Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2023 – 02:15 PM JST

PDB ID	:	8I7X
Title	:	Crystal structure of human ClpP in complex with ZG36
Authors	:	Wang, P.Y.; Gan, J.H.; Yang, C.-G.
Deposited on	:	2023-02-02
Resolution	:	1.99 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:

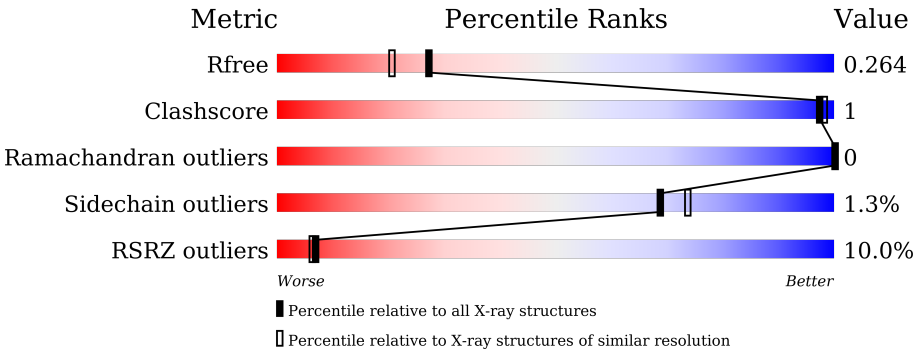
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	221	5% 69% · 27%
1	B	221	4% 70% · 27%
1	C	221	10% 70% · 27%
1	D	221	6% 73% · 26%
1	E	221	9% 70% · 27%
1	F	221	5% 72% · 26%

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Mol	Chain	Length	Quality of chain
1	G	221	10% 73% 26%
1	H	221	6% 68% 5% 27%
1	I	221	5% 71% 27%
1	J	221	10% 72% 26%
1	K	221	8% 71% 27%
1	L	221	10% 71% 27%
1	M	221	9% 71% 27%
1	N	221	7% 72% 26%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18730 atoms, of which 0 are hydrogens and 0 are deuteriums.

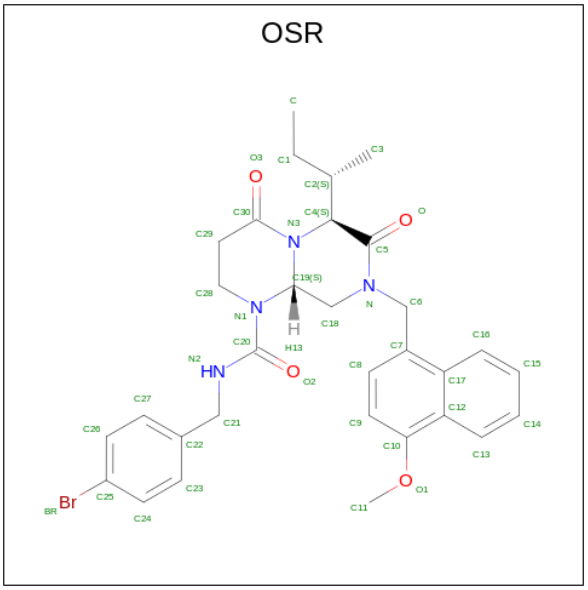
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1259	804	214	228	13			
1	B	162	Total	C	N	O	S	0	0	0
			1247	795	212	227	13			
1	C	162	Total	C	N	O	S	0	0	0
			1250	799	213	225	13			
1	D	163	Total	C	N	O	S	0	0	0
			1257	802	215	227	13			
1	E	161	Total	C	N	O	S	0	0	0
			1245	794	212	226	13			
1	F	164	Total	C	N	O	S	0	0	0
			1269	810	216	230	13			
1	G	164	Total	C	N	O	S	0	0	0
			1275	814	217	231	13			
1	H	161	Total	C	N	O	S	0	0	0
			1251	797	216	225	13			
1	I	161	Total	C	N	O	S	0	0	0
			1253	798	215	227	13			
1	J	163	Total	C	N	O	S	0	0	0
			1272	812	218	229	13			
1	K	161	Total	C	N	O	S	0	0	0
			1244	794	210	227	13			
1	L	161	Total	C	N	O	S	0	0	0
			1235	791	209	222	13			
1	M	162	Total	C	N	O	S	0	0	0
			1246	792	214	227	13			
1	N	163	Total	C	N	O	S	0	0	0
			1272	812	218	229	13			

- Molecule 2 is (6S,9aS)-N-[(4-bromophenyl)methyl]-6-[(2S)-butan-2-yl]-8-[(4-methoxynaphthalen-1-yl)methyl]-4,7-bis(oxidanylidene)-3,6,9,9a-tetrahydro-2H-pyrazino[1,2-a]pyrimidine-1-carboxamide (three-letter code: OSR) (formula: $C_{31}H_{35}BrN_4O_4$) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	B	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	C	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	D	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	F	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	G	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	G	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	H	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	I	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	J	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	K	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	K	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		
2	L	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	Br	C	N	O	0	0
			40	1	31	4	4		

- Molecule 3 is water.

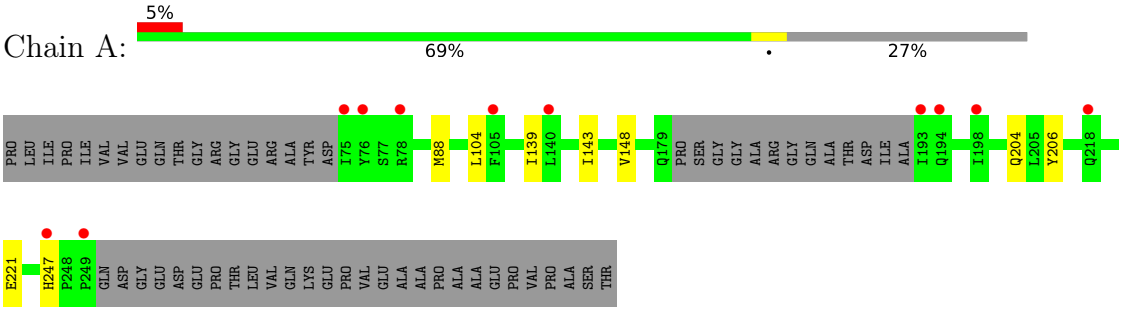
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	33	Total	O	0	0
			33	33		
3	C	25	Total	O	0	0
			25	25		
3	D	48	Total	O	0	0
			48	48		
3	E	53	Total	O	0	0
			53	53		
3	F	73	Total	O	0	0
			73	73		
3	G	52	Total	O	0	0
			52	52		
3	H	47	Total	O	0	0
			47	47		
3	I	44	Total	O	0	0
			44	44		
3	J	39	Total	O	0	0
			39	39		
3	K	29	Total	O	0	0
			29	29		
3	L	28	Total	O	0	0
			28	28		
3	M	52	Total	O	0	0
			52	52		
3	N	36	Total	O	0	0
			36	36		

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.

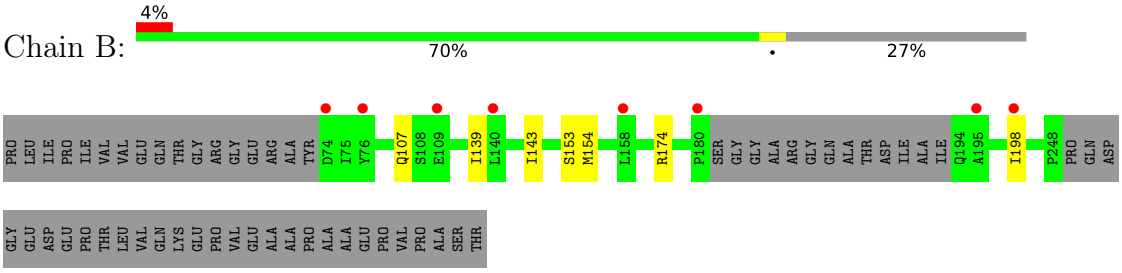
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



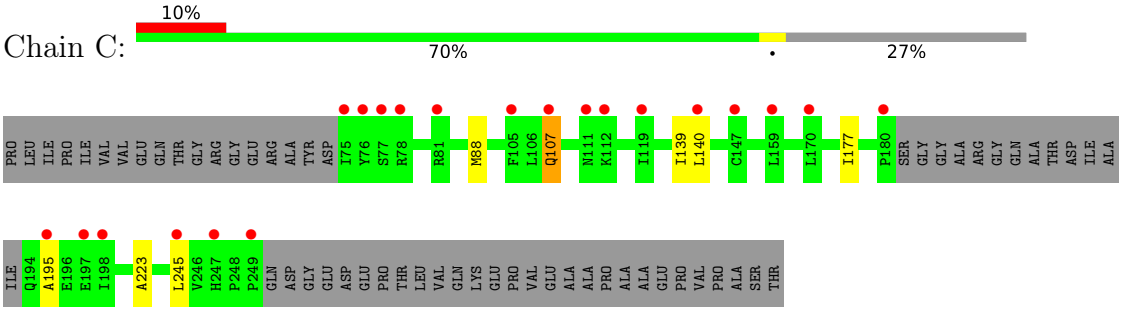
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



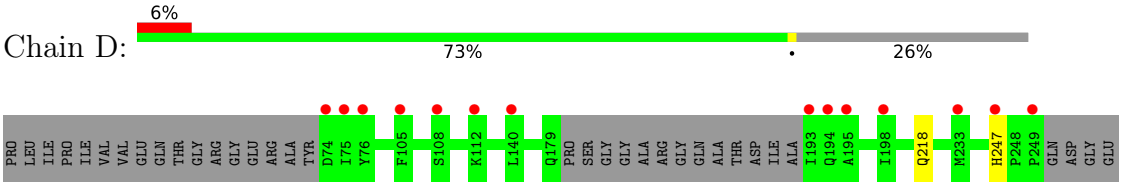
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

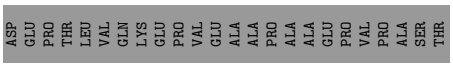
Chain C:



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

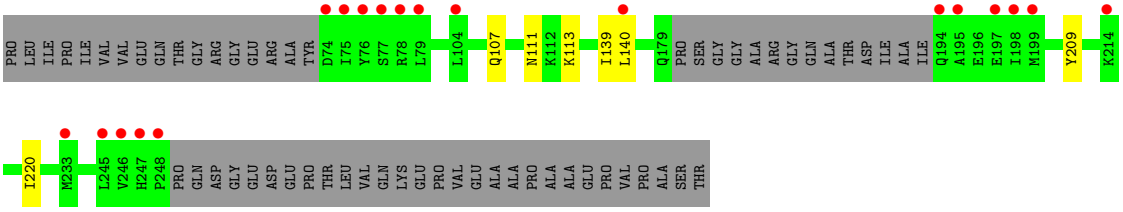
Chain D:





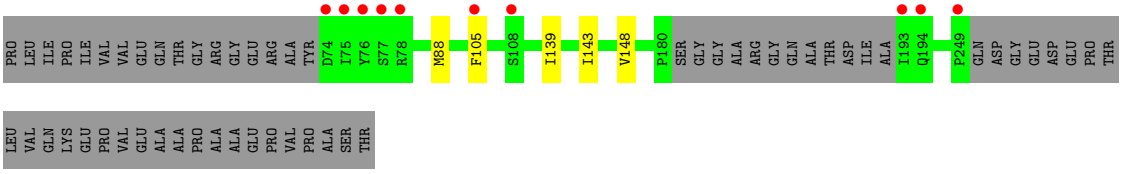
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



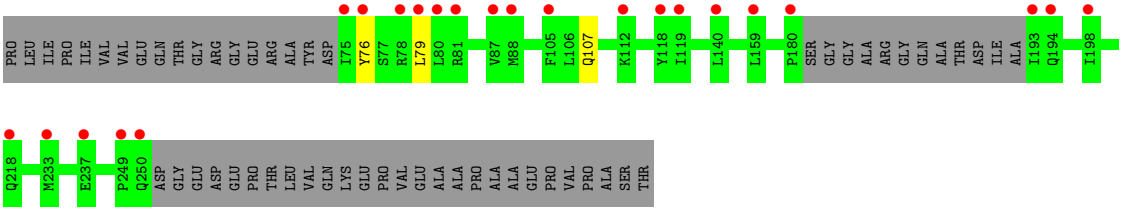
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



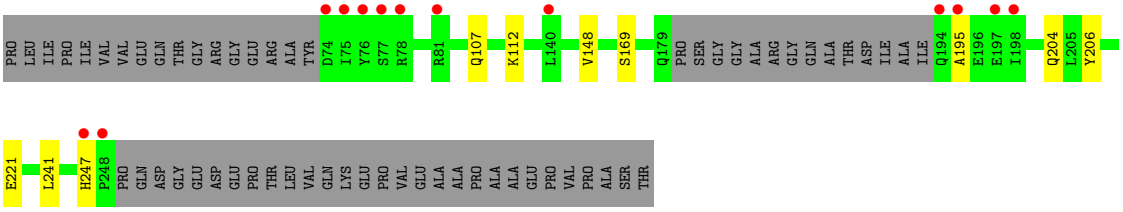
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:



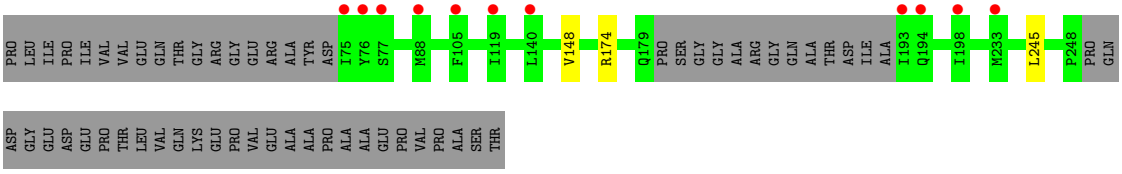
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain H:



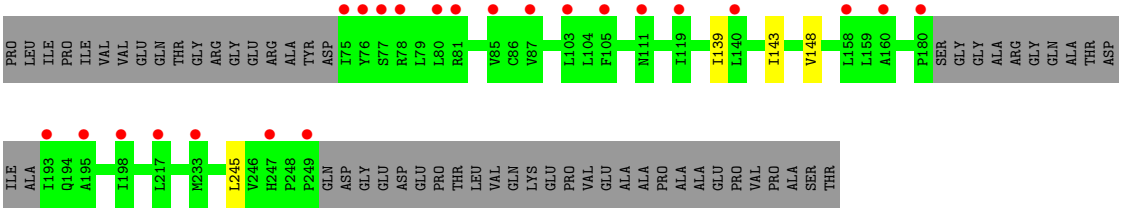
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain I:



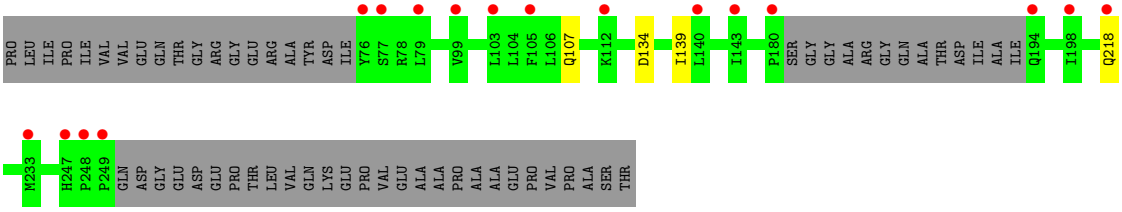
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain J:



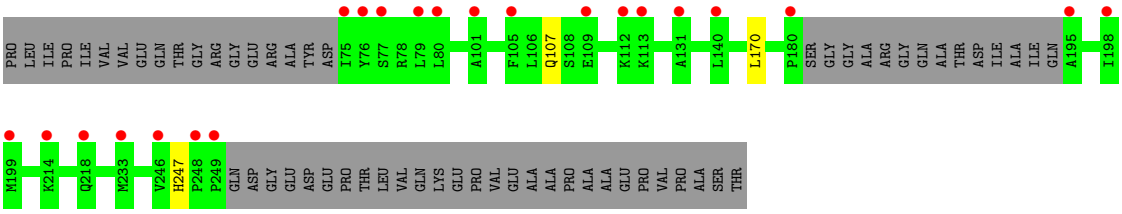
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain K:



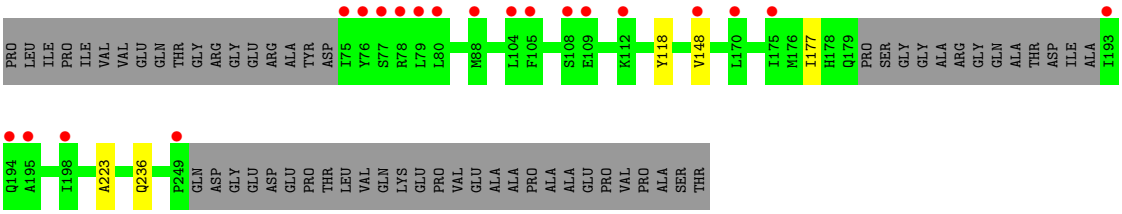
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain L:



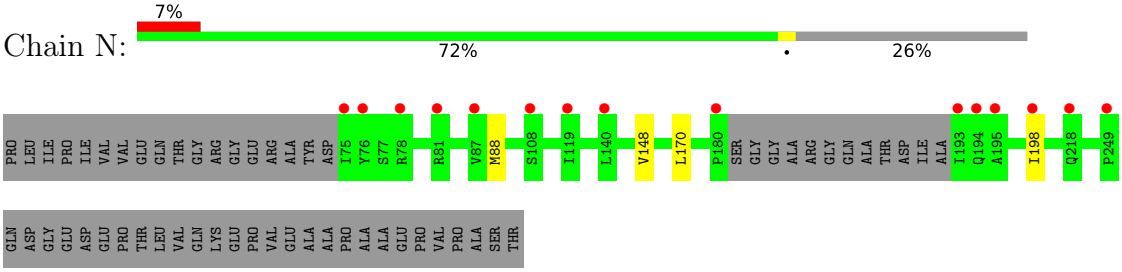
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain M:



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

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	113.24Å 96.08Å 127.00Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	30.85 – 1.99 30.85 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.85-1.99) 99.0 (30.85-1.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.260 0.237 , 0.264	Depositor DCC
R_{free} test set	9417 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18730	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: OSR

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	0.34	0/1282	0.57	0/1733
1	B	0.33	0/1270	0.54	0/1719
1	C	0.34	0/1274	0.55	0/1724
1	D	0.34	0/1280	0.55	0/1731
1	E	0.34	0/1267	0.57	0/1712
1	F	0.34	0/1292	0.57	0/1747
1	G	0.34	0/1299	0.56	0/1757
1	H	0.34	0/1273	0.56	0/1719
1	I	0.34	0/1275	0.57	0/1722
1	J	0.34	0/1296	0.56	0/1752
1	K	0.33	0/1268	0.54	0/1716
1	L	0.34	0/1259	0.54	0/1705
1	M	0.34	0/1268	0.54	0/1714
1	N	0.33	0/1296	0.55	0/1752
All	All	0.34	0/17899	0.56	0/24203

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	1259	0	1294	4	0
1	B	1247	0	1266	4	0
1	C	1250	0	1280	6	0
1	D	1257	0	1283	0	0
1	E	1245	0	1272	3	0
1	F	1269	0	1297	2	0
1	G	1275	0	1309	1	0
1	H	1251	0	1285	4	0
1	I	1253	0	1282	1	0
1	J	1272	0	1312	1	0
1	K	1244	0	1268	2	0
1	L	1235	0	1263	1	0
1	M	1246	0	1269	3	0
1	N	1272	0	1312	2	0
2	B	80	0	0	1	0
2	C	40	0	0	0	0
2	D	40	0	0	0	0
2	F	40	0	0	0	0
2	G	80	0	0	1	0
2	H	40	0	0	0	0
2	I	40	0	0	0	0
2	J	40	0	0	0	0
2	K	80	0	0	0	0
2	L	40	0	0	0	0
2	M	40	0	0	0	0
3	A	36	0	0	0	0
3	B	33	0	0	0	0
3	C	25	0	0	0	0
3	D	48	0	0	0	0
3	E	53	0	0	0	0
3	F	73	0	0	0	0
3	G	52	0	0	0	0
3	H	47	0	0	0	0
3	I	44	0	0	0	0
3	J	39	0	0	0	0
3	K	29	0	0	0	0
3	L	28	0	0	0	0
3	M	52	0	0	0	0
3	N	36	0	0	0	0
All	All	18730	0	17992	29	0

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

All (29) 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:E:111:ASN:HD22	1:E:140:LEU:HD13	1.56	0.71
1:E:107:GLN:NE2	1:E:139:ILE:HG22	2.21	0.55
1:C:195:ALA:HB2	1:N:198:ILE:HG22	1.89	0.55
1:H:204:GLN:HE22	1:I:174:ARG:HD3	1.72	0.54
1:C:177:ILE:HD11	1:C:223:ALA:CB	2.38	0.53
1:C:177:ILE:HD11	1:C:223:ALA:HB3	1.93	0.51
1:A:204:GLN:HE22	1:B:174:ARG:HD3	1.77	0.50
1:B:153:SER:OG	1:B:154:MET:N	2.45	0.48
1:C:107:GLN:NE2	1:C:139:ILE:HB	2.28	0.48
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.94	0.48
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.96	0.47
1:K:134:ASP:HB3	1:L:170:LEU:HD23	1.96	0.47
1:M:118:TYR:CE2	1:M:148:VAL:HG21	2.51	0.46
1:K:107:GLN:NE2	1:K:139:ILE:HG22	2.31	0.45
1:N:148:VAL:HG22	1:N:170:LEU:HD23	1.98	0.45
1:B:198:ILE:HG22	1:H:195:ALA:HB2	1.99	0.45
1:J:139:ILE:HD11	1:J:143:ILE:HD11	1.99	0.45
1:B:139:ILE:HD11	1:B:143:ILE:HD11	1.99	0.45
1:G:76:TYR:HA	1:G:79:LEU:HD12	1.99	0.44
1:E:209:TYR:HB3	1:E:220:ILE:HD12	1.98	0.44
1:M:177:ILE:HD11	1:M:223:ALA:CB	2.48	0.44
1:A:104:LEU:HD11	2:B:302:OSR:C12	2.48	0.44
1:H:169:SER:HB2	1:H:241:LEU:HD22	2.01	0.42
1:M:118:TYR:CE2	1:M:148:VAL:CG2	3.04	0.41
1:A:206:TYR:CE2	1:A:221:GLU:HG2	2.55	0.41
1:C:107:GLN:HE22	1:C:140:LEU:H	1.69	0.41
1:H:206:TYR:CE2	1:H:221:GLU:HG3	2.56	0.40
1:F:105:PHE:HB2	2:G:302:OSR:BR	2.77	0.40
1:C:107:GLN:HE21	1:C:107:GLN:HB2	1.55	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	158/221 (72%)	154 (98%)	4 (2%)	0	100	100
1	B	158/221 (72%)	156 (99%)	2 (1%)	0	100	100
1	C	158/221 (72%)	156 (99%)	2 (1%)	0	100	100
1	D	159/221 (72%)	157 (99%)	2 (1%)	0	100	100
1	E	157/221 (71%)	154 (98%)	3 (2%)	0	100	100
1	F	160/221 (72%)	158 (99%)	2 (1%)	0	100	100
1	G	160/221 (72%)	157 (98%)	3 (2%)	0	100	100
1	H	157/221 (71%)	154 (98%)	3 (2%)	0	100	100
1	I	157/221 (71%)	154 (98%)	3 (2%)	0	100	100
1	J	159/221 (72%)	156 (98%)	3 (2%)	0	100	100
1	K	157/221 (71%)	153 (98%)	4 (2%)	0	100	100
1	L	157/221 (71%)	153 (98%)	4 (2%)	0	100	100
1	M	158/221 (72%)	156 (99%)	2 (1%)	0	100	100
1	N	159/221 (72%)	157 (99%)	2 (1%)	0	100	100
All	All	2214/3094 (72%)	2175 (98%)	39 (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	140/185 (76%)	137 (98%)	3 (2%)	53	57
1	B	137/185 (74%)	136 (99%)	1 (1%)	84	88
1	C	138/185 (75%)	135 (98%)	3 (2%)	52	55
1	D	138/185 (75%)	136 (99%)	2 (1%)	67	72
1	E	137/185 (74%)	136 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	140/185 (76%)	138 (99%)	2 (1%)	67 72
1	G	142/185 (77%)	141 (99%)	1 (1%)	84 88
1	H	138/185 (75%)	134 (97%)	4 (3%)	42 43
1	I	138/185 (75%)	136 (99%)	2 (1%)	67 72
1	J	142/185 (77%)	140 (99%)	2 (1%)	67 72
1	K	138/185 (75%)	137 (99%)	1 (1%)	84 88
1	L	136/185 (74%)	134 (98%)	2 (2%)	65 69
1	M	137/185 (74%)	136 (99%)	1 (1%)	84 88
1	N	142/185 (77%)	141 (99%)	1 (1%)	84 88
All	All	1943/2590 (75%)	1917 (99%)	26 (1%)	69 74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	MET
1	A	148	VAL
1	A	247	HIS
1	B	107	GLN
1	C	88	MET
1	C	107	GLN
1	C	245	LEU
1	D	218	GLN
1	D	247	HIS
1	E	113	LYS
1	F	88	MET
1	F	148	VAL
1	G	107	GLN
1	H	107	GLN
1	H	112	LYS
1	H	148	VAL
1	H	247	HIS
1	I	148	VAL
1	I	245	LEU
1	J	148	VAL
1	J	245	LEU
1	K	218	GLN
1	L	107	GLN
1	L	247	HIS
1	M	236	GLN

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Mol	Chain	Res	Type
1	N	88	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	107	GLN
1	A	204	GLN
1	A	236	GLN
1	B	102	GLN
1	C	107	GLN
1	D	102	GLN
1	G	179	GLN
1	G	194	GLN
1	H	102	GLN
1	H	204	GLN
1	I	102	GLN
1	I	150	GLN
1	I	218	GLN
1	K	102	GLN
1	K	194	GLN
1	L	111	ASN
1	M	111	ASN
1	N	179	GLN
1	N	194	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 (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OSR	B	301	-	42,44,44	0.27	0	55,63,63	0.71	1 (1%)
2	OSR	G	302	-	42,44,44	0.27	0	55,63,63	0.63	0
2	OSR	F	301	-	42,44,44	0.27	0	55,63,63	0.68	1 (1%)
2	OSR	H	301	-	42,44,44	0.26	0	55,63,63	0.79	2 (3%)
2	OSR	C	301	-	42,44,44	0.27	0	55,63,63	0.70	1 (1%)
2	OSR	J	301	-	42,44,44	0.27	0	55,63,63	0.66	0
2	OSR	K	302	-	42,44,44	0.28	0	55,63,63	0.74	2 (3%)
2	OSR	L	301	-	42,44,44	0.29	0	55,63,63	0.79	2 (3%)
2	OSR	G	301	-	42,44,44	0.29	0	55,63,63	0.77	2 (3%)
2	OSR	K	301	-	42,44,44	0.28	0	55,63,63	0.63	1 (1%)
2	OSR	B	302	-	42,44,44	0.27	0	55,63,63	0.63	1 (1%)
2	OSR	I	301	-	42,44,44	0.28	0	55,63,63	0.76	2 (3%)
2	OSR	D	301	-	42,44,44	0.28	0	55,63,63	0.65	2 (3%)
2	OSR	M	301	-	42,44,44	0.29	0	55,63,63	0.66	1 (1%)

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	OSR	B	301	-	-	4/21/54/54	0/5/5/5
2	OSR	G	302	-	-	2/21/54/54	0/5/5/5
2	OSR	F	301	-	-	2/21/54/54	0/5/5/5
2	OSR	H	301	-	-	6/21/54/54	0/5/5/5
2	OSR	C	301	-	-	2/21/54/54	0/5/5/5
2	OSR	J	301	-	-	5/21/54/54	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OSR	K	302	-	-	0/21/54/54	0/5/5/5
2	OSR	L	301	-	-	0/21/54/54	0/5/5/5
2	OSR	G	301	-	-	2/21/54/54	0/5/5/5
2	OSR	K	301	-	-	2/21/54/54	0/5/5/5
2	OSR	B	302	-	-	2/21/54/54	0/5/5/5
2	OSR	I	301	-	-	2/21/54/54	0/5/5/5
2	OSR	D	301	-	-	2/21/54/54	0/5/5/5
2	OSR	M	301	-	-	2/21/54/54	0/5/5/5

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	OSR	C19-C18-N	-3.78	106.20	111.02
2	H	301	OSR	C18-C19-N1	3.55	118.67	112.59
2	G	301	OSR	C19-C18-N	-3.52	106.54	111.02
2	L	301	OSR	C19-C18-N	-3.51	106.55	111.02
2	F	301	OSR	C19-C18-N	-3.28	106.84	111.02
2	K	302	OSR	C19-C18-N	-3.25	106.88	111.02
2	B	301	OSR	C19-C18-N	-3.19	106.96	111.02
2	C	301	OSR	C21-N2-C20	3.07	123.61	120.84
2	B	302	OSR	C19-C18-N	-2.85	107.39	111.02
2	L	301	OSR	C18-C19-N1	2.69	117.19	112.59
2	G	301	OSR	C18-C19-N1	2.65	117.12	112.59
2	D	301	OSR	C19-C18-N	-2.45	107.90	111.02
2	M	301	OSR	C19-C18-N	-2.16	108.27	111.02
2	H	301	OSR	C21-N2-C20	2.13	122.76	120.84
2	K	302	OSR	C18-C19-N1	2.11	116.20	112.59
2	K	301	OSR	C19-C18-N	-2.09	108.36	111.02
2	I	301	OSR	C18-C19-N1	2.08	116.16	112.59
2	D	301	OSR	C18-C19-N1	2.00	116.02	112.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	OSR	N2-C20-N1-C28
2	C	301	OSR	O2-C20-N1-C28
2	G	302	OSR	N2-C20-N1-C28
2	G	302	OSR	O2-C20-N1-C28

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Mol	Chain	Res	Type	Atoms
2	H	301	OSR	N2-C20-N1-C28
2	H	301	OSR	O2-C20-N1-C28
2	J	301	OSR	N2-C20-N1-C28
2	J	301	OSR	O2-C20-N1-C28
2	B	301	OSR	O2-C20-N1-C28
2	B	302	OSR	O2-C20-N1-C28
2	D	301	OSR	O2-C20-N1-C28
2	F	301	OSR	C12-C10-O1-C11
2	B	301	OSR	N2-C20-N1-C28
2	J	301	OSR	C12-C10-O1-C11
2	B	301	OSR	C12-C10-O1-C11
2	F	301	OSR	C9-C10-O1-C11
2	H	301	OSR	C-C1-C2-C4
2	B	302	OSR	N2-C20-N1-C28
2	D	301	OSR	N2-C20-N1-C28
2	J	301	OSR	C9-C10-O1-C11
2	G	301	OSR	C12-C10-O1-C11
2	I	301	OSR	C12-C10-O1-C11
2	B	301	OSR	C9-C10-O1-C11
2	K	301	OSR	C12-C10-O1-C11
2	M	301	OSR	C12-C10-O1-C11
2	H	301	OSR	C12-C10-O1-C11
2	H	301	OSR	C-C1-C2-C3
2	K	301	OSR	C9-C10-O1-C11
2	G	301	OSR	C9-C10-O1-C11
2	I	301	OSR	C9-C10-O1-C11
2	M	301	OSR	C9-C10-O1-C11
2	J	301	OSR	C22-C21-N2-C20
2	H	301	OSR	C9-C10-O1-C11

There are no ring outliers.

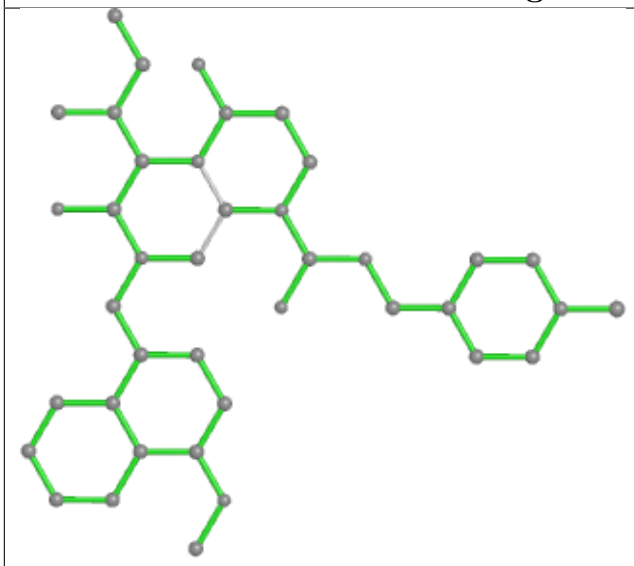
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	302	OSR	1	0
2	B	302	OSR	1	0

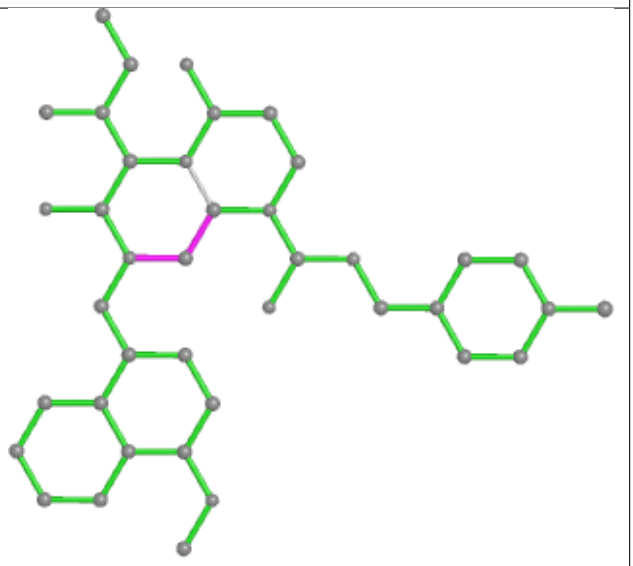
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

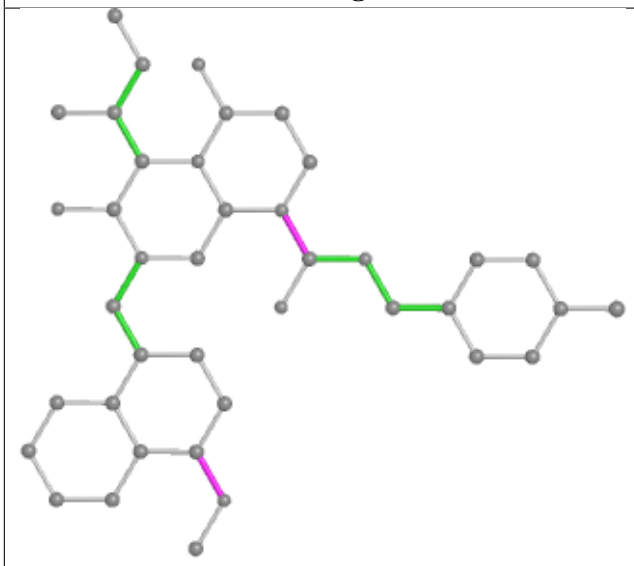
Ligand OSR B 301



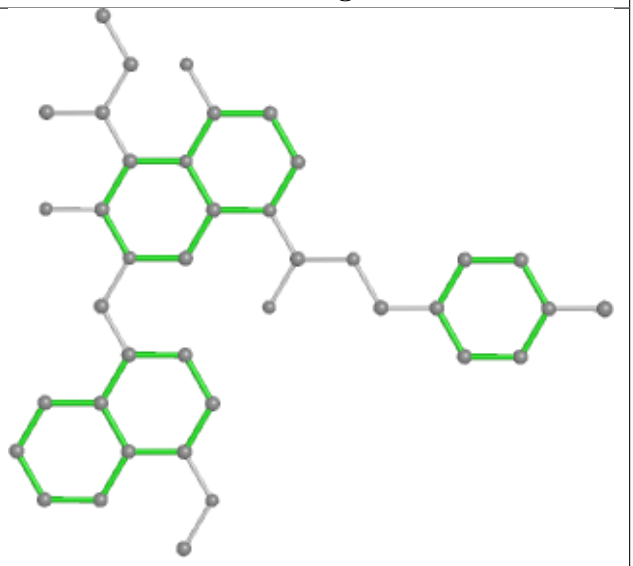
Bond lengths



Bond angles

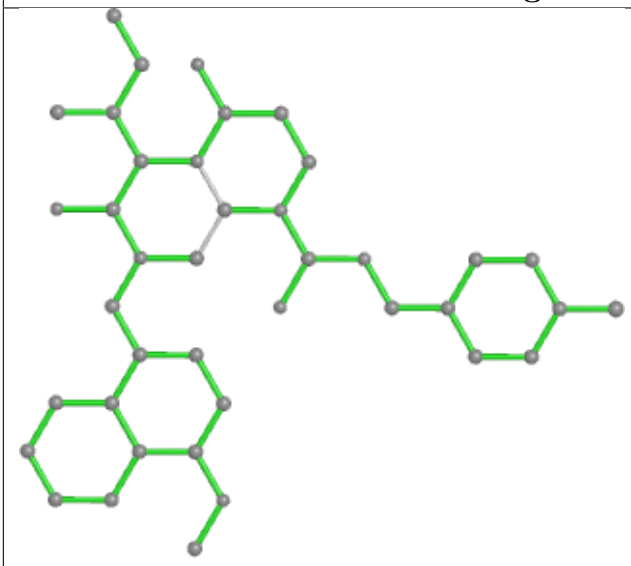


Torsions



Rings

Ligand OSR G 302



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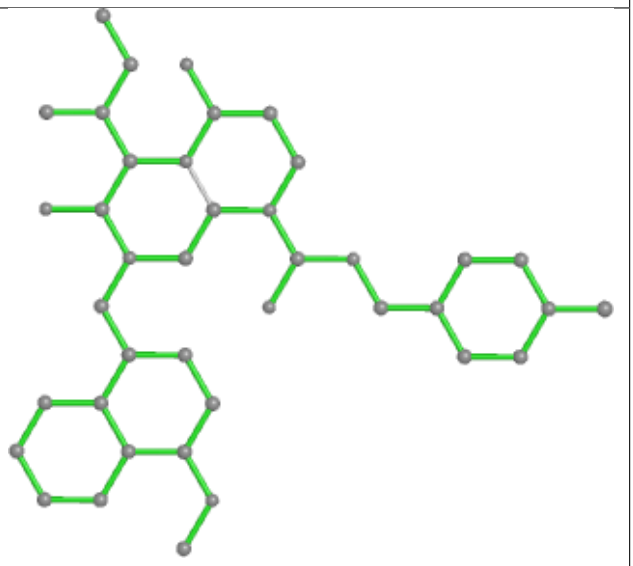
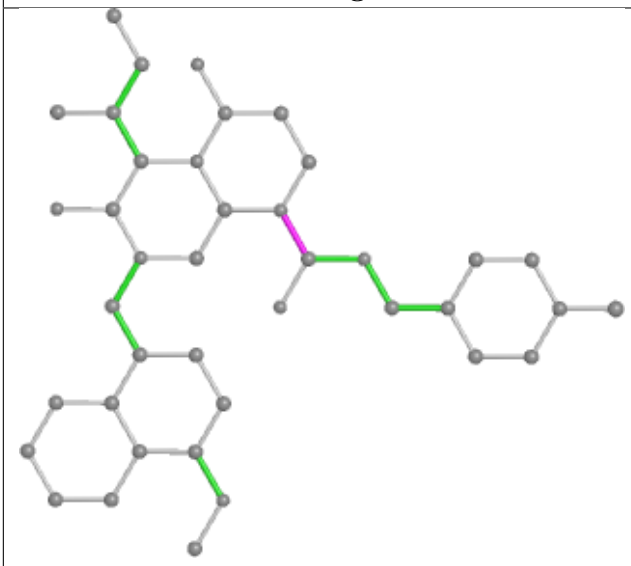


Bond angles



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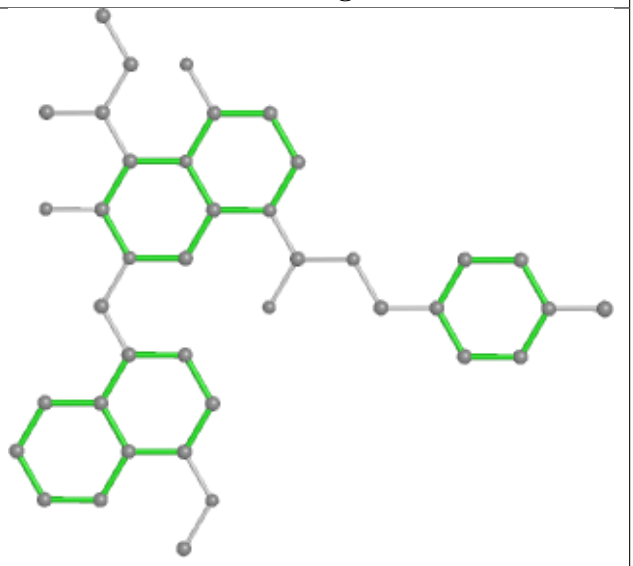
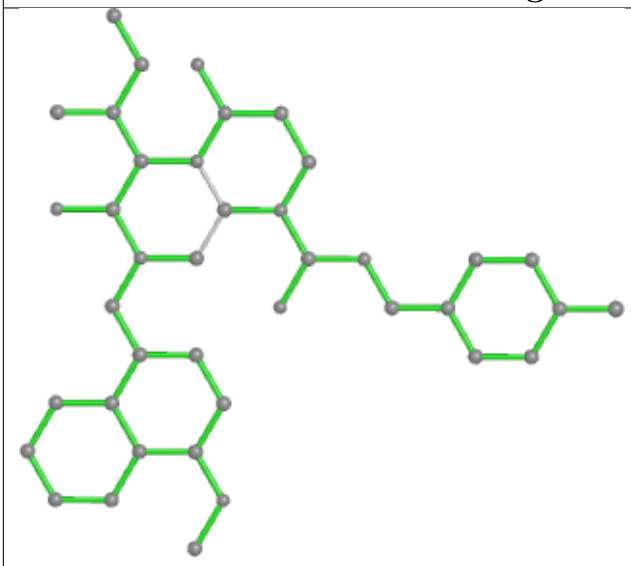
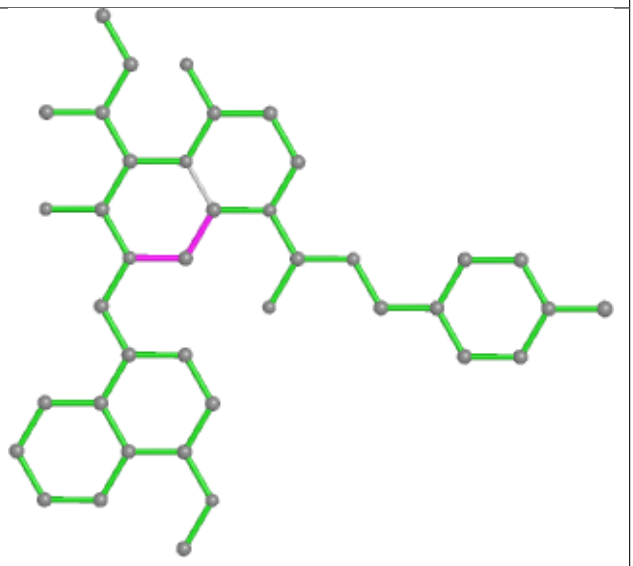


Rings

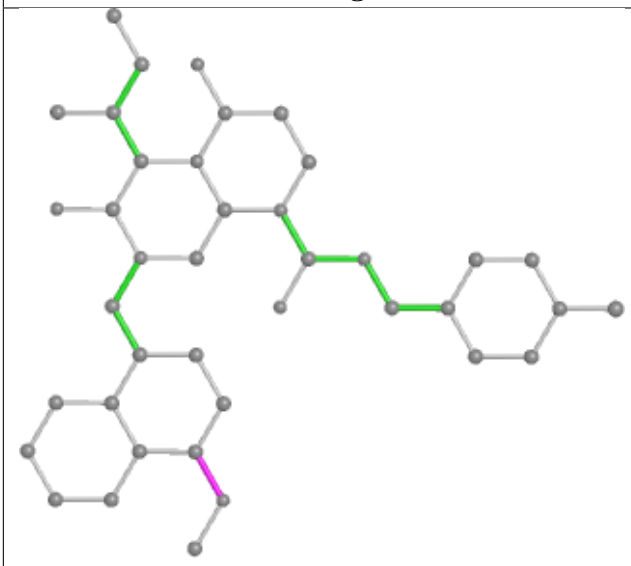
Ligand OSR F 301



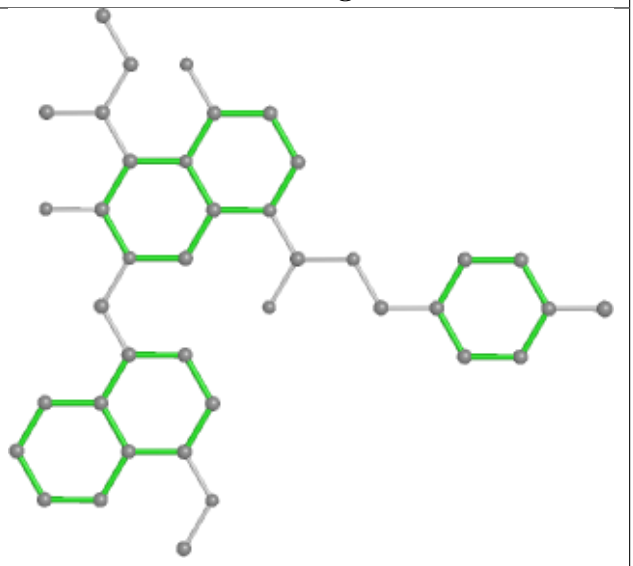
Bond lengths



Bond angles

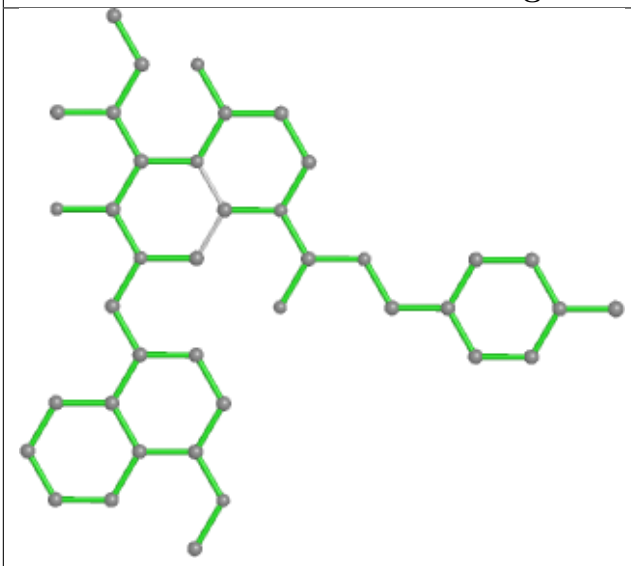


Torsions

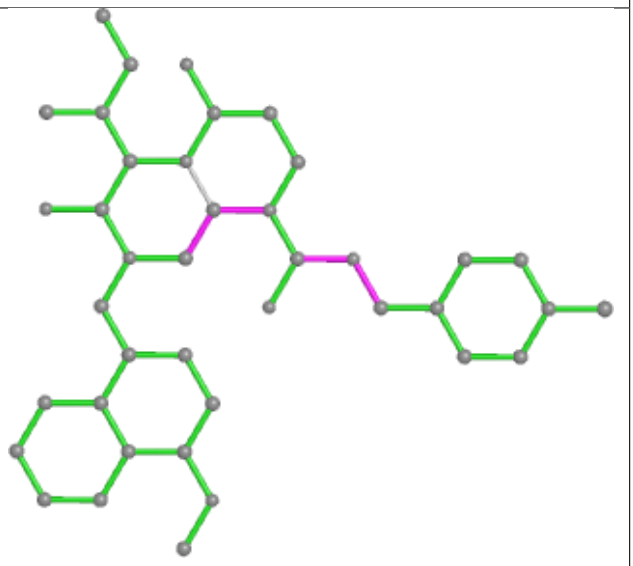


Rings

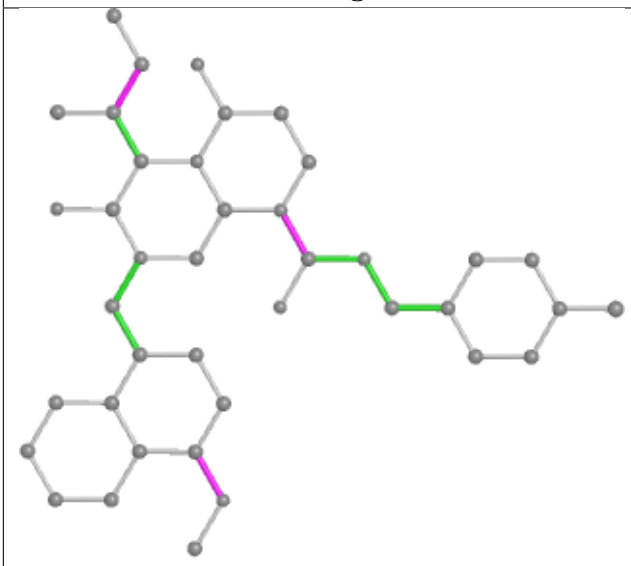
Ligand OSR H 301



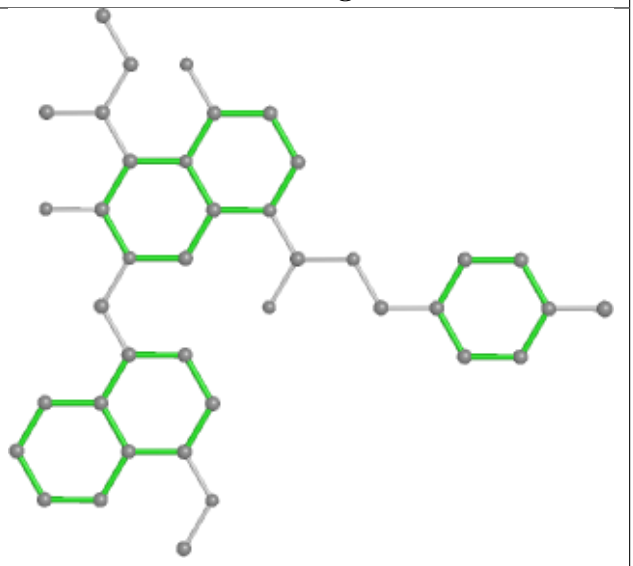
Bond lengths



Bond angles

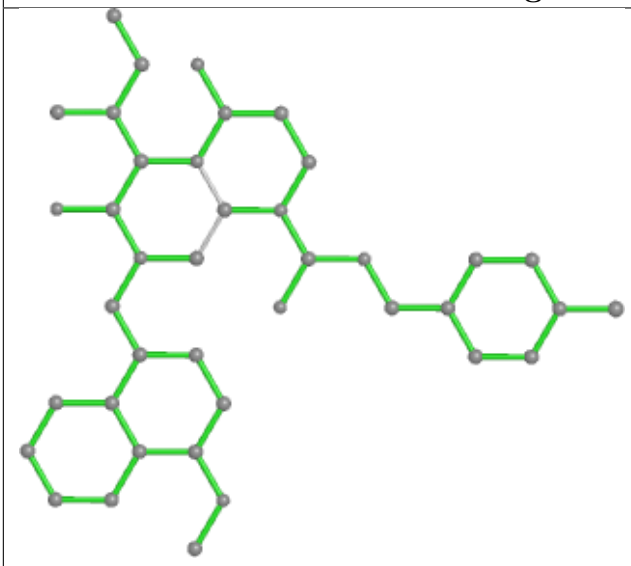


Torsions

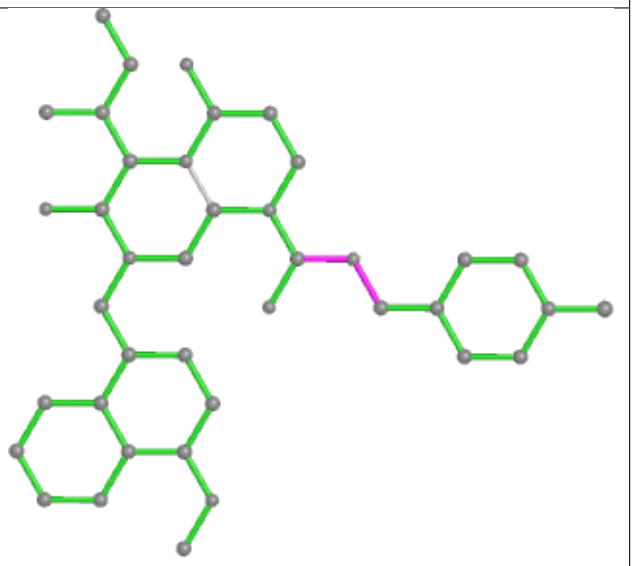


Rings

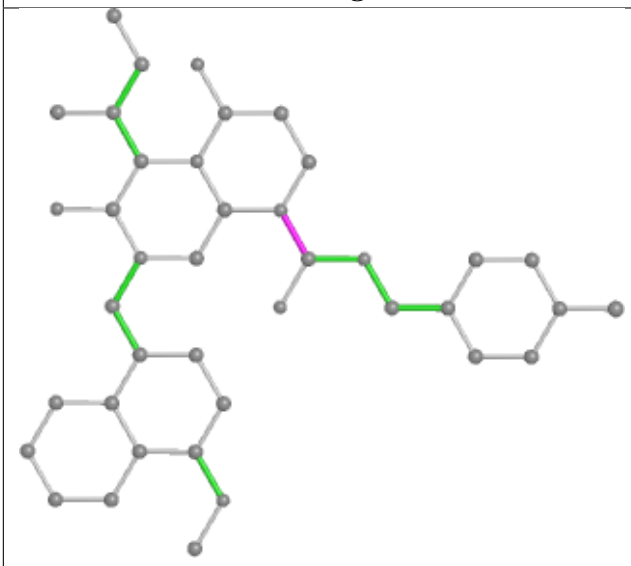
Ligand OSR C 301



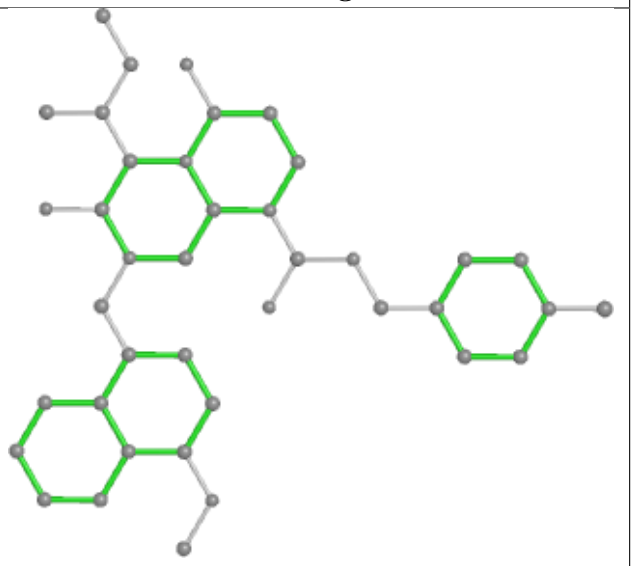
Bond lengths



Bond angles

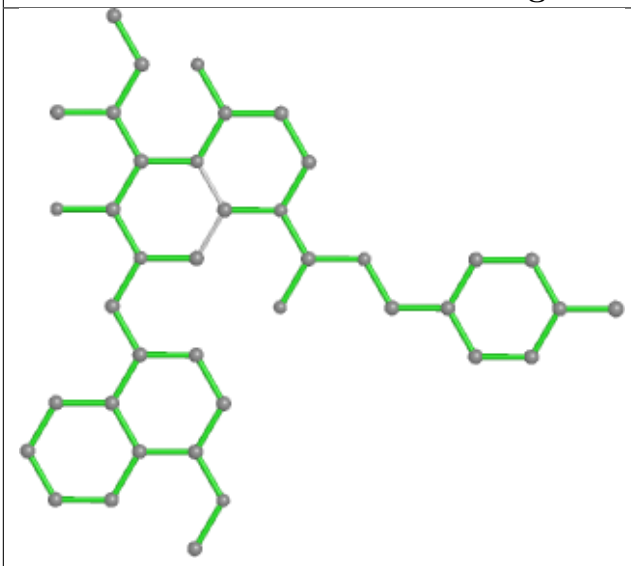


Torsions

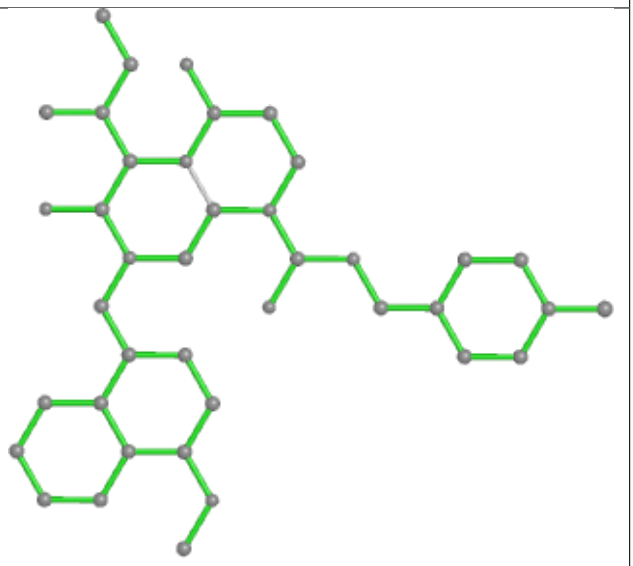


Rings

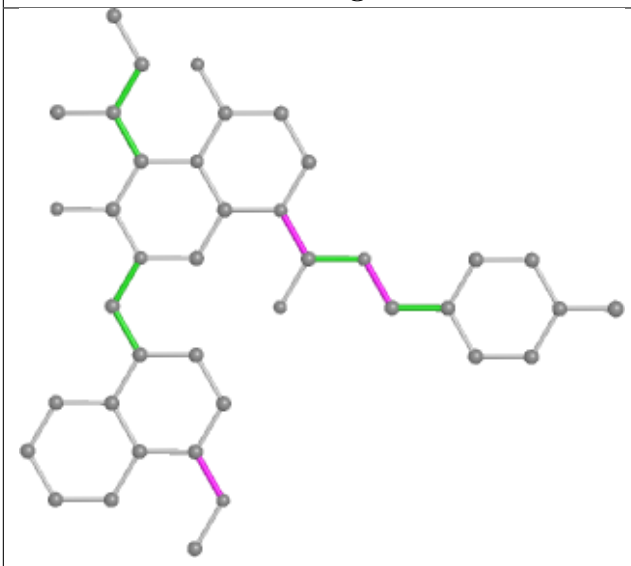
Ligand OSR J 301



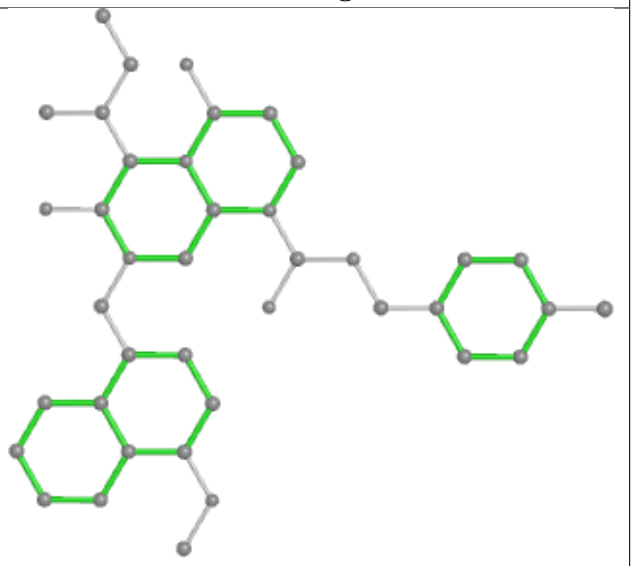
Bond lengths



Bond angles

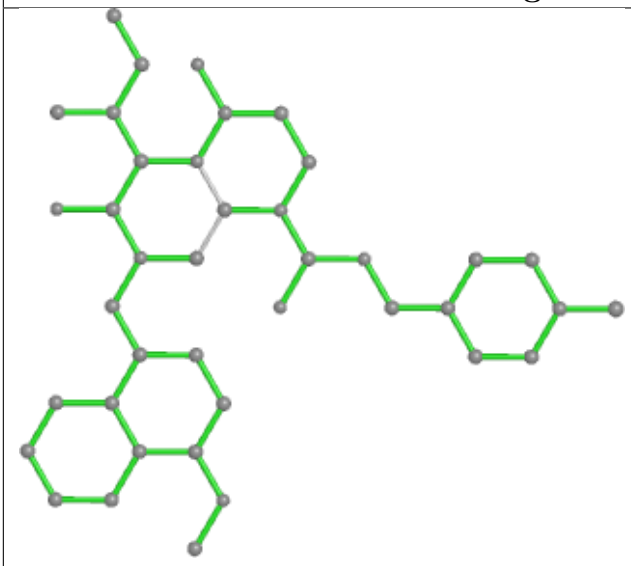


Torsions

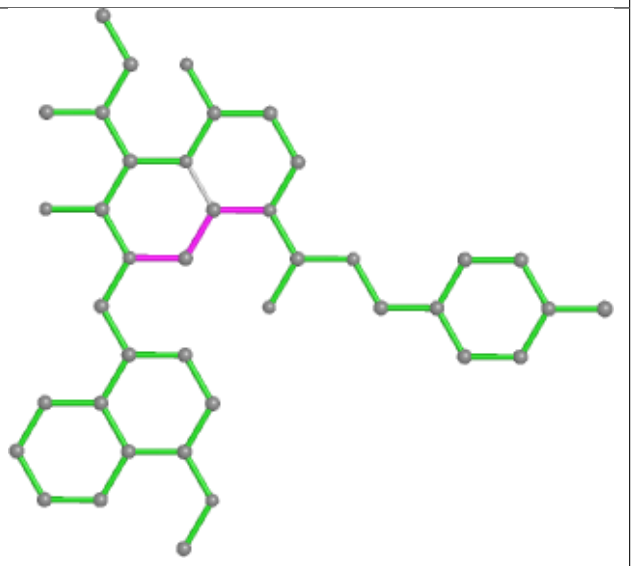


Rings

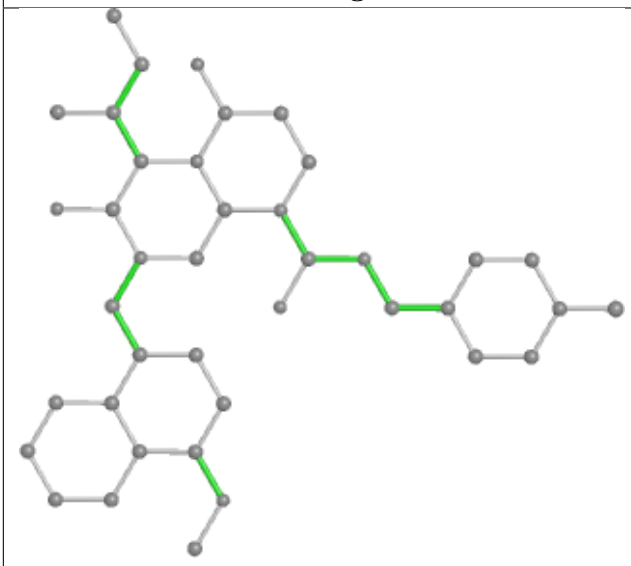
Ligand OSR K 302



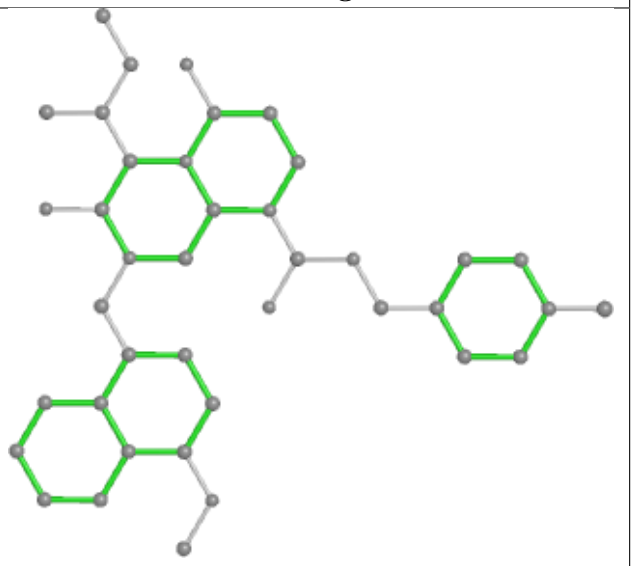
Bond lengths



Bond angles

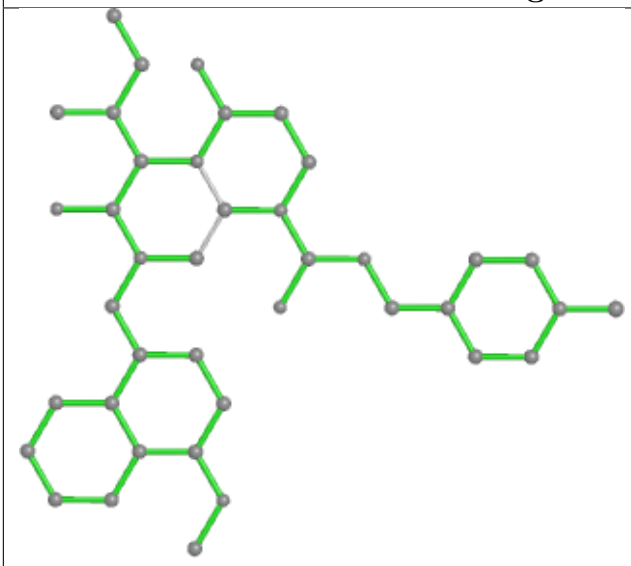


Torsions

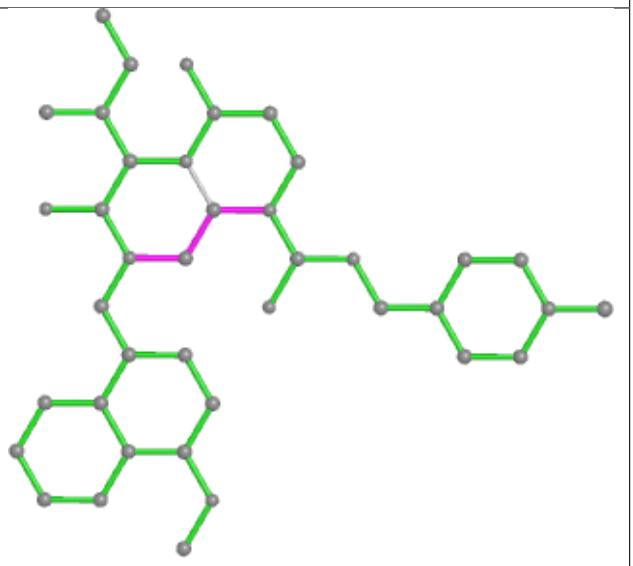


Rings

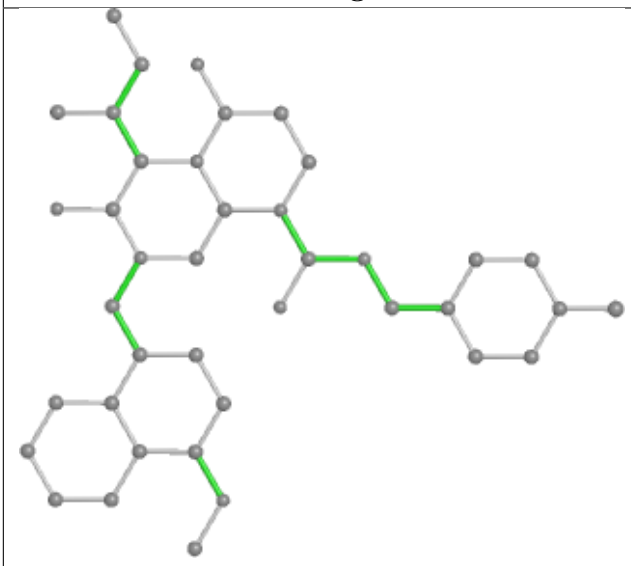
Ligand OSR L 301



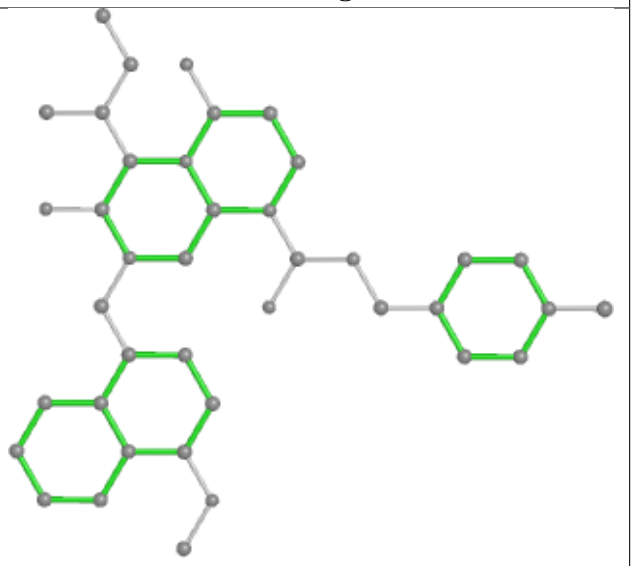
Bond lengths



Bond angles

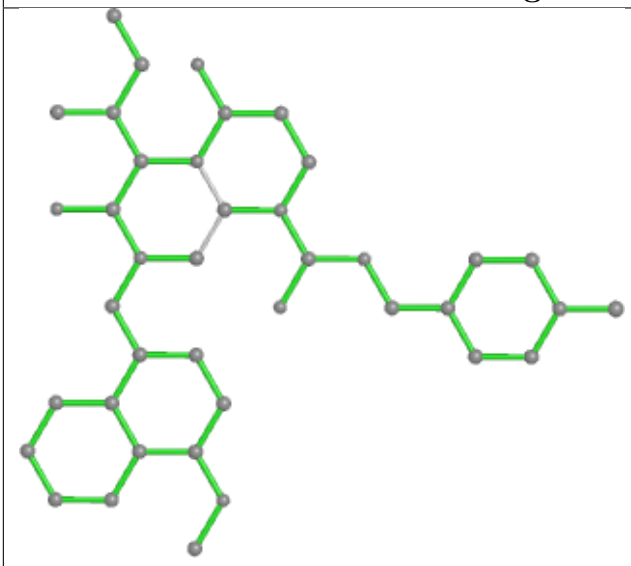


Torsions

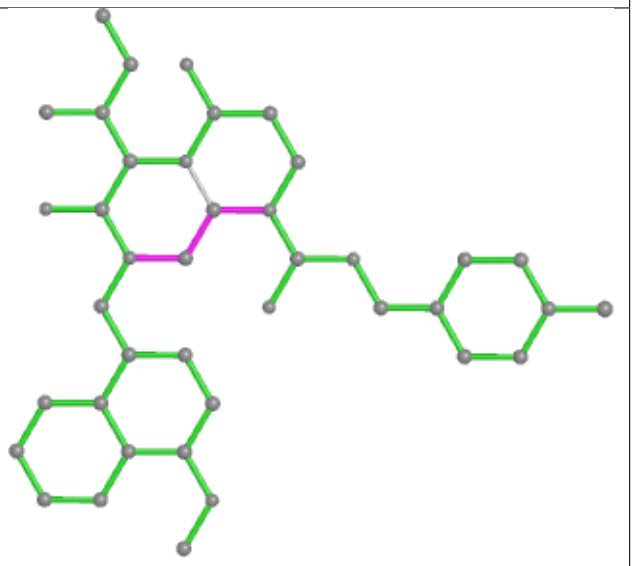


Rings

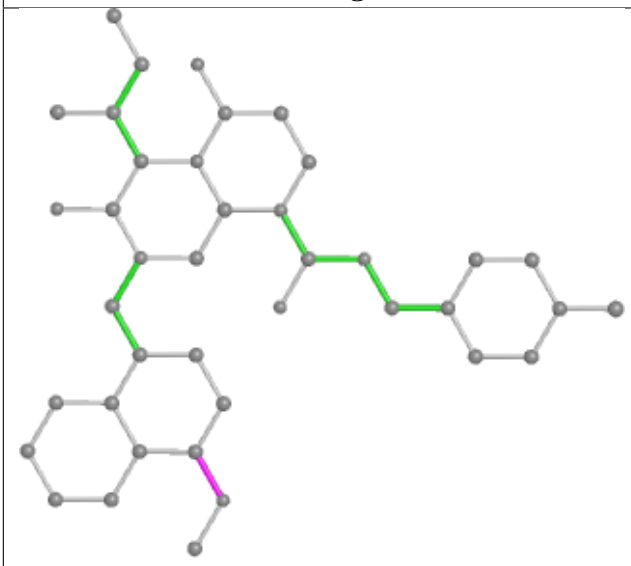
Ligand OSR G 301



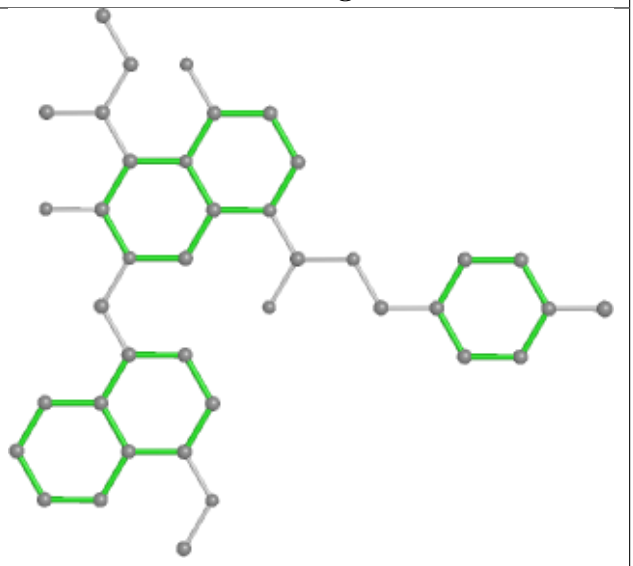
Bond lengths



Bond angles

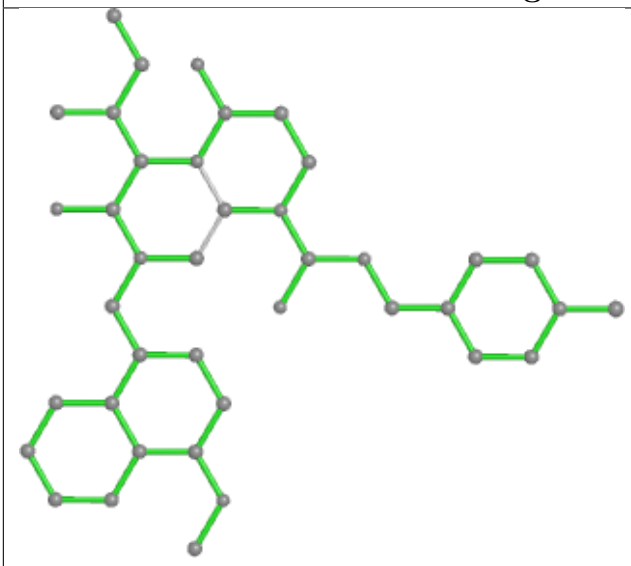


Torsions

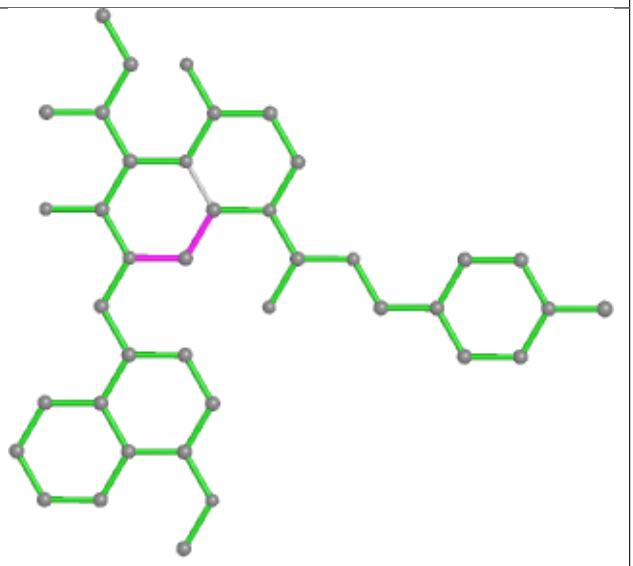


Rings

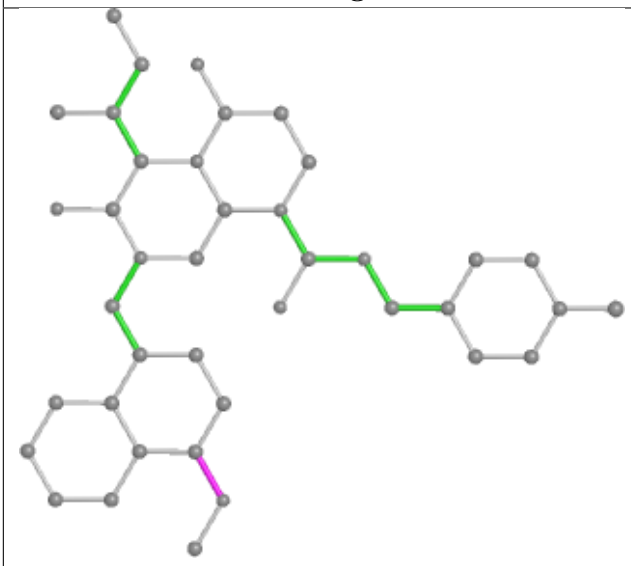
Ligand OSR K 301



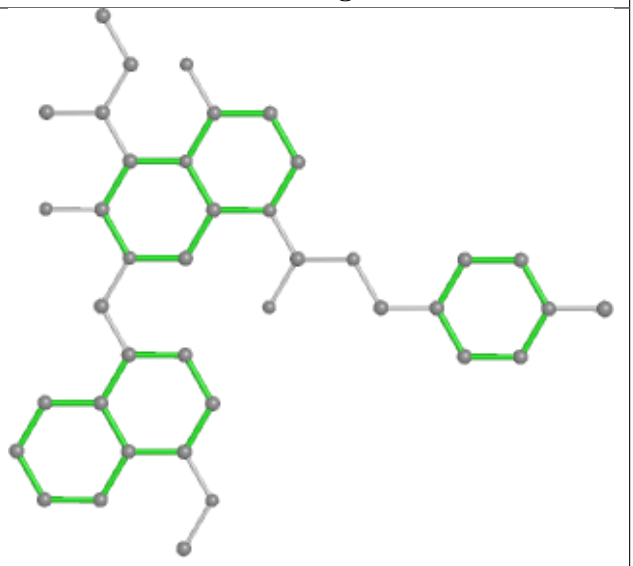
Bond lengths



Bond angles

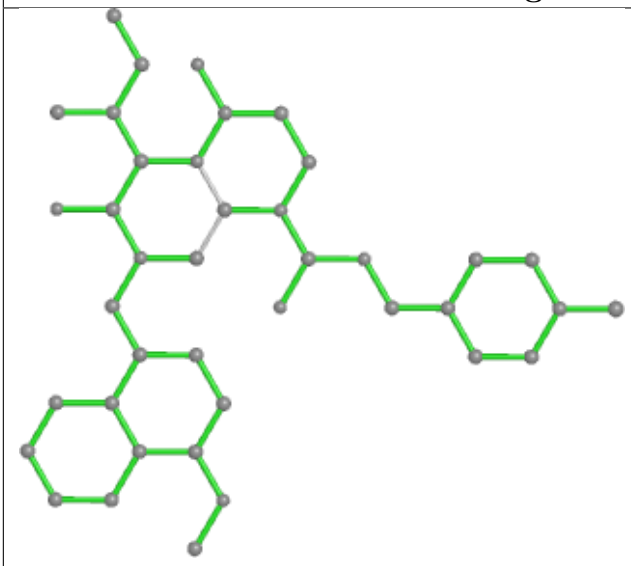


Torsions

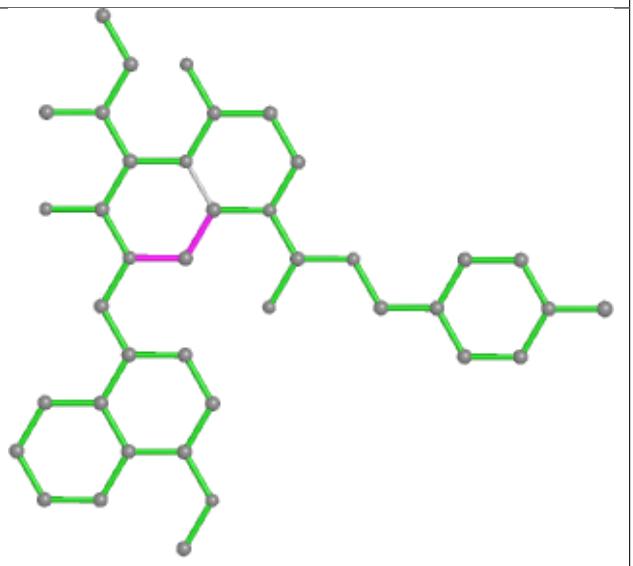


Rings

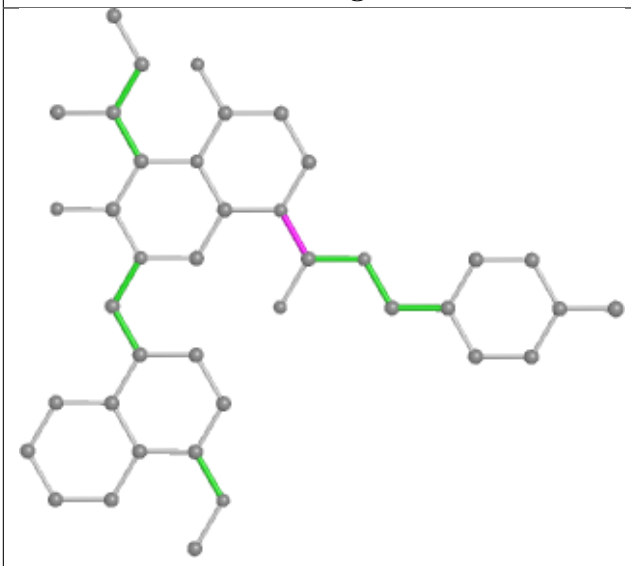
Ligand OSR B 302



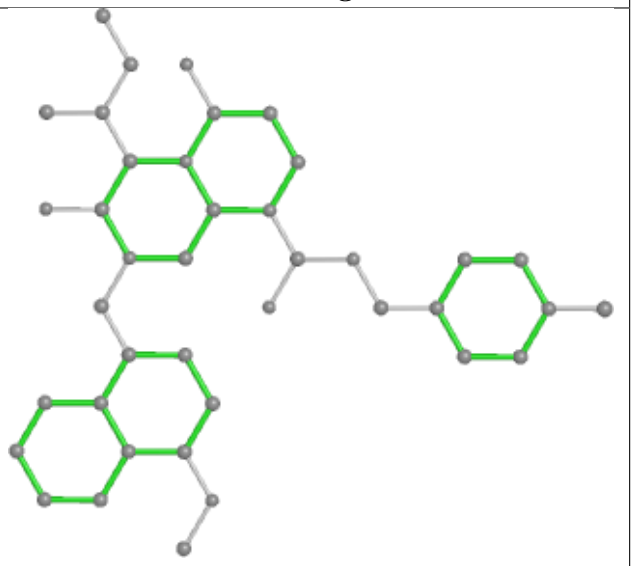
Bond lengths



Bond angles

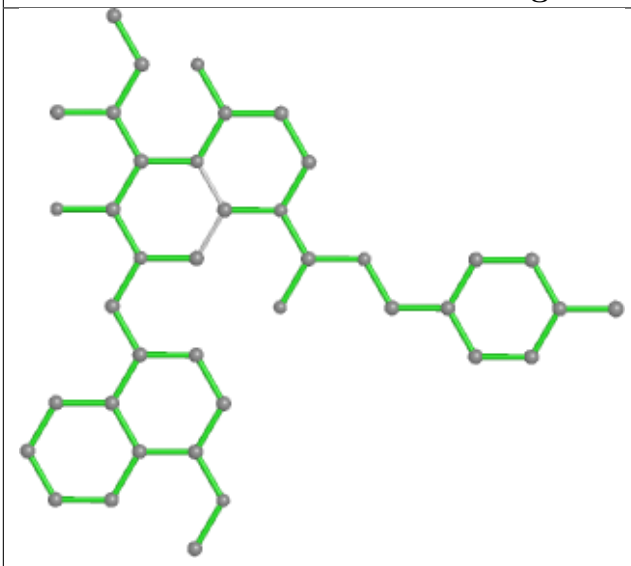


Torsions

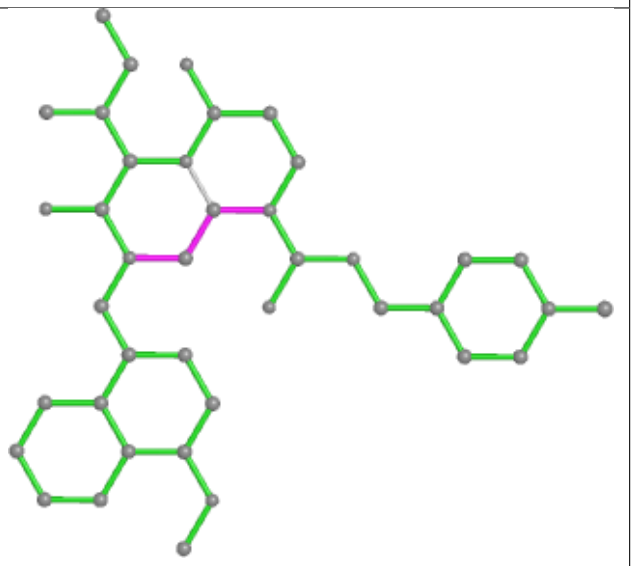


Rings

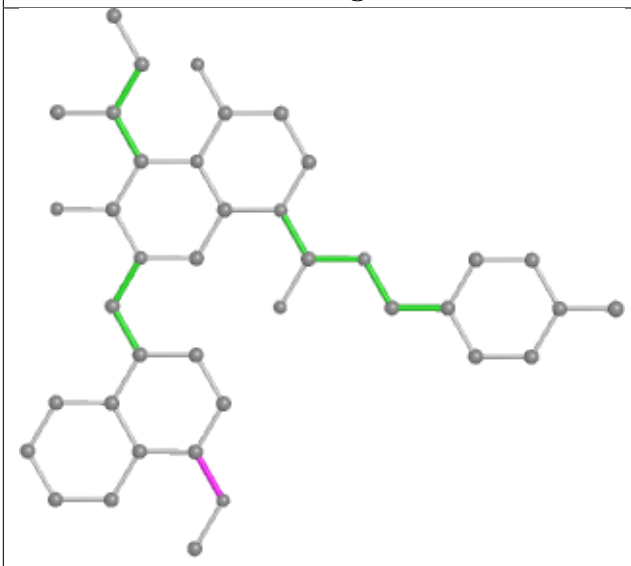
Ligand OSR I 301



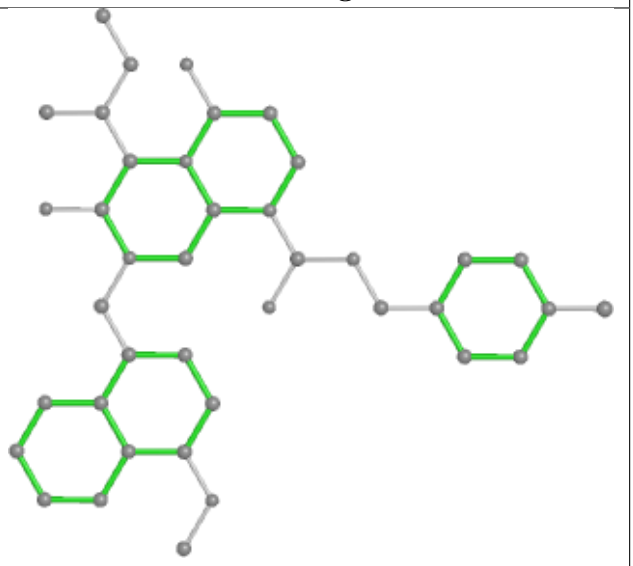
Bond lengths



Bond angles

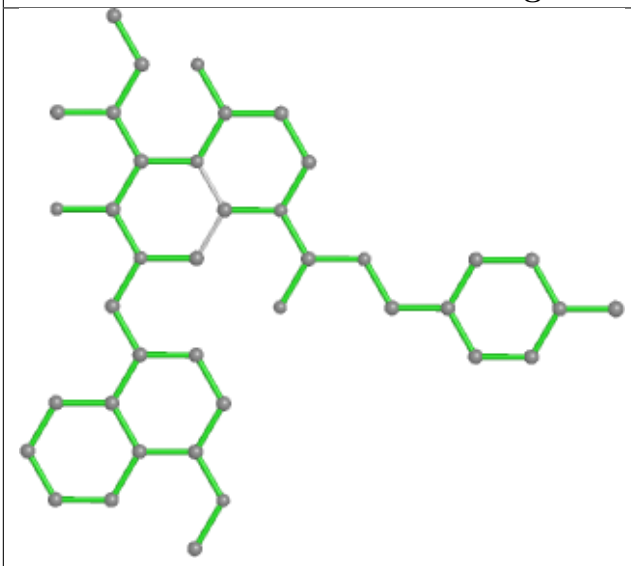


Torsions

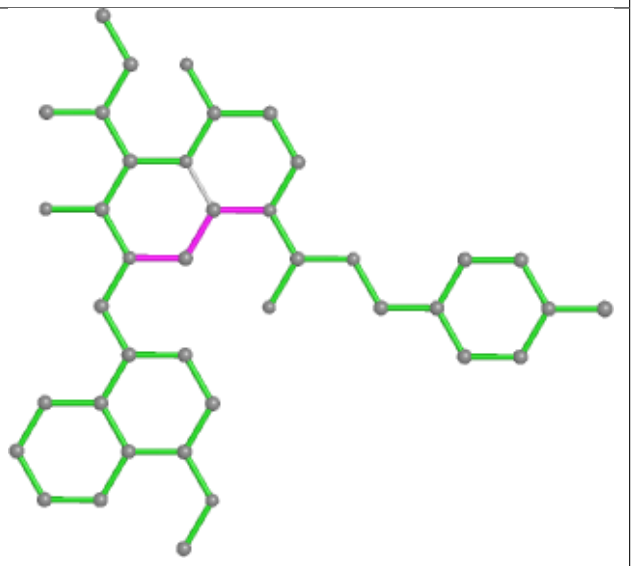


Rings

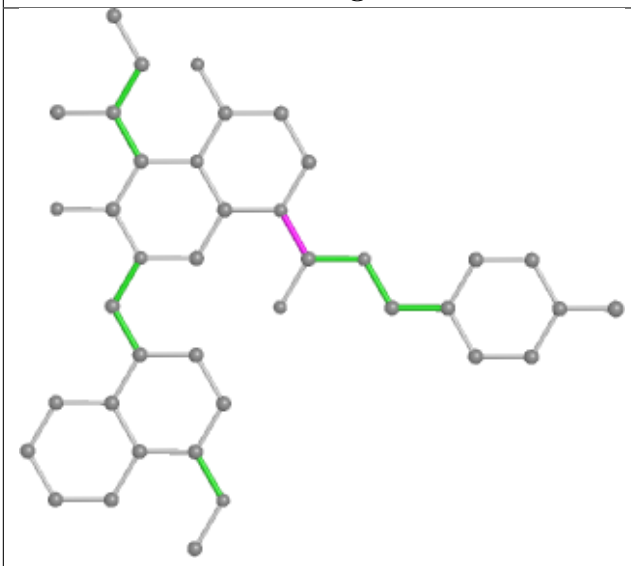
Ligand OSR D 301



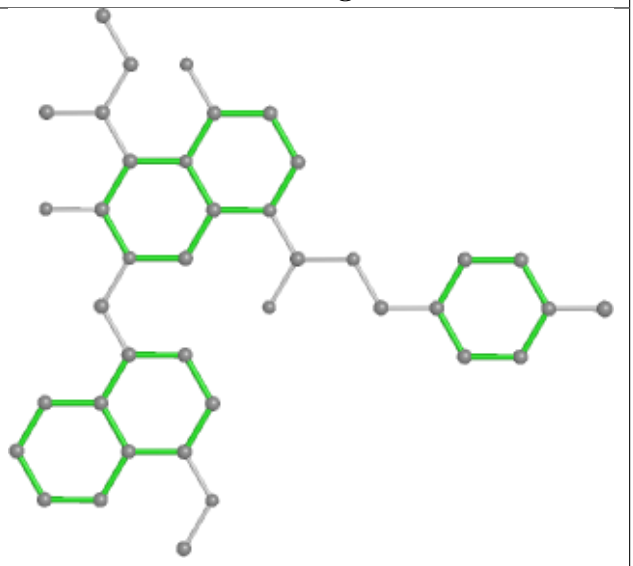
Bond lengths



Bond angles

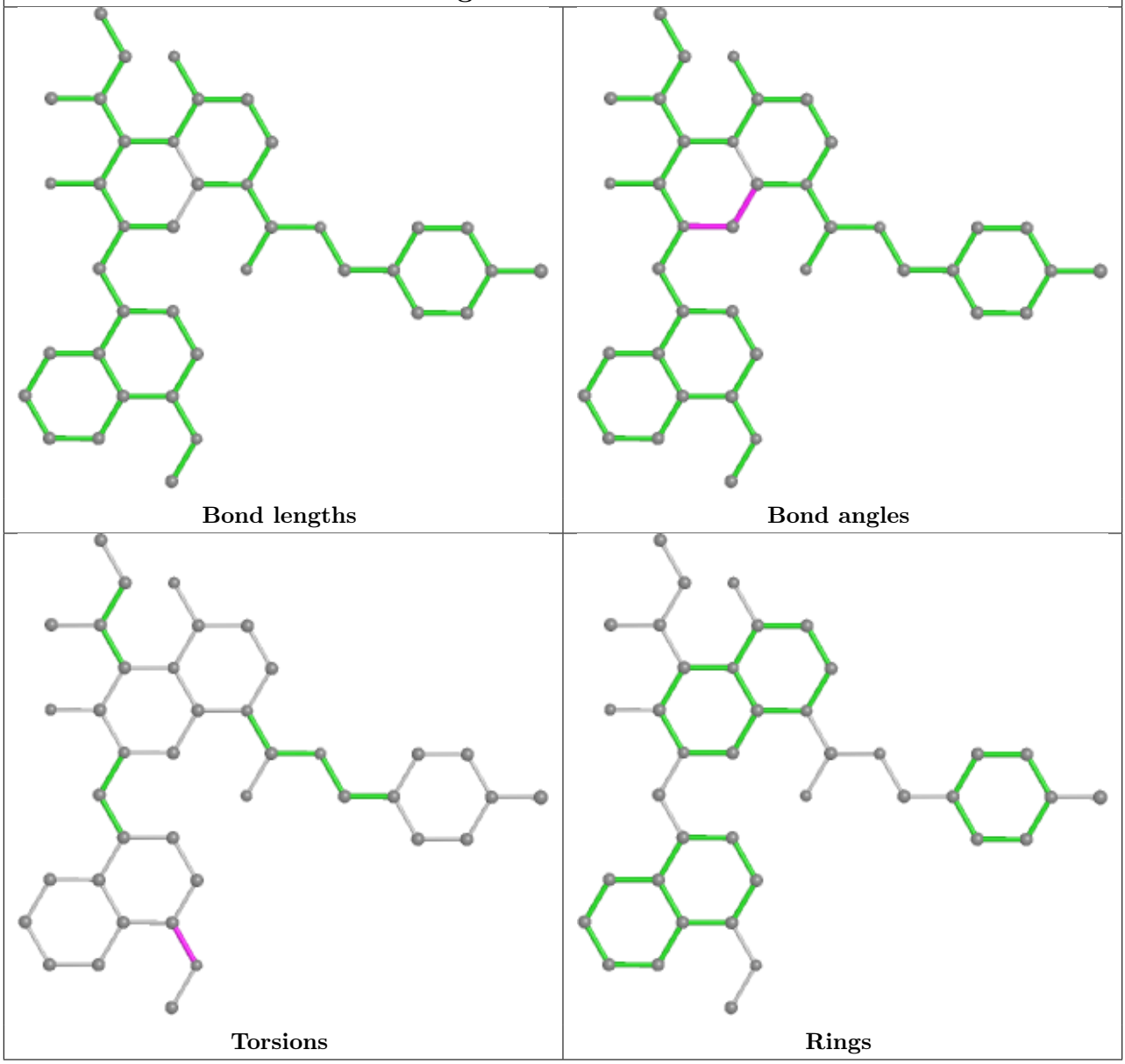


Torsions



Rings

Ligand OSR M 301



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	162/221 (73%)	0.53	11 (6%) 17 16	19, 28, 45, 60	0
1	B	162/221 (73%)	0.64	8 (4%) 29 28	21, 29, 48, 72	0
1	C	162/221 (73%)	0.87	21 (12%) 3 3	21, 30, 54, 74	0
1	D	163/221 (73%)	0.57	14 (8%) 10 9	18, 27, 47, 60	0
1	E	161/221 (72%)	0.62	19 (11%) 4 4	14, 23, 49, 75	0
1	F	164/221 (74%)	0.55	10 (6%) 21 20	13, 21, 41, 71	0
1	G	164/221 (74%)	0.82	23 (14%) 2 2	17, 27, 48, 59	0
1	H	161/221 (72%)	0.51	13 (8%) 12 11	17, 25, 50, 66	0
1	I	161/221 (72%)	0.58	11 (6%) 17 16	18, 26, 49, 75	0
1	J	163/221 (73%)	1.00	23 (14%) 2 2	21, 31, 53, 72	0
1	K	161/221 (72%)	0.77	17 (10%) 6 5	19, 29, 51, 66	0
1	L	161/221 (72%)	0.86	22 (13%) 3 2	19, 30, 52, 73	0
1	M	162/221 (73%)	0.83	20 (12%) 4 3	16, 23, 54, 80	0
1	N	163/221 (73%)	0.69	15 (9%) 9 8	18, 28, 47, 63	0
All	All	2270/3094 (73%)	0.70	227 (10%) 7 6	13, 27, 51, 80	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	193	ILE	9.4
1	I	193	ILE	7.9
1	D	193	ILE	7.9
1	M	193	ILE	7.6
1	K	249	PRO	7.1
1	B	74	ASP	6.7
1	F	193	ILE	6.6
1	C	81	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	198	ILE	5.9
1	J	193	ILE	5.9
1	C	180	PRO	5.6
1	C	75	ILE	5.5
1	F	74	ASP	5.5
1	J	249	PRO	5.4
1	L	180	PRO	5.4
1	A	193	ILE	5.4
1	E	76	TYR	5.3
1	B	76	TYR	5.2
1	I	76	TYR	5.2
1	G	193	ILE	5.2
1	B	195	ALA	5.2
1	H	76	TYR	5.1
1	L	76	TYR	5.1
1	C	195	ALA	5.1
1	J	75	ILE	5.1
1	C	77	SER	5.0
1	K	180	PRO	5.0
1	G	180	PRO	4.9
1	E	75	ILE	4.7
1	L	249	PRO	4.7
1	M	75	ILE	4.6
1	G	250	GLN	4.6
1	B	198	ILE	4.6
1	K	76	TYR	4.6
1	B	180	PRO	4.5
1	M	76	TYR	4.5
1	H	75	ILE	4.5
1	I	140	LEU	4.4
1	C	76	TYR	4.4
1	N	76	TYR	4.4
1	C	198	ILE	4.3
1	L	195	ALA	4.3
1	A	75	ILE	4.2
1	C	140	LEU	4.1
1	I	75	ILE	4.1
1	D	112	LYS	4.1
1	E	248	PRO	4.0
1	E	77	SER	4.0
1	M	105	PHE	4.0
1	G	249	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	76	TYR	3.9
1	J	76	TYR	3.9
1	D	249	PRO	3.9
1	G	76	TYR	3.9
1	J	81	ARG	3.9
1	N	75	ILE	3.9
1	A	249	PRO	3.8
1	J	140	LEU	3.8
1	K	77	SER	3.7
1	J	105	PHE	3.7
1	J	77	SER	3.7
1	E	195	ALA	3.7
1	N	195	ALA	3.7
1	H	140	LEU	3.7
1	N	180	PRO	3.7
1	M	77	SER	3.6
1	L	105	PHE	3.5
1	G	119	ILE	3.5
1	M	249	PRO	3.5
1	F	75	ILE	3.5
1	L	75	ILE	3.5
1	A	76	TYR	3.4
1	M	78	ARG	3.4
1	H	78	ARG	3.4
1	M	112	LYS	3.4
1	M	195	ALA	3.4
1	J	119	ILE	3.4
1	E	74	ASP	3.3
1	M	79	LEU	3.3
1	C	111	ASN	3.3
1	I	194	GLN	3.3
1	E	140	LEU	3.2
1	H	81	ARG	3.2
1	F	77	SER	3.2
1	C	112	LYS	3.2
1	J	233	MET	3.2
1	F	194	GLN	3.1
1	D	198	ILE	3.1
1	E	245	LEU	3.1
1	G	140	LEU	3.1
1	G	75	ILE	3.1
1	M	148	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	105	PHE	3.0
1	G	105	PHE	3.0
1	H	248	PRO	3.0
1	G	194	GLN	3.0
1	L	77	SER	3.0
1	D	233	MET	3.0
1	E	194	GLN	2.9
1	D	247	HIS	2.9
1	K	248	PRO	2.9
1	H	195	ALA	2.9
1	M	80	LEU	2.9
1	N	194	GLN	2.9
1	K	233	MET	2.9
1	D	105	PHE	2.9
1	E	78	ARG	2.8
1	G	78	ARG	2.8
1	J	158	LEU	2.8
1	M	109	GLU	2.8
1	H	194	GLN	2.8
1	E	79	LEU	2.8
1	C	249	PRO	2.8
1	D	194	GLN	2.8
1	C	78	ARG	2.8
1	K	79	LEU	2.7
1	D	195	ALA	2.7
1	C	159	LEU	2.7
1	L	80	LEU	2.7
1	K	194	GLN	2.7
1	E	247	HIS	2.7
1	J	85	VAL	2.7
1	G	79	LEU	2.7
1	A	198	ILE	2.6
1	L	198	ILE	2.6
1	L	248	PRO	2.6
1	M	198	ILE	2.6
1	C	105	PHE	2.6
1	K	218	GLN	2.6
1	N	218	GLN	2.6
1	J	87	VAL	2.6
1	C	170	LEU	2.6
1	K	103	LEU	2.6
1	I	198	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	108	SER	2.6
1	J	111	ASN	2.6
1	G	87	VAL	2.6
1	E	214	LYS	2.5
1	G	112	LYS	2.5
1	J	78	ARG	2.5
1	D	76	TYR	2.5
1	A	247	HIS	2.5
1	K	198	ILE	2.5
1	H	77	SER	2.5
1	L	113	LYS	2.5
1	J	103	LEU	2.5
1	D	74	ASP	2.5
1	L	112	LYS	2.5
1	N	198	ILE	2.5
1	N	249	PRO	2.5
1	E	199	MET	2.5
1	A	105	PHE	2.5
1	J	180	PRO	2.4
1	G	218	GLN	2.4
1	C	119	ILE	2.4
1	E	246	VAL	2.4
1	K	140	LEU	2.4
1	J	160	ALA	2.4
1	H	198	ILE	2.4
1	A	78	ARG	2.4
1	M	104	LEU	2.4
1	G	233	MET	2.4
1	C	147	CYS	2.4
1	C	247	HIS	2.4
1	N	119	ILE	2.4
1	K	112	LYS	2.4
1	K	105	PHE	2.4
1	B	158	LEU	2.3
1	L	79	LEU	2.3
1	H	247	HIS	2.3
1	D	75	ILE	2.3
1	G	198	ILE	2.3
1	L	246	VAL	2.3
1	N	87	VAL	2.3
1	L	109	GLU	2.3
1	H	74	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	140	LEU	2.3
1	J	247	HIS	2.3
1	L	131	ALA	2.3
1	A	218	GLN	2.3
1	L	218	GLN	2.3
1	M	88	MET	2.2
1	G	159	LEU	2.2
1	J	198	ILE	2.2
1	E	197	GLU	2.2
1	J	80	LEU	2.2
1	K	247	HIS	2.2
1	M	170	LEU	2.2
1	L	233	MET	2.2
1	C	107	GLN	2.2
1	N	81	ARG	2.2
1	G	237	GLU	2.2
1	I	119	ILE	2.2
1	D	108	SER	2.2
1	J	217	LEU	2.2
1	I	105	PHE	2.2
1	F	249	PRO	2.1
1	K	143	ILE	2.1
1	A	140	LEU	2.1
1	F	108	SER	2.1
1	N	78	ARG	2.1
1	E	233	MET	2.1
1	D	140	LEU	2.1
1	N	140	LEU	2.1
1	J	195	ALA	2.1
1	G	81	ARG	2.1
1	I	77	SER	2.1
1	L	199	MET	2.1
1	M	175	ILE	2.1
1	E	104	LEU	2.1
1	L	140	LEU	2.1
1	A	194	GLN	2.1
1	C	197	GLU	2.1
1	H	197	GLU	2.1
1	G	118	TYR	2.1
1	I	233	MET	2.1
1	L	101	ALA	2.1
1	L	214	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	108	SER	2.0
1	F	78	ARG	2.0
1	C	245	LEU	2.0
1	G	88	MET	2.0
1	M	194	GLN	2.0
1	K	99	VAL	2.0
1	B	109	GLU	2.0
1	G	80	LEU	2.0
1	I	88	MET	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)

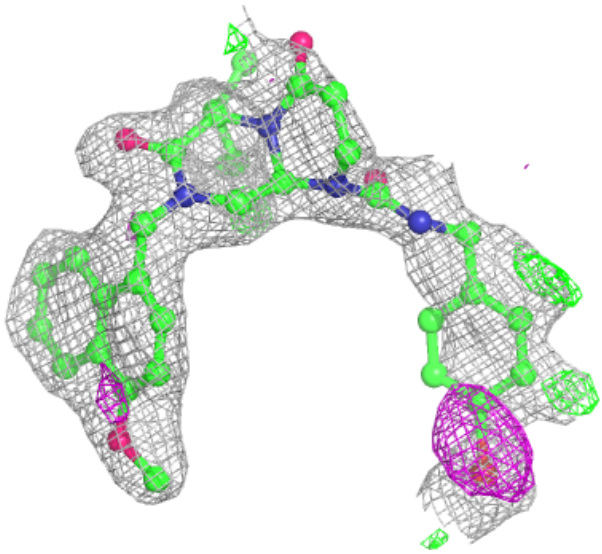
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

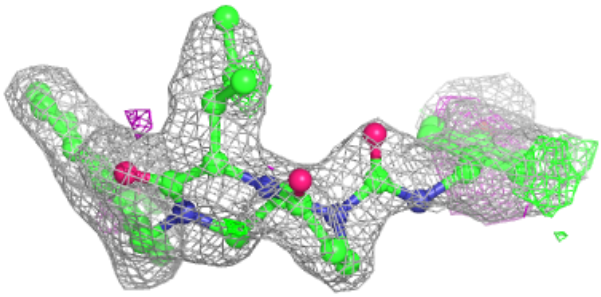
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OSR	C	301	40/40	0.71	0.23	45,55,87,99	0
2	OSR	K	301	40/40	0.79	0.20	44,53,71,80	0
2	OSR	M	301	40/40	0.80	0.28	40,52,65,69	0
2	OSR	G	302	40/40	0.83	0.19	32,39,52,60	0
2	OSR	B	302	40/40	0.83	0.19	37,50,59,64	0
2	OSR	B	301	40/40	0.83	0.18	37,46,60,67	0
2	OSR	L	301	40/40	0.84	0.18	35,42,53,60	0
2	OSR	J	301	40/40	0.84	0.20	41,48,60,66	0
2	OSR	K	302	40/40	0.86	0.18	35,48,62,68	0
2	OSR	H	301	40/40	0.87	0.15	31,37,49,56	0
2	OSR	D	301	40/40	0.88	0.17	30,38,49,57	0
2	OSR	I	301	40/40	0.90	0.13	28,35,48,54	0
2	OSR	G	301	40/40	0.90	0.16	31,37,43,48	0
2	OSR	F	301	40/40	0.91	0.14	23,29,39,45	0

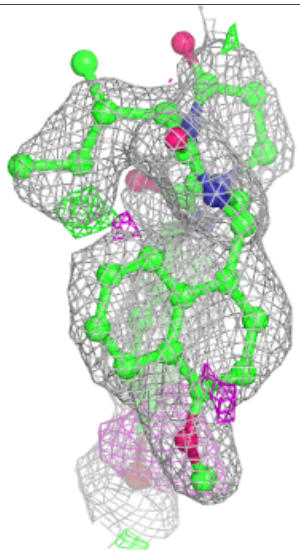
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OSR 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)

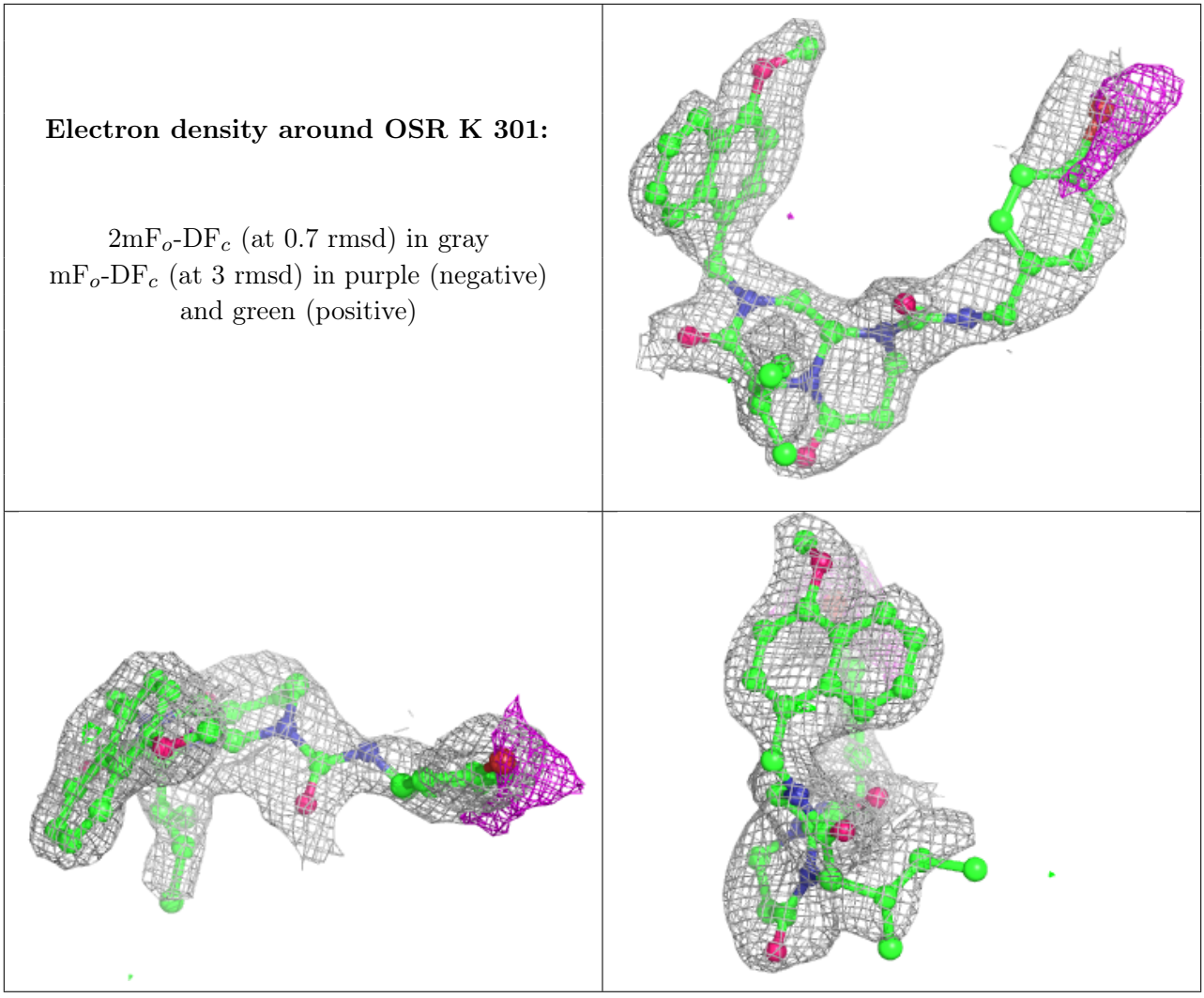






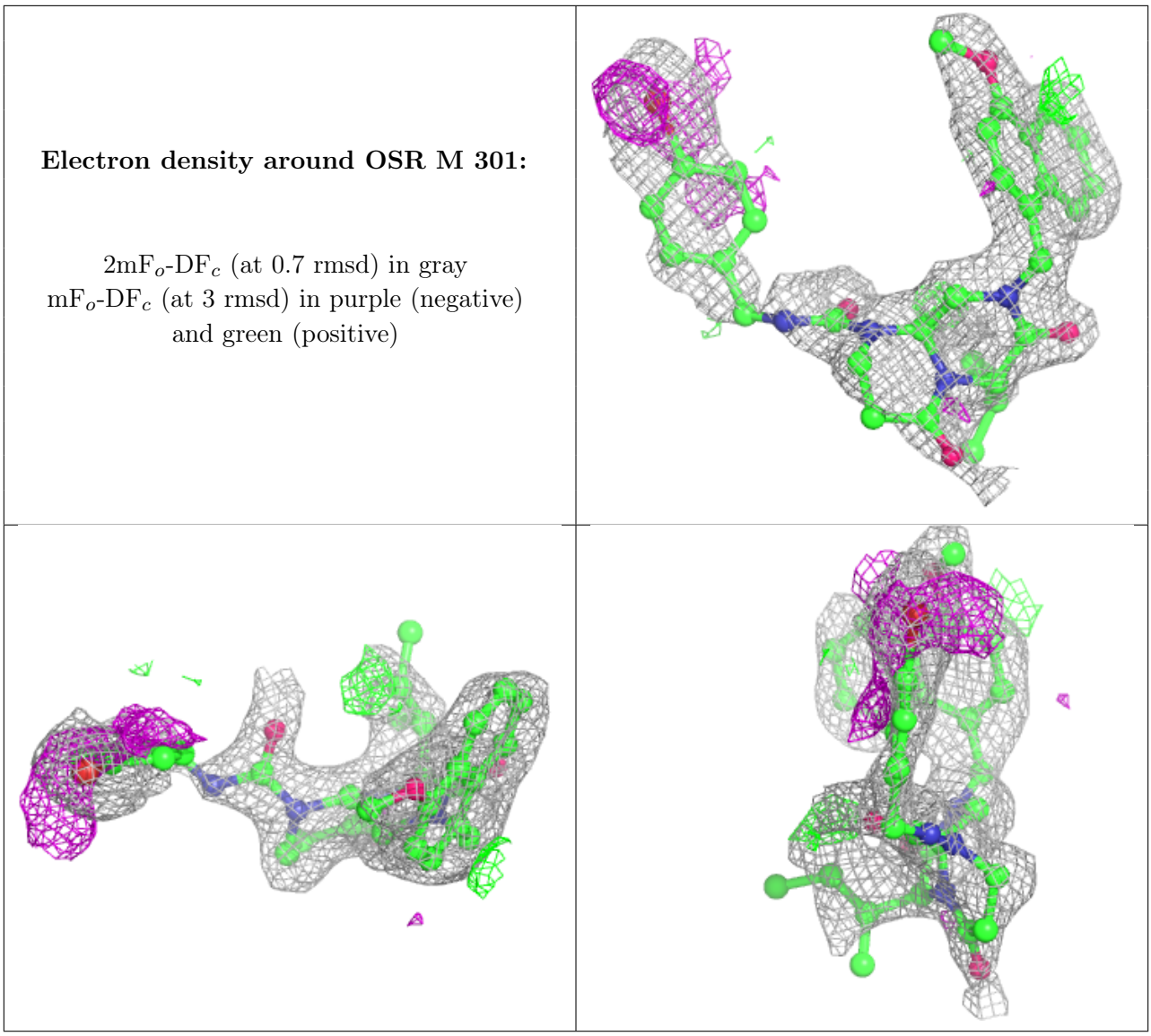
Electron density around OSR K 301:

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



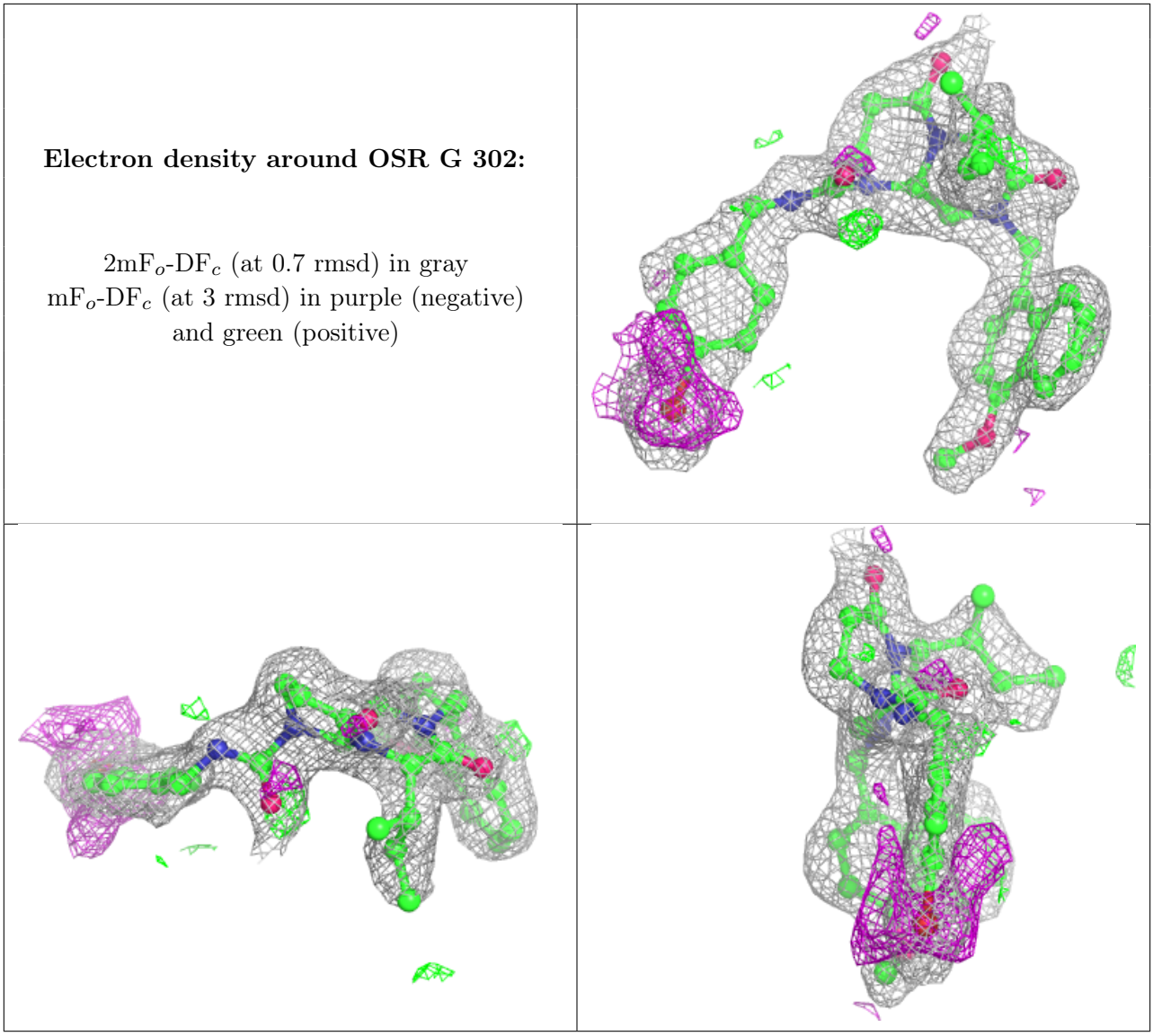
Electron density around OSR M 301:

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



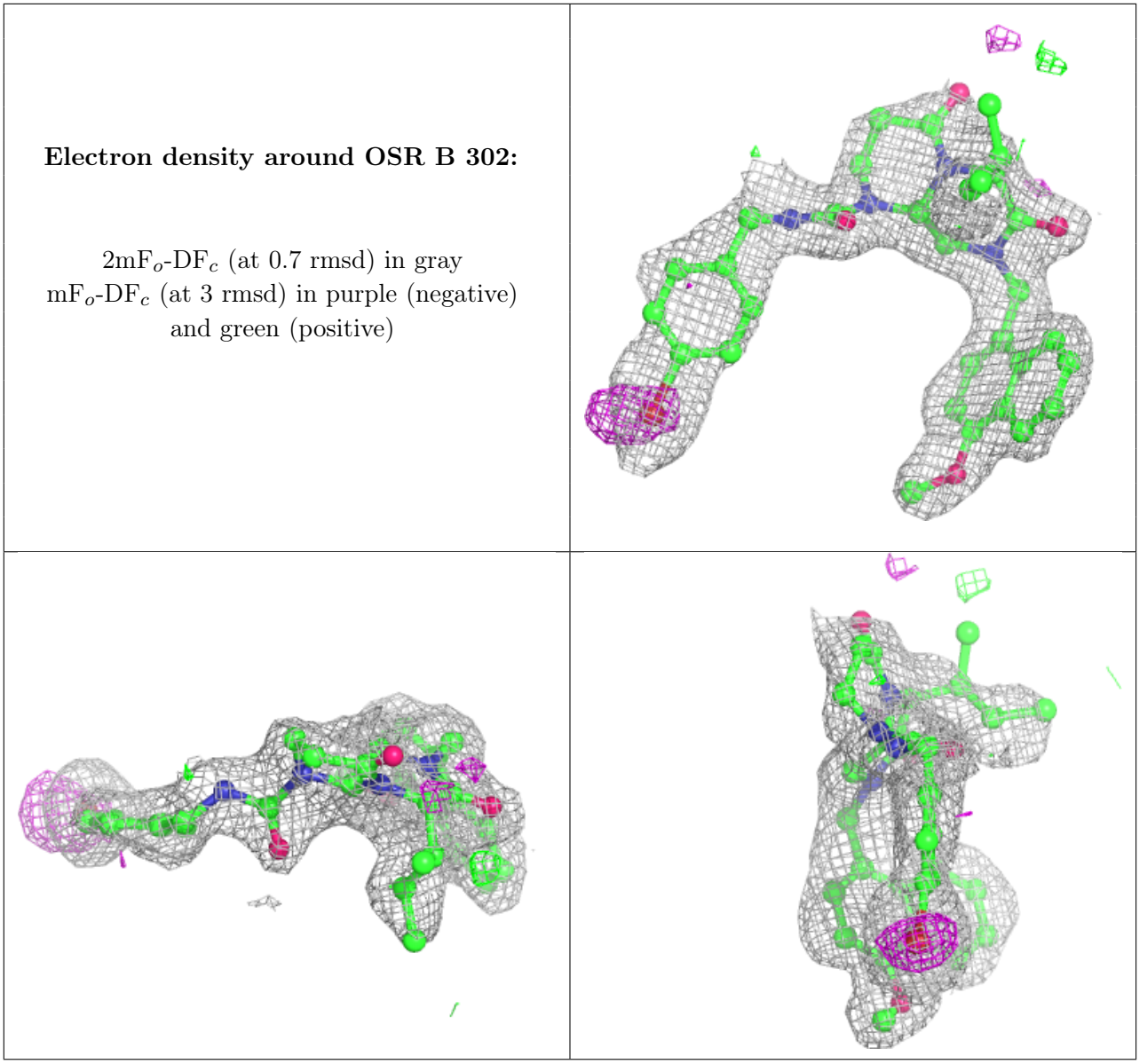
Electron density around OSR G 302:

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



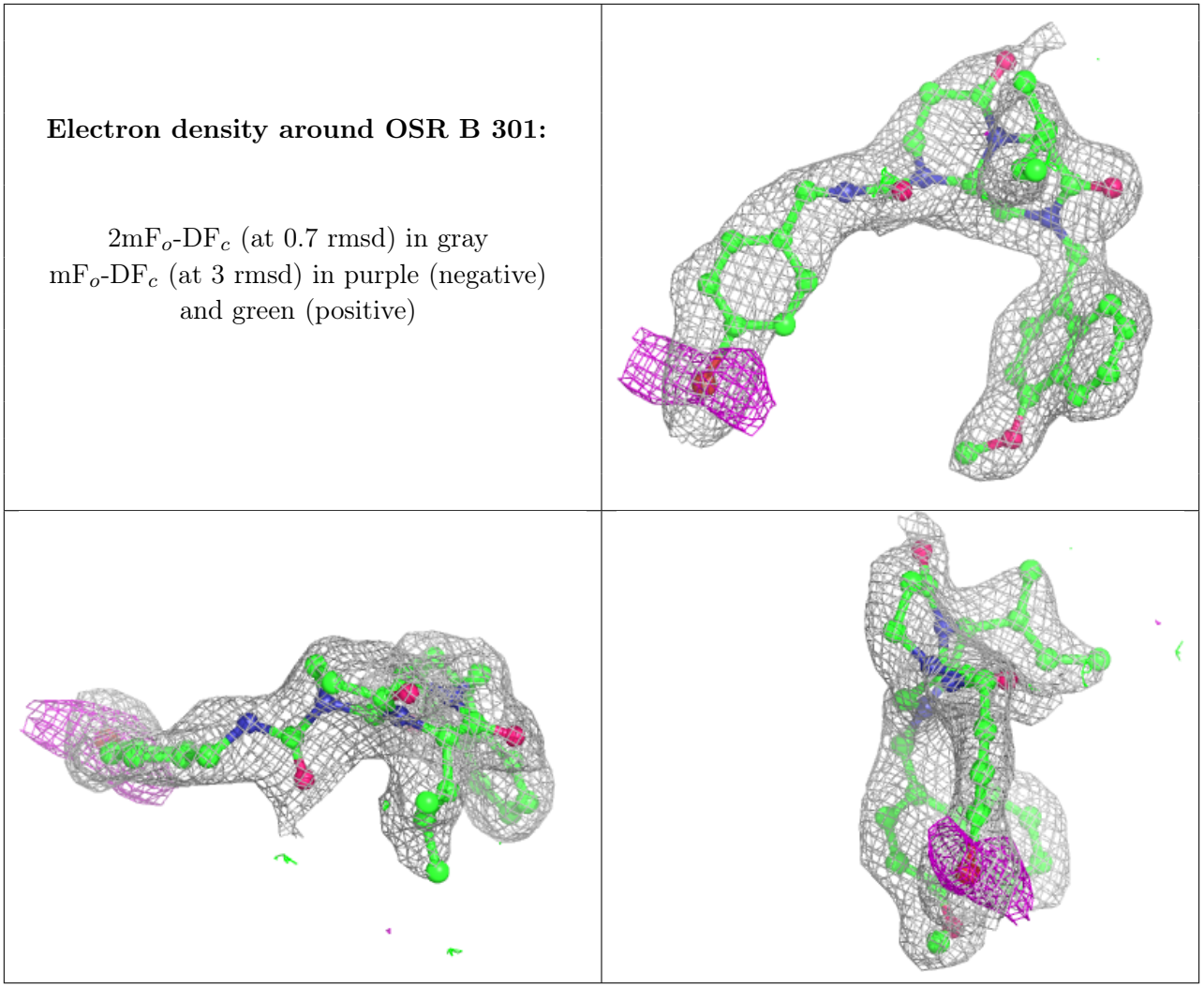
Electron density around OSR B 302:

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



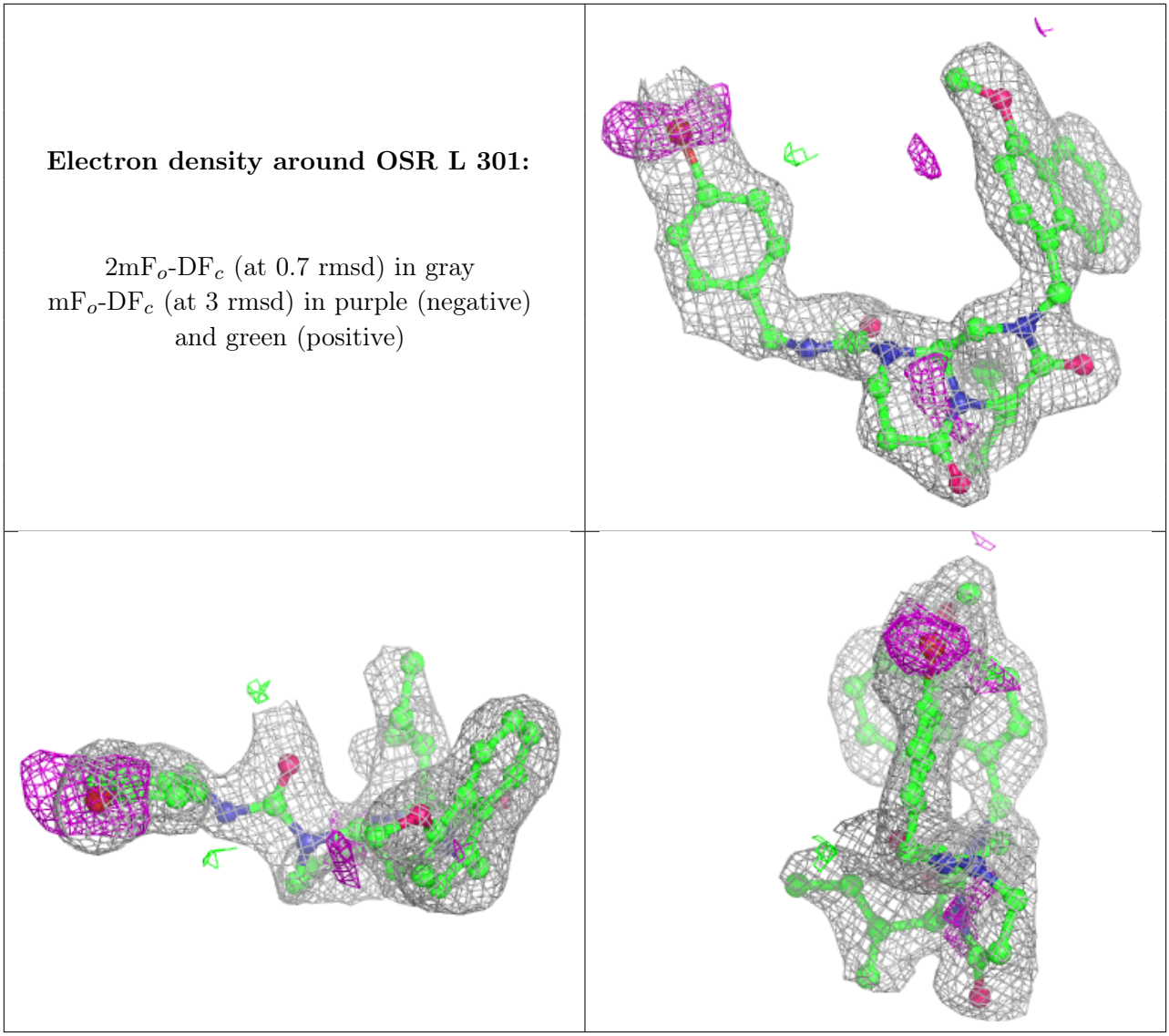
Electron density around OSR B 301:

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



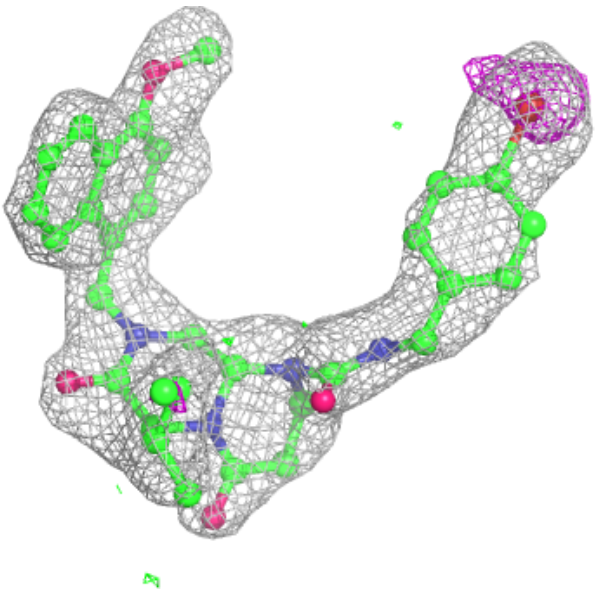
Electron density around OSR L 301:

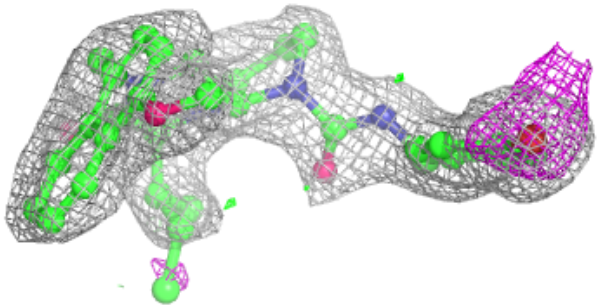
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

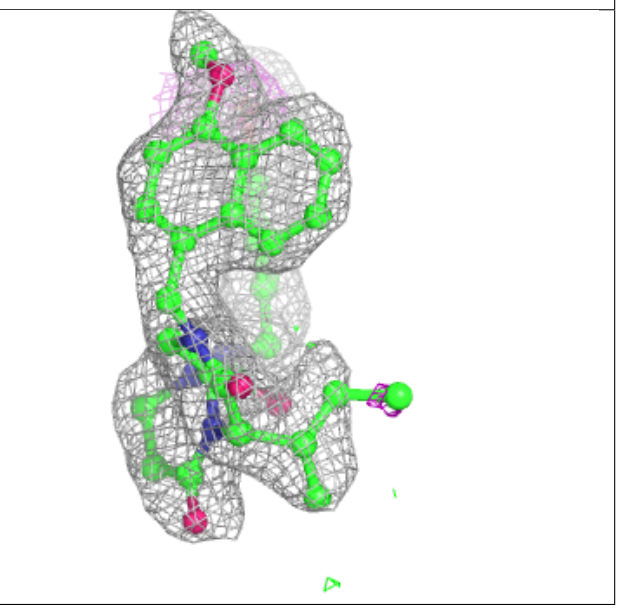


Electron density around OSR J 301:

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

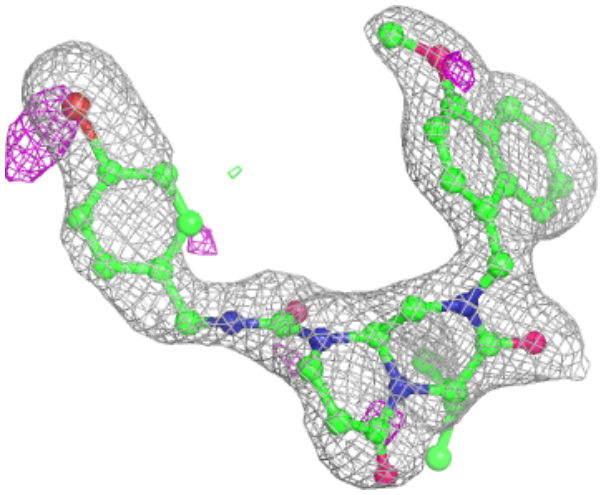


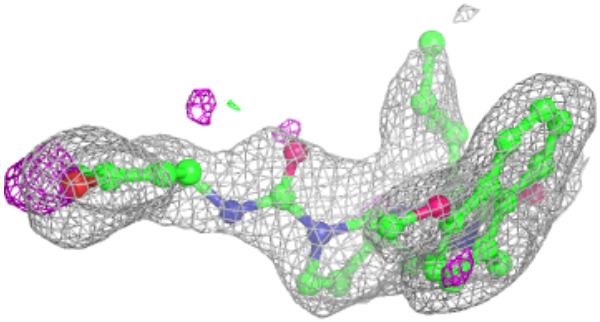


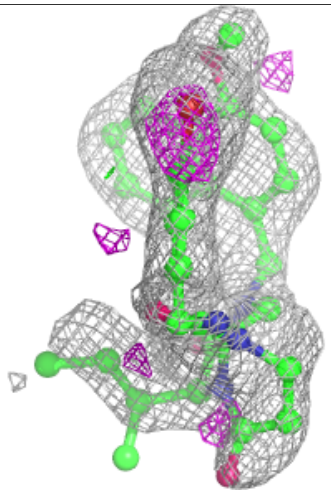


Electron density around OSR K 302:

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

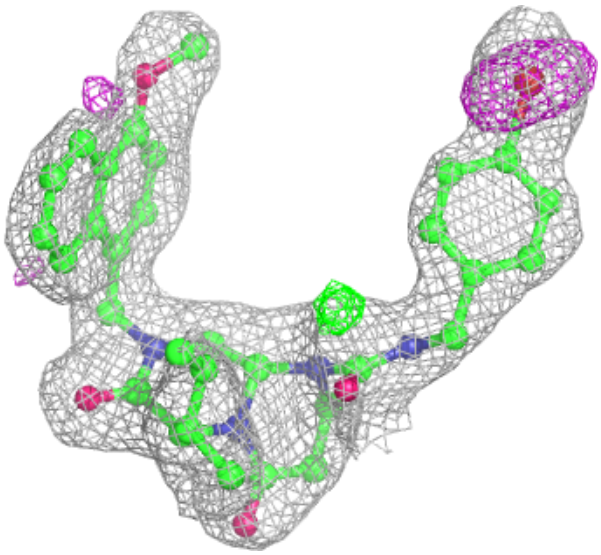


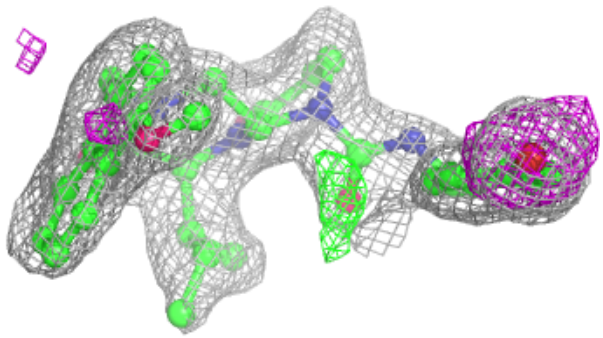


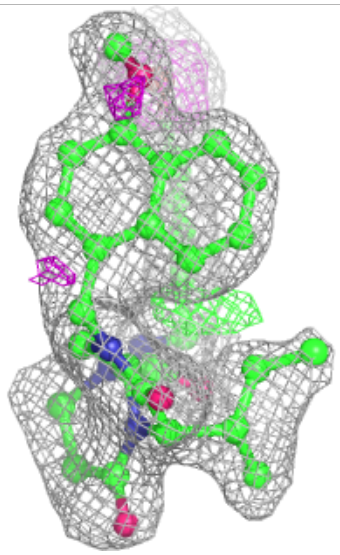


Electron density around OSR H 301:

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

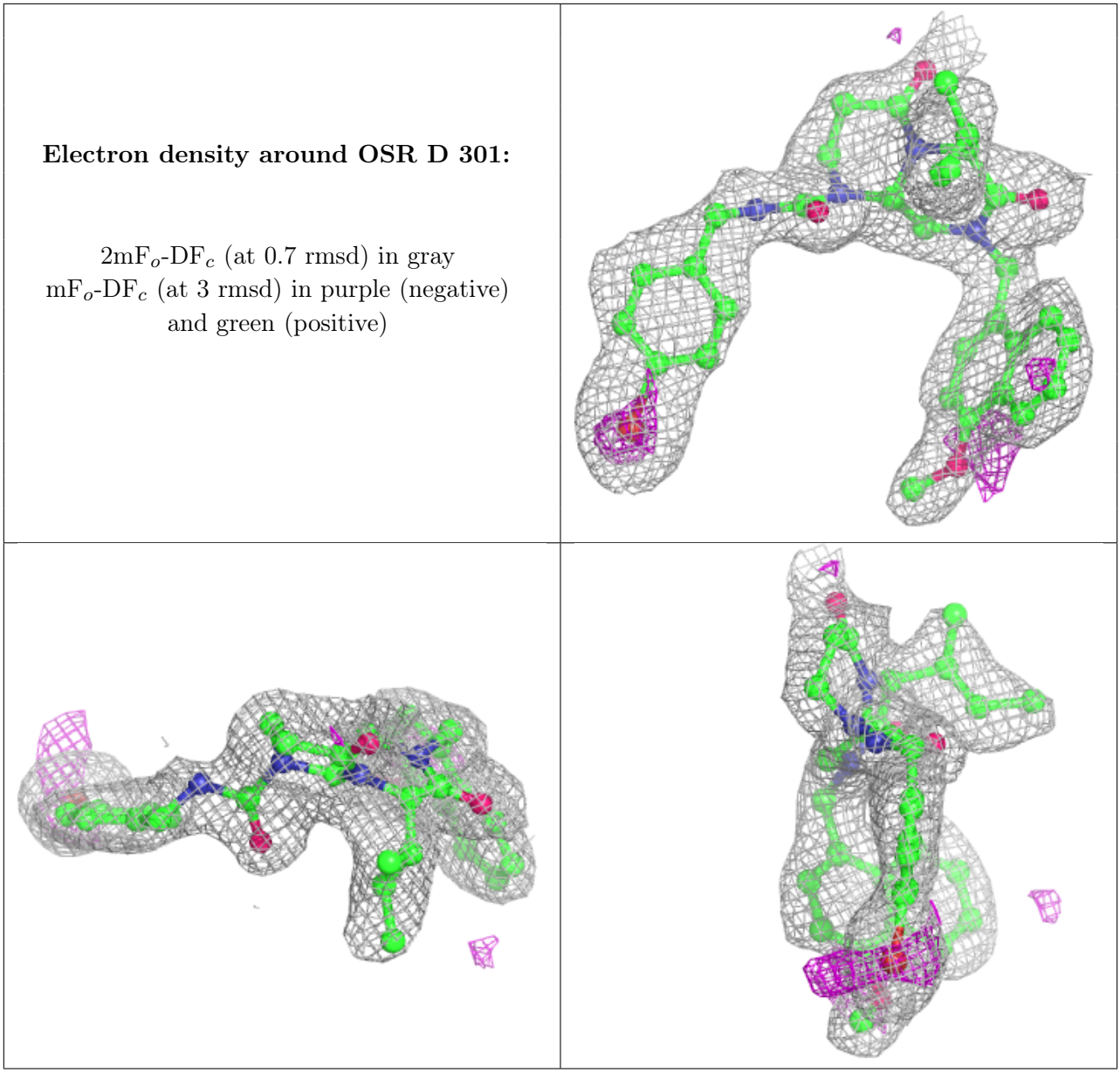






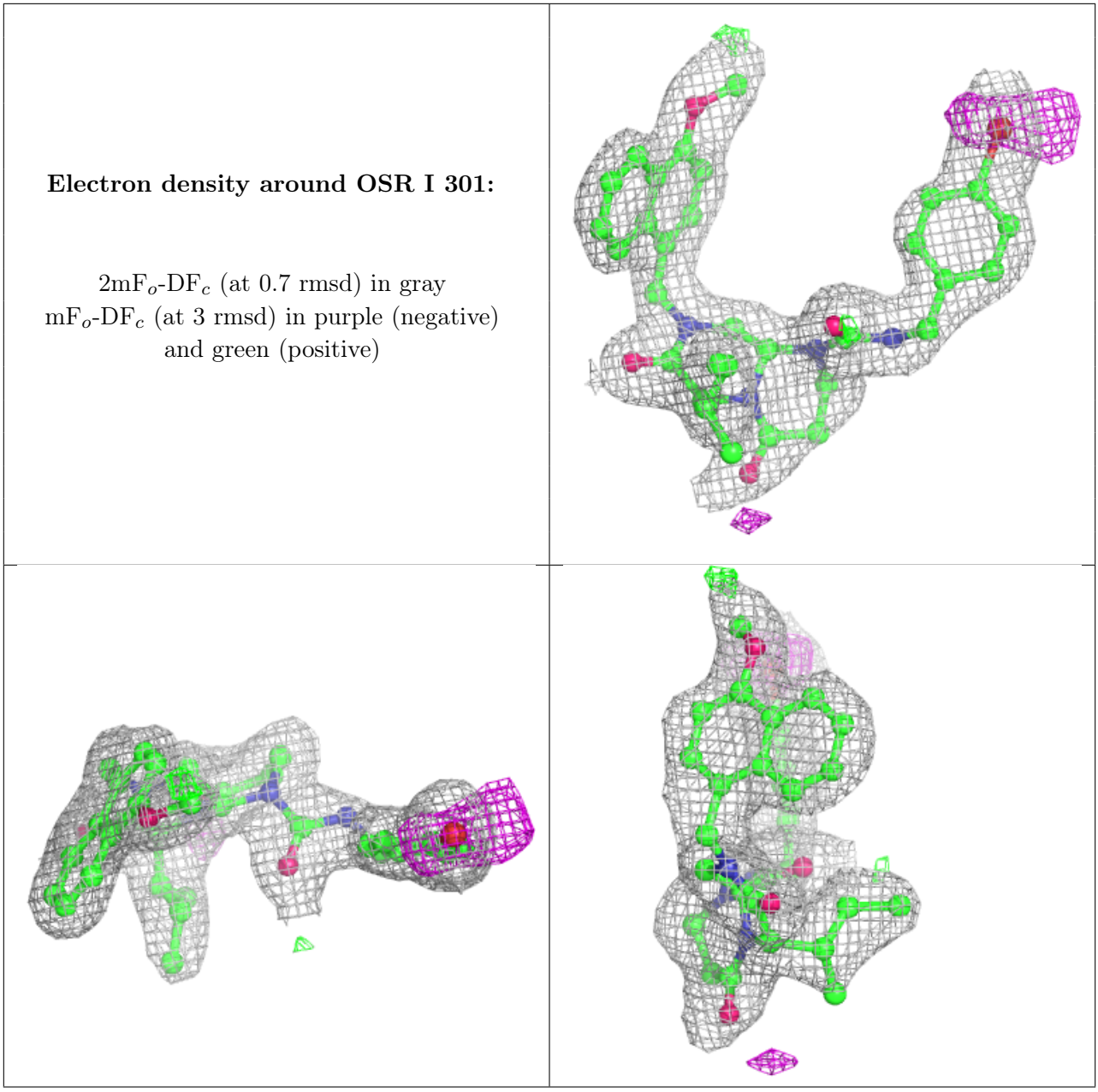
Electron density around OSR D 301:

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



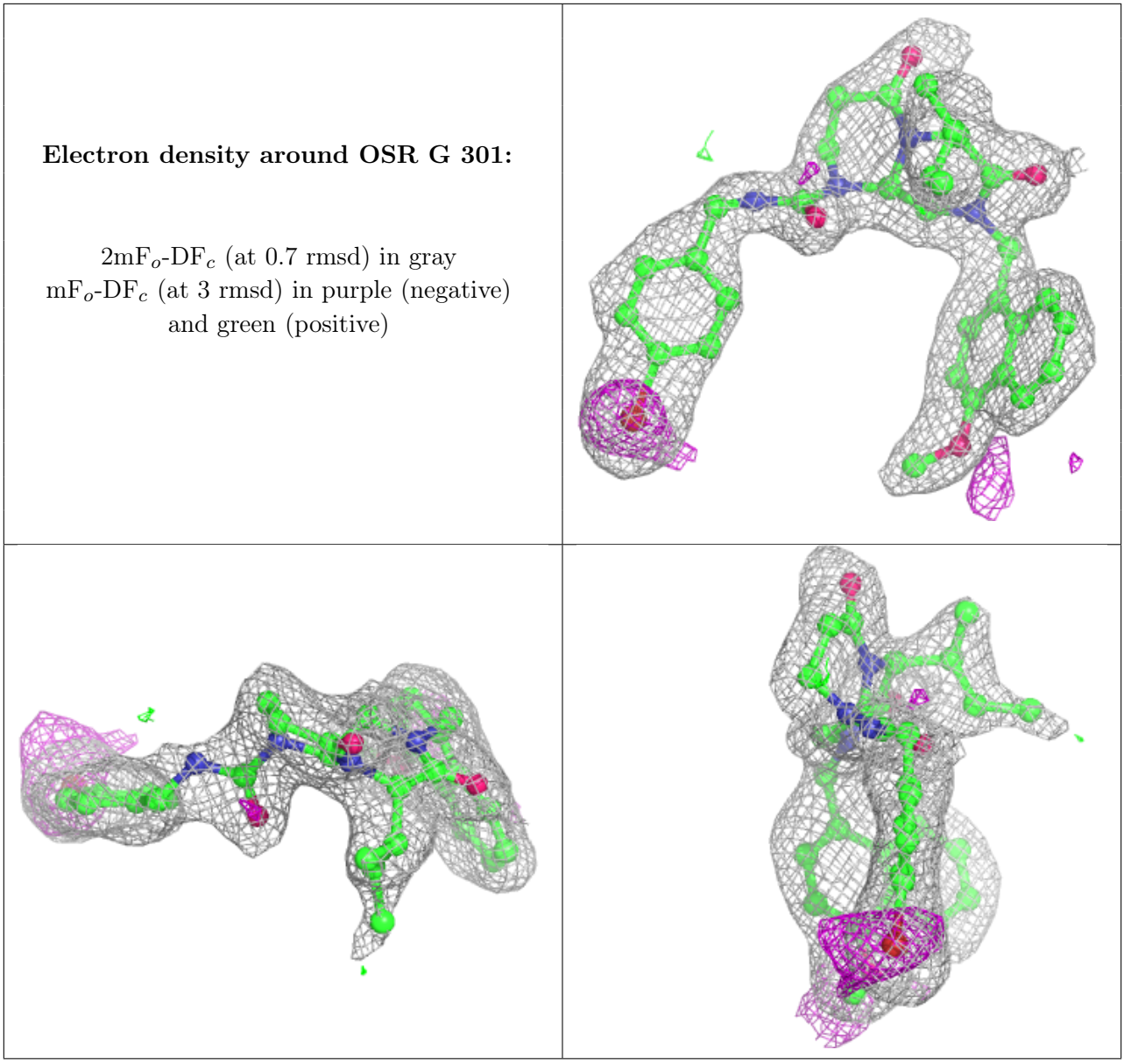
Electron density around OSR I 301:

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



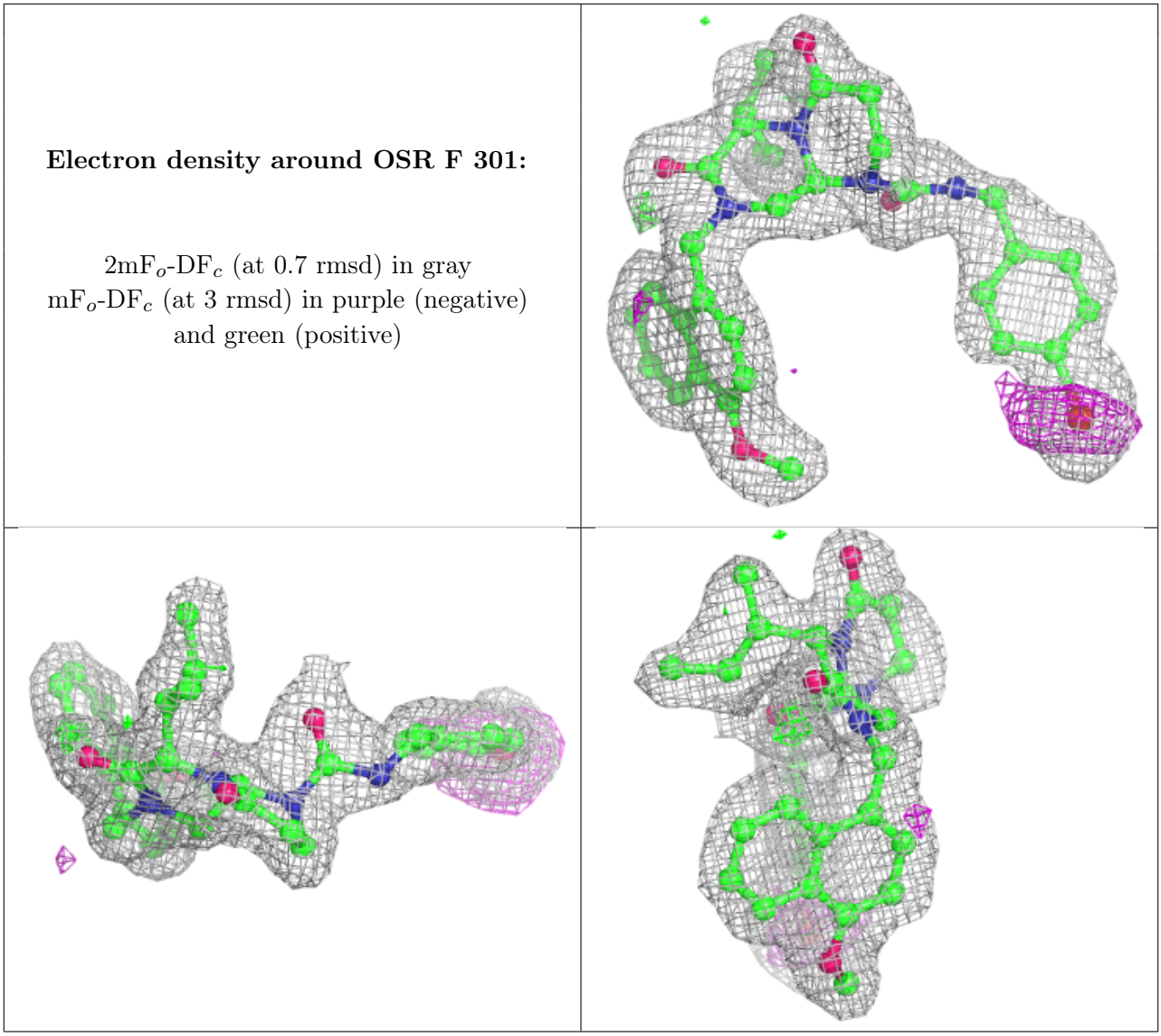
Electron density around OSR G 301:

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



Electron density around OSR F 301:

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



6.5 Other polymers

There are no such residues in this entry.