



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 PM UTC

PDB ID : 8I7X / pdb_00008i7x
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

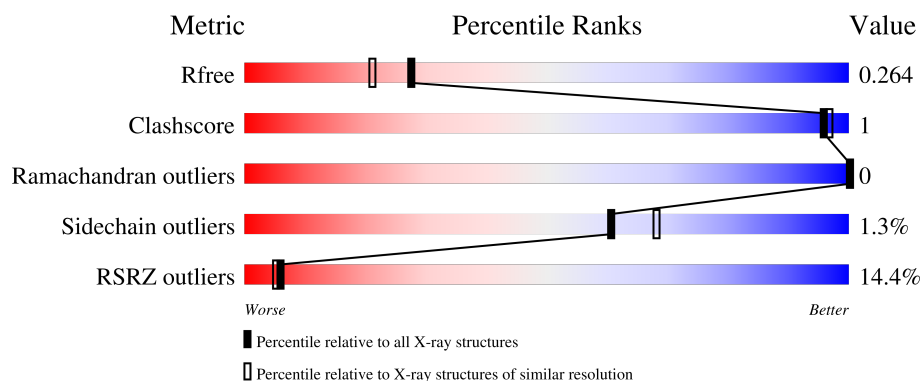
1 Overall quality at a glance

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.



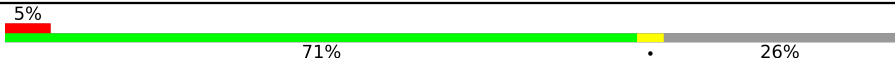
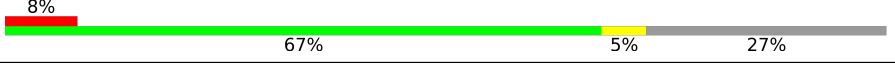
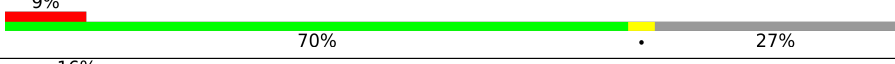
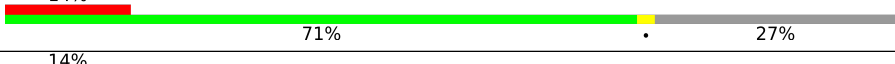
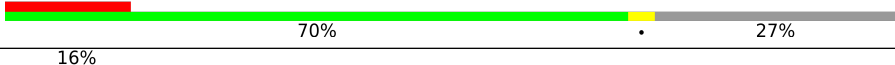
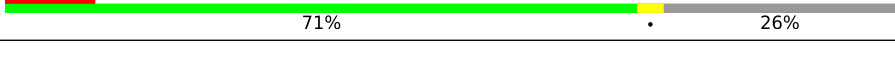
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	8% 69% 27%
1	B	221	8% 69% 5% 27%
1	C	221	15% 70% 27%
1	D	221	9% 74% 26%
1	E	221	9% 70% 27%

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Mol	Chain	Length	Quality of chain
1	F	221	
1	G	221	
1	H	221	
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	

2 Entry composition

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

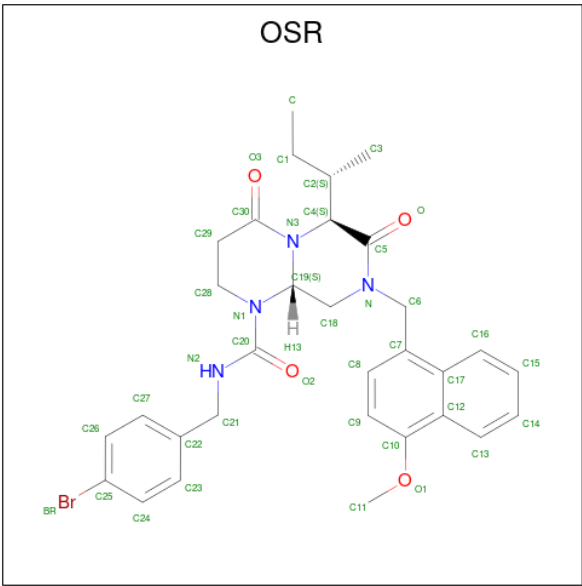
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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 (CCD ID: OSR) (formula: C₃₁H₃₅BrN₄O₄) (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		

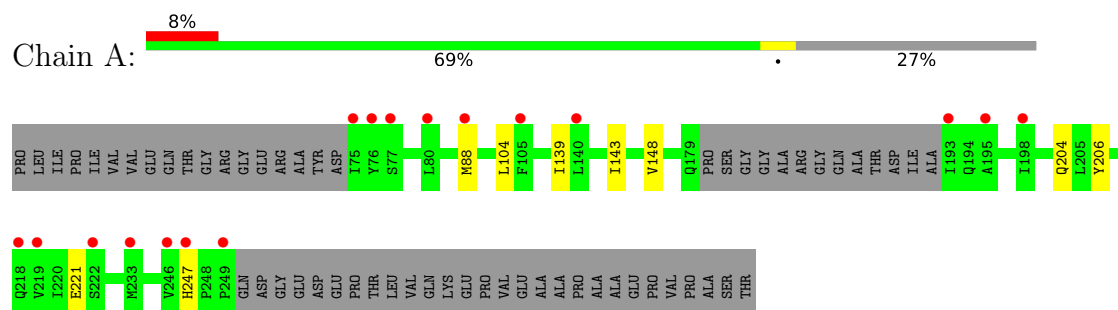
- Molecule 3 is water.

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		

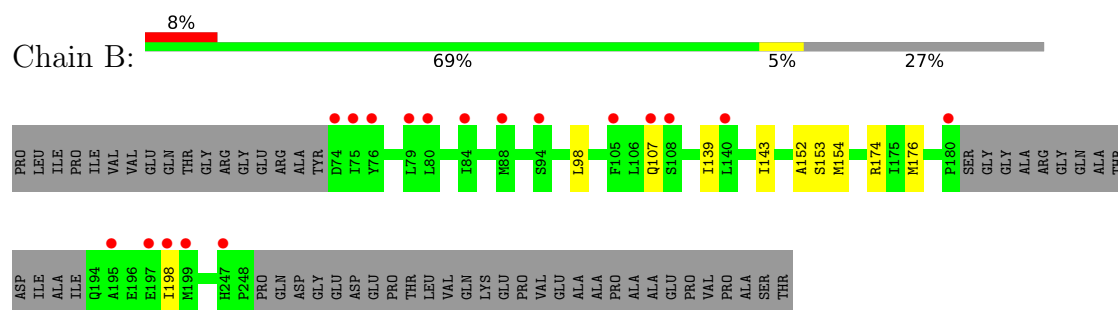
3 Residue-property plots [i](#)

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.

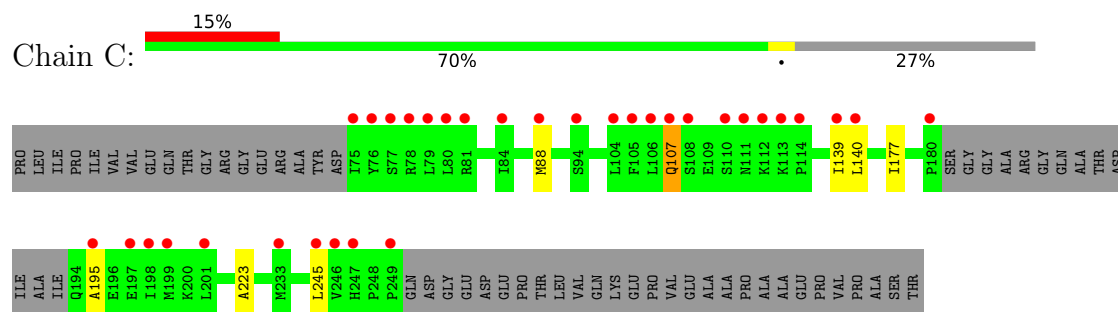
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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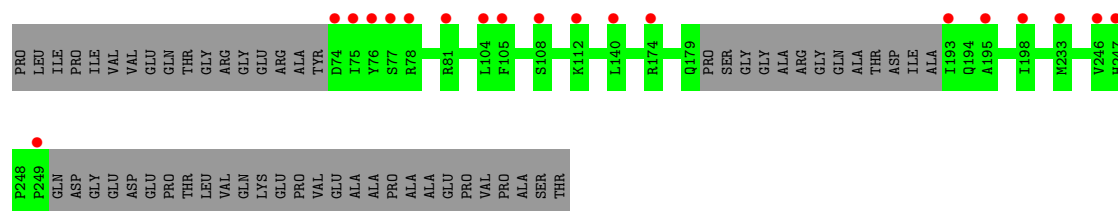


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

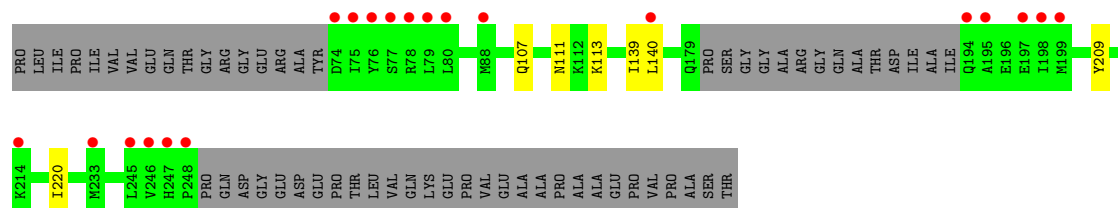


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

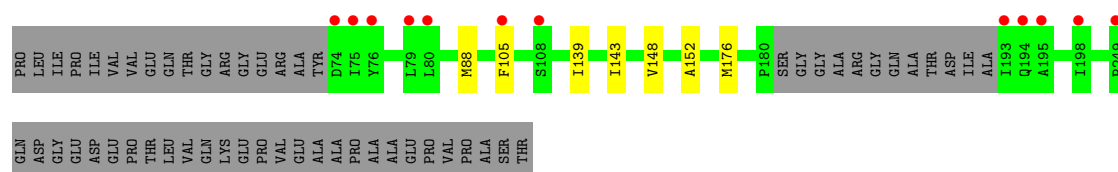




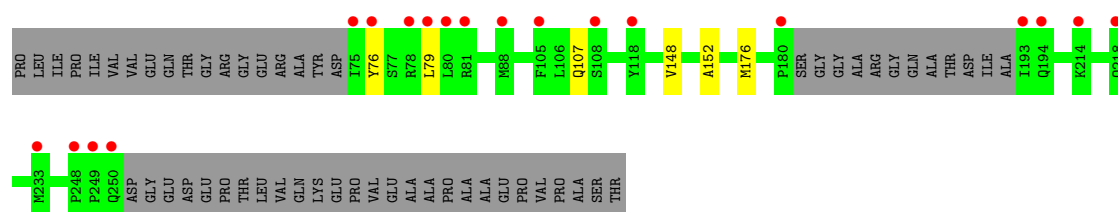
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



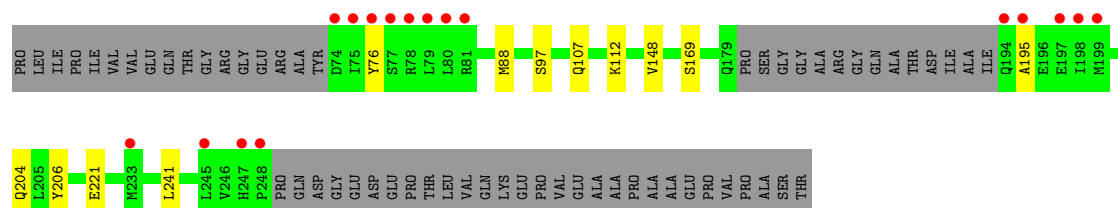
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



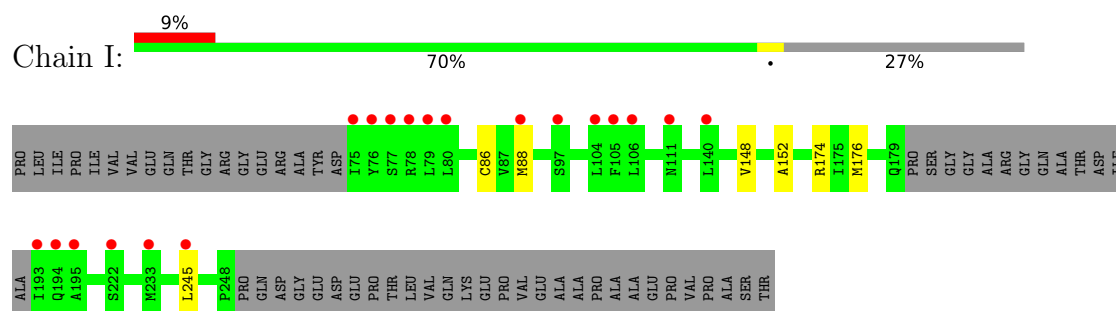
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



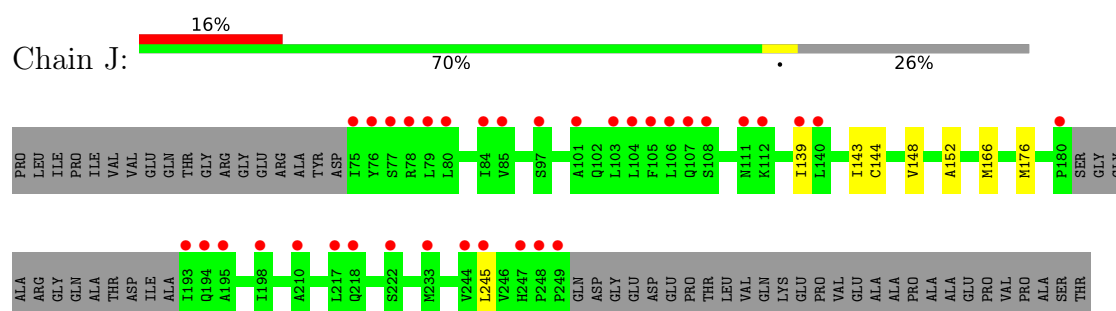
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



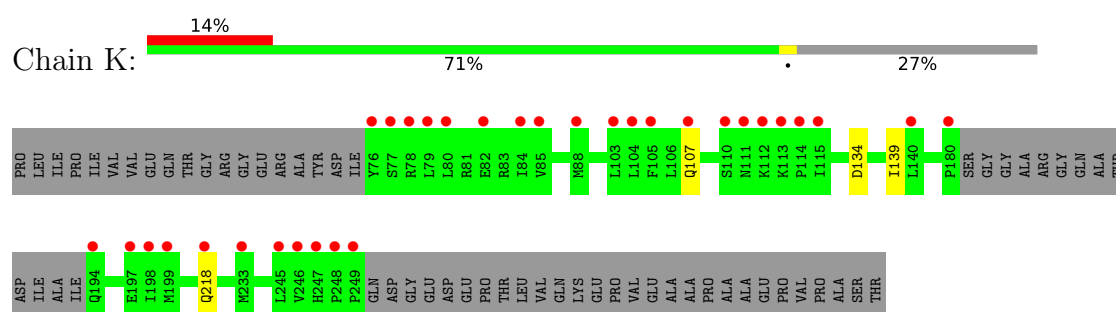
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



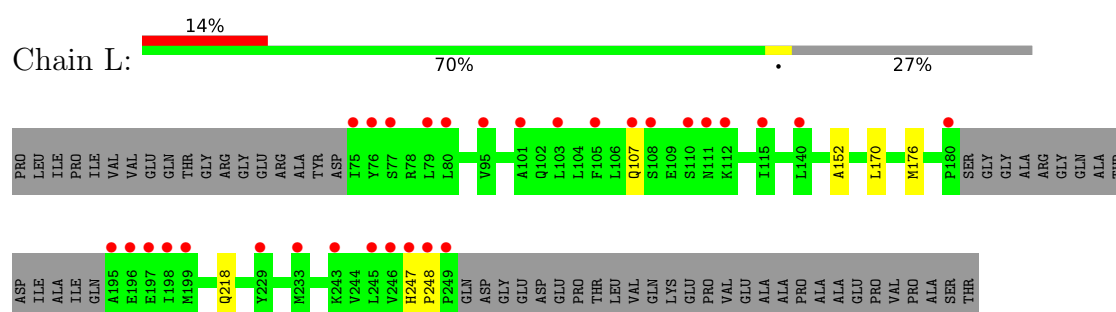
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



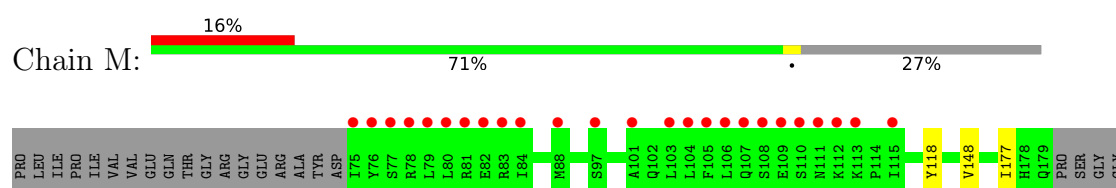
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.52	0/1282	0.77	0/1733
1	B	0.50	0/1270	0.76	0/1719
1	C	0.54	0/1274	0.78	0/1724
1	D	0.54	0/1280	0.80	0/1731
1	E	0.53	0/1267	0.77	0/1712
1	F	0.53	0/1292	0.78	0/1747
1	G	0.51	0/1299	0.78	0/1757
1	H	0.51	0/1273	0.75	0/1719
1	I	0.50	0/1275	0.77	0/1722
1	J	0.52	0/1296	0.79	0/1752
1	K	0.52	0/1268	0.76	0/1716
1	L	0.54	1/1259 (0.1%)	0.77	0/1705
1	M	0.52	0/1268	0.76	0/1714
1	N	0.51	0/1296	0.76	0/1752
All	All	0.52	1/17899 (0.0%)	0.77	0/24203

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	248	PRO	CA-C	5.54	1.54	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1259	0	1294	4	0
1	B	1247	0	1266	5	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	3	0
1	G	1275	0	1309	2	0
1	H	1251	0	1285	6	0
1	I	1253	0	1282	4	0
1	J	1272	0	1312	3	0
1	K	1244	0	1268	2	0
1	L	1235	0	1263	2	0
1	M	1246	0	1269	3	0
1	N	1272	0	1312	3	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	40	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 (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:SER:HB2	1:I:88:MET:HE2	1.67	0.76
1:E:111:ASN:HD22	1:E:140:LEU:HD13	1.56	0.71
1:N:152:ALA:HB1	1:N:176:MET:HE2	1.73	0.71
1:I:152:ALA:HB1	1:I:176:MET:HE2	1.80	0.62
1:J:152:ALA:HB1	1:J:176:MET:HE2	1.84	0.59
1:L:152:ALA:HB1	1:L:176:MET:HE2	1.85	0.58
1:G:152:ALA:HB1	1:G:176:MET:HE2	1.85	0.58
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: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:H:76:TYR:CE1	1:H:88:MET:HE1	2.49	0.47
1:K:134:ASP:HB3	1:L:170:LEU:HD23	1.96	0.47
1:B:153:SER:OG	1:B:154:MET:N	2.45	0.47
1:M:118:TYR:CE2	1:M:148:VAL:HG21	2.51	0.46
1:J:144:CYS:SG	1:J:166:MET:HE2	2.56	0.46
1:B:152:ALA:HB1	1:B:176:MET:HE2	1.98	0.45
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:I:86:CYS:SG	1:I:88:MET:HE3	2.57	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:F:152:ALA:HB1	1:F:176:MET:HE2	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

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%)	47	52
1	B	137/185 (74%)	135 (98%)	2 (2%)	57	64
1	C	138/185 (75%)	135 (98%)	3 (2%)	45	50
1	D	138/185 (75%)	138 (100%)	0	100	100
1	E	137/185 (74%)	136 (99%)	1 (1%)	76	82
1	F	140/185 (76%)	138 (99%)	2 (1%)	59	66
1	G	142/185 (77%)	140 (99%)	2 (1%)	59	66
1	H	138/185 (75%)	135 (98%)	3 (2%)	45	50
1	I	138/185 (75%)	136 (99%)	2 (1%)	59	66
1	J	142/185 (77%)	140 (99%)	2 (1%)	59	66
1	K	138/185 (75%)	137 (99%)	1 (1%)	76	82
1	L	136/185 (74%)	133 (98%)	3 (2%)	45	50
1	M	137/185 (74%)	136 (99%)	1 (1%)	76	82
1	N	142/185 (77%)	141 (99%)	1 (1%)	76	82
All	All	1943/2590 (75%)	1917 (99%)	26 (1%)	61	68

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	98	LEU
1	B	107	GLN
1	C	88	MET
1	C	107	GLN
1	C	245	LEU
1	E	113	LYS
1	F	88	MET
1	F	148	VAL

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Mol	Chain	Res	Type
1	G	107	GLN
1	G	148	VAL
1	H	107	GLN
1	H	112	LYS
1	H	148	VAL
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	218	GLN
1	L	247	HIS
1	M	236	GLN
1	N	88	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	107	GLN
1	A	120	ASN
1	A	204	GLN
1	A	207	ASN
1	A	236	GLN
1	B	102	GLN
1	B	107	GLN
1	B	150	GLN
1	C	107	GLN
1	C	137	GLN
1	C	179	GLN
1	C	194	GLN
1	D	102	GLN
1	D	194	GLN
1	E	111	ASN
1	E	179	GLN
1	F	168	HIS
1	F	194	GLN
1	G	107	GLN
1	G	120	ASN
1	G	179	GLN
1	H	102	GLN

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Mol	Chain	Res	Type
1	H	107	GLN
1	H	204	GLN
1	I	102	GLN
1	I	150	GLN
1	I	236	GLN
1	I	247	HIS
1	J	236	GLN
1	K	102	GLN
1	K	107	GLN
1	K	194	GLN
1	L	107	GLN
1	L	179	GLN
1	M	111	ASN
1	N	137	GLN
1	N	179	GLN
1	N	247	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OSR	H	301	-	43,44,44	0.28	0	55,63,63	0.75	1 (1%)
2	OSR	I	301	-	43,44,44	0.32	0	55,63,63	0.81	2 (3%)
2	OSR	L	301	-	43,44,44	0.32	0	55,63,63	0.82	2 (3%)
2	OSR	M	301	-	43,44,44	0.32	0	55,63,63	0.70	1 (1%)
2	OSR	B	301	-	43,44,44	0.31	0	55,63,63	0.75	1 (1%)
2	OSR	G	302	-	43,44,44	0.29	0	55,63,63	0.63	0
2	OSR	C	301	-	43,44,44	0.29	0	55,63,63	0.66	1 (1%)
2	OSR	B	302	-	43,44,44	0.31	0	55,63,63	0.70	2 (3%)
2	OSR	G	301	-	43,44,44	0.33	0	55,63,63	0.80	2 (3%)
2	OSR	J	301	-	43,44,44	0.29	0	55,63,63	0.63	1 (1%)
2	OSR	K	301	-	43,44,44	0.31	0	55,63,63	0.65	1 (1%)
2	OSR	D	301	-	43,44,44	0.31	0	55,63,63	0.71	2 (3%)
2	OSR	K	302	-	43,44,44	0.29	0	55,63,63	0.73	2 (3%)
2	OSR	F	301	-	43,44,44	0.30	0	55,63,63	0.71	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	H	301	-	-	5/21/54/54	0/5/5/5
2	OSR	I	301	-	-	2/21/54/54	0/5/5/5
2	OSR	L	301	-	-	0/21/54/54	0/5/5/5
2	OSR	M	301	-	-	2/21/54/54	0/5/5/5
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	C	301	-	-	2/21/54/54	0/5/5/5
2	OSR	B	302	-	-	2/21/54/54	0/5/5/5
2	OSR	G	301	-	-	2/21/54/54	0/5/5/5
2	OSR	J	301	-	-	5/21/54/54	0/5/5/5
2	OSR	K	301	-	-	2/21/54/54	0/5/5/5
2	OSR	D	301	-	-	2/21/54/54	0/5/5/5
2	OSR	K	302	-	-	0/21/54/54	0/5/5/5
2	OSR	F	301	-	-	2/21/54/54	0/5/5/5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	OSR	C19-C18-N	-4.05	106.20	111.04
2	G	301	OSR	C19-C18-N	-3.77	106.54	111.04
2	L	301	OSR	C19-C18-N	-3.76	106.55	111.04
2	H	301	OSR	C18-C19-N1	3.52	118.67	112.61
2	F	301	OSR	C19-C18-N	-3.52	106.84	111.04
2	K	302	OSR	C19-C18-N	-3.49	106.88	111.04
2	B	301	OSR	C19-C18-N	-3.42	106.96	111.04
2	B	302	OSR	C19-C18-N	-3.06	107.39	111.04
2	L	301	OSR	C18-C19-N1	2.66	117.19	112.61
2	D	301	OSR	C19-C18-N	-2.63	107.90	111.04
2	G	301	OSR	C18-C19-N1	2.62	117.12	112.61
2	C	301	OSR	C21-N2-C20	2.61	123.61	120.79
2	M	301	OSR	C19-C18-N	-2.32	108.27	111.04
2	D	301	OSR	C28-C29-C30	-2.26	107.38	117.67
2	K	301	OSR	C19-C18-N	-2.24	108.36	111.04
2	B	302	OSR	C28-C29-C30	-2.12	108.00	117.67
2	K	302	OSR	C18-C19-N1	2.09	116.20	112.61
2	I	301	OSR	C18-C19-N1	2.06	116.16	112.61
2	J	301	OSR	C19-C18-N	-2.04	108.61	111.04

There are no chirality outliers.

All (32) 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
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	B	301	OSR	N2-C20-N1-C28
2	B	302	OSR	N2-C20-N1-C28
2	D	301	OSR	N2-C20-N1-C28
2	F	301	OSR	C12-C10-O1-C11
2	J	301	OSR	C12-C10-O1-C11
2	H	301	OSR	C-C1-C2-C4

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

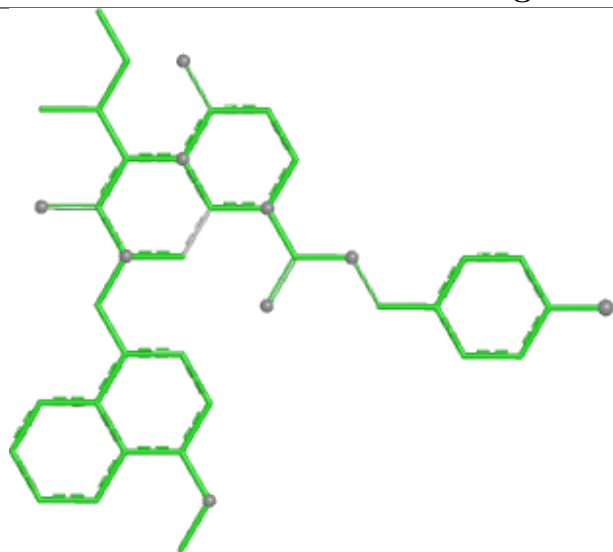
There are no ring outliers.

2 monomers are involved in 2 short contacts:

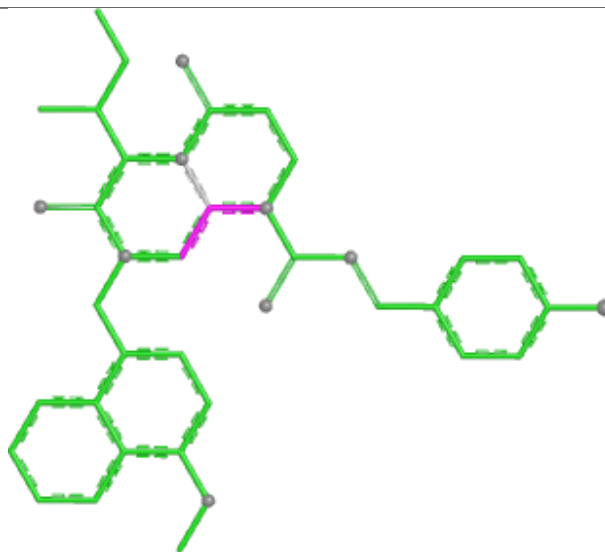
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	302	OSR	1	0
2	B	302	OSR	1	0

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 than 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.

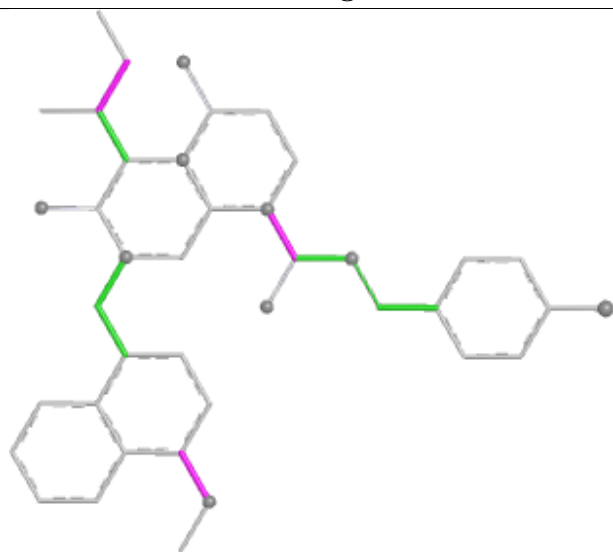
Ligand OSR H 301



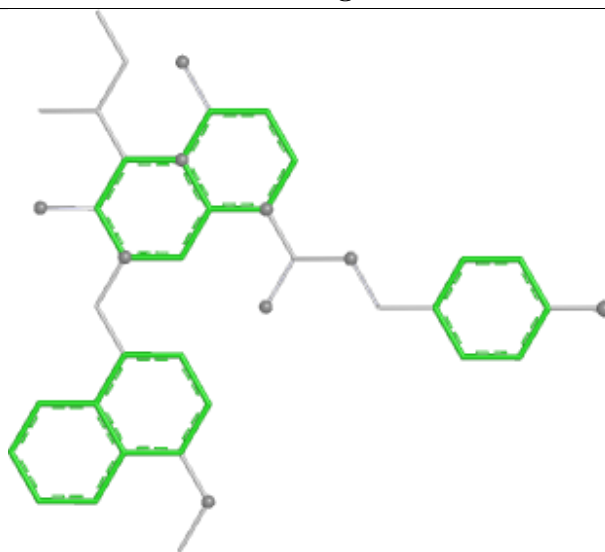
Bond lengths



Bond angles

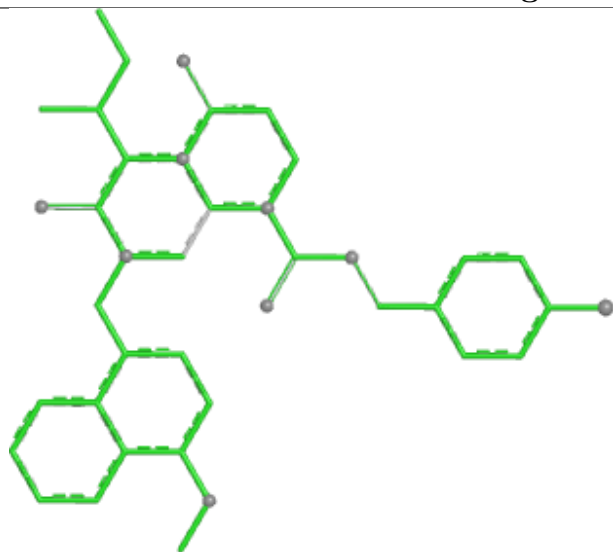


Torsions

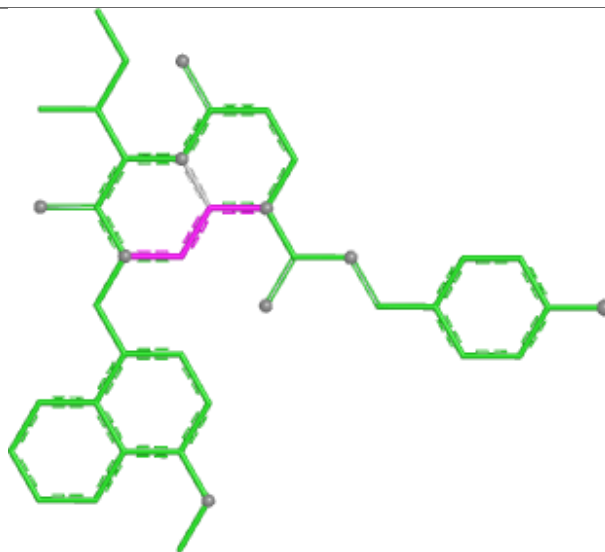


Rings

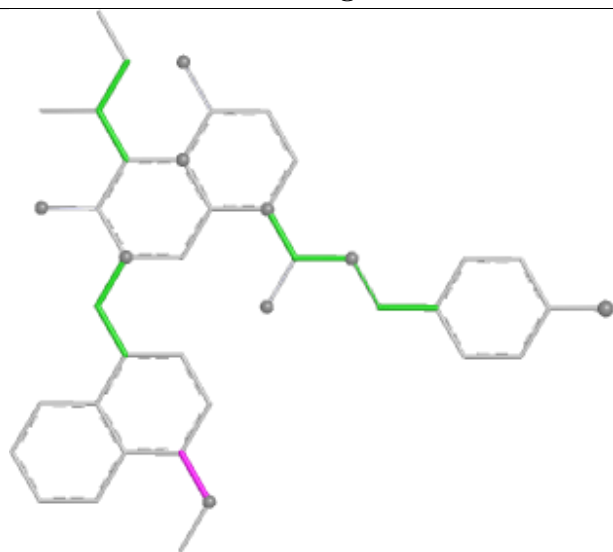
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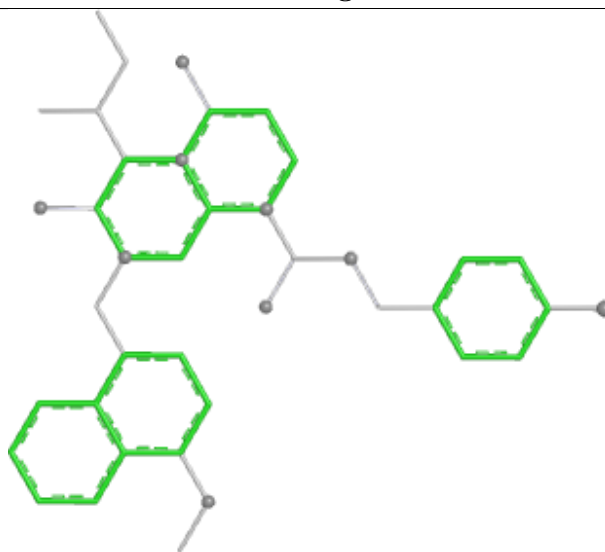
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Bond angles

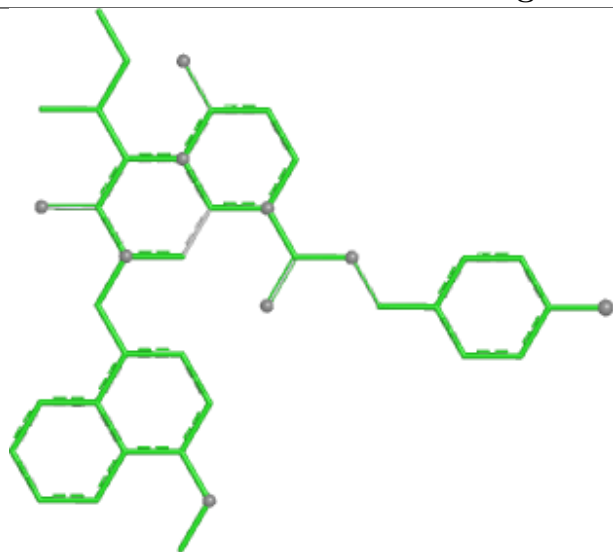


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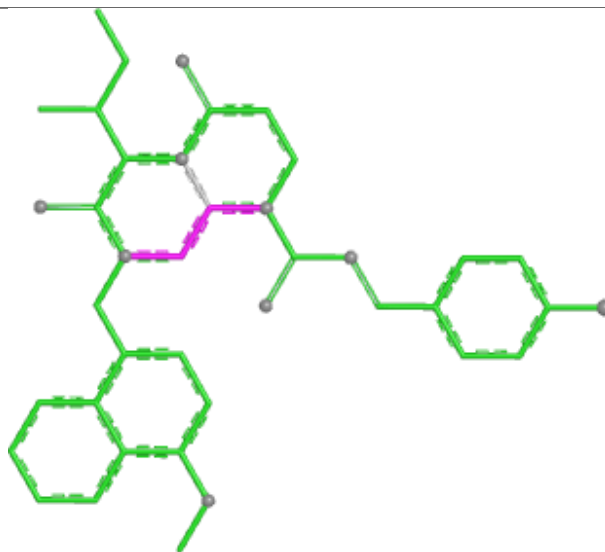


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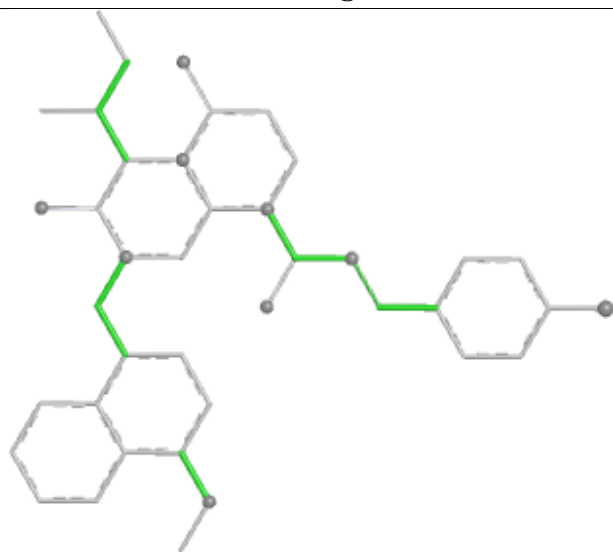
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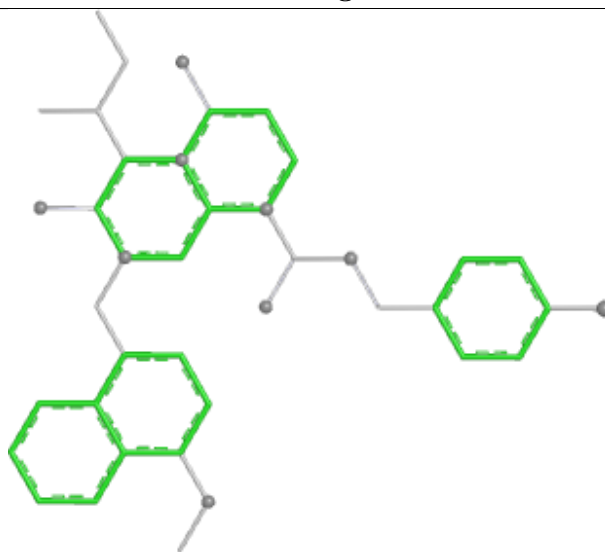
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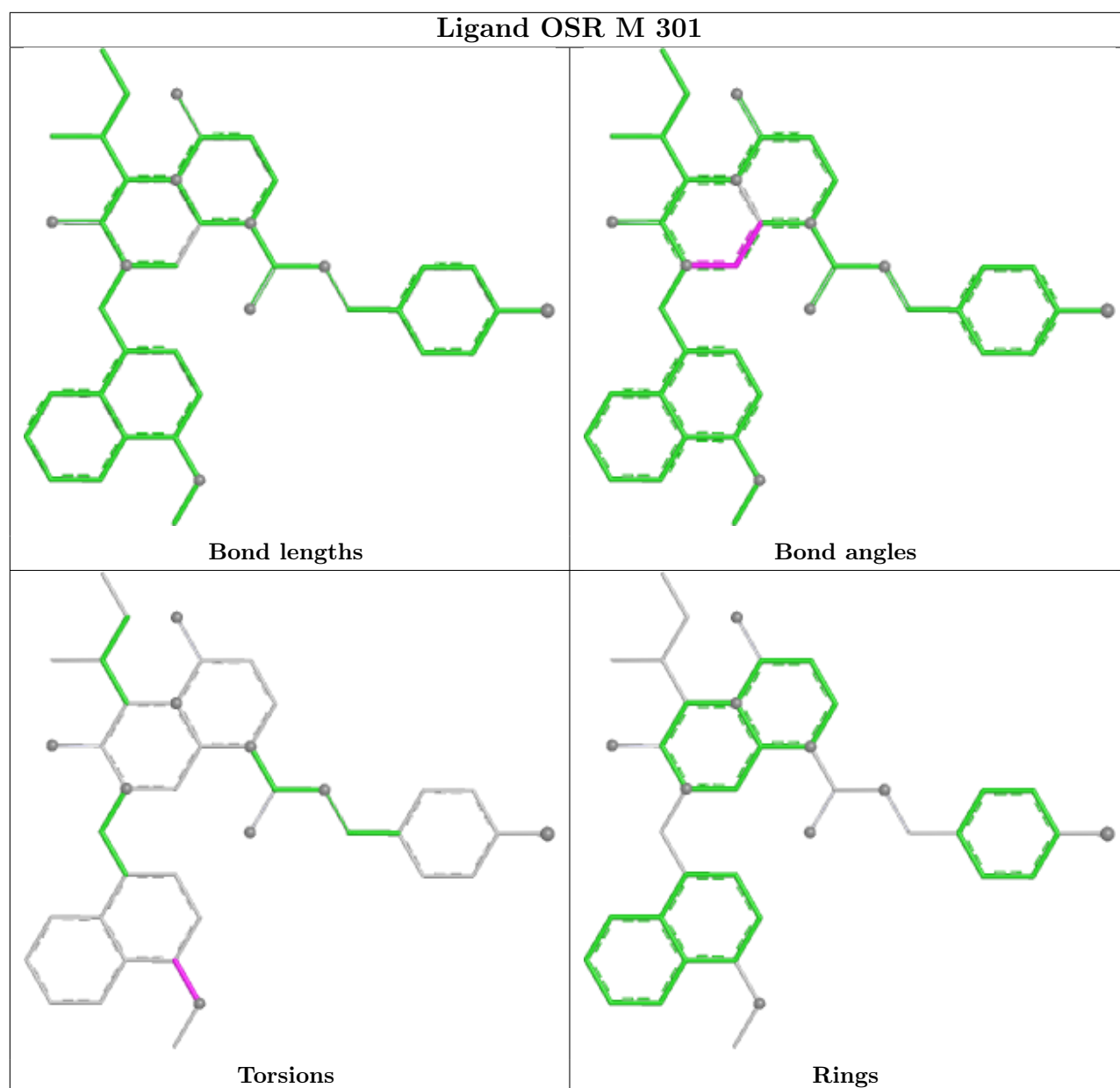
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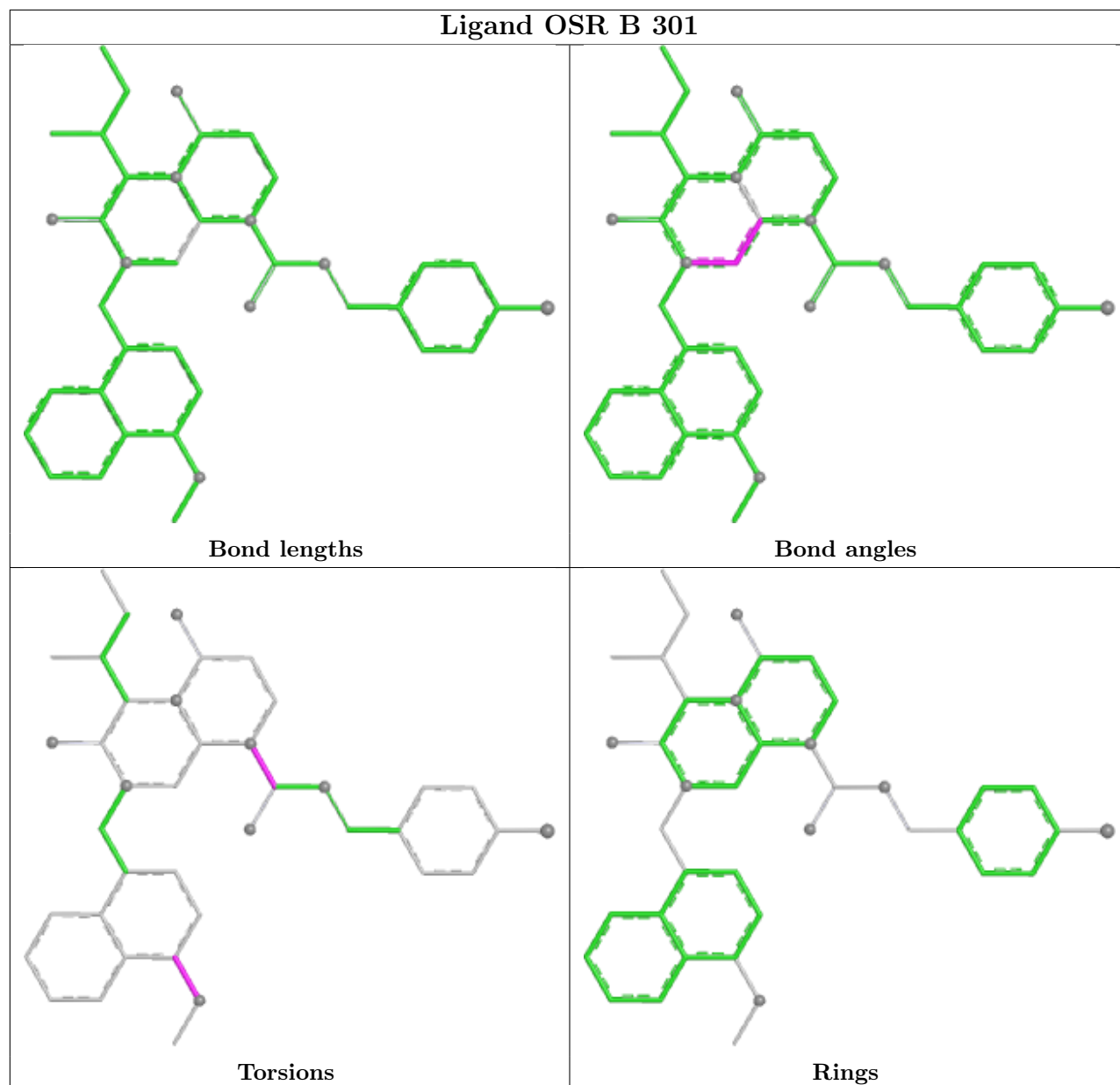


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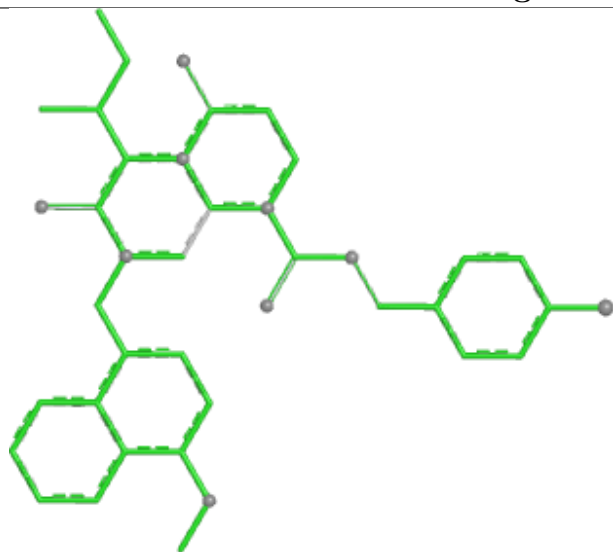


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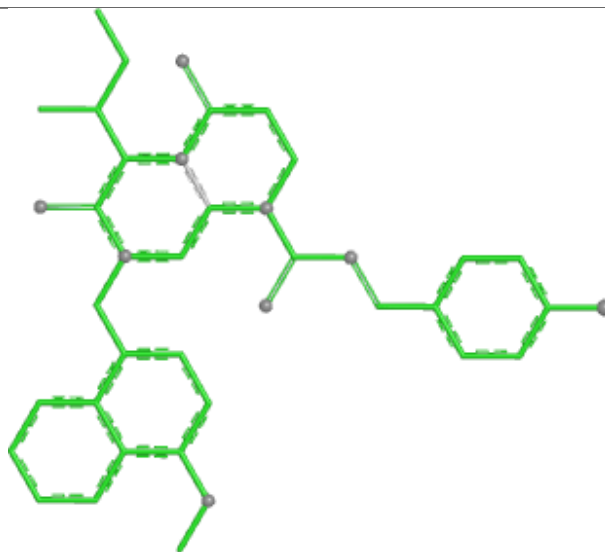




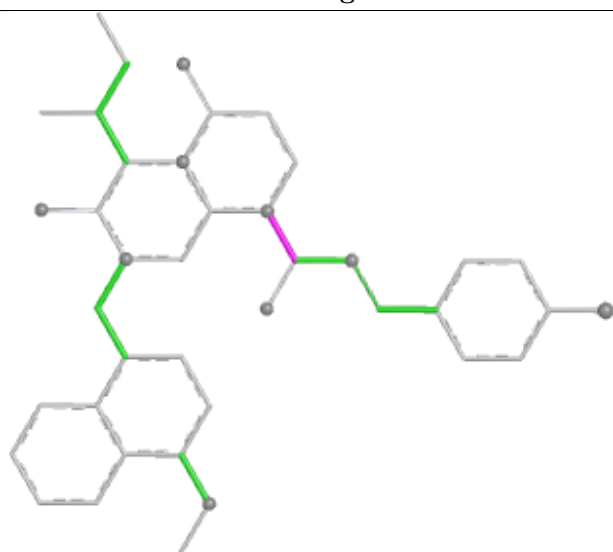
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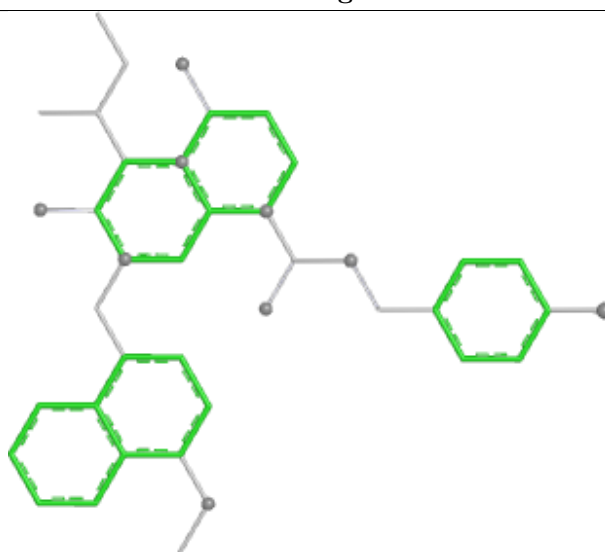
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Bond angles

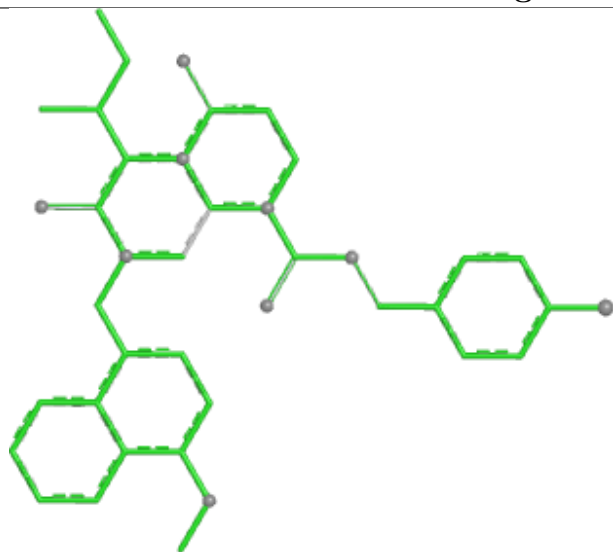


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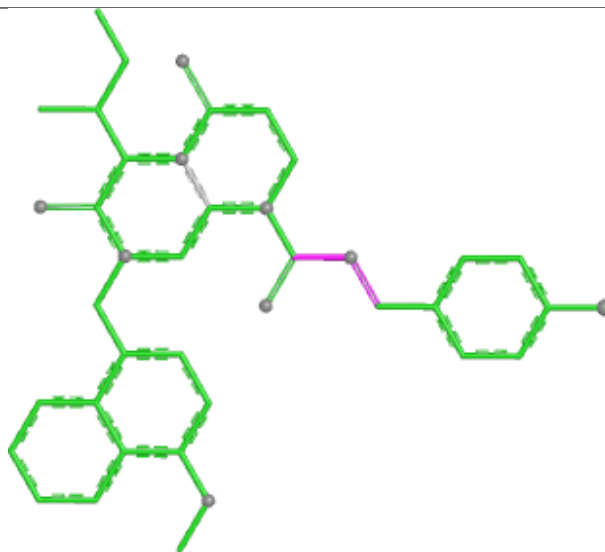


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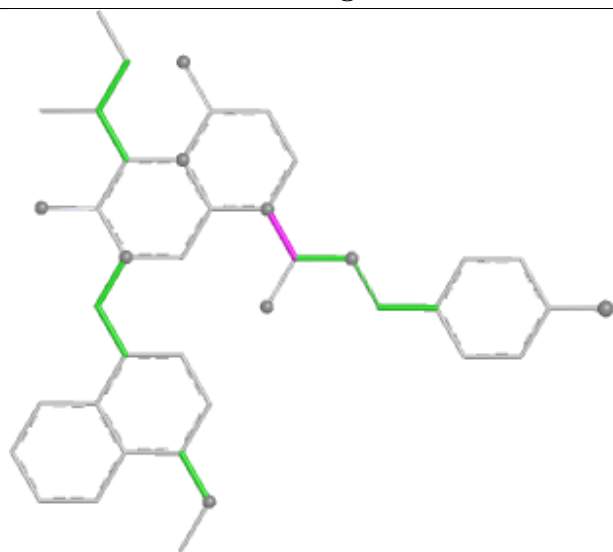
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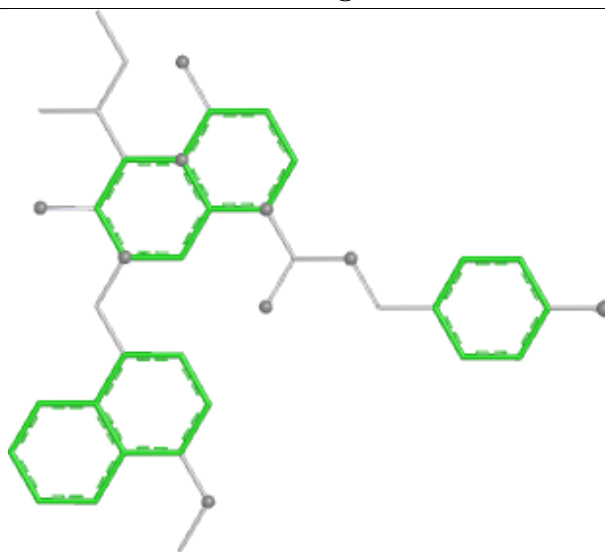
Bond lengths



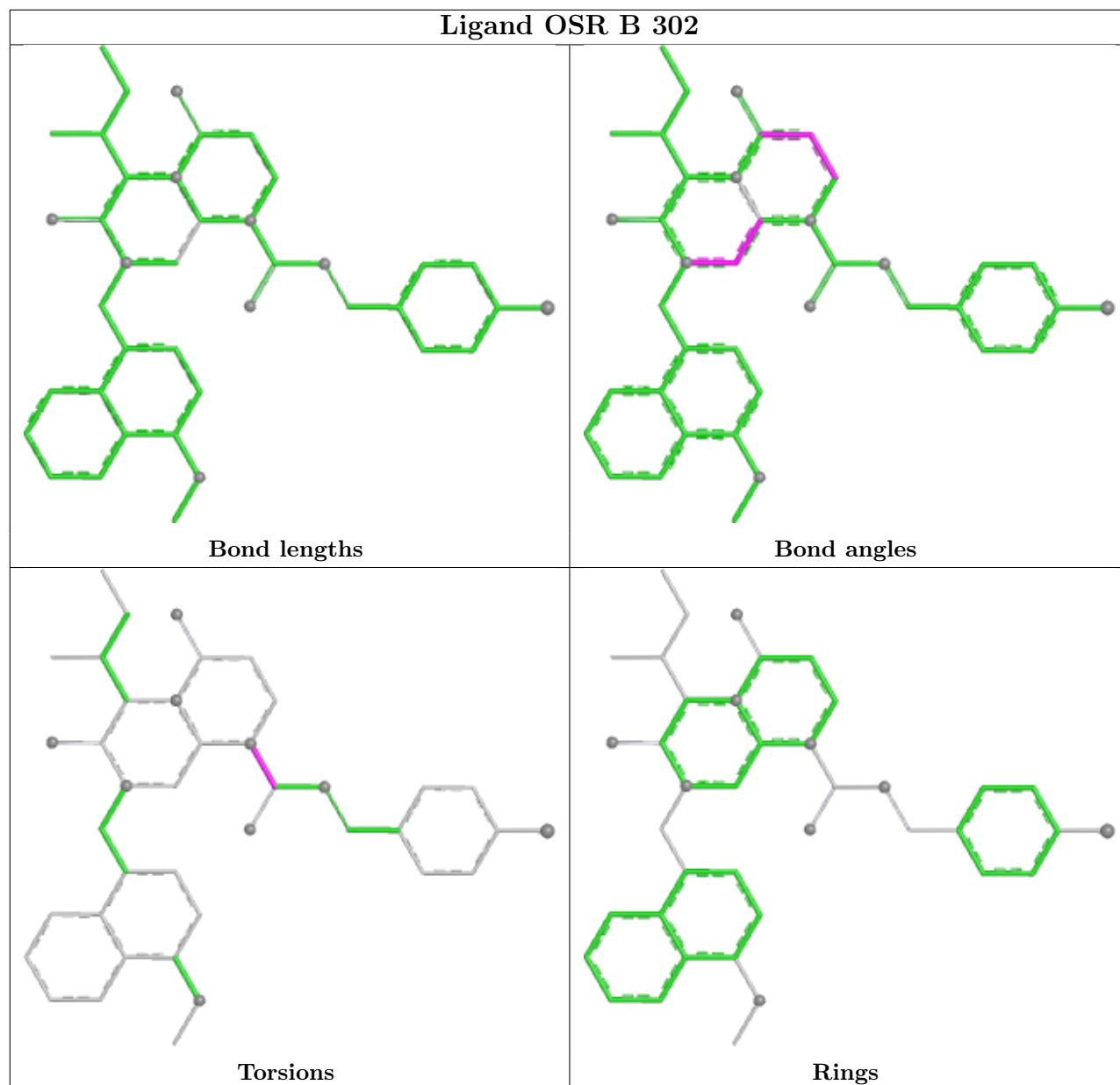
Bond angles



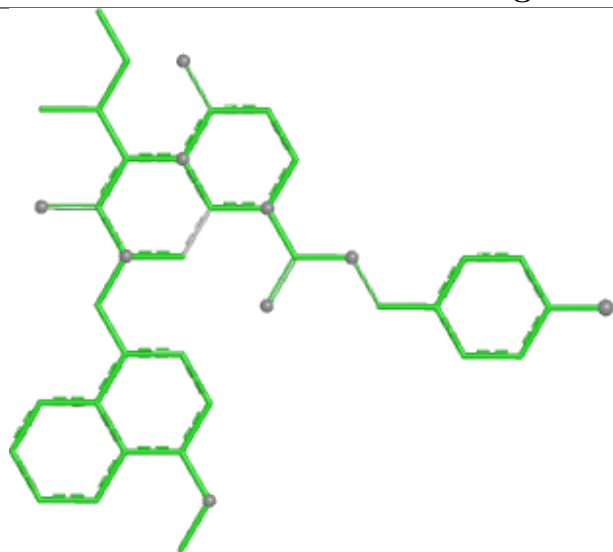
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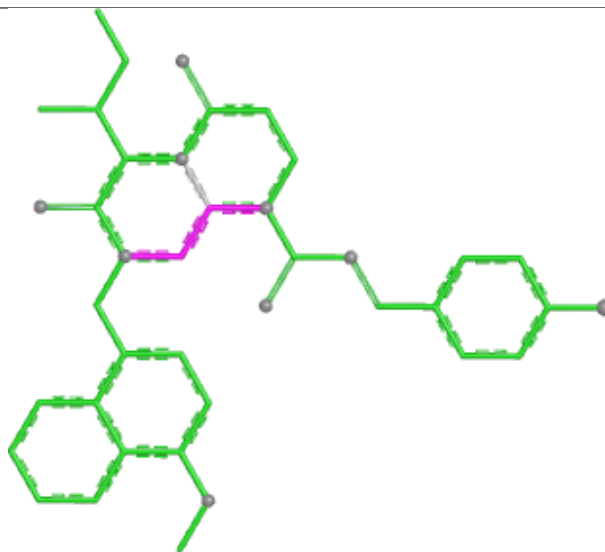
Rings



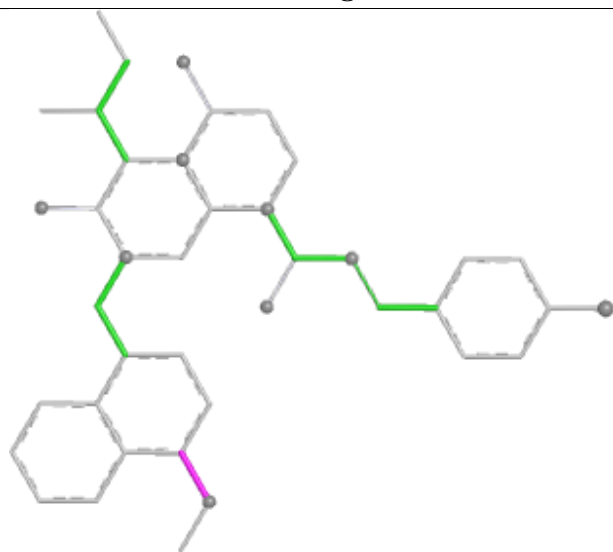
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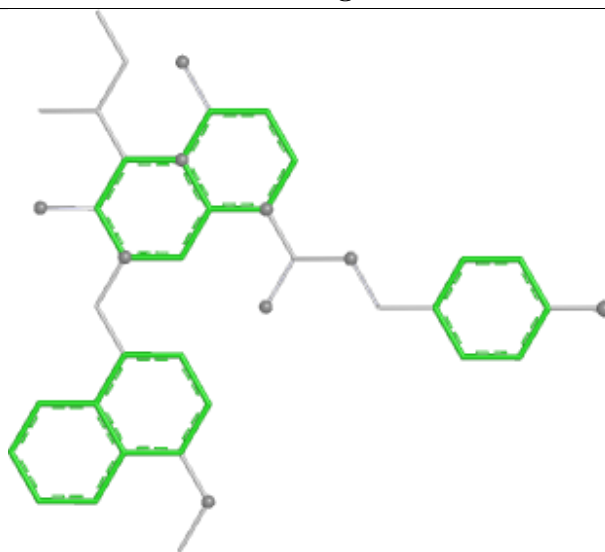
Bond lengths



Bond angles

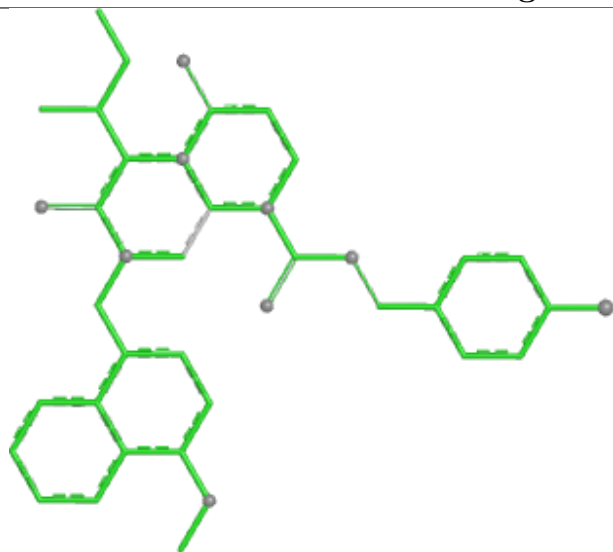


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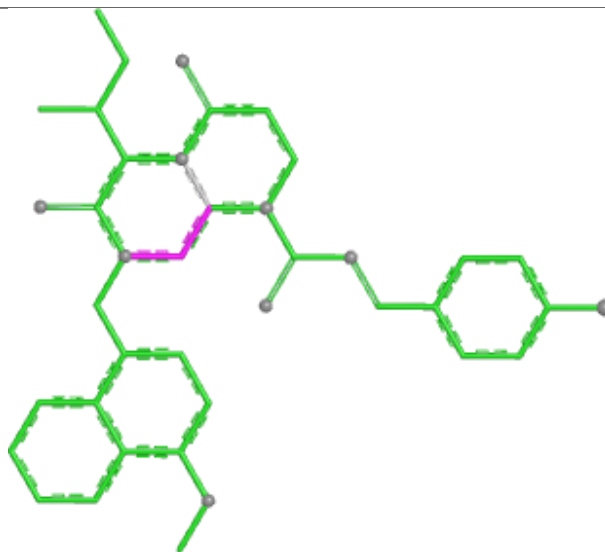


Rings

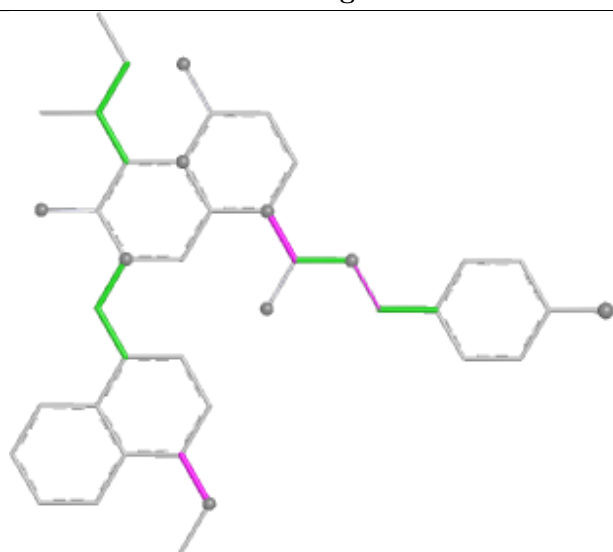
Ligand OSR J 301



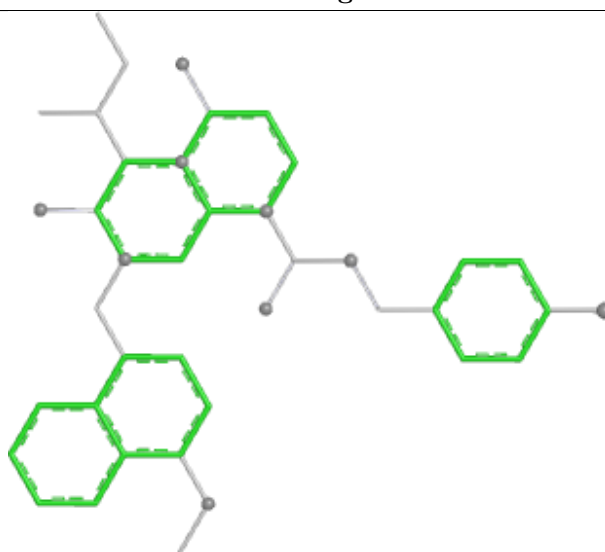
Bond lengths



Bond angles

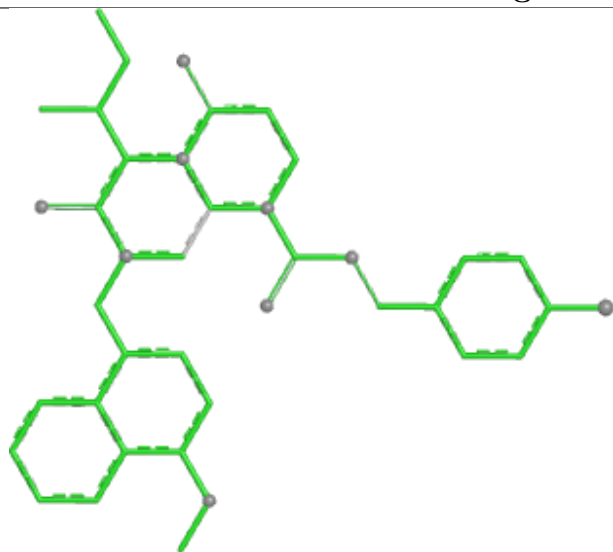


Torsions

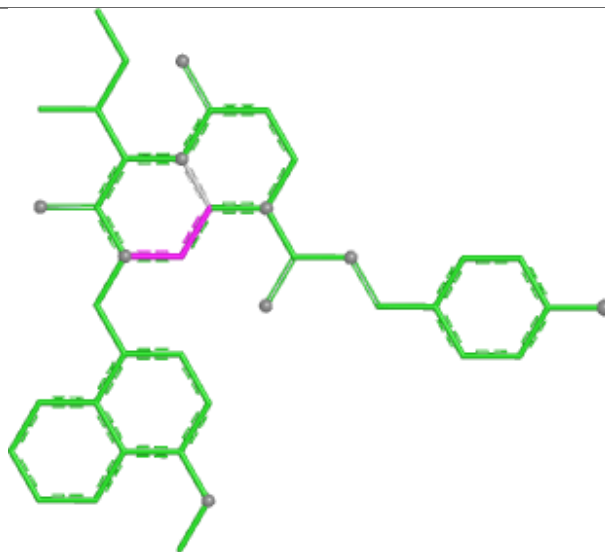


Rings

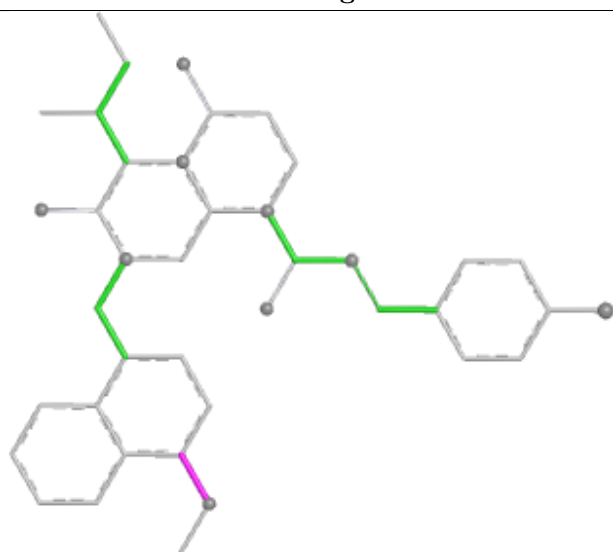
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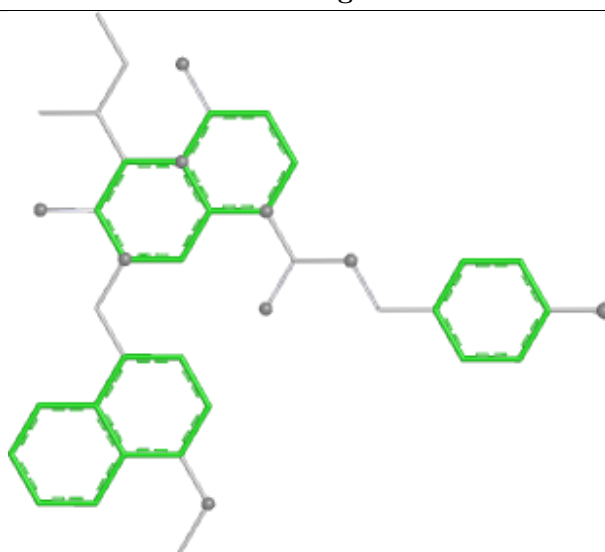
Bond lengths



Bond angles

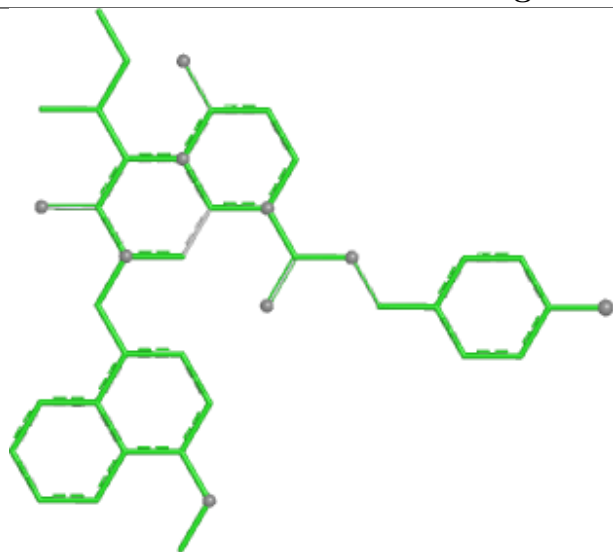


Torsions

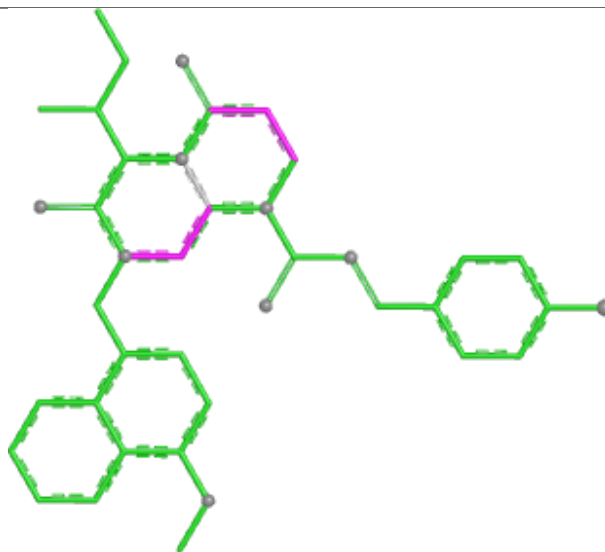


Rings

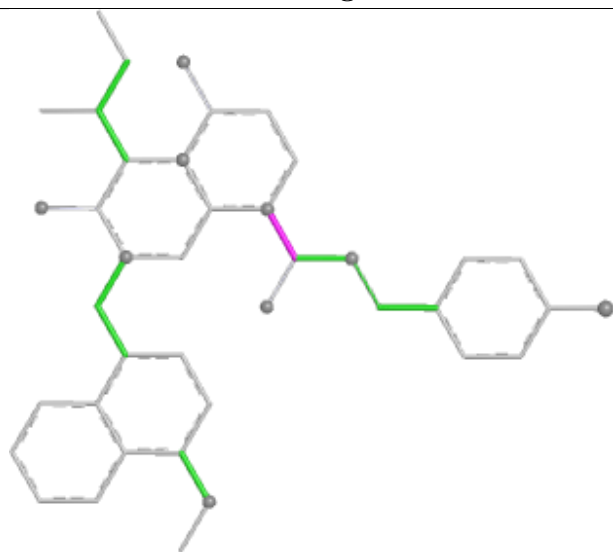
Ligand OSR D 301



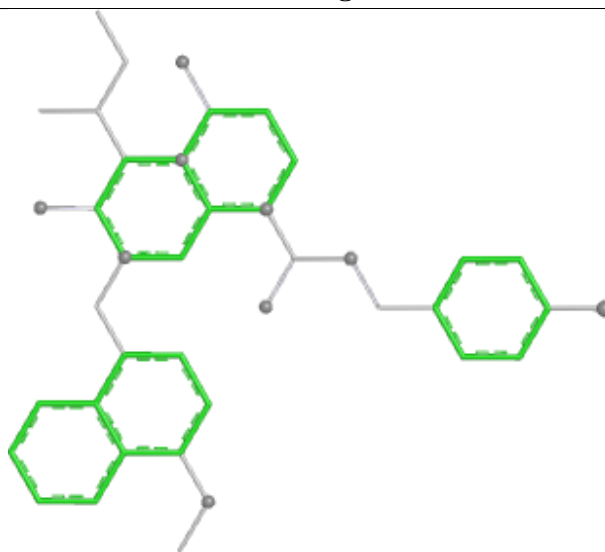
Bond lengths



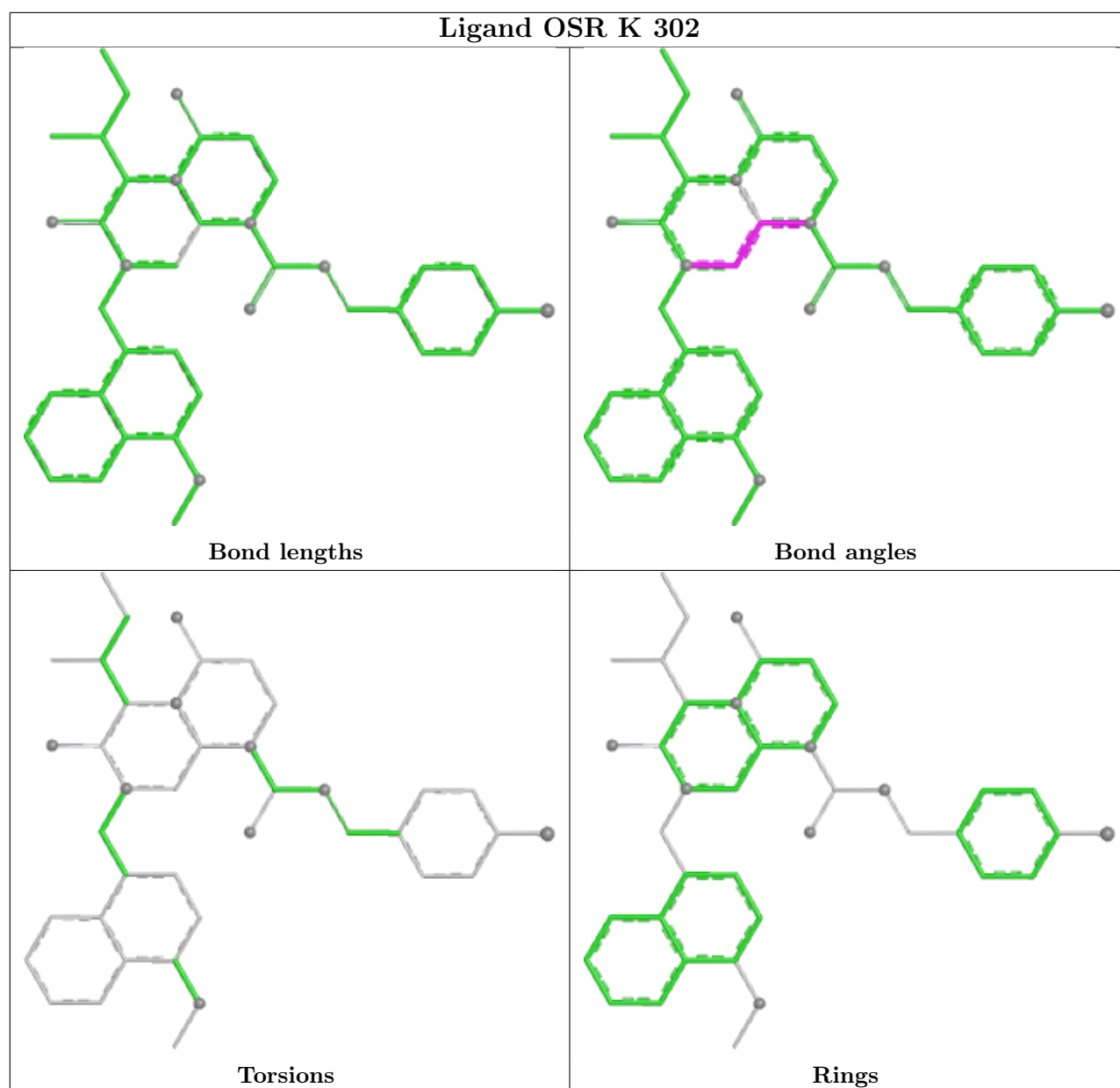
Bond angles

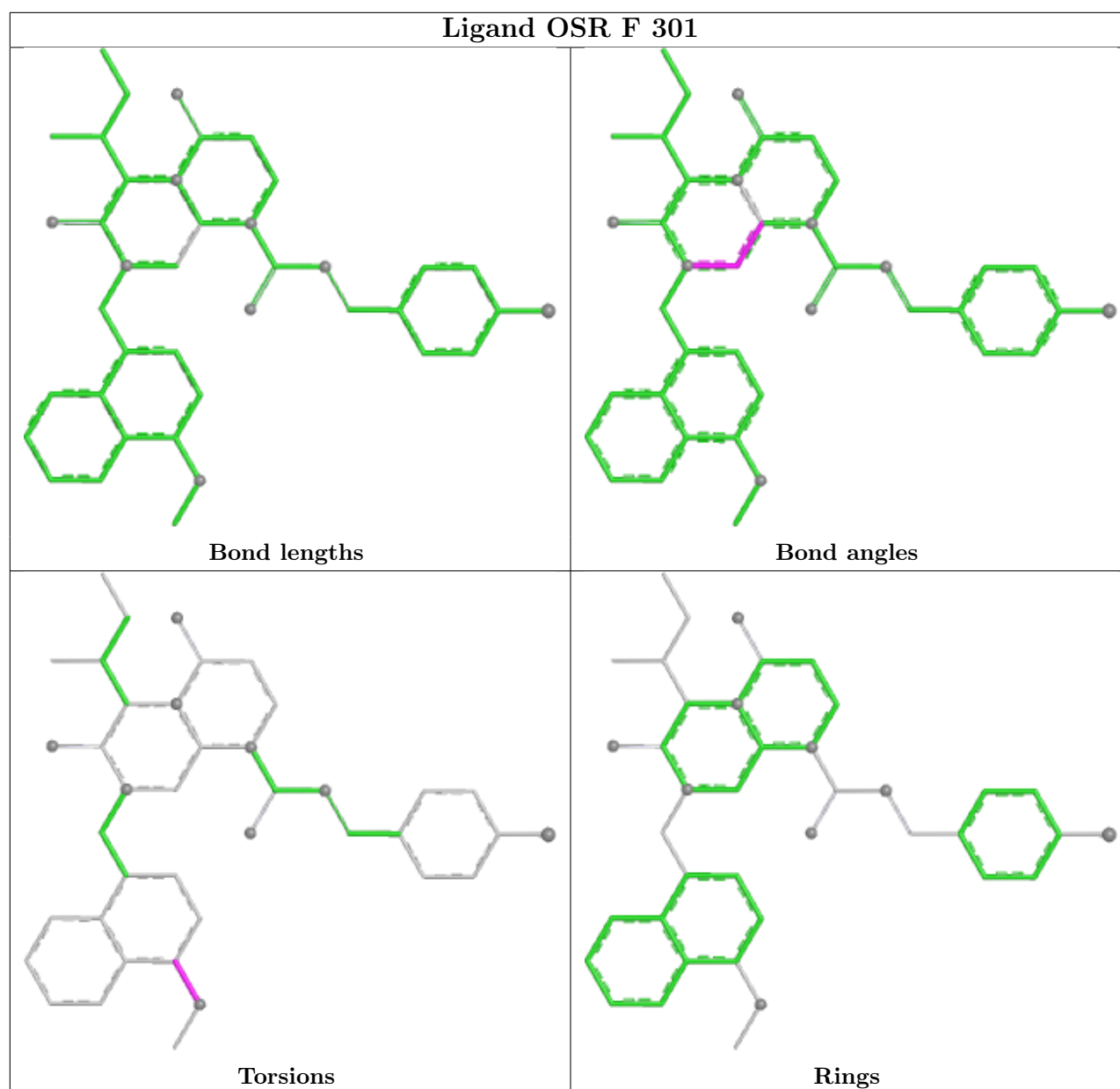


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	0.79	17 (10%) 11 10	19, 28, 45, 60	0
1	B	162/221 (73%)	0.86	18 (11%) 10 9	21, 29, 48, 72	0
1	C	162/221 (73%)	1.16	33 (20%) 3 2	21, 30, 54, 74	0
1	D	163/221 (73%)	0.79	19 (11%) 9 8	18, 27, 47, 60	0
1	E	161/221 (72%)	0.68	20 (12%) 8 7	14, 23, 49, 75	0
1	F	164/221 (74%)	0.47	12 (7%) 21 19	13, 21, 41, 71	0
1	G	164/221 (74%)	0.85	19 (11%) 9 8	17, 27, 48, 59	0
1	H	161/221 (72%)	0.62	17 (10%) 11 10	17, 25, 50, 66	0
1	I	161/221 (72%)	0.74	19 (11%) 9 8	18, 26, 49, 75	0
1	J	163/221 (73%)	1.25	35 (21%) 2 2	21, 31, 53, 72	0
1	K	161/221 (72%)	1.08	32 (19%) 3 2	19, 29, 51, 66	0
1	L	161/221 (72%)	1.12	30 (18%) 3 3	19, 30, 52, 73	0
1	M	162/221 (73%)	1.03	35 (21%) 2 2	16, 23, 54, 80	0
1	N	163/221 (73%)	0.83	22 (13%) 7 6	18, 28, 47, 63	0
All	All	2270/3094 (73%)	0.88	328 (14%) 6 5	13, 27, 51, 80	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	ILE	6.6
1	M	193	ILE	6.5
1	M	76	TYR	6.2
1	N	193	ILE	6.0
1	J	75	ILE	5.9
1	L	180	PRO	5.8
1	K	180	PRO	5.6
1	M	75	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	L	76	TYR	5.5
1	L	75	ILE	5.5
1	E	246	VAL	5.3
1	I	75	ILE	5.3
1	E	75	ILE	5.3
1	I	76	TYR	5.2
1	C	140	LEU	5.2
1	M	79	LEU	5.2
1	J	193	ILE	5.2
1	B	76	TYR	5.1
1	B	180	PRO	5.1
1	E	76	TYR	5.1
1	E	198	ILE	5.0
1	F	75	ILE	5.0
1	M	80	LEU	4.9
1	A	75	ILE	4.8
1	N	180	PRO	4.8
1	F	193	ILE	4.7
1	C	75	ILE	4.7
1	N	75	ILE	4.7
1	E	74	ASP	4.7
1	G	180	PRO	4.5
1	M	105	PHE	4.5
1	L	79	LEU	4.5
1	C	249	PRO	4.5
1	E	248	PRO	4.4
1	C	76	TYR	4.4
1	G	76	TYR	4.4
1	J	140	LEU	4.4
1	C	180	PRO	4.4
1	C	195	ALA	4.4
1	K	76	TYR	4.3
1	B	195	ALA	4.3
1	M	249	PRO	4.3
1	I	193	ILE	4.3
1	J	76	TYR	4.3
1	M	106	LEU	4.2
1	D	74	ASP	4.2
1	E	245	LEU	4.2
1	M	108	SER	4.1
1	H	76	TYR	4.1
1	B	198	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	76	TYR	4.1
1	K	249	PRO	4.1
1	A	140	LEU	4.1
1	J	79	LEU	4.1
1	H	74	ASP	4.0
1	N	76	TYR	4.0
1	L	196	GLU	3.9
1	C	80	LEU	3.9
1	G	80	LEU	3.9
1	G	75	ILE	3.9
1	G	81	ARG	3.9
1	E	79	LEU	3.9
1	E	77	SER	3.8
1	C	77	SER	3.8
1	K	79	LEU	3.8
1	C	245	LEU	3.7
1	C	111	ASN	3.7
1	G	193	ILE	3.7
1	J	111	ASN	3.7
1	B	79	LEU	3.7
1	C	81	ARG	3.7
1	L	105	PHE	3.7
1	J	80	LEU	3.6
1	D	233	MET	3.6
1	C	198	ILE	3.6
1	J	180	PRO	3.6
1	G	79	LEU	3.6
1	M	195	ALA	3.6
1	M	77	SER	3.6
1	K	77	SER	3.5
1	L	248	PRO	3.5
1	H	75	ILE	3.5
1	C	107	GLN	3.4
1	F	249	PRO	3.4
1	F	76	TYR	3.4
1	M	78	ARG	3.4
1	L	80	LEU	3.4
1	E	194	GLN	3.4
1	H	195	ALA	3.4
1	L	101	ALA	3.4
1	C	79	LEU	3.4
1	G	249	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	249	PRO	3.4
1	A	247	HIS	3.3
1	B	74	ASP	3.3
1	F	74	ASP	3.3
1	L	198	ILE	3.3
1	M	97	SER	3.3
1	L	195	ALA	3.3
1	A	80	LEU	3.3
1	F	80	LEU	3.3
1	I	80	LEU	3.3
1	M	104	LEU	3.3
1	H	248	PRO	3.3
1	I	140	LEU	3.3
1	N	118	TYR	3.3
1	M	109	GLU	3.3
1	L	246	VAL	3.3
1	M	107	GLN	3.2
1	C	78	ARG	3.2
1	M	110	SER	3.2
1	I	88	MET	3.2
1	M	88	MET	3.2
1	I	194	GLN	3.2
1	J	78	ARG	3.2
1	K	198	ILE	3.2
1	E	195	ALA	3.2
1	L	245	LEU	3.2
1	L	199	MET	3.2
1	L	247	HIS	3.2
1	K	113	LYS	3.1
1	M	113	LYS	3.1
1	K	233	MET	3.1
1	J	245	LEU	3.1
1	K	78	ARG	3.1
1	C	105	PHE	3.1
1	C	84	ILE	3.1
1	D	75	ILE	3.1
1	J	103	LEU	3.1
1	G	250	GLN	3.1
1	D	249	PRO	3.1
1	H	197	GLU	3.1
1	K	248	PRO	3.1
1	J	195	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	ILE	3.0
1	K	140	LEU	3.0
1	L	140	LEU	3.0
1	B	75	ILE	3.0
1	N	198	ILE	3.0
1	E	247	HIS	3.0
1	G	78	ARG	3.0
1	C	197	GLU	3.0
1	K	245	LEU	3.0
1	H	194	GLN	3.0
1	J	105	PHE	3.0
1	J	249	PRO	3.0
1	E	197	GLU	3.0
1	I	245	LEU	2.9
1	K	246	VAL	2.9
1	N	195	ALA	2.9
1	E	140	LEU	2.9
1	J	107	GLN	2.9
1	E	233	MET	2.9
1	N	233	MET	2.9
1	L	77	SER	2.9
1	C	106	LEU	2.9
1	D	195	ALA	2.9
1	E	199	MET	2.9
1	H	80	LEU	2.9
1	K	103	LEU	2.9
1	D	112	LYS	2.8
1	K	112	LYS	2.8
1	G	233	MET	2.8
1	M	84	ILE	2.8
1	N	80	LEU	2.8
1	N	247	HIS	2.8
1	F	195	ALA	2.8
1	H	77	SER	2.8
1	J	210	ALA	2.8
1	F	79	LEU	2.8
1	H	78	ARG	2.8
1	D	105	PHE	2.8
1	M	81	ARG	2.8
1	C	112	LYS	2.8
1	K	104	LEU	2.8
1	H	198	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	246	VAL	2.8
1	G	105	PHE	2.7
1	N	249	PRO	2.7
1	B	105	PHE	2.7
1	A	193	ILE	2.7
1	C	139	ILE	2.7
1	M	112	LYS	2.7
1	C	247	HIS	2.7
1	B	88	MET	2.6
1	F	105	PHE	2.6
1	M	248	PRO	2.6
1	C	104	LEU	2.6
1	K	107	GLN	2.6
1	B	140	LEU	2.6
1	C	88	MET	2.6
1	H	81	ARG	2.6
1	H	199	MET	2.6
1	M	199	MET	2.6
1	F	194	GLN	2.6
1	I	222	SER	2.6
1	K	110	SER	2.6
1	L	229	TYR	2.6
1	J	104	LEU	2.6
1	J	233	MET	2.6
1	D	108	SER	2.6
1	L	108	SER	2.6
1	M	247	HIS	2.5
1	A	249	PRO	2.5
1	K	114	PRO	2.5
1	H	245	LEU	2.5
1	I	79	LEU	2.5
1	K	84	ILE	2.5
1	K	111	ASN	2.5
1	A	222	SER	2.5
1	C	110	SER	2.5
1	N	97	SER	2.5
1	K	247	HIS	2.5
1	G	118	TYR	2.5
1	L	110	SER	2.5
1	K	199	MET	2.5
1	M	233	MET	2.5
1	L	112	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	80	LEU	2.5
1	J	77	SER	2.5
1	M	198	ILE	2.5
1	N	88	MET	2.5
1	A	105	PHE	2.4
1	K	105	PHE	2.4
1	G	88	MET	2.4
1	I	233	MET	2.4
1	K	88	MET	2.4
1	I	195	ALA	2.4
1	J	101	ALA	2.4
1	M	197	GLU	2.4
1	N	194	GLN	2.4
1	A	77	SER	2.4
1	H	79	LEU	2.4
1	I	104	LEU	2.4
1	J	106	LEU	2.4
1	J	217	LEU	2.4
1	N	77	SER	2.4
1	M	83	ARG	2.4
1	J	194	GLN	2.4
1	H	247	HIS	2.4
1	I	97	SER	2.4
1	N	78	ARG	2.4
1	M	82	GLU	2.4
1	B	107	GLN	2.4
1	C	114	PRO	2.4
1	C	199	MET	2.4
1	L	233	MET	2.4
1	K	80	LEU	2.3
1	I	105	PHE	2.3
1	K	194	GLN	2.3
1	J	84	ILE	2.3
1	B	108	SER	2.3
1	K	197	GLU	2.3
1	G	194	GLN	2.3
1	G	218	GLN	2.3
1	C	113	LYS	2.3
1	C	94	SER	2.3
1	K	85	VAL	2.3
1	L	107	GLN	2.3
1	D	140	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	247	HIS	2.3
1	B	199	MET	2.3
1	C	233	MET	2.3
1	E	88	MET	2.3
1	D	77	SER	2.3
1	L	197	GLU	2.3
1	N	87	VAL	2.3
1	L	103	LEU	2.3
1	D	76	TYR	2.2
1	J	108	SER	2.2
1	A	246	VAL	2.2
1	C	201	LEU	2.2
1	E	80	LEU	2.2
1	I	77	SER	2.2
1	N	108	SER	2.2
1	K	115	ILE	2.2
1	A	233	MET	2.2
1	L	243	LYS	2.2
1	E	78	ARG	2.2
1	J	218	GLN	2.2
1	C	108	SER	2.2
1	F	108	SER	2.2
1	J	222	SER	2.2
1	F	198	ILE	2.2
1	H	233	MET	2.2
1	L	111	ASN	2.2
1	L	95	VAL	2.2
1	M	103	LEU	2.2
1	N	199	MET	2.1
1	B	197	GLU	2.1
1	K	82	GLU	2.1
1	C	246	VAL	2.1
1	G	108	SER	2.1
1	J	248	PRO	2.1
1	A	195	ALA	2.1
1	L	115	ILE	2.1
1	A	219	VAL	2.1
1	E	214	LYS	2.1
1	A	88	MET	2.1
1	B	247	HIS	2.1
1	G	248	PRO	2.1
1	J	247	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	106	LEU	2.1
1	I	111	ASN	2.1
1	M	101	ALA	2.1
1	N	105	PHE	2.1
1	B	84	ILE	2.1
1	D	198	ILE	2.1
1	D	78	ARG	2.1
1	J	85	VAL	2.1
1	J	112	LYS	2.0
1	J	198	ILE	2.0
1	M	115	ILE	2.0
1	M	196	GLU	2.0
1	M	111	ASN	2.0
1	D	104	LEU	2.0
1	N	170	LEU	2.0
1	D	174	ARG	2.0
1	I	78	ARG	2.0
1	N	109	GLU	2.0
1	G	214	LYS	2.0
1	B	94	SER	2.0
1	J	97	SER	2.0
1	J	139	ILE	2.0
1	A	218	GLN	2.0
1	K	218	GLN	2.0
1	D	81	ARG	2.0
1	J	244	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

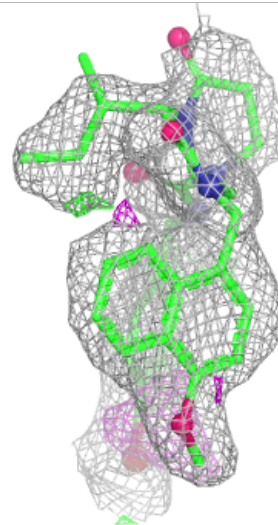
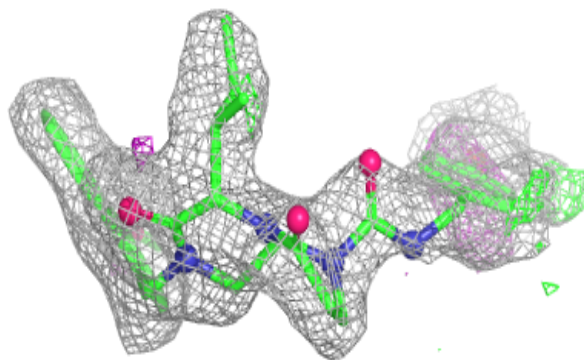
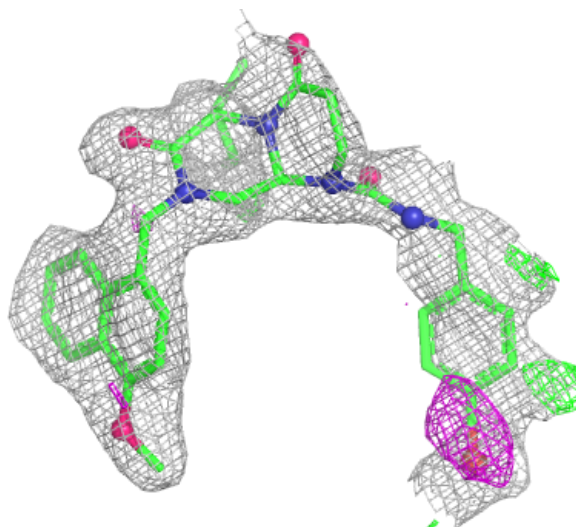
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OSR	C	301	40/40	0.71	0.22	45,55,87,99	0
2	OSR	M	301	40/40	0.81	0.17	40,52,65,69	0
2	OSR	K	301	40/40	0.82	0.17	44,53,71,80	0
2	OSR	G	302	40/40	0.86	0.14	32,39,52,60	0
2	OSR	B	302	40/40	0.86	0.15	37,50,59,64	0
2	OSR	B	301	40/40	0.86	0.14	37,46,60,67	0
2	OSR	K	302	40/40	0.87	0.15	35,48,62,68	0
2	OSR	L	301	40/40	0.87	0.14	35,42,53,60	0
2	OSR	J	301	40/40	0.87	0.14	41,48,60,66	0
2	OSR	H	301	40/40	0.88	0.12	31,37,49,56	0
2	OSR	D	301	40/40	0.90	0.12	30,38,49,57	0
2	OSR	G	301	40/40	0.92	0.11	31,37,43,48	0
2	OSR	I	301	40/40	0.93	0.10	28,35,48,54	0
2	OSR	F	301	40/40	0.93	0.10	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.

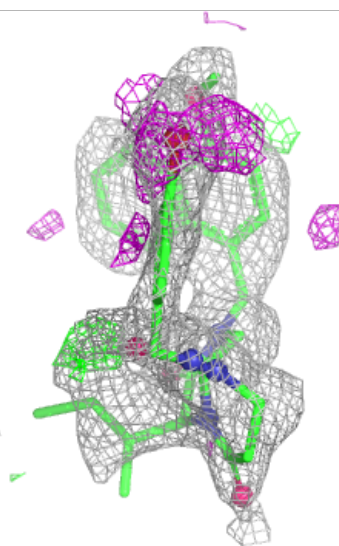
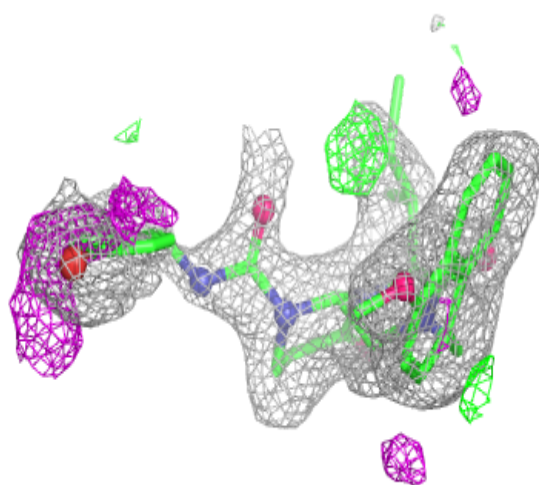
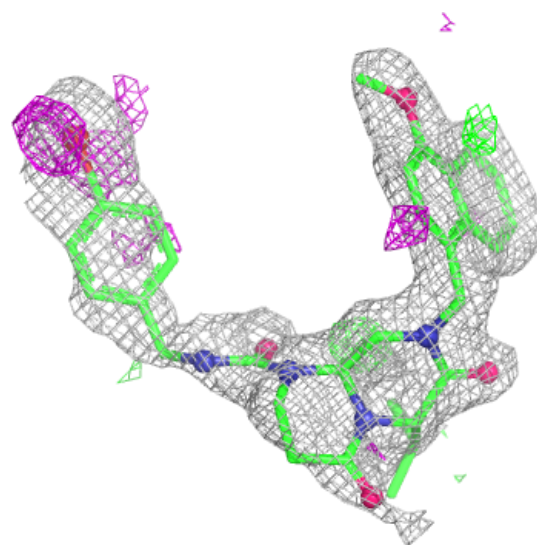
Electron density around OSR C 301:

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



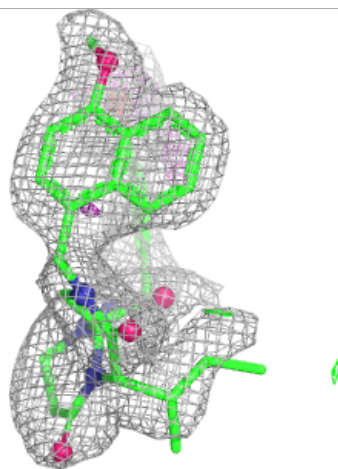
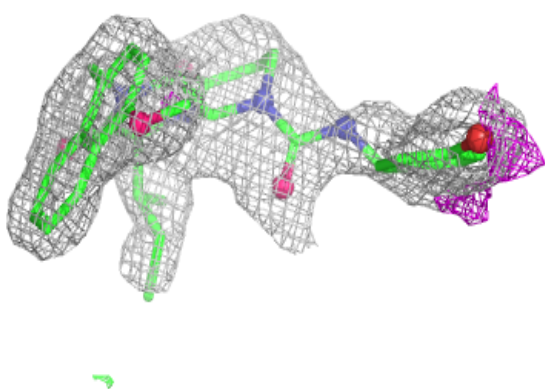
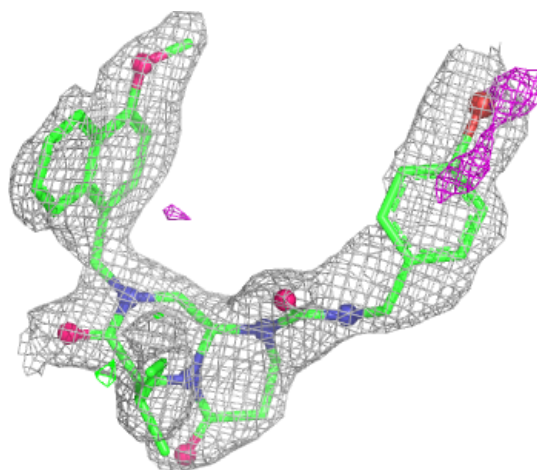
Electron density around OSR M 301:

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



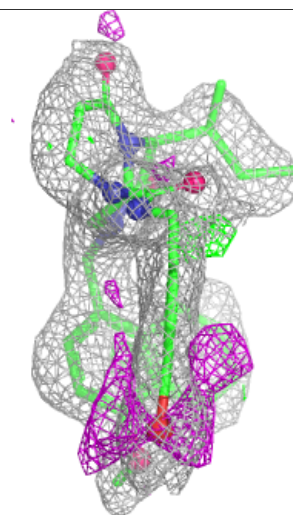
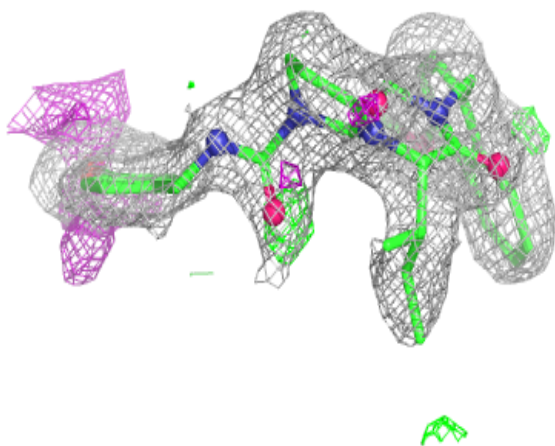
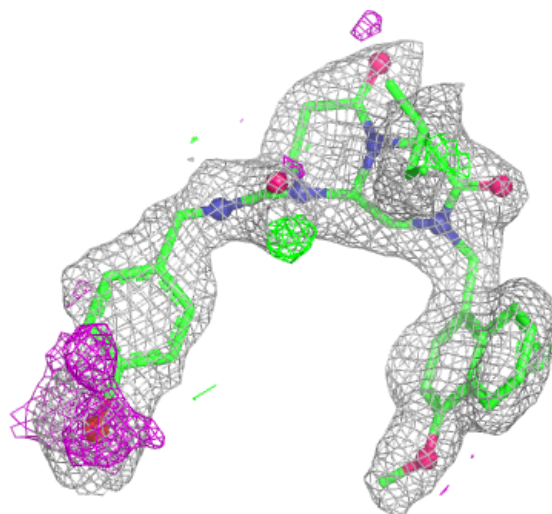
Electron density around OSR K 301:

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



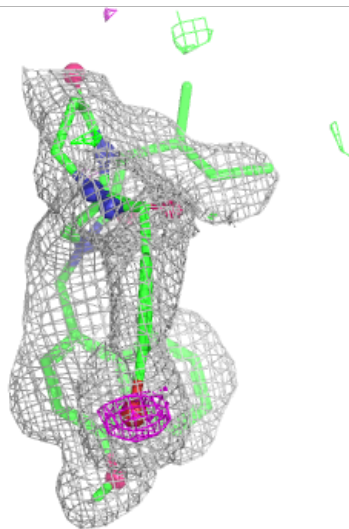
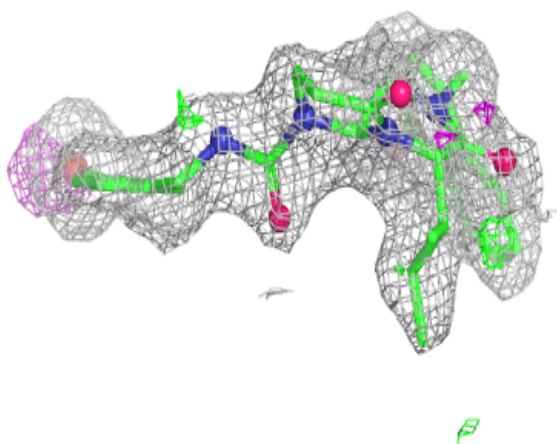
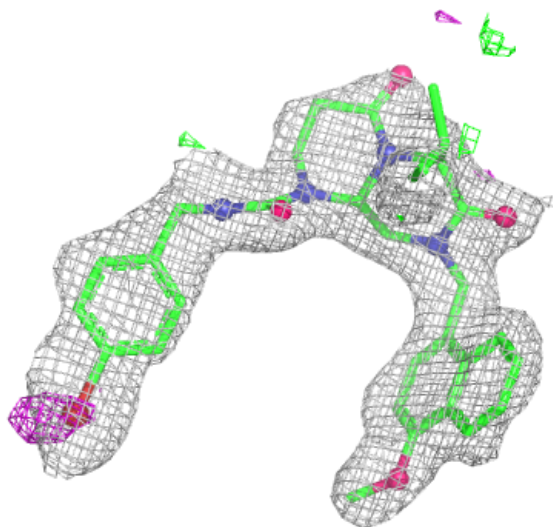
Electron density around OSR G 302:

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



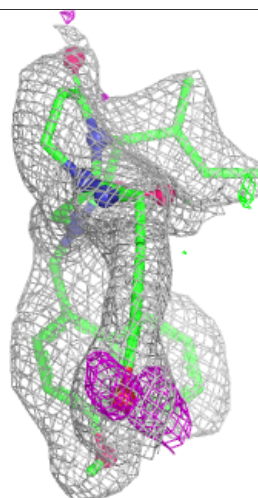
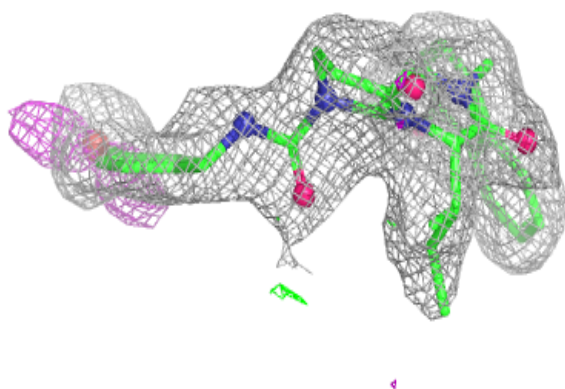
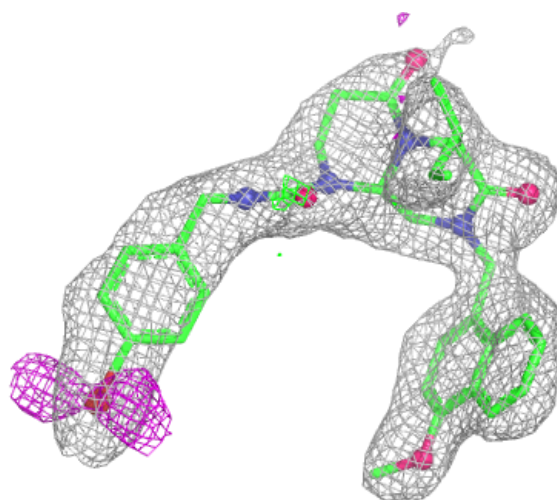
Electron density around OSR B 302:

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



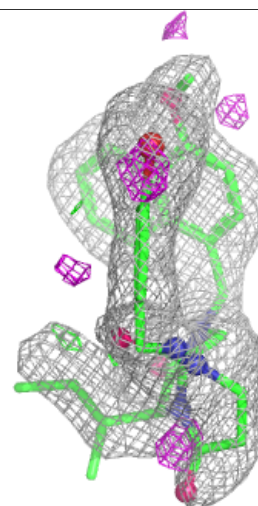
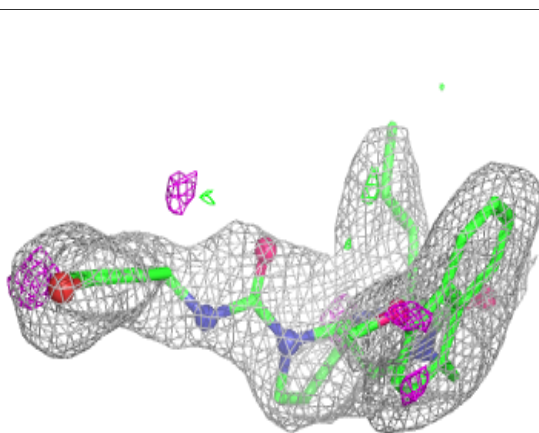
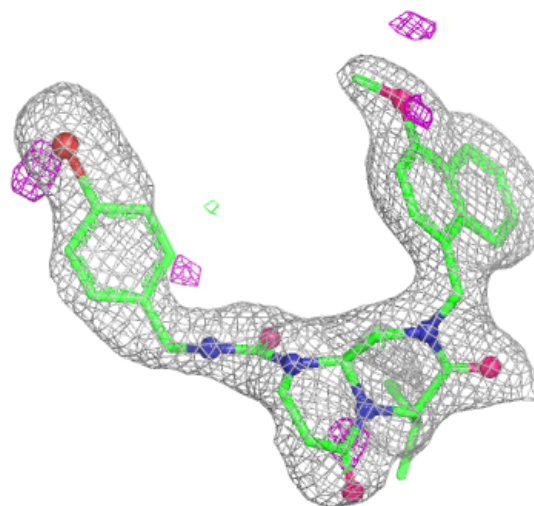
Electron density around OSR B 301:

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



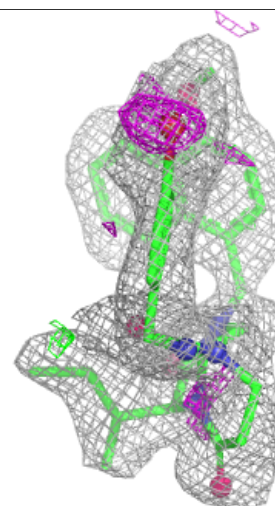
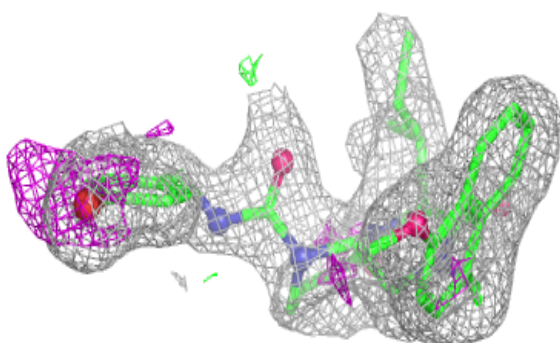
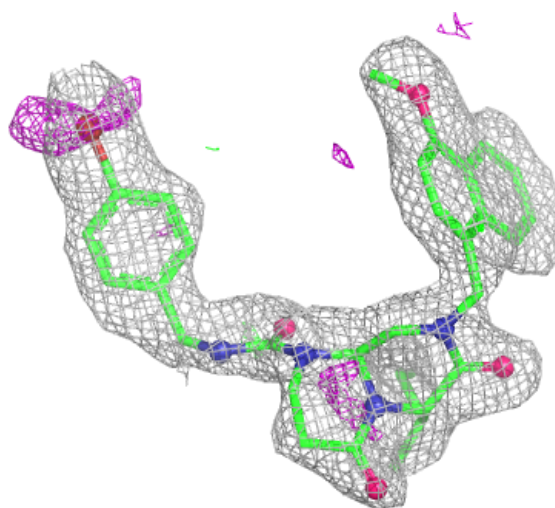
Electron density around OSR K 302:

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



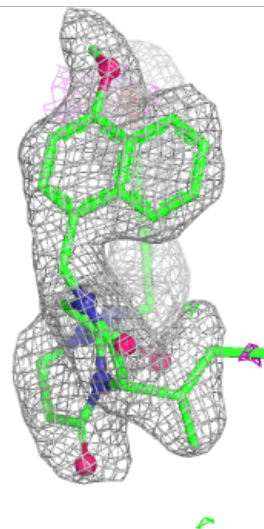
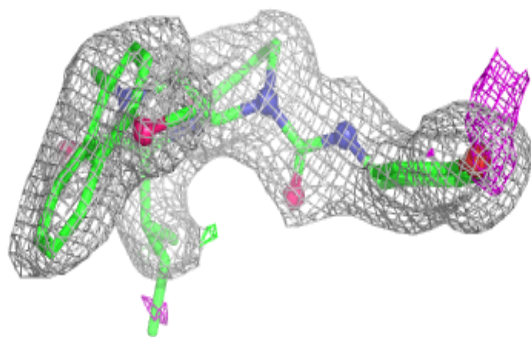
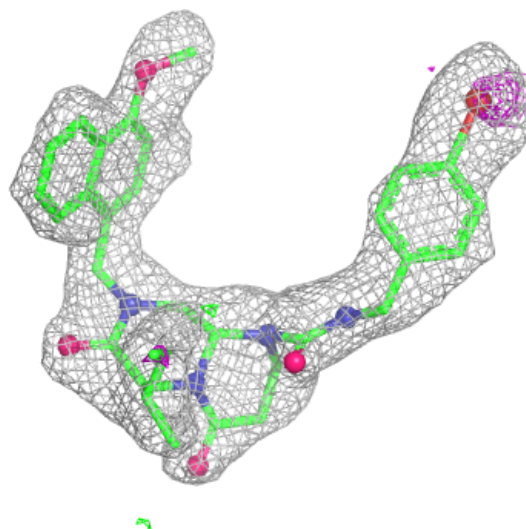
Electron density around OSR L 301:

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



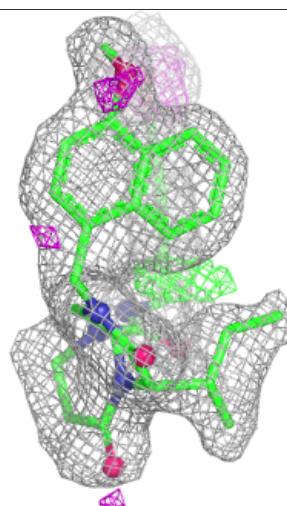
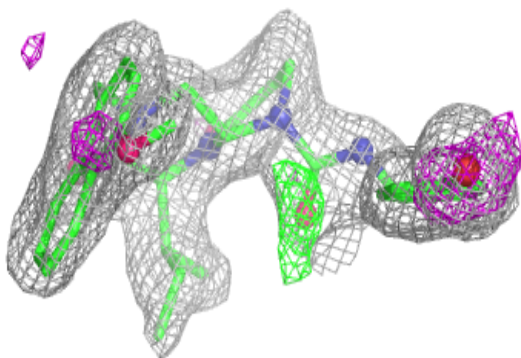
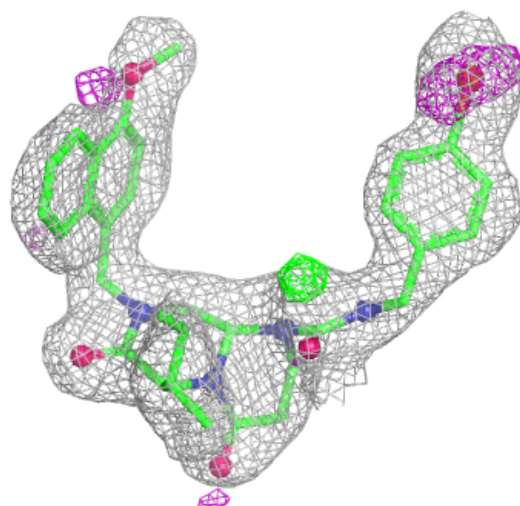
Electron density around OSR J 301:

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



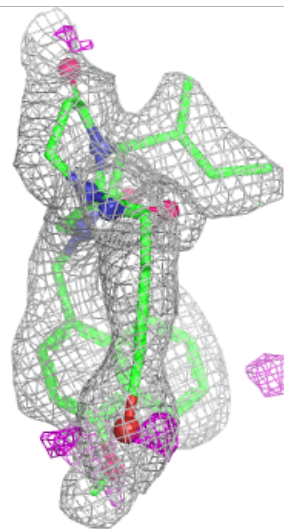
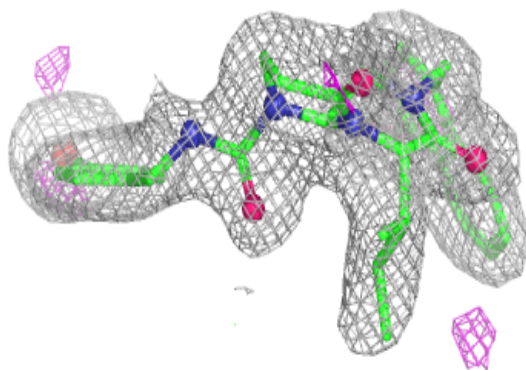
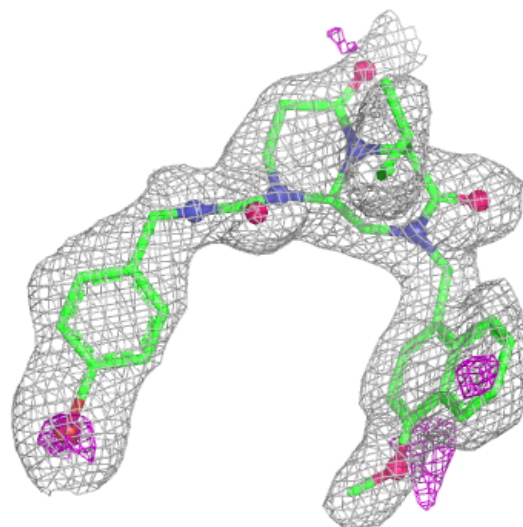
Electron density around OSR H 301:

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



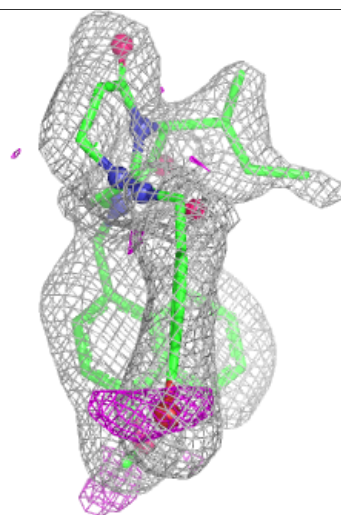
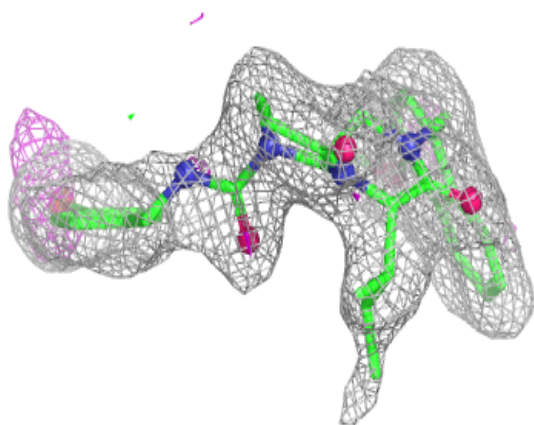
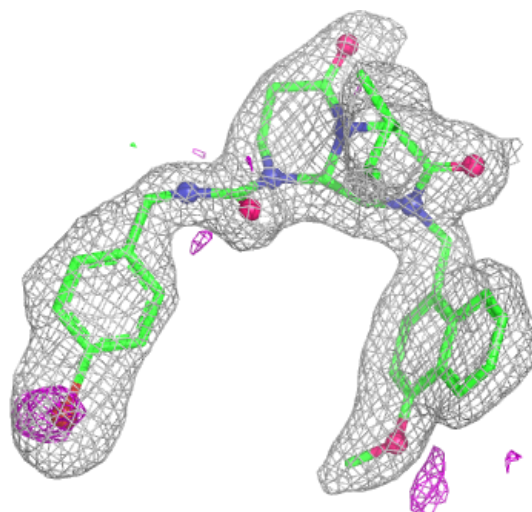
Electron density around OSR D 301:

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



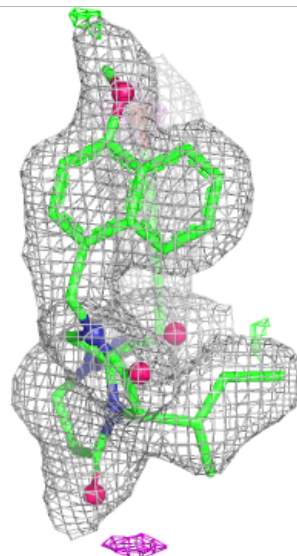
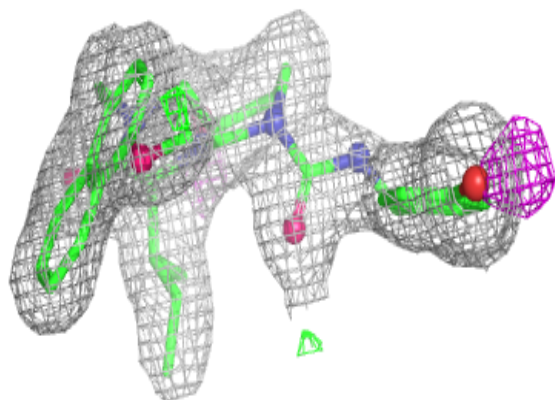
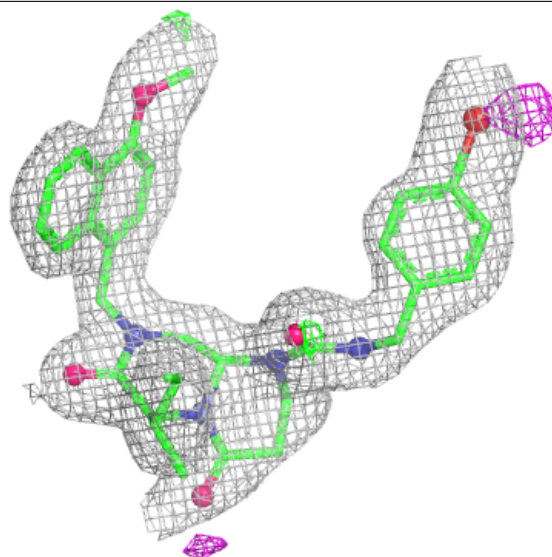
Electron density around OSR G 301:

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



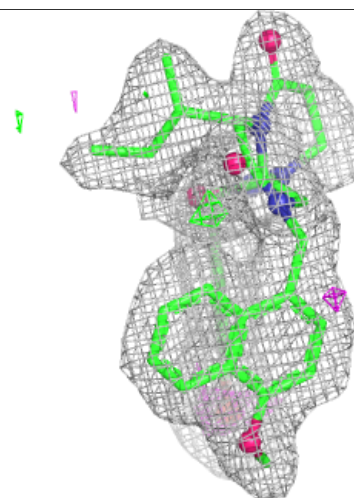
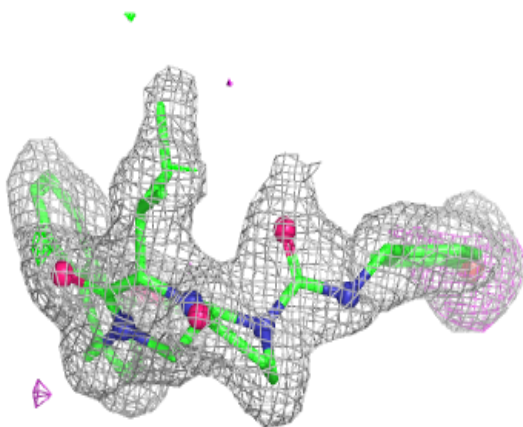
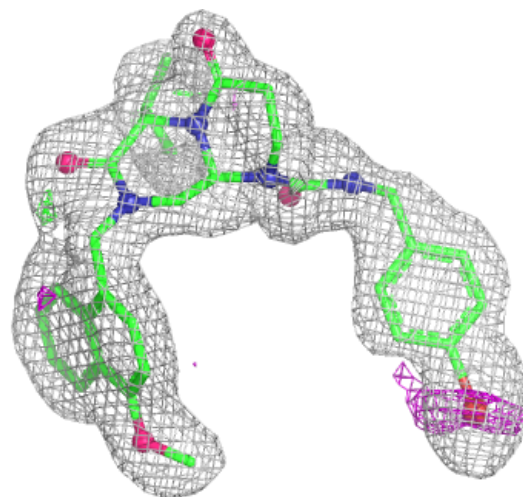
Electron density around OSR I 301:

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



Electron density around OSR F 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.