



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2024 – 03:09 PM EST

PDB ID : 4Q50
Title : The Estrogen Receptor Alpha Ligand Binding Domain D538G Mutant in Complex with 4-hydroxytamoxifen
Authors : Fanning, S.W.; Greene, G.L.
Deposited on : 2014-04-15
Resolution : 3.07 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

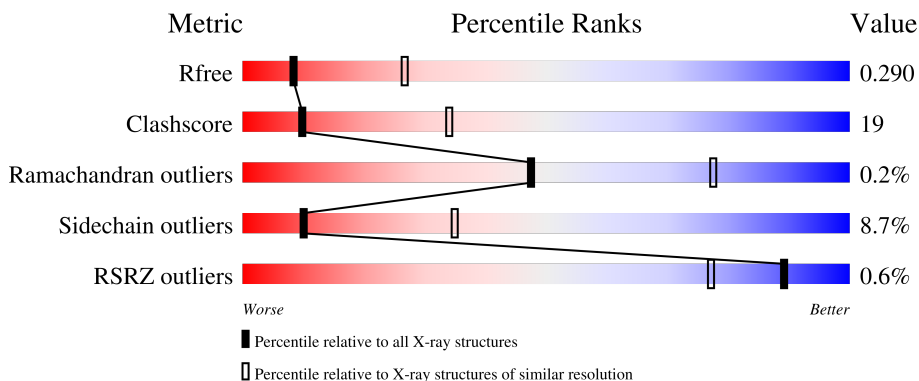
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	260	 45% 30% 5% 19%
1	B	260	 51% 26% 2% 20%
1	C	260	 51% 30% 1% 15%
1	D	260	 51% 30% 1% 17%
1	E	260	 53% 27% 1% 16%

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Mol	Chain	Length	Quality of chain
1	F	260	<p>%</p> <p>60% 22% 15%</p>
1	G	260	<p>55% 27% 16%</p>
1	H	260	<p>%</p> <p>54% 24% 5% 16%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	602	-	X	-	-
3	SO4	H	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14071 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	Total 1675	C 1078	N 286	O 295	S 16	0	0	0
1	B	209	Total 1669	C 1071	N 285	O 295	S 18	0	1	0
1	C	220	Total 1745	C 1120	N 296	O 312	S 17	0	0	0
1	D	216	Total 1716	C 1100	N 293	O 305	S 18	0	0	0
1	E	218	Total 1750	C 1126	N 297	O 309	S 18	0	1	0
1	F	220	Total 1757	C 1129	N 296	O 315	S 17	0	1	0
1	G	219	Total 1754	C 1126	N 295	O 313	S 20	0	4	0
1	H	218	Total 1751	C 1127	N 294	O 312	S 18	0	4	0

There are 40 discrepancies between the modelled and reference sequences:

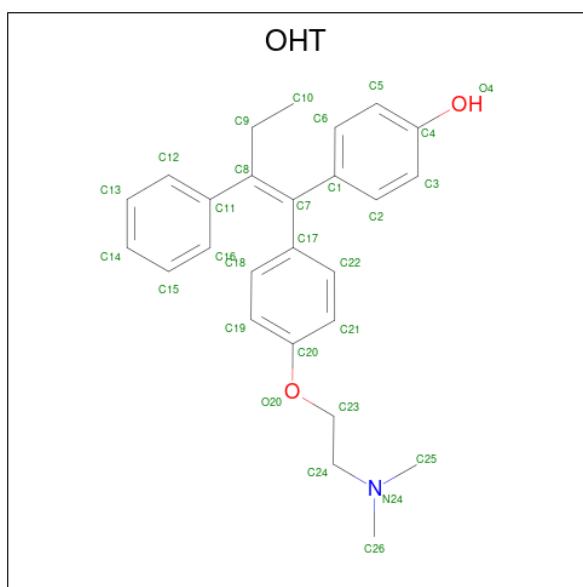
Chain	Residue	Modelled	Actual	Comment	Reference
A	295	SER	-	expression tag	UNP P03372
A	296	ASN	-	expression tag	UNP P03372
A	297	ALA	-	expression tag	UNP P03372
A	298	MET	-	expression tag	UNP P03372
A	538	GLY	ASP	engineered mutation	UNP P03372
B	295	SER	-	expression tag	UNP P03372
B	296	ASN	-	expression tag	UNP P03372
B	297	ALA	-	expression tag	UNP P03372
B	298	MET	-	expression tag	UNP P03372
B	538	GLY	ASP	engineered mutation	UNP P03372
C	295	SER	-	expression tag	UNP P03372
C	296	ASN	-	expression tag	UNP P03372
C	297	ALA	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
C	298	MET	-	expression tag	UNP P03372
C	538	GLY	ASP	engineered mutation	UNP P03372
D	295	SER	-	expression tag	UNP P03372
D	296	ASN	-	expression tag	UNP P03372
D	297	ALA	-	expression tag	UNP P03372
D	298	MET	-	expression tag	UNP P03372
D	538	GLY	ASP	engineered mutation	UNP P03372
E	295	SER	-	expression tag	UNP P03372
E	296	ASN	-	expression tag	UNP P03372
E	297	ALA	-	expression tag	UNP P03372
E	298	MET	-	expression tag	UNP P03372
E	538	GLY	ASP	engineered mutation	UNP P03372
F	295	SER	-	expression tag	UNP P03372
F	296	ASN	-	expression tag	UNP P03372
F	297	ALA	-	expression tag	UNP P03372
F	298	MET	-	expression tag	UNP P03372
F	538	GLY	ASP	engineered mutation	UNP P03372
G	295	SER	-	expression tag	UNP P03372
G	296	ASN	-	expression tag	UNP P03372
G	297	ALA	-	expression tag	UNP P03372
G	298	MET	-	expression tag	UNP P03372
G	538	GLY	ASP	engineered mutation	UNP P03372
H	295	SER	-	expression tag	UNP P03372
H	296	ASN	-	expression tag	UNP P03372
H	297	ALA	-	expression tag	UNP P03372
H	298	MET	-	expression tag	UNP P03372
H	538	GLY	ASP	engineered mutation	UNP P03372

- Molecule 2 is 4-HYDROXYTAMOXIFEN (three-letter code: OHT) (formula: C₂₆H₂₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	29	26	1	2	0	0
2	B	1	29	26	1	2	0	0
2	C	1	29	26	1	2	0	0
2	D	1	29	26	1	2	0	0
2	E	1	29	26	1	2	0	0
2	F	1	29	26	1	2	0	0
2	G	1	29	26	1	2	0	0
2	H	1	29	26	1	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

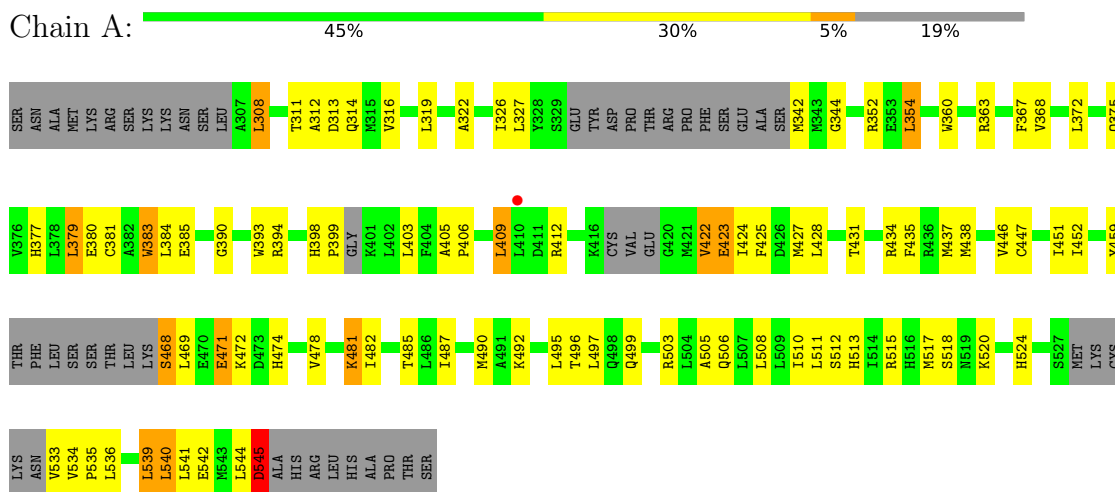
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	1	Total O 1 1	0	0
4	C	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	G	2	Total O 2 2	0	0

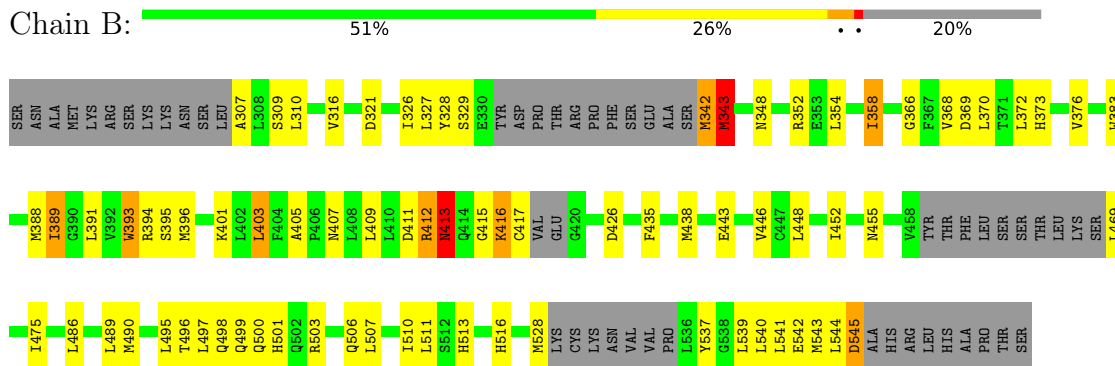
3 Residue-property plots

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.

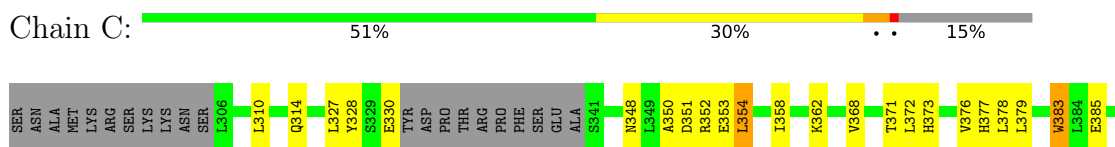
- Molecule 1: Estrogen receptor

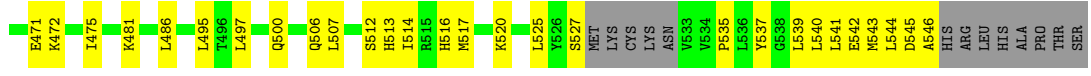
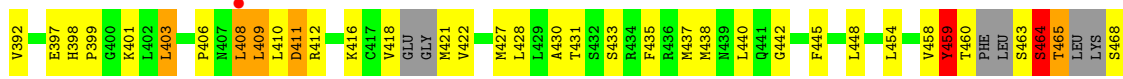


- Molecule 1: Estrogen receptor

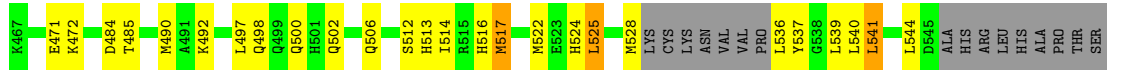
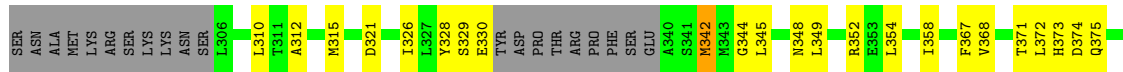


- Molecule 1: Estrogen receptor

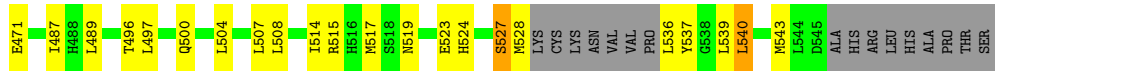
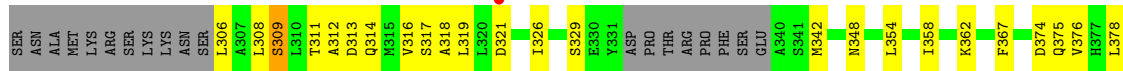




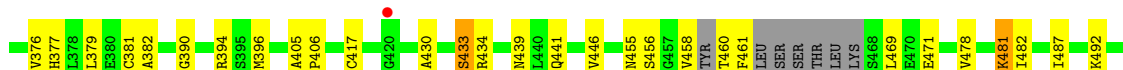
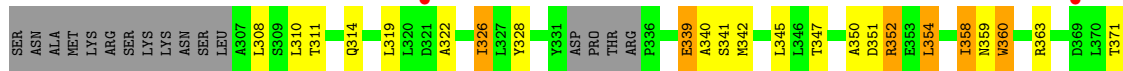
• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor

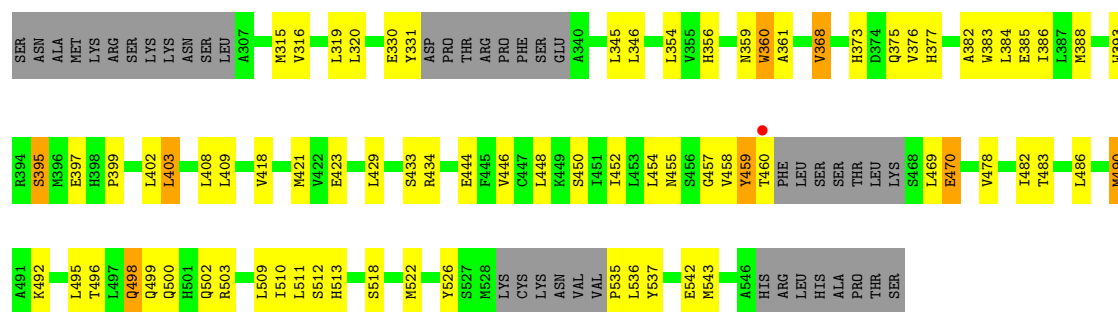


• Molecule 1: Estrogen receptor



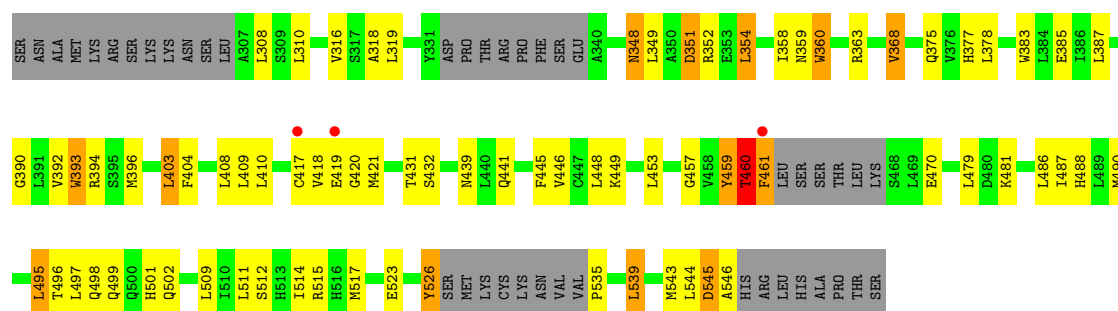
• Molecule 1: Estrogen receptor

Chain G:  55% 27% 16%



• Molecule 1: Estrogen receptor

Chain H:  54% 24% 5% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.65Å 165.24Å 191.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.07 48.74 – 3.07	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-3.07) 95.7 (48.74-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.07Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.283 0.225 , 0.290	Depositor DCC
R_{free} test set	3034 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14071	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3182e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, OHT

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	0.73	2/1701 (0.1%)	0.93	1/2292 (0.0%)
1	B	0.77	2/1697 (0.1%)	0.95	4/2284 (0.2%)
1	C	0.71	1/1771 (0.1%)	1.02	7/2388 (0.3%)
1	D	0.76	2/1742 (0.1%)	0.96	2/2346 (0.1%)
1	E	0.67	0/1779	0.98	7/2397 (0.3%)
1	F	0.70	1/1789 (0.1%)	0.88	3/2410 (0.1%)
1	G	0.69	3/1795 (0.2%)	0.91	1/2420 (0.0%)
1	H	0.67	2/1793 (0.1%)	0.91	4/2418 (0.2%)
All	All	0.71	13/14067 (0.1%)	0.94	29/18955 (0.2%)

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	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	TRP	CD2-CE2	5.93	1.48	1.41
1	F	360	TRP	CD2-CE2	5.91	1.48	1.41
1	B	393	TRP	CD2-CE2	5.82	1.48	1.41
1	C	383	TRP	CD2-CE2	5.74	1.48	1.41
1	H	393	TRP	CD2-CE2	5.60	1.48	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	398	HIS	C-N-CD	-16.83	83.58	120.60
1	C	465	THR	N-CA-CB	16.43	141.51	110.30
1	C	464	SER	CB-CA-C	10.65	130.33	110.10
1	E	528	MET	N-CA-CB	-9.85	92.87	110.60
1	H	460	THR	N-CA-C	9.68	137.13	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	LEU	Peptide

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	1675	0	1725	75	0
1	B	1669	0	1724	74	0
1	C	1745	0	1799	102	0
1	D	1716	0	1774	67	0
1	E	1750	0	1794	62	0
1	F	1757	0	1798	38	0
1	G	1754	0	1808	82	0
1	H	1751	0	1803	75	0
2	A	29	0	28	4	0
2	B	29	0	28	2	0
2	C	29	0	29	7	0
2	D	29	0	28	5	0
2	E	29	0	29	3	0
2	F	29	0	29	4	0
2	G	29	0	28	5	0
2	H	29	0	29	4	0
3	B	5	0	0	0	0
3	H	5	0	0	2	0
4	A	3	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	G	2	0	0	0	0
All	All	14071	0	14453	548	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 19.

The worst 5 of 548 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:460:THR:O	1:H:461:PHE:CD1	1.75	1.40
1:G:377:HIS:NE2	1:G:460:THR:HG23	1.57	1.19
1:B:540:LEU:O	1:B:544:LEU:HD12	1.40	1.16
1:H:460:THR:O	1:H:461:PHE:HD1	0.83	1.15
1:C:459:TYR:CE2	1:G:513:HIS:CG	2.36	1.12

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	198/260 (76%)	187 (94%)	11 (6%)	0	100	100
1	B	200/260 (77%)	184 (92%)	16 (8%)	0	100	100
1	C	208/260 (80%)	195 (94%)	13 (6%)	0	100	100
1	D	208/260 (80%)	196 (94%)	11 (5%)	1 (0%)	29	61
1	E	209/260 (80%)	193 (92%)	15 (7%)	1 (0%)	29	61
1	F	211/260 (81%)	194 (92%)	16 (8%)	1 (0%)	29	61
1	G	215/260 (83%)	198 (92%)	17 (8%)	0	100	100
1	H	214/260 (82%)	205 (96%)	8 (4%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1663/2080 (80%)	1552 (93%)	107 (6%)	4 (0%)	47 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	419	GLU
1	F	340	ALA
1	D	416	LYS
1	E	399	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	187/233 (80%)	162 (87%)	25 (13%)	4 15
1	B	187/233 (80%)	171 (91%)	16 (9%)	10 36
1	C	197/233 (84%)	184 (93%)	13 (7%)	16 45
1	D	192/233 (82%)	171 (89%)	21 (11%)	6 24
1	E	195/233 (84%)	179 (92%)	16 (8%)	11 37
1	F	197/233 (84%)	183 (93%)	14 (7%)	14 43
1	G	198/233 (85%)	185 (93%)	13 (7%)	16 45
1	H	197/233 (84%)	179 (91%)	18 (9%)	9 31
All	All	1550/1864 (83%)	1414 (91%)	136 (9%)	10 34

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	512[A]	SER
1	H	310	LEU
1	H	509	LEU
1	C	437	MET
1	C	422	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	377	HIS
1	H	348	ASN
1	H	524	HIS
1	C	502	GLN
1	C	414	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	OHT	A	1000	-	31,31,31	0.52	0	41,41,41	1.45	8 (19%)
2	OHT	F	1000	-	31,31,31	0.60	0	41,41,41	1.31	7 (17%)
3	SO4	B	602	-	4,4,4	2.77	3 (75%)	6,6,6	2.10	3 (50%)
2	OHT	H	601	-	31,31,31	0.65	0	41,41,41	1.91	11 (26%)
2	OHT	G	1000	-	31,31,31	0.55	0	41,41,41	1.65	8 (19%)
2	OHT	B	601	-	31,31,31	0.68	0	41,41,41	1.24	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	602	-	4,4,4	0.25	0	6,6,6	0.59	0
2	OHT	E	1000	-	31,31,31	0.70	0	41,41,41	1.00	2 (4%)
2	OHT	C	1000	-	31,31,31	0.78	0	41,41,41	1.43	6 (14%)
2	OHT	D	1000	-	31,31,31	0.79	1 (3%)	41,41,41	1.74	10 (24%)

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	OHT	A	1000	-	-	5/24/24/24	0/3/3/3
2	OHT	F	1000	-	-	4/24/24/24	0/3/3/3
2	OHT	H	601	-	-	3/24/24/24	0/3/3/3
2	OHT	G	1000	-	-	4/24/24/24	0/3/3/3
2	OHT	B	601	-	-	6/24/24/24	0/3/3/3
2	OHT	E	1000	-	-	6/24/24/24	0/3/3/3
2	OHT	C	1000	-	-	6/24/24/24	0/3/3/3
2	OHT	D	1000	-	-	5/24/24/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	SO4	O2-S	3.86	1.66	1.46
3	B	602	SO4	O4-S	2.72	1.70	1.47
3	B	602	SO4	O3-S	-2.40	1.28	1.47
2	D	1000	OHT	C22-C21	2.07	1.42	1.38

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	OHT	C2-C1-C7	-4.93	113.09	120.91
2	G	1000	OHT	C23-C24-N24	-4.06	103.85	114.56
2	D	1000	OHT	C11-C8-C7	-4.04	118.18	122.33
2	H	601	OHT	C1-C7-C8	-3.93	118.46	122.86
2	H	601	OHT	C16-C11-C8	-3.92	115.98	121.01

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

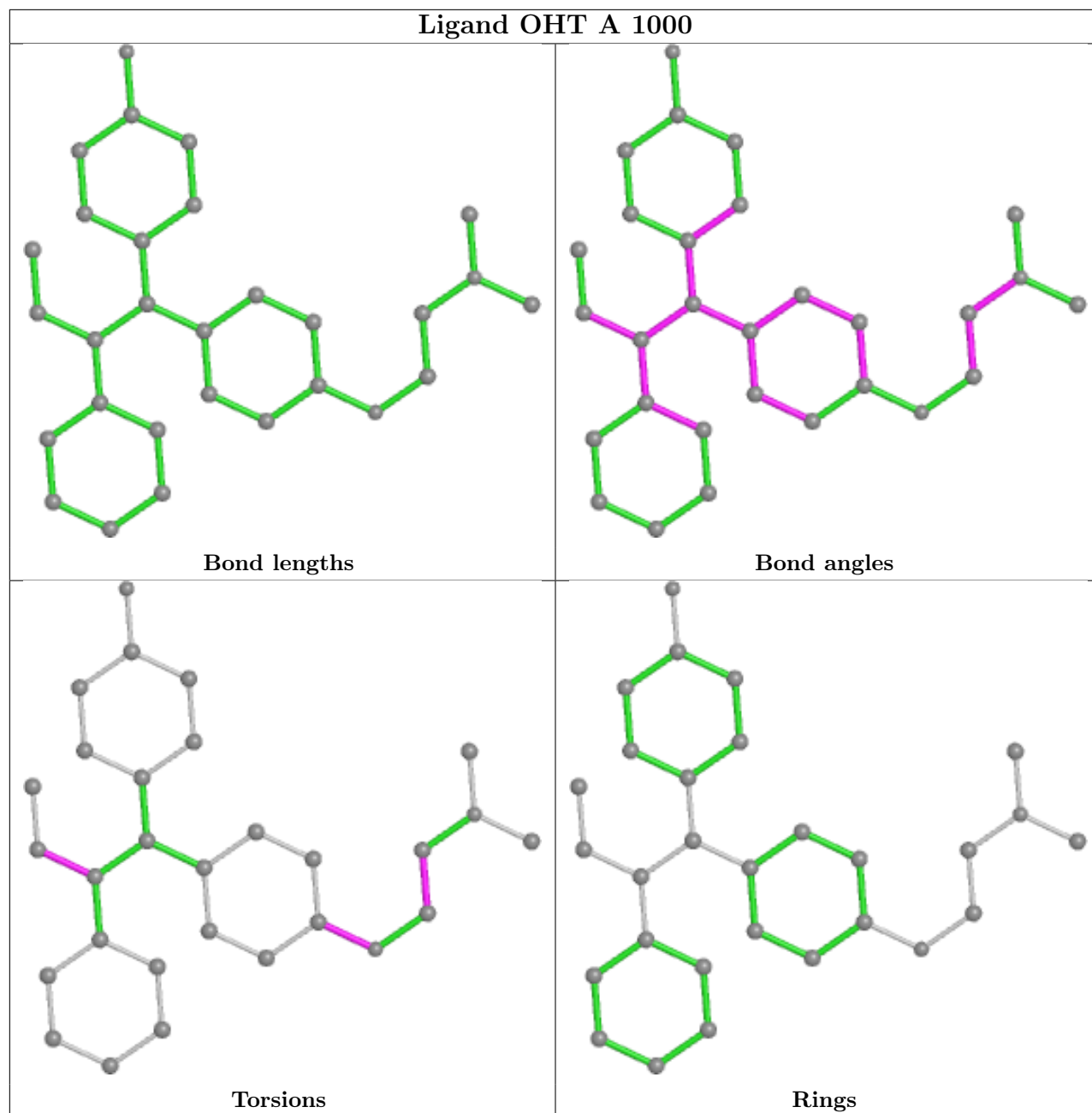
Mol	Chain	Res	Type	Atoms
2	A	1000	OHT	C11-C8-C9-C10
2	A	1000	OHT	C7-C8-C9-C10
2	B	601	OHT	C11-C8-C9-C10
2	B	601	OHT	C7-C8-C9-C10
2	C	1000	OHT	C11-C8-C9-C10

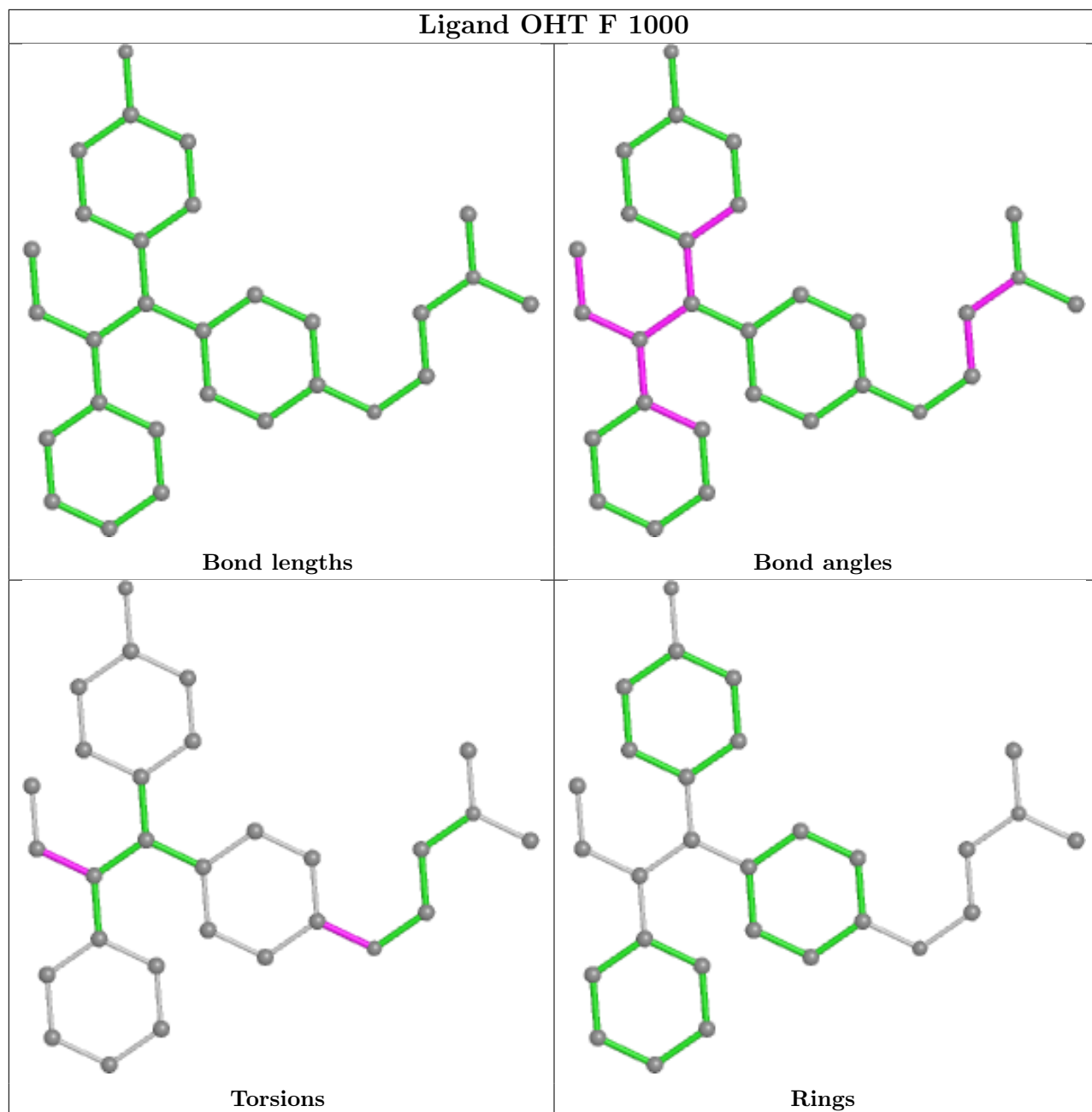
There are no ring outliers.

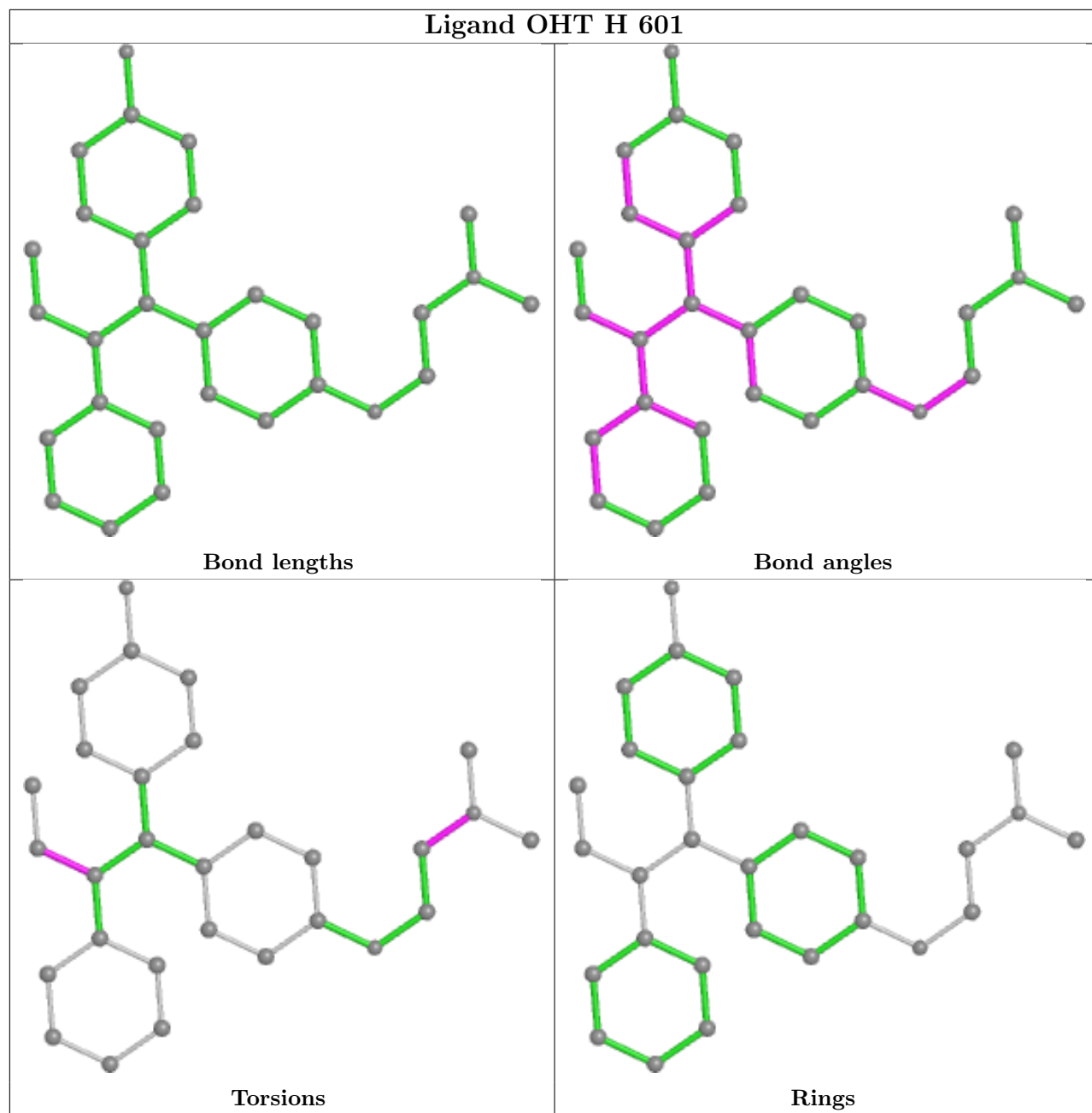
9 monomers are involved in 36 short contacts:

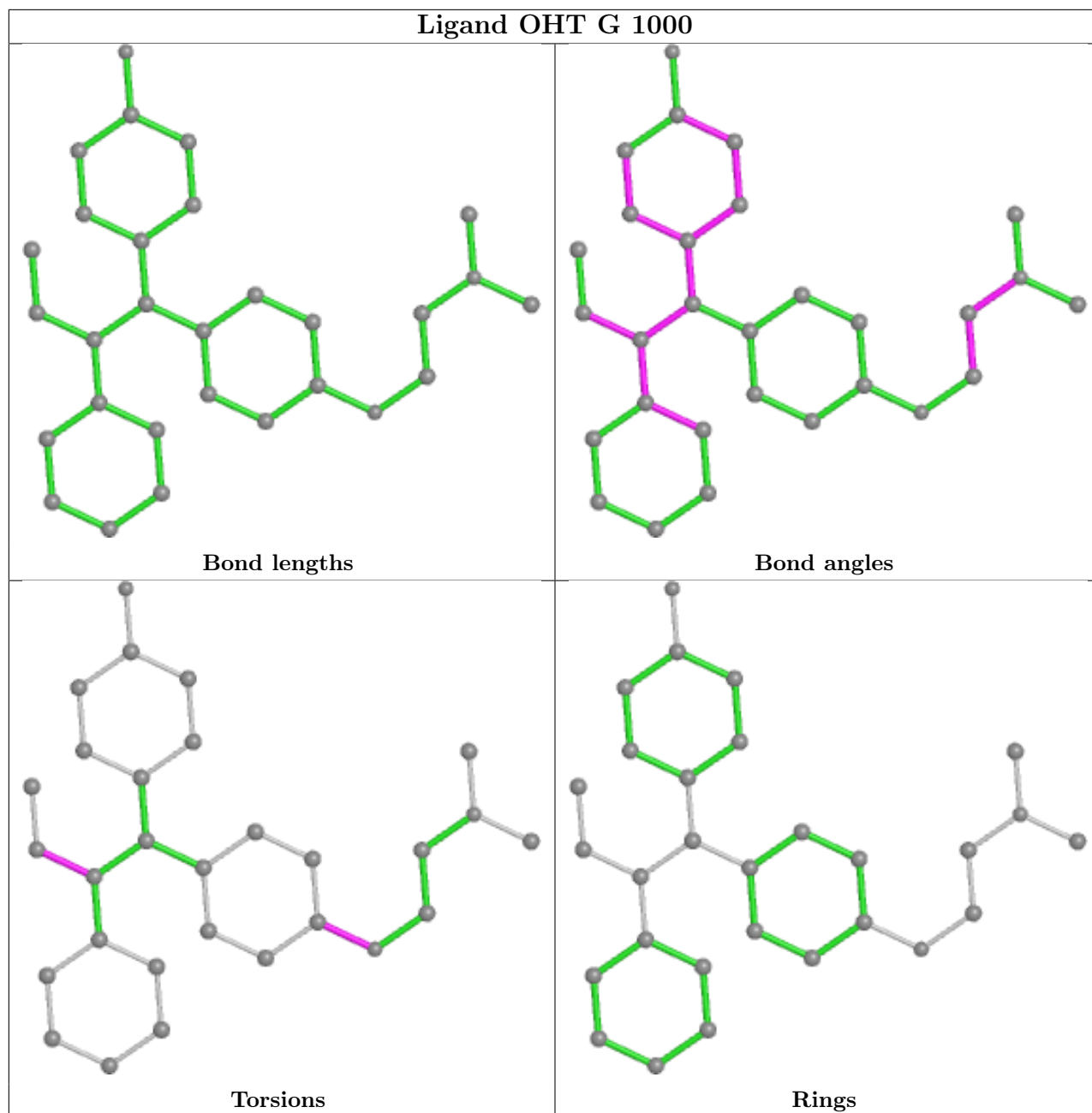
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	OHT	4	0
2	F	1000	OHT	4	0
2	H	601	OHT	4	0
2	G	1000	OHT	5	0
2	B	601	OHT	2	0
3	H	602	SO4	2	0
2	E	1000	OHT	3	0
2	C	1000	OHT	7	0
2	D	1000	OHT	5	0

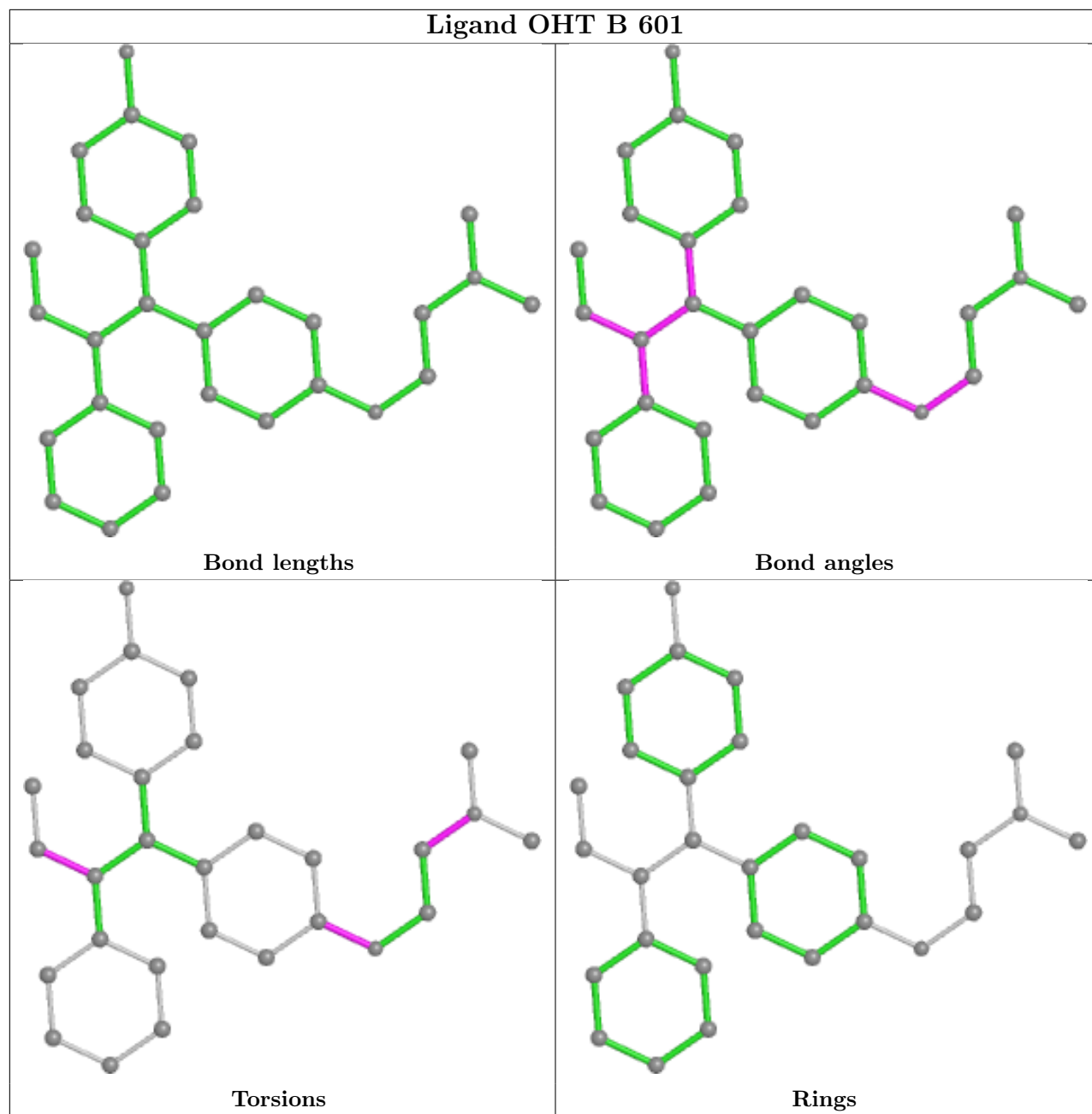
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

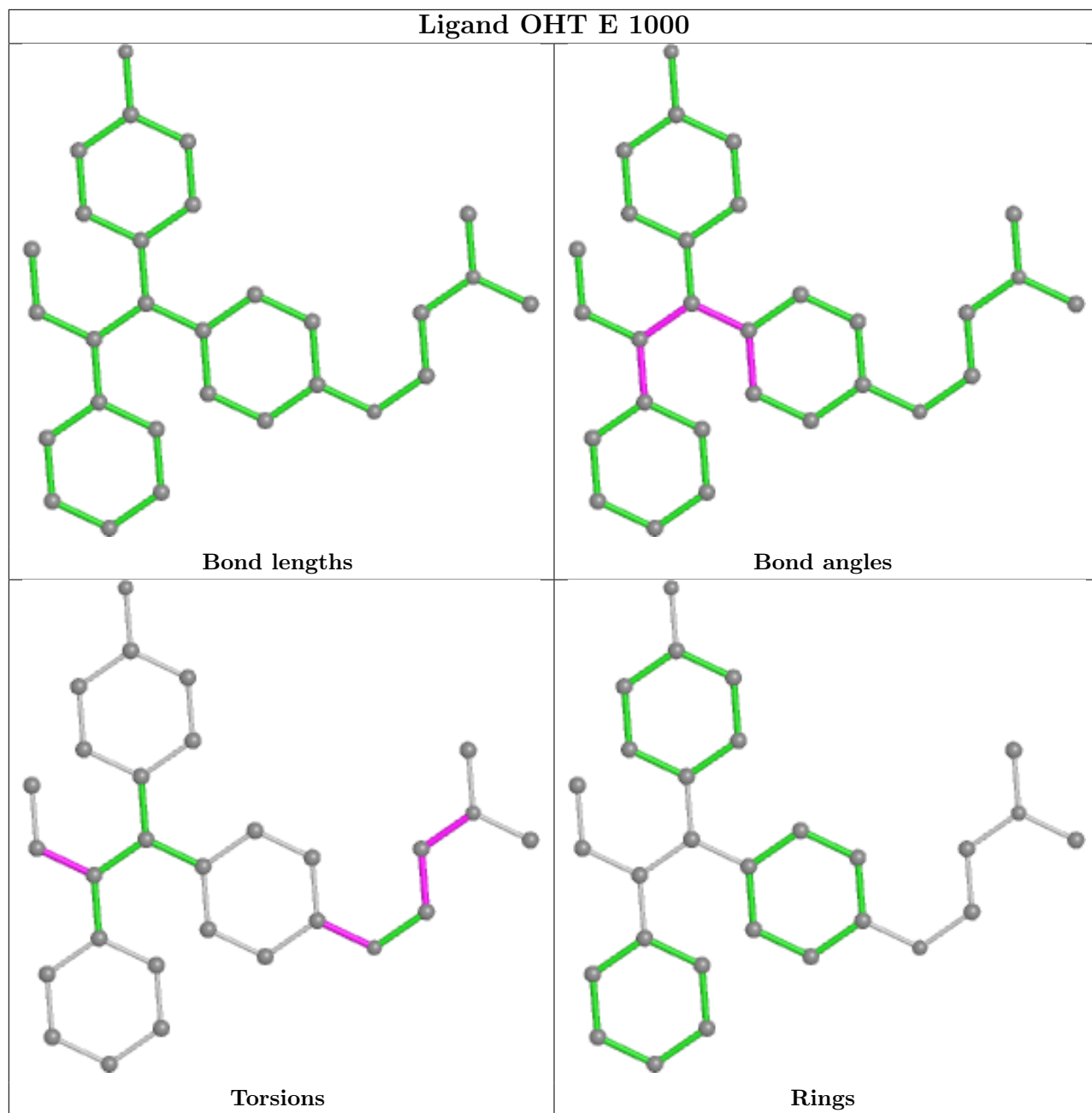


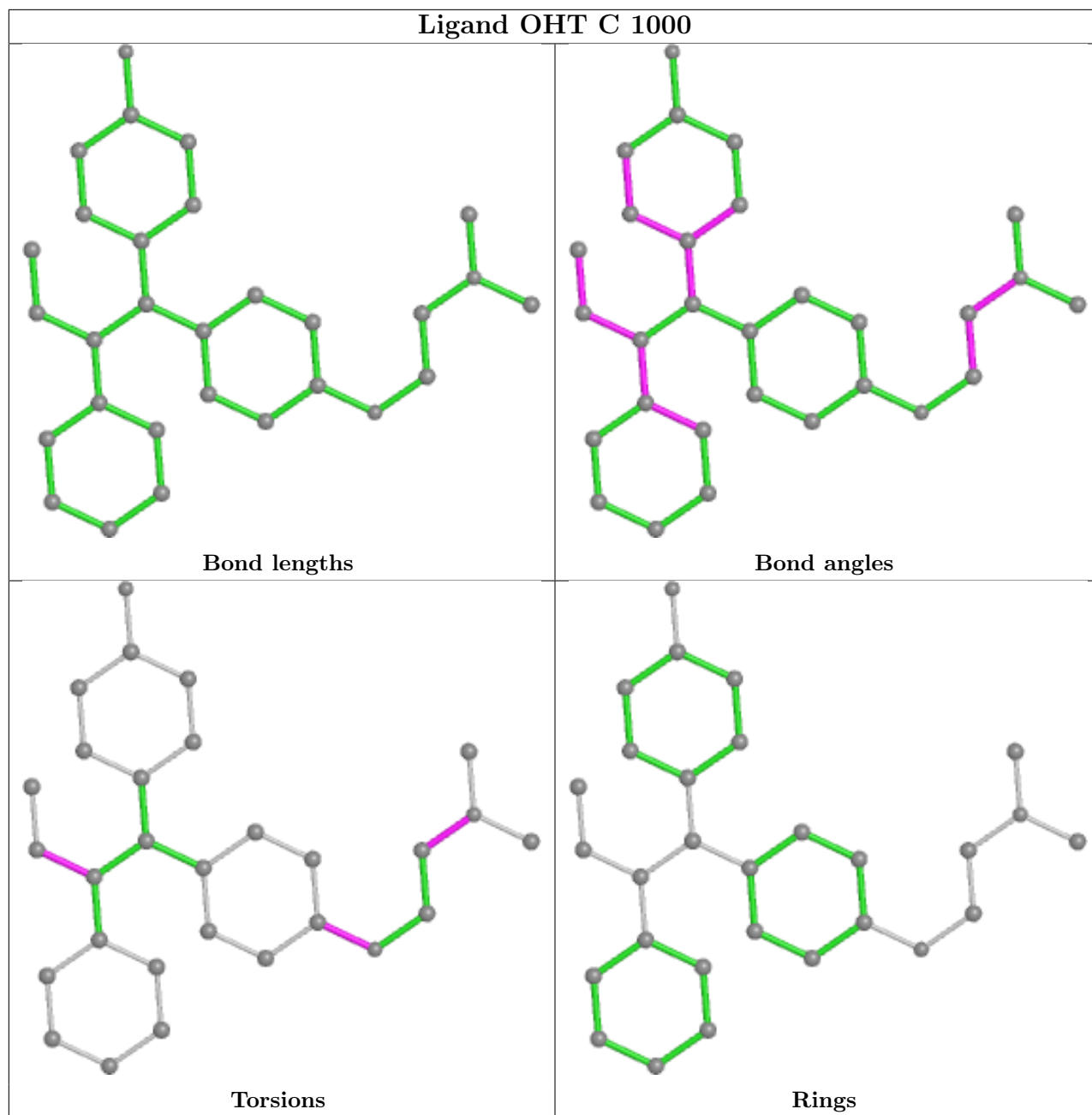


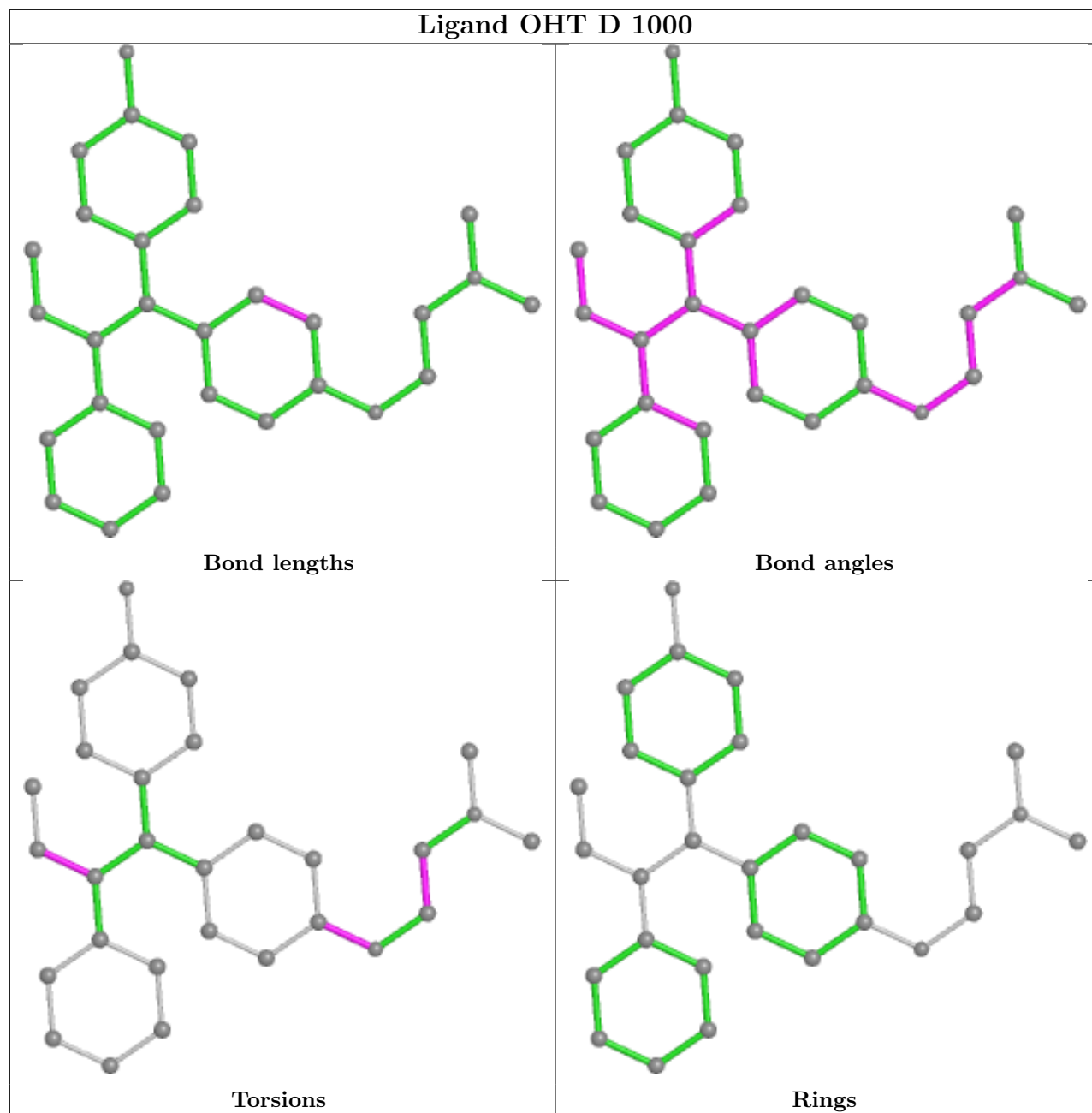












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	210/260 (80%)	-0.32	1 (0%) 91 80	33, 52, 84, 109	2 (0%)
1	B	209/260 (80%)	-0.41	0 100 100	29, 50, 82, 101	2 (0%)
1	C	220/260 (84%)	-0.28	1 (0%) 91 80	29, 52, 87, 114	2 (0%)
1	D	216/260 (83%)	-0.42	0 100 100	28, 49, 87, 113	2 (0%)
1	E	218/260 (83%)	-0.18	1 (0%) 91 80	35, 69, 103, 124	2 (0%)
1	F	220/260 (84%)	-0.24	3 (1%) 75 55	31, 57, 90, 122	2 (0%)
1	G	219/260 (84%)	-0.22	1 (0%) 91 80	33, 55, 92, 126	2 (0%)
1	H	218/260 (83%)	-0.10	3 (1%) 75 55	32, 64, 100, 139	2 (0%)
All	All	1730/2080 (83%)	-0.27	10 (0%) 89 77	28, 56, 94, 139	16 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	419	GLU	3.8
1	G	460	THR	3.0
1	H	461	PHE	3.0
1	A	410	LEU	2.6
1	F	420	GLY	2.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

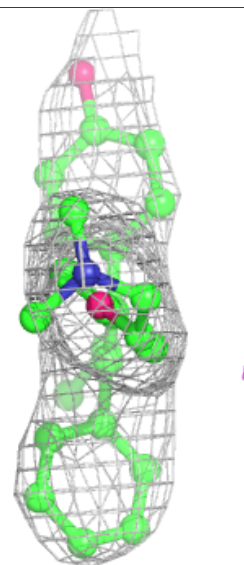
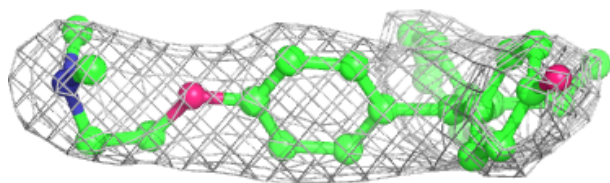
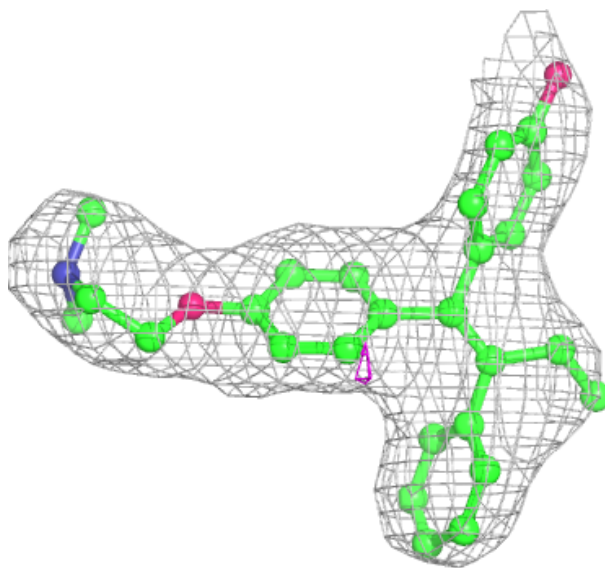
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	602	5/5	0.80	0.35	259,262,265,272	0
2	OHT	H	601	29/29	0.95	0.23	45,51,59,61	0
2	OHT	G	1000	29/29	0.96	0.20	44,48,52,53	0
2	OHT	C	1000	29/29	0.96	0.23	43,50,55,57	0
2	OHT	F	1000	29/29	0.96	0.19	41,48,52,52	0
2	OHT	D	1000	29/29	0.97	0.20	39,44,52,54	0
2	OHT	E	1000	29/29	0.97	0.20	43,51,58,61	0
2	OHT	B	601	29/29	0.97	0.20	39,43,54,58	0
2	OHT	A	1000	29/29	0.98	0.27	42,46,51,53	0
3	SO4	H	602	5/5	0.98	0.36	91,95,100,102	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.

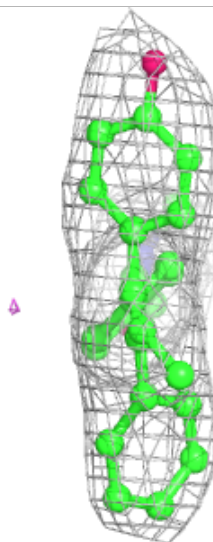
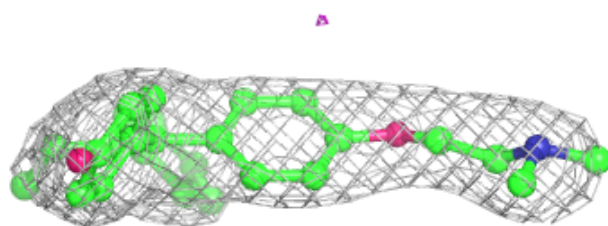
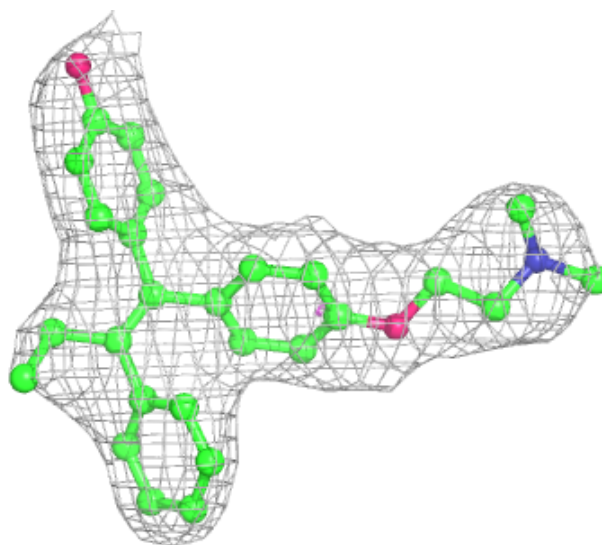
Electron density around OHT H 601:

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



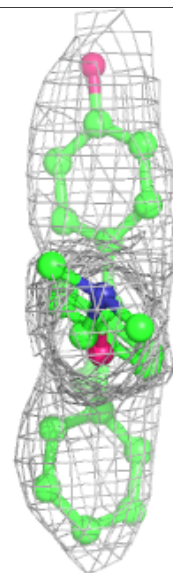
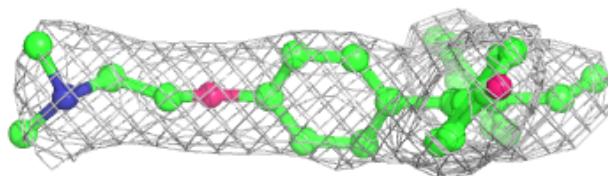
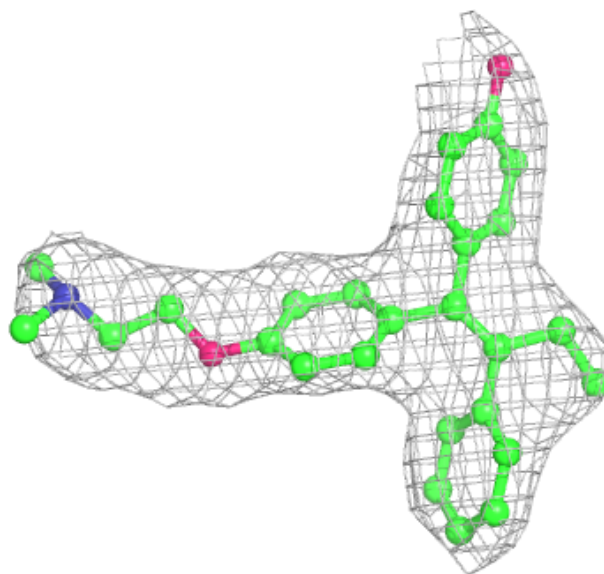
Electron density around OHT G 1000:

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



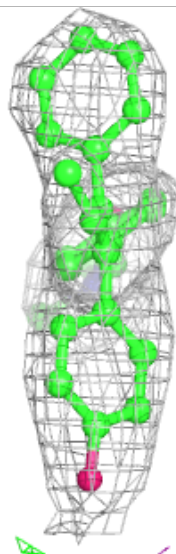
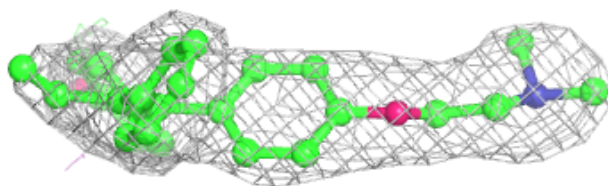
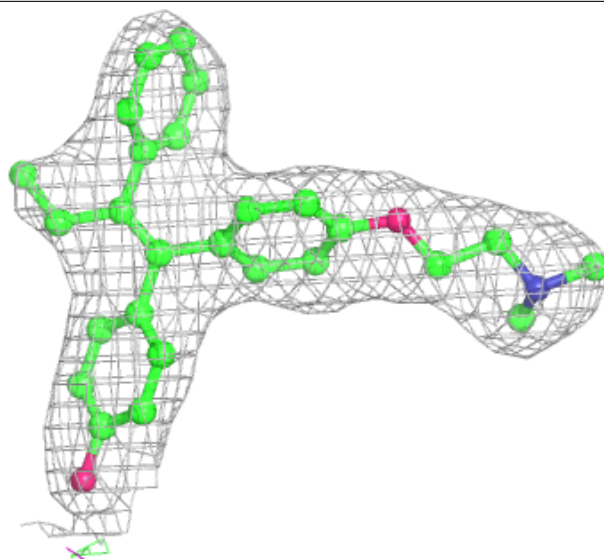
Electron density around OHT C 1000:

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



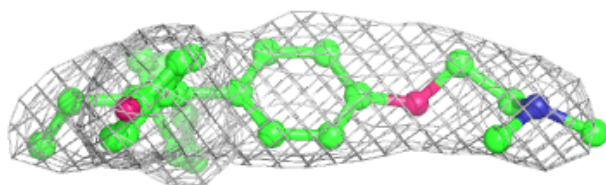
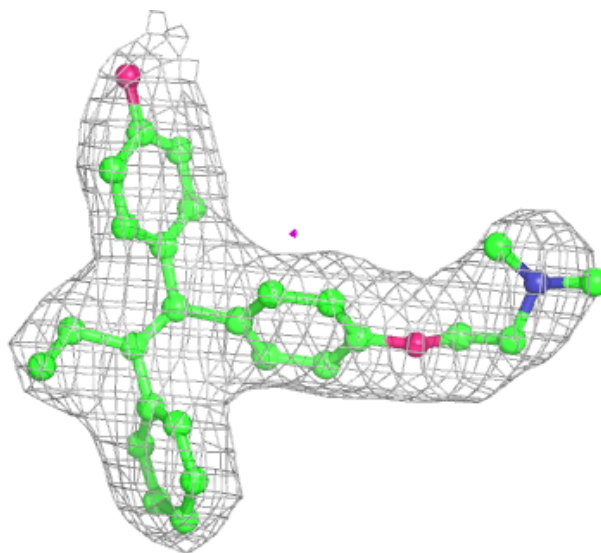
Electron density around OHT F 1000:

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



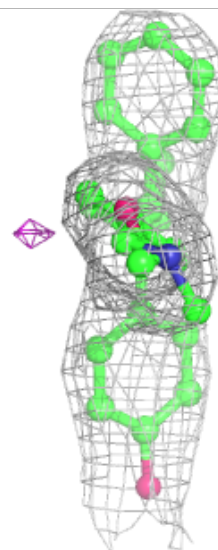
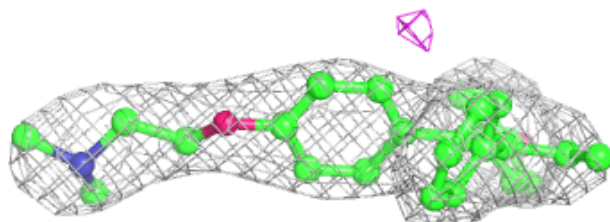
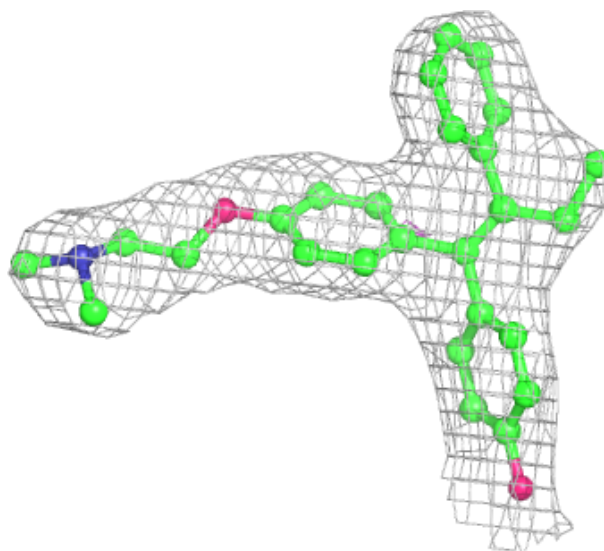
Electron density around OHT D 1000:

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



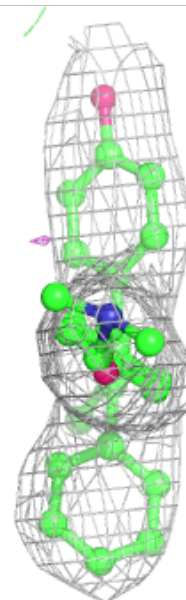
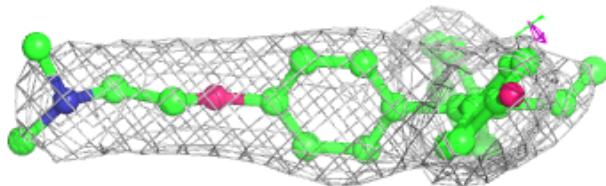
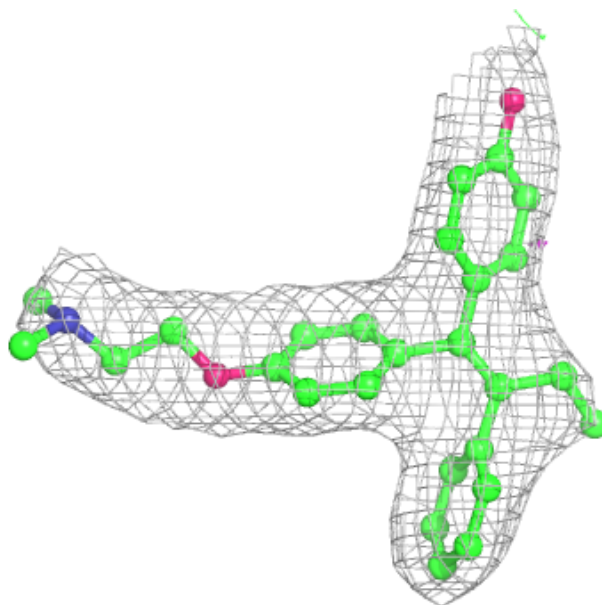
Electron density around OHT E 1000:

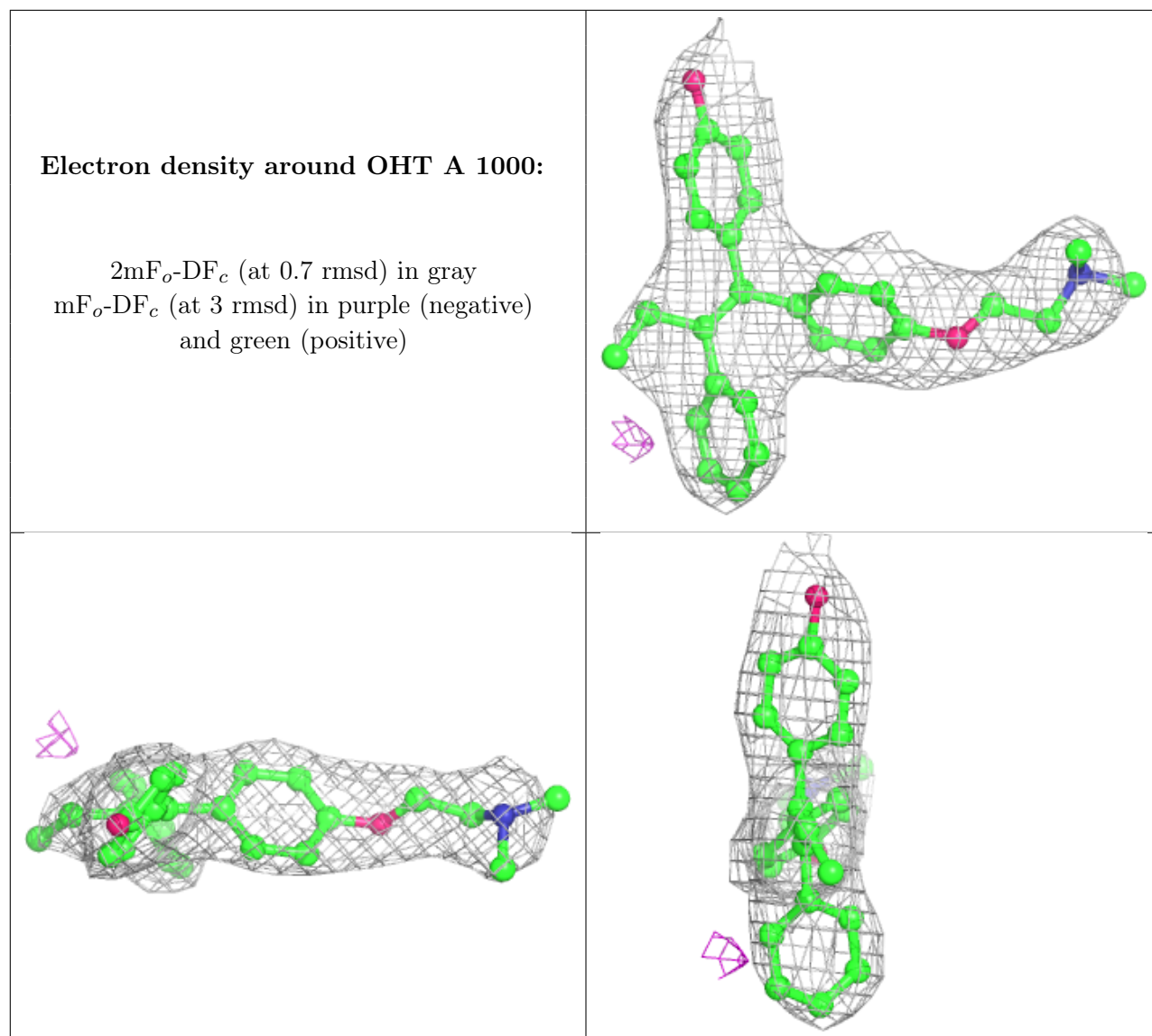
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHT B 601:

$2mF_o-DF_c$ (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.