



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:53 PM UTC

PDB ID : 9ESJ / pdb_00009esj
Title : CDK2-cyclin A in complex with FragLite 31
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on : 2024-03-26
Resolution : 2.37 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

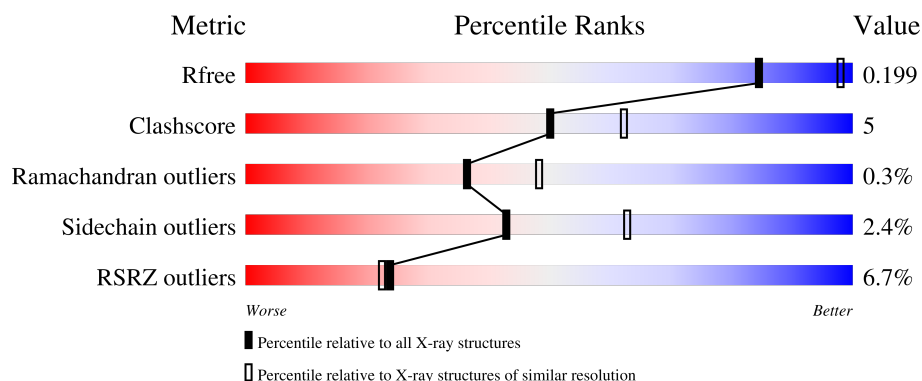
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	302	7% 80% 17% ..
1	C	302	7% 76% 13% 11%
2	B	268	% 88% 9% .
2	D	268	10% 90% 7% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9356 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	P	S	0	1	0
			2413	1565	410	429	1	8			
1	C	270	Total	C	N	O	P	S	0	1	0
			2172	1406	370	388	1	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	2	0
			2126	1374	347	395	10			
2	D	262	Total	C	N	O	S	0	0	0
			2110	1366	344	390	10			

There are 14 discrepancies between the modelled and reference sequences:

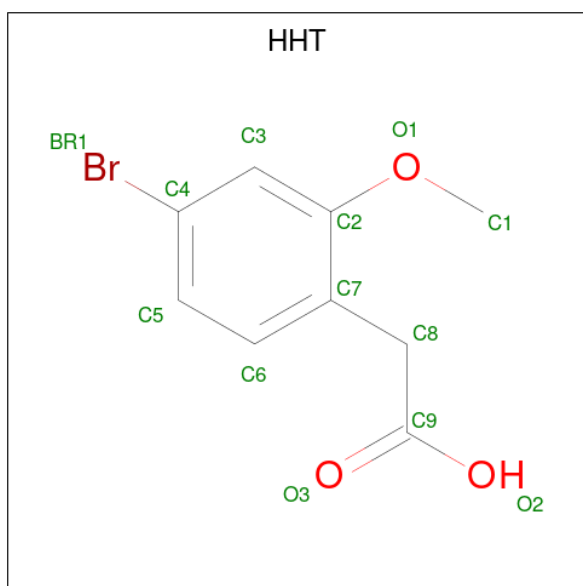
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is 2-(4-bromanyl-2-methoxy-phenyl)ethanoic acid (CCD ID: HHT) (formula: $C_9H_9BrO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	O	0	0
			13	1	9	3		
3	A	1	Total	Br	C	O	0	0
			13	1	9	3		
3	A	1	Total	Br	C	O	0	0
			13	1	9	3		
3	A	1	Total	Br	C	O	0	1
			26	2	18	6		
3	B	1	Total	Br	C	O	0	1
			39	3	27	9		
3	B	1	Total	Br	C	O	0	0
			13	1	9	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 13	Br 1	C 9	O 3	0	0
3	C	1	Total 13	Br 1	C 9	O 3	0	0
3	C	1	Total 13	Br 1	C 9	O 3	0	0
3	D	1	Total 13	Br 1	C 9	O 3	0	0

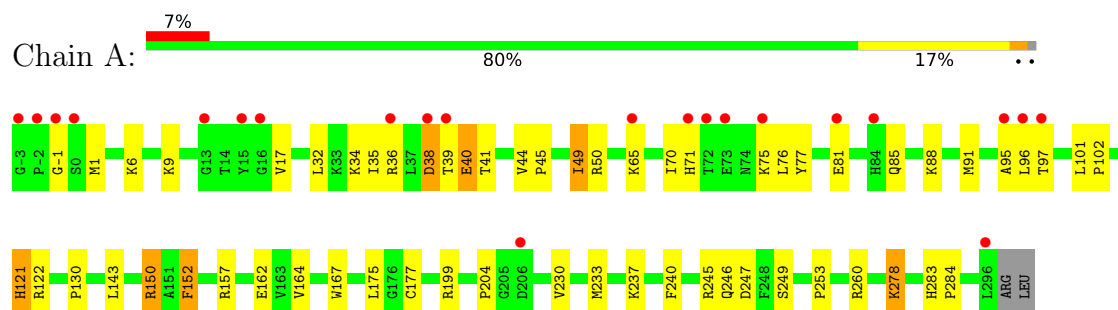
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	120	Total 120	O 120	0	0
4	C	60	Total 60	O 60	0	0
4	D	51	Total 51	O 51	0	0

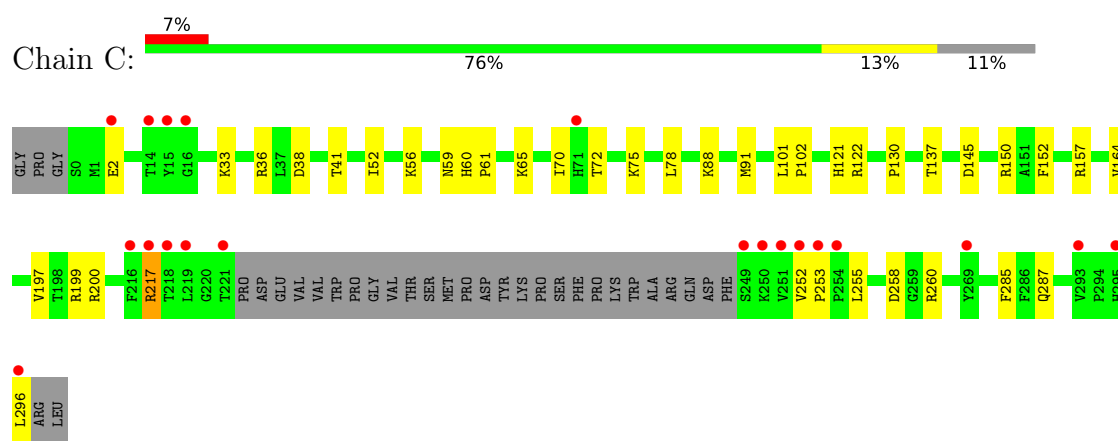
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

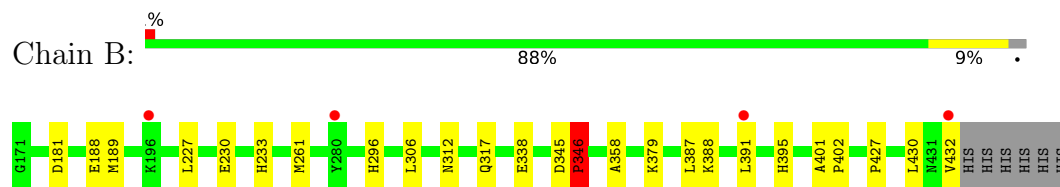
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 1: Cyclin-dependent kinase 2

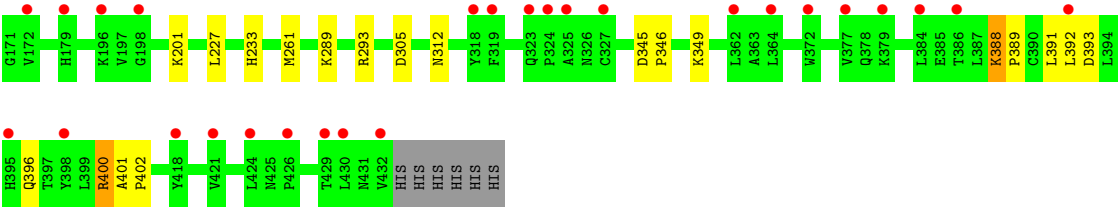


• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.01Å 134.16Å 147.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.50 – 2.37 99.30 – 2.37	Depositor EDS
% Data completeness (in resolution range)	88.3 (99.50-2.37) 88.3 (99.30-2.37)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.218 , 0.223 0.202 , 0.199	Depositor DCC
R_{free} test set	2923 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9356	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, HHT

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	0.69	0/2465	1.20	10/3345 (0.3%)
1	C	0.60	0/2209	1.09	1/2990 (0.0%)
2	B	0.65	0/2176	1.12	2/2959 (0.1%)
2	D	0.59	0/2160	1.10	0/2937
All	All	0.64	0/9010	1.13	13/12231 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	4
2	D	0	1
All	All	0	8

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	PRO	N-CA-CB	-11.37	90.10	102.60
1	A	39	THR	N-CA-C	-6.61	105.08	113.01
1	A	253	PRO	N-CA-C	6.48	118.61	110.70
1	A	247	ASP	CB-CA-C	6.30	119.30	109.84
1	A	152	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	85	GLN	N-CA-CB	-5.53	102.99	111.56
2	B	188	GLU	CB-CA-C	5.42	119.47	110.90
1	A	162	GLU	CB-CG-CD	5.42	121.81	112.60
1	C	253	PRO	N-CA-C	5.24	117.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	278	LYS	CB-CA-C	5.16	118.99	110.88
1	A	246	GLN	CB-CA-C	5.09	117.94	109.53
1	A	40	GLU	N-CA-C	-5.06	106.03	113.61

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	50	ARG	Sidechain
1	C	150	ARG	Sidechain
1	C	157	ARG	Sidechain
1	C	217	ARG	Sidechain
1	C	36	ARG	Sidechain
2	D	293	ARG	Sidechain

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	2413	0	2449	37	0
1	C	2172	0	2226	28	0
2	B	2126	0	2136	19	0
2	D	2110	0	2128	10	0
3	A	65	0	0	6	0
3	B	52	0	0	1	0
3	C	39	0	0	1	0
3	D	13	0	0	0	0
4	A	135	0	0	4	0
4	B	120	0	0	4	0
4	C	60	0	0	1	0
4	D	51	0	0	1	0
All	All	9356	0	8939	95	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 5.

All (95) 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)
3:A:604[B]:HHT:O1	3:A:604[B]:HHT:O2	1.60	1.18
1:A:177:CYS:SG	1:A:233:MET:HE3	1.83	1.16
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.46	0.97
1:A:177:CYS:SG	1:A:233:MET:CE	2.71	0.76
1:A:121:HIS:O	1:A:122:ARG:HG3	1.87	0.75
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.70	0.73
1:A:34:LYS:HE2	1:A:75:LYS:HG2	1.73	0.70
1:A:121:HIS:C	1:A:122:ARG:HG3	2.18	0.68
2:B:387:LEU:O	2:B:391:LEU:HG	1.93	0.68
1:A:65:LYS:HE3	4:A:751:HOH:O	1.99	0.62
2:D:233:HIS:HD2	4:D:629:HOH:O	1.81	0.62
1:C:88:LYS:HA	1:C:91:MET:HE2	1.81	0.62
1:C:59:ASN:HD21	1:C:65:LYS:HZ2	1.47	0.61
1:C:59:ASN:ND2	1:C:65:LYS:NZ	2.48	0.61
1:A:1:MET:HA	1:A:1:MET:HE2	1.82	0.60
1:A:32:LEU:HD12	3:A:603:HHT:BR1	2.56	0.59
1:A:177:CYS:SG	1:A:233:MET:HG2	2.42	0.59
1:A:95:ALA:O	1:A:199:ARG:NH1	2.37	0.57
1:A:249:SER:HA	1:A:260:ARG:HD2	1.86	0.56
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.35	0.56
2:D:227:LEU:HD12	2:D:261:MET:HE3	1.88	0.55
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.55
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.29	0.55
4:A:727:HOH:O	2:B:189:MET:HE2	2.07	0.53
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.37	0.52
2:D:393:ASP:HA	2:D:396:GLN:OE1	2.10	0.52
2:B:358:ALA:HB1	2:B:391:LEU:HD23	1.91	0.52
1:A:177:CYS:HB2	4:A:735:HOH:O	2.09	0.52
2:D:346:PRO:O	2:D:349:LYS:HG2	2.10	0.51
2:B:230:GLU:OE1	2:B:312[B]:ASN:ND2	2.43	0.51
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.46	0.51
1:C:75:LYS:NZ	4:C:602:HOH:O	2.43	0.51
2:B:233:HIS:HE1	4:B:630:HOH:O	1.93	0.51
1:A:65:LYS:HD2	1:A:81:GLU:OE1	2.10	0.50
2:B:388:LYS:HA	2:B:391:LEU:HD12	1.94	0.50
1:A:-1:GLY:HA3	1:A:70:ILE:HD11	1.94	0.50
2:D:392:LEU:O	2:D:396:GLN:HG3	2.11	0.50
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.94	0.49
1:A:237:LYS:HE2	1:A:240:PHE:HE1	1.77	0.49
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.95	0.49
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.94	0.49
2:B:317:GLN:HB3	2:B:379:LYS:NZ	2.28	0.49
1:C:59:ASN:HD21	1:C:65:LYS:NZ	2.09	0.49
2:B:430:LEU:HB3	2:B:432:VAL:HG23	1.94	0.49
1:C:137:THR:HA	1:C:296:LEU:HD12	1.94	0.49
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.95	0.48
1:C:121:HIS:O	1:C:122:ARG:HG3	2.13	0.48
1:A:237:LYS:HE2	1:A:240:PHE:CE1	2.50	0.47
1:A:38:ASP:C	1:A:41:THR:H	2.23	0.47
1:A:101:LEU:N	1:A:102:PRO:CD	2.78	0.47
3:A:604[B]:HHT:O1	3:A:604[B]:HHT:C9	2.50	0.47
1:C:59:ASN:ND2	1:C:65:LYS:HZ3	2.11	0.47
2:B:358:ALA:HA	2:B:391:LEU:HD21	1.97	0.47
1:A:9:LYS:HE2	1:A:17:VAL:HG23	1.97	0.46
2:B:345:ASP:HA	2:B:346:PRO:HA	1.75	0.45
1:A:71:HIS:HD2	1:A:76:LEU:HD13	1.81	0.45
2:B:233:HIS:HD2	4:B:670:HOH:O	1.99	0.45
1:C:56:LYS:HZ3	2:D:305:ASP:CG	2.25	0.45
1:A:65:LYS:HG3	4:A:751:HOH:O	2.16	0.45
1:A:230:VAL:HA	1:A:233:MET:SD	2.57	0.44
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.51	0.44
2:B:387:LEU:HB2	2:B:391:LEU:HD11	2.00	0.44
2:D:401:ALA:HB3	2:D:402:PRO:HD3	2.00	0.44
2:D:396:GLN:HB3	2:D:400:ARG:CZ	2.47	0.44
1:A:88:LYS:HB2	1:A:130:PRO:HB2	2.00	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.83	0.44
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.53	0.43
1:A:77:TYR:OH	3:A:602:HHT:O3	2.34	0.43
1:A:88:LYS:HA	1:A:91:MET:CE	2.48	0.43
1:C:91:MET:HE1	1:C:130:PRO:HG2	2.01	0.43
3:A:604[A]:HHT:C6	3:A:604[A]:HHT:O2	2.65	0.43
1:C:33:LYS:NZ	3:C:501:HHT:O2	2.48	0.43
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.54	0.43
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.54	0.43
2:B:227:LEU:HD12	2:B:261:MET:HE3	2.00	0.42
2:B:401:ALA:N	2:B:402:PRO:CD	2.82	0.42
3:B:502:HHT:C1	4:B:616:HOH:O	2.67	0.42
1:C:38:ASP:HB3	1:C:41:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.86	0.42
1:C:52:ILE:HD11	1:C:78:LEU:HD21	2.01	0.42
1:C:56:LYS:HB3	1:C:56:LYS:HE2	1.63	0.42
1:C:121:HIS:C	1:C:122:ARG:HG3	2.44	0.42
1:A:34:LYS:HZ2	1:A:36:ARG:HH11	1.67	0.41
1:C:255:LEU:O	1:C:260:ARG:NH1	2.53	0.41
1:A:175:LEU:CD1	1:A:233:MET:HE2	2.50	0.41
1:C:258:ASP:HB3	1:C:285:PHE:HB2	2.02	0.41
1:C:101:LEU:HD13	1:C:101:LEU:O	2.20	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41
2:D:388:LYS:O	2:D:389:PRO:C	2.62	0.41
1:A:6:LYS:HB3	1:A:6:LYS:HE2	1.94	0.41
2:B:338:GLU:HG3	4:B:630:HOH:O	2.21	0.41
1:C:122:ARG:HA	1:C:152:PHE:CZ	2.56	0.40
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.89	0.40
3:A:603:HHT:O1	3:A:603:HHT:C9	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	298/302 (99%)	290 (97%)	7 (2%)	1 (0%)	36	48
1	C	266/302 (88%)	249 (94%)	15 (6%)	2 (1%)	16	23
2	B	262/268 (98%)	258 (98%)	4 (2%)	0	100	100
2	D	260/268 (97%)	256 (98%)	4 (2%)	0	100	100
All	All	1086/1140 (95%)	1053 (97%)	30 (3%)	3 (0%)	36	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
1	C	145	ASP

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	263/264 (100%)	254 (97%)	9 (3%)	32	51
1	C	237/264 (90%)	229 (97%)	8 (3%)	32	51
2	B	236/240 (98%)	235 (100%)	1 (0%)	84	91
2	D	234/240 (98%)	228 (97%)	6 (3%)	40	60
All	All	970/1008 (96%)	946 (98%)	24 (2%)	43	61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	38	ASP
1	A	40	GLU
1	A	49	ILE
1	A	96	LEU
1	A	97	THR
1	A	143	LEU
1	A	150	ARG
1	A	157	ARG
2	B	346	PRO
1	C	2[A]	GLU
1	C	2[B]	GLU
1	C	70	ILE
1	C	72	THR
1	C	199	ARG
1	C	200	ARG
1	C	217	ARG
1	C	287	GLN
2	D	201	LYS

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Mol	Chain	Res	Type
2	D	289	LYS
2	D	312	ASN
2	D	388	LYS
2	D	391	LEU
2	D	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	378	GLN
2	B	395	HIS
2	B	403	GLN
1	C	59	ASN
1	C	265	GLN
1	C	287	GLN
2	D	254	GLN
2	D	406	GLN
2	D	419	HIS
2	D	431	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	C	160	1	8,10,11	1.02	0	10,14,16	1.04	0
1	TPO	A	160	1	8,10,11	0.72	0	10,14,16	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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
3	HHT	A	602	-	13,13,13	0.95	0	17,17,17	1.36	2 (11%)
3	HHT	B	501[A]	-	13,13,13	1.02	1 (7%)	17,17,17	0.78	0
3	HHT	A	604[A]	-	13,13,13	0.70	0	17,17,17	1.03	1 (5%)
3	HHT	A	601	-	13,13,13	1.02	1 (7%)	17,17,17	0.89	0
3	HHT	C	502	-	13,13,13	0.85	0	17,17,17	1.03	2 (11%)
3	HHT	A	603	-	13,13,13	0.90	0	17,17,17	0.95	0
3	HHT	B	501[B]	-	13,13,13	0.71	0	17,17,17	0.64	0
3	HHT	B	501[C]	-	13,13,13	0.91	0	17,17,17	1.96	3 (17%)
3	HHT	C	503	-	13,13,13	0.84	0	17,17,17	0.80	0
3	HHT	C	501	-	13,13,13	0.94	1 (7%)	17,17,17	0.84	0
3	HHT	D	501	-	13,13,13	1.17	1 (7%)	17,17,17	0.82	0
3	HHT	A	604[B]	-	13,13,13	0.94	1 (7%)	17,17,17	1.52	2 (11%)
3	HHT	B	502	-	13,13,13	1.18	1 (7%)	17,17,17	1.43	3 (17%)

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
3	HHT	A	602	-	-	0/6/6/6	0/1/1/1
3	HHT	B	501[A]	-	-	2/6/6/6	0/1/1/1
3	HHT	A	604[A]	-	-	2/6/6/6	0/1/1/1
3	HHT	A	601	-	-	2/6/6/6	0/1/1/1
3	HHT	C	502	-	-	0/6/6/6	0/1/1/1
3	HHT	A	603	-	-	3/6/6/6	0/1/1/1
3	HHT	B	501[B]	-	-	4/6/6/6	0/1/1/1
3	HHT	B	501[C]	-	-	4/6/6/6	0/1/1/1
3	HHT	C	503	-	-	0/6/6/6	0/1/1/1
3	HHT	C	501	-	-	0/6/6/6	0/1/1/1
3	HHT	D	501	-	-	2/6/6/6	0/1/1/1
3	HHT	A	604[B]	-	-	4/6/6/6	0/1/1/1
3	HHT	B	502	-	-	3/6/6/6	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	HHT	C2-C7	3.36	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	HHT	C2-C7	2.53	1.44	1.39
3	B	501[A]	HHT	C2-C7	2.43	1.43	1.39
3	C	501	HHT	O2-C9	-2.18	1.23	1.30
3	A	601	HHT	O2-C9	-2.12	1.23	1.30
3	A	604[B]	HHT	C2-C7	2.06	1.43	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501[C]	HHT	C1-O1-C2	-6.43	108.08	117.51
3	A	604[B]	HHT	C1-O1-C2	-4.74	110.56	117.51
3	A	602	HHT	C1-O1-C2	4.37	123.92	117.51
3	B	502	HHT	C7-C8-C9	-3.25	106.11	113.10
3	B	501[C]	HHT	C7-C8-C9	-2.83	107.00	113.10
3	B	502	HHT	C1-O1-C2	2.74	121.53	117.51
3	A	604[A]	HHT	C7-C8-C9	-2.59	107.52	113.10
3	B	502	HHT	O1-C2-C7	-2.21	112.67	115.96
3	C	502	HHT	C1-O1-C2	2.20	120.73	117.51
3	B	501[C]	HHT	O1-C2-C7	-2.19	112.70	115.96
3	A	602	HHT	C7-C8-C9	-2.16	108.45	113.10
3	A	604[B]	HHT	C7-C8-C9	2.15	117.74	113.10
3	C	502	HHT	O3-C9-C8	-2.07	116.70	122.94

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604[B]	HHT	C6-C7-C8-C9
3	A	604[B]	HHT	C2-C7-C8-C9
3	B	502	HHT	C3-C2-O1-C1
3	B	502	HHT	C7-C2-O1-C1
3	B	501[C]	HHT	C7-C2-O1-C1
3	B	501[A]	HHT	C6-C7-C8-C9
3	B	501[B]	HHT	C3-C2-O1-C1
3	B	501[C]	HHT	C3-C2-O1-C1
3	B	501[B]	HHT	C7-C2-O1-C1
3	A	604[A]	HHT	C2-C7-C8-C9
3	B	501[A]	HHT	C2-C7-C8-C9
3	A	604[A]	HHT	C6-C7-C8-C9
3	A	603	HHT	C7-C2-O1-C1
3	B	501[B]	HHT	C7-C8-C9-O2
3	A	601	HHT	C7-C8-C9-O2

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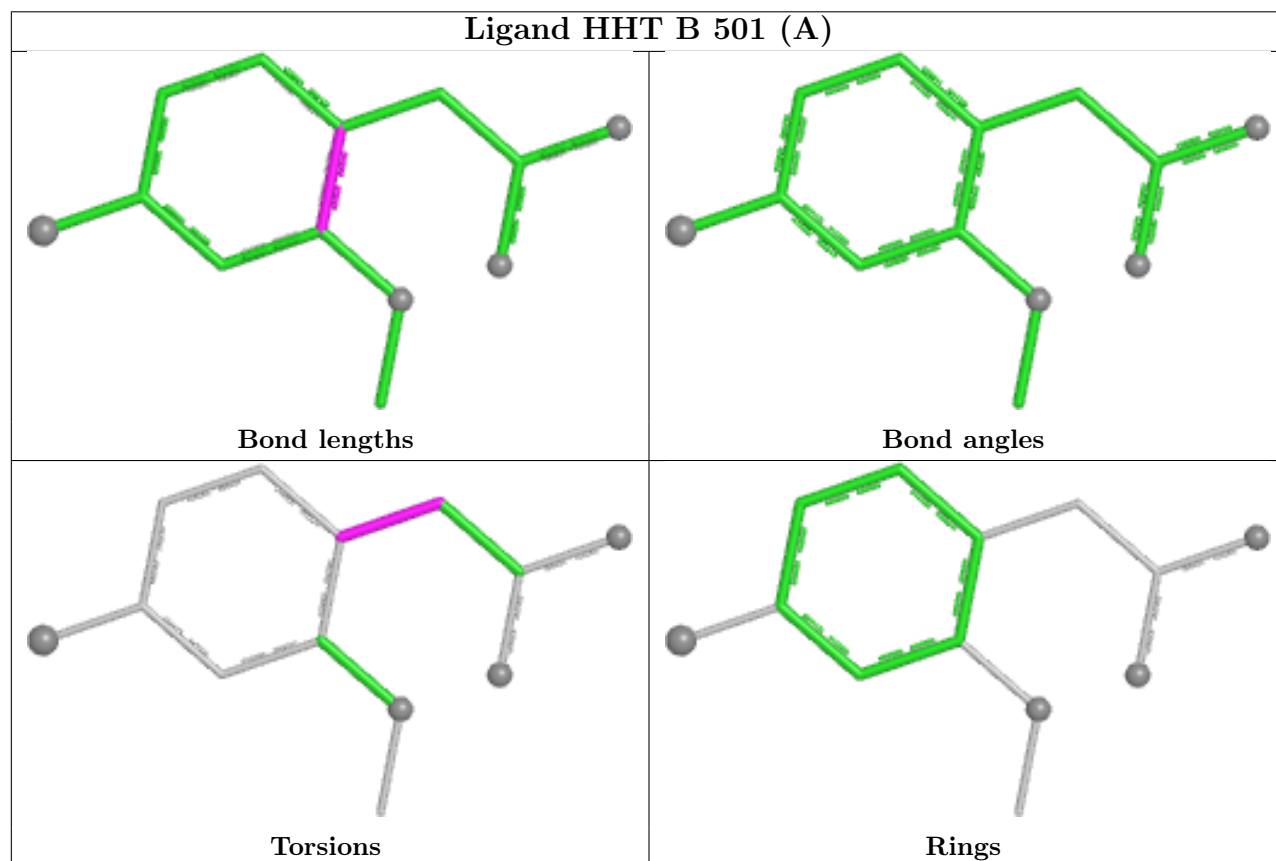
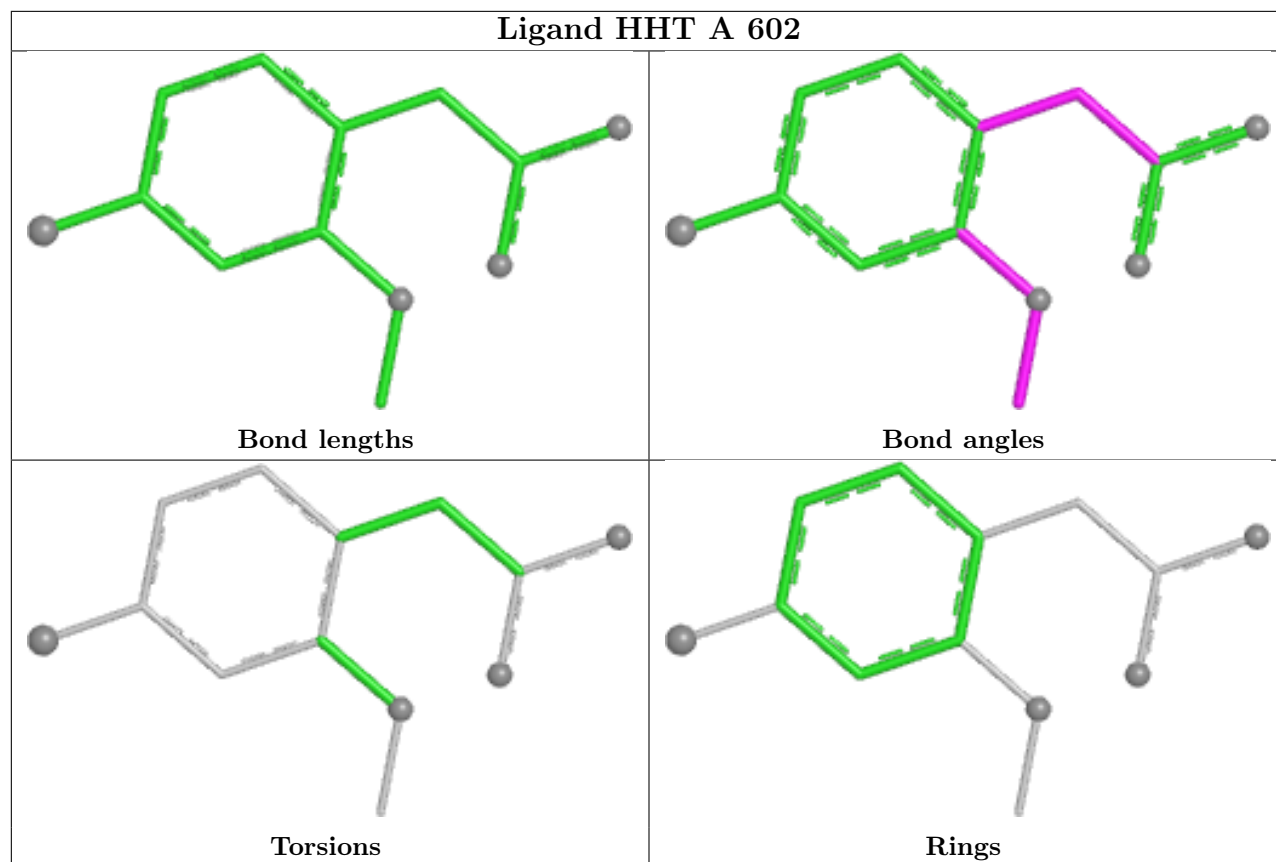
Mol	Chain	Res	Type	Atoms
3	B	501[B]	HHT	C7-C8-C9-O3
3	A	601	HHT	C7-C8-C9-O3
3	A	603	HHT	C2-C7-C8-C9
3	A	603	HHT	C6-C7-C8-C9
3	B	501[C]	HHT	C7-C8-C9-O2
3	A	604[B]	HHT	C7-C8-C9-O2
3	A	604[B]	HHT	C7-C8-C9-O3
3	B	501[C]	HHT	C7-C8-C9-O3
3	D	501	HHT	C6-C7-C8-C9
3	D	501	HHT	C7-C8-C9-O2
3	B	502	HHT	C7-C8-C9-O3

There are no ring outliers.

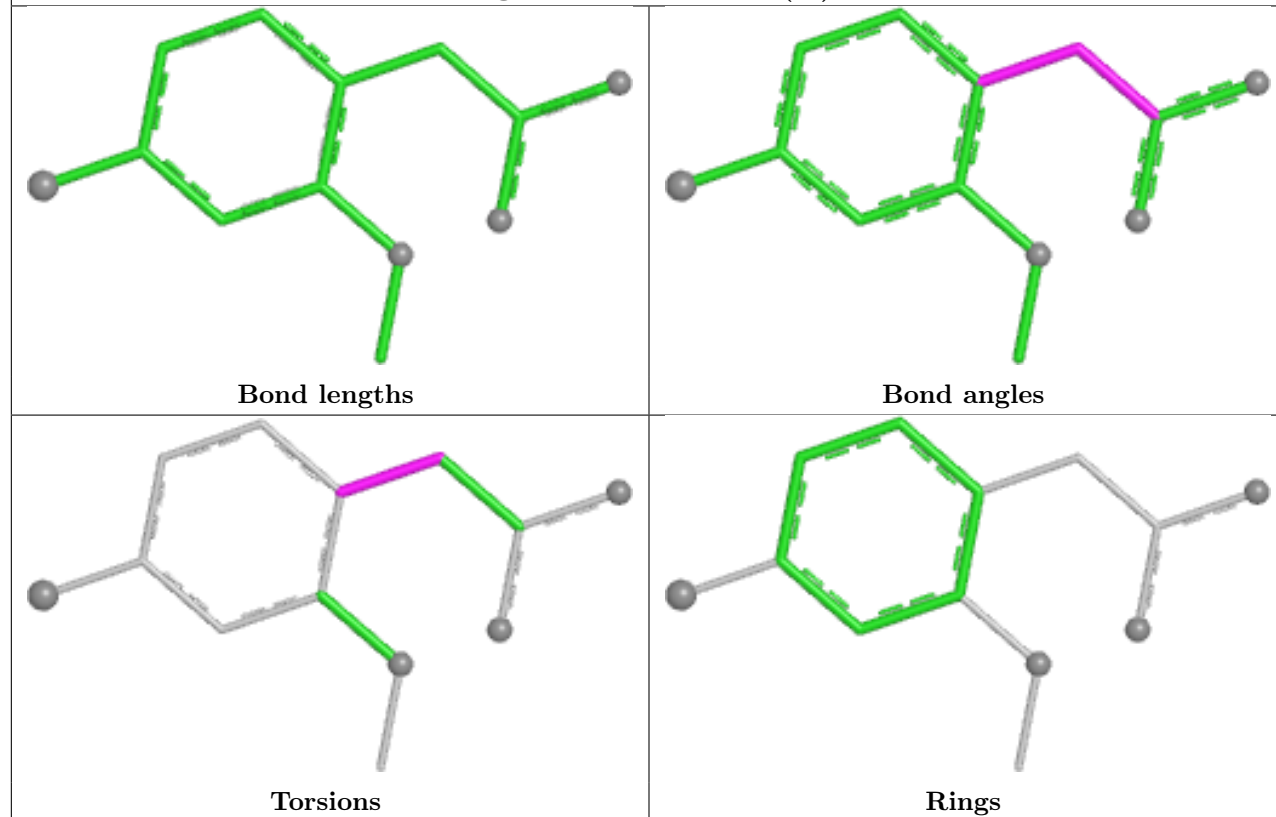
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HHT	1	0
3	A	604[A]	HHT	1	0
3	A	603	HHT	2	0
3	C	501	HHT	1	0
3	A	604[B]	HHT	2	0
3	B	502	HHT	1	0

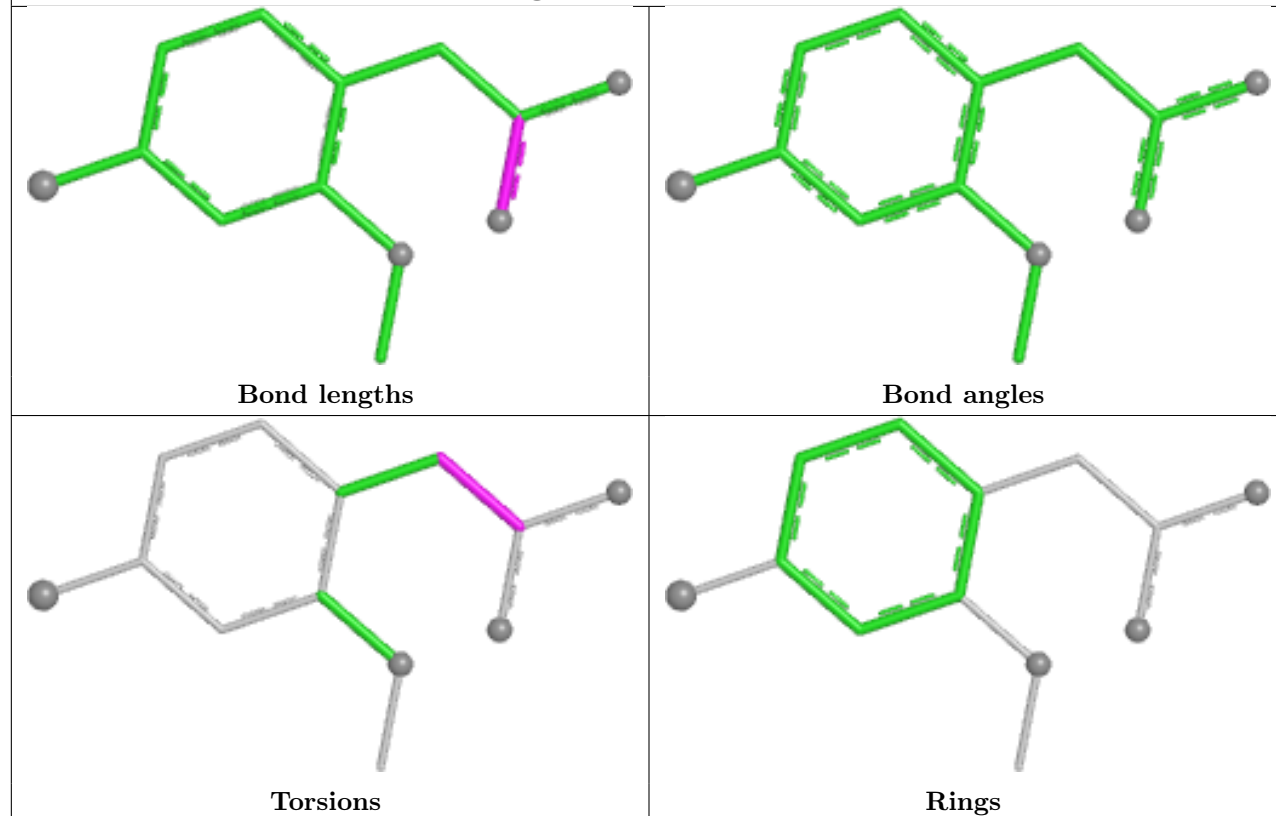
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

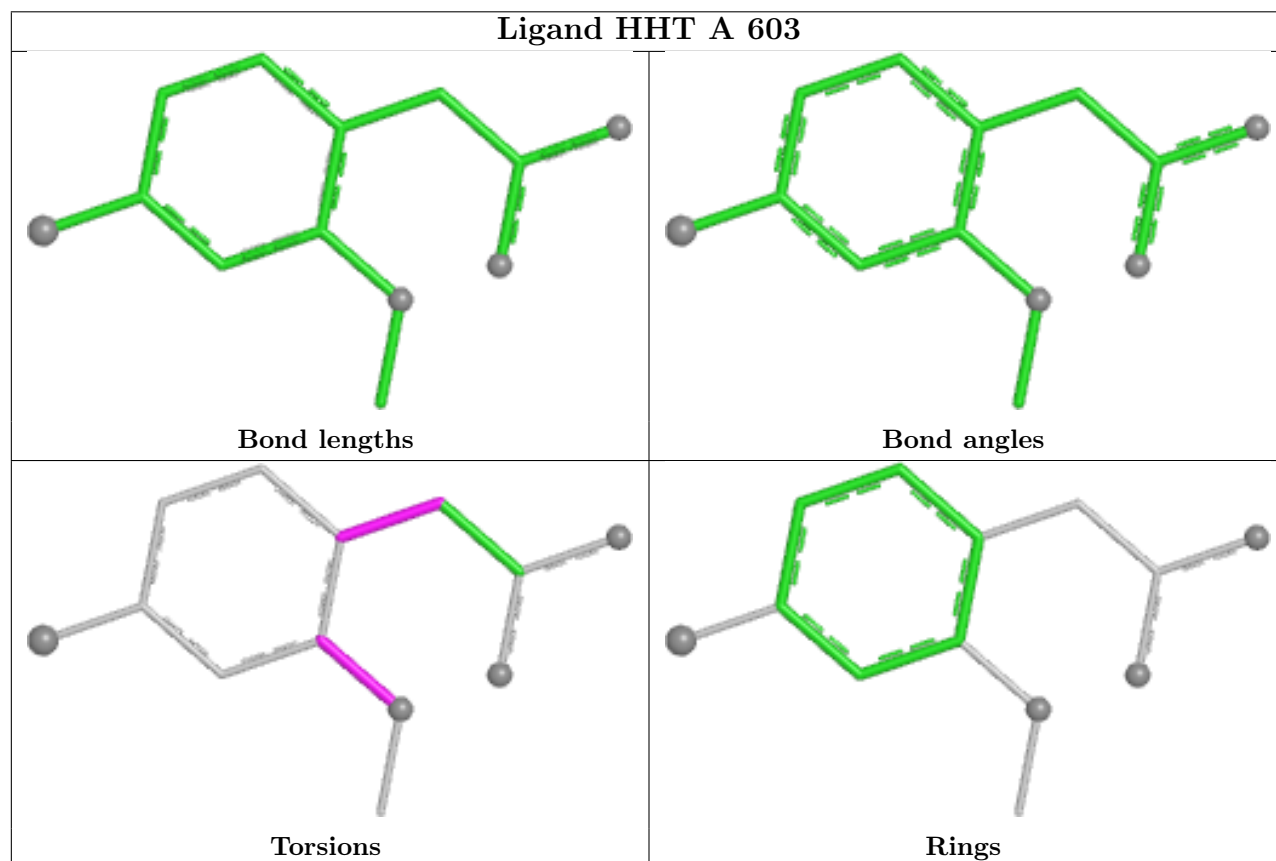
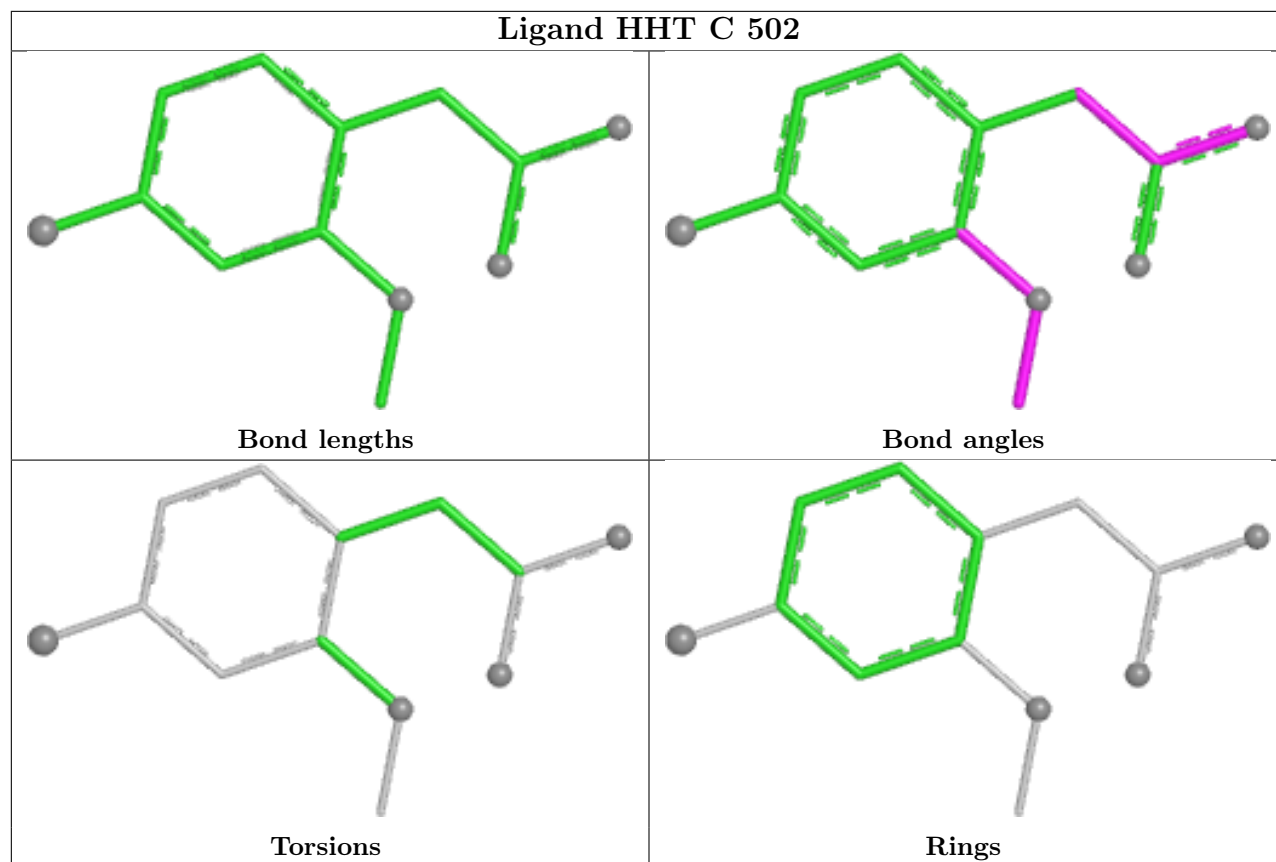


Ligand HHT A 604 (A)

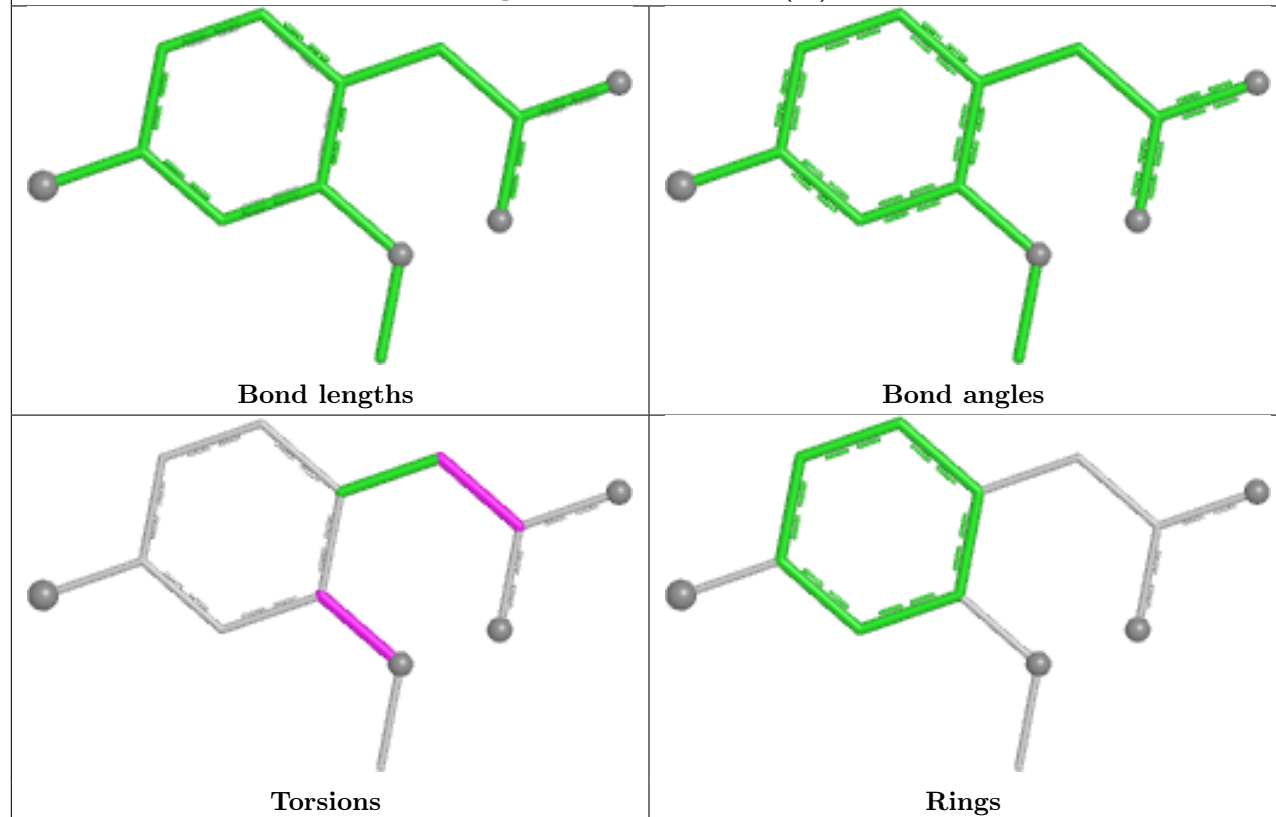


Ligand HHT A 601

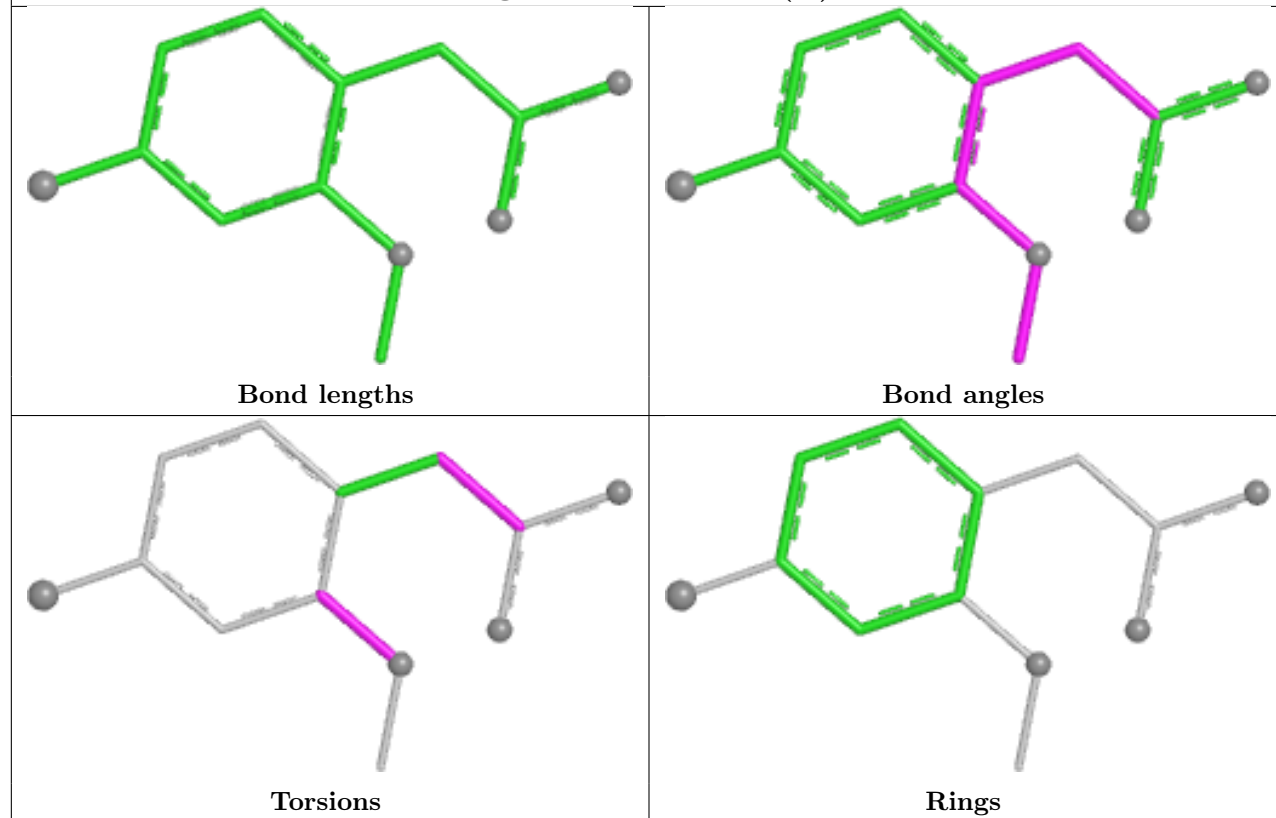


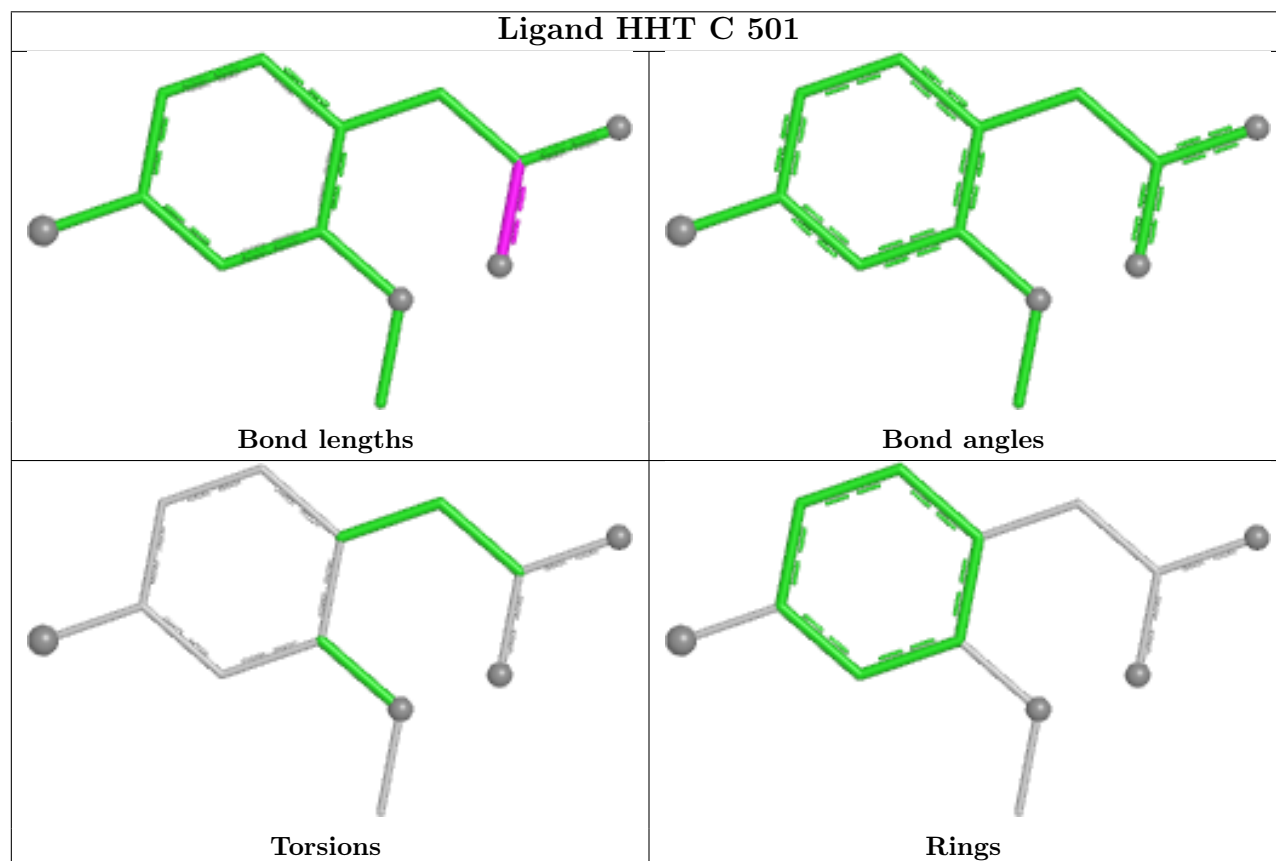
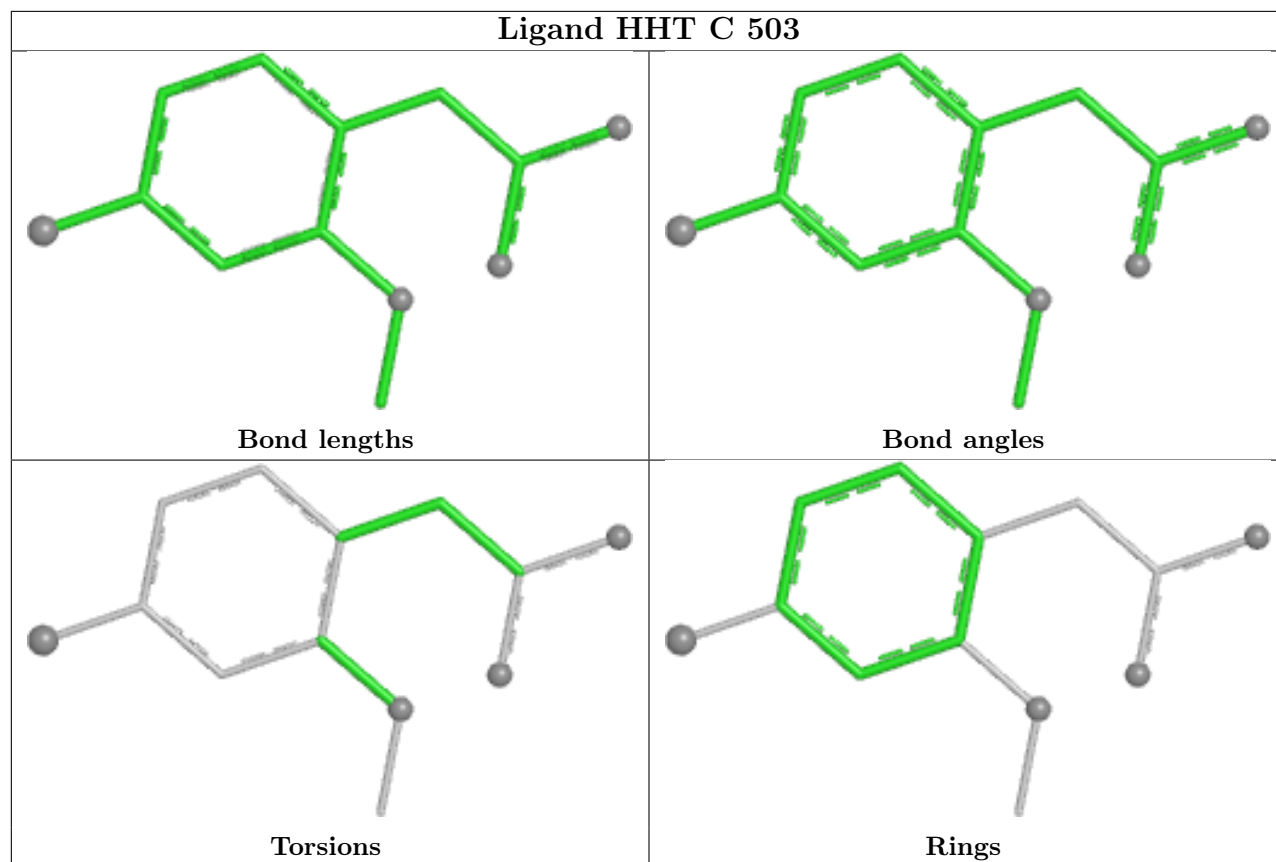


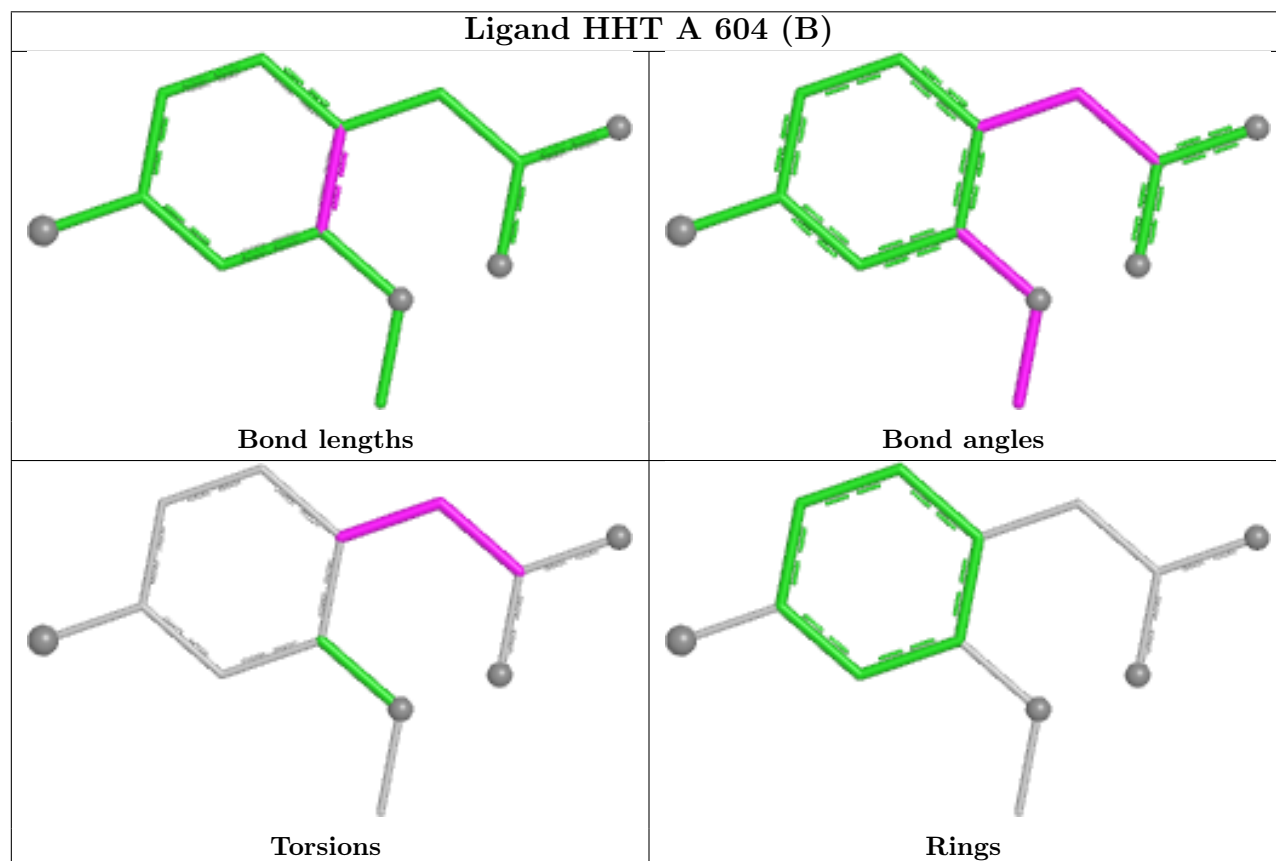
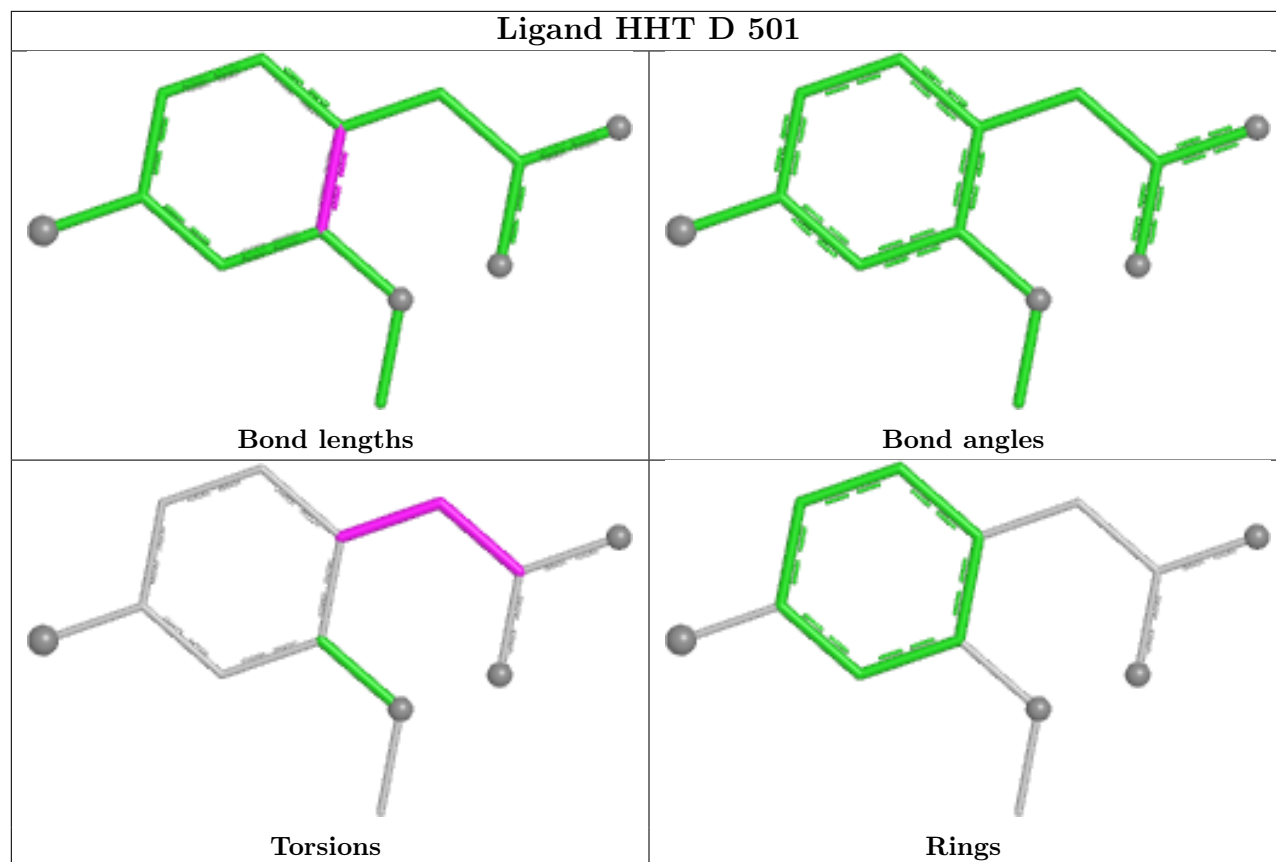
Ligand HHT B 501 (B)

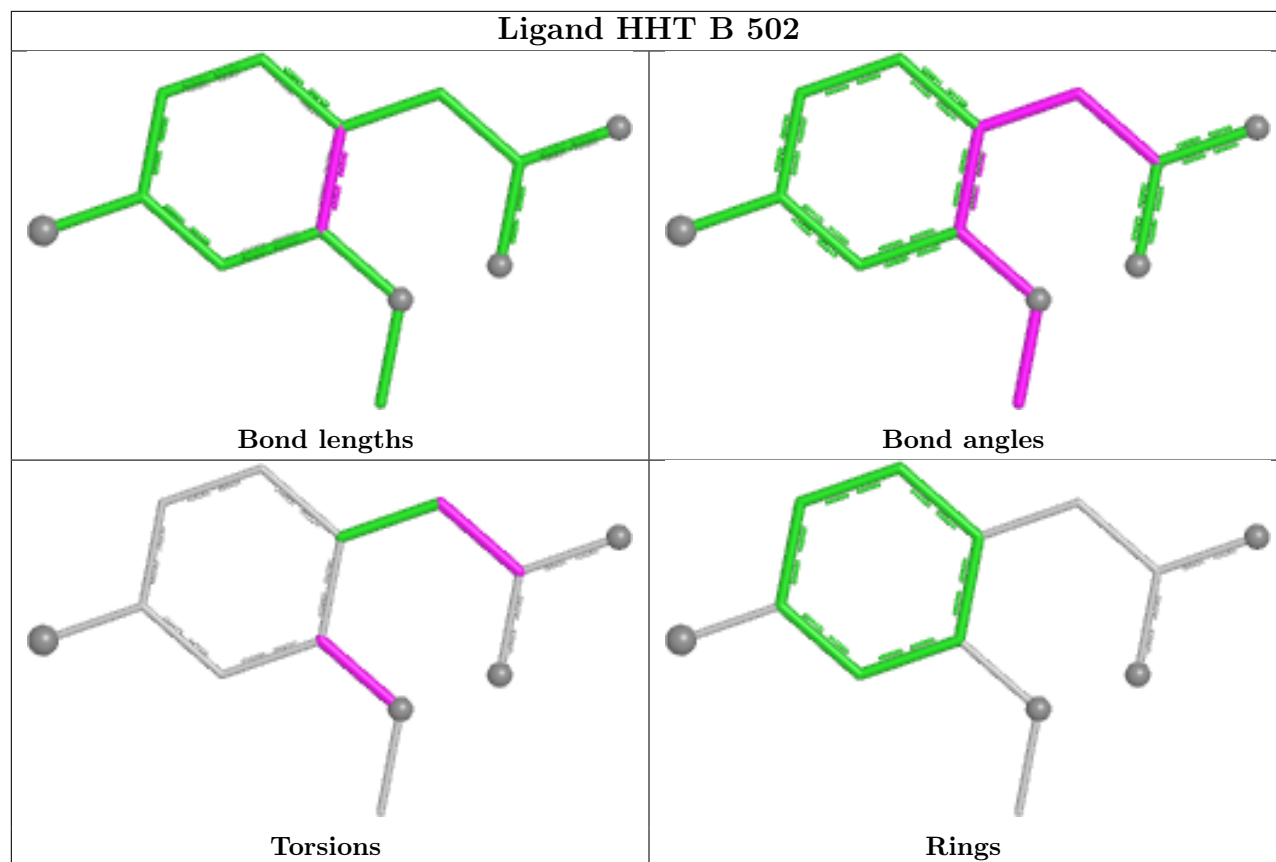


Ligand HHT B 501 (C)









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	299/302 (99%)	0.10	22 (7%)	20 19	24, 44, 110, 171	1 (0%)
1	C	269/302 (89%)	0.46	20 (7%)	20 19	37, 58, 106, 133	1 (0%)
2	B	262/268 (97%)	-0.07	4 (1%)	72 71	19, 46, 75, 106	2 (0%)
2	D	262/268 (97%)	0.68	27 (10%)	12 10	38, 65, 106, 144	0
All	All	1092/1140 (95%)	0.29	73 (6%)	24 22	19, 53, 104, 171	4 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	VAL	5.9
1	A	-2	PRO	5.5
1	C	269	TYR	5.3
1	C	15	TYR	5.1
1	C	71	HIS	4.6
1	C	251	VAL	4.6
1	A	96	LEU	4.1
1	A	15	TYR	4.0
1	A	72	THR	3.8
1	C	249	SER	3.8
1	A	39	THR	3.5
1	A	81	GLU	3.3
1	A	84[A]	HIS	3.2
1	A	13	GLY	3.1
2	D	384	LEU	3.1
1	A	-3	GLY	3.0
2	D	426	PRO	3.0
2	B	391	LEU	3.0
2	D	318	TYR	3.0
2	D	418	TYR	3.0
1	C	250	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	172	VAL	2.9
1	A	16	GLY	2.9
1	A	95	ALA	2.9
2	D	424	LEU	2.8
1	A	36	ARG	2.8
1	C	293	VAL	2.8
1	C	221	THR	2.7
1	C	16	GLY	2.7
1	C	296	LEU	2.7
2	D	323	GLN	2.7
2	D	324	PRO	2.7
2	D	430	LEU	2.7
2	D	196	LYS	2.7
2	D	429	THR	2.7
2	D	398	TYR	2.6
1	C	218	THR	2.6
1	C	252	VAL	2.6
2	B	432	VAL	2.6
2	D	198	GLY	2.6
2	D	386	THR	2.6
1	A	38	ASP	2.6
1	A	73	GLU	2.6
1	C	216	PHE	2.6
1	A	296	LEU	2.5
2	D	362	LEU	2.5
1	A	71	HIS	2.5
2	D	392	LEU	2.5
1	A	-1	GLY	2.4
1	A	65	LYS	2.4
2	D	364	LEU	2.4
1	A	0	SER	2.3
1	C	2[A]	GLU	2.3
1	A	206	ASP	2.3
2	B	280	TYR	2.3
1	A	97	THR	2.3
1	A	75	LYS	2.3
2	D	379	LYS	2.3
2	D	325	ALA	2.2
2	D	421	VAL	2.2
1	C	254	PRO	2.2
2	D	395	HIS	2.2
1	C	219	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	377	VAL	2.1
1	C	253	PRO	2.1
2	D	179	HIS	2.1
2	D	327	CYS	2.1
1	C	217	ARG	2.1
2	D	372	TRP	2.1
1	C	295	HIS	2.1
2	D	319	PHE	2.1
2	B	196	LYS	2.0
1	C	14	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.97	0.06	50,56,59,60	0
1	TPO	A	160	11/12	0.98	0.06	37,40,43,43	0

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.

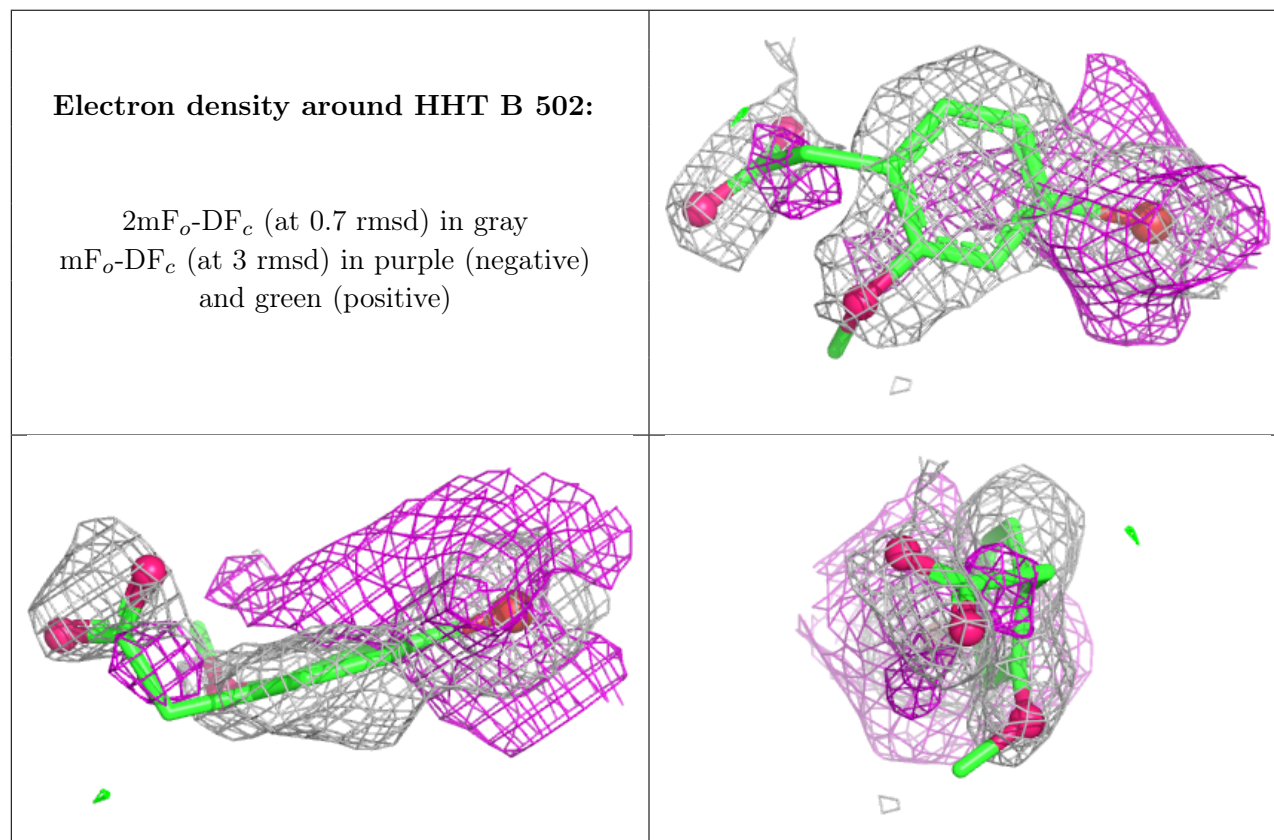
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HHT	B	502	13/13	0.81	0.20	67,95,109,110	0
3	HHT	D	501	13/13	0.83	0.18	87,113,135,140	0
3	HHT	A	604[A]	13/13	0.84	0.29	62,98,113,117	13
3	HHT	A	604[B]	13/13	0.84	0.29	74,102,201,203	13
3	HHT	B	501[C]	13/13	0.88	0.59	75,85,100,104	13
3	HHT	B	501[A]	13/13	0.88	0.59	87,128,191,296	13

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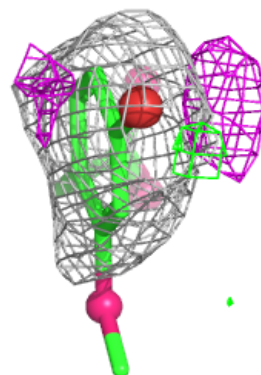
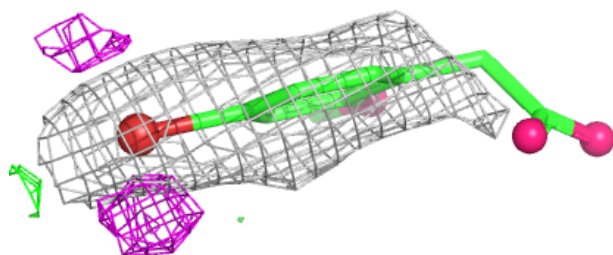
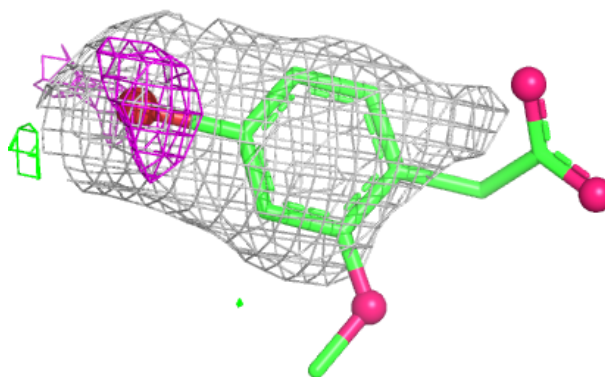
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HHT	B	501[B]	13/13	0.88	0.59	75,85,100,104	13
3	HHT	A	603	13/13	0.90	0.13	92,112,128,131	0
3	HHT	C	503	13/13	0.91	0.13	81,96,122,126	0
3	HHT	C	502	13/13	0.97	0.10	61,70,94,94	0
3	HHT	A	602	13/13	0.97	0.11	71,87,114,129	0
3	HHT	A	601	13/13	0.97	0.09	51,53,59,66	0
3	HHT	C	501	13/13	0.99	0.07	48,53,57,60	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.



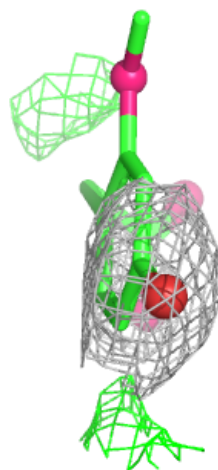
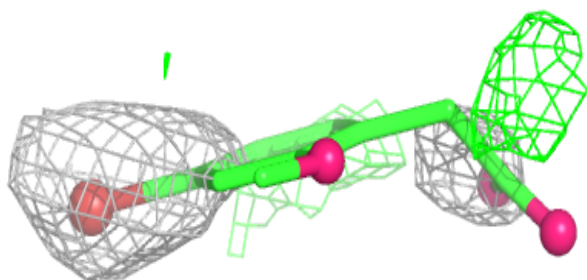
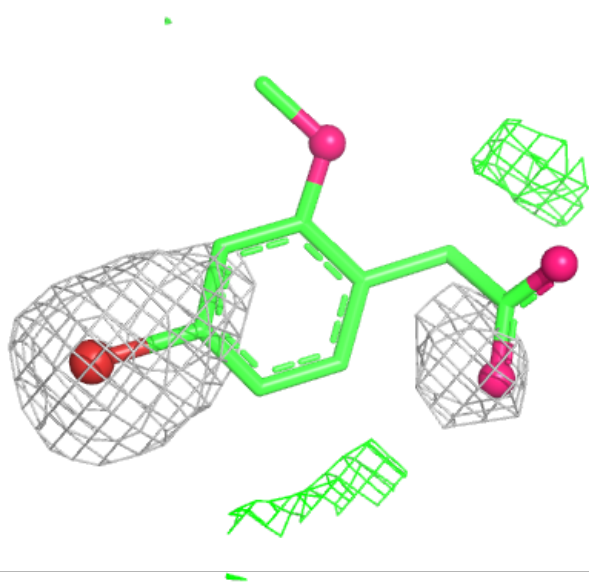
Electron density around HHT D 501:

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



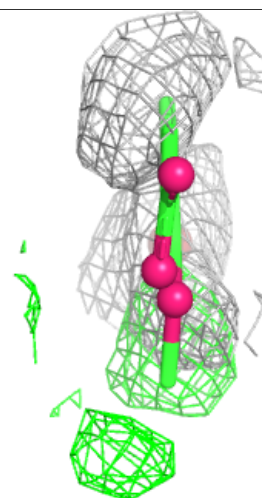
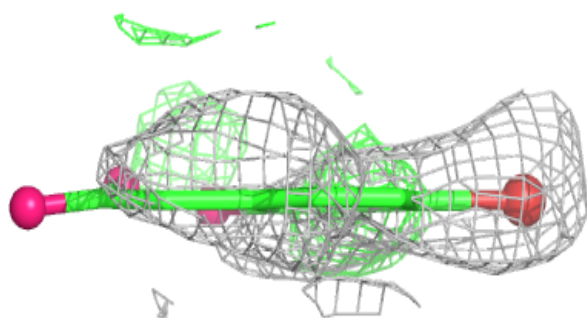
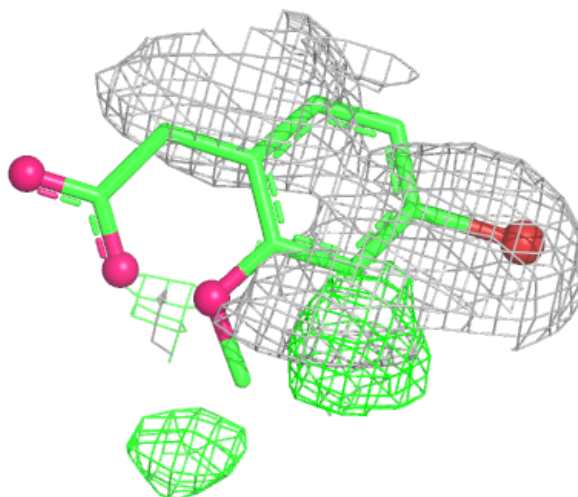
Electron density around HHT A 604 (A):

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



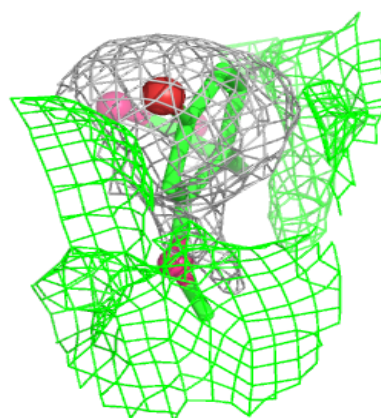
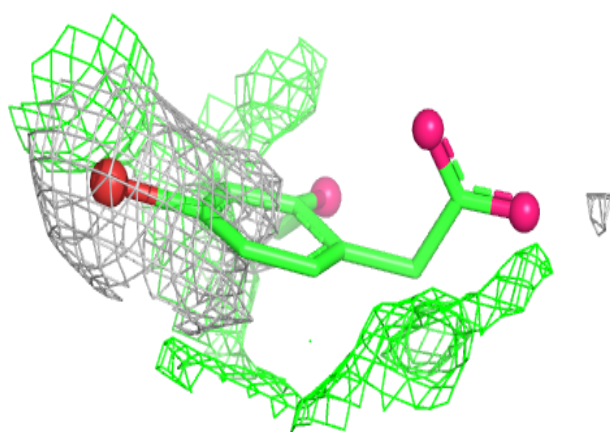
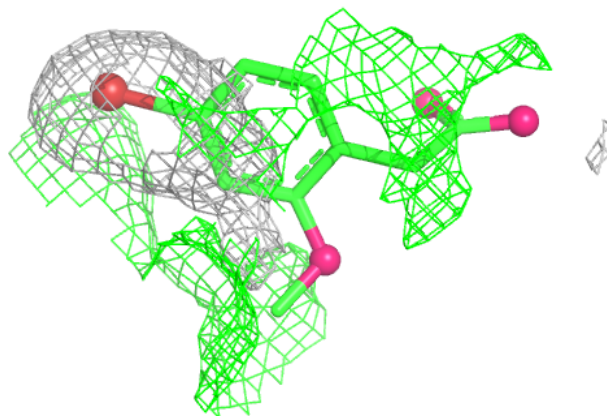
Electron density around HHT A 604 (B):

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



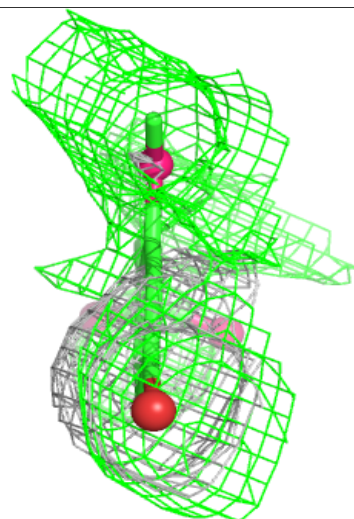
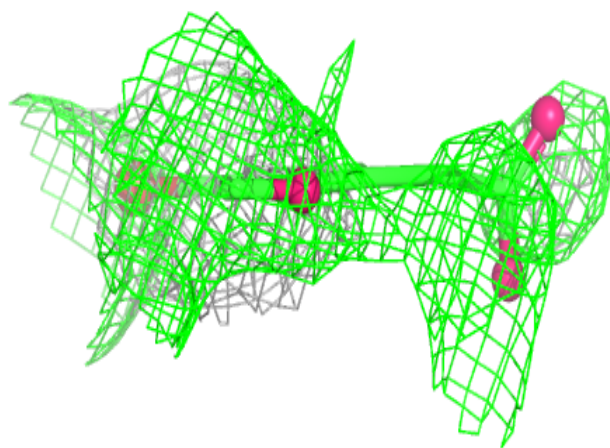
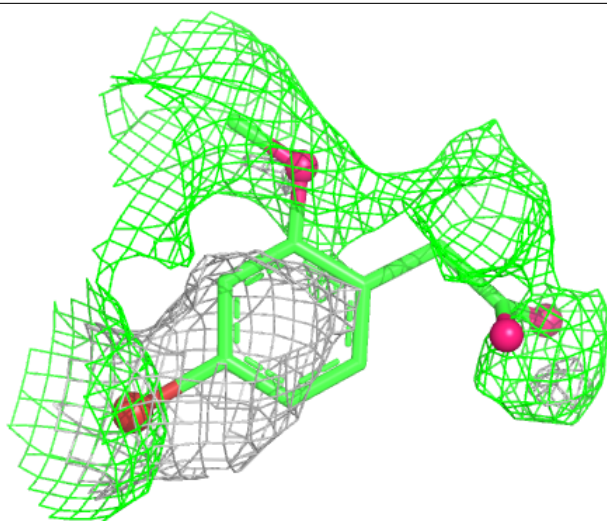
Electron density around HHT B 501 (C):

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



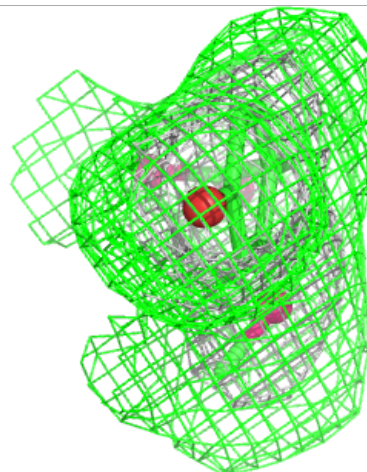
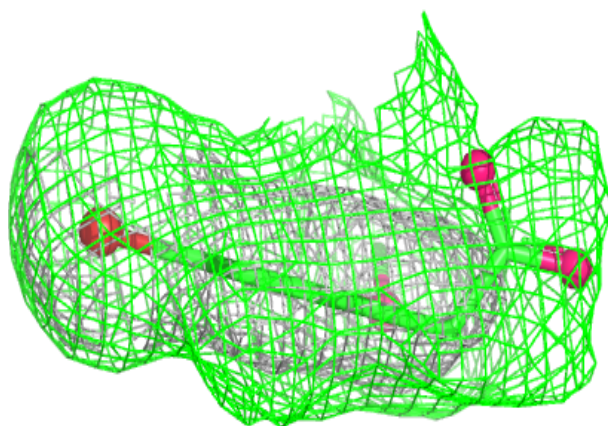
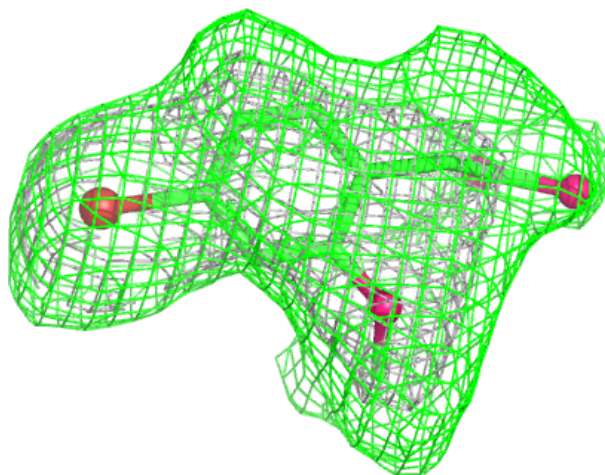
Electron density around HHT B 501 (A):

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



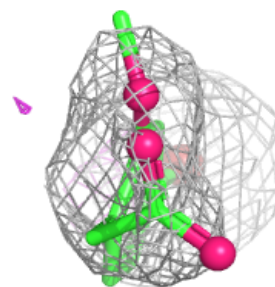
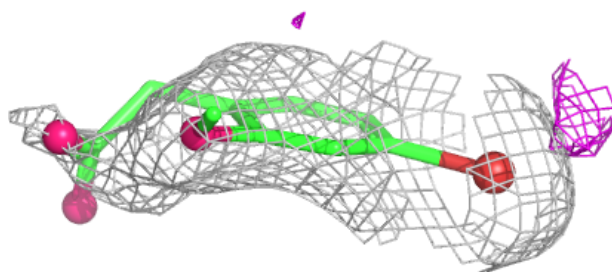
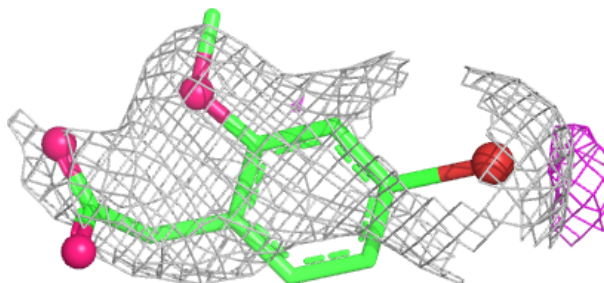
Electron density around HHT B 501 (B):

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

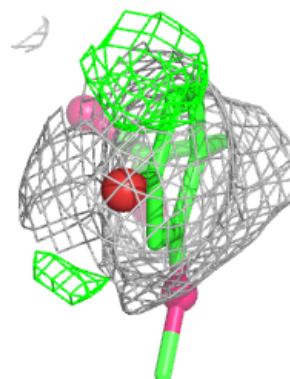
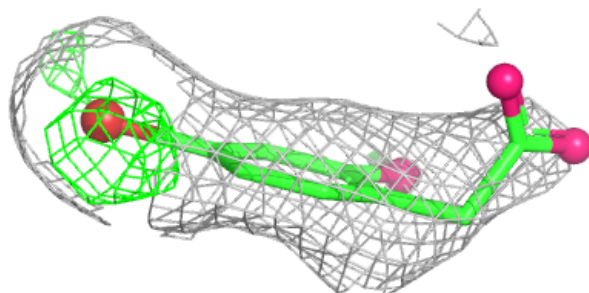
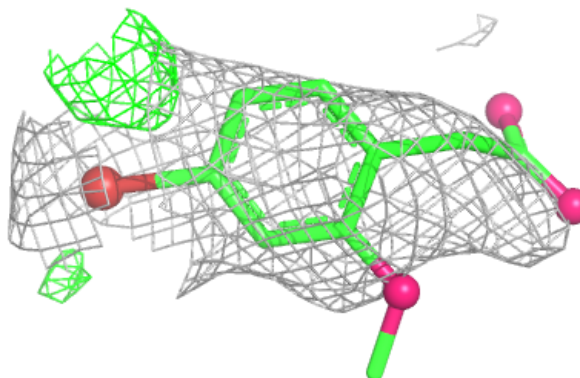


Electron density around HHT A 603:

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

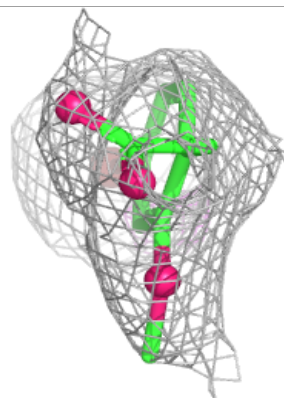
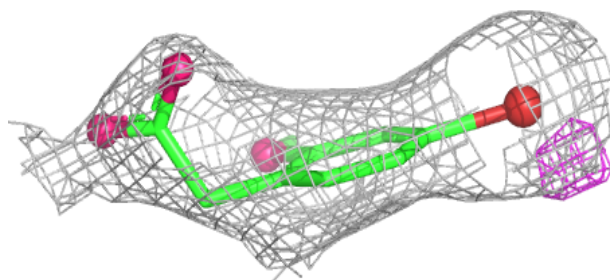
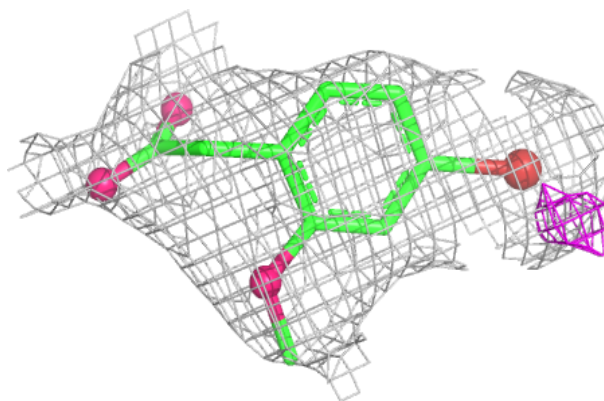
**Electron density around HHT C 503:**

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

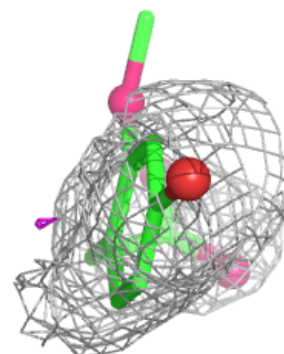
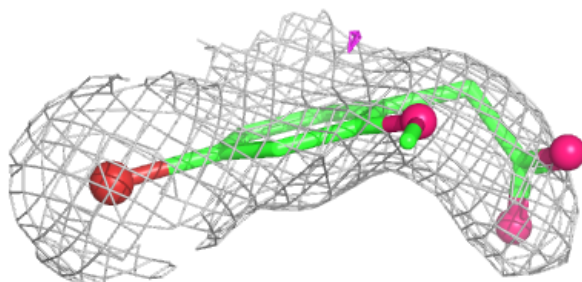
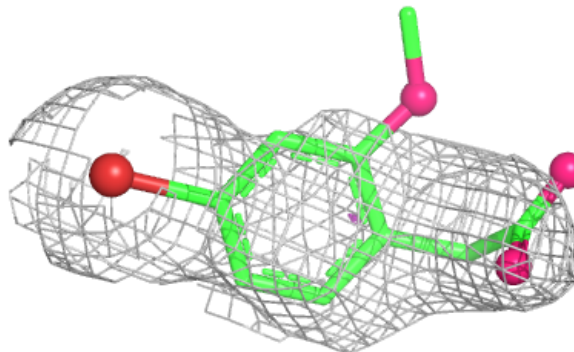


Electron density around HHT C 502:

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

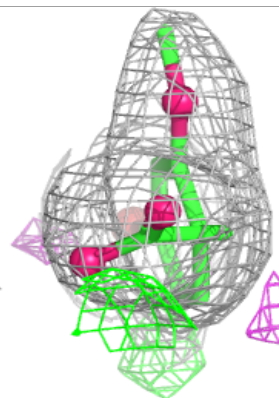
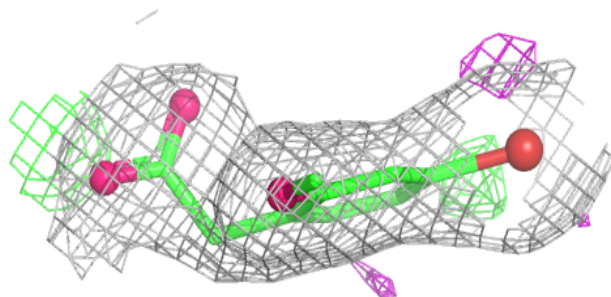
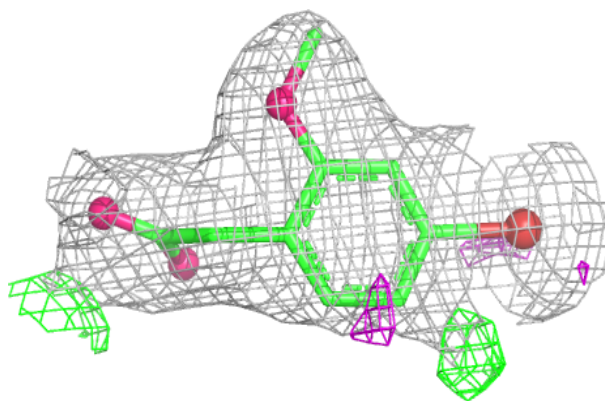
**Electron density around HHT A 602:**

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

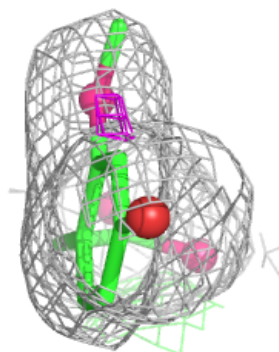
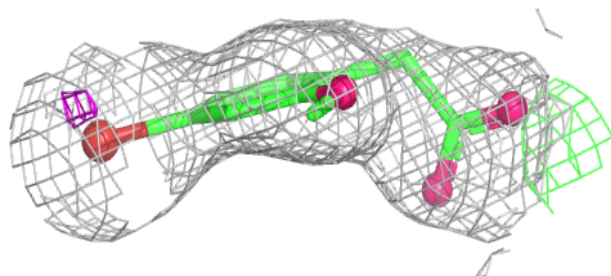
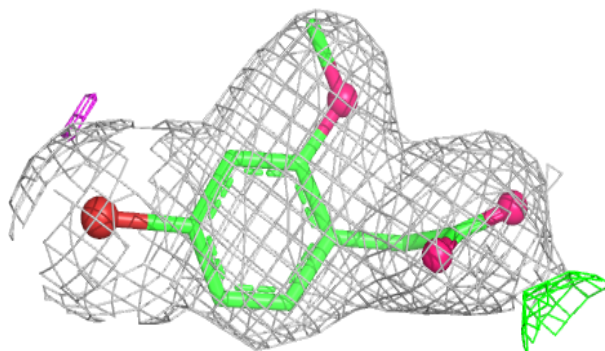


Electron density around HHT A 601:

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

**Electron density around HHT C 501:**

$2mF_o-DF_c$ (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.