Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 01:56 PM JST

PDB ID	:	7XBZ
Title	:	Crystal structure of Staphylococcus aureus ClpP in complex with R-ZG197
Authors	:	Wei, B.Y.; Gan, J.H.; Yang, C.-G.
Deposited on	:	2022-03-22
Resolution	:	2.15 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:

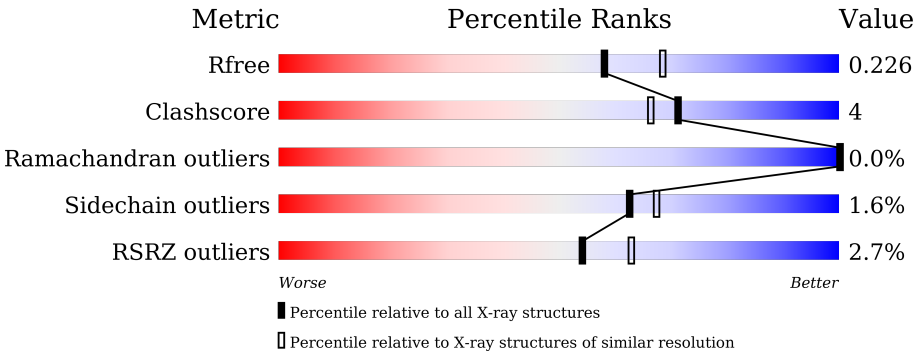
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	195	2% 89% 6% 5%
1	B	195	3% 92%
1	C	195	3% 89% 6% 5%
1	D	195	% 85% 7% 8%
1	E	195	3% 87% 5% 8%
1	F	195	3% 89% 7%

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Mol	Chain	Length	Quality of chain
1	G	195	2% 87% 6% • 7%
1	H	195	4% 89% 6% • 5%
1	I	195	3% 86% 8% • 6%
1	J	195	4% 86% 5% • 8%
1	K	195	% 89% • 8%
1	L	195	3% 87% 5% • 8%
1	M	195	3% 87% • 9%
1	N	195	2% 84% 8% • 8%

2 Entry composition (i)

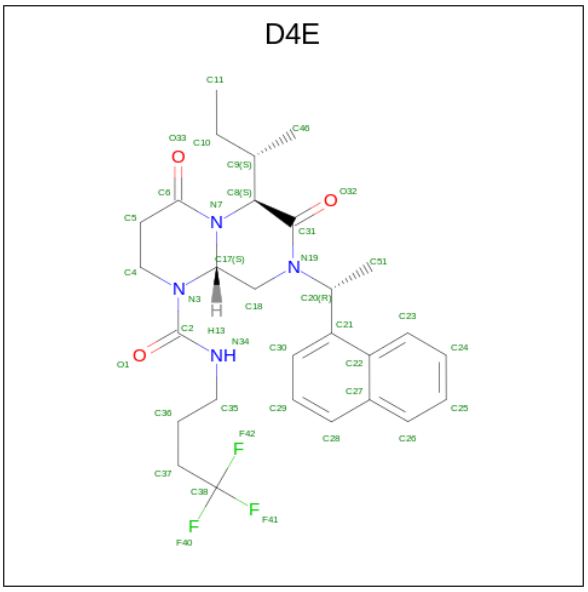
There are 5 unique types of molecules in this entry. The entry contains 20434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			1409	889	238	276	6			
1	B	187	Total	C	N	O	S	0	0	0
			1407	887	239	275	6			
1	C	185	Total	C	N	O	S	0	1	0
			1410	892	237	275	6			
1	D	179	Total	C	N	O	S	0	0	0
			1363	858	232	267	6			
1	E	179	Total	C	N	O	S	0	0	0
			1372	866	233	267	6			
1	F	181	Total	C	N	O	S	0	1	0
			1377	869	234	268	6			
1	G	182	Total	C	N	O	S	0	3	0
			1372	866	233	265	8			
1	H	185	Total	C	N	O	S	0	1	0
			1404	888	237	272	7			
1	I	184	Total	C	N	O	S	0	0	0
			1399	883	236	274	6			
1	J	179	Total	C	N	O	S	0	1	0
			1369	862	231	270	6			
1	K	180	Total	C	N	O	S	0	1	0
			1371	863	234	268	6			
1	L	180	Total	C	N	O	S	0	1	0
			1370	868	233	263	6			
1	M	177	Total	C	N	O	S	0	0	0
			1353	851	231	265	6			
1	N	179	Total	C	N	O	S	0	1	0
			1379	872	232	269	6			

- Molecule 2 is (6S,9aS)-6-[(2S)-butan-2-yl]-8-[(1R)-1-naphthalen-1-ylethyl]-4,7-bis(oxidanylidene)-N-[4,4,4-tris(fluoranyl)butyl]-3,6,9,9a-tetrahydro-2H-pyrazino[1,2-a]pyrimidine-1-carboxamide (three-letter code: D4E) (formula: $C_{28}H_{35}F_3N_4O_3$) (labeled as "Ligand of Interest" by depositor).

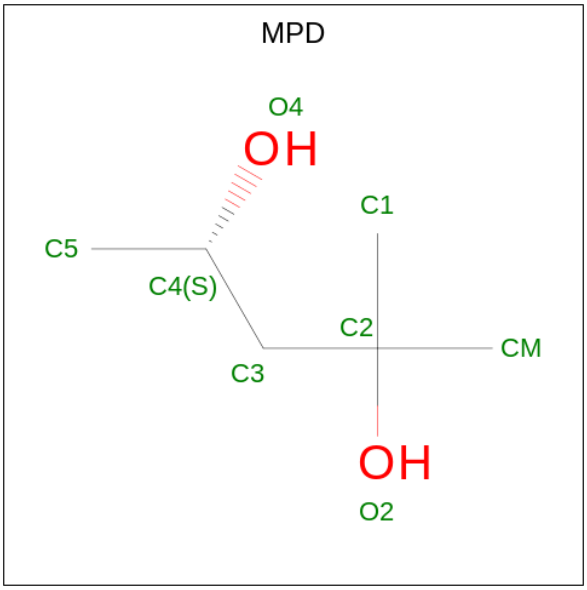


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	C	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	E	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	E	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	G	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	I	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	I	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	K	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	L	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	M	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	N	1	Total	C	F	N	O	0	0
			38	28	3	4	3		
2	N	1	Total	C	F	N	O	0	0
			38	28	3	4	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	H	1	Total C O 8 6 2	0	0
4	I	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0
4	K	1	Total C O 8 6 2	0	0
4	L	1	Total C O 8 6 2	0	0
4	M	1	Total C O 8 6 2	0	0
4	N	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	B	54	Total O 54 54	0	0
5	C	33	Total O 33 33	0	0
5	D	25	Total O 25 25	0	0
5	E	23	Total O 23 23	0	0

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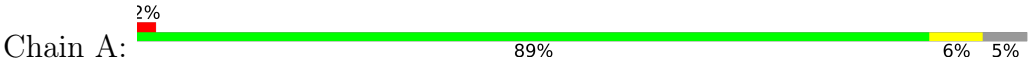
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	28	Total O 28 28	0	0
5	G	48	Total O 48 48	0	0
5	H	52	Total O 52 52	0	0
5	I	59	Total O 59 59	0	0
5	J	30	Total O 30 30	0	0
5	K	17	Total O 17 17	0	0
5	L	10	Total O 10 10	0	0
5	M	17	Total O 17 17	0	0
5	N	39	Total O 39 39	0	0

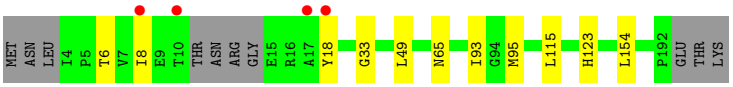
3 Residue-property plots (i)

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

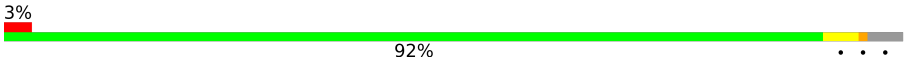
Chain A:





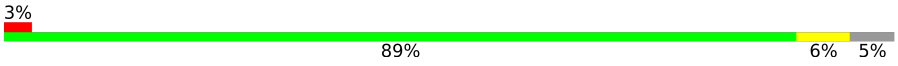
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

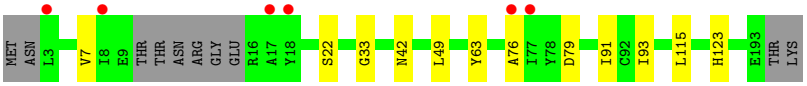
Chain B:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



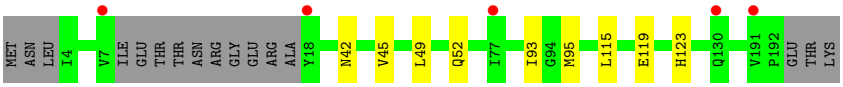


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:

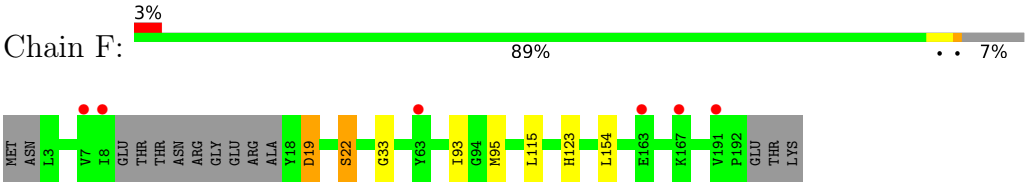
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



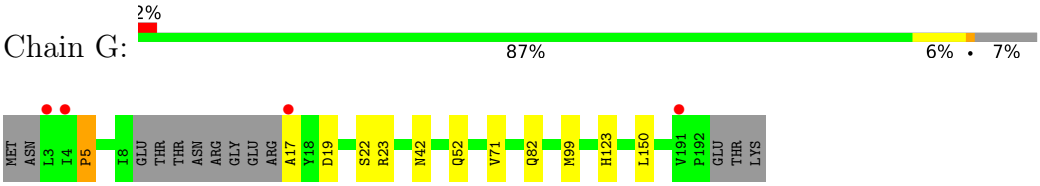
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



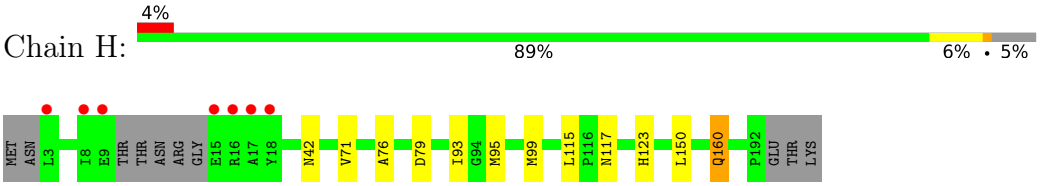
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



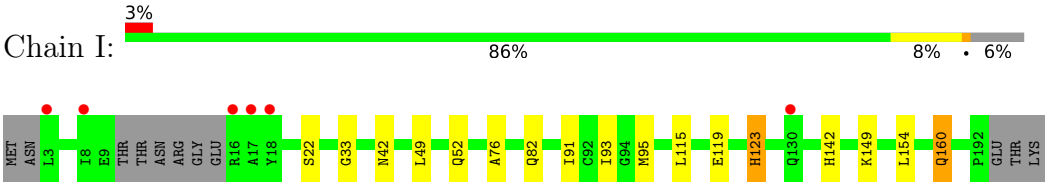
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



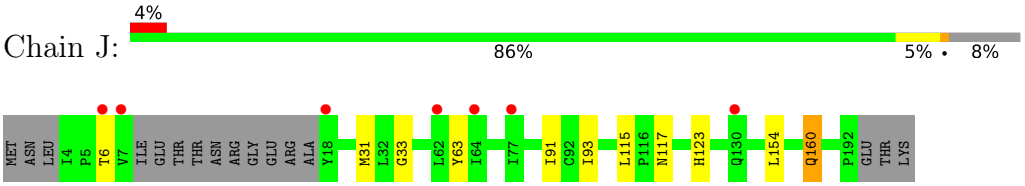
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



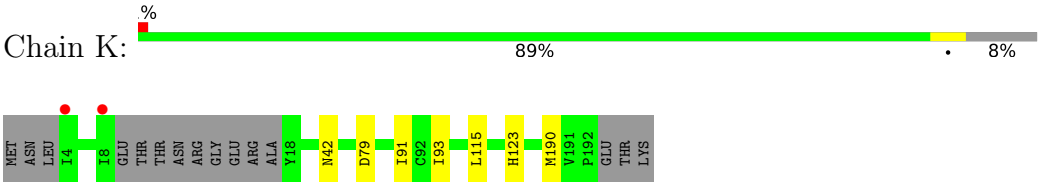
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



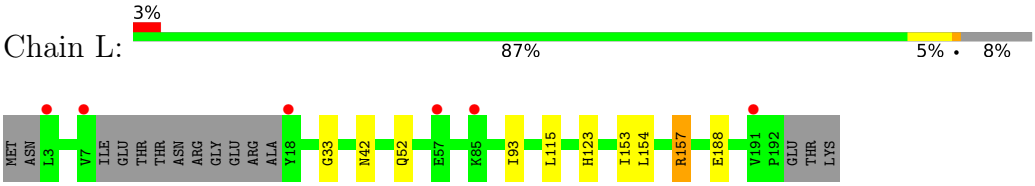
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



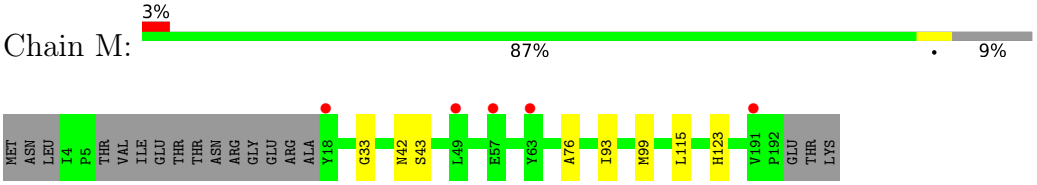
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



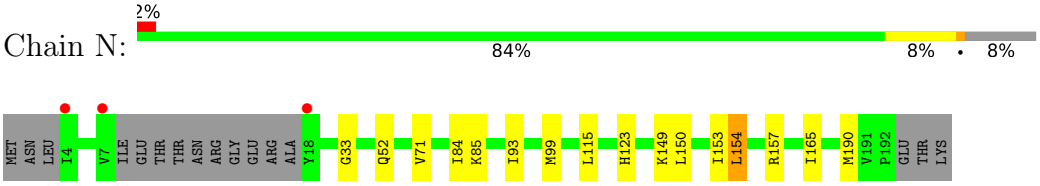
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

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	93.90Å 125.65Å 145.23Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.78 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.15) 94.1 (29.78-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.221 0.202 , 0.226	Depositor DCC
R_{free} test set	8841 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20434	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: D4E, MPD, MG

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	0.57	0/1430	0.70	0/1934
1	B	0.55	0/1425	0.71	0/1929
1	C	0.55	0/1431	0.67	0/1935
1	D	0.46	0/1381	0.67	0/1867
1	E	0.49	0/1390	0.66	0/1878
1	F	0.53	0/1397	0.69	0/1889
1	G	0.57	0/1397	0.71	0/1889
1	H	0.53	0/1425	0.67	0/1927
1	I	0.54	0/1417	0.71	0/1917
1	J	0.52	0/1390	0.66	0/1880
1	K	0.44	0/1391	0.65	0/1881
1	L	0.48	0/1391	0.65	0/1879
1	M	0.46	0/1370	0.67	0/1849
1	N	0.51	0/1400	0.65	0/1892
All	All	0.52	0/19635	0.68	0/26546

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1409	0	1405	8	0
1	B	1407	0	1390	12	0
1	C	1410	0	1412	26	0
1	D	1363	0	1354	13	0
1	E	1372	0	1381	10	0
1	F	1377	0	1380	6	0
1	G	1372	0	1357	11	0
1	H	1404	0	1401	16	0
1	I	1399	0	1391	19	0
1	J	1369	0	1361	11	0
1	K	1371	0	1371	7	0
1	L	1370	0	1383	8	0
1	M	1353	0	1355	7	0
1	N	1379	0	1389	16	0
2	A	38	0	0	1	0
2	C	38	0	0	1	0
2	E	76	0	0	6	0
2	G	38	0	0	0	0
2	I	76	0	0	2	0
2	K	38	0	0	3	0
2	L	38	0	0	0	0
2	M	38	0	0	2	0
2	N	76	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	8	0	14	0	0
4	B	16	0	28	1	0
4	C	8	0	14	0	0
4	D	8	0	14	1	0
4	E	8	0	14	0	0
4	F	8	0	14	0	0
4	G	8	0	14	2	0
4	H	8	0	14	4	0
4	I	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	8	0	14	0	0
4	K	8	0	14	0	0
4	L	8	0	14	0	0
4	M	8	0	14	1	0
4	N	8	0	14	4	0
5	A	56	0	0	1	0
5	B	54	0	0	2	0
5	C	33	0	0	0	0
5	D	25	0	0	1	0
5	E	23	0	0	2	0
5	F	28	0	0	1	0
5	G	48	0	0	0	0
5	H	52	0	0	2	0
5	I	59	0	0	3	0
5	J	30	0	0	0	0
5	K	17	0	0	0	0
5	L	10	0	0	1	0
5	M	17	0	0	1	0
5	N	39	0	0	0	0
All	All	20434	0	19540	138	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 4.

All (138) 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:A:8:ILE:HD12	1:G:17:ALA:N	1.75	1.01
1:I:95:MET:HG3	5:I:309:HOH:O	1.64	0.97
1:E:49:LEU:HD21	2:E:202:D4E:C25	1.98	0.94
1:C:63:TYR:CD2	1:C:93:ILE:HD12	2.05	0.92
1:C:63:TYR:HD2	1:C:93:ILE:HD12	1.34	0.91
1:D:91:ILE:HD11	1:D:115:LEU:CD1	2.00	0.91
1:E:49:LEU:HD11	2:E:202:D4E:C26	2.02	0.89
1:B:42:ASN:HB3	5:B:352:HOH:O	1.76	0.85
1:H:99[A]:MET:CE	4:H:202:MPD:H53	2.07	0.84
1:I:160:GLN:HE21	1:I:160:GLN:HA	1.44	0.83
1:H:160:GLN:HE21	1:H:160:GLN:HA	1.44	0.82
1:J:160:GLN:HE21	1:J:160:GLN:HA	1.44	0.81
1:K:91:ILE:HG12	2:K:201:D4E:C51	2.15	0.77
1:G:150:LEU:HD13	4:G:203:MPD:H53	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:LEU:HD13	4:N:204:MPD:H52	1.66	0.77
1:B:42:ASN:ND2	1:C:33:GLY:HA3	2.00	0.77
1:A:95:MET:HG3	5:A:353:HOH:O	1.84	0.76
1:H:42:ASN:OD1	1:I:33:GLY:HA3	1.90	0.72
1:H:99[A]:MET:HE2	4:H:202:MPD:H53	1.72	0.71
1:N:99:MET:CE	4:N:204:MPD:H53	2.21	0.71
1:D:95:MET:HG3	5:D:308:HOH:O	1.91	0.70
1:H:95:MET:HG3	5:H:317:HOH:O	1.91	0.69
1:H:42:ASN:HB3	5:H:344:HOH:O	1.94	0.68
1:D:91:ILE:HD11	1:D:115:LEU:HD11	1.75	0.67
1:C:42:ASN:ND2	1:D:33:GLY:HA3	2.11	0.65
1:H:150:LEU:HD13	4:H:202:MPD:H52	1.79	0.64
1:L:52:GLN:HE22	2:M:201:D4E:C11	2.11	0.64
1:F:95:MET:HG3	5:F:307:HOH:O	1.99	0.62
1:L:42:ASN:ND2	1:M:33:GLY:HA3	2.16	0.61
1:E:49:LEU:HD21	2:E:202:D4E:C24	2.30	0.61
1:E:95:MET:HG3	5:E:313:HOH:O	2.01	0.60
1:I:142:HIS:ND1	5:I:301:HOH:O	2.30	0.60
1:C:63:TYR:CE2	1:C:93:ILE:CD1	2.85	0.60
1:C:63:TYR:CD2	1:C:93:ILE:CD1	2.83	0.59
1:B:42:ASN:ND2	1:C:33:GLY:O	2.29	0.59
1:E:52:GLN:HE22	2:E:202:D4E:C11	2.15	0.59
1:F:93:ILE:HG12	1:F:115:LEU:HD22	1.84	0.59
1:M:93:ILE:HG12	1:M:115:LEU:HD22	1.84	0.59
1:D:93:ILE:HG12	1:D:115:LEU:HD22	1.83	0.59
1:D:91:ILE:HD11	1:D:115:LEU:HD12	1.84	0.58
1:N:99:MET:HE1	4:N:204:MPD:H53	1.86	0.57
1:F:19:ASP:C	1:F:19:ASP:OD2	2.43	0.57
1:C:63:TYR:CE2	1:C:91:ILE:HG21	2.40	0.56
1:E:42:ASN:ND2	1:F:33:GLY:HA3	2.21	0.56
1:G:71:VAL:HG22	1:G:99[A]:MET:HE3	1.88	0.55
1:M:42:ASN:ND2	1:N:33:GLY:HA3	2.21	0.55
1:N:52:GLN:HE21	1:N:85:LYS:H	1.56	0.54
1:G:99[A]:MET:HE2	4:G:203:MPD:O4	2.07	0.53
1:N:71:VAL:HG22	1:N:99:MET:CE	2.38	0.53
1:C:63:TYR:CD2	1:C:91:ILE:CG2	2.92	0.53
1:C:63:TYR:CE2	1:C:93:ILE:HD12	2.44	0.53
1:K:42:ASN:ND2	1:L:33:GLY:HA3	2.24	0.53
1:H:99[A]:MET:HE1	4:H:202:MPD:H53	1.89	0.52
1:F:22:SER:OG	1:G:5:PRO:HA	2.10	0.52
1:G:71:VAL:HG22	1:G:99[A]:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:GLN:NE2	2:M:201:D4E:C11	2.73	0.52
1:I:42:ASN:ND2	1:J:33:GLY:O	2.41	0.52
1:I:42:ASN:ND2	1:J:33:GLY:HA3	2.25	0.52
1:H:71:VAL:HG22	1:H:99[A]:MET:CE	2.39	0.51
1:B:42:ASN:HD21	1:C:33:GLY:C	2.12	0.51
1:N:99:MET:HE2	4:N:204:MPD:H53	1.91	0.50
1:J:160:GLN:HA	1:J:160:GLN:NE2	2.22	0.50
1:M:99:MET:CE	4:M:203:MPD:H53	2.41	0.50
1:I:49:LEU:HD13	2:I:202:D4E:C25	2.42	0.49
1:D:49:LEU:HD13	2:E:201:D4E:C25	2.42	0.49
1:C:22:SER:OG	1:D:6:THR:N	2.36	0.49
1:N:153:ILE:O	1:N:157:ARG:HG2	2.13	0.49
1:K:91:ILE:CD1	2:K:201:D4E:C51	2.91	0.49
1:N:52:GLN:HG3	1:N:84:ILE:HB	1.95	0.49
1:B:42:ASN:ND2	1:C:33:GLY:CA	2.72	0.48
1:K:91:ILE:CG1	2:K:201:D4E:C51	2.89	0.48
1:C:63:TYR:CD2	1:C:91:ILE:HG23	2.49	0.48
1:H:79:ASP:HB3	1:I:115:LEU:HD13	1.96	0.48
1:A:93:ILE:HG12	1:A:115:LEU:HD12	1.96	0.47
1:N:93:ILE:HG12	1:N:115:LEU:HD12	1.96	0.47
1:C:93:ILE:HG12	1:C:115:LEU:HD12	1.96	0.47
1:E:93:ILE:HG12	1:E:115:LEU:HD12	1.96	0.47
1:D:65:ASN:HD22	1:D:95:MET:H	1.62	0.47
1:I:22:SER:HB3	1:J:6:THR:O	2.14	0.47
1:B:93:ILE:HG12	1:B:115:LEU:HD12	1.96	0.47
1:C:63:TYR:HA	1:C:91:ILE:HG23	1.97	0.47
1:H:93:ILE:HG12	1:H:115:LEU:HD12	1.96	0.47
1:K:93:ILE:HG12	1:K:115:LEU:HD12	1.97	0.47
1:A:49:LEU:HD13	2:A:201:D4E:C25	2.46	0.46
1:L:93:ILE:HG12	1:L:115:LEU:HD12	1.96	0.46
1:C:63:TYR:CD2	1:C:91:ILE:HG21	2.50	0.46
1:D:150:LEU:HD13	4:D:201:MPD:H52	1.96	0.46
1:L:153:ILE:O	1:L:157:ARG:HG2	2.16	0.46
1:G:82:GLN:HE21	1:G:82:GLN:HA	1.81	0.46
1:A:33:GLY:HA3	1:G:42:ASN:ND2	2.31	0.46
1:C:63:TYR:HE2	1:C:93:ILE:CD1	2.28	0.46
1:J:93:ILE:HG12	1:J:115:LEU:HD12	1.97	0.46
1:N:71:VAL:HG22	1:N:99:MET:HE1	1.97	0.46
1:A:65:ASN:HD22	1:A:95:MET:H	1.63	0.45
1:I:82:GLN:HE21	1:I:82:GLN:HA	1.81	0.45
1:I:93:ILE:HG12	1:I:115:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PHE:CZ	1:C:7:VAL:HG11	2.51	0.45
1:B:76:ALA:HB1	1:C:93:ILE:HG22	1.98	0.45
1:C:79:ASP:HB3	1:D:115:LEU:HD23	1.99	0.45
1:E:119:GLU:HG2	5:E:313:HOH:O	2.15	0.45
1:H:71:VAL:HG22	1:H:99[A]:MET:HE1	1.97	0.45
1:M:99:MET:HA	1:M:99:MET:HE2	1.99	0.45
1:H:160:GLN:HA	1:H:160:GLN:NE2	2.23	0.45
1:I:22:SER:OG	1:J:6:THR:N	2.44	0.45
1:B:42:ASN:HD21	1:C:33:GLY:CA	2.29	0.44
1:I:123:HIS:O	4:I:204:MPD:H12	2.17	0.44
1:B:42:ASN:CB	5:B:352:HOH:O	2.51	0.44
1:D:4:ILE:HA	1:D:5:PRO:HD3	1.90	0.44
1:C:76:ALA:HB1	1:D:93:ILE:HG22	2.00	0.44
1:G:17:ALA:CB	1:G:23:ARG:HA	2.48	0.44
1:K:79:ASP:HB3	1:L:115:LEU:HD13	2.00	0.44
1:G:82:GLN:HA	1:G:82:GLN:NE2	2.33	0.43
1:I:82:GLN:HA	1:I:82:GLN:NE2	2.33	0.43
1:H:117:ASN:HD22	1:N:149:LYS:HD2	1.82	0.43
1:I:76:ALA:HB1	1:J:93:ILE:HG22	2.00	0.43
1:M:43:SER:HB2	5:M:305:HOH:O	2.18	0.43
1:N:154:LEU:HB3	1:N:165:ILE:HD13	2.00	0.43
1:I:91:ILE:HD13	2:I:201:D4E:C30	2.49	0.43
1:M:76:ALA:HB1	1:N:93:ILE:HG22	2.00	0.43
1:J:31:MET:HE1	1:J:63:TYR:CD2	2.54	0.43
1:C:63:TYR:HE2	1:C:93:ILE:HD11	1.84	0.42
1:E:52:GLN:NE2	2:E:202:D4E:C11	2.81	0.42
1:N:71:VAL:HG22	1:N:99:MET:HE3	2.01	0.42
1:H:71:VAL:HG22	1:H:99[A]:MET:HE3	2.01	0.41
1:C:49:LEU:HD13	2:C:201:D4E:C25	2.49	0.41
1:B:123:HIS:O	4:B:202:MPD:HM1	2.21	0.41
1:A:6:THR:O	1:G:22:SER:HB3	2.21	0.41
1:A:18:TYR:CZ	1:B:8:ILE:HD12	2.55	0.41
1:F:19:ASP:OD2	1:F:22:SER:OG	2.31	0.41
1:H:76:ALA:HB1	1:I:93:ILE:HG22	2.03	0.41
1:E:45:VAL:O	1:E:49:LEU:HG	2.20	0.40
1:I:119:GLU:HG3	5:I:313:HOH:O	2.21	0.40
1:L:188:GLU:CG	5:L:310:HOH:O	2.68	0.40
1:N:115:LEU:HD23	1:N:190:MET:HB2	2.04	0.40
1:C:63:TYR:HA	1:C:91:ILE:CG2	2.51	0.40
1:I:149:LYS:HD2	1:J:117:ASN:HD22	1.86	0.40
1:K:115:LEU:HD23	1:K:190:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:TYR:HA	1:J:91:ILE:HG23	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	182/195 (93%)	180 (99%)	2 (1%)	0	100	100
1	B	183/195 (94%)	180 (98%)	3 (2%)	0	100	100
1	C	182/195 (93%)	179 (98%)	3 (2%)	0	100	100
1	D	175/195 (90%)	172 (98%)	3 (2%)	0	100	100
1	E	175/195 (90%)	172 (98%)	3 (2%)	0	100	100
1	F	178/195 (91%)	175 (98%)	3 (2%)	0	100	100
1	G	181/195 (93%)	177 (98%)	3 (2%)	1 (1%)	25	18
1	H	182/195 (93%)	180 (99%)	2 (1%)	0	100	100
1	I	180/195 (92%)	177 (98%)	3 (2%)	0	100	100
1	J	176/195 (90%)	173 (98%)	3 (2%)	0	100	100
1	K	177/195 (91%)	174 (98%)	3 (2%)	0	100	100
1	L	177/195 (91%)	174 (98%)	3 (2%)	0	100	100
1	M	173/195 (89%)	170 (98%)	3 (2%)	0	100	100
1	N	176/195 (90%)	173 (98%)	3 (2%)	0	100	100
All	All	2497/2730 (92%)	2456 (98%)	40 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	5	PRO

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	149/163 (91%)	147 (99%)	2 (1%)	69	74
1	B	146/163 (90%)	144 (99%)	2 (1%)	67	72
1	C	149/163 (91%)	148 (99%)	1 (1%)	84	89
1	D	144/163 (88%)	141 (98%)	3 (2%)	53	57
1	E	147/163 (90%)	146 (99%)	1 (1%)	84	89
1	F	146/163 (90%)	142 (97%)	4 (3%)	44	46
1	G	141/163 (86%)	138 (98%)	3 (2%)	53	57
1	H	147/163 (90%)	145 (99%)	2 (1%)	67	72
1	I	147/163 (90%)	143 (97%)	4 (3%)	44	46
1	J	146/163 (90%)	143 (98%)	3 (2%)	53	57
1	K	146/163 (90%)	145 (99%)	1 (1%)	84	89
1	L	145/163 (89%)	142 (98%)	3 (2%)	53	57
1	M	144/163 (88%)	143 (99%)	1 (1%)	84	89
1	N	148/163 (91%)	146 (99%)	2 (1%)	67	72
All	All	2045/2282 (90%)	2013 (98%)	32 (2%)	62	67

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	154	LEU
1	B	123	HIS
1	B	154	LEU
1	C	123	HIS
1	D	52	GLN
1	D	123	HIS
1	D	154	LEU
1	E	123	HIS
1	F	19	ASP
1	F	22	SER

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Mol	Chain	Res	Type
1	F	123	HIS
1	F	154	LEU
1	G	19	ASP
1	G	52	GLN
1	G	123	HIS
1	H	123	HIS
1	H	160	GLN
1	I	52	GLN
1	I	123	HIS
1	I	154	LEU
1	I	160	GLN
1	J	123	HIS
1	J	154	LEU
1	J	160	GLN
1	K	123	HIS
1	L	123	HIS
1	L	154	LEU
1	L	157	ARG
1	M	123	HIS
1	N	123	HIS
1	N	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	42	ASN
1	D	65	ASN
1	E	52	GLN
1	F	117	ASN
1	F	151	ASN
1	G	82	GLN
1	H	42	ASN
1	H	117	ASN
1	H	160	GLN
1	I	82	GLN
1	I	160	GLN
1	J	89	GLN
1	J	117	ASN
1	J	160	GLN
1	K	117	ASN
1	L	52	GLN

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Mol	Chain	Res	Type
1	L	83	HIS
1	L	89	GLN
1	M	89	GLN
1	N	52	GLN
1	N	89	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 12 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MPD	J	202	-	7,7,7	0.33	0	9,10,10	0.64	0
4	MPD	D	201	-	7,7,7	0.29	0	9,10,10	0.57	0
4	MPD	A	204	-	7,7,7	0.25	0	9,10,10	0.73	0
4	MPD	H	202	-	7,7,7	0.32	0	9,10,10	1.01	0
2	D4E	K	201	-	39,41,41	1.72	8 (20%)	51,60,60	1.79	13 (25%)
4	MPD	C	203	-	7,7,7	0.33	0	9,10,10	0.51	0
4	MPD	M	203	-	7,7,7	0.23	0	9,10,10	0.85	0
2	D4E	N	202	-	39,41,41	0.83	1 (2%)	51,60,60	1.67	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MPD	N	204	-	7,7,7	0.39	0	9,10,10	0.52	0
4	MPD	K	203	-	7,7,7	0.28	0	9,10,10	0.76	0
4	MPD	G	203	-	7,7,7	0.31	0	9,10,10	0.53	0
2	D4E	I	201	-	39,41,41	0.95	2 (5%)	51,60,60	1.91	10 (19%)
2	D4E	E	201	-	39,41,41	0.82	1 (2%)	51,60,60	1.28	5 (9%)
4	MPD	B	202	-	7,7,7	0.30	0	9,10,10	0.63	0
2	D4E	I	202	-	39,41,41	1.05	3 (7%)	51,60,60	1.37	6 (11%)
2	D4E	N	201	-	39,41,41	1.02	2 (5%)	51,60,60	1.36	8 (15%)
4	MPD	E	203	-	7,7,7	0.33	0	9,10,10	0.80	0
2	D4E	G	201	-	39,41,41	0.92	2 (5%)	51,60,60	1.34	7 (13%)
2	D4E	E	202	-	39,41,41	0.83	1 (2%)	51,60,60	1.52	9 (17%)
2	D4E	C	201	-	39,41,41	0.84	0	51,60,60	1.27	3 (5%)
2	D4E	M	201	-	39,41,41	0.78	1 (2%)	51,60,60	1.73	9 (17%)
2	D4E	A	201	-	39,41,41	0.92	1 (2%)	51,60,60	1.97	12 (23%)
4	MPD	I	204	-	7,7,7	0.36	0	9,10,10	0.60	0
4	MPD	B	203	-	7,7,7	0.34	0	9,10,10	0.35	0
4	MPD	L	202	-	7,7,7	0.29	0	9,10,10	0.75	0
4	MPD	F	202	-	7,7,7	0.38	0	9,10,10	0.38	0
2	D4E	L	201	-	39,41,41	0.79	1 (2%)	51,60,60	1.42	8 (15%)

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
4	MPD	J	202	-	-	0/5/5/5	-
4	MPD	D	201	-	-	0/5/5/5	-
4	MPD	A	204	-	-	0/5/5/5	-
4	MPD	H	202	-	-	0/5/5/5	-
2	D4E	K	201	-	-	11/26/59/59	0/4/4/4
4	MPD	C	203	-	-	0/5/5/5	-
4	MPD	M	203	-	-	0/5/5/5	-
2	D4E	N	202	-	-	5/26/59/59	0/4/4/4
4	MPD	N	204	-	-	0/5/5/5	-
4	MPD	K	203	-	-	0/5/5/5	-
4	MPD	G	203	-	-	2/5/5/5	-
2	D4E	I	201	-	-	2/26/59/59	0/4/4/4
2	D4E	E	201	-	-	9/26/59/59	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	B	202	-	-	0/5/5/5	-
2	D4E	I	202	-	-	3/26/59/59	0/4/4/4
2	D4E	N	201	-	-	6/26/59/59	0/4/4/4
4	MPD	E	203	-	-	0/5/5/5	-
2	D4E	G	201	-	-	2/26/59/59	0/4/4/4
2	D4E	E	202	-	-	6/26/59/59	0/4/4/4
2	D4E	C	201	-	-	5/26/59/59	0/4/4/4
2	D4E	M	201	-	-	7/26/59/59	0/4/4/4
2	D4E	A	201	-	-	10/26/59/59	0/4/4/4
4	MPD	I	204	-	-	0/5/5/5	-
4	MPD	B	203	-	-	0/5/5/5	-
4	MPD	L	202	-	-	0/5/5/5	-
4	MPD	F	202	-	-	0/5/5/5	-
2	D4E	L	201	-	-	5/26/59/59	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	D4E	C21-C20	-5.30	1.46	1.52
2	K	201	D4E	C22-C27	-4.17	1.35	1.43
2	K	201	D4E	C21-C22	-3.56	1.37	1.43
2	I	202	D4E	C6-N7	3.26	1.38	1.35
2	N	201	D4E	C18-N19	2.83	1.50	1.46
2	G	201	D4E	C18-N19	2.59	1.50	1.46
2	K	201	D4E	C20-N19	-2.57	1.44	1.48
2	K	201	D4E	C23-C22	-2.55	1.37	1.42
2	I	202	D4E	C18-N19	2.51	1.50	1.46
2	I	201	D4E	C30-C21	2.42	1.41	1.37
2	K	201	D4E	C17-N3	-2.30	1.44	1.46
2	N	201	D4E	C6-N7	2.29	1.37	1.35
2	E	202	D4E	C18-N19	2.26	1.49	1.46
2	L	201	D4E	C30-C21	2.23	1.41	1.37
2	A	201	D4E	C30-C21	2.20	1.41	1.37
2	N	202	D4E	C30-C21	2.18	1.41	1.37
2	K	201	D4E	C4-N3	-2.07	1.43	1.47
2	G	201	D4E	C25-C26	2.07	1.41	1.36
2	I	201	D4E	C24-C23	2.04	1.41	1.36
2	E	201	D4E	C17-N3	2.04	1.49	1.46
2	I	202	D4E	C30-C21	2.02	1.41	1.37
2	K	201	D4E	C8-C31	-2.02	1.48	1.52
2	M	201	D4E	C30-C21	2.01	1.41	1.37

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	201	D4E	C51-C20-N19	-8.41	101.62	110.38
2	A	201	D4E	C9-C8-N7	-6.46	100.89	111.76
2	N	202	D4E	C51-C20-N19	-6.39	103.73	110.38
2	M	201	D4E	C51-C20-N19	-6.03	104.10	110.38
2	E	202	D4E	C51-C20-N19	-5.54	104.61	110.38
2	K	201	D4E	C31-C8-N7	-4.90	100.41	112.33
2	K	201	D4E	C51-C20-N19	-4.67	105.51	110.38
2	A	201	D4E	C9-C8-C31	4.59	120.31	110.81
2	I	202	D4E	C21-C20-N19	4.46	116.33	110.29
2	A	201	D4E	C51-C20-N19	-4.36	105.84	110.38
2	C	201	D4E	C21-C20-N19	4.26	116.06	110.29
2	M	201	D4E	C21-C20-N19	4.14	115.90	110.29
2	A	201	D4E	C18-C17-N3	4.04	119.50	112.59
2	M	201	D4E	C35-N34-C2	4.00	124.56	120.84
2	A	201	D4E	C46-C9-C8	3.80	118.99	110.46
2	N	201	D4E	C35-N34-C2	3.77	124.35	120.84
2	E	201	D4E	C51-C20-N19	-3.63	106.59	110.38
2	I	201	D4E	C18-N19-C20	-3.61	111.96	117.09
2	K	201	D4E	C21-C20-N19	3.59	115.16	110.29
2	L	201	D4E	C51-C20-N19	-3.50	106.73	110.38
2	G	201	D4E	C37-C36-C35	-3.49	106.41	112.46
2	K	201	D4E	C5-C4-N3	-3.33	100.63	111.61
2	I	201	D4E	C51-C20-C21	3.30	121.01	114.21
2	M	201	D4E	C9-C8-N7	3.29	117.29	111.76
2	K	201	D4E	C9-C8-C31	-3.28	104.01	110.81
2	E	201	D4E	C21-C20-N19	3.21	114.63	110.29
2	I	201	D4E	C18-N19-C31	3.21	129.76	122.88
2	A	201	D4E	C37-C36-C35	-3.11	107.06	112.46
2	N	202	D4E	C18-N19-C31	3.09	129.51	122.88
2	L	201	D4E	C18-N19-C20	-3.07	112.73	117.09
2	N	202	D4E	C35-N34-C2	3.07	123.70	120.84
2	L	201	D4E	C35-N34-C2	3.07	123.69	120.84
2	C	201	D4E	C18-C17-N3	3.04	117.79	112.59
2	A	201	D4E	F41-C38-C37	-2.99	101.76	112.82
2	K	201	D4E	C18-N19-C20	2.94	121.28	117.09
2	N	202	D4E	C18-N19-C20	-2.94	112.91	117.09
2	E	202	D4E	C35-N34-C2	2.91	123.55	120.84
2	K	201	D4E	C35-N34-C2	2.86	123.50	120.84
2	A	201	D4E	C35-N34-C2	2.82	123.46	120.84
2	G	201	D4E	C51-C20-N19	-2.81	107.45	110.38
2	I	201	D4E	C21-C20-N19	2.80	114.08	110.29
2	M	201	D4E	C18-N19-C31	2.79	128.87	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	201	D4E	C37-C36-C35	-2.77	107.65	112.46
2	I	202	D4E	C35-N34-C2	2.73	123.38	120.84
2	N	202	D4E	C51-C20-C21	2.72	119.82	114.21
2	N	202	D4E	O33-C6-N7	2.66	125.66	122.28
2	N	202	D4E	C46-C9-C8	2.65	116.42	110.46
2	A	201	D4E	C5-C4-N3	-2.64	102.92	111.61
2	N	202	D4E	C21-C20-N19	2.61	113.83	110.29
2	E	202	D4E	C21-C20-N19	2.59	113.79	110.29
2	E	202	D4E	C51-C20-C21	2.58	119.52	114.21
2	N	201	D4E	C5-C4-N3	-2.57	103.15	111.61
2	N	202	D4E	C5-C6-N7	-2.57	114.35	117.97
2	I	202	D4E	C5-C4-N3	-2.55	103.20	111.61
2	E	202	D4E	C18-N19-C31	2.52	128.29	122.88
2	E	202	D4E	C18-C17-N3	2.45	116.78	112.59
2	K	201	D4E	C8-C31-N19	-2.43	112.01	117.56
2	I	202	D4E	C18-C17-N3	2.42	116.73	112.59
2	K	201	D4E	C18-C17-N3	-2.42	108.46	112.59
2	M	201	D4E	C18-N19-C20	-2.41	113.68	117.09
2	E	202	D4E	C26-C27-C28	-2.39	117.60	123.19
2	K	201	D4E	C51-C20-C21	-2.39	109.30	114.21
2	M	201	D4E	C26-C27-C28	-2.38	117.63	123.19
2	A	201	D4E	C26-C27-C28	-2.37	117.65	123.19
2	C	201	D4E	C26-C27-C28	-2.34	117.72	123.19
2	E	201	D4E	C35-N34-C2	2.34	123.01	120.84
2	L	201	D4E	C26-C27-C28	-2.33	117.75	123.19
2	I	201	D4E	C4-N3-C2	2.32	130.51	122.00
2	N	201	D4E	O1-C2-N34	-2.30	117.37	123.53
2	I	202	D4E	C26-C27-C28	-2.29	117.84	123.19
2	I	201	D4E	C5-C4-N3	-2.29	104.08	111.61
2	G	201	D4E	C21-C20-N19	2.28	113.37	110.29
2	G	201	D4E	C18-C17-N3	2.27	116.48	112.59
2	I	201	D4E	C26-C27-C28	-2.27	117.89	123.19
2	L	201	D4E	C9-C8-C31	2.25	115.47	110.81
2	L	201	D4E	C51-C20-C21	2.24	118.82	114.21
2	I	201	D4E	C36-C37-C38	-2.21	108.92	113.84
2	N	201	D4E	O33-C6-C5	-2.20	116.23	121.32
2	K	201	D4E	C37-C36-C35	-2.19	108.65	112.46
2	G	201	D4E	C5-C4-N3	-2.16	104.49	111.61
2	A	201	D4E	C36-C35-N34	-2.15	106.07	112.21
2	M	201	D4E	C51-C20-C21	2.14	118.61	114.21
2	I	202	D4E	O33-C6-C5	-2.14	116.38	121.32
2	G	201	D4E	C26-C27-C28	-2.13	118.20	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	201	D4E	F41-C38-F40	2.13	114.26	106.43
2	I	201	D4E	C28-C29-C30	-2.13	117.60	120.99
2	E	202	D4E	C18-N19-C20	-2.11	114.09	117.09
2	N	201	D4E	C18-C17-N3	2.11	116.20	112.59
2	N	202	D4E	C31-C8-N7	-2.09	107.25	112.33
2	L	201	D4E	C10-C9-C8	2.09	115.37	111.48
2	E	201	D4E	C18-N19-C31	2.08	127.35	122.88
2	N	202	D4E	C26-C27-C28	-2.08	118.33	123.19
2	E	201	D4E	C26-C27-C28	-2.08	118.34	123.19
2	G	201	D4E	O32-C31-C8	-2.07	115.66	119.95
2	L	201	D4E	O33-C6-C5	-2.04	116.60	121.32
2	E	202	D4E	C5-C6-N7	-2.04	115.09	117.97
2	A	201	D4E	C18-N19-C20	-2.04	114.20	117.09
2	K	201	D4E	C10-C9-C8	2.02	115.26	111.48
2	N	201	D4E	C26-C27-C28	-2.02	118.47	123.19
2	M	201	D4E	C18-C17-N3	-2.01	109.15	112.59
2	K	201	D4E	C30-C21-C22	2.01	121.12	118.72

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	D4E	N7-C8-C9-C10
2	A	201	D4E	N7-C8-C9-C46
2	A	201	D4E	C31-C8-C9-C46
2	E	201	D4E	N7-C8-C9-C10
2	E	201	D4E	C31-C8-C9-C10
2	E	201	D4E	C31-C8-C9-C46
2	E	202	D4E	C36-C37-C38-F42
2	K	201	D4E	C51-C20-N19-C18
2	K	201	D4E	C21-C20-N19-C18
2	K	201	D4E	C51-C20-N19-C31
2	K	201	D4E	C21-C20-N19-C31
2	K	201	D4E	C51-C20-C21-C22
2	M	201	D4E	C36-C37-C38-F42
4	G	203	MPD	C2-C3-C4-O4
4	G	203	MPD	C2-C3-C4-C5
2	L	201	D4E	N34-C35-C36-C37
2	I	201	D4E	C11-C10-C9-C46
2	A	201	D4E	C11-C10-C9-C8
2	C	201	D4E	C11-C10-C9-C8
2	G	201	D4E	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	I	202	D4E	C11-C10-C9-C8
2	K	201	D4E	C11-C10-C9-C8
2	E	202	D4E	C11-C10-C9-C46
2	C	201	D4E	N34-C35-C36-C37
2	E	202	D4E	N34-C35-C36-C37
2	M	201	D4E	N34-C35-C36-C37
2	K	201	D4E	C36-C35-N34-C2
2	L	201	D4E	C36-C35-N34-C2
2	I	201	D4E	C11-C10-C9-C8
2	C	201	D4E	C36-C35-N34-C2
2	M	201	D4E	C36-C35-N34-C2
2	K	201	D4E	C51-C20-C21-C30
2	E	202	D4E	C11-C10-C9-C8
2	K	201	D4E	N19-C20-C21-C30
2	K	201	D4E	N19-C20-C21-C22
2	A	201	D4E	C36-C37-C38-F42
2	E	202	D4E	C36-C37-C38-F41
2	L	201	D4E	C36-C37-C38-F42
2	L	201	D4E	C36-C37-C38-F40
2	L	201	D4E	C36-C37-C38-F41
2	M	201	D4E	C36-C37-C38-F40
2	N	201	D4E	C11-C10-C9-C8
2	N	201	D4E	C36-C37-C38-F41
2	E	201	D4E	N7-C8-C9-C46
2	I	202	D4E	C11-C10-C9-C46
2	C	201	D4E	C11-C10-C9-C46
2	G	201	D4E	C11-C10-C9-C46
2	N	201	D4E	N34-C35-C36-C37
2	E	201	D4E	N34-C35-C36-C37
2	E	202	D4E	C36-C37-C38-F40
2	M	201	D4E	C36-C37-C38-F41
2	N	201	D4E	C36-C37-C38-F42
2	N	201	D4E	C36-C37-C38-F40
2	C	201	D4E	C35-C36-C37-C38
2	I	202	D4E	C35-C36-C37-C38
2	M	201	D4E	C35-C36-C37-C38
2	E	201	D4E	C11-C10-C9-C46
2	A	201	D4E	C11-C10-C9-C46
2	N	201	D4E	C11-C10-C9-C46
2	A	201	D4E	C36-C37-C38-F41
2	A	201	D4E	C31-C8-C9-C10
2	K	201	D4E	C11-C10-C9-C46

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Mol	Chain	Res	Type	Atoms
2	E	201	D4E	N3-C2-N34-C35
2	M	201	D4E	C11-C10-C9-C8
2	A	201	D4E	C36-C37-C38-F40
2	E	201	D4E	C36-C37-C38-F40
2	N	202	D4E	C36-C37-C38-F40
2	N	202	D4E	C36-C37-C38-F41
2	A	201	D4E	N34-C35-C36-C37
2	N	202	D4E	N34-C35-C36-C37
2	N	202	D4E	C31-C8-C9-C46
2	E	201	D4E	C36-C37-C38-F41
2	N	202	D4E	C36-C37-C38-F42

There are no ring outliers.

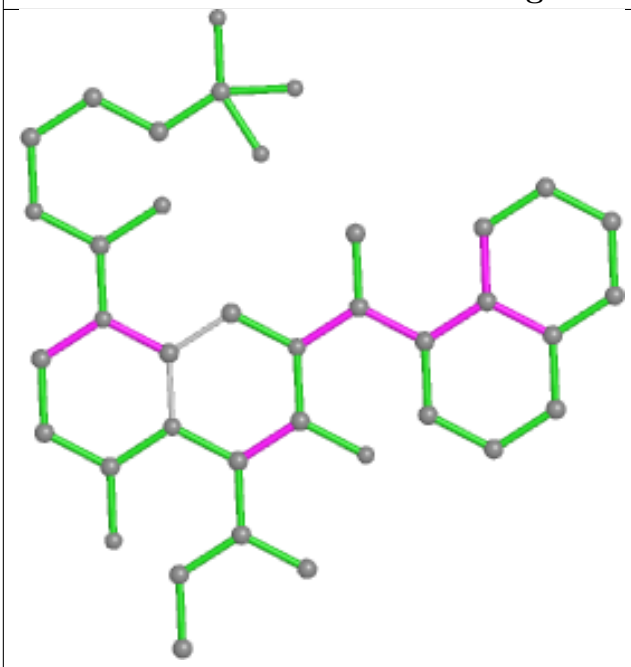
15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	MPD	1	0
4	H	202	MPD	4	0
2	K	201	D4E	3	0
4	M	203	MPD	1	0
4	N	204	MPD	4	0
4	G	203	MPD	2	0
2	I	201	D4E	1	0
2	E	201	D4E	1	0
4	B	202	MPD	1	0
2	I	202	D4E	1	0
2	E	202	D4E	5	0
2	C	201	D4E	1	0
2	M	201	D4E	2	0
2	A	201	D4E	1	0
4	I	204	MPD	1	0

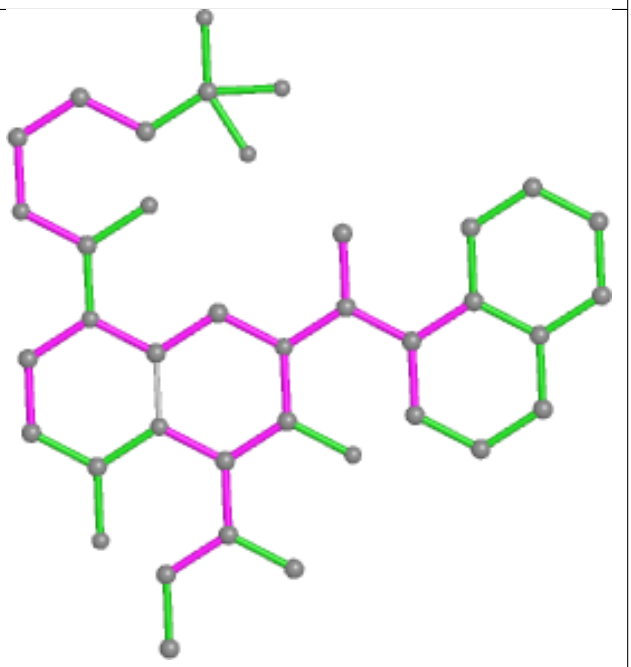
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

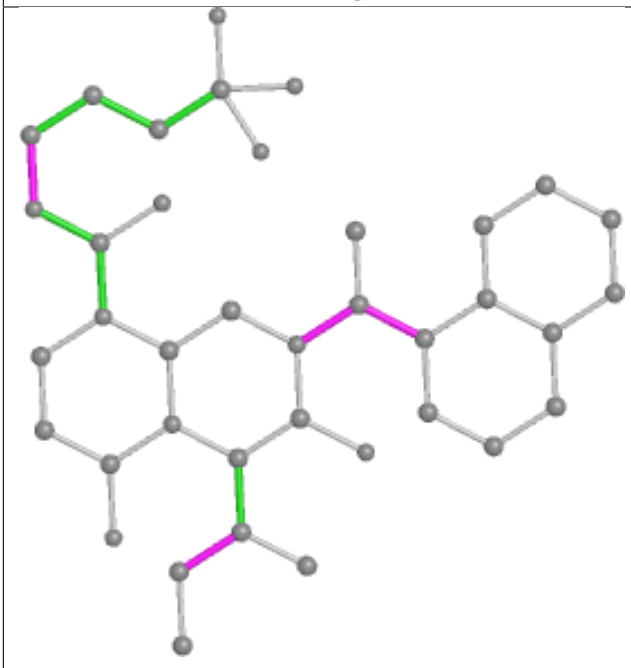
Ligand D4E K 201



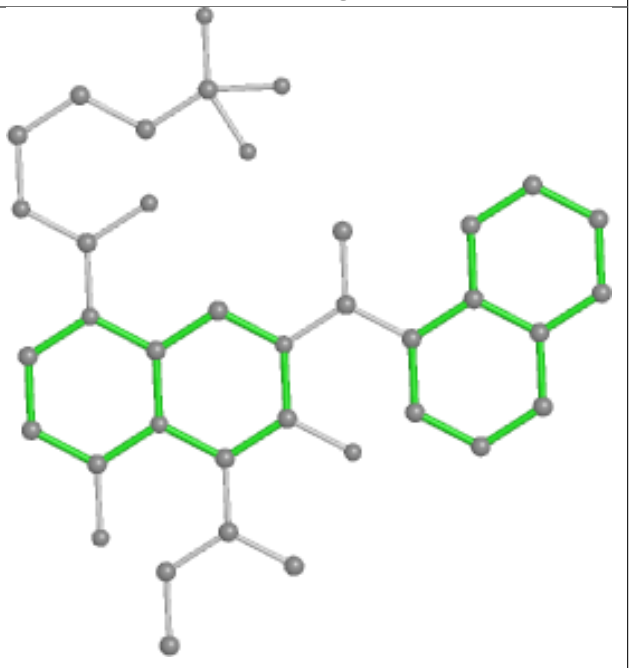
Bond lengths



Bond angles

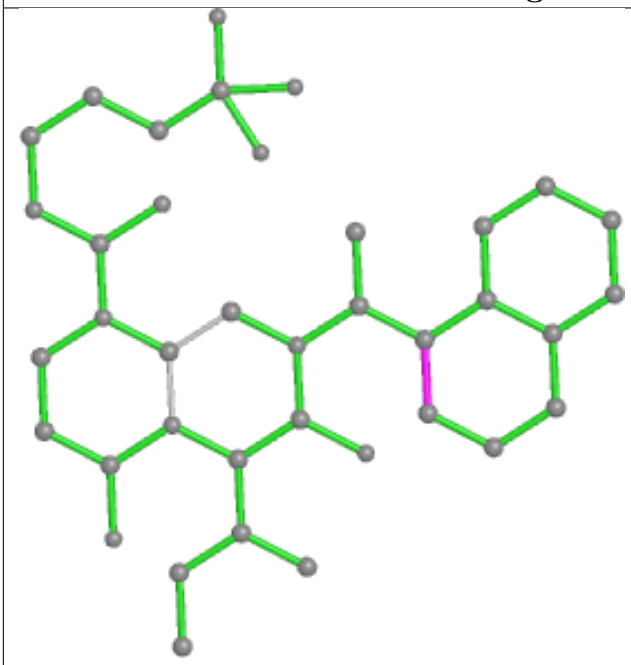


Torsions

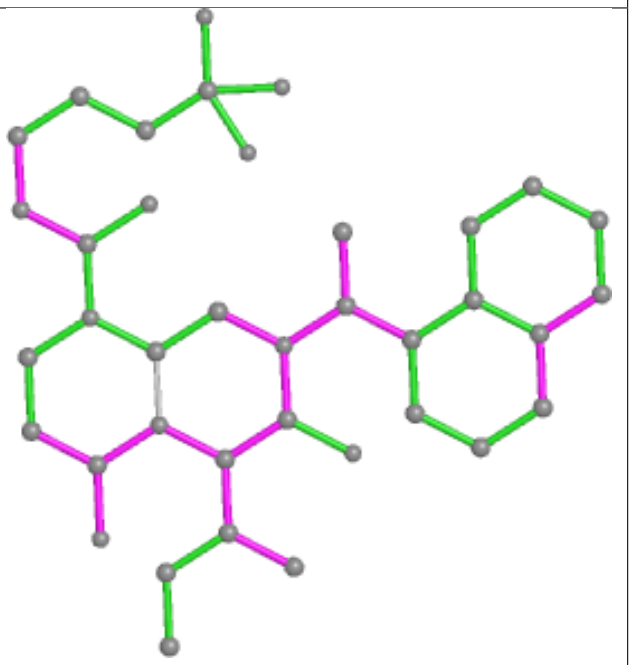


Rings

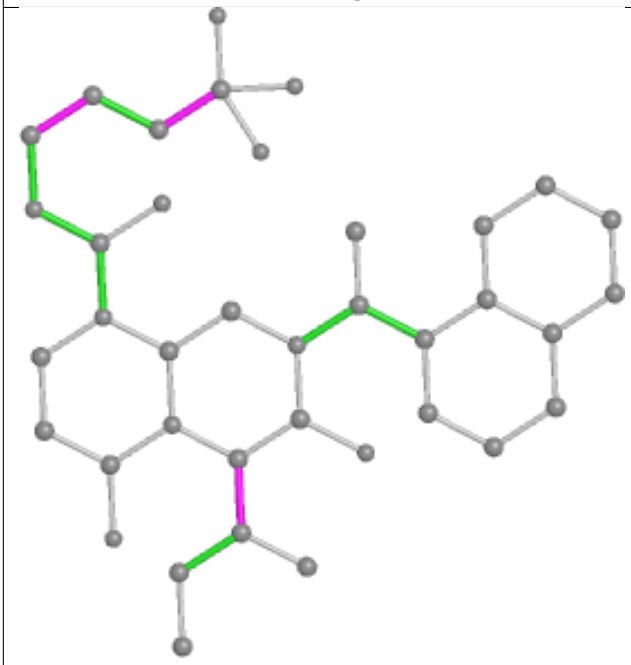
Ligand D4E N 202



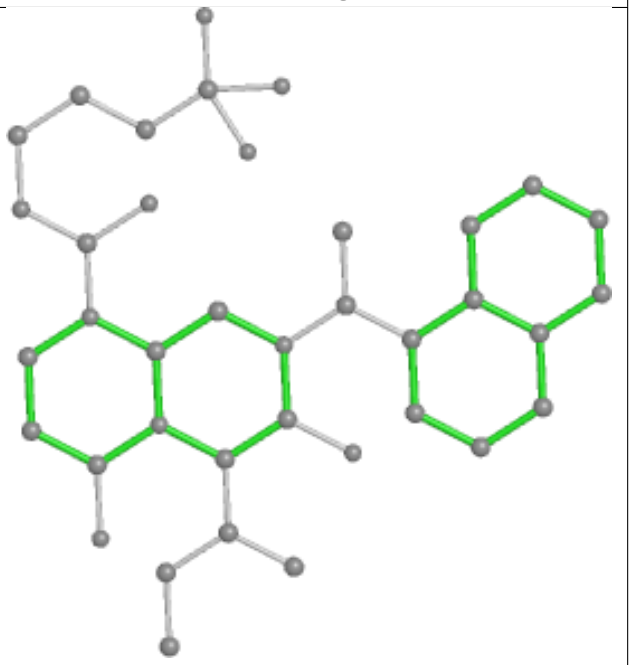
Bond lengths



Bond angles

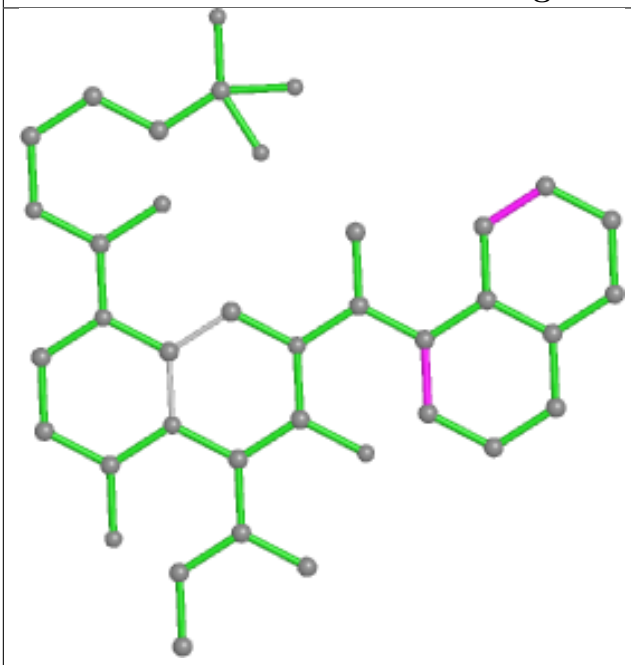


Torsions

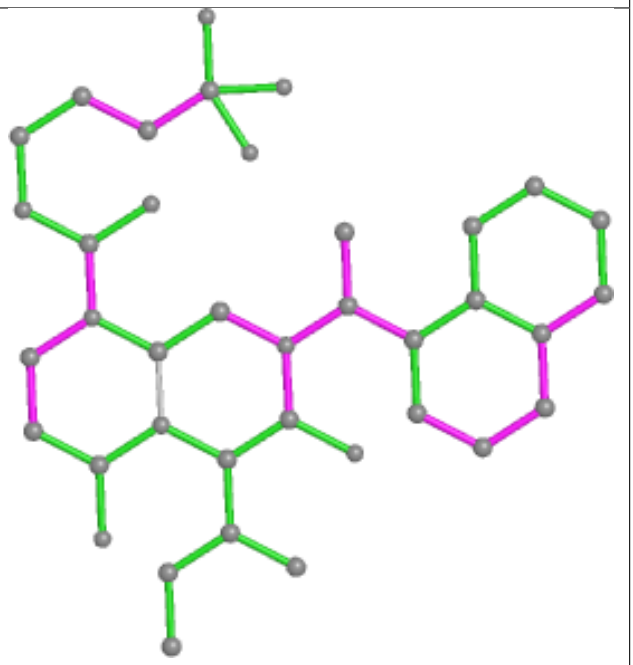


Rings

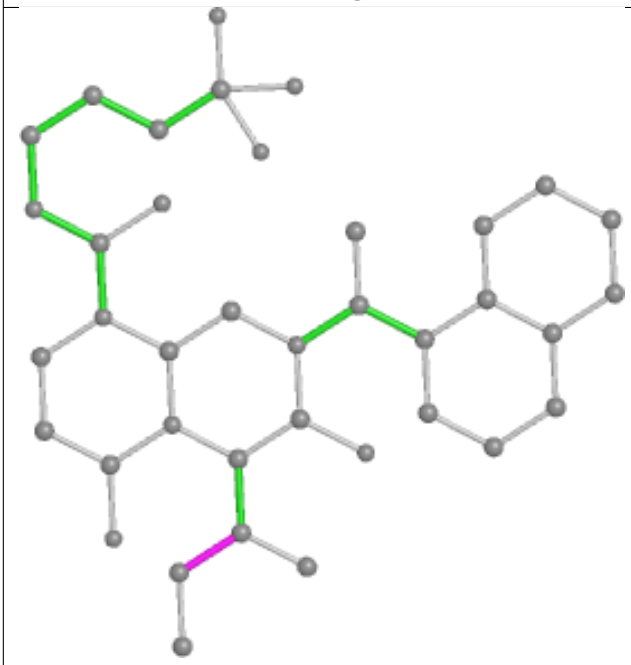
Ligand D4E I 201



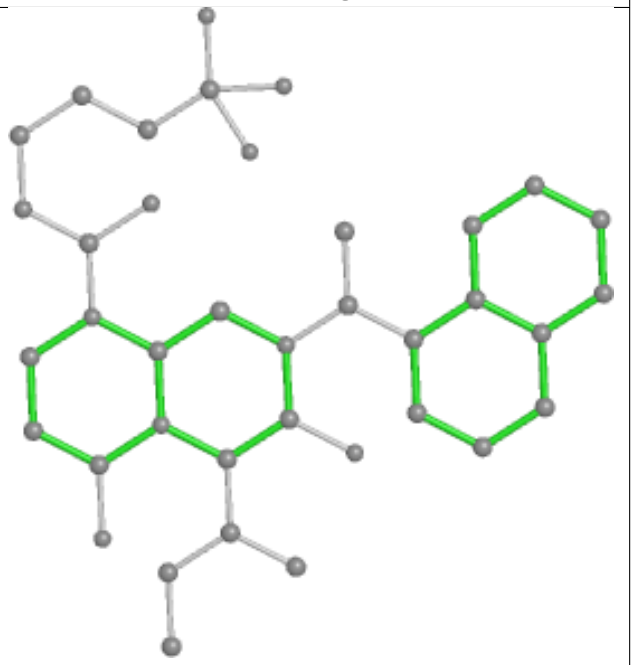
Bond lengths



Bond angles

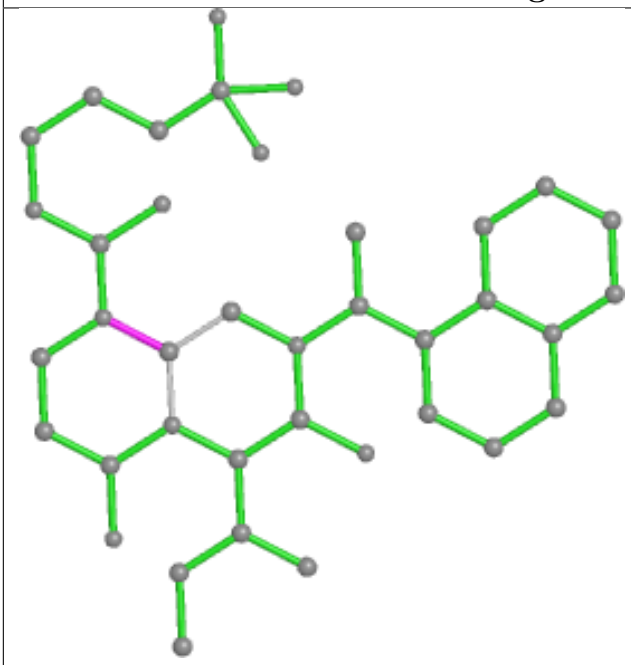


Torsions

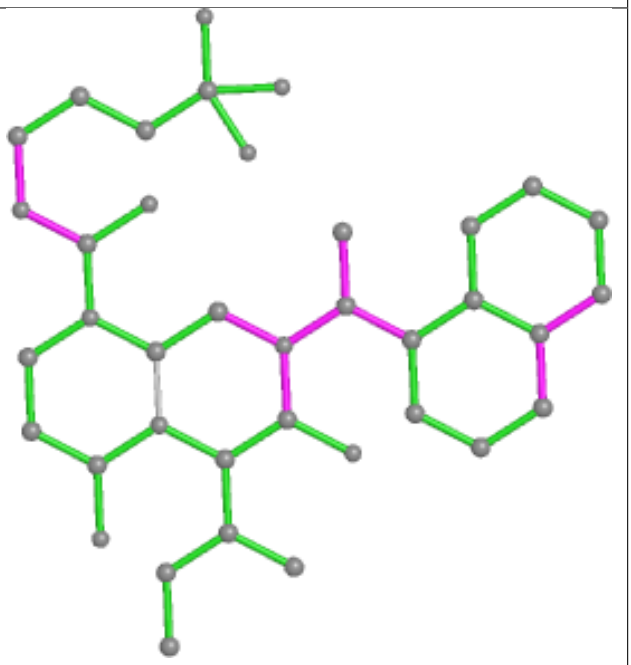


Rings

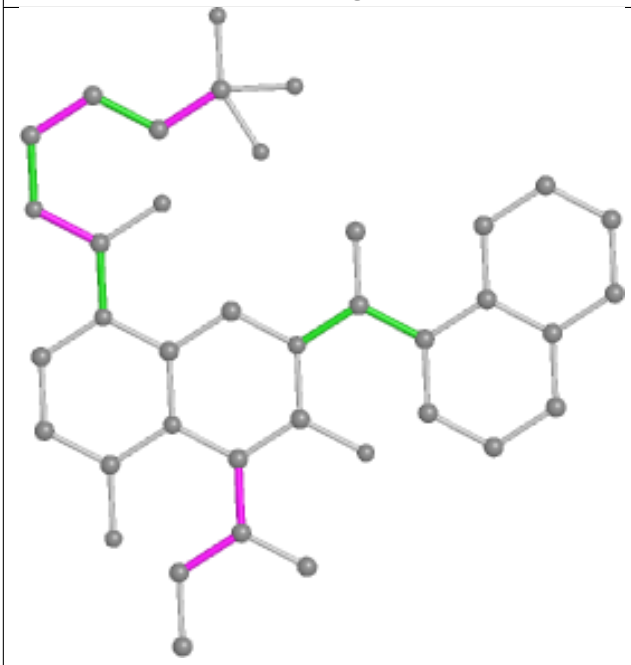
Ligand D4E E 201



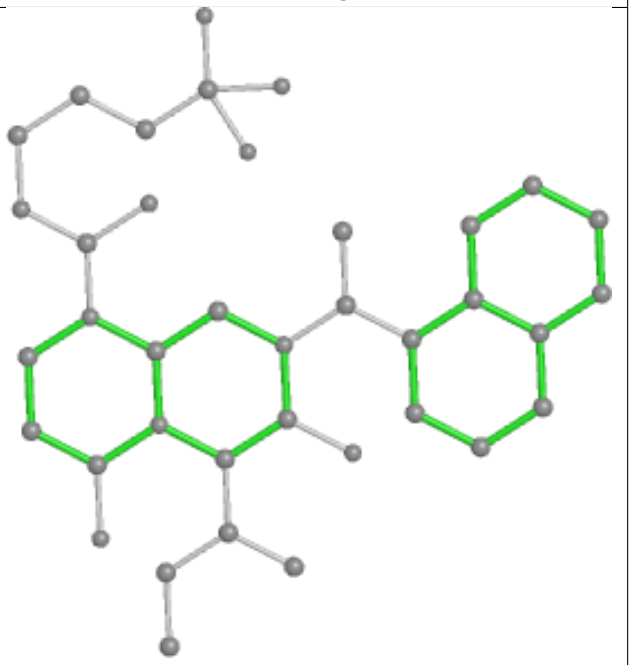
Bond lengths



Bond angles

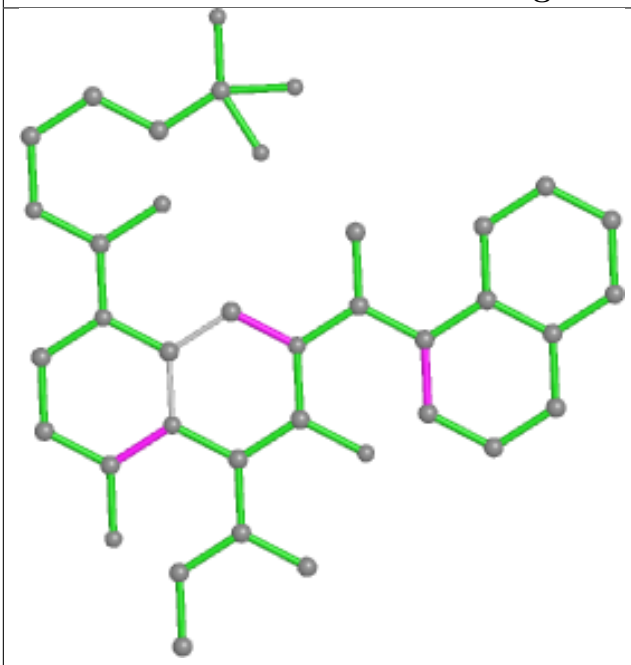


Torsions

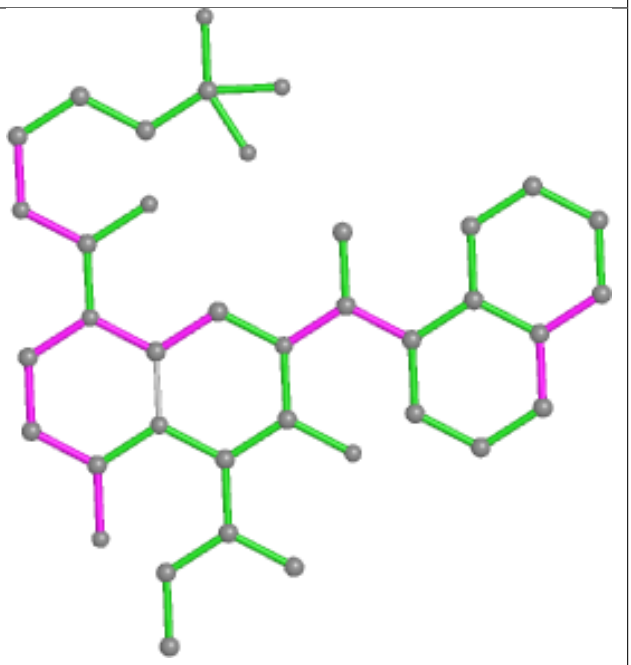


Rings

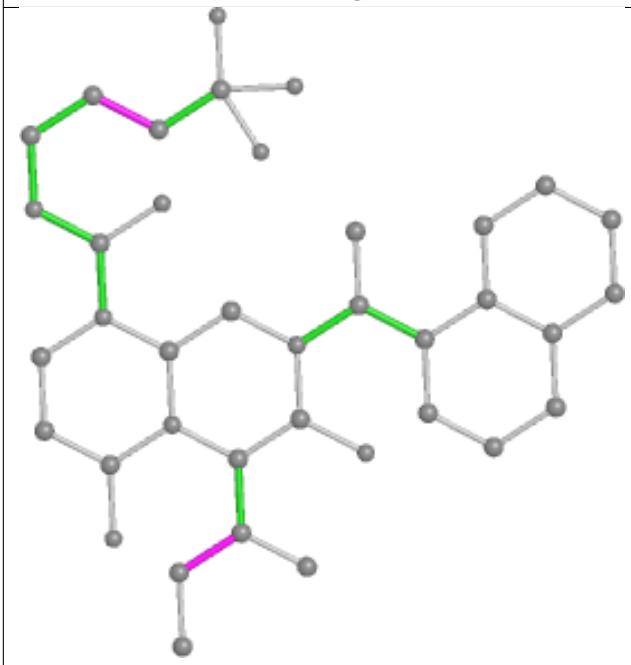
Ligand D4E I 202



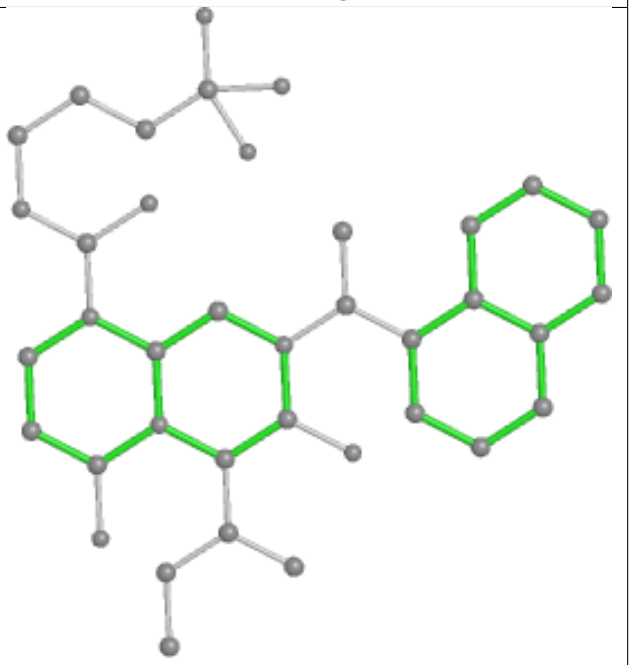
Bond lengths



Bond angles

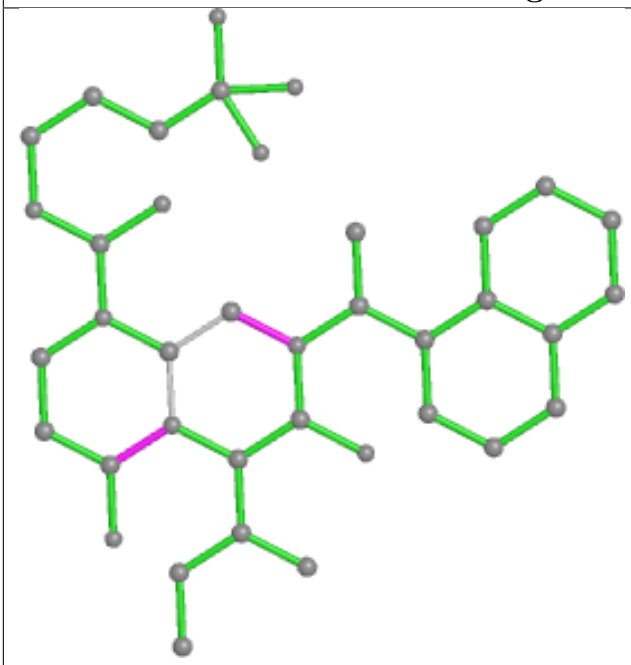


Torsions

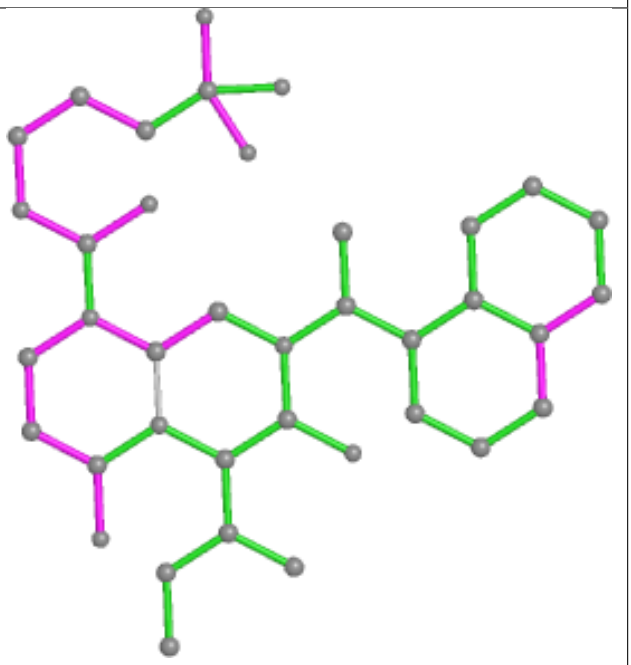


Rings

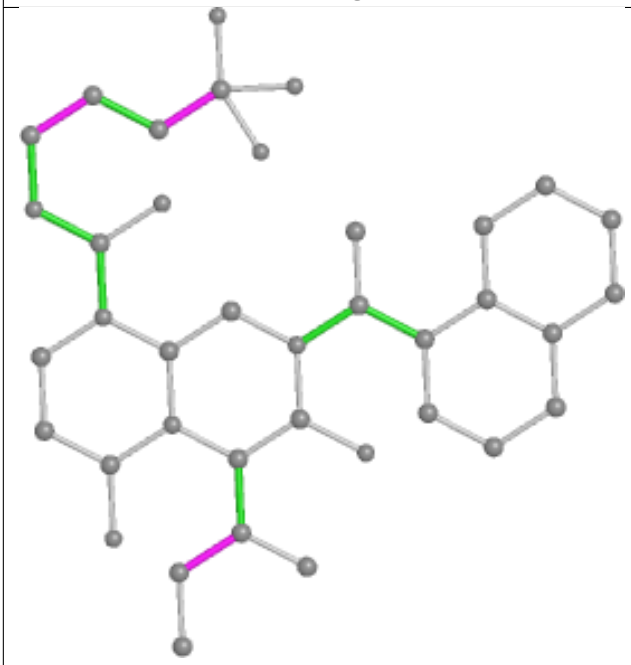
Ligand D4E N 201



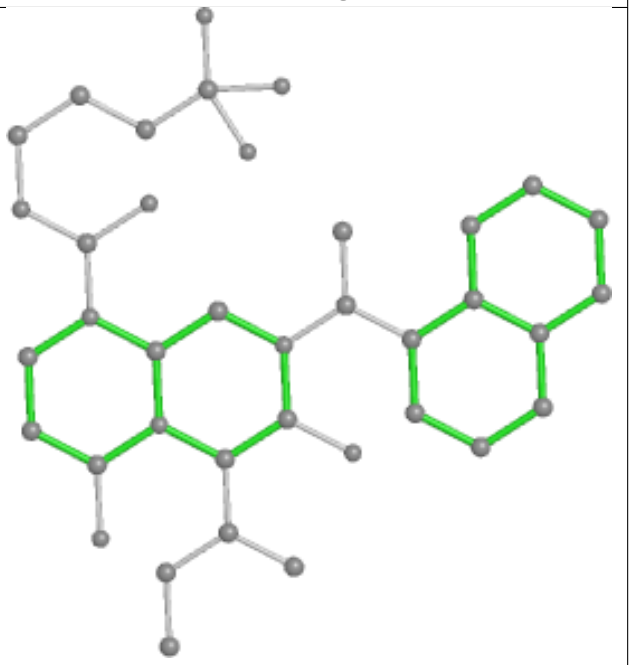
Bond lengths



Bond angles

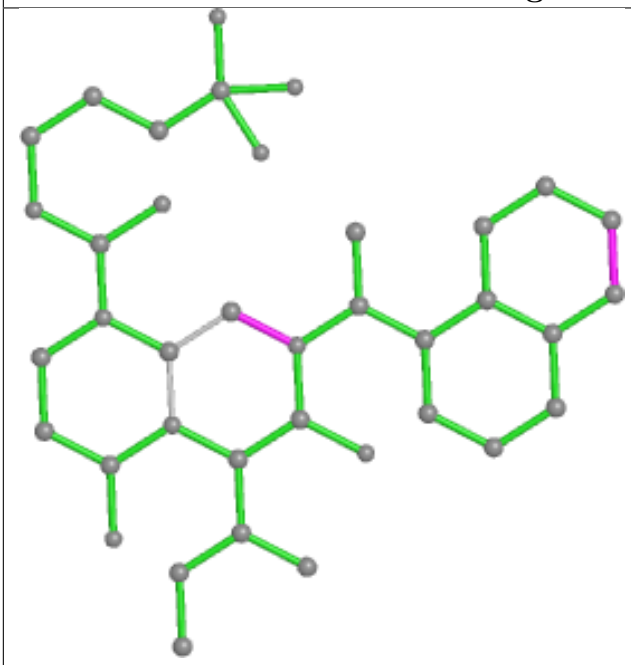


Torsions

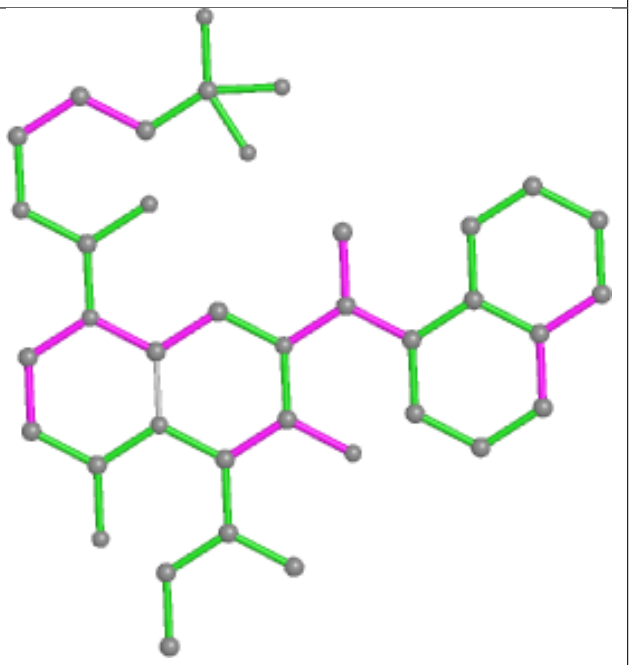


Rings

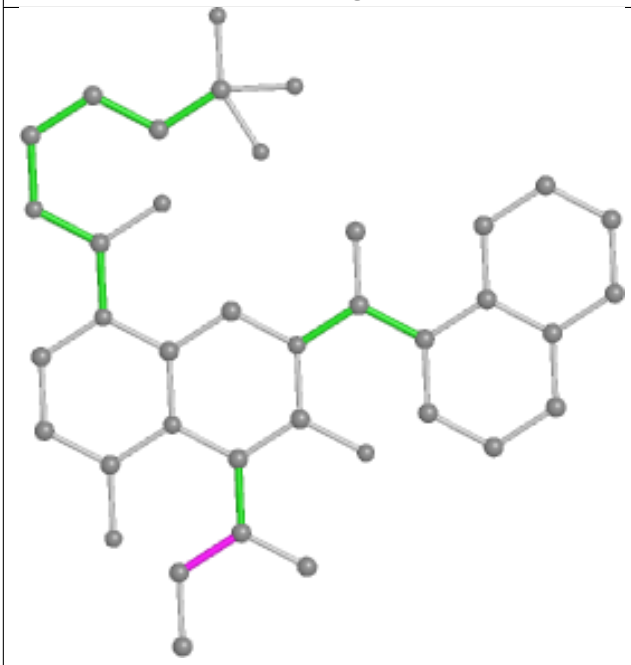
Ligand D4E G 201



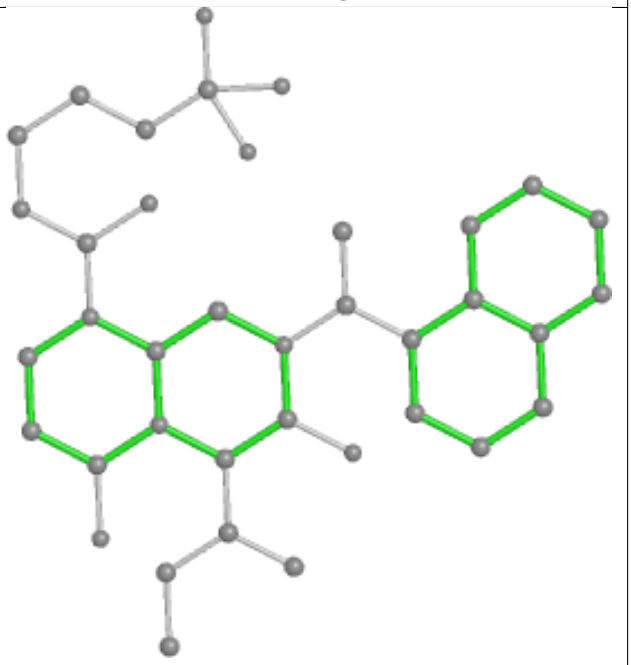
Bond lengths



Bond angles

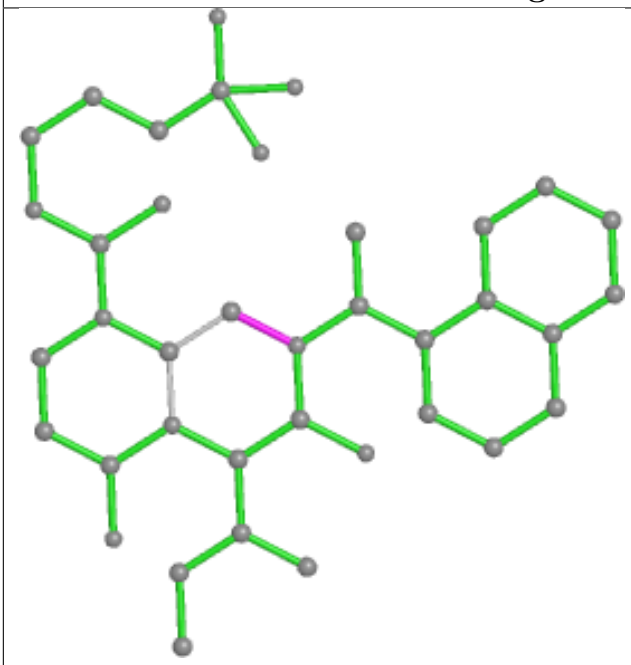


Torsions

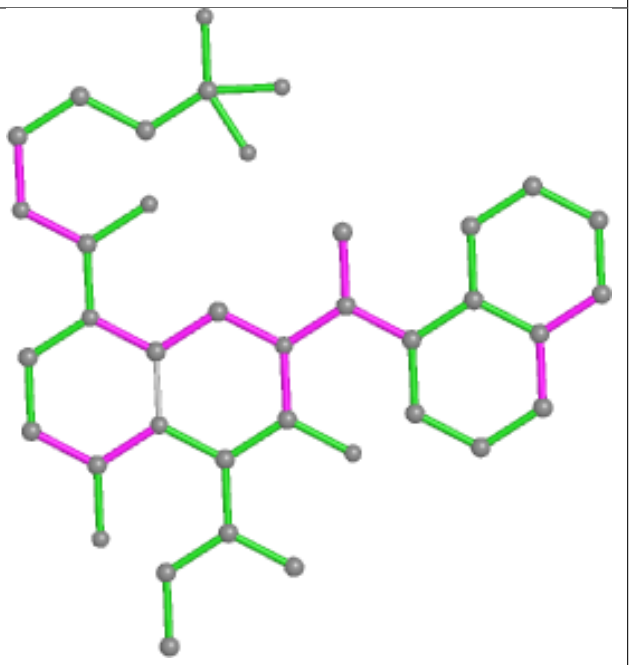


Rings

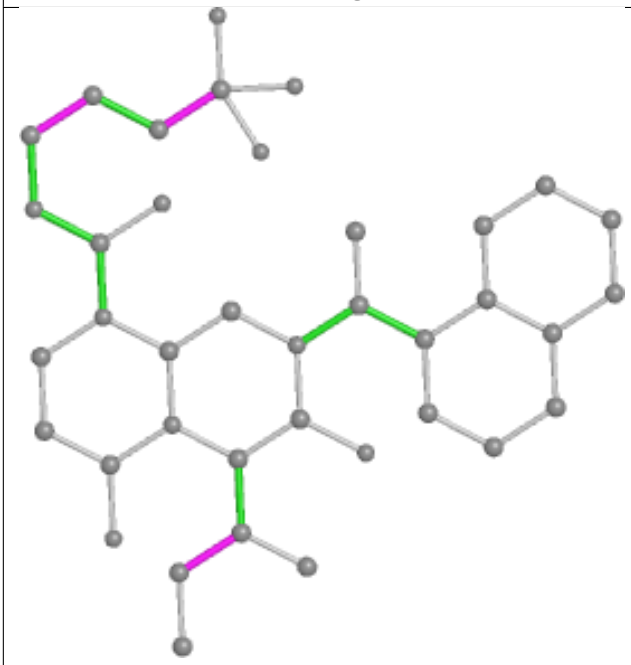
Ligand D4E E 202



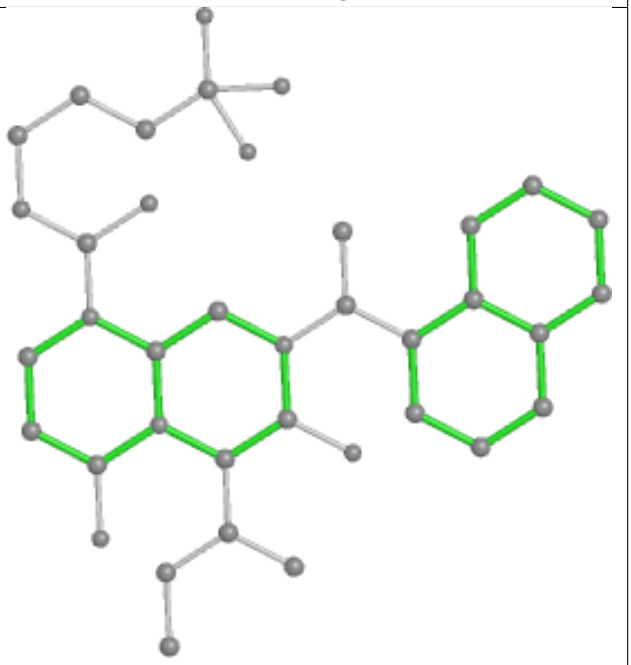
Bond lengths



Bond angles

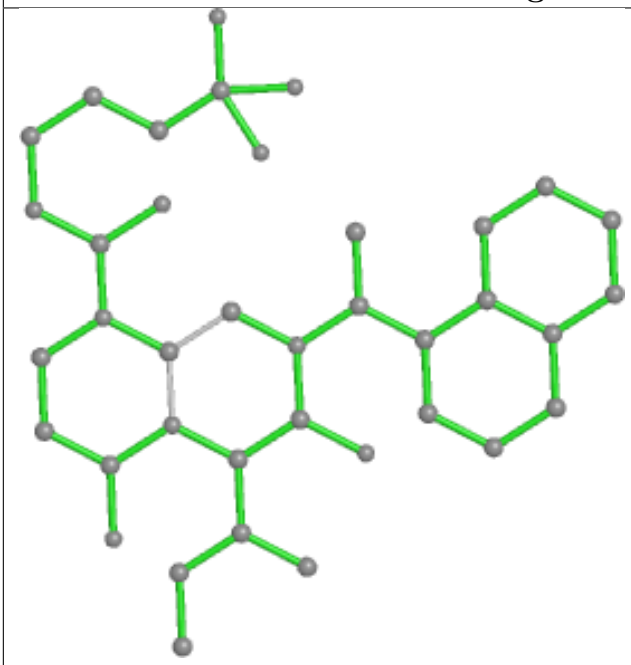


Torsions

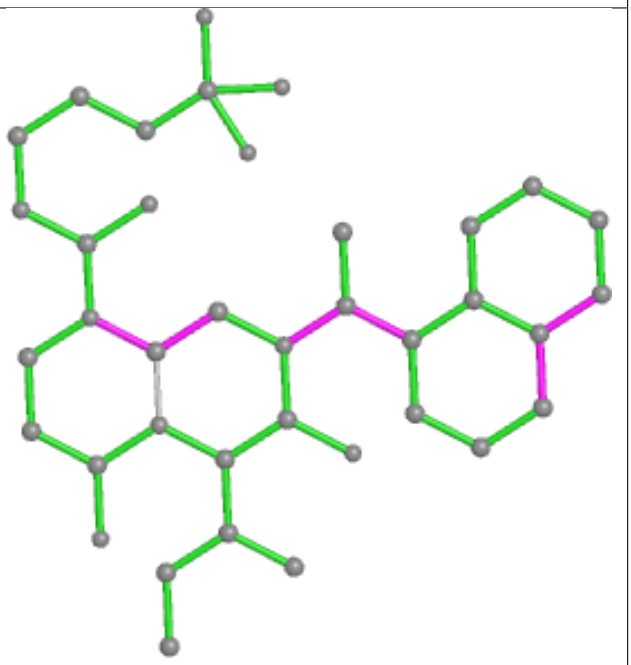


Rings

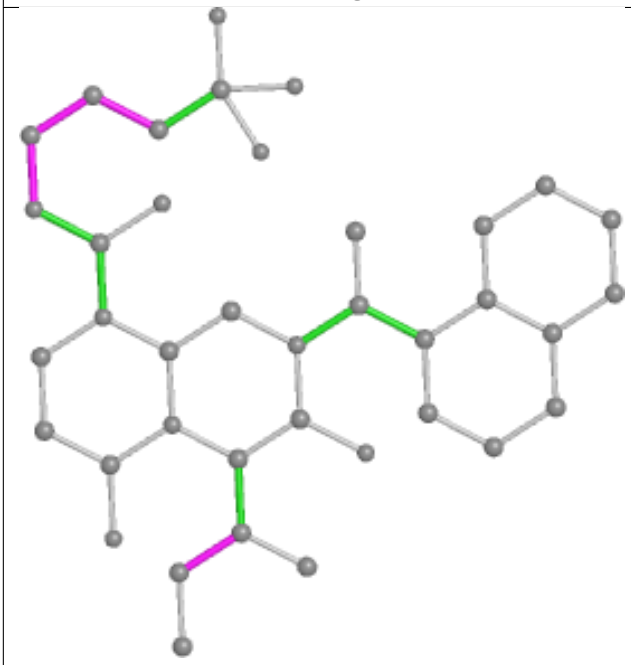
Ligand D4E C 201



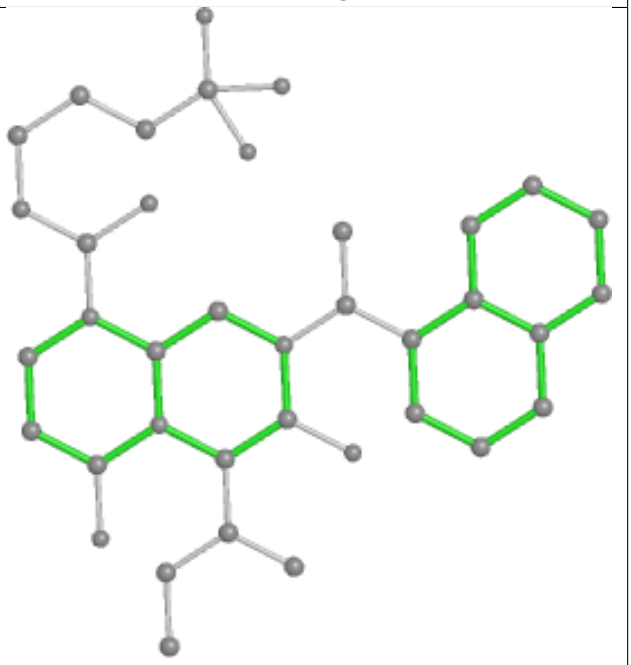
Bond lengths



Bond angles

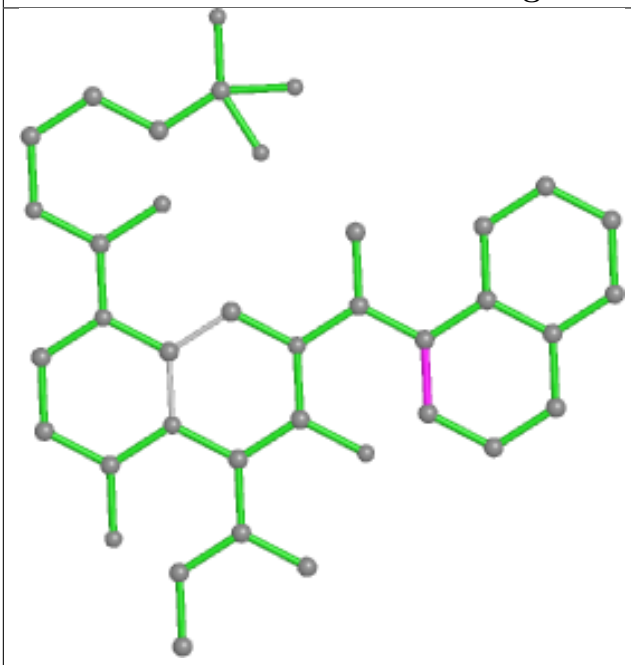


Torsions

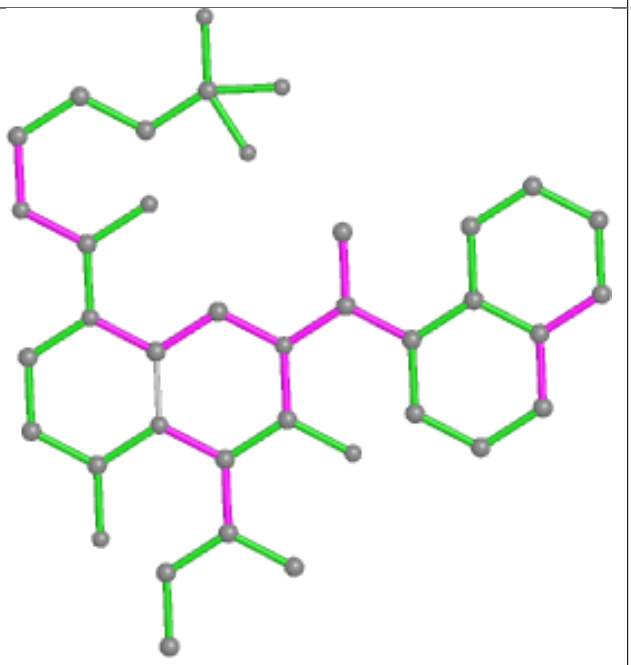


Rings

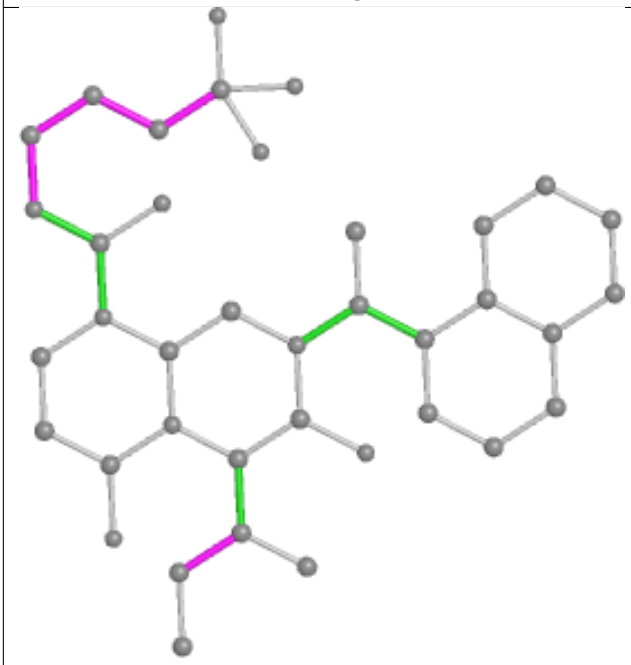
Ligand D4E M 201



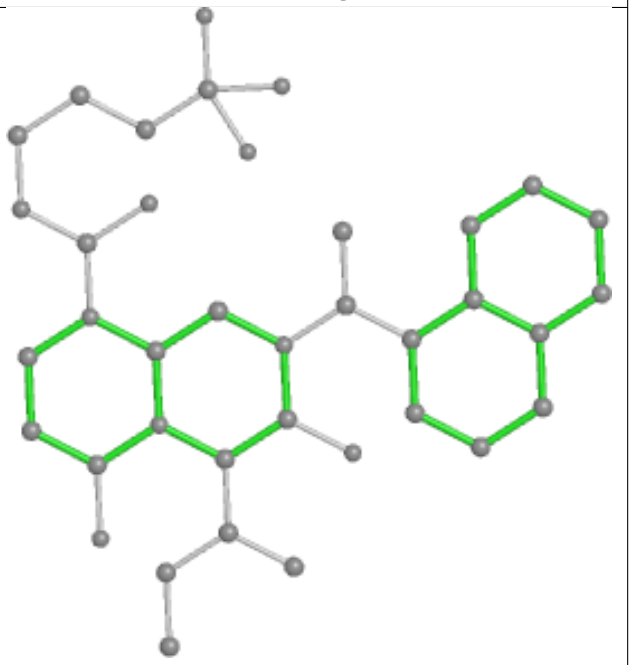
Bond lengths



Bond angles

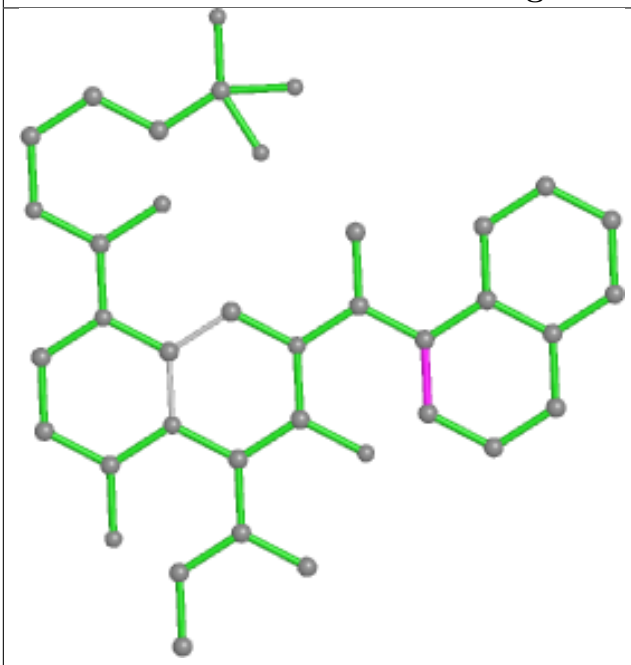


Torsions

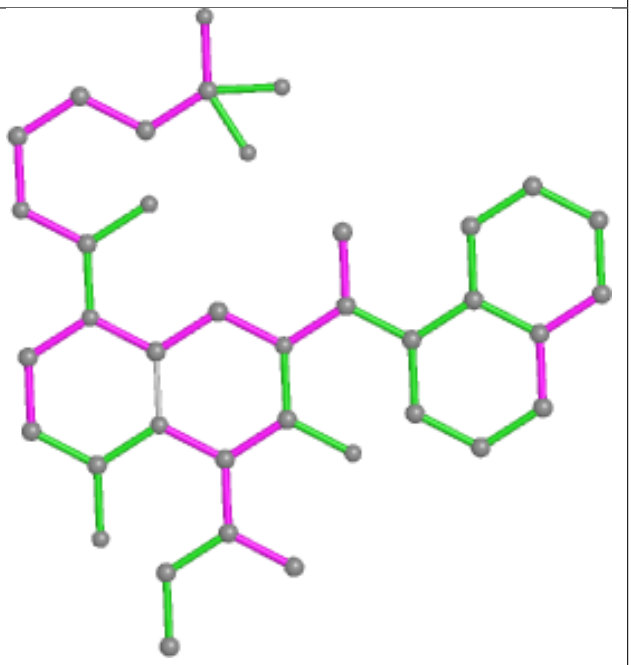


Rings

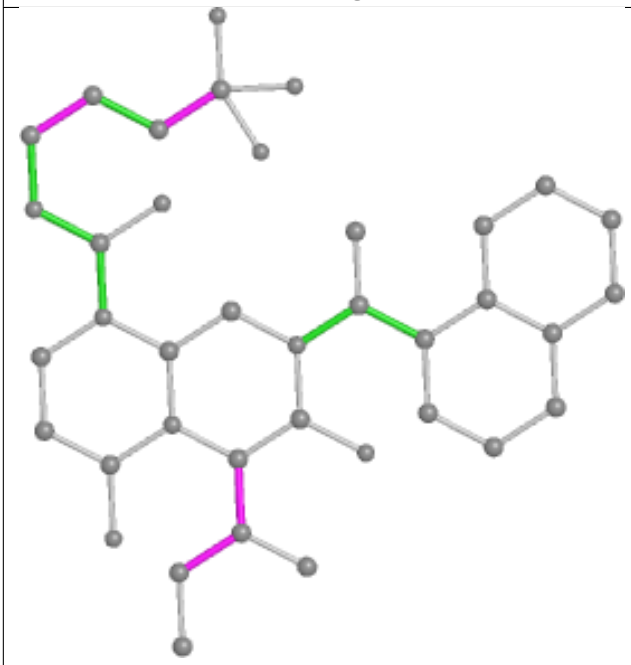
Ligand D4E A 201



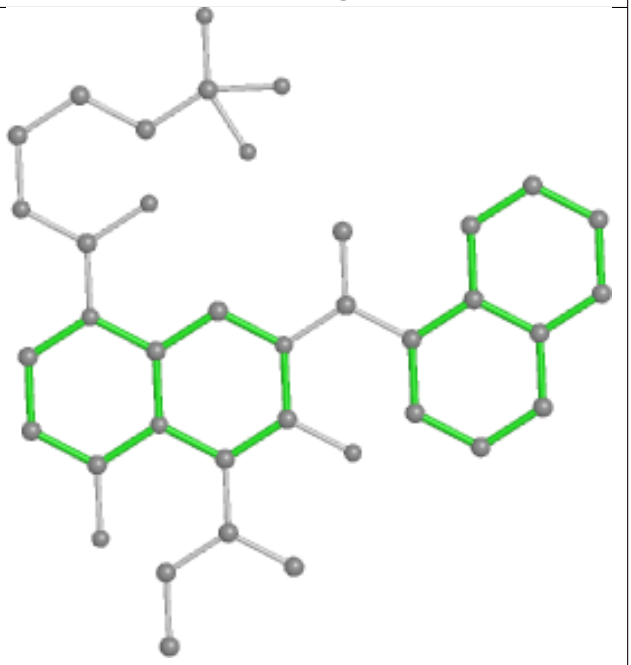
Bond lengths



Bond angles

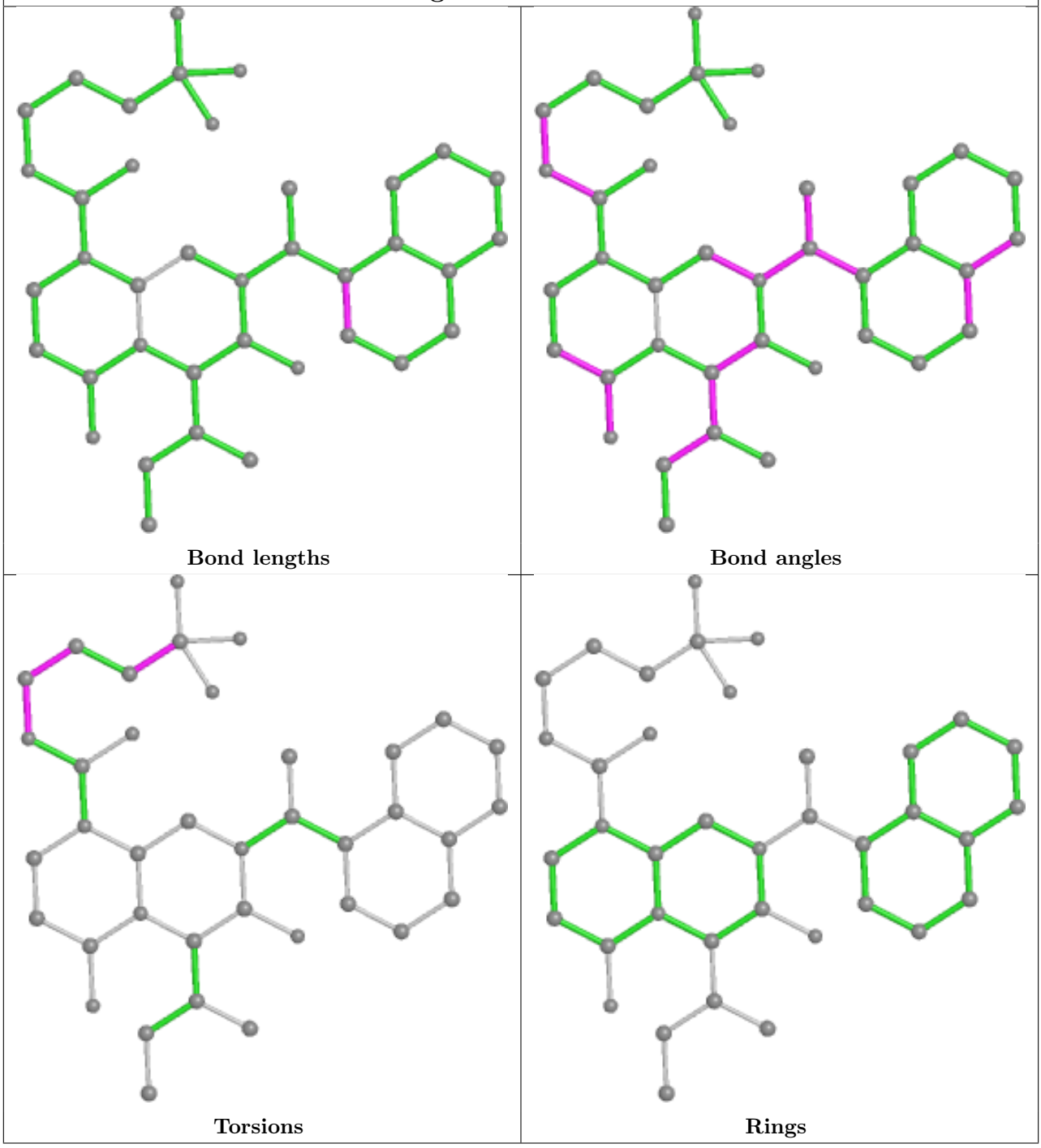


Torsions



Rings

Ligand D4E L 201



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	185/195 (94%)	-0.03	4 (2%)	62	69	21, 28, 50, 87	0
1	B	187/195 (95%)	-0.04	5 (2%)	54	63	20, 28, 46, 92	0
1	C	185/195 (94%)	0.05	6 (3%)	47	56	25, 33, 52, 69	0
1	D	179/195 (91%)	0.07	2 (1%)	80	85	30, 40, 58, 90	0
1	E	179/195 (91%)	0.21	5 (2%)	53	62	30, 39, 57, 70	0
1	F	181/195 (92%)	0.11	6 (3%)	46	55	26, 39, 55, 76	0
1	G	182/195 (93%)	-0.11	4 (2%)	62	69	23, 30, 54, 82	0
1	H	185/195 (94%)	-0.03	7 (3%)	40	49	20, 29, 51, 92	0
1	I	184/195 (94%)	-0.10	6 (3%)	46	55	22, 29, 49, 80	0
1	J	179/195 (91%)	0.03	7 (3%)	39	48	26, 34, 50, 75	0
1	K	180/195 (92%)	0.24	2 (1%)	80	85	35, 44, 59, 86	0
1	L	180/195 (92%)	0.25	6 (3%)	46	55	34, 45, 63, 84	0
1	M	177/195 (90%)	0.23	5 (2%)	53	62	30, 44, 62, 73	0
1	N	179/195 (91%)	-0.02	3 (1%)	70	76	23, 32, 53, 78	0
All	All	2542/2730 (93%)	0.06	68 (2%)	54	63	20, 36, 58, 92	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	17	ALA	7.7
1	D	18	TYR	6.4
1	K	8	ILE	6.4
1	J	18	TYR	6.1
1	A	17	ALA	6.0
1	N	18	TYR	5.5
1	I	17	ALA	5.3
1	J	7	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	L	7	VAL	4.4
1	H	15	GLU	4.1
1	C	17	ALA	3.8
1	G	4	ILE	3.7
1	G	3	LEU	3.7
1	C	8	ILE	3.6
1	L	3	LEU	3.6
1	H	9	GLU	3.5
1	I	16	ARG	3.5
1	I	8	ILE	3.2
1	I	3	LEU	3.2
1	A	8	ILE	3.2
1	M	191	VAL	3.1
1	H	8	ILE	3.0
1	M	57	GLU	2.9
1	G	191	VAL	2.9
1	K	4	ILE	2.9
1	C	3	LEU	2.9
1	B	10	THR	2.9
1	F	8	ILE	2.9
1	F	191	VAL	2.8
1	L	18	TYR	2.8
1	B	17	ALA	2.7
1	H	16	ARG	2.7
1	J	77	ILE	2.7
1	F	63	TYR	2.7
1	L	57	GLU	2.7
1	L	191	VAL	2.7
1	C	77	ILE	2.7
1	H	18	TYR	2.6
1	E	7	VAL	2.6
1	B	14	GLY	2.6
1	A	10	THR	2.6
1	E	130	GLN	2.5
1	E	18	TYR	2.5
1	N	7	VAL	2.5
1	B	9	GLU	2.5
1	J	130	GLN	2.5
1	J	62	LEU	2.4
1	F	7	VAL	2.4
1	I	18	TYR	2.4
1	M	49	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	77	ILE	2.3
1	M	18	TYR	2.3
1	I	130	GLN	2.3
1	F	167	LYS	2.3
1	F	163	GLU	2.3
1	J	6	THR	2.3
1	C	18	TYR	2.2
1	A	18	TYR	2.2
1	B	15	GLU	2.2
1	L	85	LYS	2.2
1	E	191	VAL	2.1
1	D	6	THR	2.1
1	G	17	ALA	2.1
1	H	3	LEU	2.1
1	N	4	ILE	2.1
1	J	64	ILE	2.0
1	M	63	TYR	2.0
1	C	76	ALA	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	D4E	M	201	38/38	0.74	0.34	88,101,110,113	0
2	D4E	L	201	38/38	0.76	0.24	78,95,111,112	0
2	D4E	K	201	38/38	0.77	0.27	63,78,103,109	0
2	D4E	C	201	38/38	0.78	0.27	69,78,84,86	0
2	D4E	N	202	38/38	0.79	0.26	58,71,96,102	0

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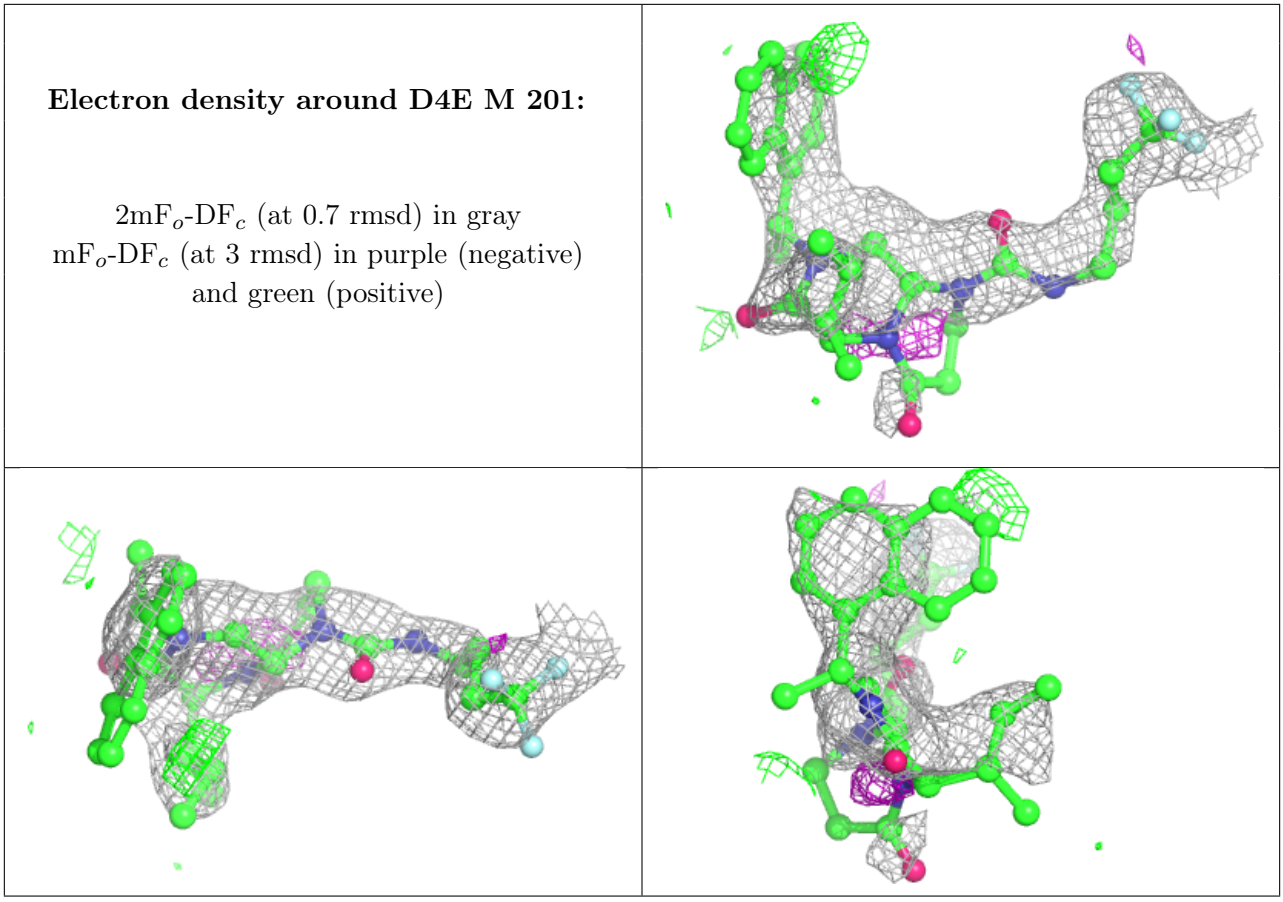
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	D4E	E	202	38/38	0.80	0.30	69,90,107,108	0
2	D4E	I	202	38/38	0.80	0.25	45,64,75,84	0
2	D4E	I	201	38/38	0.81	0.27	43,60,72,74	0
3	MG	A	203	1/1	0.82	0.13	50,50,50,50	0
3	MG	F	201	1/1	0.83	0.14	51,51,51,51	0
3	MG	C	202	1/1	0.86	0.15	41,41,41,41	0
2	D4E	E	201	38/38	0.86	0.17	55,70,81,87	0
3	MG	N	203	1/1	0.87	0.10	47,47,47,47	0
2	D4E	N	201	38/38	0.89	0.18	41,49,57,63	0
2	D4E	A	201	38/38	0.89	0.15	31,38,45,47	0
4	MPD	N	204	8/8	0.89	0.18	36,41,54,56	0
2	D4E	G	201	38/38	0.90	0.17	40,49,57,59	0
3	MG	K	202	1/1	0.90	0.27	59,59,59,59	0
4	MPD	K	203	8/8	0.91	0.21	42,49,53,62	0
4	MPD	M	203	8/8	0.92	0.20	48,57,67,69	0
4	MPD	C	203	8/8	0.92	0.17	40,47,50,61	0
4	MPD	F	202	8/8	0.93	0.16	41,44,48,55	0
4	MPD	D	201	8/8	0.94	0.13	42,46,52,58	0
4	MPD	E	203	8/8	0.94	0.17	45,50,57,62	0
4	MPD	B	203	8/8	0.94	0.13	55,57,58,58	0
4	MPD	A	204	8/8	0.95	0.17	33,36,40,48	0
4	MPD	H	202	8/8	0.95	0.18	35,36,44,51	0
4	MPD	J	202	8/8	0.95	0.15	37,41,48,56	0
3	MG	M	202	1/1	0.96	0.30	57,57,57,57	0
4	MPD	I	204	8/8	0.96	0.14	33,36,43,53	0
4	MPD	G	203	8/8	0.96	0.15	43,46,53,54	0
3	MG	G	202	1/1	0.97	0.10	39,39,39,39	0
4	MPD	L	202	8/8	0.97	0.12	45,50,57,58	0
3	MG	H	201	1/1	0.97	0.21	39,39,39,39	0
4	MPD	B	202	8/8	0.97	0.11	29,33,38,42	0
3	MG	B	201	1/1	0.98	0.07	36,36,36,36	0
3	MG	J	201	1/1	0.98	0.24	49,49,49,49	0
3	MG	I	203	1/1	0.99	0.18	35,35,35,35	0
3	MG	A	202	1/1	0.99	0.17	41,41,41,41	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.

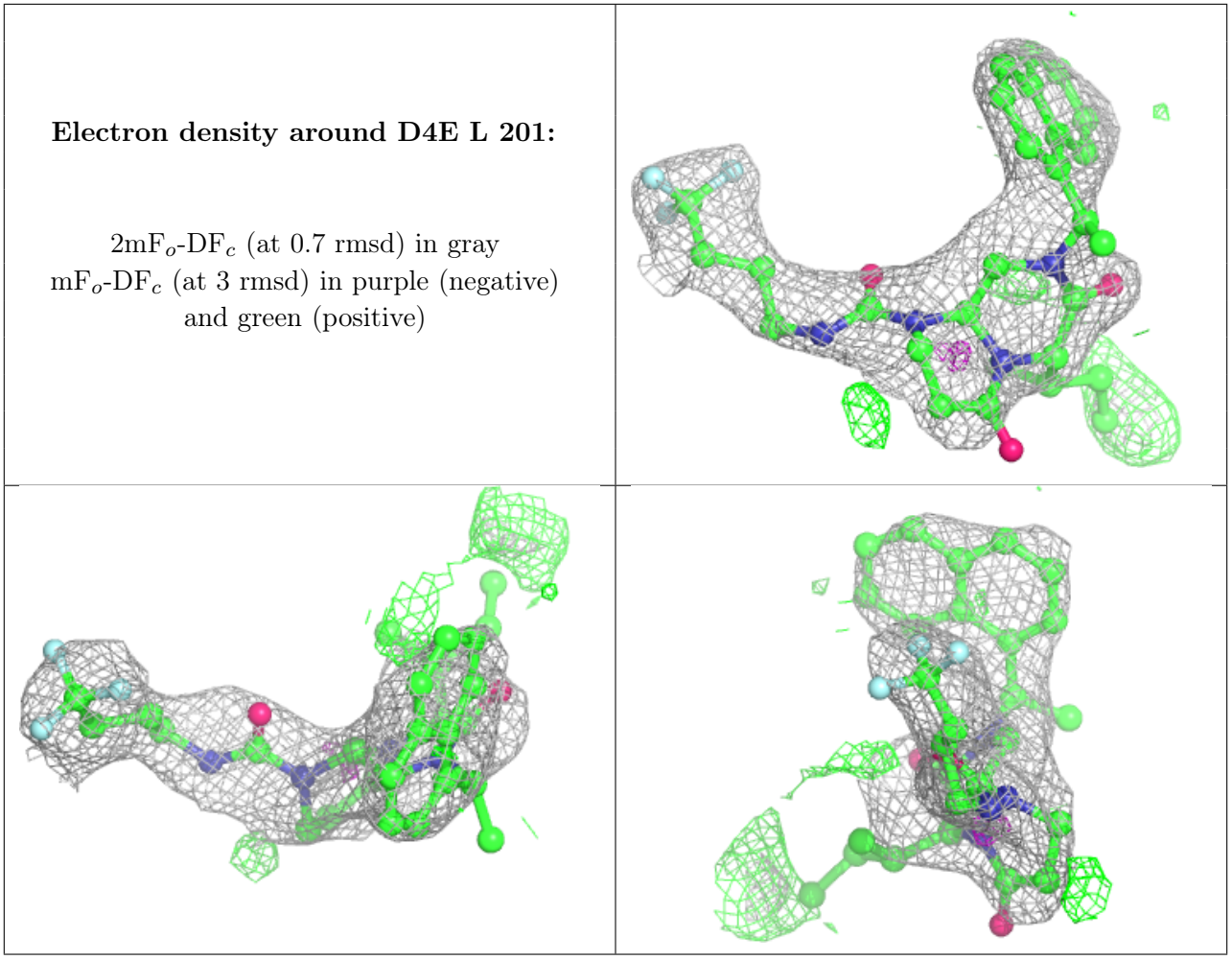
Electron density around D4E M 201:

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



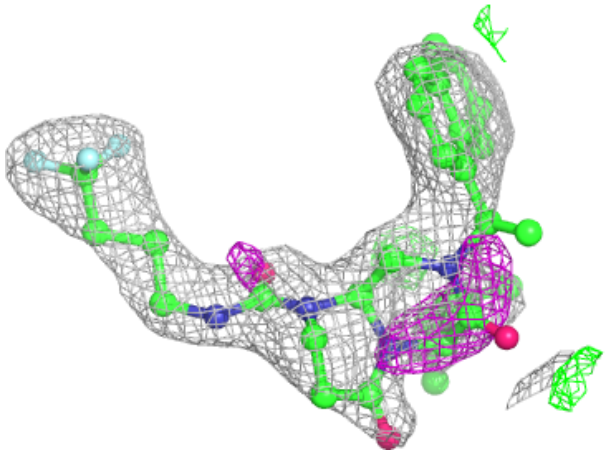
Electron density around D4E L 201:

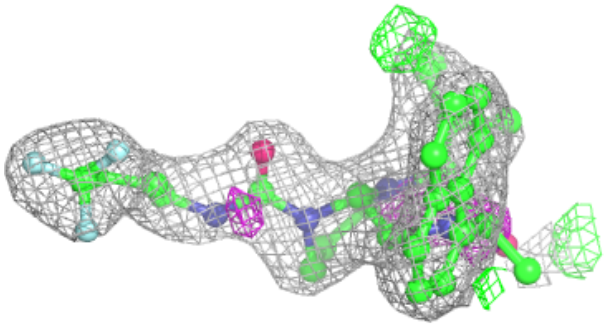
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

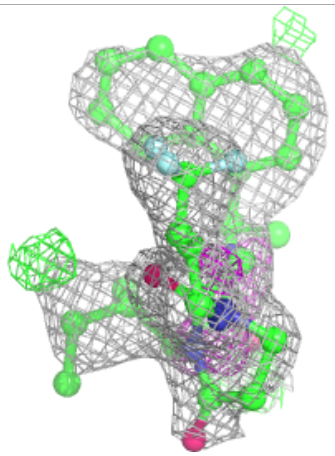


Electron density around D4E K 201:

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

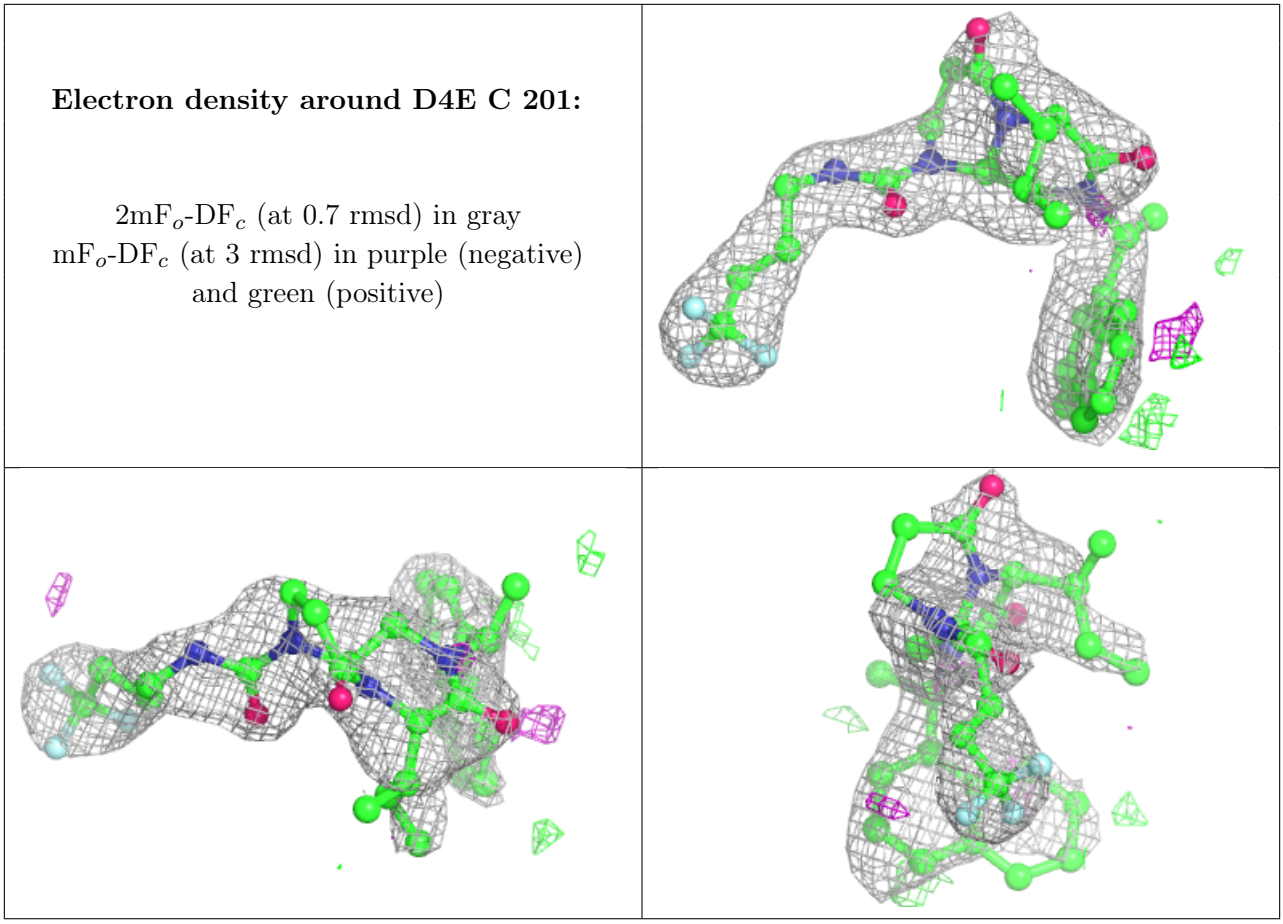






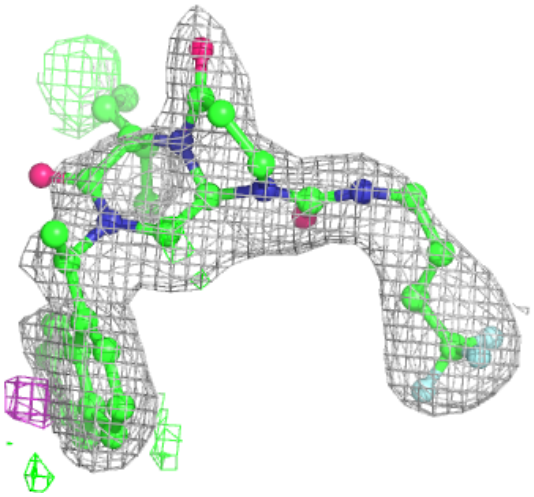
Electron density around D4E C 201:

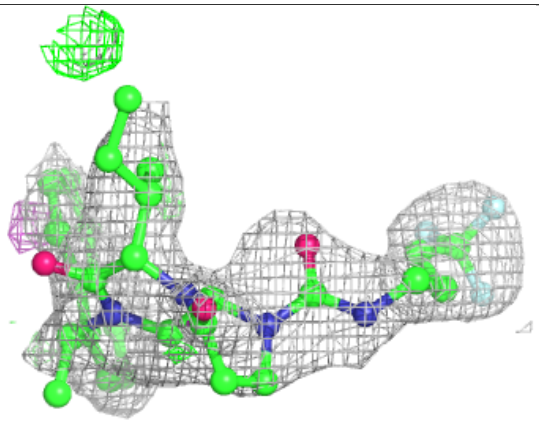
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

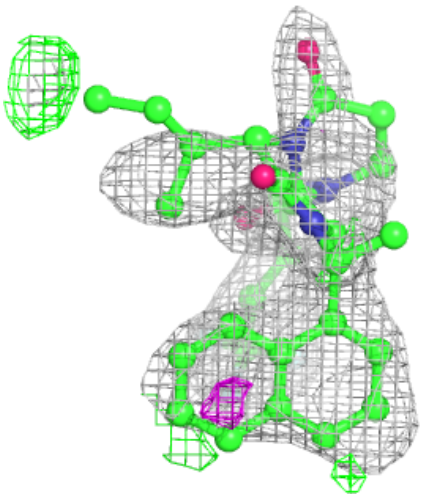


Electron density around D4E N 202:

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

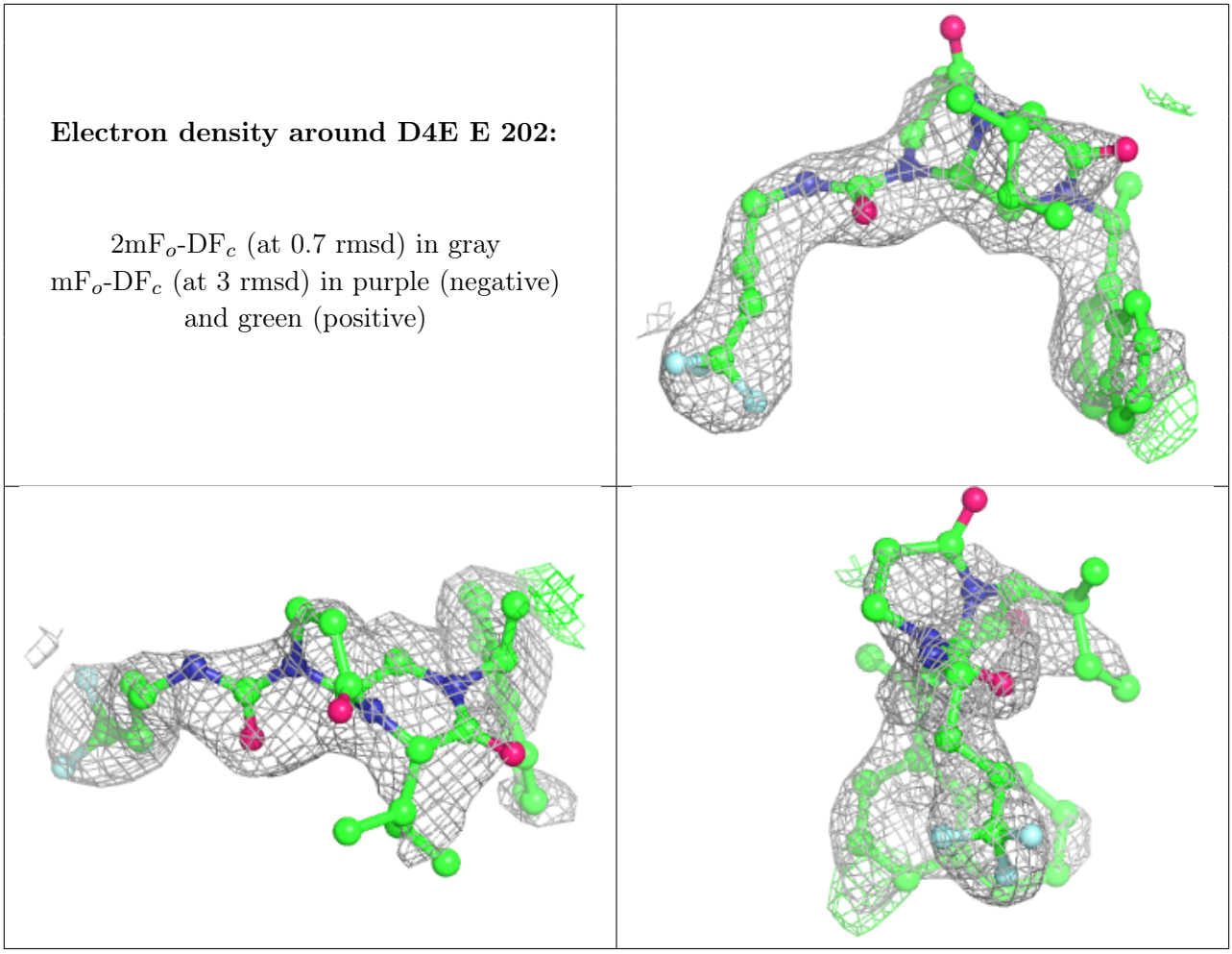






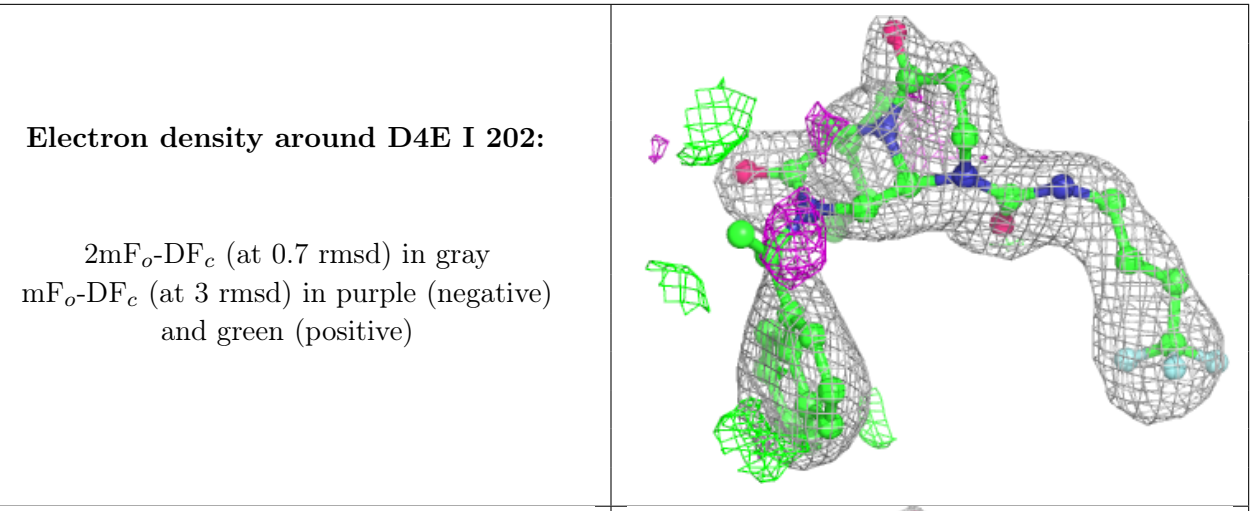
Electron density around D4E E 202:

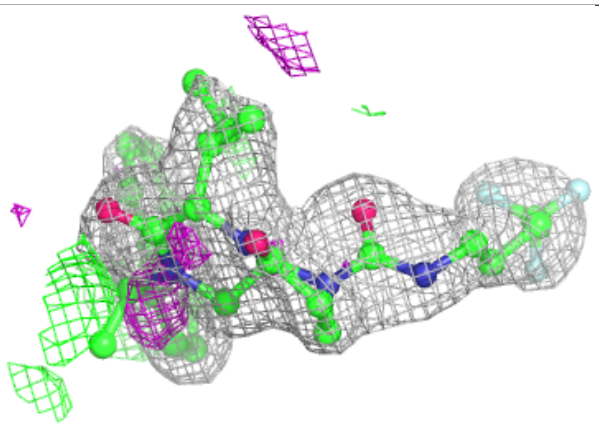
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

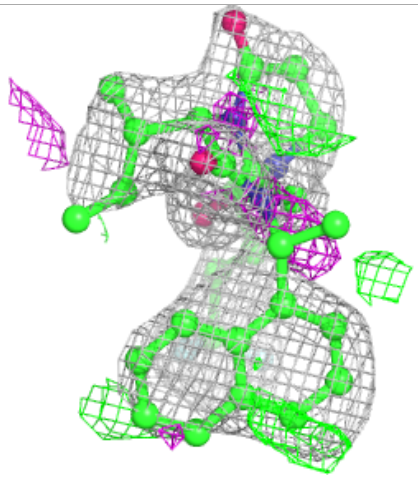


Electron density around D4E I 202:

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

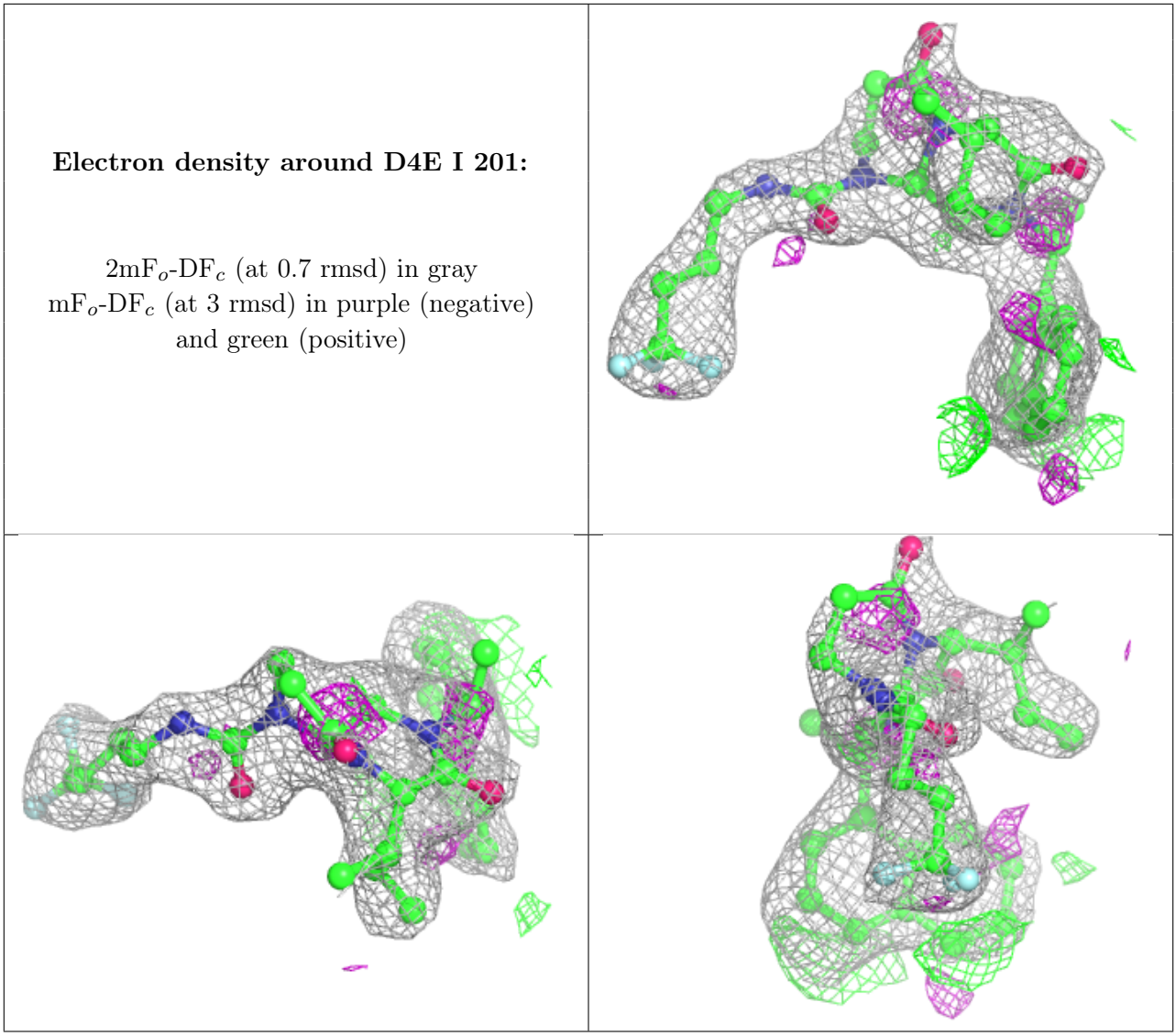






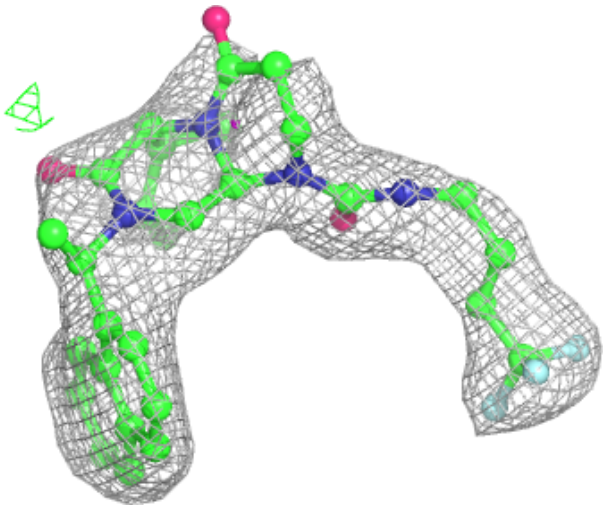
Electron density around D4E I 201:

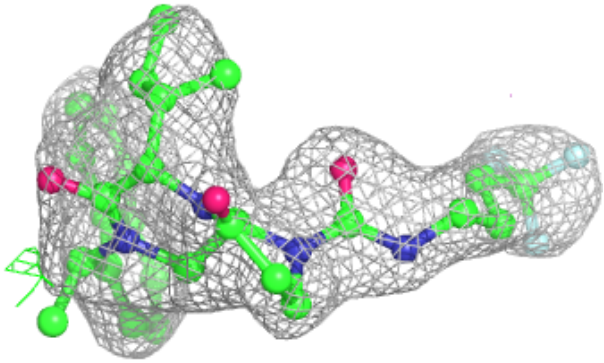
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

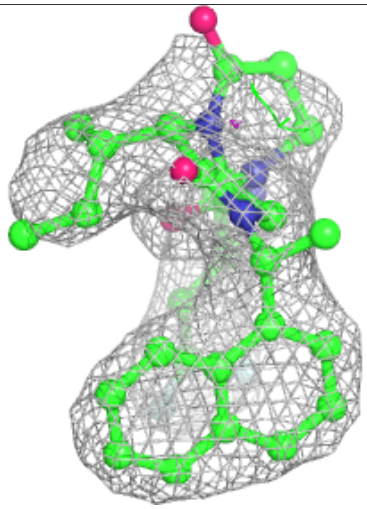


Electron density around D4E E 201:

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

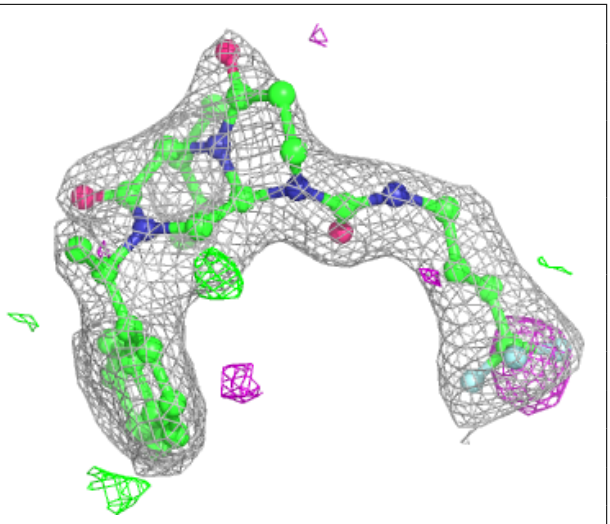


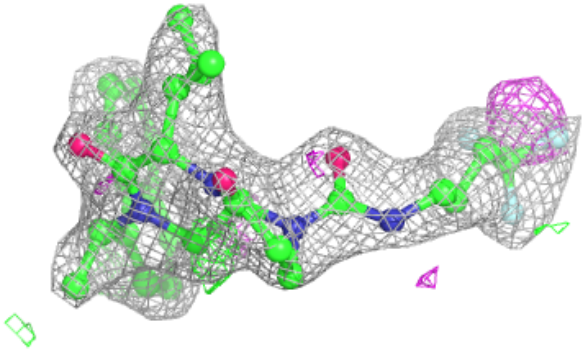


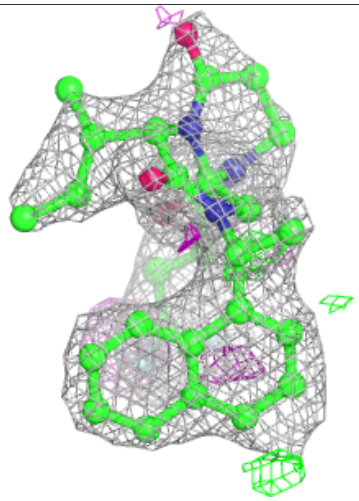


Electron density around D4E N 201:

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

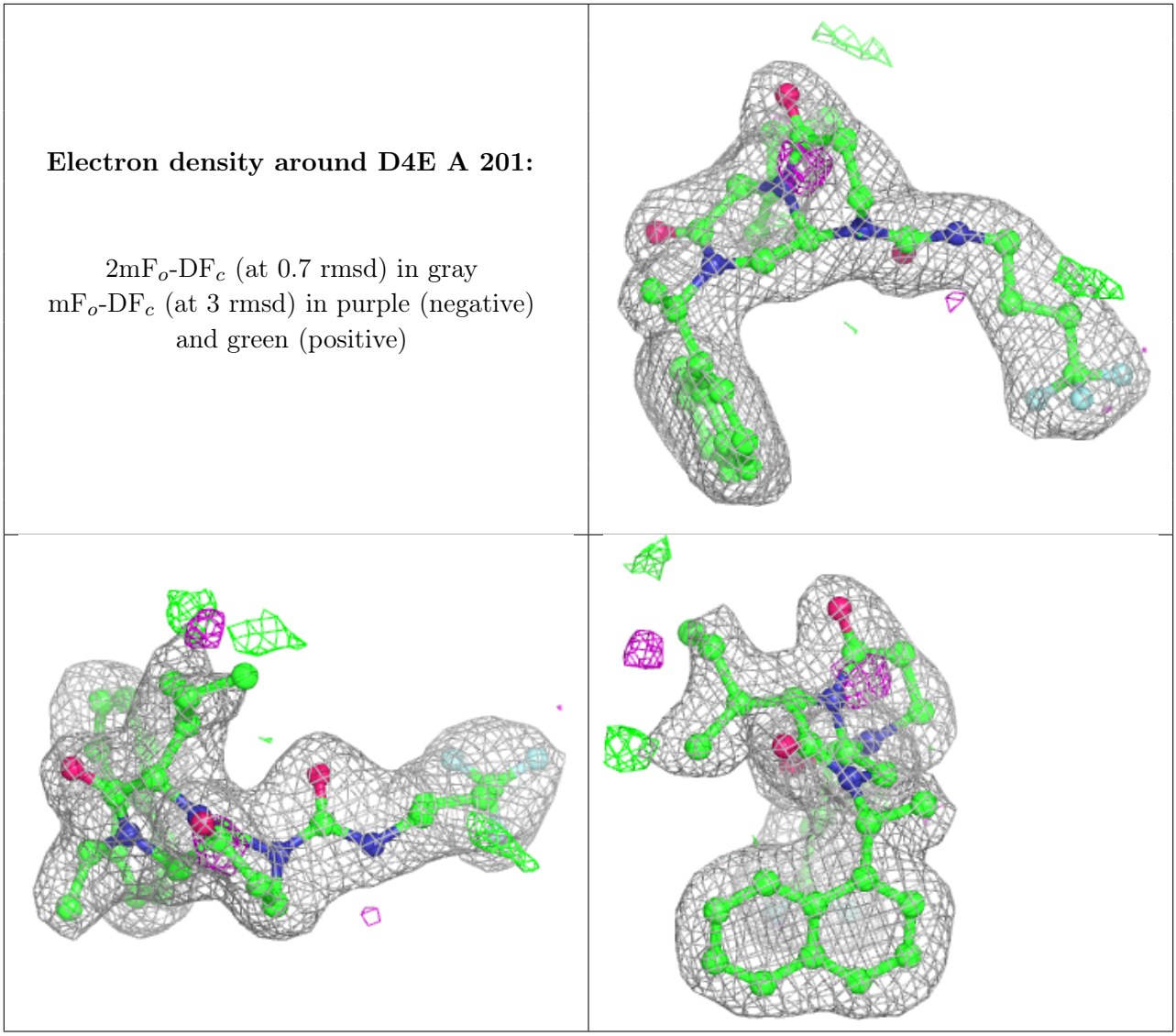






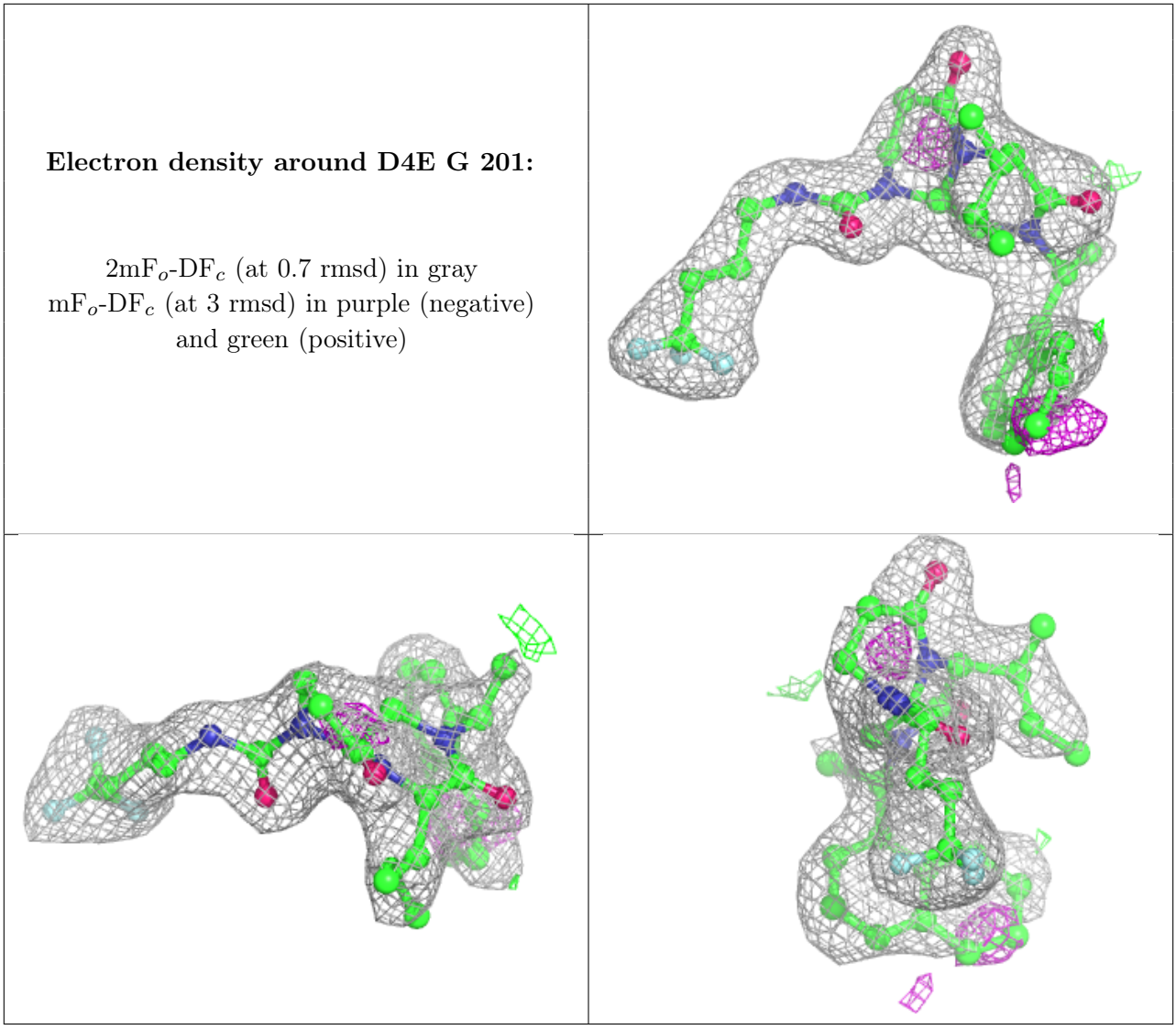
Electron density around D4E A 201:

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



Electron density around D4E G 201:

$2mF_o$-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.