Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:19 PM JST

PDB ID	:	9K2A
Title	:	Structure of ClpP from Staphylococcus aureus in complex with ZY27
Authors	:	Wei, B.Y.; Wang, P.Y.; Wu, W.; Zhang, T.; Yang, C.-G.
Deposited on	:	2024-10-17
Resolution	:	2.19 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

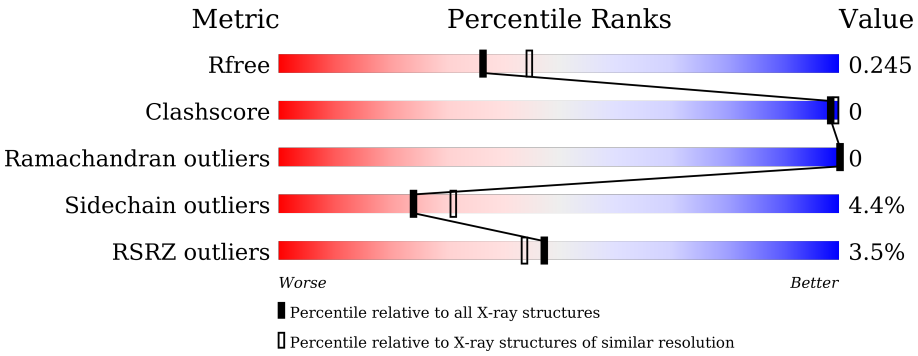
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & 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 2.19 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 88% · 8%
1	B	201	3% 87% 6% 7%
1	C	201	5% 87% 5% 7%
1	D	201	6% 89% · 7%
1	E	201	6% 92% · 5%
1	F	201	5% 91% · 5%

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Mol	Chain	Length	Quality of chain
1	G	201	2% 87% 5% 8%
1	H	201	3% 91% 7%
1	I	201	3% 91% 5%
1	J	201	90% 5% 5%
1	K	201	% 89% 7%
1	L	201	% 88% 7%
1	M	201	4% 88% 8%
1	N	201	2% 86% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20690 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	185	Total	C	N	O	S	0	1	0
			1425	900	241	278	6			
1	B	186	Total	C	N	O	S	0	0	0
			1424	899	242	277	6			
1	C	186	Total	C	N	O	S	0	0	0
			1416	894	241	275	6			
1	D	187	Total	C	N	O	S	0	0	0
			1433	904	243	280	6			
1	E	191	Total	C	N	O	S	0	0	0
			1456	914	247	289	6			
1	F	190	Total	C	N	O	S	0	1	0
			1455	916	249	284	6			
1	G	184	Total	C	N	O	S	0	0	0
			1408	889	239	274	6			
1	H	187	Total	C	N	O	S	0	0	0
			1419	895	241	277	6			
1	I	190	Total	C	N	O	S	0	0	0
			1440	906	245	283	6			
1	J	191	Total	C	N	O	S	0	0	0
			1462	919	249	288	6			
1	K	186	Total	C	N	O	S	0	0	0
			1417	893	240	278	6			
1	L	186	Total	C	N	O	S	0	1	0
			1430	903	243	278	6			
1	M	185	Total	C	N	O	S	0	0	0
			1415	893	240	276	6			
1	N	182	Total	C	N	O	S	0	0	0
			1394	881	237	270	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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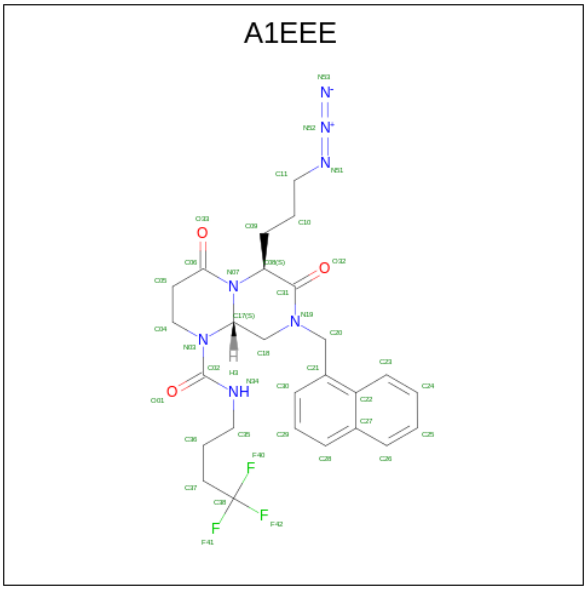
Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	-	expression tag	UNP A7WZR9
H	198	HIS	-	expression tag	UNP A7WZR9
H	199	HIS	-	expression tag	UNP A7WZR9
H	200	HIS	-	expression tag	UNP A7WZR9
H	201	HIS	-	expression tag	UNP A7WZR9
I	196	HIS	-	expression tag	UNP A7WZR9
I	197	HIS	-	expression tag	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-(3-azidopropyl)-8-(naphthalen-1-ylmethyl)-4,7-bis(oxida

nylidene)- {N}-[4,4,4-tris(fluoranyl)butyl]-3,6,9,9 {a}-tetrahydro-2 {H}-pyrazino[1,2-a]pyrimidine-1-carboxamide (three-letter code: A1EEE) (formula: $C_{26}H_{30}F_3N_7O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	B	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	C	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	D	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	E	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	F	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	G	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	H	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	I	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	I	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	K	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	L	1	Total	C	F	N	O	0	0
			39	26	3	7	3		

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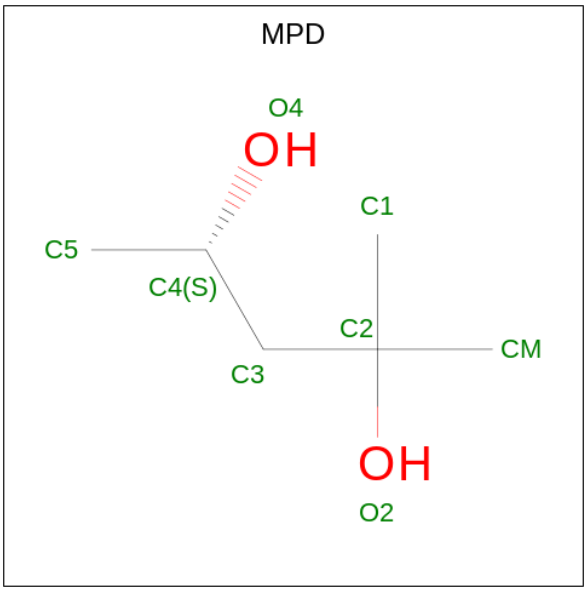
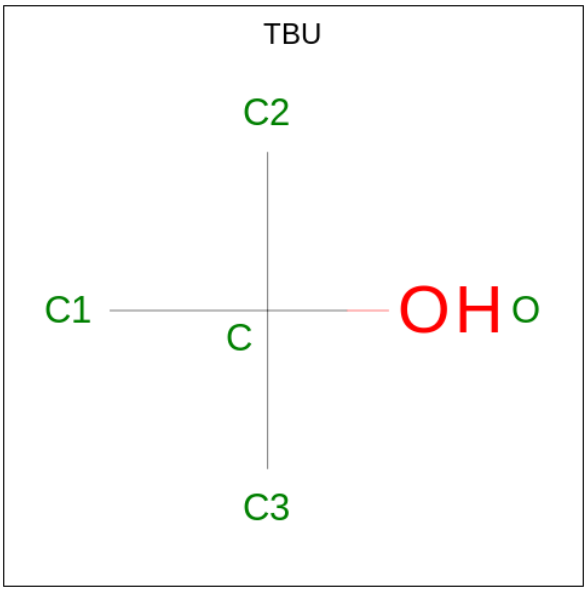
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	N	1	Total	C	F	N	O	0	0
			39	26	3	7	3		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is TERTIARY-BUTYL ALCOHOL (three-letter code: TBU) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	4	Total O 4 4	0	0
5	C	3	Total O 3 3	0	0
5	D	5	Total O 5 5	0	0
5	E	7	Total O 7 7	0	0
5	F	10	Total O 10 10	0	0
5	G	15	Total O 15 15	0	0
5	H	13	Total O 13 13	0	0
5	I	14	Total O 14 14	0	0
5	J	17	Total O 17 17	0	0
5	K	12	Total O 12 12	0	0

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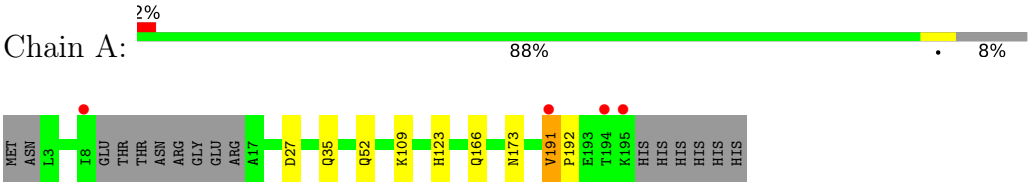
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	8	Total O 8 8	0	0
5	M	2	Total O 2 2	0	0
5	N	3	Total O 3 3	0	0

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.

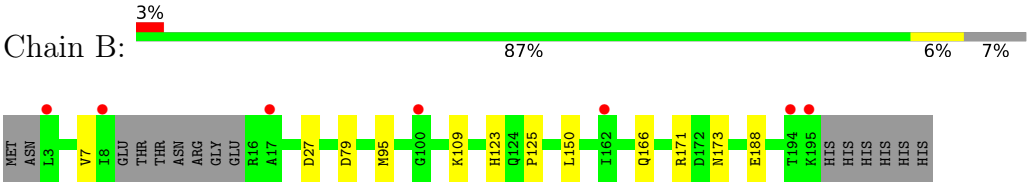
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



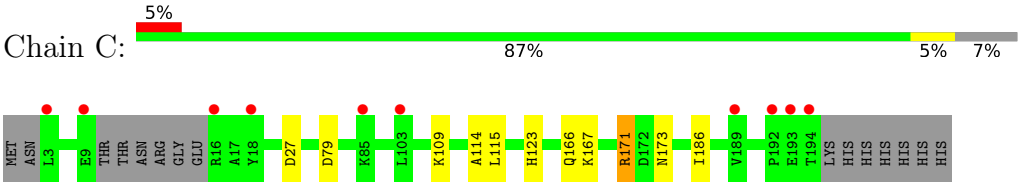
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



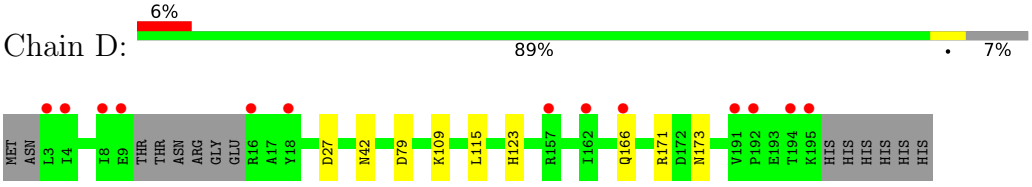
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



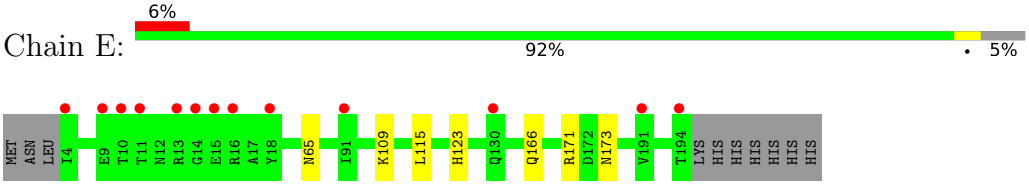
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



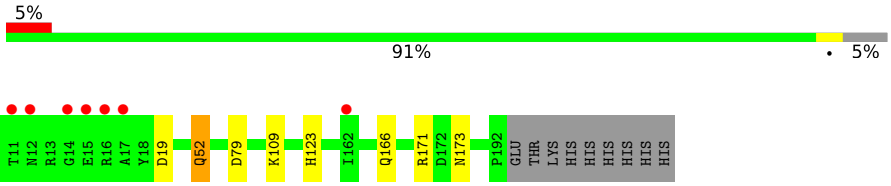
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



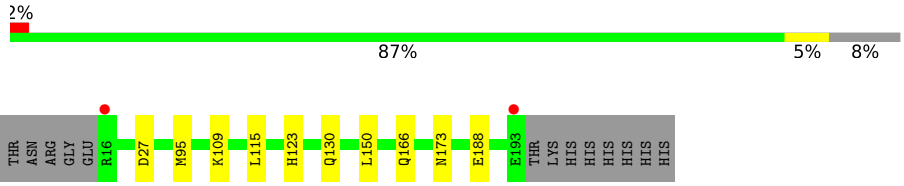
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



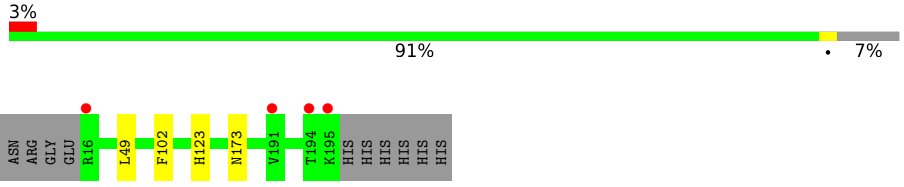
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



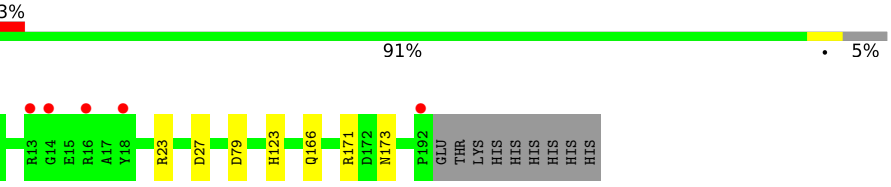
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



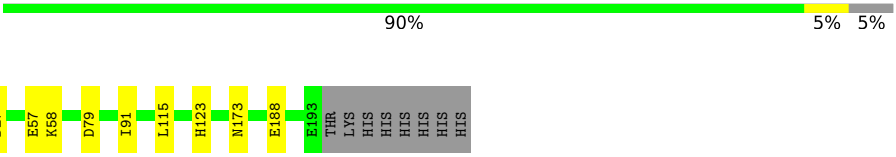
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



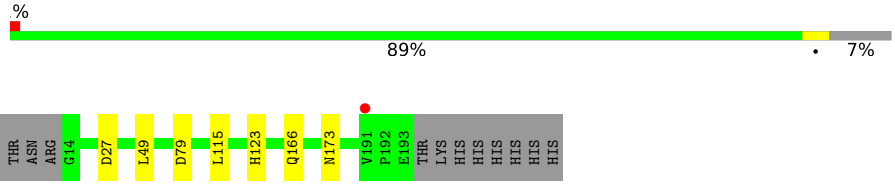
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



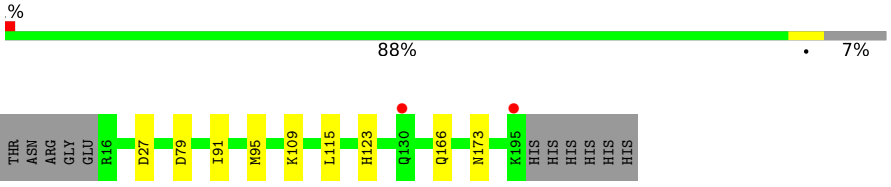
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



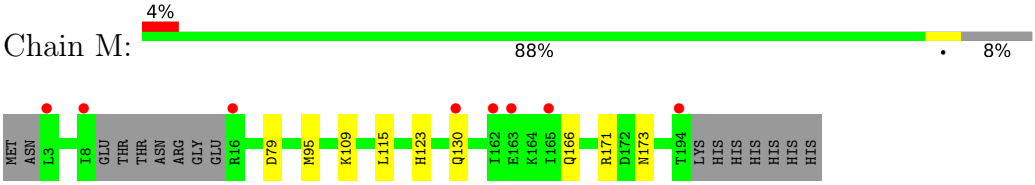
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



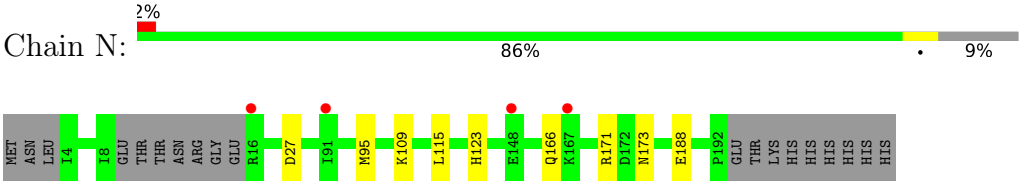
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

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	94.42Å 190.26Å 96.20Å 90.00° 117.82° 90.00°	Depositor
Resolution (Å)	95.13 – 2.19 95.13 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.5 (95.13-2.19) 97.5 (95.13-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.214 , 0.244 0.217 , 0.245	Depositor DCC
R_{free} test set	7904 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 12.4	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 0.028 for h,-k,-h-l 0.033 for -h-l,-k,l 0.032 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20690	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: TBU, A1EEE, MPD

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	0.36	0/1446	0.57	0/1952
1	B	0.36	0/1442	0.57	0/1947
1	C	0.35	0/1434	0.54	0/1938
1	D	0.37	0/1451	0.57	0/1959
1	E	0.37	0/1475	0.59	0/1995
1	F	0.36	0/1477	0.57	0/1998
1	G	0.37	0/1426	0.58	0/1926
1	H	0.36	0/1437	0.58	0/1943
1	I	0.38	0/1459	0.59	0/1975
1	J	0.37	0/1481	0.59	0/2003
1	K	0.38	0/1435	0.59	0/1939
1	L	0.36	0/1451	0.56	0/1959
1	M	0.36	0/1433	0.57	0/1936
1	N	0.37	0/1412	0.57	0/1907
All	All	0.37	0/20259	0.58	0/27377

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	ARG	Sidechain
1	F	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	1425	0	1442	2	0
1	B	1424	0	1438	3	0
1	C	1416	0	1423	3	0
1	D	1433	0	1444	3	0
1	E	1456	0	1452	2	0
1	F	1455	0	1463	2	0
1	G	1408	0	1418	2	0
1	H	1419	0	1413	1	0
1	I	1440	0	1435	1	0
1	J	1462	0	1465	2	0
1	K	1417	0	1416	2	0
1	L	1430	0	1446	2	0
1	M	1415	0	1425	2	0
1	N	1394	0	1410	1	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
2	C	39	0	0	0	0
2	D	39	0	0	0	0
2	E	39	0	0	0	0
2	F	39	0	0	0	0
2	G	39	0	0	0	0
2	H	39	0	0	0	0
2	I	78	0	0	0	0
2	K	39	0	0	0	0
2	L	39	0	0	0	0
2	M	39	0	0	0	0
2	N	39	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	3	0
3	G	8	0	14	1	0
4	H	5	0	10	1	0
5	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	0	0
5	E	7	0	0	0	0
5	F	10	0	0	0	0
5	G	15	0	0	0	0
5	H	13	0	0	0	0
5	I	14	0	0	0	0
5	J	17	0	0	0	0
5	K	12	0	0	0	0
5	L	8	0	0	0	0
5	M	2	0	0	0	0
5	N	3	0	0	0	0
All	All	20690	0	20142	19	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 0.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:LEU:HD13	3:G:302:MPD:H52	1.79	0.62
1:A:191:VAL:HG22	1:A:192:PRO:HD2	1.88	0.55
1:C:114:ALA:HB3	1:C:186:ILE:HD13	1.94	0.50
1:I:79:ASP:HB3	1:J:115:LEU:HD23	1.93	0.50
1:D:42:ASN:HD21	1:E:65:ASN:HD22	1.61	0.49
1:B:125:PRO:HD3	3:B:302:MPD:HM3	1.97	0.47
1:B:79:ASP:HB3	1:C:115:LEU:HD23	1.97	0.46
3:B:302:MPD:H12	3:B:302:MPD:H4	1.75	0.46
1:A:52[B]:GLN:HE21	1:A:52[B]:GLN:HB3	1.57	0.45
1:B:150:LEU:HD22	3:B:302:MPD:H11	1.97	0.45
1:M:79:ASP:HB3	1:N:115:LEU:HD23	2.00	0.44
1:F:52[A]:GLN:HE21	1:F:52[A]:GLN:HB3	1.59	0.43
1:K:79:ASP:HB3	1:L:115:LEU:HD23	2.01	0.42
1:C:79:ASP:HB3	1:D:115:LEU:HD23	2.01	0.42
1:H:102:PHE:HB2	4:H:302:TBU:H11	2.01	0.42
1:D:79:ASP:HB3	1:E:115:LEU:HD13	2.01	0.41
1:F:79:ASP:HB3	1:G:115:LEU:HD23	2.02	0.41
1:J:79:ASP:HB3	1:K:115:LEU:HD23	2.02	0.41
1:L:79:ASP:HB3	1:M:115:LEU:HD23	2.04	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	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
1	B	182/201 (90%)	178 (98%)	4 (2%)	0	100	100
1	C	182/201 (90%)	177 (97%)	5 (3%)	0	100	100
1	D	183/201 (91%)	181 (99%)	2 (1%)	0	100	100
1	E	189/201 (94%)	187 (99%)	2 (1%)	0	100	100
1	F	189/201 (94%)	185 (98%)	4 (2%)	0	100	100
1	G	180/201 (90%)	178 (99%)	2 (1%)	0	100	100
1	H	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
1	I	188/201 (94%)	186 (99%)	2 (1%)	0	100	100
1	J	189/201 (94%)	186 (98%)	3 (2%)	0	100	100
1	K	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
1	L	183/201 (91%)	181 (99%)	2 (1%)	0	100	100
1	M	181/201 (90%)	178 (98%)	3 (2%)	0	100	100
1	N	178/201 (89%)	176 (99%)	2 (1%)	0	100	100
All	All	2571/2814 (91%)	2533 (98%)	38 (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%)	146 (95%)	7 (5%)	23	30
1	B	152/169 (90%)	143 (94%)	9 (6%)	16	20
1	C	150/169 (89%)	143 (95%)	7 (5%)	22	29
1	D	153/169 (90%)	147 (96%)	6 (4%)	27	37
1	E	155/169 (92%)	150 (97%)	5 (3%)	34	45
1	F	155/169 (92%)	148 (96%)	7 (4%)	23	30
1	G	150/169 (89%)	142 (95%)	8 (5%)	19	24
1	H	149/169 (88%)	146 (98%)	3 (2%)	50	65
1	I	152/169 (90%)	145 (95%)	7 (5%)	23	30
1	J	156/169 (92%)	148 (95%)	8 (5%)	20	25
1	K	150/169 (89%)	145 (97%)	5 (3%)	33	44
1	L	153/169 (90%)	146 (95%)	7 (5%)	23	30
1	M	151/169 (89%)	144 (95%)	7 (5%)	23	30
1	N	149/169 (88%)	141 (95%)	8 (5%)	18	23
All	All	2128/2366 (90%)	2034 (96%)	94 (4%)	24	31

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	35	GLN
1	A	109	LYS
1	A	123	HIS
1	A	166	GLN
1	A	173	ASN
1	A	191	VAL
1	B	7	VAL
1	B	27	ASP
1	B	95	MET
1	B	109	LYS
1	B	123	HIS
1	B	166	GLN
1	B	171	ARG
1	B	173	ASN
1	B	188	GLU
1	C	27	ASP
1	C	109	LYS
1	C	123	HIS

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Mol	Chain	Res	Type
1	C	166	GLN
1	C	167	LYS
1	C	171	ARG
1	C	173	ASN
1	D	27	ASP
1	D	109	LYS
1	D	123	HIS
1	D	166	GLN
1	D	171	ARG
1	D	173	ASN
1	E	109	LYS
1	E	123	HIS
1	E	166	GLN
1	E	171	ARG
1	E	173	ASN
1	F	19	ASP
1	F	52[A]	GLN
1	F	52[B]	GLN
1	F	109	LYS
1	F	123	HIS
1	F	166	GLN
1	F	173	ASN
1	G	27	ASP
1	G	95	MET
1	G	109	LYS
1	G	123	HIS
1	G	130	GLN
1	G	166	GLN
1	G	173	ASN
1	G	188	GLU
1	H	49	LEU
1	H	123	HIS
1	H	173	ASN
1	I	6	THR
1	I	23	ARG
1	I	27	ASP
1	I	123	HIS
1	I	166	GLN
1	I	171	ARG
1	I	173	ASN
1	J	9	GLU
1	J	27	ASP

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Mol	Chain	Res	Type
1	J	57	GLU
1	J	58	LYS
1	J	91	ILE
1	J	123	HIS
1	J	173	ASN
1	J	188	GLU
1	K	27	ASP
1	K	49	LEU
1	K	123	HIS
1	K	166	GLN
1	K	173	ASN
1	L	27	ASP
1	L	91	ILE
1	L	95	MET
1	L	109	LYS
1	L	123	HIS
1	L	166	GLN
1	L	173	ASN
1	M	95	MET
1	M	109	LYS
1	M	123	HIS
1	M	130	GLN
1	M	166	GLN
1	M	171	ARG
1	M	173	ASN
1	N	27	ASP
1	N	95	MET
1	N	109	LYS
1	N	123	HIS
1	N	166	GLN
1	N	171	ARG
1	N	173	ASN
1	N	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	82	GLN
1	A	117	ASN
1	A	124	GLN
1	A	173	ASN

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Mol	Chain	Res	Type
1	B	82	GLN
1	B	117	ASN
1	B	124	GLN
1	B	173	ASN
1	C	117	ASN
1	C	124	GLN
1	C	166	GLN
1	C	173	ASN
1	D	42	ASN
1	D	82	GLN
1	D	124	GLN
1	D	173	ASN
1	E	42	ASN
1	E	82	GLN
1	E	117	ASN
1	E	124	GLN
1	E	173	ASN
1	F	82	GLN
1	F	117	ASN
1	F	124	GLN
1	F	173	ASN
1	G	124	GLN
1	G	166	GLN
1	G	173	ASN
1	H	42	ASN
1	H	82	GLN
1	H	83	HIS
1	H	117	ASN
1	H	124	GLN
1	H	173	ASN
1	I	82	GLN
1	I	117	ASN
1	I	124	GLN
1	I	130	GLN
1	I	173	ASN
1	J	42	ASN
1	J	82	GLN
1	J	124	GLN
1	J	151	ASN
1	J	166	GLN
1	J	173	ASN
1	K	82	GLN

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Mol	Chain	Res	Type
1	K	117	ASN
1	K	124	GLN
1	K	173	ASN
1	L	42	ASN
1	L	82	GLN
1	L	124	GLN
1	L	173	ASN
1	M	42	ASN
1	M	82	GLN
1	M	117	ASN
1	M	124	GLN
1	M	173	ASN
1	N	42	ASN
1	N	82	GLN
1	N	117	ASN
1	N	124	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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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	A1EEE	G	301	-	39,42,42	4.95	16 (41%)	49,59,59	2.22	5 (10%)
2	A1EEE	D	301	-	39,42,42	4.95	14 (35%)	49,59,59	2.21	5 (10%)
2	A1EEE	H	301	-	39,42,42	5.02	14 (35%)	49,59,59	2.23	7 (14%)
2	A1EEE	A	301	-	39,42,42	4.98	13 (33%)	49,59,59	2.15	4 (8%)
2	A1EEE	I	302	-	39,42,42	4.96	14 (35%)	49,59,59	2.16	6 (12%)
2	A1EEE	K	301	-	39,42,42	4.91	16 (41%)	49,59,59	2.25	7 (14%)
2	A1EEE	I	301	-	39,42,42	4.93	14 (35%)	49,59,59	2.23	6 (12%)
3	MPD	G	302	-	7,7,7	0.23	0	9,10,10	0.32	0
2	A1EEE	M	301	-	39,42,42	4.95	13 (33%)	49,59,59	2.10	3 (6%)
2	A1EEE	B	301	-	39,42,42	4.98	13 (33%)	49,59,59	2.15	5 (10%)
3	MPD	B	302	-	7,7,7	0.27	0	9,10,10	0.39	0
3	MPD	A	302	-	7,7,7	0.20	0	9,10,10	0.36	0
2	A1EEE	L	301	-	39,42,42	4.98	15 (38%)	49,59,59	2.18	5 (10%)
2	A1EEE	E	301	-	39,42,42	4.89	15 (38%)	49,59,59	2.15	4 (8%)
2	A1EEE	N	301	-	39,42,42	4.96	14 (35%)	49,59,59	2.22	5 (10%)
2	A1EEE	C	301	-	39,42,42	4.92	13 (33%)	49,59,59	2.19	5 (10%)
2	A1EEE	F	301	-	39,42,42	4.95	15 (38%)	49,59,59	2.22	6 (12%)
4	TBU	H	302	-	4,4,4	0.37	0	6,6,6	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EEE	G	301	-	-	5/22/55/55	0/4/4/4
2	A1EEE	D	301	-	-	4/22/55/55	0/4/4/4
2	A1EEE	H	301	-	-	7/22/55/55	0/4/4/4
2	A1EEE	A	301	-	-	3/22/55/55	0/4/4/4
2	A1EEE	I	302	-	-	6/22/55/55	0/4/4/4
2	A1EEE	K	301	-	-	2/22/55/55	0/4/4/4
2	A1EEE	I	301	-	-	6/22/55/55	0/4/4/4
3	MPD	G	302	-	-	0/5/5/5	-
2	A1EEE	M	301	-	-	2/22/55/55	0/4/4/4
2	A1EEE	B	301	-	-	5/22/55/55	0/4/4/4
3	MPD	B	302	-	-	0/5/5/5	-
3	MPD	A	302	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EEE	L	301	-	-	1/22/55/55	0/4/4/4
2	A1EEE	E	301	-	-	6/22/55/55	0/4/4/4
2	A1EEE	N	301	-	-	4/22/55/55	0/4/4/4
2	A1EEE	C	301	-	-	5/22/55/55	0/4/4/4
2	A1EEE	F	301	-	-	4/22/55/55	0/4/4/4

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	A1EEE	C08-N07	-19.42	1.15	1.47
2	L	301	A1EEE	C08-N07	-19.20	1.16	1.47
2	C	301	A1EEE	C08-N07	-18.92	1.16	1.47
2	A	301	A1EEE	C08-N07	-18.85	1.16	1.47
2	I	302	A1EEE	C08-N07	-18.83	1.16	1.47
2	E	301	A1EEE	C08-N07	-18.80	1.16	1.47
2	D	301	A1EEE	C08-N07	-18.77	1.17	1.47
2	M	301	A1EEE	C08-N07	-18.71	1.17	1.47
2	B	301	A1EEE	C08-N07	-18.69	1.17	1.47
2	H	301	A1EEE	C08-N07	-18.69	1.17	1.47
2	N	301	A1EEE	C08-N07	-18.59	1.17	1.47
2	K	301	A1EEE	C08-N07	-18.57	1.17	1.47
2	F	301	A1EEE	C08-N07	-18.46	1.17	1.47
2	I	301	A1EEE	C08-N07	-18.44	1.17	1.47
2	H	301	A1EEE	C06-N07	18.37	1.51	1.35
2	B	301	A1EEE	C06-N07	18.23	1.51	1.35
2	A	301	A1EEE	C06-N07	18.11	1.51	1.35
2	I	302	A1EEE	C06-N07	18.10	1.51	1.35
2	M	301	A1EEE	C06-N07	18.09	1.51	1.35
2	F	301	A1EEE	C06-N07	18.04	1.51	1.35
2	N	301	A1EEE	C06-N07	17.99	1.50	1.35
2	D	301	A1EEE	C06-N07	17.98	1.50	1.35
2	I	301	A1EEE	C06-N07	17.88	1.50	1.35
2	L	301	A1EEE	C06-N07	17.87	1.50	1.35
2	C	301	A1EEE	C06-N07	17.70	1.50	1.35
2	K	301	A1EEE	C06-N07	17.68	1.50	1.35
2	G	301	A1EEE	C06-N07	17.57	1.50	1.35
2	E	301	A1EEE	C06-N07	17.12	1.50	1.35
2	F	301	A1EEE	N52-N51	10.53	1.51	1.23
2	K	301	A1EEE	N52-N51	10.52	1.51	1.23
2	A	301	A1EEE	N52-N51	10.51	1.51	1.23
2	N	301	A1EEE	N52-N51	10.50	1.51	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1EEE	N52-N51	10.50	1.51	1.23
2	H	301	A1EEE	N52-N51	10.46	1.50	1.23
2	B	301	A1EEE	N52-N51	10.46	1.50	1.23
2	D	301	A1EEE	N52-N51	10.43	1.50	1.23
2	M	301	A1EEE	N52-N51	10.39	1.50	1.23
2	E	301	A1EEE	N52-N51	10.38	1.50	1.23
2	I	302	A1EEE	N52-N51	10.38	1.50	1.23
2	G	301	A1EEE	N52-N51	10.34	1.50	1.23
2	C	301	A1EEE	N52-N51	10.32	1.50	1.23
2	L	301	A1EEE	N52-N51	10.29	1.50	1.23
2	L	301	A1EEE	C18-N19	-5.30	1.40	1.46
2	H	301	A1EEE	C18-N19	-5.28	1.40	1.46
2	A	301	A1EEE	C18-N19	-5.16	1.40	1.46
2	B	301	A1EEE	C18-N19	-4.99	1.41	1.46
2	I	301	A1EEE	C18-N19	-4.95	1.41	1.46
2	E	301	A1EEE	C18-N19	-4.92	1.41	1.46
2	K	301	A1EEE	C18-N19	-4.89	1.41	1.46
2	F	301	A1EEE	C18-N19	-4.80	1.41	1.46
2	I	302	A1EEE	C18-N19	-4.74	1.41	1.46
2	N	301	A1EEE	C18-N19	-4.73	1.41	1.46
2	H	301	A1EEE	C09-C08	4.72	1.60	1.53
2	C	301	A1EEE	C18-N19	-4.60	1.41	1.46
2	I	301	A1EEE	C09-C08	4.57	1.60	1.53
2	F	301	A1EEE	C09-C08	4.53	1.60	1.53
2	G	301	A1EEE	C18-N19	-4.40	1.41	1.46
2	N	301	A1EEE	C09-C08	4.36	1.60	1.53
2	M	301	A1EEE	C09-C08	4.36	1.60	1.53
2	M	301	A1EEE	C18-N19	-4.26	1.41	1.46
2	B	301	A1EEE	C31-N19	4.19	1.44	1.35
2	L	301	A1EEE	C09-C08	4.19	1.60	1.53
2	D	301	A1EEE	C18-N19	-4.18	1.42	1.46
2	N	301	A1EEE	C17-N03	4.16	1.51	1.46
2	A	301	A1EEE	C31-N19	4.15	1.44	1.35
2	D	301	A1EEE	C09-C08	4.11	1.60	1.53
2	I	302	A1EEE	C31-N19	4.08	1.44	1.35
2	F	301	A1EEE	C31-N19	4.08	1.44	1.35
2	M	301	A1EEE	C31-N19	4.07	1.44	1.35
2	E	301	A1EEE	C31-N19	4.02	1.44	1.35
2	I	301	A1EEE	C31-N19	4.02	1.44	1.35
2	B	301	A1EEE	C09-C08	4.02	1.59	1.53
2	E	301	A1EEE	C09-C08	4.02	1.59	1.53
2	K	301	A1EEE	C09-C08	4.02	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	A1EEE	C31-N19	4.01	1.44	1.35
2	C	301	A1EEE	C09-C08	4.00	1.59	1.53
2	G	301	A1EEE	C09-C08	3.99	1.59	1.53
2	D	301	A1EEE	C17-N03	3.98	1.51	1.46
2	H	301	A1EEE	C31-N19	3.97	1.44	1.35
2	K	301	A1EEE	C31-N19	3.97	1.44	1.35
2	E	301	A1EEE	C02-N03	3.95	1.50	1.37
2	C	301	A1EEE	C31-N19	3.94	1.44	1.35
2	F	301	A1EEE	C02-N03	3.94	1.50	1.37
2	L	301	A1EEE	C31-N19	3.92	1.44	1.35
2	D	301	A1EEE	C02-N03	3.92	1.50	1.37
2	N	301	A1EEE	C02-N03	3.91	1.50	1.37
2	B	301	A1EEE	C17-N03	3.90	1.51	1.46
2	A	301	A1EEE	C09-C08	3.90	1.59	1.53
2	I	302	A1EEE	C09-C08	3.88	1.59	1.53
2	M	301	A1EEE	C02-N03	3.83	1.50	1.37
2	K	301	A1EEE	C02-N03	3.82	1.50	1.37
2	H	301	A1EEE	C02-N03	3.82	1.50	1.37
2	B	301	A1EEE	C02-N03	3.79	1.50	1.37
2	I	302	A1EEE	C02-N03	3.79	1.50	1.37
2	D	301	A1EEE	C31-N19	3.79	1.43	1.35
2	E	301	A1EEE	C17-N03	3.78	1.51	1.46
2	I	301	A1EEE	C02-N03	3.76	1.50	1.37
2	F	301	A1EEE	C17-N03	3.75	1.51	1.46
2	M	301	A1EEE	C17-N03	3.73	1.51	1.46
2	G	301	A1EEE	C02-N03	3.73	1.50	1.37
2	I	302	A1EEE	C17-N03	3.71	1.51	1.46
2	H	301	A1EEE	C17-N03	3.71	1.51	1.46
2	G	301	A1EEE	C31-N19	3.70	1.43	1.35
2	L	301	A1EEE	C02-N03	3.65	1.49	1.37
2	C	301	A1EEE	C02-N03	3.65	1.49	1.37
2	A	301	A1EEE	C02-N03	3.63	1.49	1.37
2	K	301	A1EEE	C17-N03	3.60	1.51	1.46
2	A	301	A1EEE	C37-C36	-3.60	1.39	1.52
2	I	301	A1EEE	C17-N03	3.60	1.50	1.46
2	A	301	A1EEE	C17-N03	3.57	1.50	1.46
2	D	301	A1EEE	C37-C36	-3.57	1.39	1.52
2	E	301	A1EEE	C37-C36	-3.56	1.39	1.52
2	G	301	A1EEE	C37-C36	-3.56	1.39	1.52
2	H	301	A1EEE	C37-C36	-3.55	1.39	1.52
2	M	301	A1EEE	C37-C36	-3.55	1.39	1.52
2	K	301	A1EEE	C37-C36	-3.53	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	A1EEE	C37-C36	-3.50	1.39	1.52
2	I	301	A1EEE	C37-C36	-3.49	1.39	1.52
2	C	301	A1EEE	C37-C36	-3.46	1.39	1.52
2	I	302	A1EEE	C37-C36	-3.46	1.39	1.52
2	F	301	A1EEE	C37-C36	-3.45	1.39	1.52
2	B	301	A1EEE	C37-C36	-3.44	1.39	1.52
2	N	301	A1EEE	C37-C36	-3.42	1.40	1.52
2	C	301	A1EEE	C17-N03	3.35	1.50	1.46
2	G	301	A1EEE	C17-N03	3.32	1.50	1.46
2	L	301	A1EEE	C17-N03	3.26	1.50	1.46
2	B	301	A1EEE	C02-N34	2.99	1.47	1.34
2	N	301	A1EEE	C02-N34	2.98	1.47	1.34
2	E	301	A1EEE	C02-N34	2.95	1.47	1.34
2	I	302	A1EEE	C02-N34	2.93	1.47	1.34
2	A	301	A1EEE	C02-N34	2.92	1.47	1.34
2	D	301	A1EEE	C37-C38	-2.91	1.38	1.49
2	D	301	A1EEE	C02-N34	2.90	1.47	1.34
2	C	301	A1EEE	C02-N34	2.90	1.47	1.34
2	F	301	A1EEE	C02-N34	2.89	1.47	1.34
2	L	301	A1EEE	C02-N34	2.89	1.47	1.34
2	K	301	A1EEE	C02-N34	2.89	1.47	1.34
2	M	301	A1EEE	C02-N34	2.88	1.47	1.34
2	H	301	A1EEE	C02-N34	2.86	1.47	1.34
2	I	301	A1EEE	C02-N34	2.86	1.47	1.34
2	H	301	A1EEE	C37-C38	-2.80	1.39	1.49
2	A	301	A1EEE	C37-C38	-2.79	1.39	1.49
2	G	301	A1EEE	C02-N34	2.74	1.46	1.34
2	K	301	A1EEE	C37-C38	-2.69	1.39	1.49
2	G	301	A1EEE	C37-C38	-2.69	1.39	1.49
2	C	301	A1EEE	C37-C38	-2.68	1.39	1.49
2	F	301	A1EEE	C37-C38	-2.67	1.39	1.49
2	I	302	A1EEE	C37-C38	-2.67	1.39	1.49
2	L	301	A1EEE	C37-C38	-2.66	1.39	1.49
2	E	301	A1EEE	C37-C38	-2.65	1.39	1.49
2	M	301	A1EEE	C37-C38	-2.65	1.39	1.49
2	I	301	A1EEE	C37-C38	-2.60	1.39	1.49
2	C	301	A1EEE	C22-C27	-2.60	1.38	1.43
2	N	301	A1EEE	C37-C38	-2.58	1.39	1.49
2	H	301	A1EEE	C10-C11	2.56	1.60	1.51
2	L	301	A1EEE	C22-C27	-2.55	1.38	1.43
2	G	301	A1EEE	C22-C27	-2.55	1.38	1.43
2	I	301	A1EEE	C10-C11	2.54	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1EEE	C37-C38	-2.52	1.40	1.49
2	K	301	A1EEE	C10-C11	2.50	1.60	1.51
2	I	301	A1EEE	C22-C27	-2.49	1.38	1.43
2	B	301	A1EEE	C22-C27	-2.49	1.38	1.43
2	D	301	A1EEE	C10-C11	2.49	1.60	1.51
2	B	301	A1EEE	C10-C11	2.47	1.60	1.51
2	M	301	A1EEE	C10-C11	2.47	1.60	1.51
2	A	301	A1EEE	C22-C27	-2.47	1.38	1.43
2	M	301	A1EEE	C22-C27	-2.47	1.38	1.43
2	A	301	A1EEE	C10-C11	2.46	1.60	1.51
2	F	301	A1EEE	C10-C11	2.45	1.60	1.51
2	F	301	A1EEE	C22-C27	-2.44	1.38	1.43
2	D	301	A1EEE	C22-C27	-2.43	1.38	1.43
2	E	301	A1EEE	C10-C11	2.41	1.59	1.51
2	N	301	A1EEE	C10-C11	2.41	1.59	1.51
2	I	301	A1EEE	O01-C02	-2.41	1.18	1.23
2	K	301	A1EEE	C22-C27	-2.39	1.38	1.43
2	I	302	A1EEE	C10-C11	2.39	1.59	1.51
2	L	301	A1EEE	C10-C11	2.39	1.59	1.51
2	E	301	A1EEE	C22-C27	-2.35	1.38	1.43
2	H	301	A1EEE	O01-C02	-2.34	1.18	1.23
2	C	301	A1EEE	C10-C11	2.33	1.59	1.51
2	I	302	A1EEE	C22-C27	-2.30	1.38	1.43
2	H	301	A1EEE	C22-C27	-2.29	1.38	1.43
2	G	301	A1EEE	C10-C11	2.27	1.59	1.51
2	L	301	A1EEE	O32-C31	-2.26	1.18	1.22
2	G	301	A1EEE	O32-C31	-2.22	1.18	1.22
2	I	302	A1EEE	O01-C02	-2.20	1.19	1.23
2	K	301	A1EEE	O32-C31	-2.19	1.18	1.22
2	N	301	A1EEE	C22-C27	-2.18	1.39	1.43
2	E	301	A1EEE	O01-C02	-2.16	1.19	1.23
2	E	301	A1EEE	O32-C31	-2.16	1.18	1.22
2	G	301	A1EEE	O01-C02	-2.10	1.19	1.23
2	K	301	A1EEE	O01-C02	-2.10	1.19	1.23
2	K	301	A1EEE	O33-C06	-2.06	1.18	1.23
2	D	301	A1EEE	O01-C02	-2.05	1.19	1.23
2	N	301	A1EEE	O01-C02	-2.04	1.19	1.23
2	L	301	A1EEE	O33-C06	-2.04	1.18	1.23
2	F	301	A1EEE	O32-C31	-2.03	1.18	1.22
2	F	301	A1EEE	O01-C02	-2.02	1.19	1.23
2	G	301	A1EEE	O33-C06	-2.00	1.18	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	301	A1EEE	C11-N51-N52	13.43	179.62	115.95
2	K	301	A1EEE	C11-N51-N52	13.41	179.53	115.95
2	I	301	A1EEE	C11-N51-N52	13.38	179.41	115.95
2	D	301	A1EEE	C11-N51-N52	13.35	179.24	115.95
2	F	301	A1EEE	C11-N51-N52	13.29	178.96	115.95
2	C	301	A1EEE	C11-N51-N52	13.20	178.57	115.95
2	B	301	A1EEE	C11-N51-N52	13.19	178.53	115.95
2	H	301	A1EEE	C11-N51-N52	13.14	178.26	115.95
2	E	301	A1EEE	C11-N51-N52	13.13	178.23	115.95
2	L	301	A1EEE	C11-N51-N52	13.13	178.22	115.95
2	G	301	A1EEE	C11-N51-N52	13.12	178.17	115.95
2	A	301	A1EEE	C11-N51-N52	13.01	177.63	115.95
2	I	302	A1EEE	C11-N51-N52	12.94	177.30	115.95
2	M	301	A1EEE	C11-N51-N52	12.91	177.16	115.95
2	D	301	A1EEE	C20-N19-C18	3.28	121.19	115.69
2	I	301	A1EEE	C20-N19-C18	3.16	121.00	115.69
2	K	301	A1EEE	C09-C08-C31	-3.06	103.79	111.17
2	L	301	A1EEE	C20-N19-C18	3.03	120.78	115.69
2	I	302	A1EEE	C31-C08-N07	2.99	118.24	112.29
2	G	301	A1EEE	C20-N19-C18	2.97	120.68	115.69
2	C	301	A1EEE	C20-N19-C18	2.95	120.65	115.69
2	N	301	A1EEE	C20-N19-C18	2.94	120.62	115.69
2	F	301	A1EEE	C20-N19-C18	2.92	120.59	115.69
2	D	301	A1EEE	C31-C08-N07	2.91	118.08	112.29
2	L	301	A1EEE	C08-C31-N19	2.90	123.37	116.85
2	K	301	A1EEE	C20-N19-C18	2.73	120.27	115.69
2	M	301	A1EEE	C20-N19-C18	2.72	120.25	115.69
2	N	301	A1EEE	C31-C08-N07	2.71	117.67	112.29
2	I	301	A1EEE	C09-C08-C31	-2.70	104.65	111.17
2	B	301	A1EEE	C20-N19-C18	2.69	120.21	115.69
2	A	301	A1EEE	C31-C08-N07	2.68	117.61	112.29
2	G	301	A1EEE	C31-C08-N07	2.66	117.58	112.29
2	C	301	A1EEE	C31-C08-N07	2.66	117.58	112.29
2	I	302	A1EEE	C20-N19-C18	2.65	120.14	115.69
2	H	301	A1EEE	C08-C31-N19	2.60	122.71	116.85
2	H	301	A1EEE	C31-C08-N07	2.57	117.40	112.29
2	E	301	A1EEE	C20-N19-C18	2.53	119.94	115.69
2	H	301	A1EEE	C09-C08-N07	2.50	114.98	111.45
2	H	301	A1EEE	C20-N19-C18	2.50	119.89	115.69
2	K	301	A1EEE	C08-C31-N19	2.48	122.45	116.85
2	A	301	A1EEE	C20-N19-C18	2.47	119.84	115.69
2	F	301	A1EEE	C08-C31-N19	2.46	122.40	116.85
2	E	301	A1EEE	C31-C08-N07	2.45	117.16	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	A1EEE	C09-C08-C31	-2.44	105.28	111.17
2	I	301	A1EEE	C09-C08-N07	2.42	114.87	111.45
2	B	301	A1EEE	C31-C08-N07	2.39	117.04	112.29
2	I	301	A1EEE	C31-C08-N07	2.37	117.00	112.29
2	L	301	A1EEE	C31-C08-N07	2.37	116.99	112.29
2	I	301	A1EEE	C08-C31-N19	2.37	122.18	116.85
2	N	301	A1EEE	C09-C08-C31	-2.35	105.50	111.17
2	N	301	A1EEE	C08-C31-N19	2.35	122.13	116.85
2	B	301	A1EEE	C08-C31-N19	2.34	122.13	116.85
2	A	301	A1EEE	C08-C31-N19	2.34	122.12	116.85
2	F	301	A1EEE	C09-C08-N07	2.33	114.74	111.45
2	G	301	A1EEE	C08-C31-N19	2.30	122.04	116.85
2	M	301	A1EEE	C09-C08-C31	-2.29	105.64	111.17
2	I	302	A1EEE	C08-C31-N19	2.26	121.93	116.85
2	F	301	A1EEE	C31-C08-N07	2.25	116.77	112.29
2	C	301	A1EEE	C08-C31-N19	2.25	121.92	116.85
2	K	301	A1EEE	C05-C04-N03	-2.24	104.24	111.61
2	K	301	A1EEE	C31-C08-N07	2.24	116.73	112.29
2	C	301	A1EEE	C05-C04-N03	-2.22	104.30	111.61
2	D	301	A1EEE	C08-C31-N19	2.19	121.78	116.85
2	E	301	A1EEE	C08-C31-N19	2.16	121.72	116.85
2	B	301	A1EEE	C05-C04-N03	-2.14	104.55	111.61
2	K	301	A1EEE	C09-C08-N07	2.14	114.47	111.45
2	I	302	A1EEE	C05-C04-N03	-2.12	104.63	111.61
2	I	302	A1EEE	C10-C09-C08	-2.10	108.84	113.78
2	D	301	A1EEE	C09-C08-C31	-2.08	106.15	111.17
2	H	301	A1EEE	C05-C04-N03	-2.07	104.78	111.61
2	L	301	A1EEE	O32-C31-N19	-2.05	120.06	122.49
2	G	301	A1EEE	C05-C04-N03	-2.04	104.88	111.61
2	H	301	A1EEE	C09-C08-C31	-2.04	106.23	111.17

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1EEE	C09-C10-C11-N51
2	B	301	A1EEE	C09-C10-C11-N51
2	B	301	A1EEE	N07-C08-C09-C10
2	B	301	A1EEE	C31-C08-C09-C10
2	C	301	A1EEE	C09-C10-C11-N51
2	C	301	A1EEE	N07-C08-C09-C10
2	C	301	A1EEE	C31-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
2	D	301	A1EEE	C09-C10-C11-N51
2	E	301	A1EEE	C09-C10-C11-N51
2	E	301	A1EEE	C31-C08-C09-C10
2	F	301	A1EEE	C09-C10-C11-N51
2	F	301	A1EEE	N07-C08-C09-C10
2	G	301	A1EEE	N07-C08-C09-C10
2	H	301	A1EEE	C09-C10-C11-N51
2	H	301	A1EEE	N07-C08-C09-C10
2	H	301	A1EEE	C31-C08-C09-C10
2	I	301	A1EEE	C09-C10-C11-N51
2	I	301	A1EEE	N07-C08-C09-C10
2	I	302	A1EEE	C09-C10-C11-N51
2	I	302	A1EEE	N07-C08-C09-C10
2	I	302	A1EEE	C31-C08-C09-C10
2	I	302	A1EEE	C10-C11-N51-N52
2	K	301	A1EEE	C09-C10-C11-N51
2	M	301	A1EEE	C09-C10-C11-N51
2	N	301	A1EEE	C09-C10-C11-N51
2	E	301	A1EEE	N34-C35-C36-C37
2	A	301	A1EEE	C08-C09-C10-C11
2	D	301	A1EEE	N34-C35-C36-C37
2	F	301	A1EEE	C08-C09-C10-C11
2	H	301	A1EEE	C08-C09-C10-C11
2	I	301	A1EEE	C08-C09-C10-C11
2	I	302	A1EEE	C08-C09-C10-C11
2	N	301	A1EEE	C08-C09-C10-C11
2	I	301	A1EEE	N34-C35-C36-C37
2	C	301	A1EEE	N34-C35-C36-C37
2	B	301	A1EEE	C08-C09-C10-C11
2	D	301	A1EEE	C08-C09-C10-C11
2	B	301	A1EEE	N34-C35-C36-C37
2	H	301	A1EEE	N34-C35-C36-C37
2	C	301	A1EEE	C11-N51-N52-N53
2	H	301	A1EEE	C11-N51-N52-N53
2	I	302	A1EEE	C11-N51-N52-N53
2	N	301	A1EEE	N34-C35-C36-C37
2	F	301	A1EEE	N34-C35-C36-C37
2	G	301	A1EEE	C10-C11-N51-N52
2	I	301	A1EEE	C11-N51-N52-N53
2	G	301	A1EEE	C31-C08-C09-C10
3	A	302	MPD	C1-C2-C3-C4
2	G	301	A1EEE	N34-C35-C36-C37

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	H	301	A1EEE	C10-C11-N51-N52
2	A	301	A1EEE	N34-C35-C36-C37
2	E	301	A1EEE	C11-N51-N52-N53
2	G	301	A1EEE	C11-N51-N52-N53
2	E	301	A1EEE	C10-C11-N51-N52
2	E	301	A1EEE	N07-C08-C09-C10
2	I	301	A1EEE	C10-C11-N51-N52
2	L	301	A1EEE	C10-C11-N51-N52
2	D	301	A1EEE	C11-N51-N52-N53
2	K	301	A1EEE	C11-N51-N52-N53
2	M	301	A1EEE	C11-N51-N52-N53
2	N	301	A1EEE	C11-N51-N52-N53

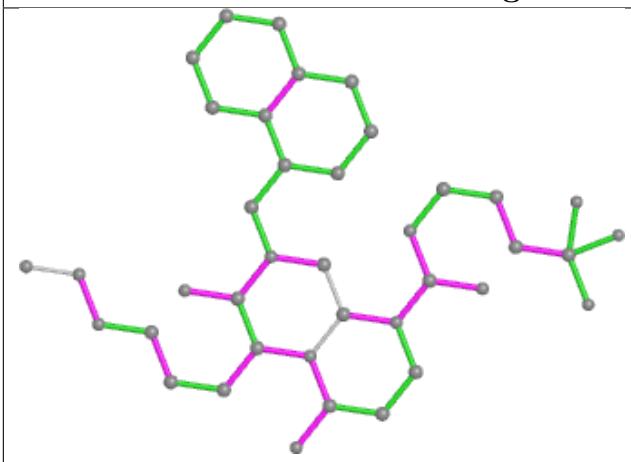
There are no ring outliers.

3 monomers are involved in 5 short contacts:

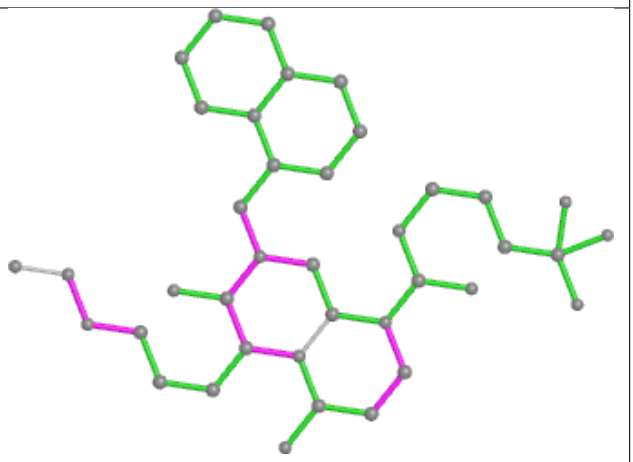
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	302	MPD	1	0
3	B	302	MPD	3	0
4	H	302	TBU	1	0

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

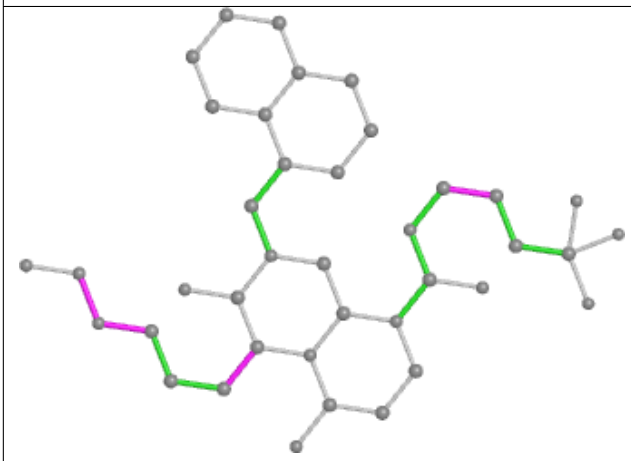
Ligand A1EEE G 301



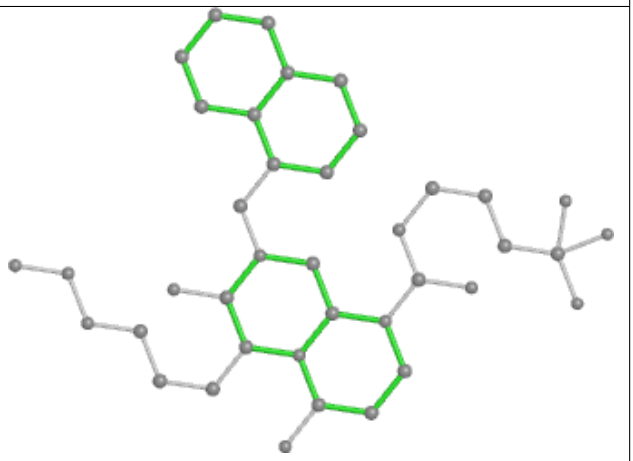
Bond lengths



Bond angles

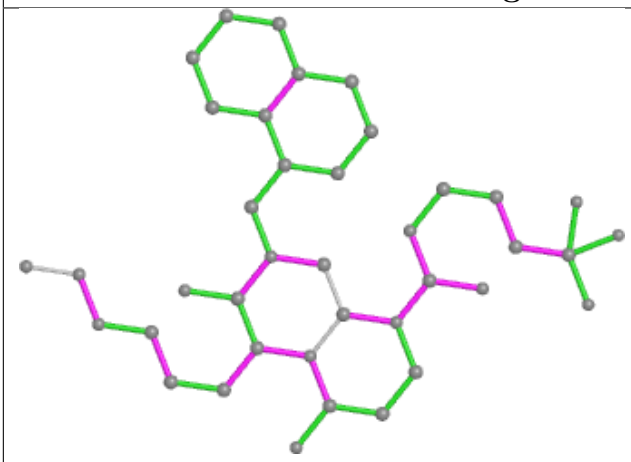


Torsions

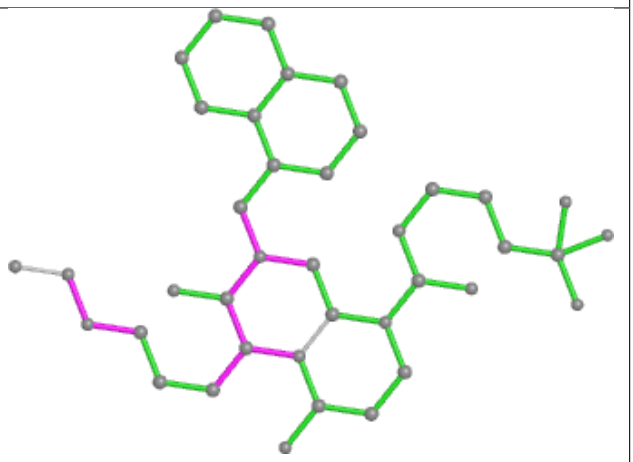


Rings

Ligand A1EEE D 301



Bond lengths



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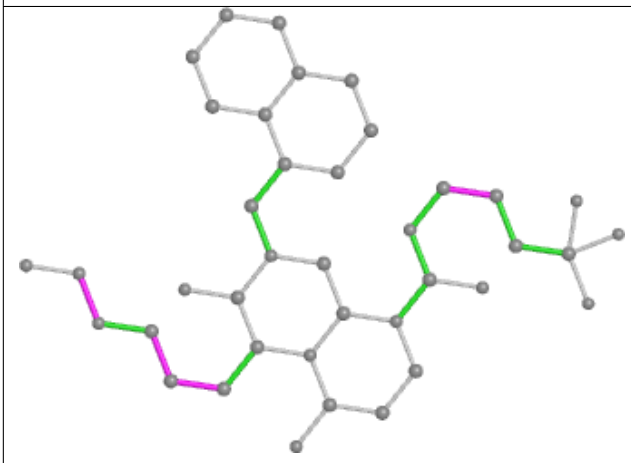

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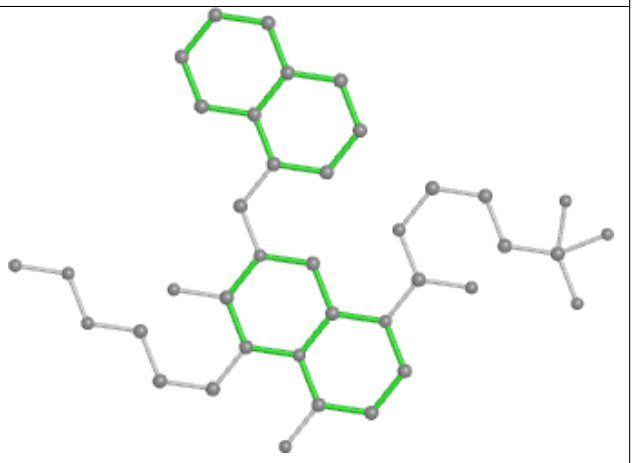
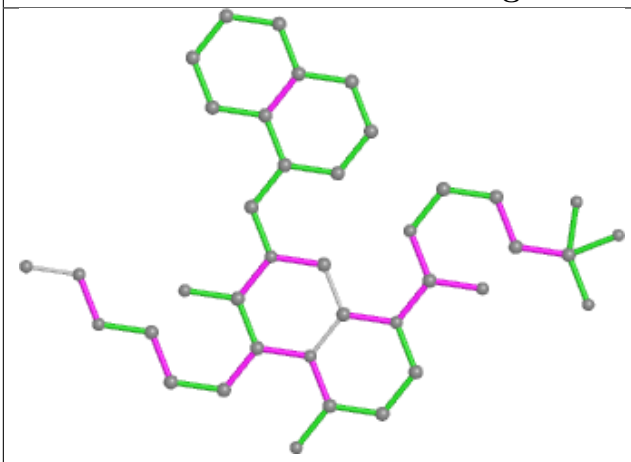
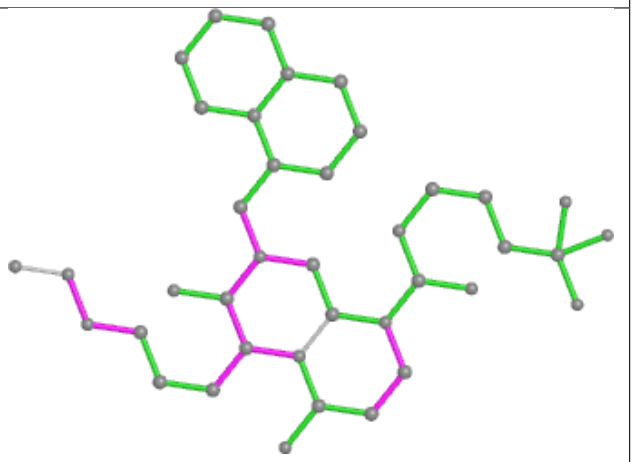


Rings

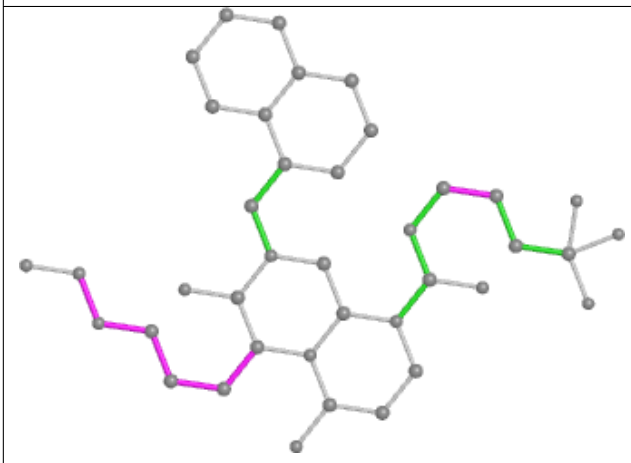
Ligand A1EEE H 301



Bond lengths



Bond angles



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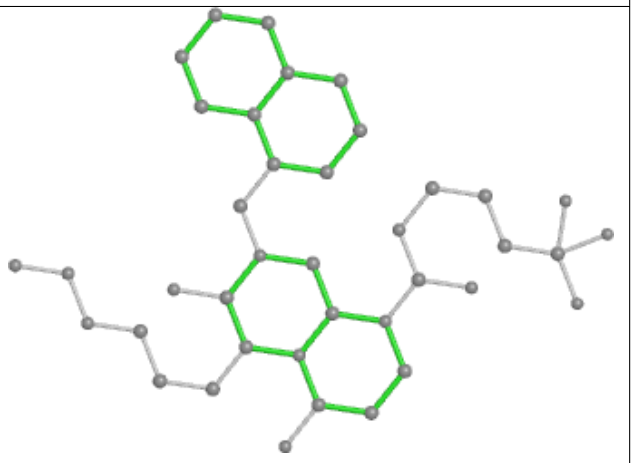
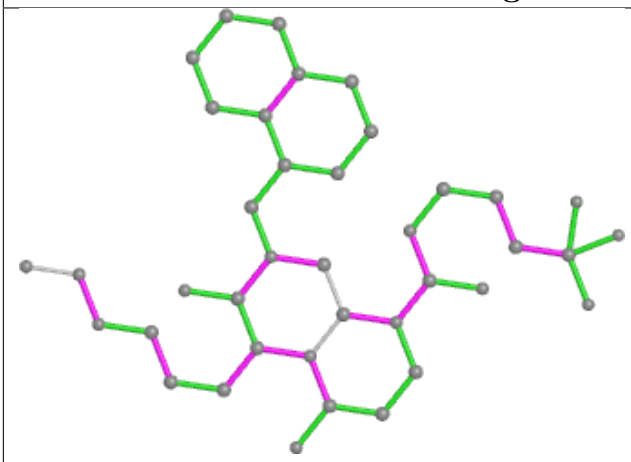


Rings

Ligand A1EEE A 301



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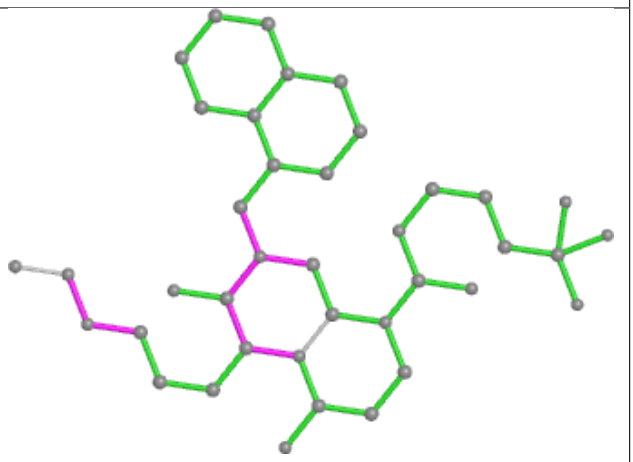

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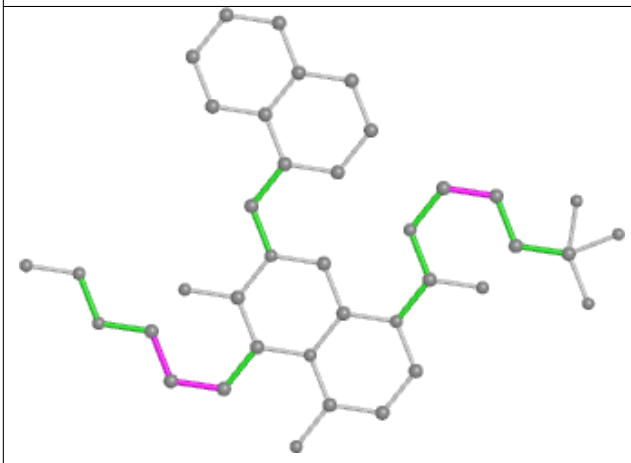

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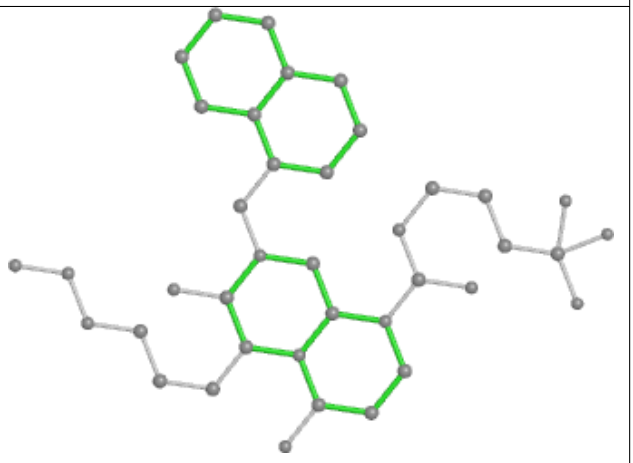
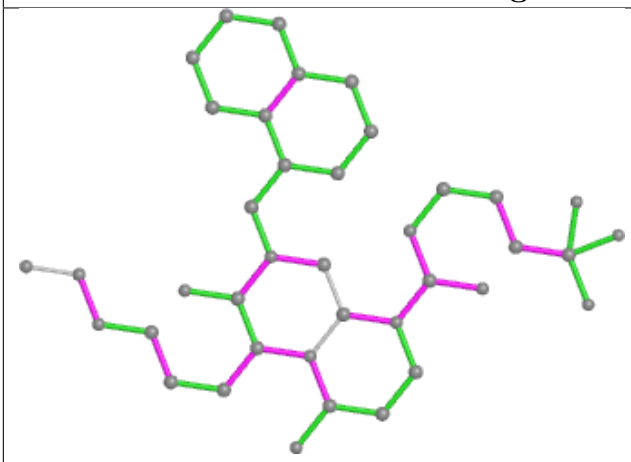


Rings

Ligand A1EEE I 302



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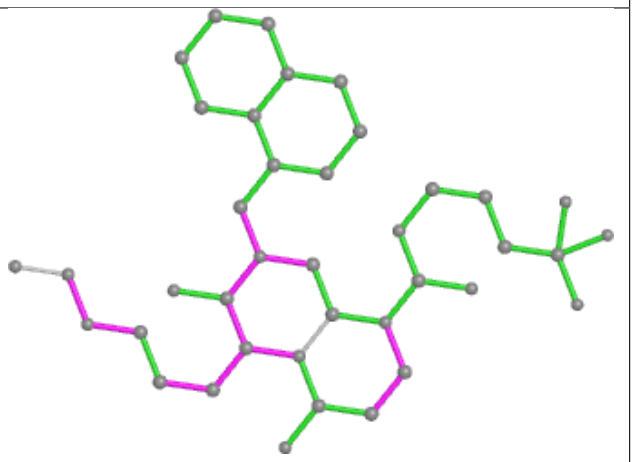

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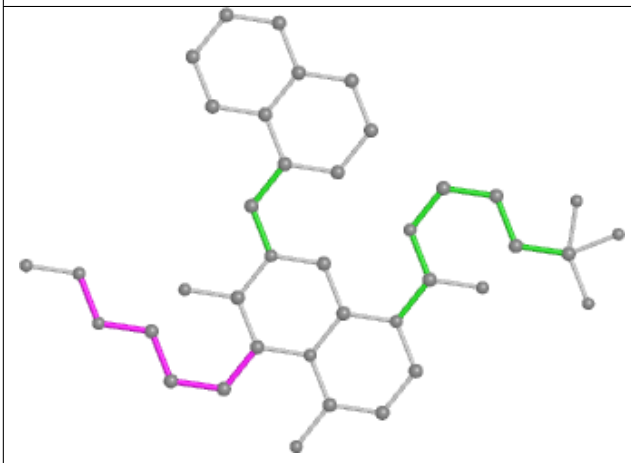

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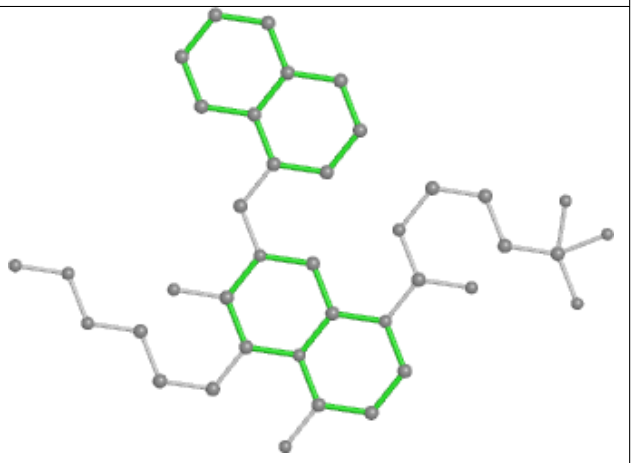
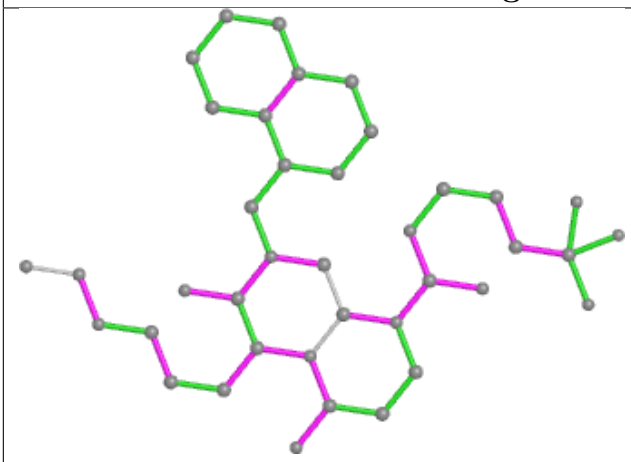


Rings

Ligand A1EEE K 301



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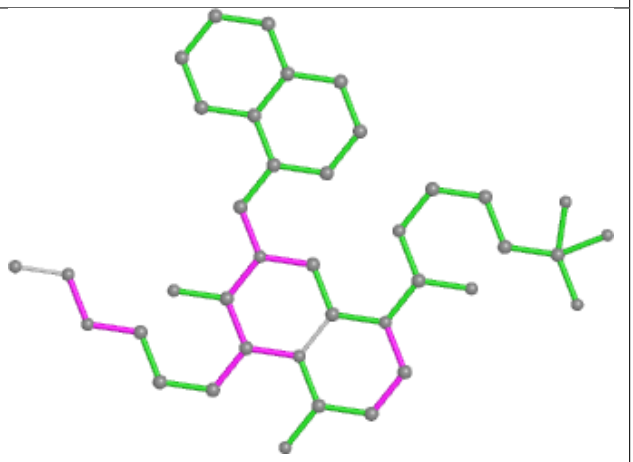

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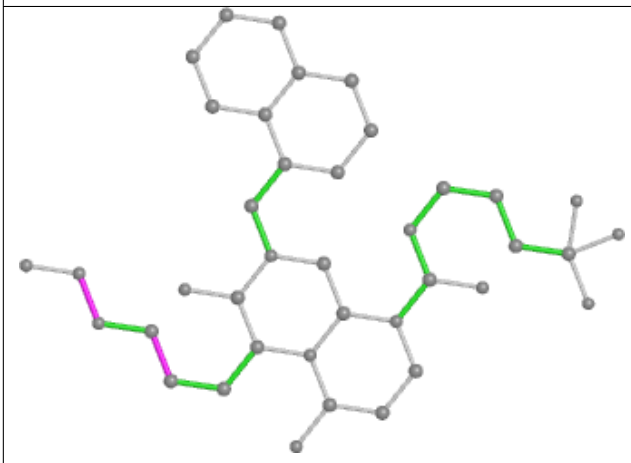

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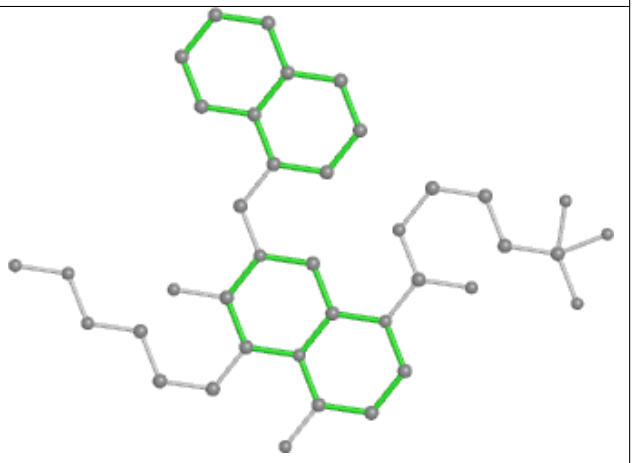
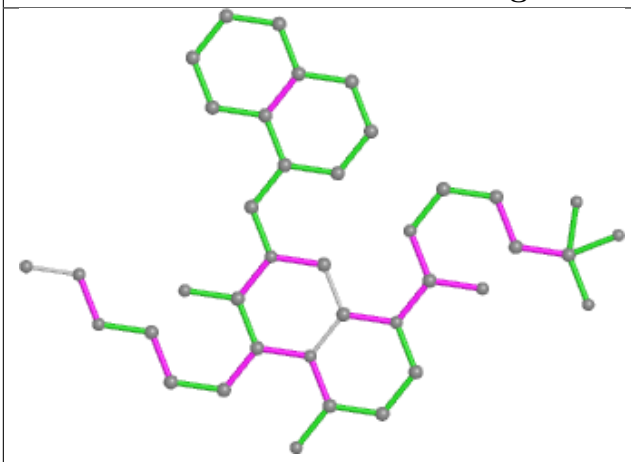


Rings

Ligand A1EEE I 301



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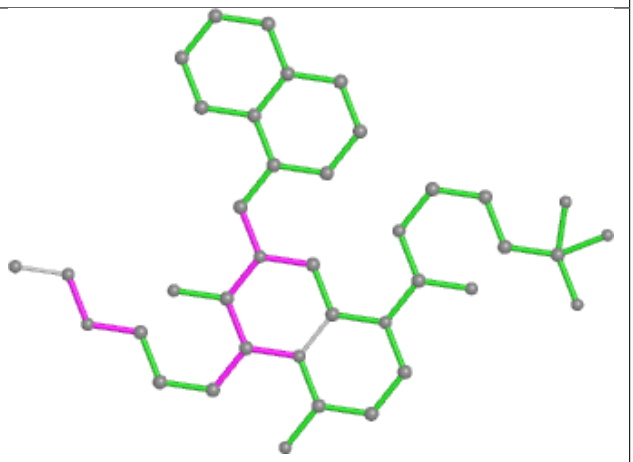

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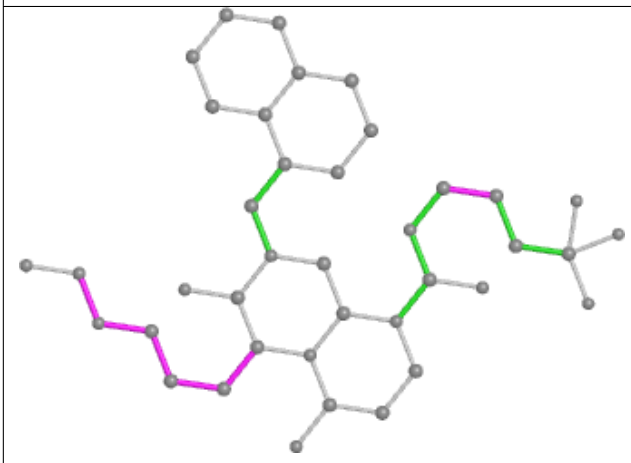

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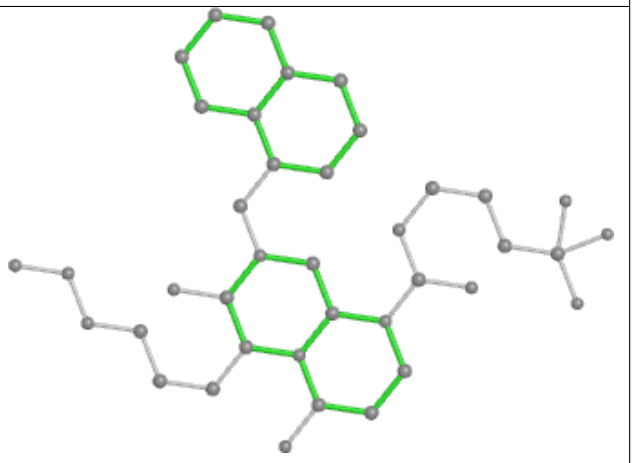
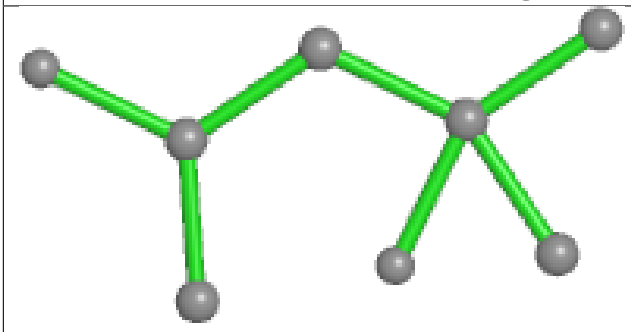


Rings

Ligand MPD G 302



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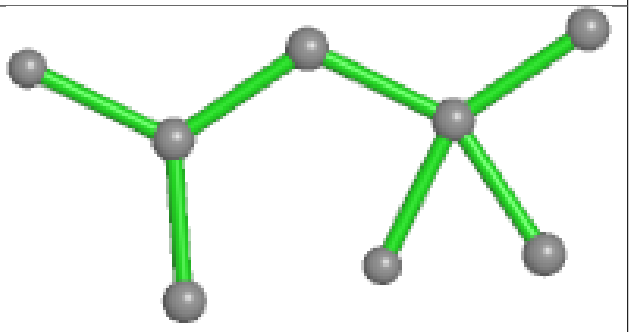

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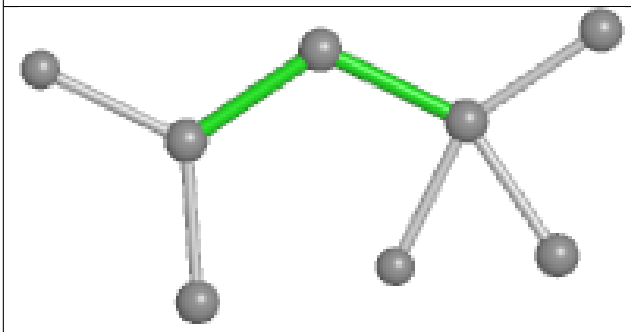

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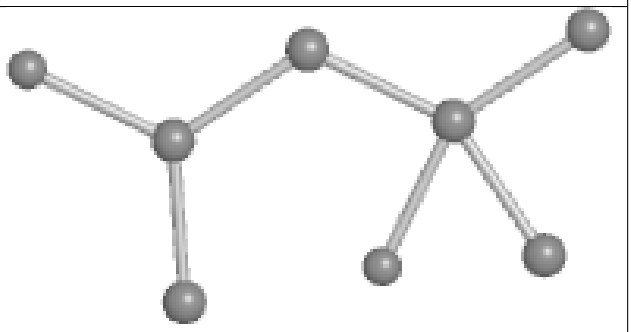
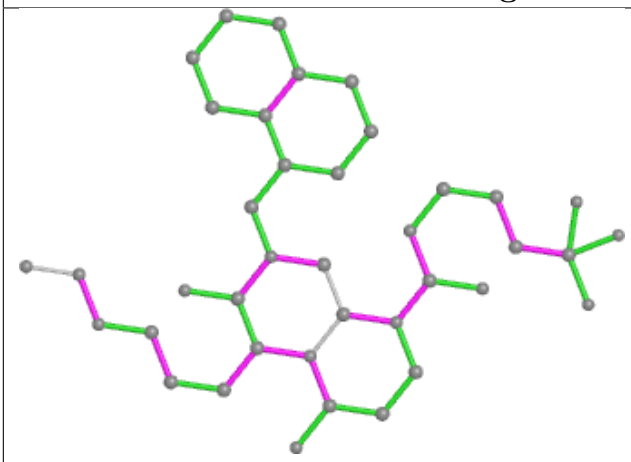


Rings

Ligand A1EEE M 301



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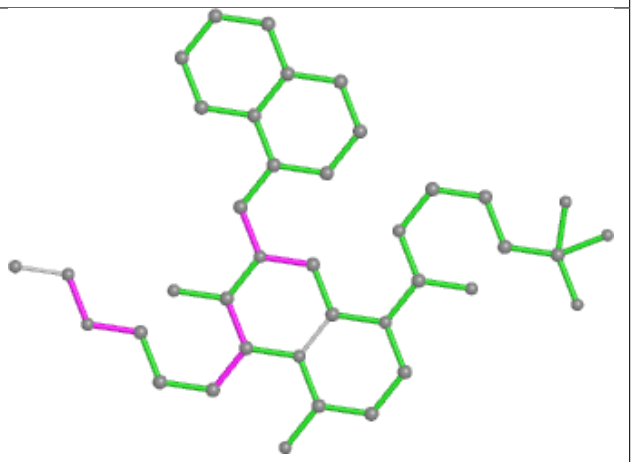

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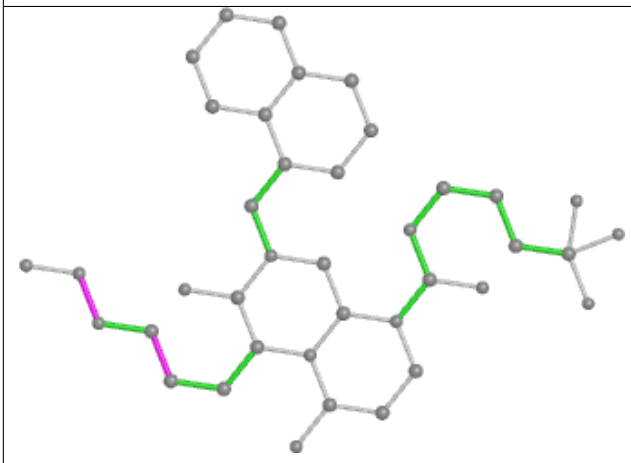

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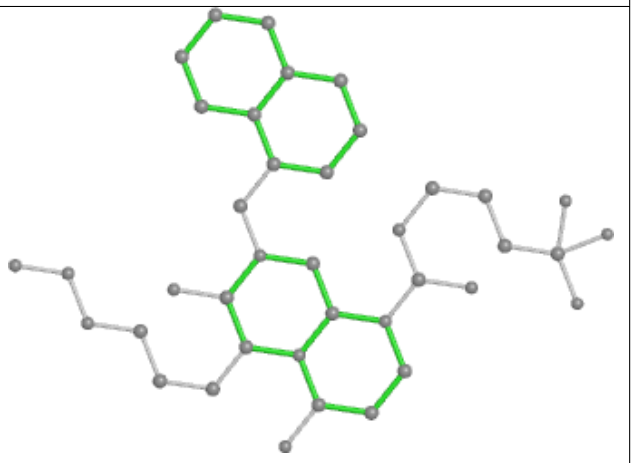
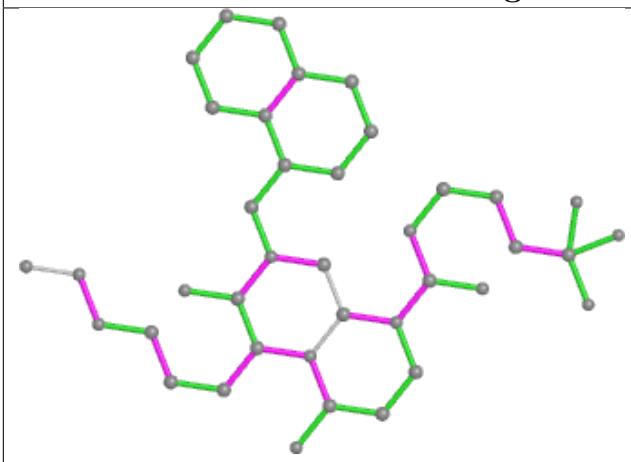


Rings

Ligand A1EEE B 301



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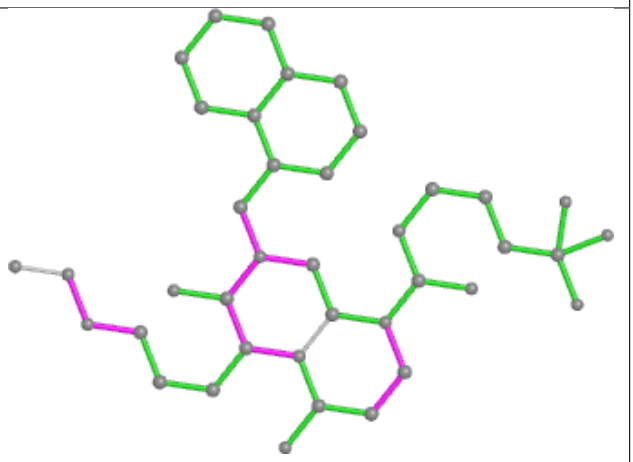

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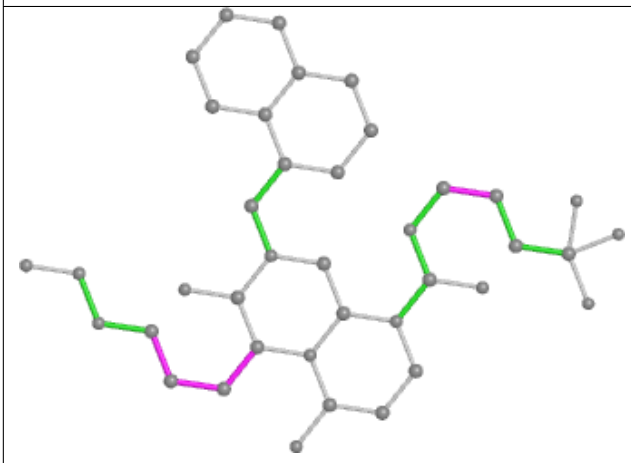

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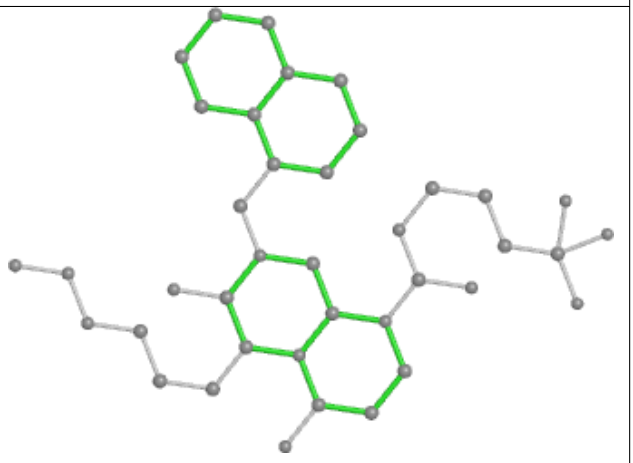
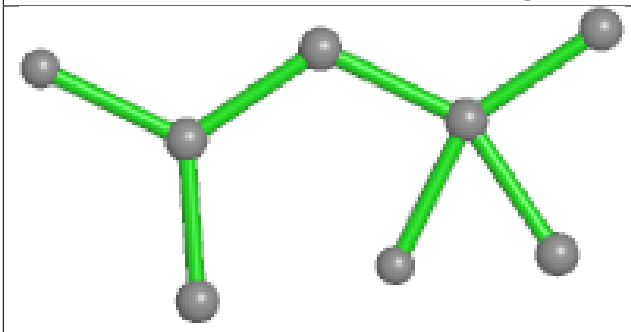


Rings

Ligand MPD B 302



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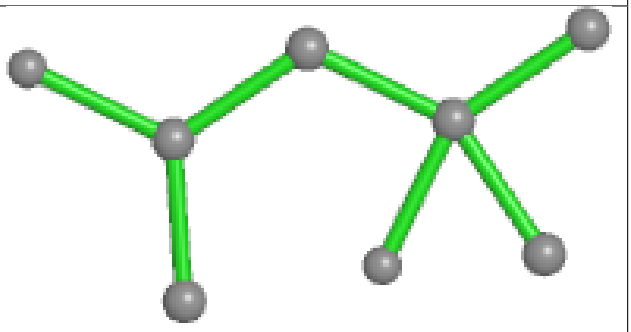
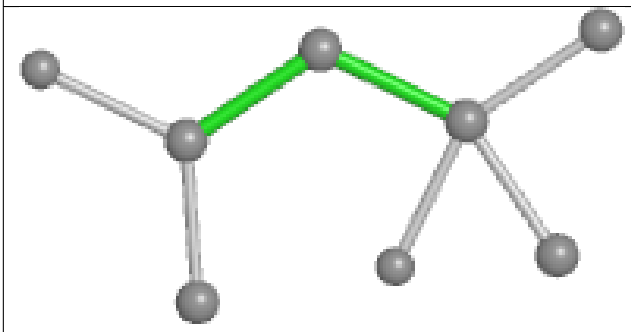


Bond angles



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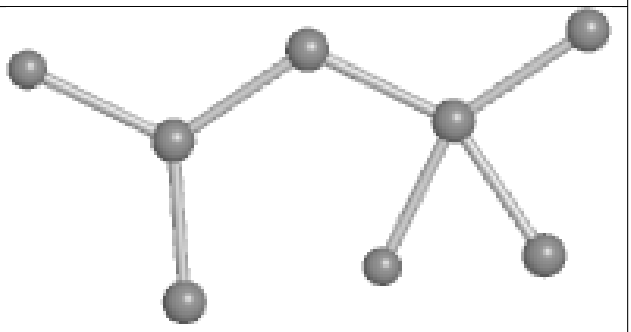
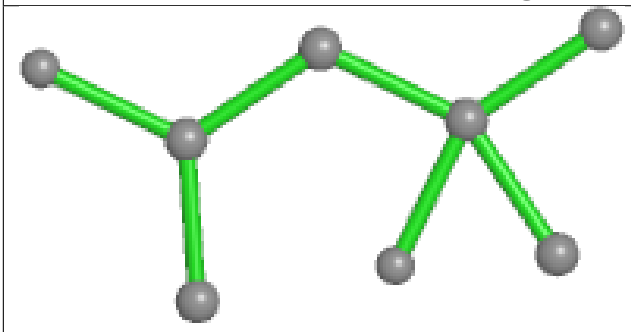


Rings

Ligand MPD A 302



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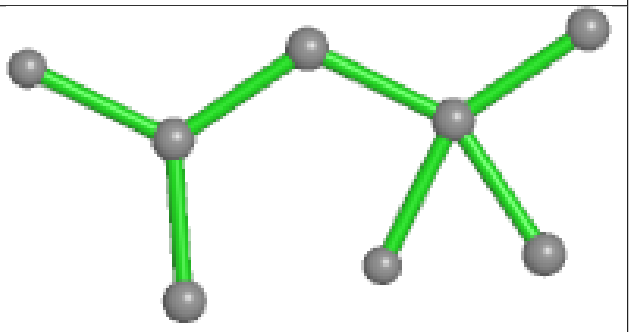
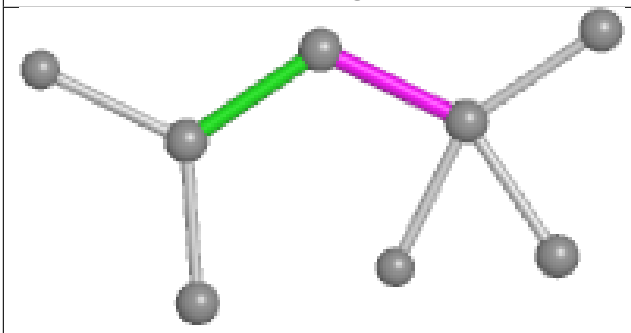
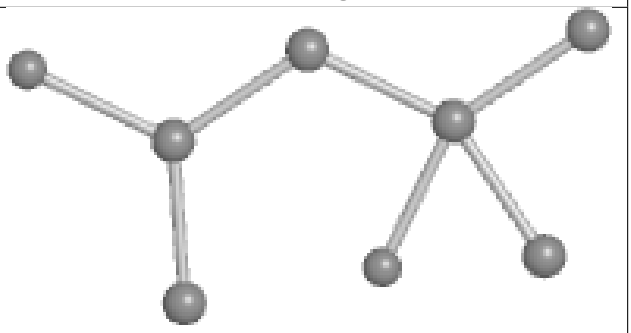


Bond angles

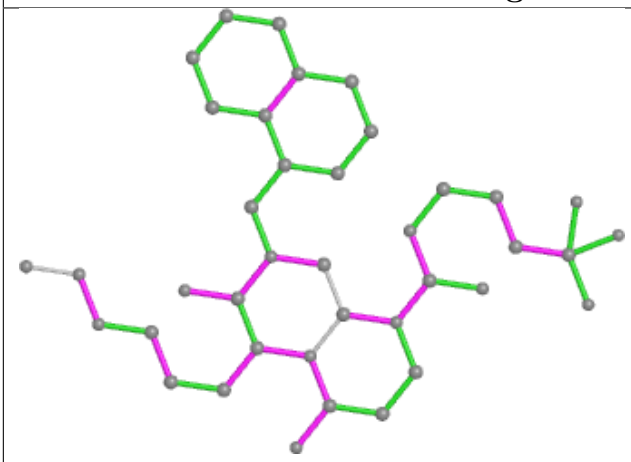


Torsions



Rings

Ligand A1EEE L 301



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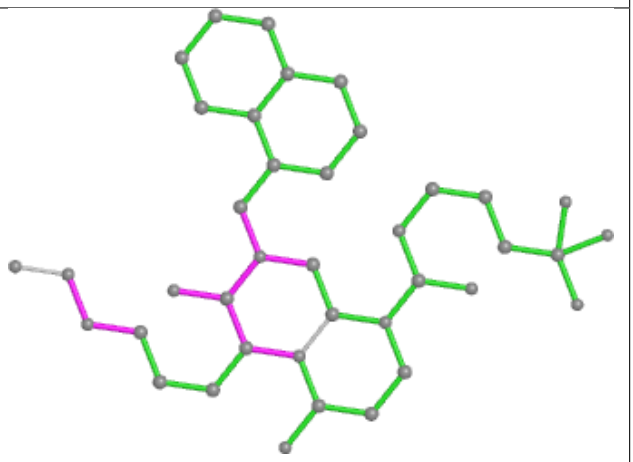
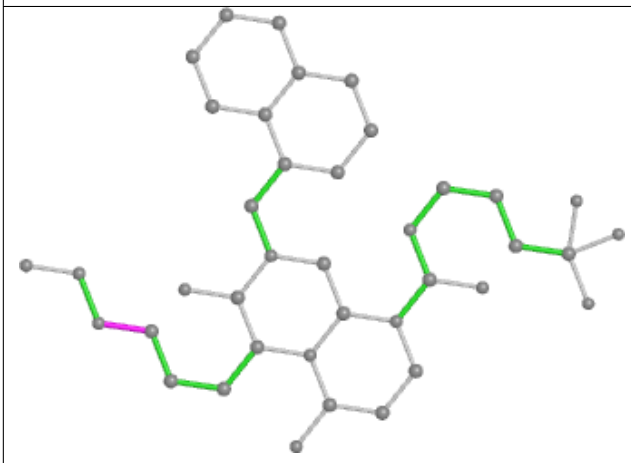
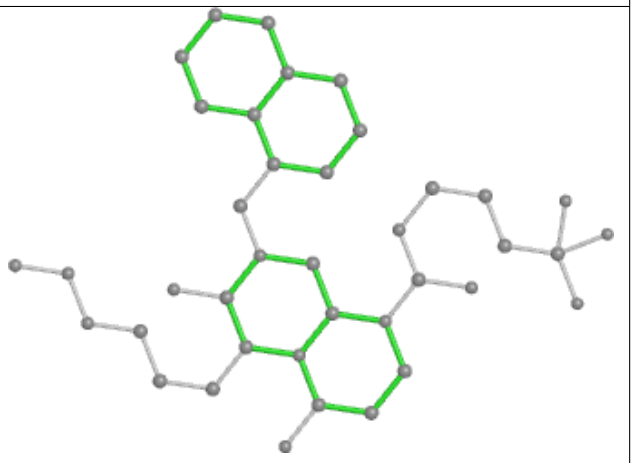


Bond angles

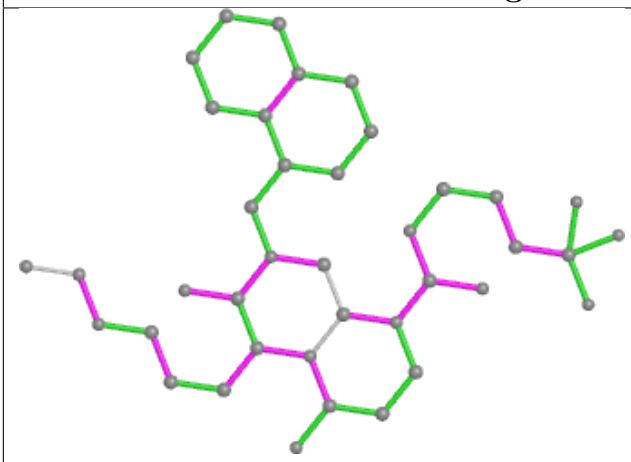


Torsions

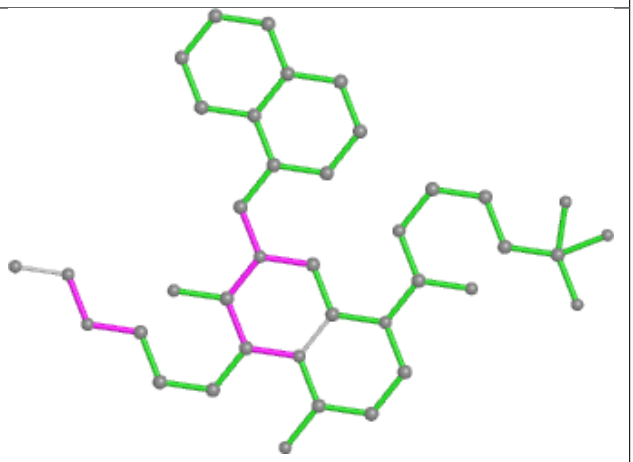


Rings

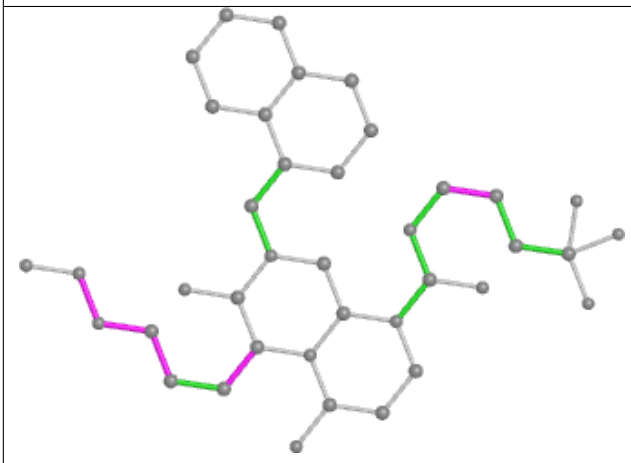
Ligand A1EEE E 301



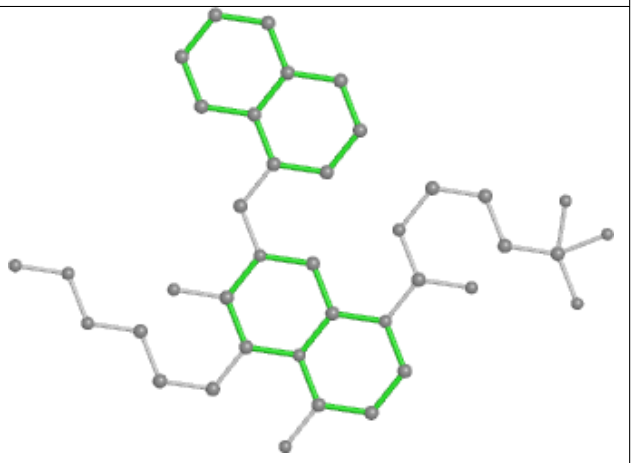
Bond lengths



Bond angles

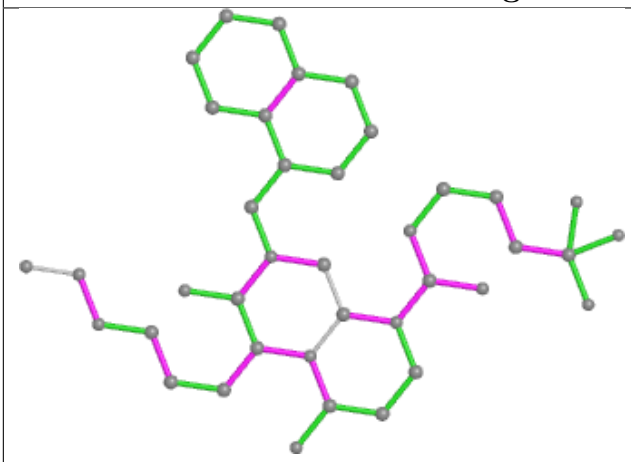


Torsions

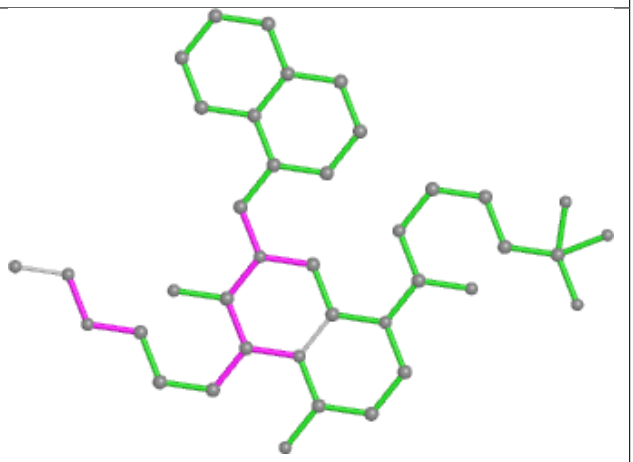


Rings

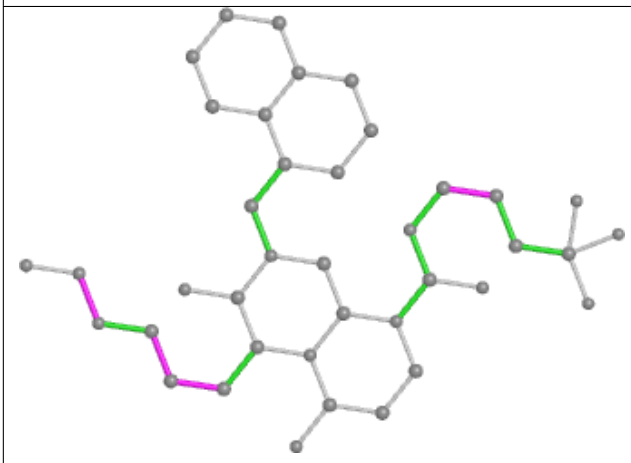
Ligand A1EEE N 301



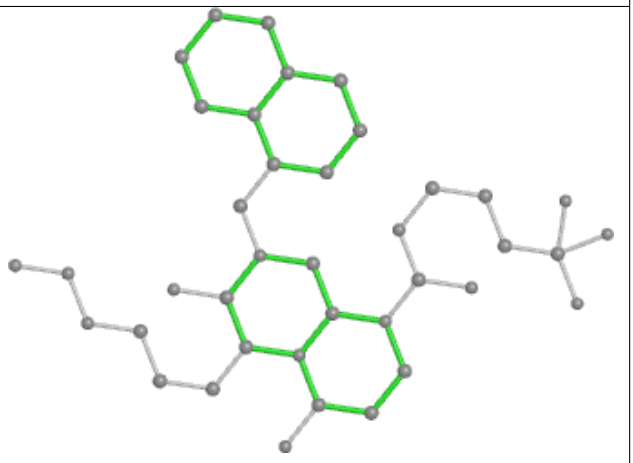
Bond lengths



Bond angles

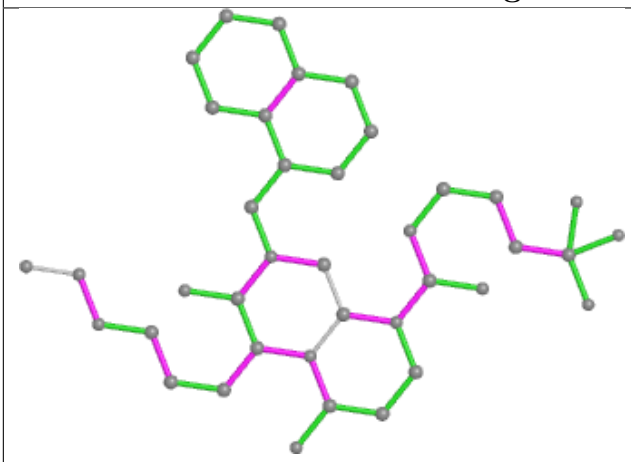


Torsions

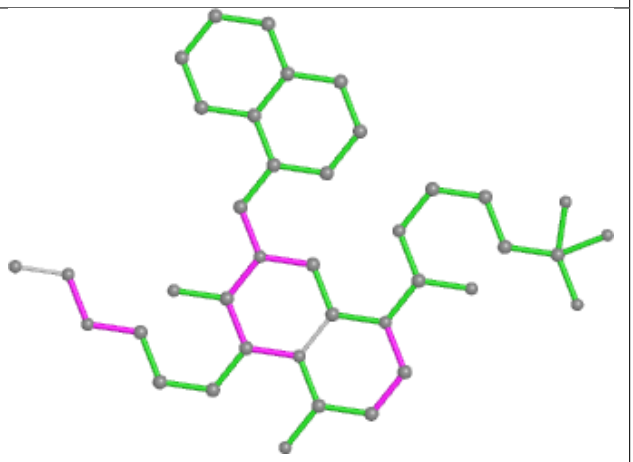


Rings

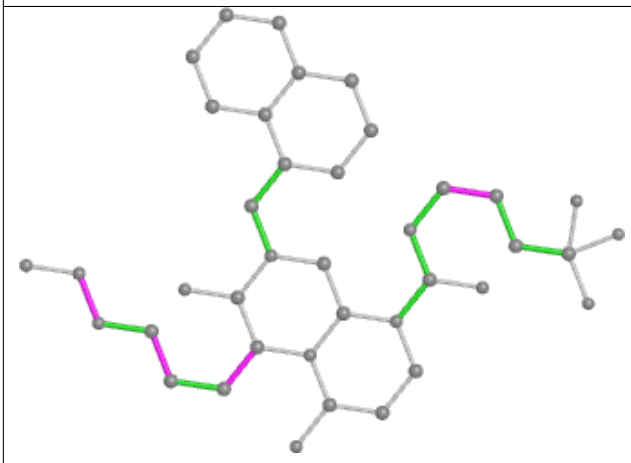
Ligand A1EEE C 301



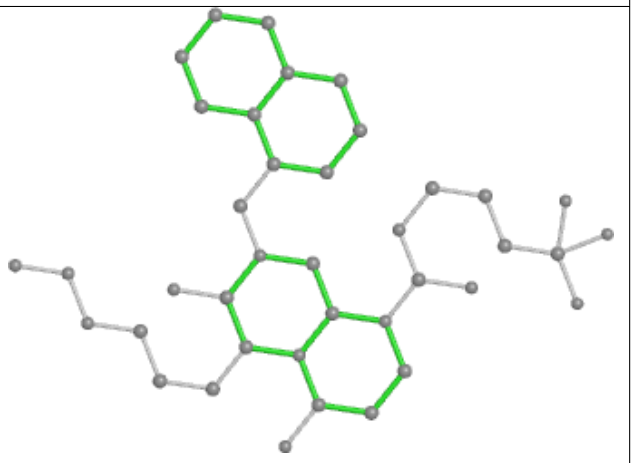
Bond lengths



Bond angles

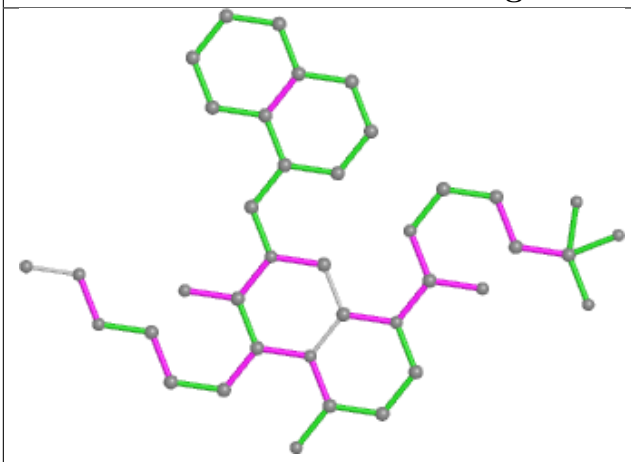


Torsions

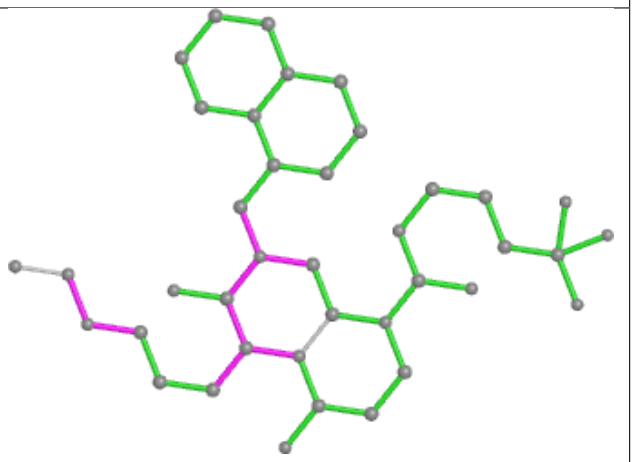


Rings

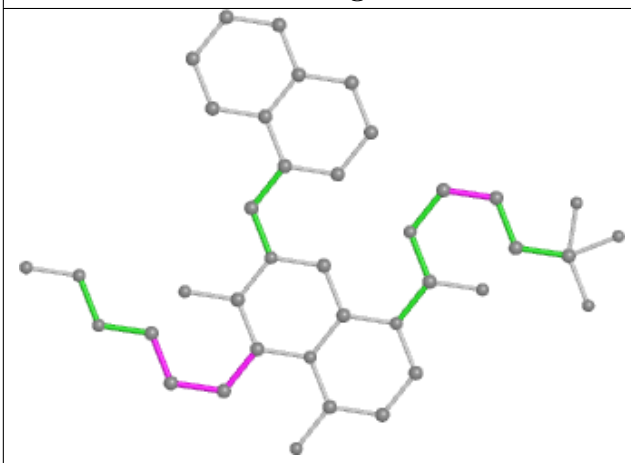
Ligand A1EEE F 301



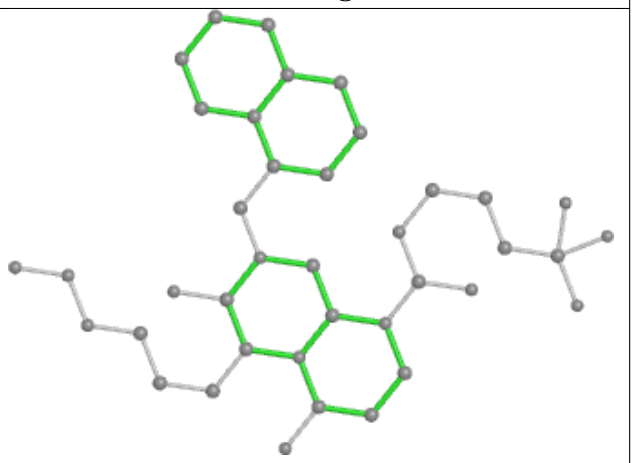
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	185/201 (92%)	-0.01	4 (2%)	62	58	25, 39, 52, 68	1 (0%)
1	B	186/201 (92%)	0.50	7 (3%)	44	41	36, 47, 64, 92	0
1	C	186/201 (92%)	0.77	10 (5%)	32	29	39, 51, 70, 105	0
1	D	187/201 (93%)	0.68	13 (6%)	24	21	36, 49, 79, 108	0
1	E	191/201 (95%)	0.13	13 (6%)	25	22	31, 41, 73, 103	0
1	F	190/201 (94%)	0.15	10 (5%)	33	30	26, 39, 71, 88	1 (0%)
1	G	184/201 (91%)	0.01	4 (2%)	62	58	31, 39, 57, 81	0
1	H	187/201 (93%)	0.03	6 (3%)	50	47	29, 38, 65, 88	0
1	I	190/201 (94%)	-0.02	6 (3%)	50	47	27, 36, 58, 73	0
1	J	191/201 (95%)	-0.07	1 (0%)	87	85	30, 37, 52, 75	0
1	K	186/201 (92%)	-0.10	3 (1%)	70	67	28, 36, 54, 78	0
1	L	186/201 (92%)	0.05	3 (1%)	70	67	28, 39, 54, 76	1 (0%)
1	M	185/201 (92%)	0.39	8 (4%)	40	36	36, 48, 64, 87	0
1	N	182/201 (90%)	0.28	4 (2%)	62	58	34, 46, 61, 67	0
All	All	2616/2814 (92%)	0.20	92 (3%)	47	44	25, 42, 63, 108	3 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	5.9
1	F	3	LEU	5.7
1	E	194	THR	4.7
1	C	9	GLU	4.5
1	B	8	ILE	4.4
1	C	194	THR	4.3
1	J	3	LEU	4.3
1	G	8	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	194	THR	3.9
1	E	10	THR	3.9
1	D	9	GLU	3.8
1	D	18	TYR	3.8
1	E	11	THR	3.7
1	C	3	LEU	3.7
1	B	162	ILE	3.6
1	B	195	LYS	3.5
1	H	9	GLU	3.5
1	H	3	LEU	3.5
1	F	12	ASN	3.5
1	D	195	LYS	3.4
1	H	16	ARG	3.4
1	G	193	GLU	3.3
1	F	16	ARG	3.3
1	D	16	ARG	3.2
1	H	195	LYS	3.2
1	B	3	LEU	3.1
1	I	13	ARG	3.1
1	I	18	TYR	3.0
1	M	16	ARG	3.0
1	F	14	GLY	2.9
1	C	193	GLU	2.9
1	B	17	ALA	2.9
1	B	194	THR	2.9
1	K	3	LEU	2.8
1	N	91	ILE	2.7
1	C	16	ARG	2.7
1	F	8	ILE	2.7
1	M	194	THR	2.7
1	L	130	GLN	2.7
1	G	16	ARG	2.7
1	D	191	VAL	2.7
1	H	191	VAL	2.7
1	L	3	LEU	2.6
1	C	85	LYS	2.6
1	N	16	ARG	2.6
1	E	15	GLU	2.6
1	F	11	THR	2.6
1	D	166	GLN	2.6
1	F	17	ALA	2.6
1	E	18	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	162	ILE	2.6
1	I	8	ILE	2.6
1	M	3	LEU	2.5
1	H	194	THR	2.5
1	E	13	ARG	2.4
1	E	191	VAL	2.4
1	L	195	LYS	2.4
1	I	14	GLY	2.4
1	M	130	GLN	2.4
1	F	10	THR	2.4
1	D	8	ILE	2.4
1	A	195	LYS	2.4
1	D	192	PRO	2.4
1	B	100	GLY	2.4
1	K	191	VAL	2.3
1	E	91	ILE	2.3
1	M	165	ILE	2.3
1	G	3	LEU	2.3
1	I	16	ARG	2.3
1	E	130	GLN	2.3
1	C	18	TYR	2.3
1	E	16	ARG	2.3
1	A	8	ILE	2.3
1	C	192	PRO	2.2
1	E	14	GLY	2.2
1	D	4	ILE	2.2
1	E	4	ILE	2.2
1	F	15	GLU	2.2
1	M	163	GLU	2.2
1	N	167	LYS	2.2
1	K	8	ILE	2.1
1	M	162	ILE	2.1
1	A	194	THR	2.1
1	M	8	ILE	2.1
1	E	9	GLU	2.1
1	D	157	ARG	2.1
1	I	192	PRO	2.1
1	N	148	GLU	2.1
1	C	103	LEU	2.1
1	A	191	VAL	2.0
1	D	162	ILE	2.0
1	C	189	VAL	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)

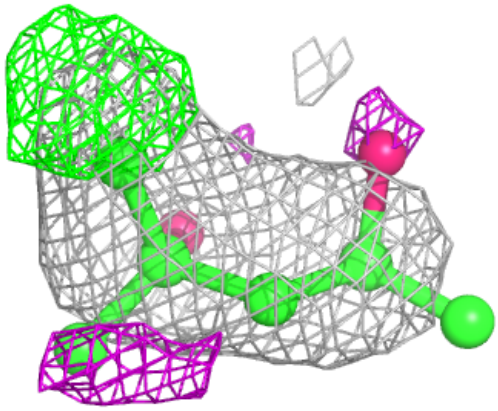
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

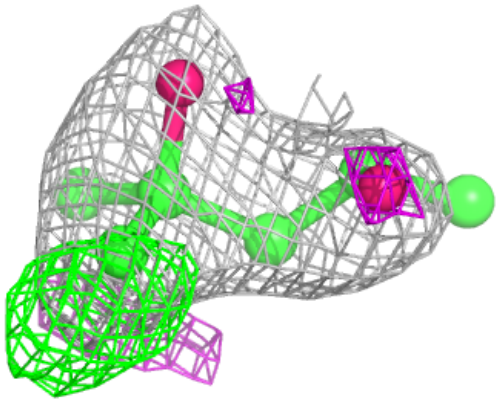
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	A	302	8/8	0.72	0.24	55,57,62,63	0
4	TBU	H	302	5/5	0.78	0.19	44,46,47,47	0
2	A1EEE	D	301	39/39	0.86	0.12	50,55,67,68	0
3	MPD	B	302	8/8	0.87	0.23	67,70,73,73	0
2	A1EEE	B	301	39/39	0.87	0.12	44,52,59,60	0
2	A1EEE	M	301	39/39	0.89	0.11	48,55,68,69	0
2	A1EEE	N	301	39/39	0.89	0.12	49,53,69,73	0
2	A1EEE	C	301	39/39	0.89	0.11	54,61,74,74	0
2	A1EEE	H	301	39/39	0.89	0.11	43,47,62,64	0
2	A1EEE	I	301	39/39	0.89	0.11	38,42,57,60	0
3	MPD	G	302	8/8	0.90	0.16	58,61,63,63	0
2	A1EEE	F	301	39/39	0.90	0.11	39,45,62,66	0
2	A1EEE	K	301	39/39	0.91	0.10	34,41,53,55	0
2	A1EEE	L	301	39/39	0.91	0.10	35,43,63,68	0
2	A1EEE	E	301	39/39	0.91	0.10	41,46,58,60	0
2	A1EEE	I	302	39/39	0.91	0.10	34,42,60,64	0
2	A1EEE	G	301	39/39	0.92	0.10	38,46,61,64	0
2	A1EEE	A	301	39/39	0.93	0.09	36,42,59,61	0

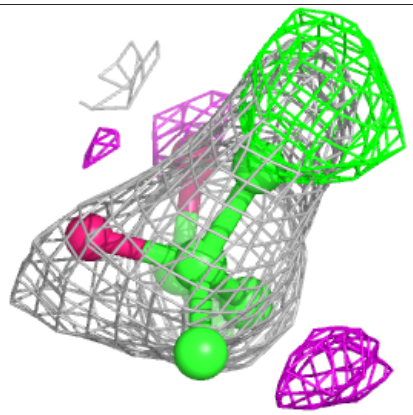
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MPD A 302:

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

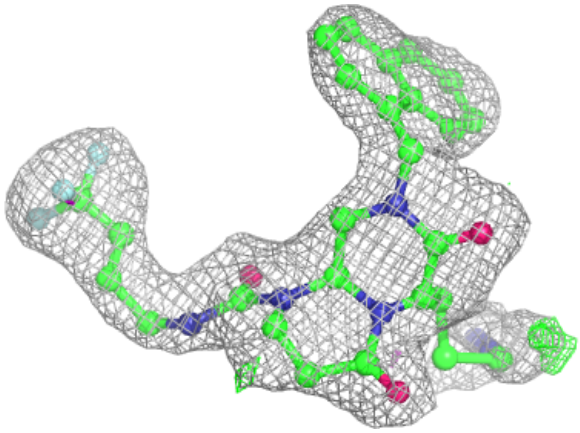


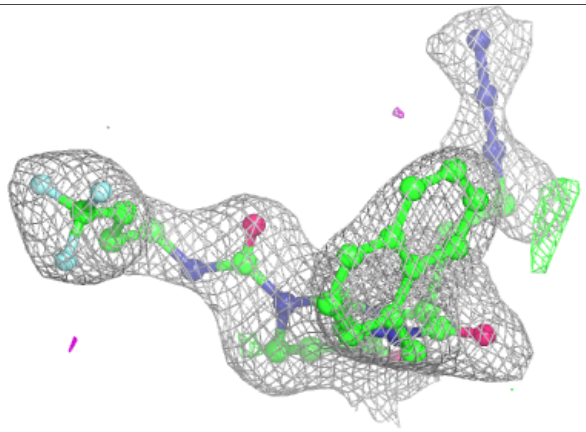


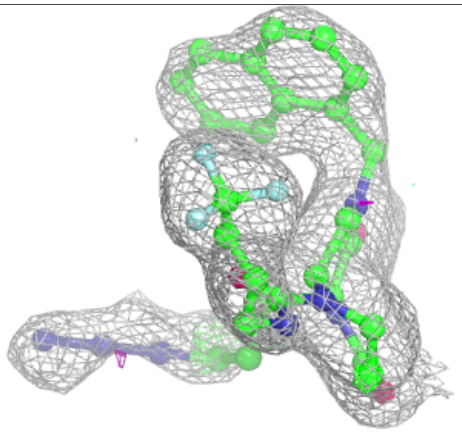


Electron density around A1EEE D 301:

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

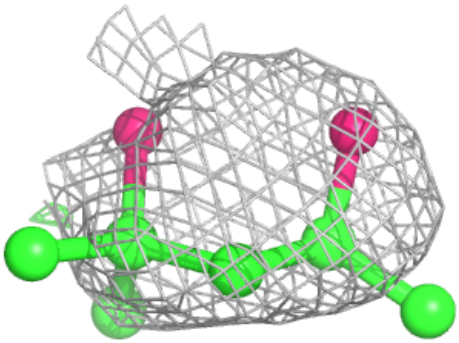


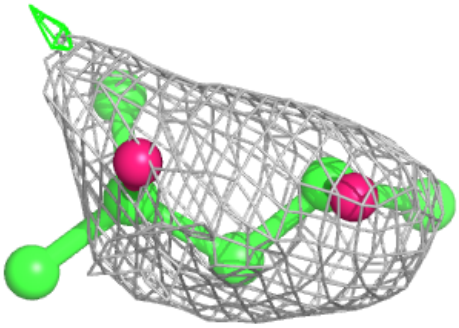


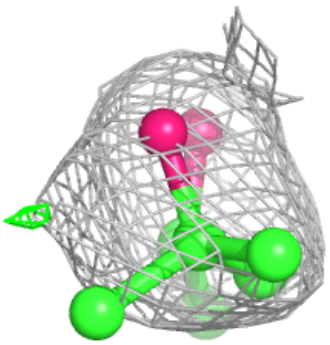


Electron density around MPD B 302:

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

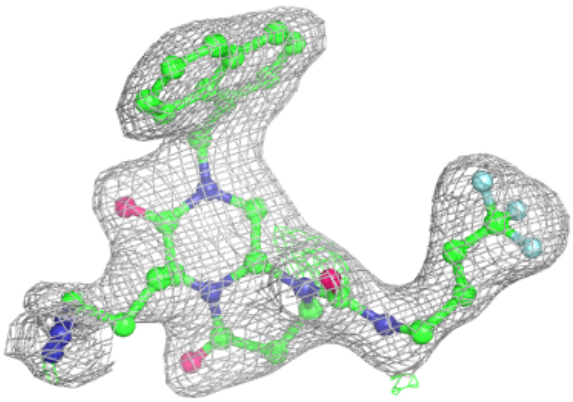


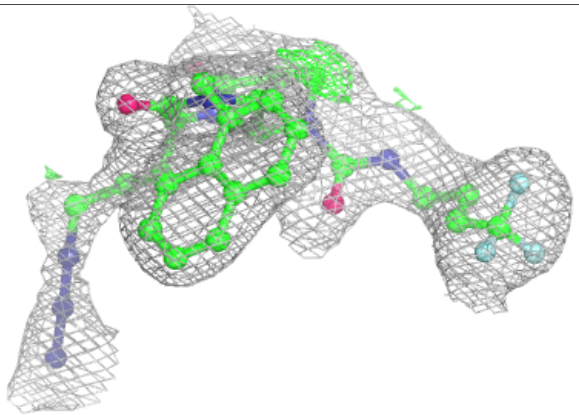


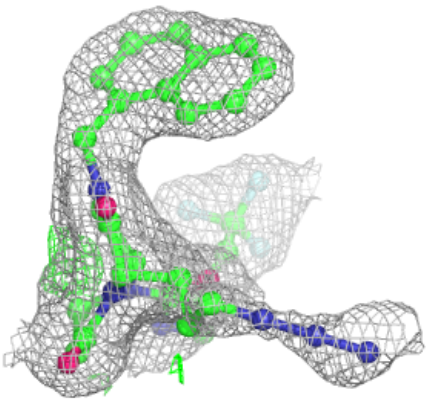


Electron density around A1EEE B 301:

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

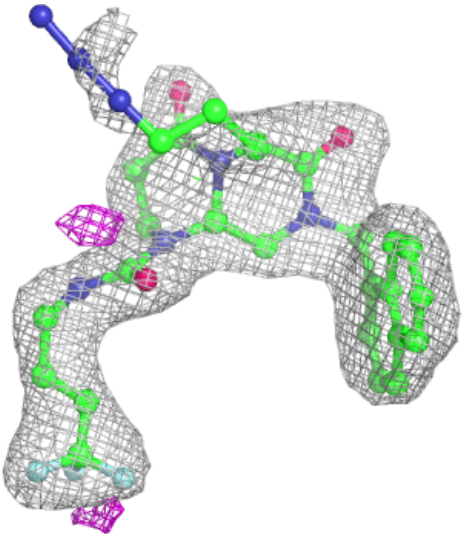


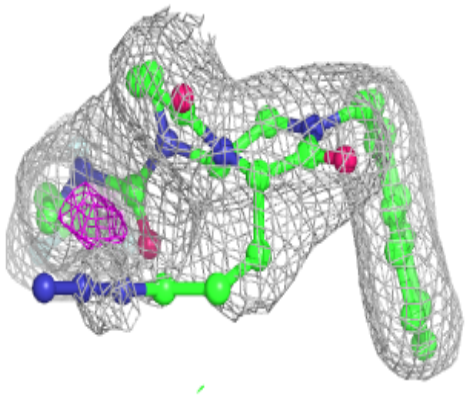


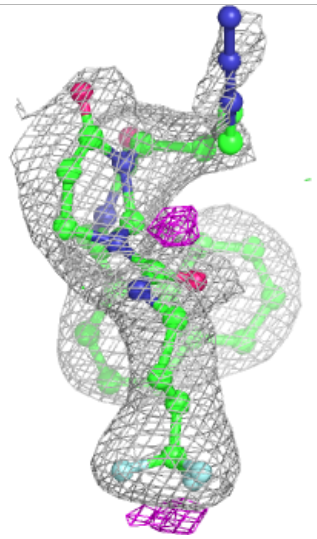


Electron density around A1EEE M 301:

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

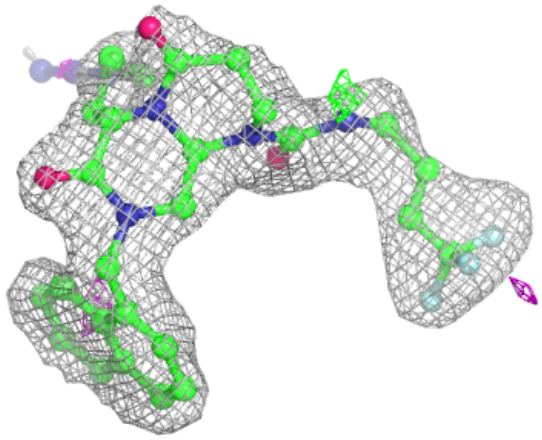


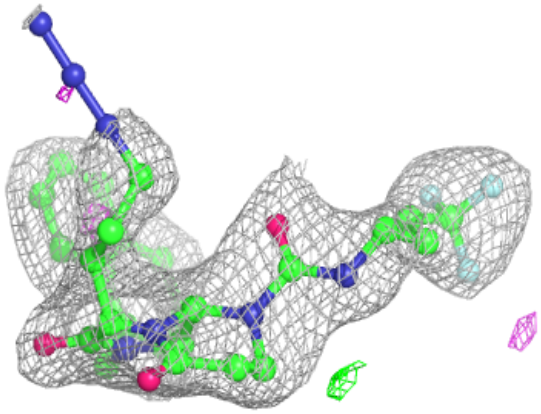


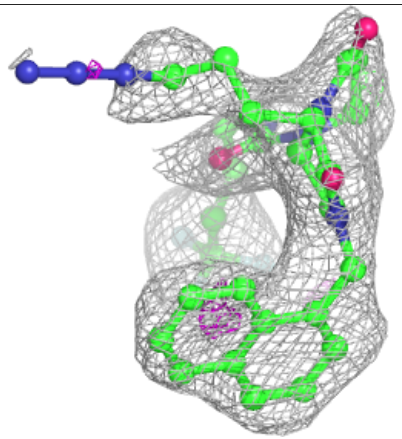


Electron density around A1EEE N 301:

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

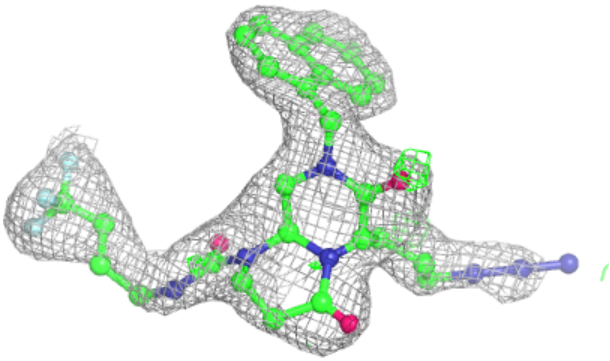


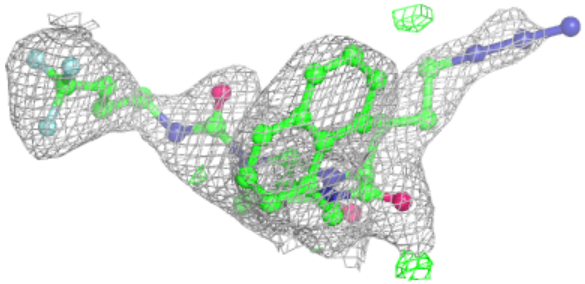


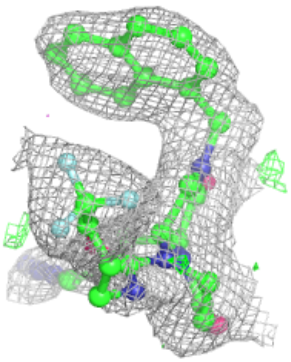


Electron density around A1EEE C 301:

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

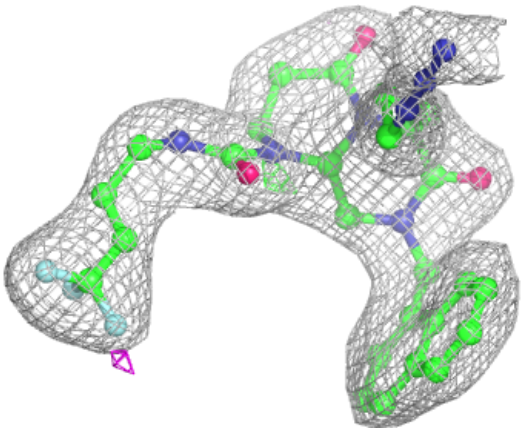


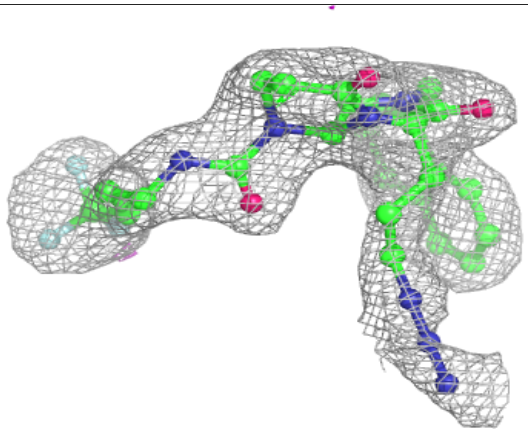


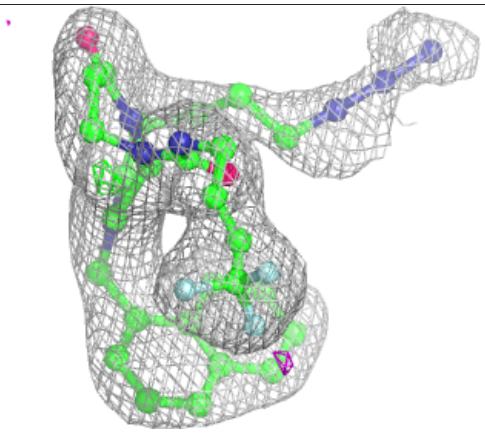


Electron density around A1EEE H 301:

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

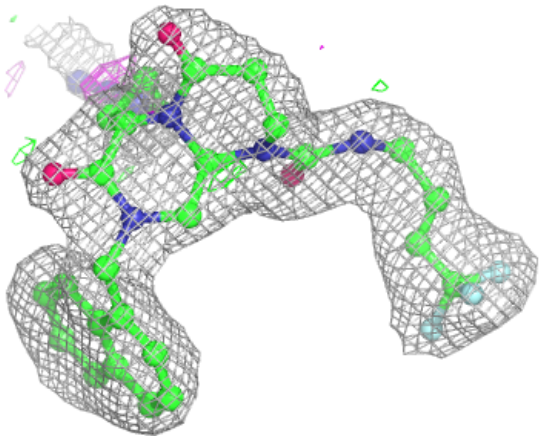


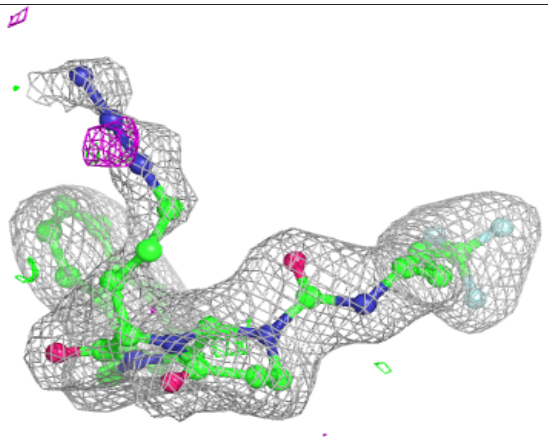


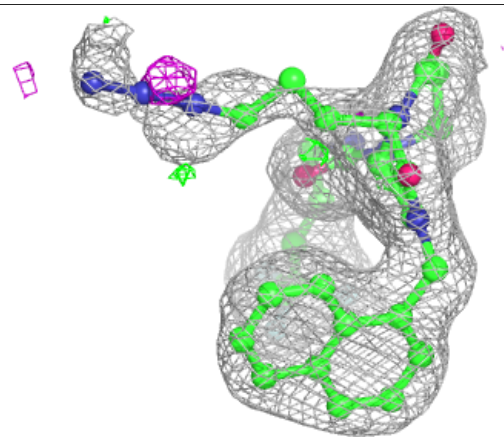


Electron density around A1EEE I 301:

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

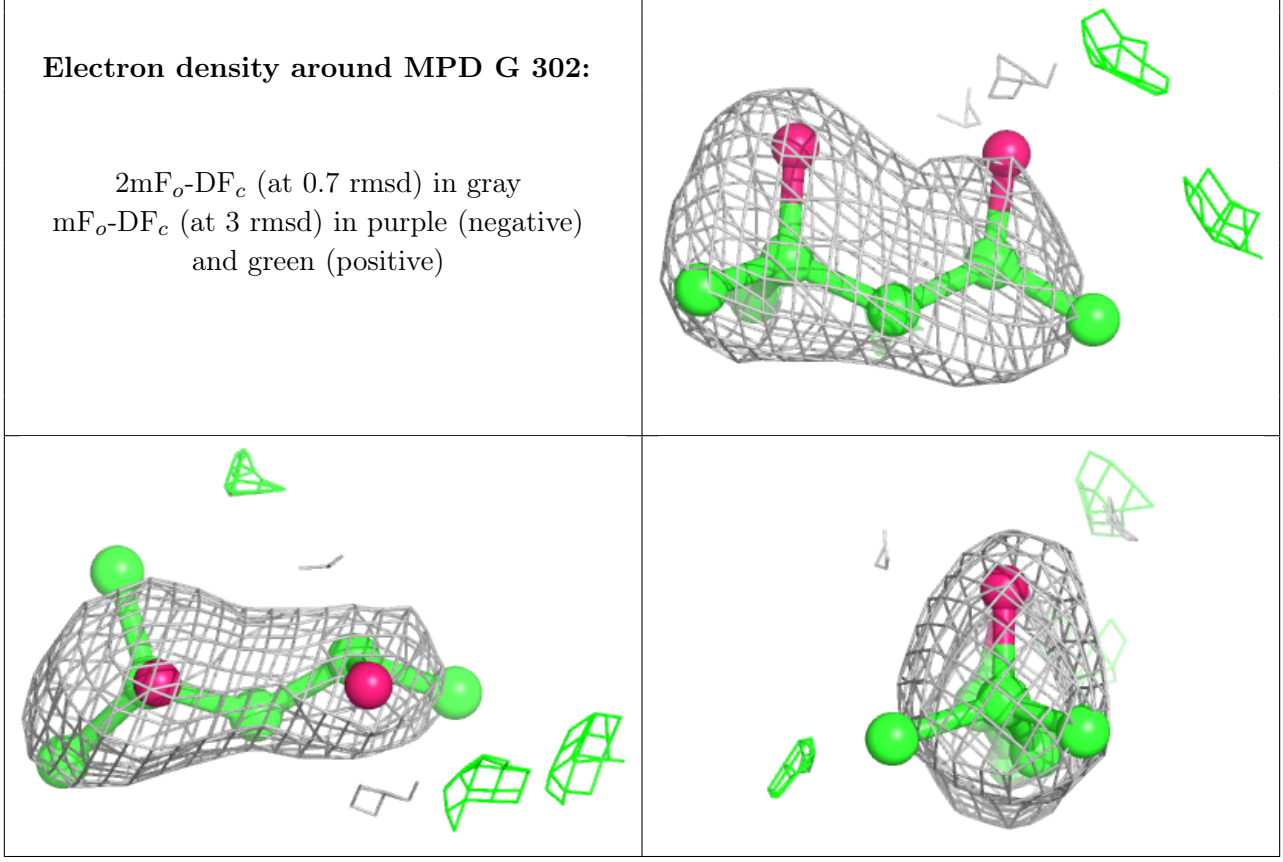






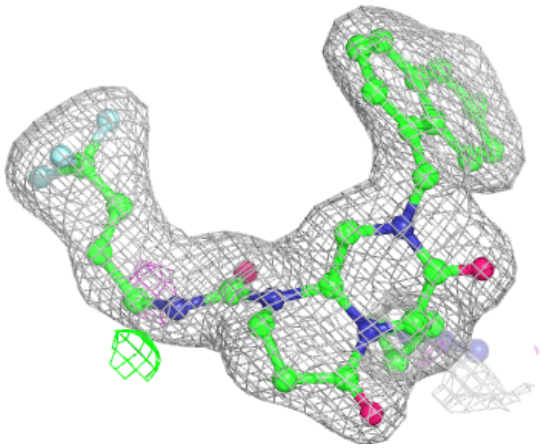
Electron density around MPD G 302:

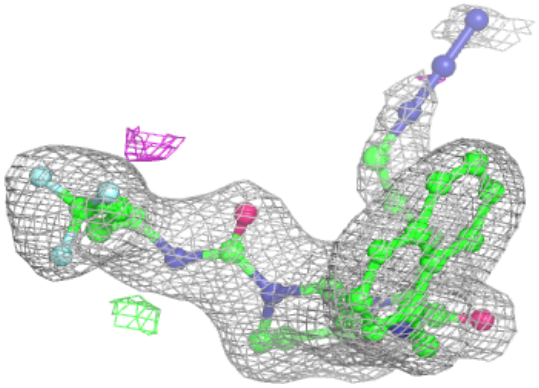
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

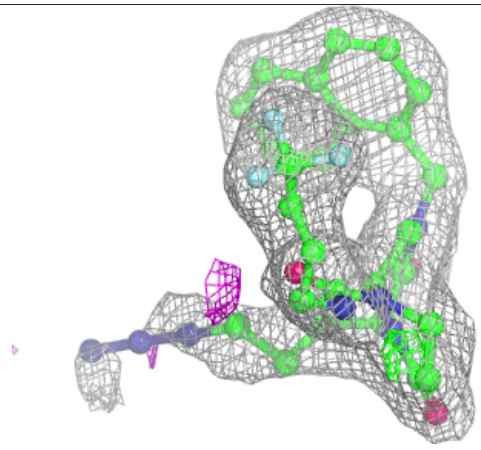


Electron density around A1EEE F 301:

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

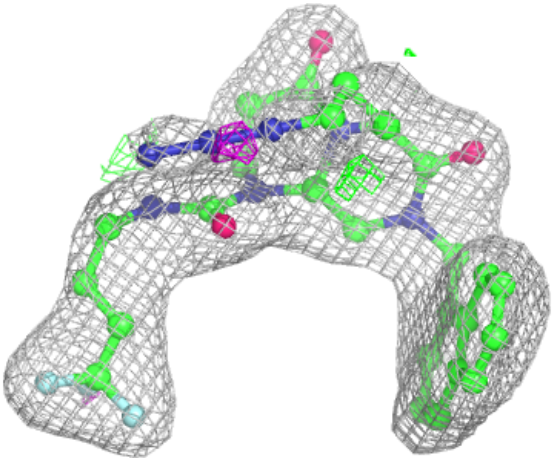


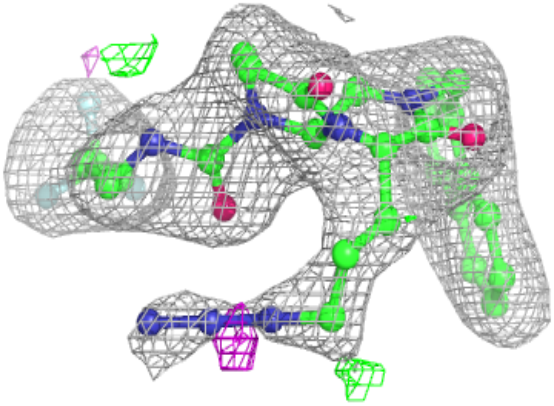


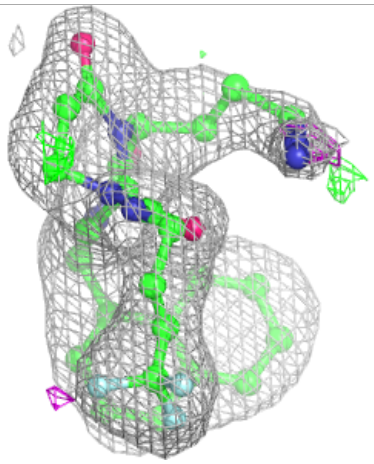


Electron density around A1EEE K 301:

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

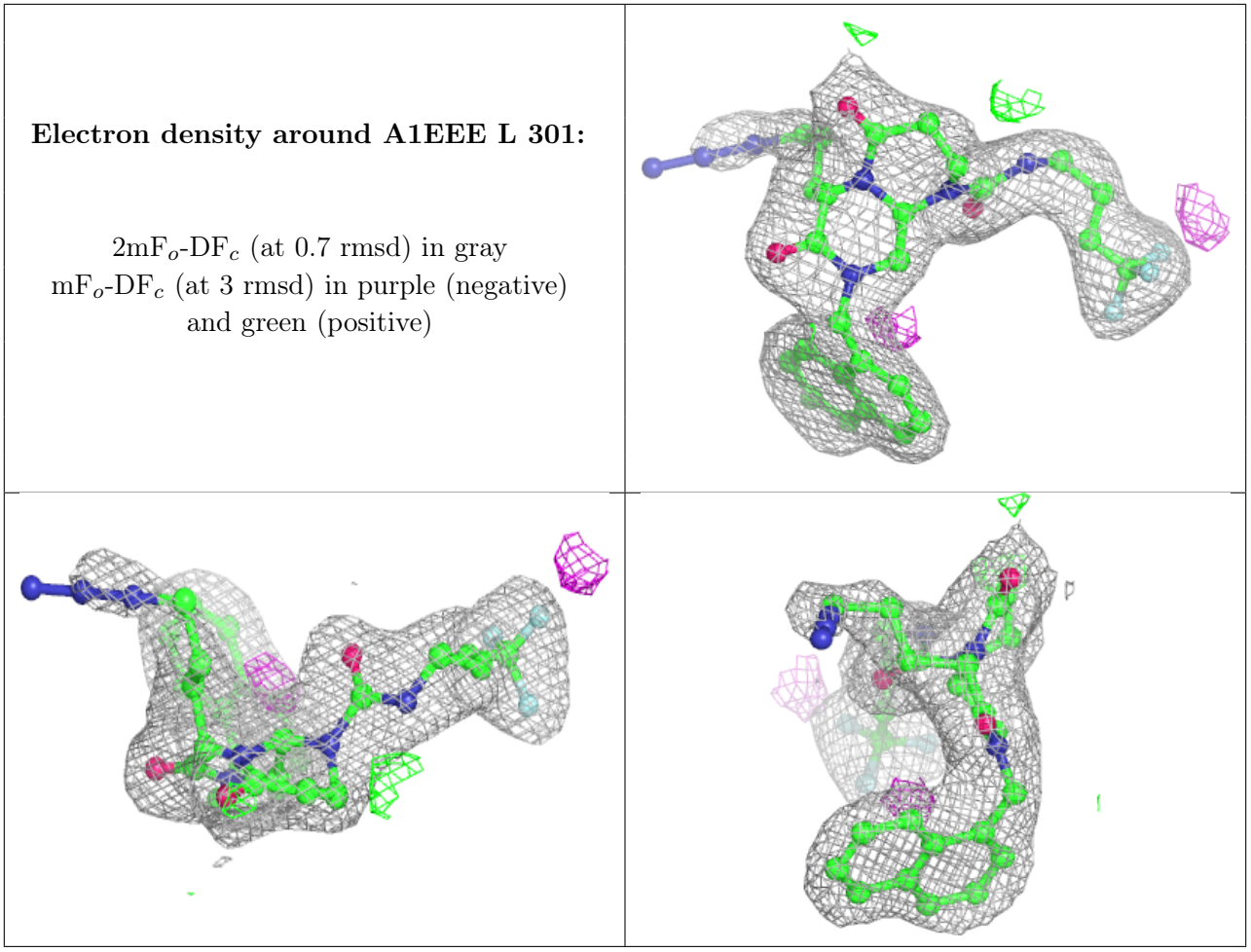






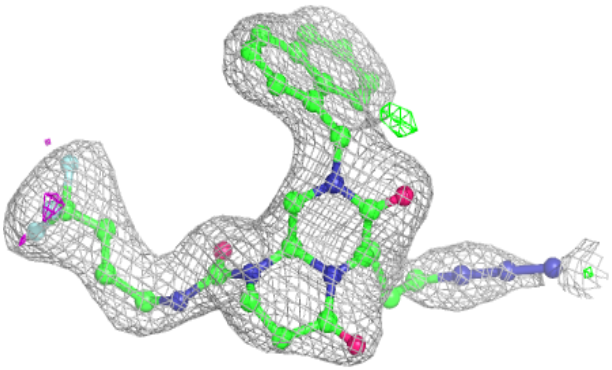
Electron density around A1EEE L 301:

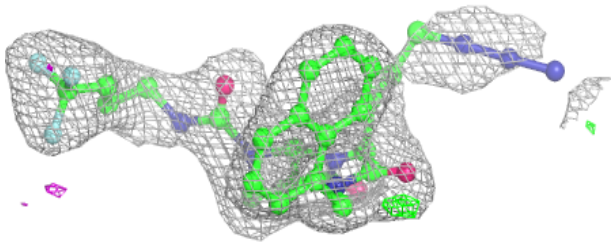
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

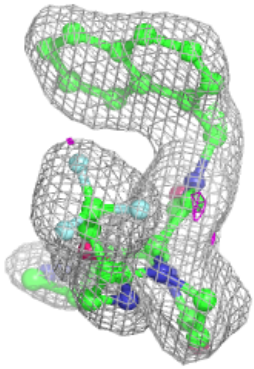


Electron density around A1EEE E 301:

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

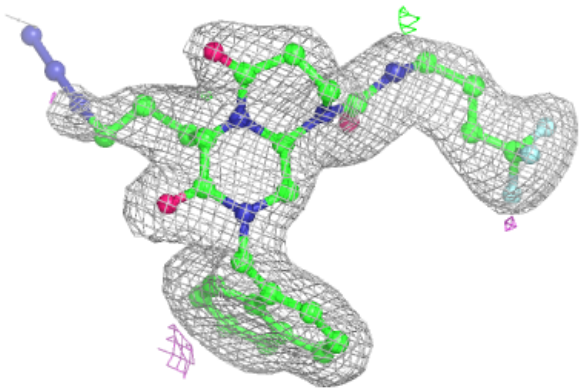


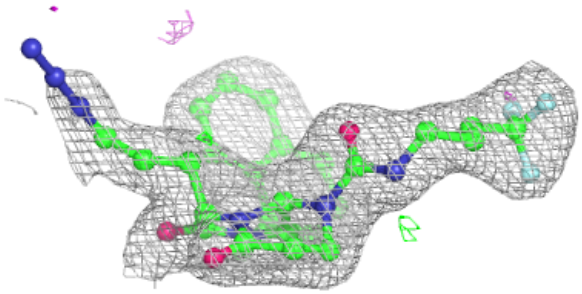


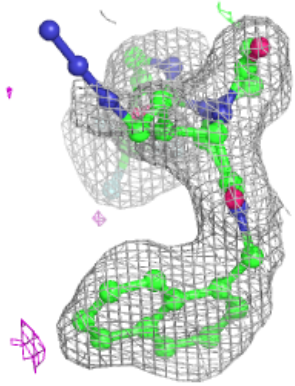


Electron density around A1EEE I 302:

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

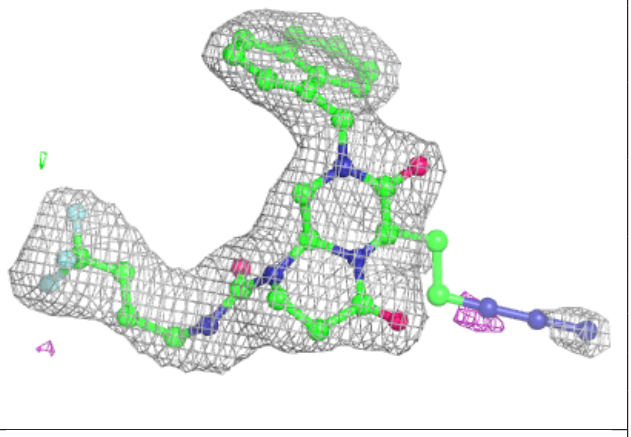


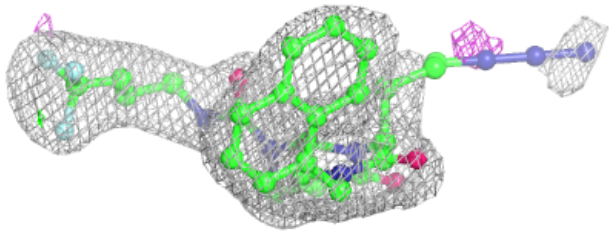


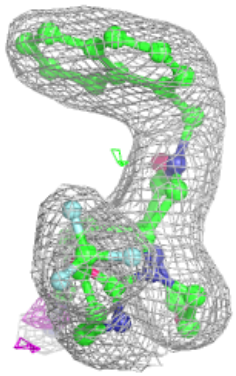


Electron density around A1EEE G 301:

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

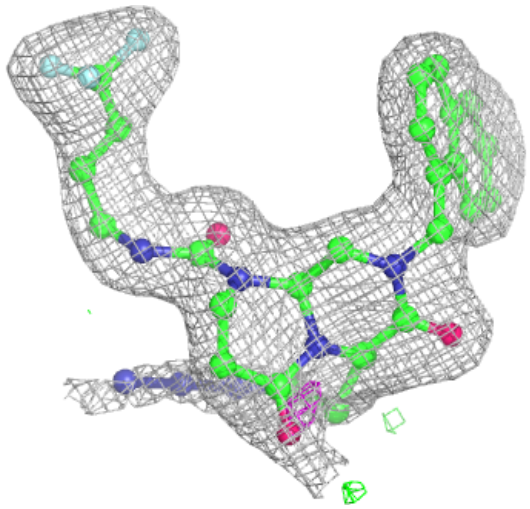


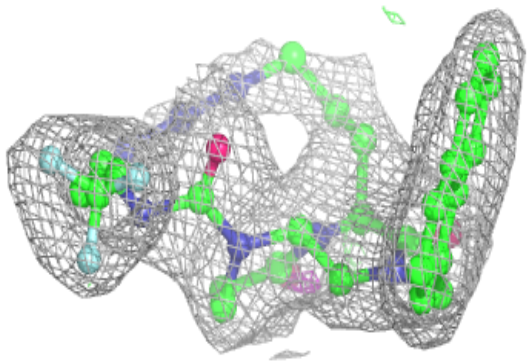


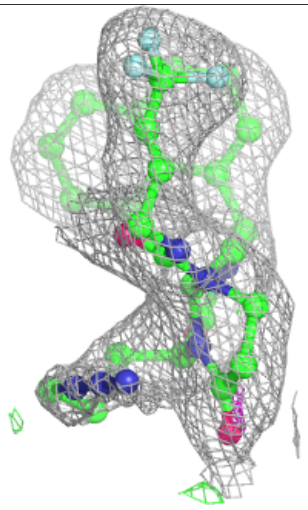


Electron density around A1EEE A 301:

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







6.5 Other polymers

There are no such residues in this entry.