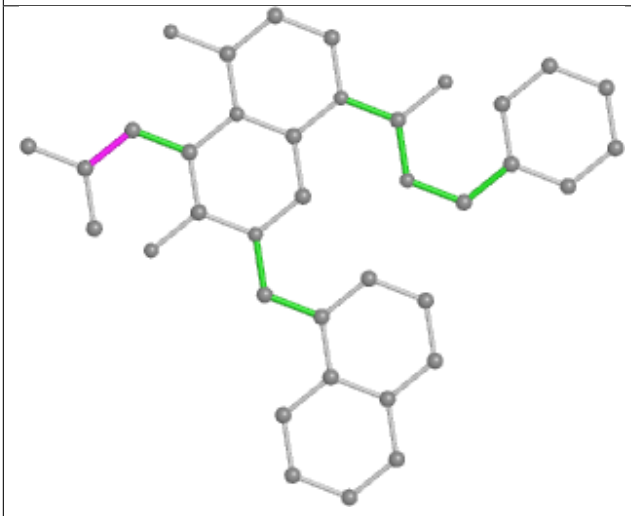

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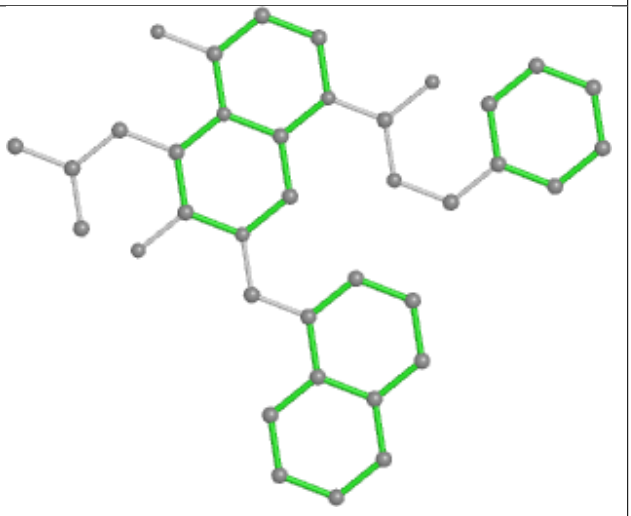
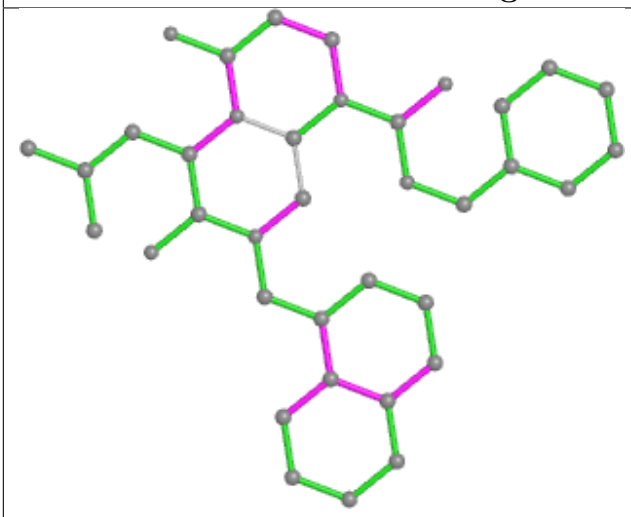


Rings

Ligand A1EEG K 301



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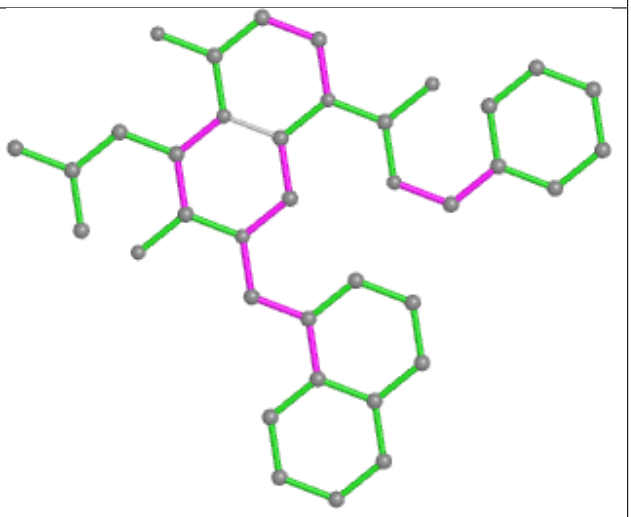
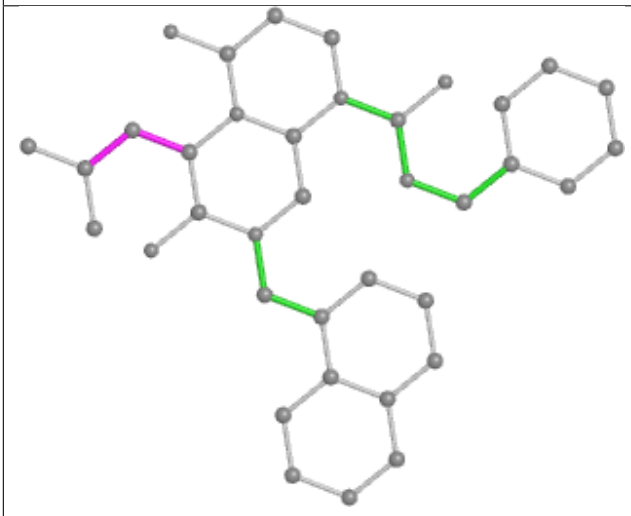


Bond angles



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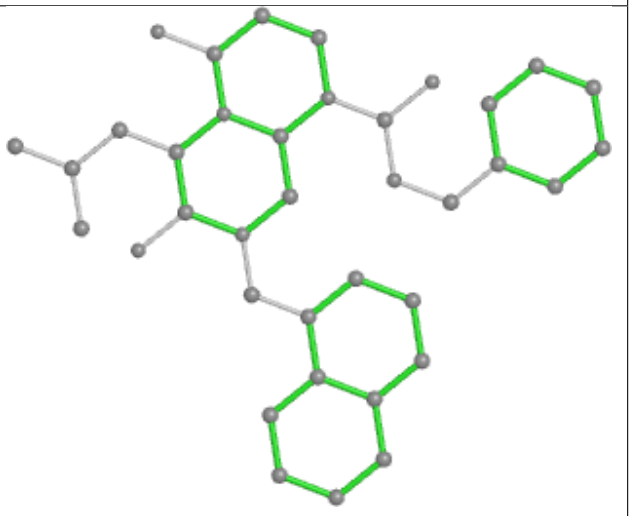
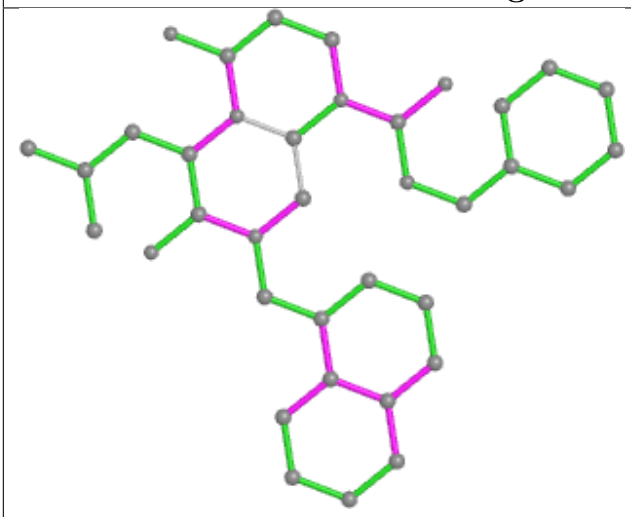


Rings

Ligand A1EEG I 301



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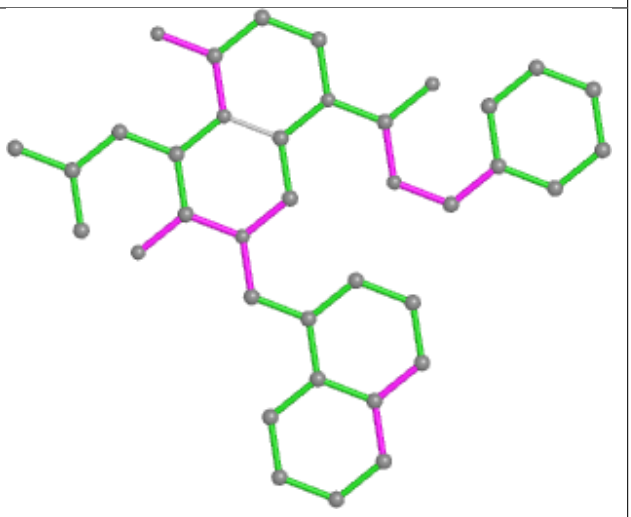

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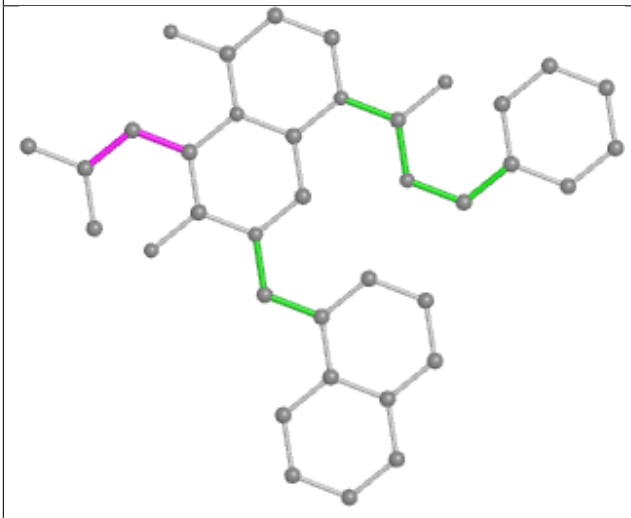

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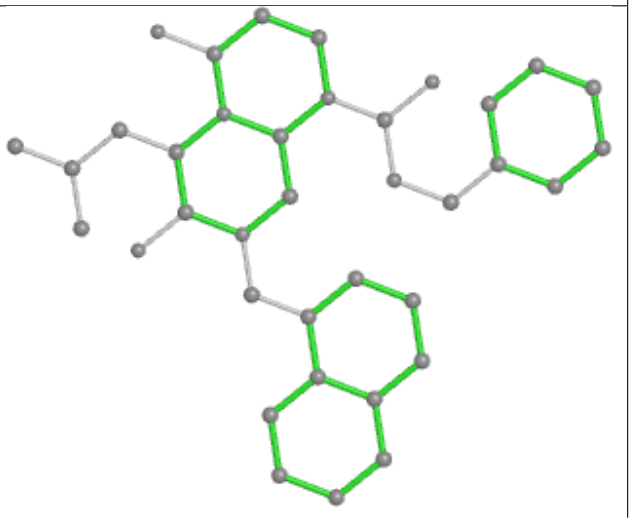
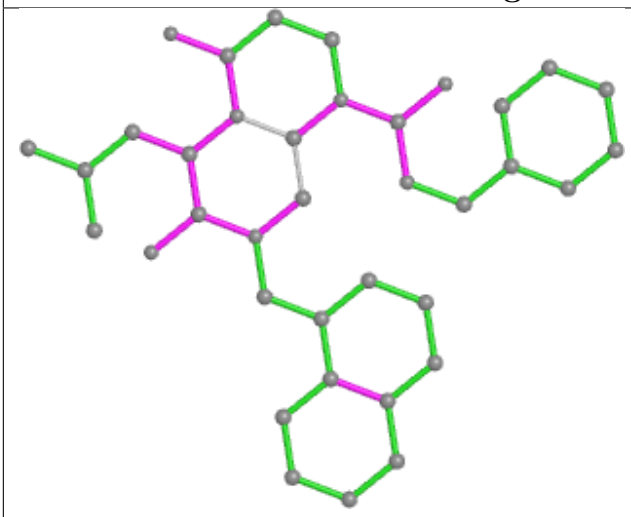


Rings

Ligand A1EEG L 301



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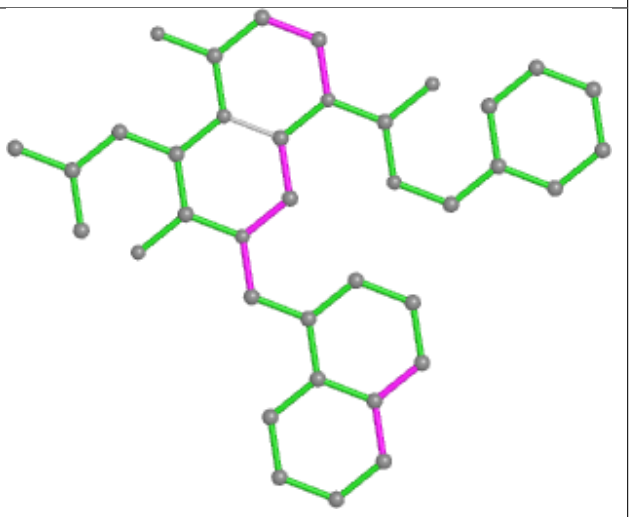

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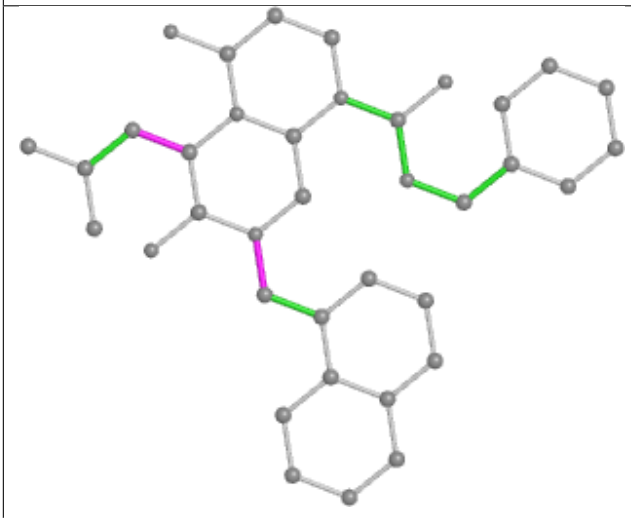

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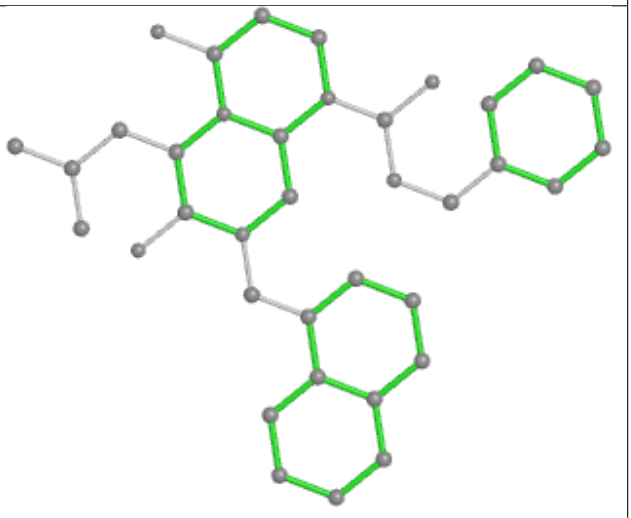
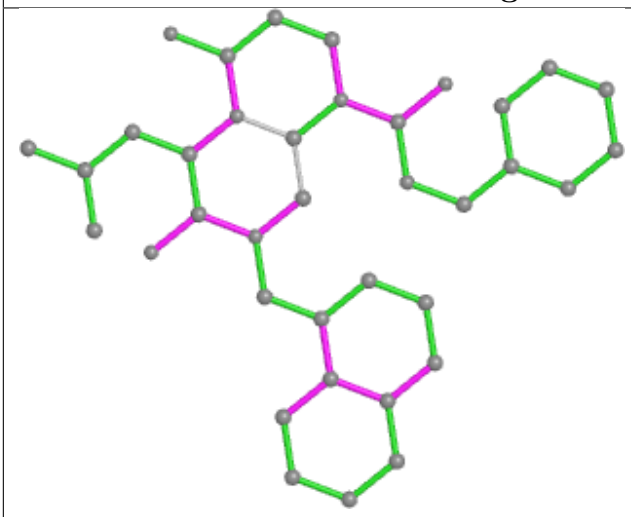


Rings

Ligand A1EEG A 301



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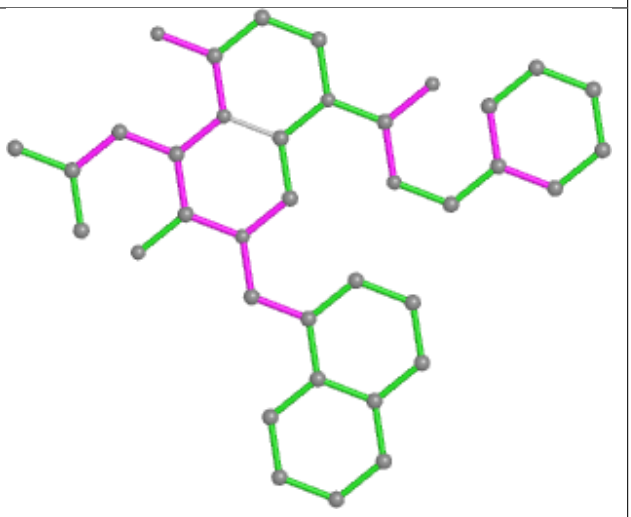

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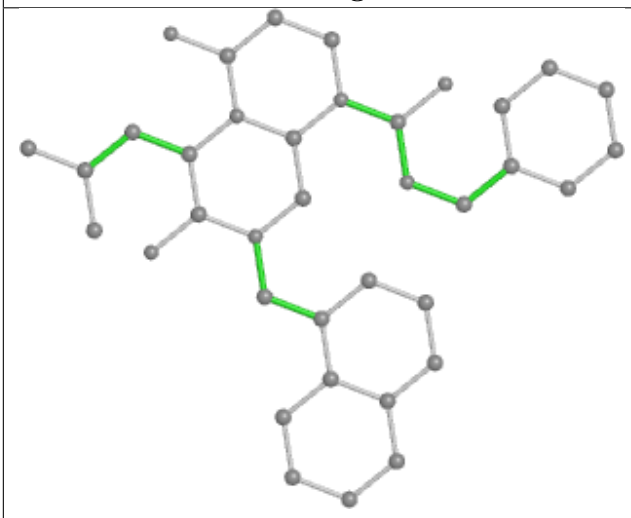

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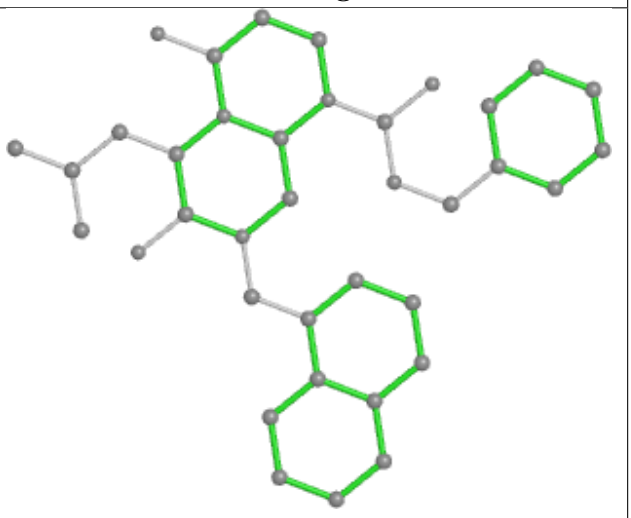
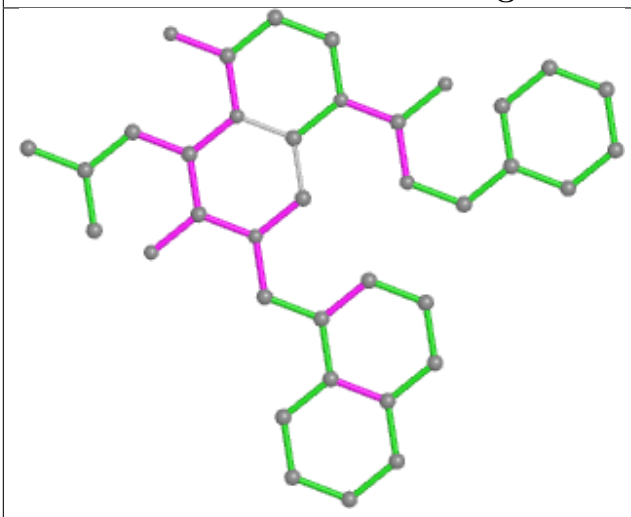


Rings

Ligand A1EEG M 301



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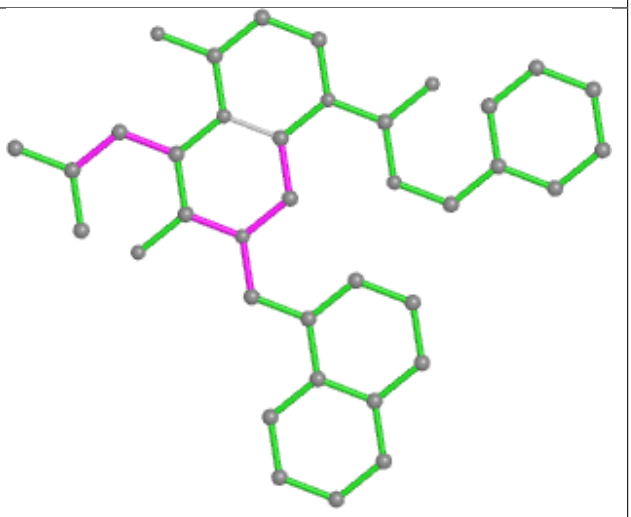

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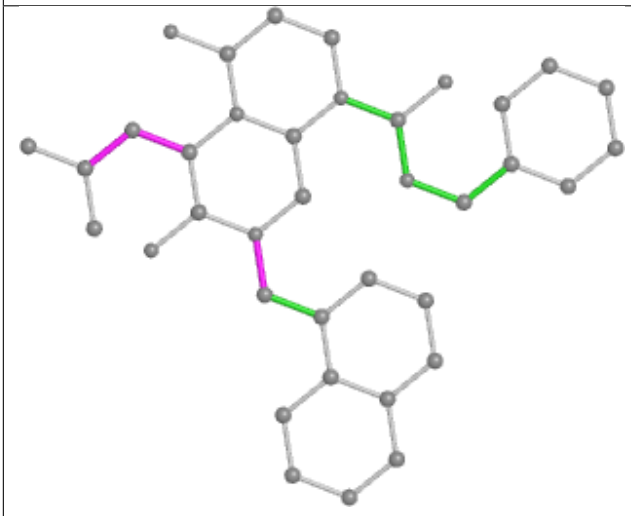

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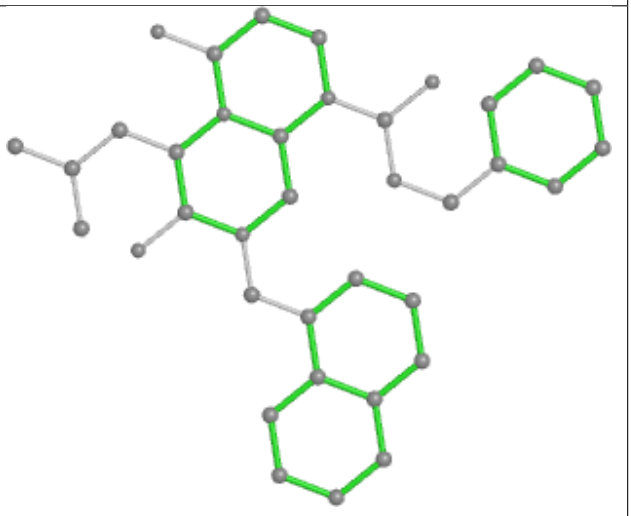
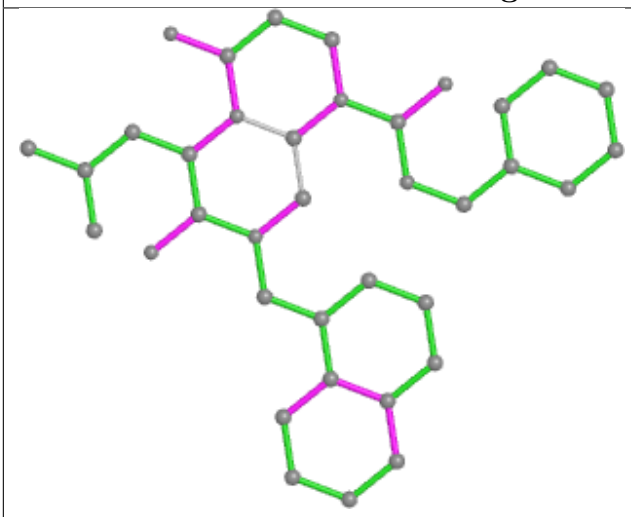


Rings

Ligand A1EEG D 301



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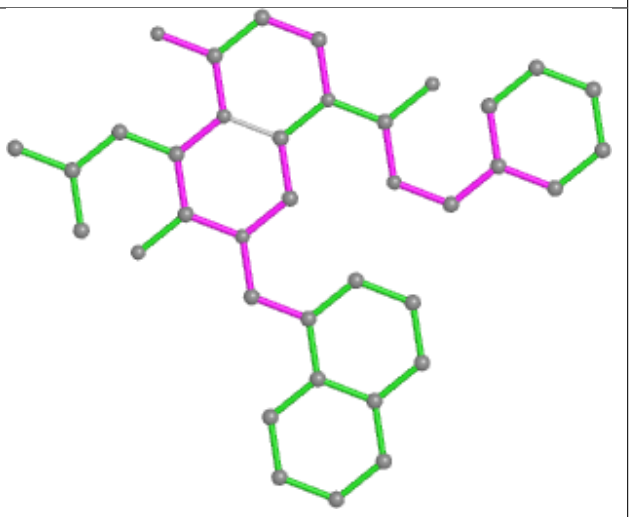

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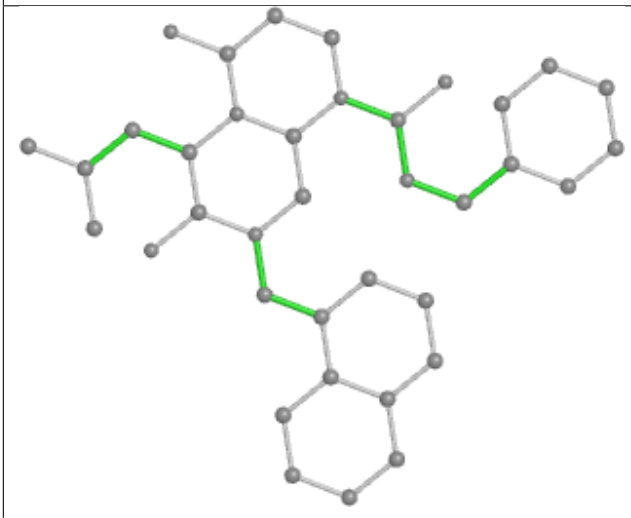

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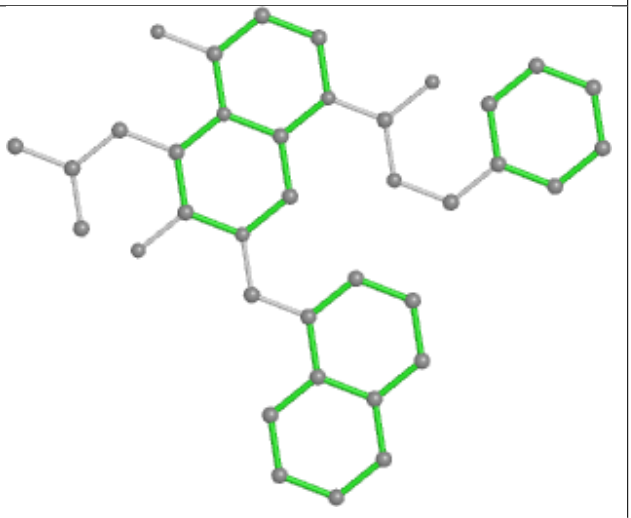
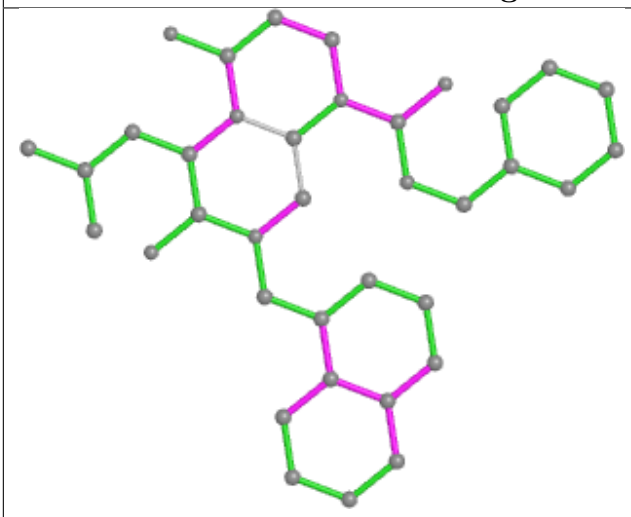


Rings

Ligand A1EEG G 301



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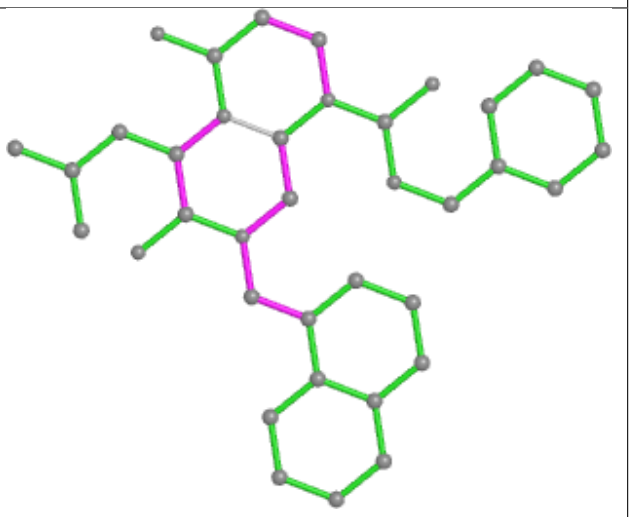

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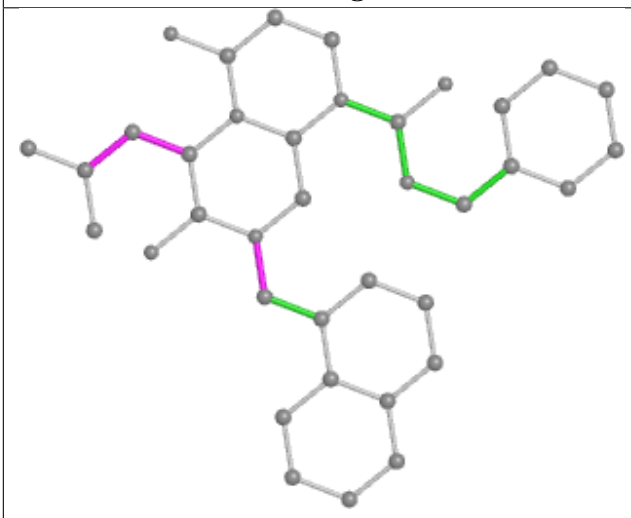

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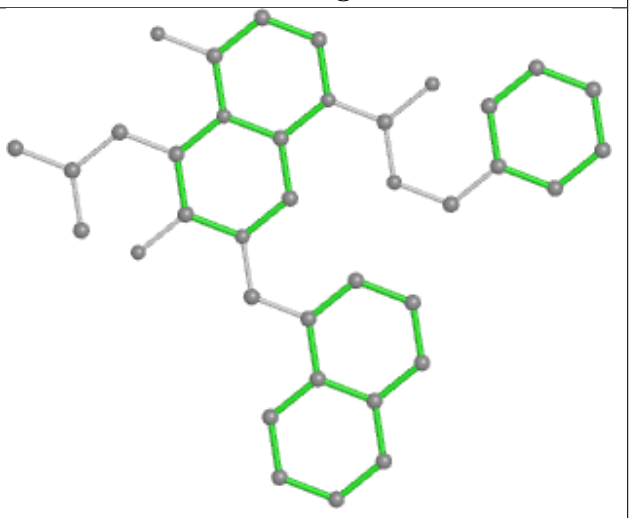
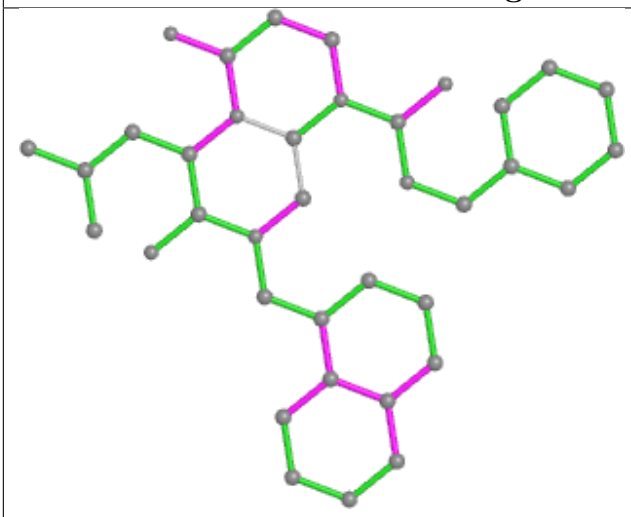


Rings

Ligand A1EEG J 301



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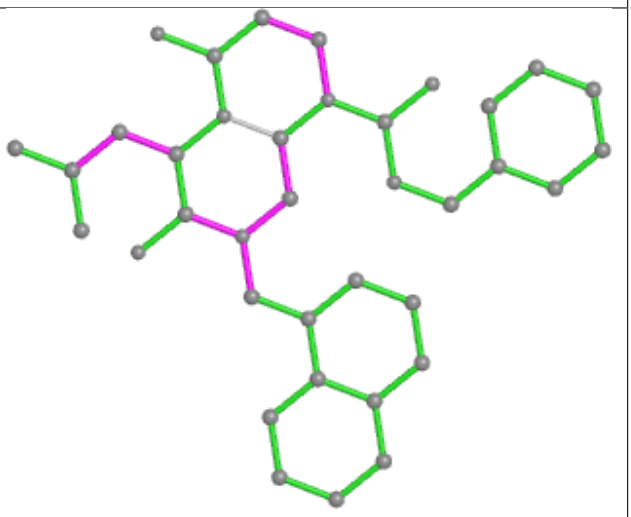

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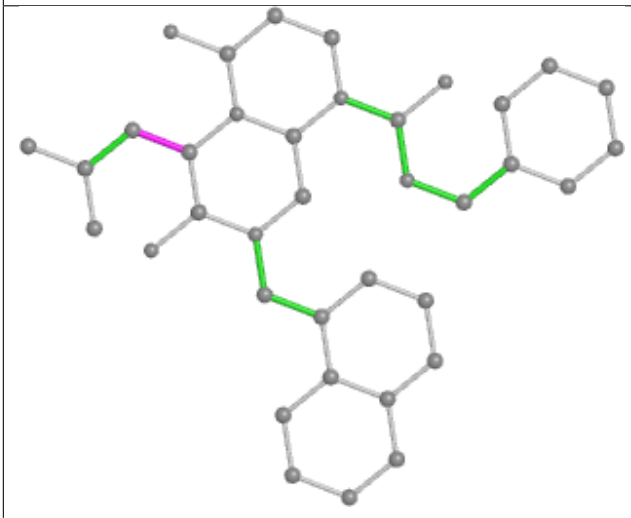

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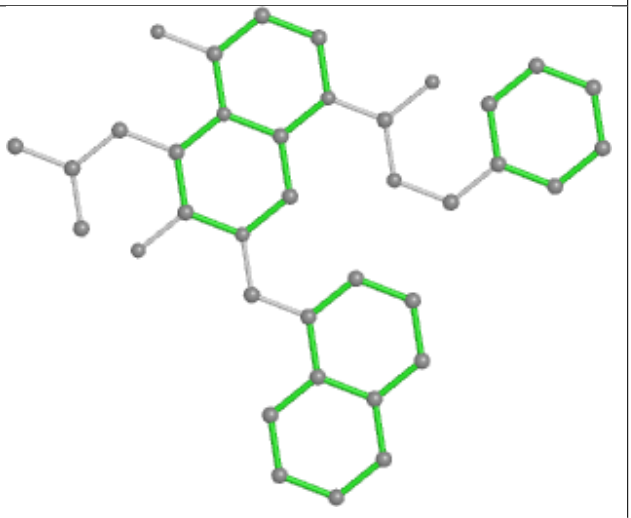
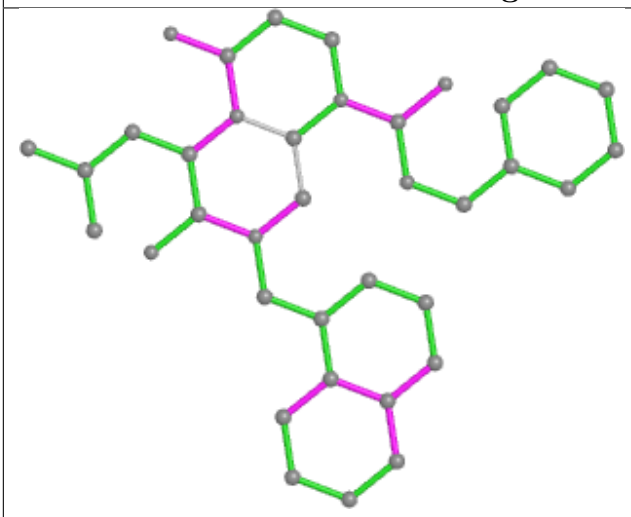


Rings

Ligand A1EEG C 301



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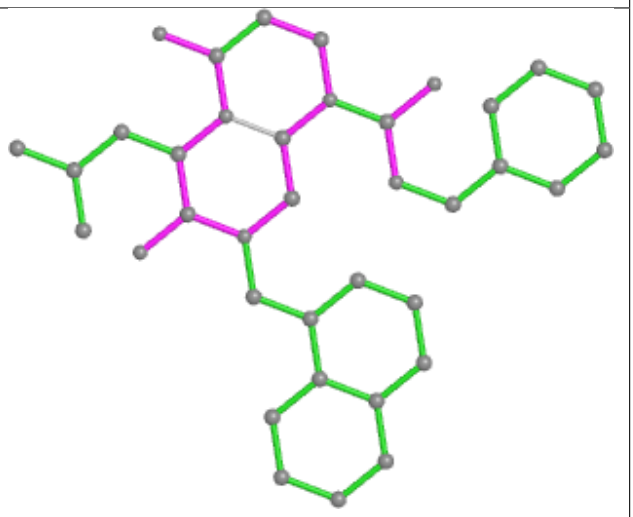

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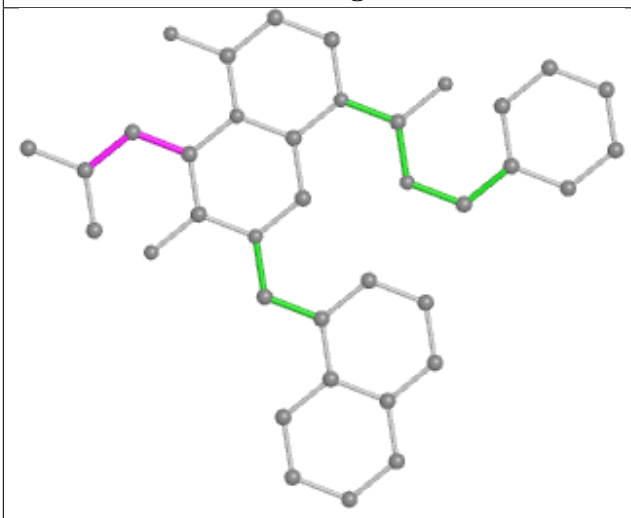

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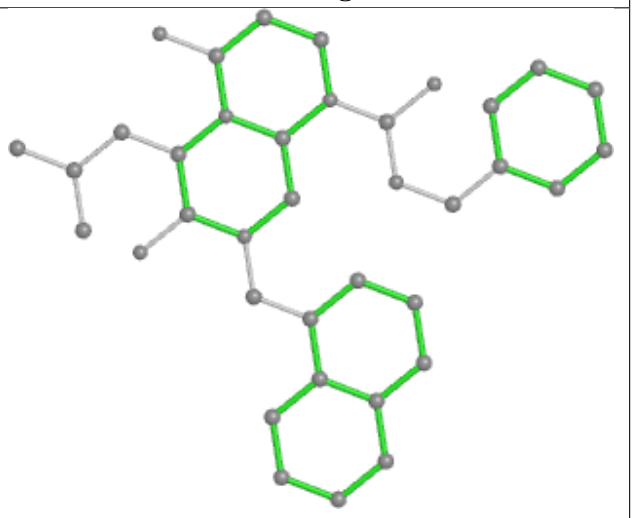
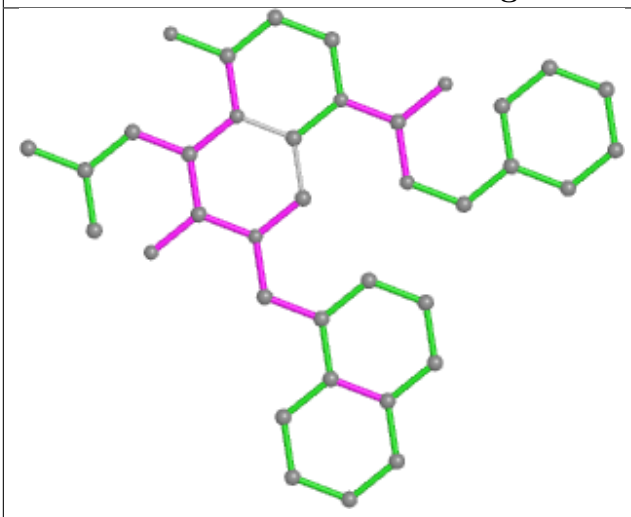


Rings

Ligand A1EEG N 301



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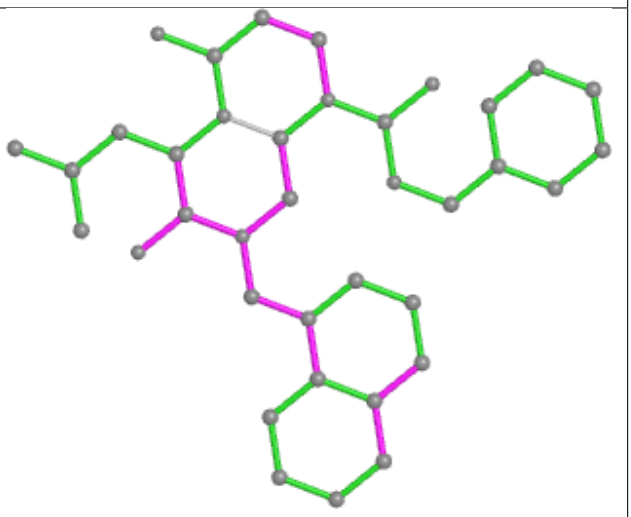
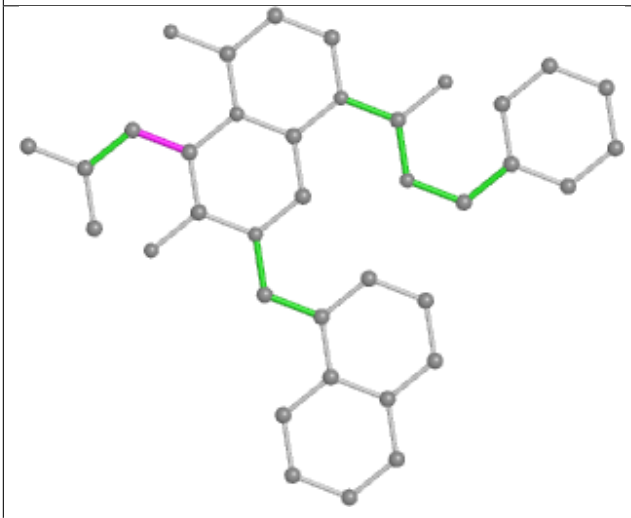


Bond angles



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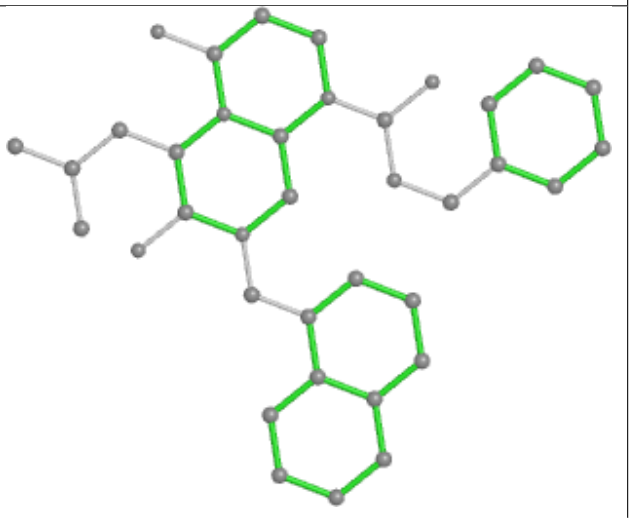
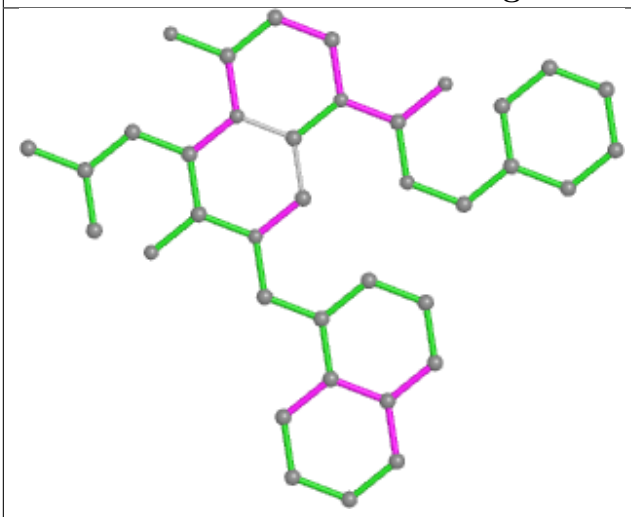


Rings

Ligand A1EEG F 301



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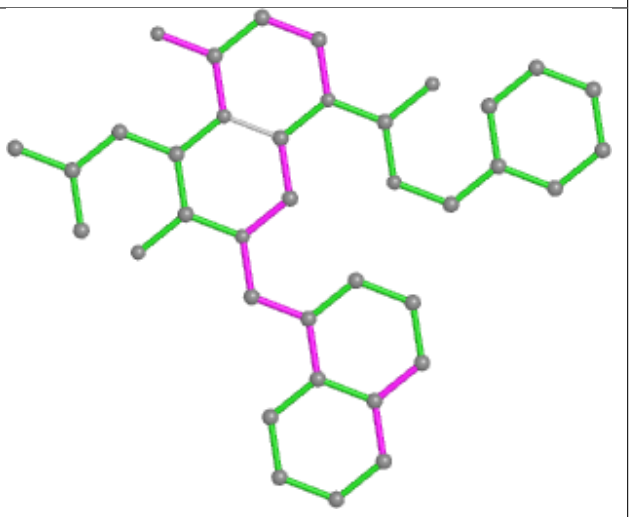
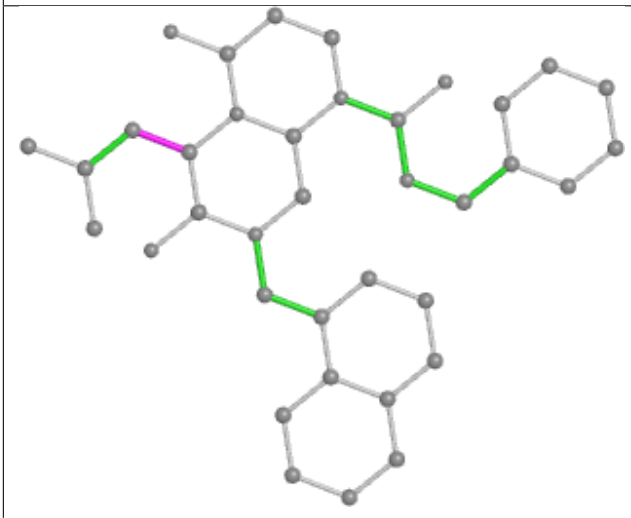


Bond angles



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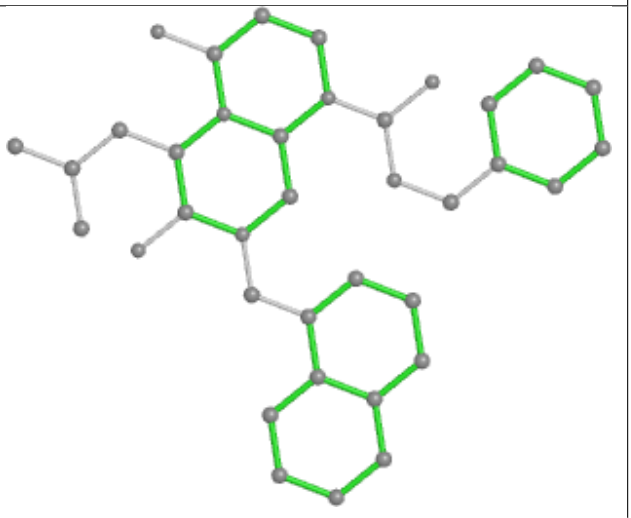
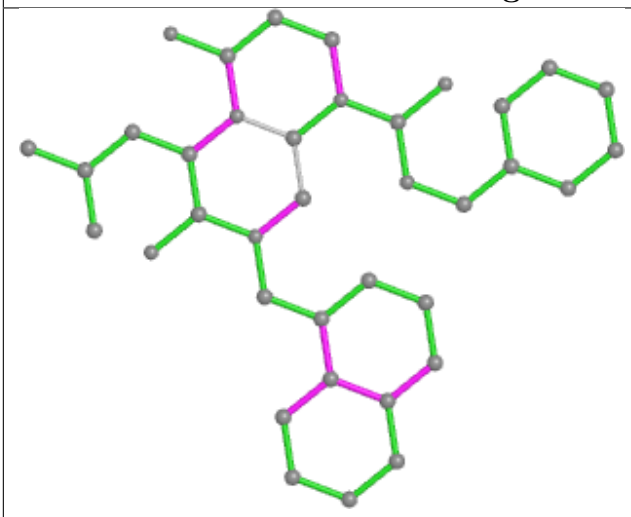
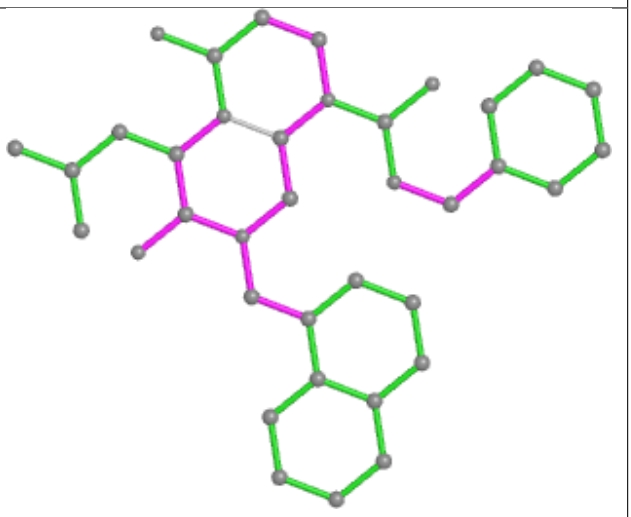


Rings

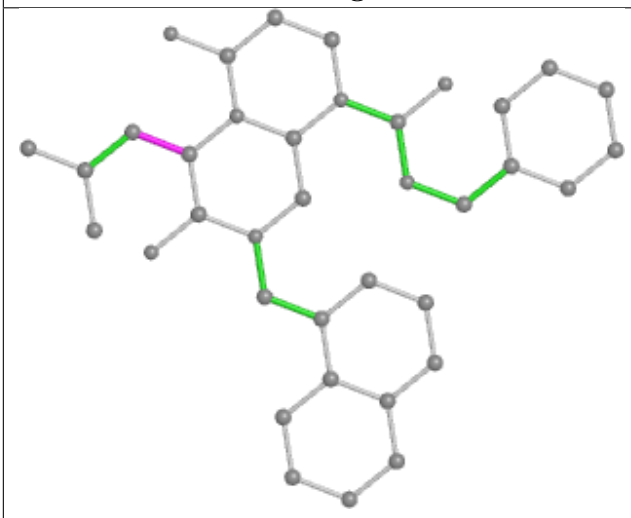
Ligand A1EEG E 301



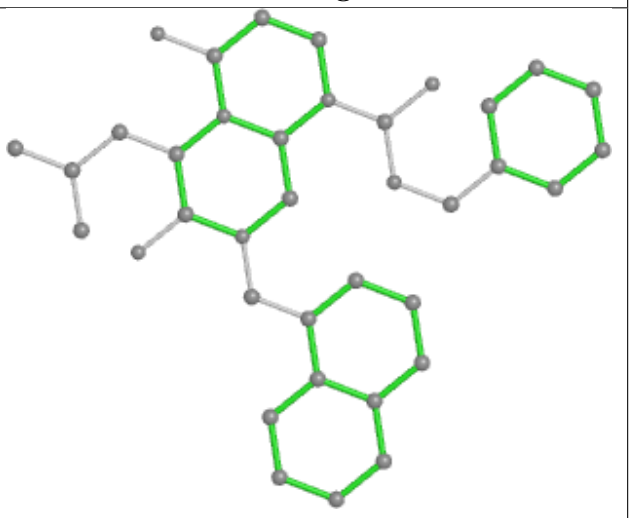
Bond lengths



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

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	184/201 (91%)	-0.10	1 (0%) 87 88	33, 48, 67, 83	0
1	B	186/201 (92%)	-0.23	0 100 100	30, 45, 65, 80	0
1	C	186/201 (92%)	-0.24	2 (1%) 77 79	26, 39, 66, 121	0
1	D	188/201 (93%)	-0.33	2 (1%) 77 79	29, 41, 63, 84	0
1	E	190/201 (94%)	-0.20	1 (0%) 87 88	30, 46, 65, 90	0
1	F	190/201 (94%)	-0.06	2 (1%) 77 79	34, 50, 74, 89	0
1	G	191/201 (95%)	-0.09	1 (0%) 87 88	32, 47, 71, 85	0
1	H	184/201 (91%)	0.02	2 (1%) 77 79	32, 50, 70, 103	0
1	I	183/201 (91%)	-0.17	1 (0%) 87 88	32, 47, 64, 90	0
1	J	189/201 (94%)	-0.10	3 (1%) 70 70	34, 48, 73, 150	0
1	K	191/201 (95%)	-0.03	6 (3%) 51 52	33, 52, 84, 138	0
1	L	190/201 (94%)	0.04	5 (2%) 57 57	38, 52, 83, 109	0
1	M	189/201 (94%)	-0.01	3 (1%) 70 70	30, 50, 74, 93	0
1	N	183/201 (91%)	0.00	1 (0%) 87 88	34, 52, 73, 108	0
All	All	2624/2814 (93%)	-0.11	30 (1%) 77 79	26, 48, 71, 150	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	192	PRO	4.6
1	J	194	THR	3.7
1	H	3	LEU	3.6
1	D	193	GLU	3.4
1	L	193	GLU	3.4
1	C	194	THR	3.3
1	F	193	GLU	3.2
1	A	193	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	193	GLU	2.9
1	G	193	GLU	2.8
1	K	194	THR	2.8
1	L	13	ARG	2.7
1	K	12	ASN	2.6
1	F	10	THR	2.4
1	K	119	GLU	2.3
1	C	193	GLU	2.3
1	K	193	GLU	2.3
1	D	12	ASN	2.3
1	M	15	GLU	2.3
1	J	193	GLU	2.2
1	M	162	ILE	2.2
1	L	192	PRO	2.1
1	I	4	ILE	2.1
1	E	192	PRO	2.1
1	L	4	ILE	2.1
1	K	10	THR	2.1
1	M	10	THR	2.1
1	K	191	VAL	2.1
1	L	35	GLN	2.0
1	J	18	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	A1EEG	M	301	37/37	0.89	0.12	43,55,71,74	0

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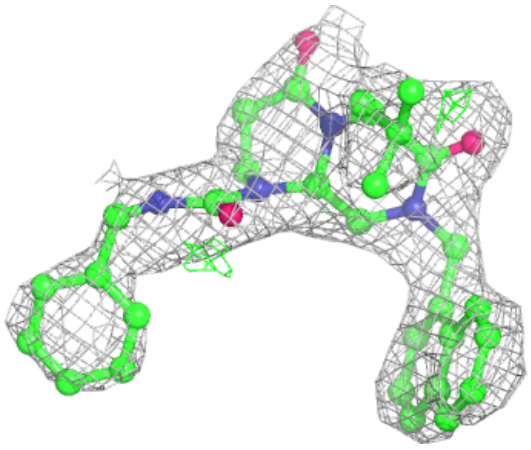
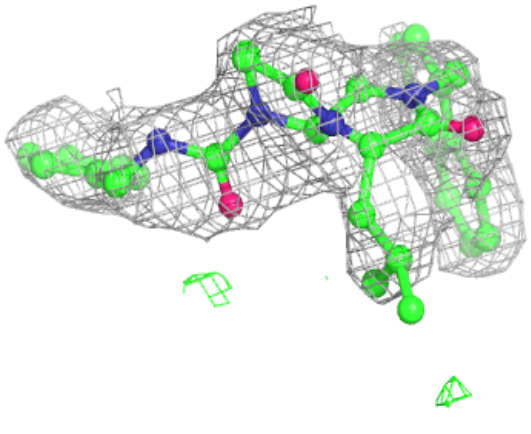
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1EEG	N	301	37/37	0.90	0.11	43,46,78,83	0
2	A1EEG	H	301	37/37	0.91	0.10	37,45,58,61	0
2	A1EEG	L	301	37/37	0.91	0.12	44,52,76,77	0
2	A1EEG	A	301	37/37	0.91	0.10	36,42,55,56	0
2	A1EEG	D	301	37/37	0.91	0.10	32,39,59,62	0
2	A1EEG	C	301	37/37	0.92	0.10	39,43,57,57	0
2	A1EEG	I	301	37/37	0.92	0.09	38,49,62,65	0
2	A1EEG	K	301	37/37	0.92	0.10	46,53,69,69	0
2	A1EEG	E	301	37/37	0.92	0.10	38,42,67,70	0
2	A1EEG	F	301	37/37	0.92	0.10	36,43,56,57	0
2	A1EEG	G	301	37/37	0.92	0.09	33,37,57,59	0
2	A1EEG	J	301	37/37	0.93	0.09	36,44,58,62	0
2	A1EEG	B	301	37/37	0.94	0.09	32,35,49,51	0

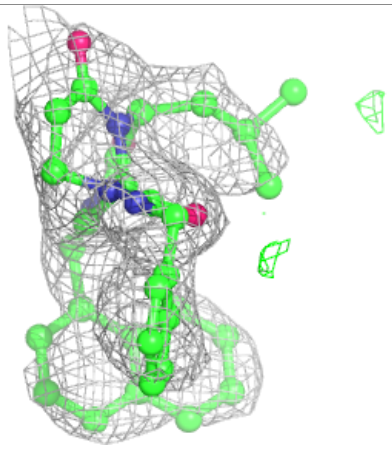
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EEG 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)

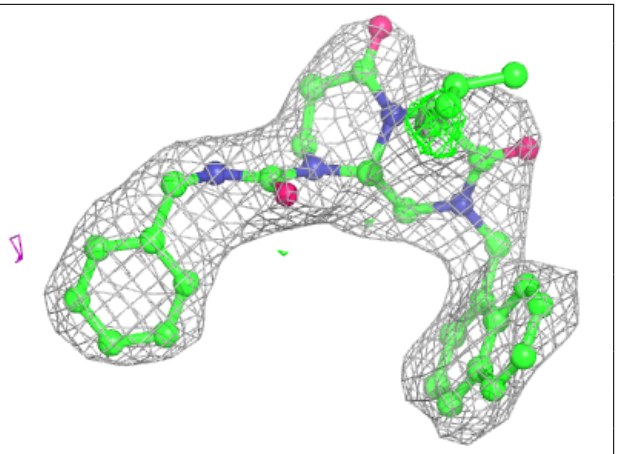


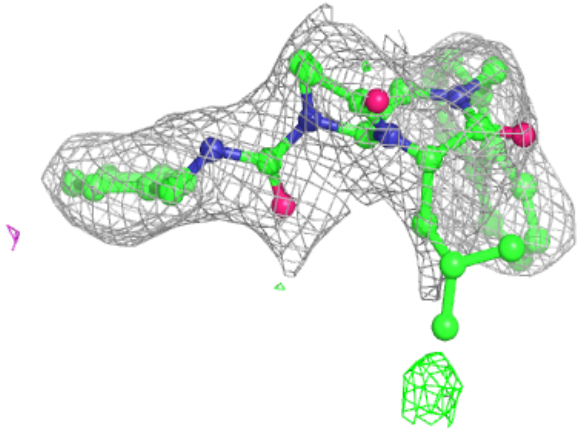


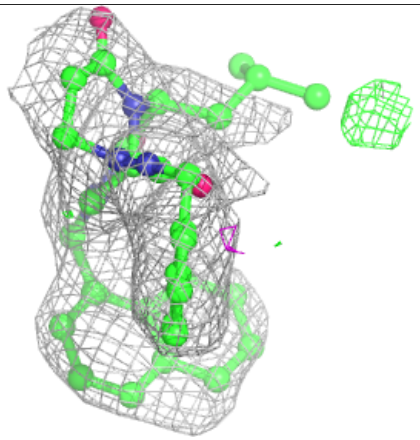


Electron density around A1EEG N 301:

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

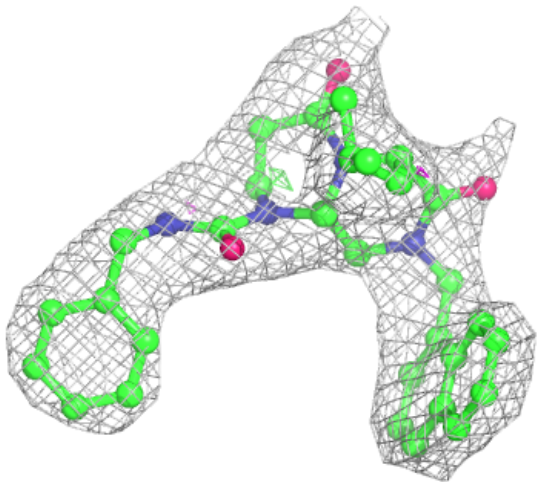


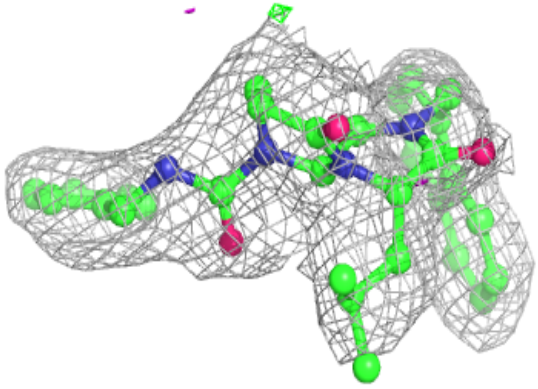


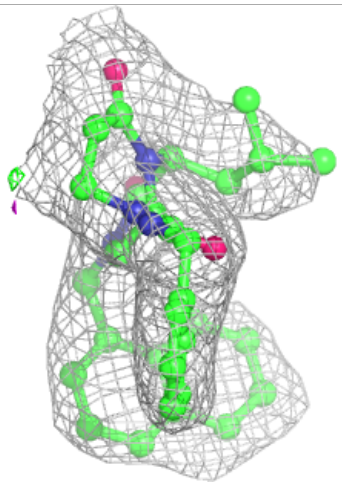


Electron density around A1EEG H 301:

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

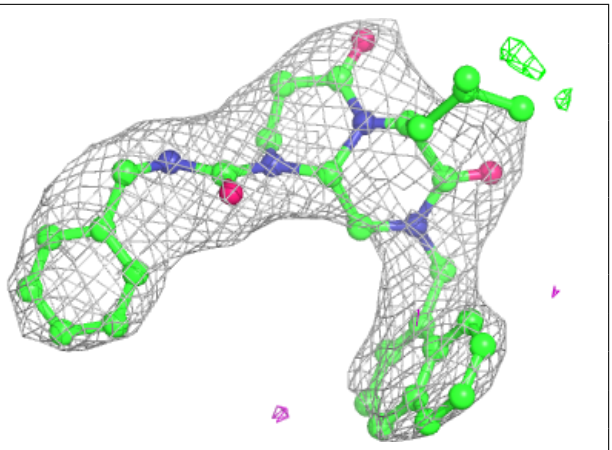


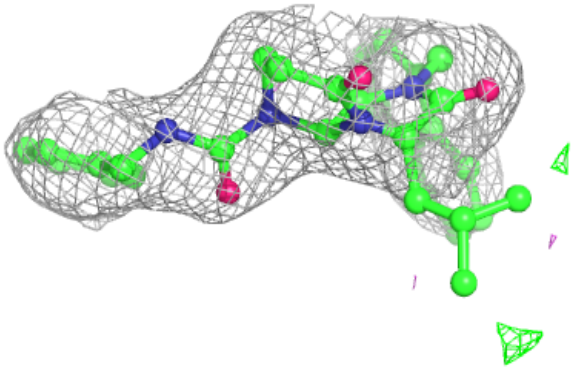


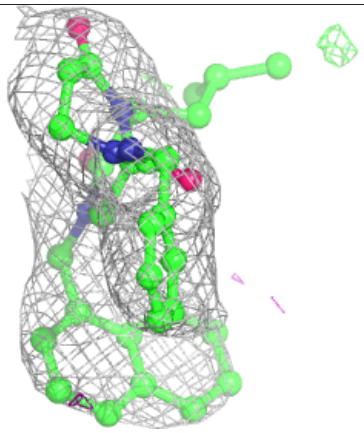


Electron density around A1EEG L 301:

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

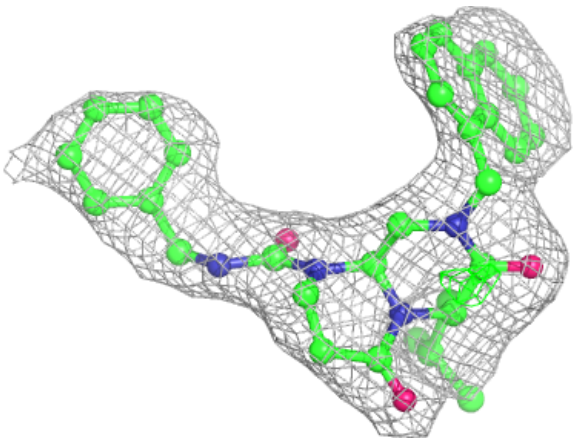


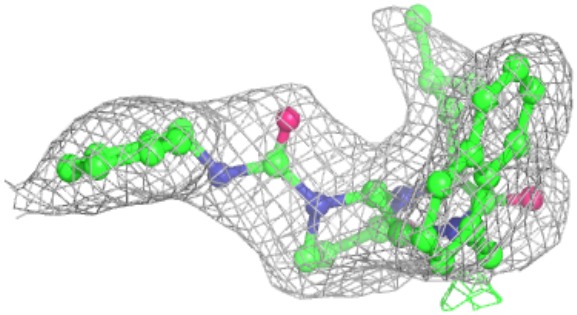


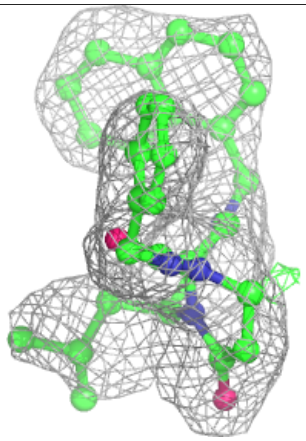


Electron density around A1EEG A 301:

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

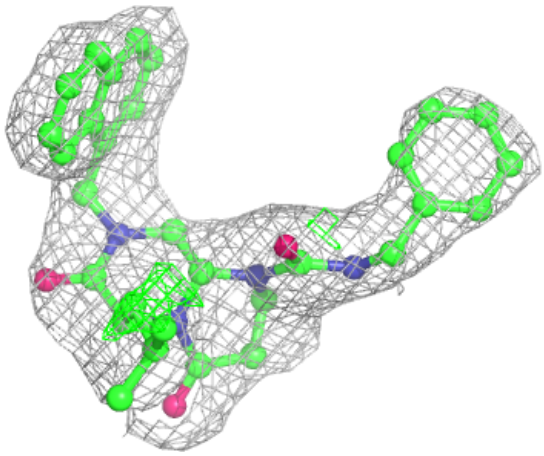


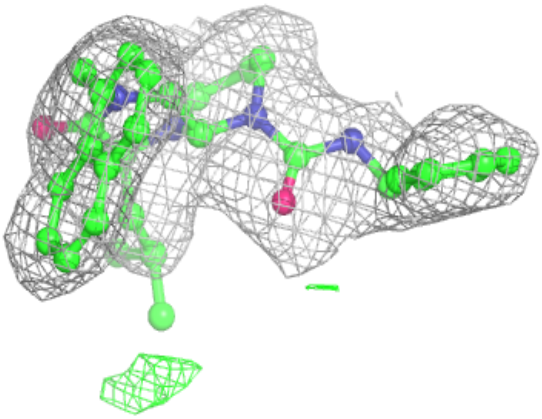


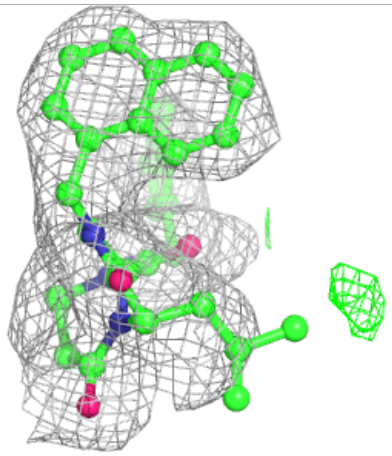


Electron density around A1EEG D 301:

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

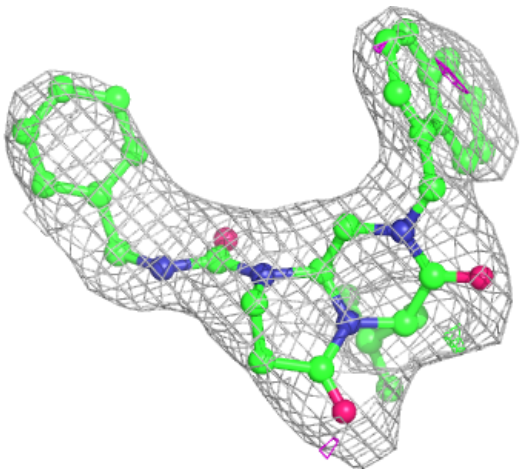


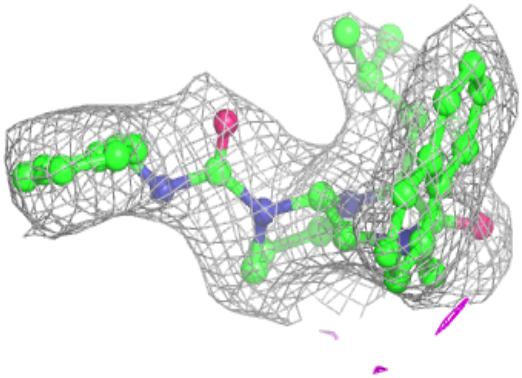


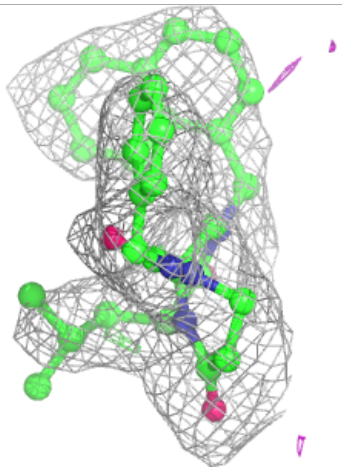


Electron density around A1EEG C 301:

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

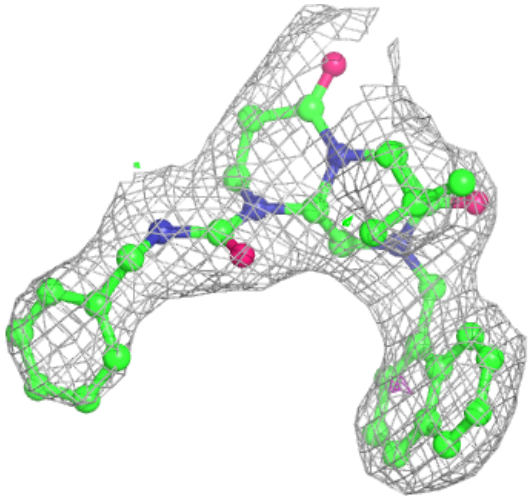


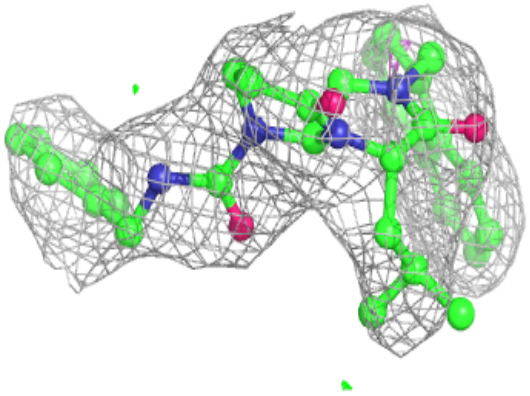


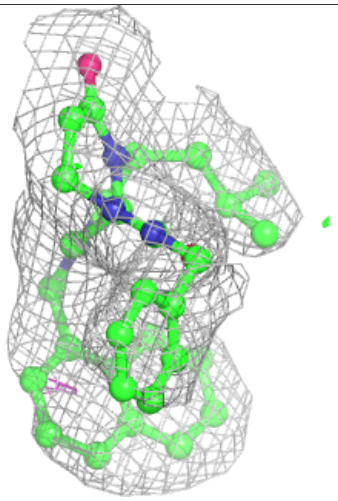


Electron density around A1EEG I 301:

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

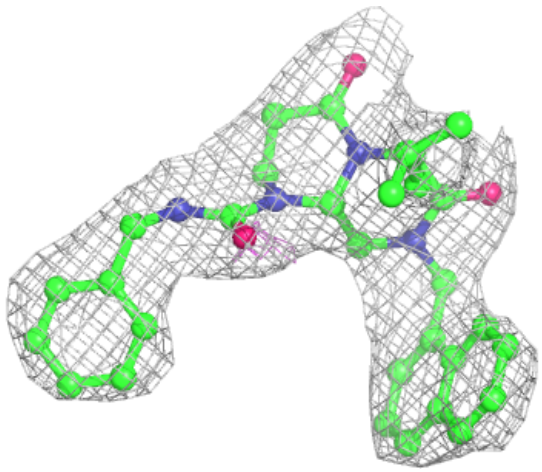


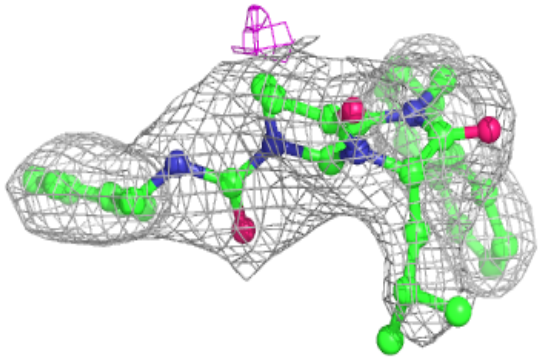


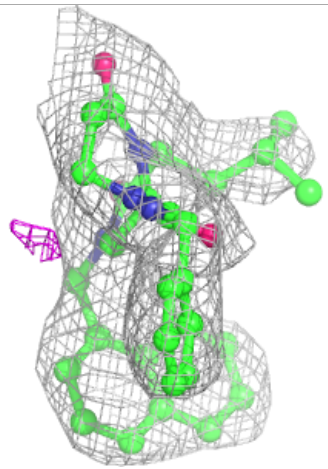


Electron density around A1EEG K 301:

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

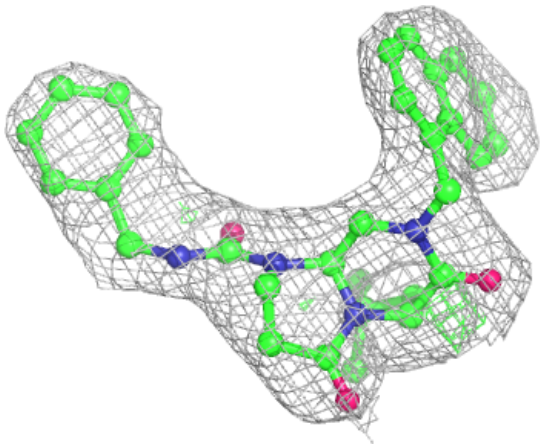


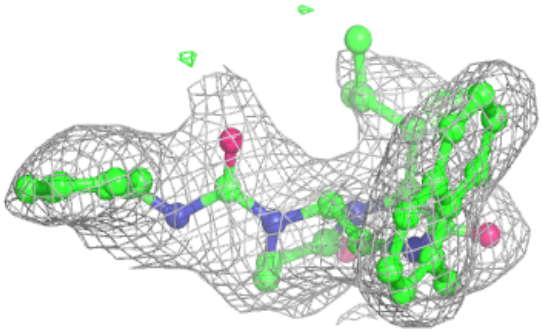


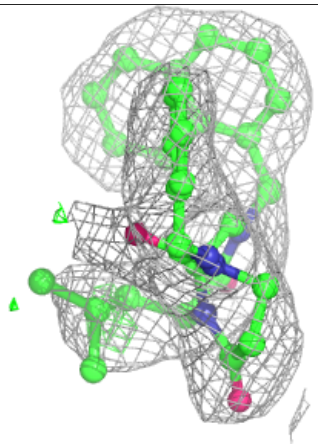


Electron density around A1EEG E 301:

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

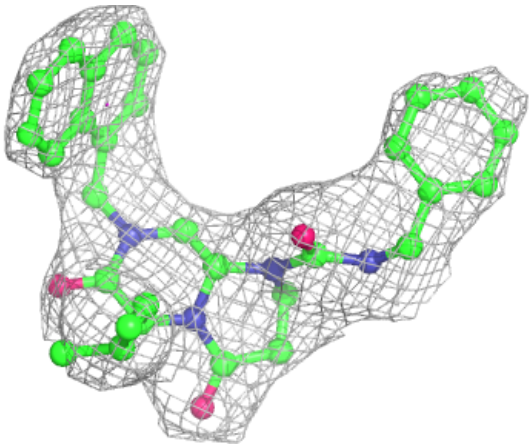


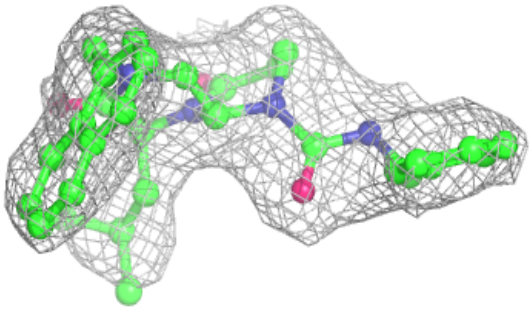


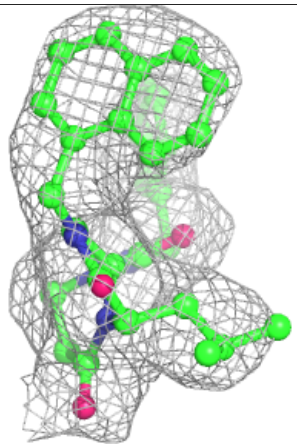


Electron density around A1EEG F 301:

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

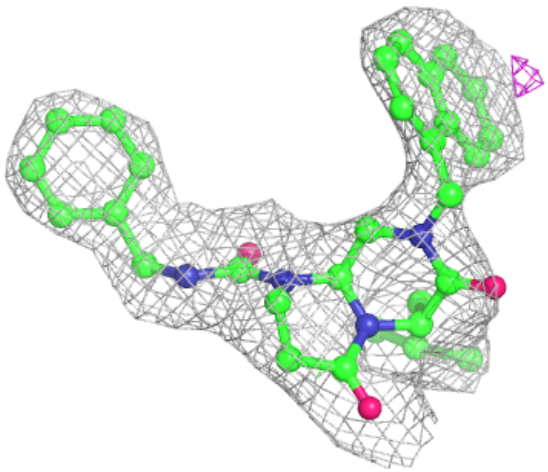


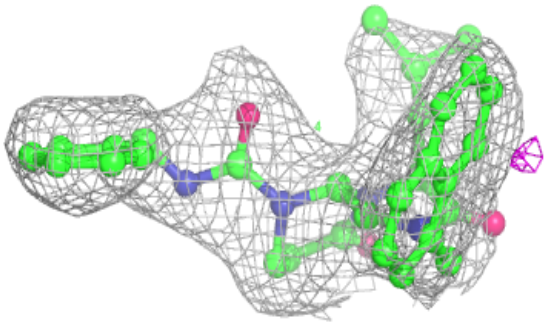


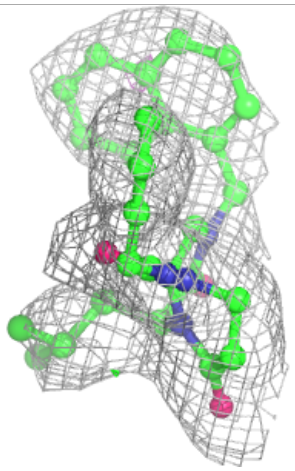


Electron density around A1EEG G 301:

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

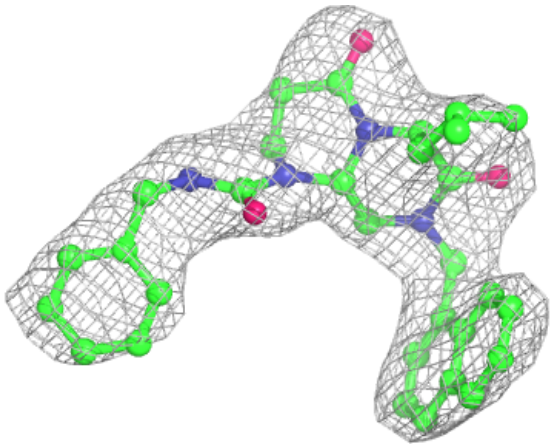


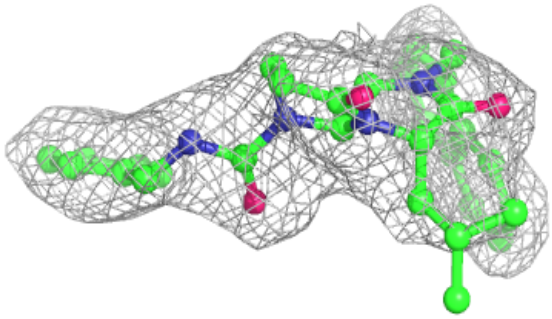


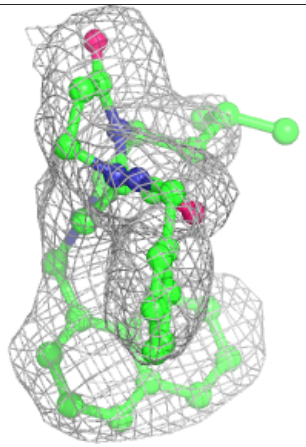


Electron density around A1EEG J 301:

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

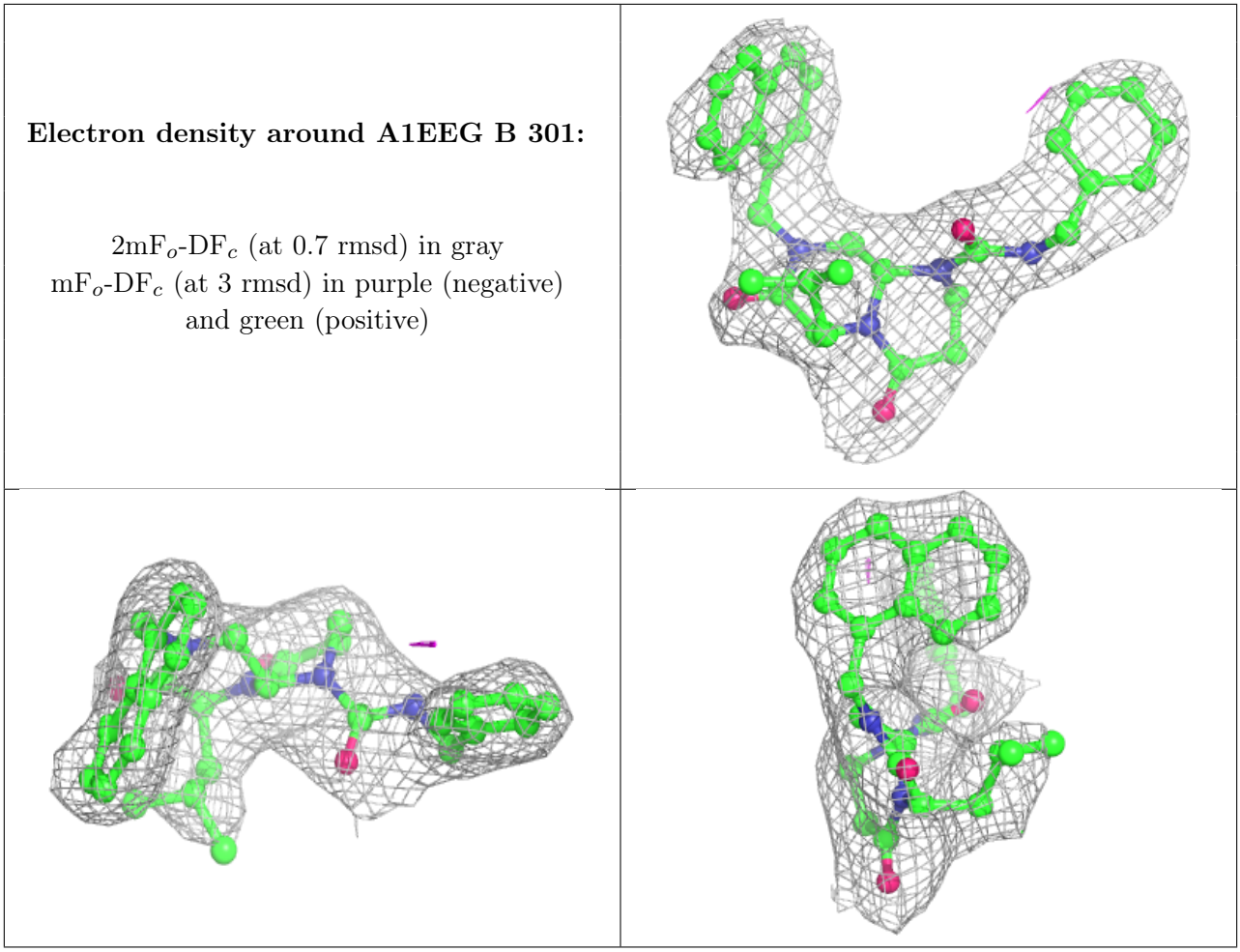






Electron density around A1EEG B 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.