



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:40 PM UTC

PDB ID : 2GPV / pdb_00002gpv
Title : Estrogen Related Receptor-gamma ligand binding domain complexed with 4-hydroxy-tamoxifen and a SMRT peptide
Authors : Wang, L.; Zuercher, W.J.; Consler, T.G.; Lambert, M.H.; Miller, A.B.; Osband-miller, L.A.; McKee, D.D.; Willson, T.M.; Nolte, R.T.
Deposited on : 2006-04-18
Resolution : 2.85 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

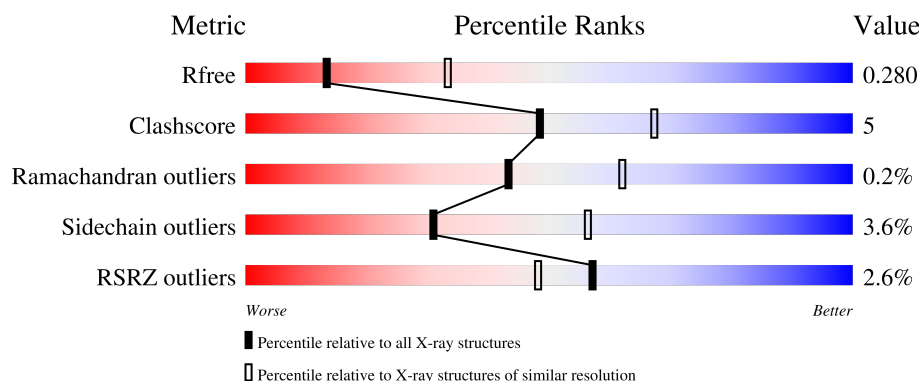
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	230	 3% 83% 13% ..
1	B	230	 3% 82% 13% ..
1	C	230	 2% 80% 16% .
1	D	230	 4% 77% 14% 9%

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Mol	Chain	Length	Quality of chain
1	E	230	% 80%10%10%
1	F	230	79%10%10%
2	G	22	41%9%5%45%
2	H	22	55%45%
2	I	22	5% 50%5%45%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10855 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.

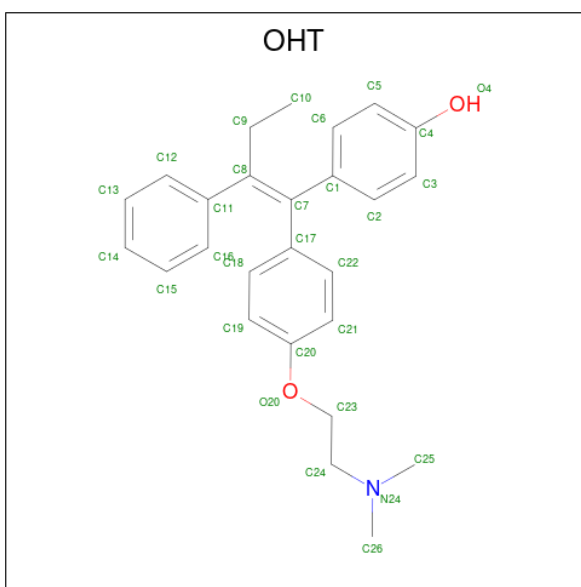
- Molecule 1 is a protein called Estrogen-related receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	3	0
			1807	1160	292	342	13			
1	B	223	Total	C	N	O	S	0	2	0
			1790	1148	289	340	13			
1	C	223	Total	C	N	O	S	0	1	0
			1780	1142	287	339	12			
1	D	209	Total	C	N	O	S	0	1	0
			1666	1067	271	318	10			
1	E	208	Total	C	N	O	S	0	0	0
			1650	1056	266	318	10			
1	F	208	Total	C	N	O	S	0	1	0
			1660	1063	269	318	10			

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	12	Total	C	N	O	S	0	0	0
			87	56	16	14	1			
2	H	12	Total	C	N	O		0	1	0
			93	59	17	17				
2	I	12	Total	C	N	O	S	0	0	0
			87	56	16	14	1			

- Molecule 3 is 4-HYDROXYTAMOXIFEN (CCD ID: OHT) (formula: C₂₆H₂₉NO₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	9	Total	O	0	0
			9	9		
4	C	6	Total	O	0	0
			6	6		
4	D	13	Total	O	0	0
			13	13		
4	E	7	Total	O	0	0
			7	7		
4	F	7	Total	O	0	0
			7	7		

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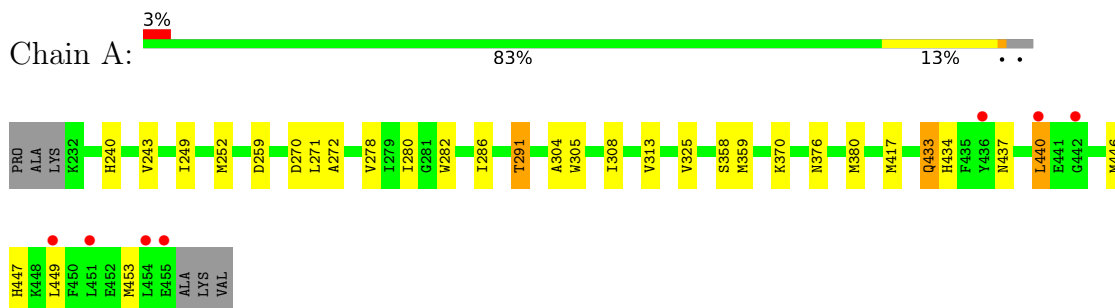
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	O	0	0
			1	1		

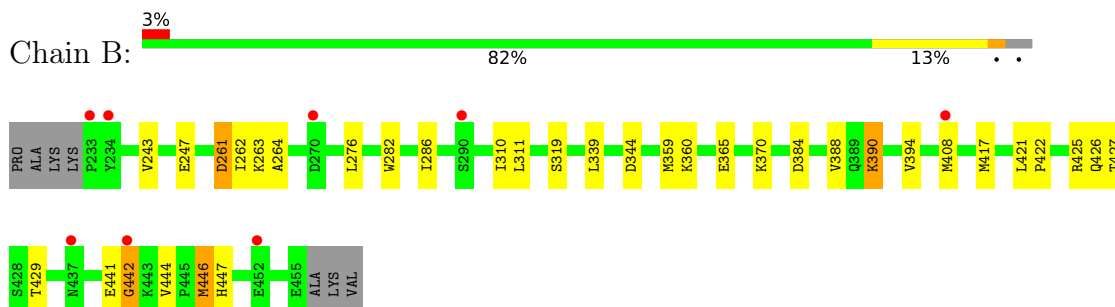
3 Residue-property plots [i](#)

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.

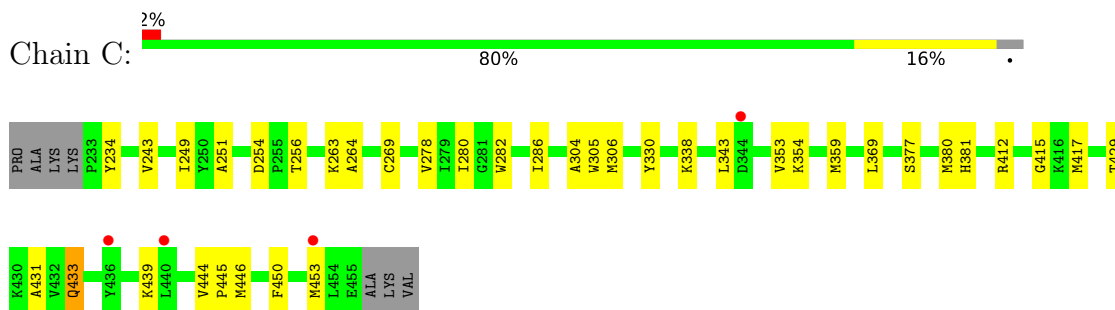
- Molecule 1: Estrogen-related receptor gamma



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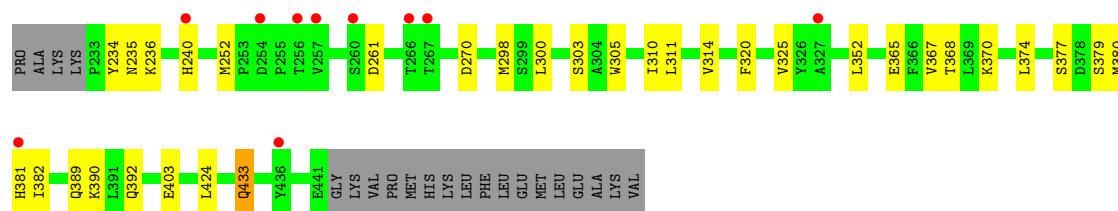


- Molecule 1: Estrogen-related receptor gamma

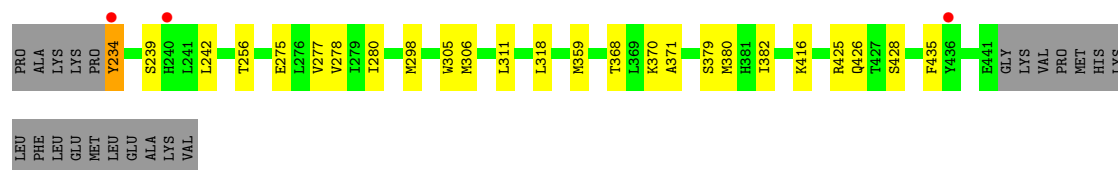
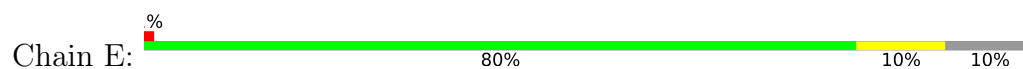


- Molecule 1: Estrogen-related receptor gamma

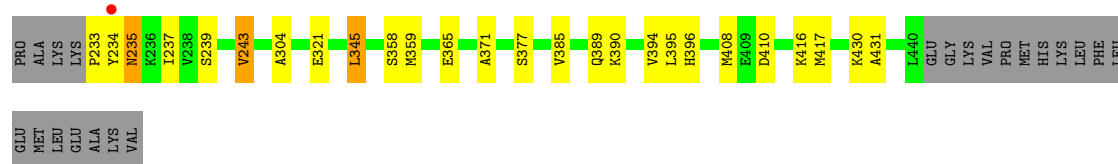
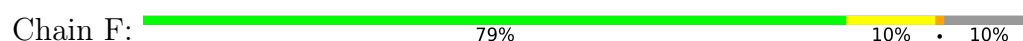




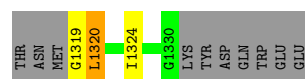
● Molecule 1: Estrogen-related receptor gamma



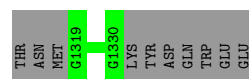
● Molecule 1: Estrogen-related receptor gamma



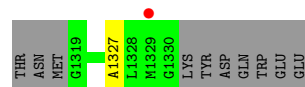
● Molecule 2: Nuclear receptor corepressor 2



● Molecule 2: Nuclear receptor corepressor 2



● Molecule 2: Nuclear receptor corepressor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.22Å 117.17Å 90.47Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	19.91 – 2.85 19.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.9 (19.91-2.85) 90.6 (19.91-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.279 0.225 , 0.280	Depositor DCC
R_{free} test set	1359 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10855	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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: 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	0.65	0/1839	0.87	1/2487 (0.0%)
1	B	0.61	0/1822	0.81	0/2464
1	C	0.60	0/1812	0.85	0/2452
1	D	0.56	0/1696	0.79	0/2297
1	E	0.61	0/1678	0.84	1/2273 (0.0%)
1	F	0.60	0/1689	0.85	0/2287
2	G	0.64	0/86	0.88	0/112
2	H	0.63	0/92	0.88	0/121
2	I	0.58	0/86	0.85	0/112
All	All	0.61	0/10800	0.84	2/14605 (0.0%)

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	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	318	LEU	N-CA-C	5.29	117.05	111.28
1	A	325	VAL	CB-CA-C	-5.16	106.79	112.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	234	TYR	Peptide
1	F	233	PRO	Peptide

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	1807	0	1842	24	0
1	B	1790	0	1820	23	0
1	C	1780	0	1805	24	0
1	D	1666	0	1687	21	0
1	E	1650	0	1668	21	0
1	F	1660	0	1686	13	0
2	G	87	0	100	3	0
2	H	93	0	98	0	0
2	I	87	0	100	2	0
3	A	29	0	29	2	0
3	B	29	0	29	2	0
3	C	29	0	29	0	0
3	D	29	0	29	2	0
3	E	29	0	29	5	0
3	F	29	0	29	1	0
4	A	18	0	0	2	0
4	B	9	0	0	0	0
4	C	6	0	0	0	0
4	D	13	0	0	2	0
4	E	7	0	0	0	0
4	F	7	0	0	1	0
4	G	1	0	0	0	0
All	All	10855	0	10980	119	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 (119) 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:D:379:SER:HB3	1:D:382:ILE:HD11	1.69	0.74
1:A:453:MET:HE2	1:E:280:ILE:HD12	1.70	0.74
1:A:359:MET:HE1	1:A:417:MET:SD	2.30	0.71
1:A:249:ILE:HD11	1:A:278:VAL:HG21	1.73	0.70
1:C:359:MET:HE2	1:C:417:MET:HE2	1.76	0.68
1:D:310:ILE:O	1:D:314:VAL:HG23	1.93	0.68
1:A:453:MET:HE2	1:E:280:ILE:CD1	2.24	0.68
1:F:410:ASP:OD2	1:F:416:LYS:NZ	2.24	0.67
1:A:453:MET:CE	1:E:280:ILE:HD12	2.27	0.65
1:D:311:LEU:HD13	1:D:424:LEU:HD22	1.80	0.64
1:F:408:MET:HE3	4:F:22:HOH:O	1.98	0.62
1:A:359:MET:CE	1:A:417:MET:SD	2.88	0.61
1:D:270:ASP:HB3	4:D:59:HOH:O	2.00	0.61
1:C:306:MET:HE3	1:C:431:ALA:HB1	1.82	0.61
1:E:359:MET:CE	1:E:416:LYS:HB3	2.32	0.59
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.59
1:B:390:LYS:O	1:B:394:VAL:HG23	2.03	0.58
1:C:380:MET:HE3	1:C:381:HIS:CE1	2.38	0.57
1:D:235:ASN:HD22	1:D:236:LYS:N	2.01	0.57
1:F:345:LEU:HD21	1:F:431:ALA:HA	1.86	0.57
1:C:338:LYS:HG2	1:C:343:LEU:HD22	1.87	0.56
1:B:426:GLN:NE2	1:E:425:ARG:HD2	2.22	0.55
3:E:504:OHT:C17	3:E:504:OHT:C12	2.84	0.55
1:B:262:ILE:HD12	1:B:444:VAL:HG22	1.89	0.55
1:D:352:LEU:HD11	1:D:424:LEU:HA	1.88	0.55
1:C:306:MET:HE3	1:C:431:ALA:CB	2.38	0.54
1:B:262:ILE:HG23	1:B:444:VAL:HG22	1.89	0.54
1:B:384:ASP:O	1:B:388:VAL:HG23	2.08	0.54
1:B:282:TRP:CH2	1:B:286:ILE:HD11	2.43	0.53
1:A:449[B]:LEU:HG	1:A:453:MET:HE1	1.91	0.53
3:E:504:OHT:C11	3:E:504:OHT:C22	2.85	0.53
1:C:280:ILE:HG21	2:I:1327:ALA:HB3	1.91	0.53
1:A:291:THR:HB	4:A:41:HOH:O	2.10	0.52
1:B:426:GLN:HE21	1:E:425:ARG:HD2	1.75	0.52
1:C:264:ALA:HA	1:C:330:TYR:OH	2.11	0.51
1:E:359:MET:HE3	1:E:416:LYS:HB3	1.93	0.51
1:A:453:MET:HE3	1:E:277:VAL:HA	1.93	0.50
1:B:261:ASP:N	1:B:261:ASP:OD1	2.44	0.50
1:A:280:ILE:HD13	2:G:1324:ILE:HA	1.93	0.50
1:A:359:MET:HE2	1:A:417:MET:CE	2.43	0.49
1:F:304:ALA:HB2	1:F:377:SER:HB3	1.95	0.49
1:E:435:PHE:CZ	3:E:504:OHT:H253	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:MET:O	1:B:360:LYS:C	2.55	0.48
1:C:446:MET:HE2	1:C:450:PHE:CE1	2.48	0.48
1:D:365:GLU:OE2	1:D:403:GLU:OE2	2.32	0.48
1:B:311:LEU:HD23	1:B:370:LYS:HG2	1.96	0.48
1:D:311:LEU:HD23	1:D:370:LYS:HG2	1.96	0.47
1:D:389:GLN:O	1:D:392:GLN:HB2	2.15	0.47
1:D:433:GLN:HE21	1:D:433:GLN:HA	1.79	0.47
1:E:311:LEU:HD23	1:E:370:LYS:CG	2.44	0.47
1:F:365:GLU:OE2	1:F:417:MET:HE3	2.13	0.47
1:B:426:GLN:NE2	1:E:425:ARG:HH11	2.12	0.47
1:C:415:GLY:HA3	1:F:396:HIS:CE1	2.49	0.47
1:C:263:LYS:O	1:C:264:ALA:C	2.57	0.47
3:E:504:OHT:C12	3:E:504:OHT:C22	2.93	0.47
1:F:235:ASN:OD1	1:F:235:ASN:C	2.57	0.47
1:B:441:GLU:O	1:B:442:GLY:C	2.57	0.46
1:B:339:LEU:HD23	1:D:381[A]:HIS:CD2	2.50	0.46
1:E:435:PHE:HB2	3:E:504:OHT:H13	1.98	0.46
1:A:376:ASN:ND2	4:A:18:HOH:O	2.49	0.46
1:E:239:SER:HA	1:E:242:LEU:HD12	1.98	0.46
1:A:282:TRP:CH2	1:A:286:ILE:HD11	2.51	0.46
1:B:365:GLU:OE2	1:B:417:MET:HE3	2.15	0.46
1:D:424:LEU:HD12	1:D:424:LEU:O	2.16	0.46
3:A:500:OHT:C22	3:A:500:OHT:C11	2.94	0.45
1:B:425:ARG:HD2	1:E:426:GLN:OE1	2.16	0.45
2:G:1319:GLY:O	2:G:1320:LEU:HB3	2.17	0.45
1:B:263:LYS:O	1:B:264:ALA:C	2.58	0.45
1:F:239:SER:O	1:F:243:VAL:HG13	2.15	0.45
1:C:251:ALA:HB3	1:C:330:TYR:HB2	1.99	0.45
1:E:379:SER:HB3	1:E:382:ILE:HD11	1.99	0.44
1:A:280:ILE:CD1	2:G:1324:ILE:HA	2.48	0.44
1:B:339:LEU:HD23	1:D:381[A]:HIS:CG	2.53	0.44
1:F:359:MET:HE2	1:F:417:MET:HE2	1.99	0.44
1:C:444:VAL:N	1:C:445:PRO:HD2	2.33	0.44
1:A:270:ASP:OD1	1:A:270:ASP:O	2.36	0.43
1:C:249:ILE:HD11	1:C:278:VAL:HG21	1.99	0.43
3:B:501:OHT:C6	3:B:501:OHT:H91	2.48	0.43
1:E:306:MET:HB3	1:E:428:SER:OG	2.19	0.43
1:A:308:ILE:HG23	1:A:370:LYS:HD2	2.00	0.43
3:A:500:OHT:C6	3:A:500:OHT:H91	2.49	0.43
1:B:446:MET:HE1	1:D:305:TRP:CH2	2.53	0.43
1:C:359:MET:HE2	1:C:417:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ARG:HB3	1:F:396:HIS:CE1	2.54	0.43
1:A:446:MET:HE1	1:E:305:TRP:CZ2	2.54	0.42
1:A:447:HIS:CD2	1:E:298:MET:HE3	2.54	0.42
1:A:304:ALA:O	1:A:305:TRP:C	2.61	0.42
1:C:282:TRP:CH2	1:C:286:ILE:HD11	2.54	0.42
1:D:303:SER:HB3	1:D:377:SER:HB2	2.01	0.42
1:B:426:GLN:HE21	1:E:425:ARG:HH11	1.67	0.42
1:C:304:ALA:O	1:C:305:TRP:C	2.62	0.42
1:C:353:VAL:O	1:C:354:LYS:C	2.63	0.42
1:A:433:GLN:C	1:A:437:ASN:HD22	2.27	0.42
3:D:503:OHT:H91	3:D:503:OHT:C6	2.49	0.42
1:F:371:ALA:HB1	1:F:395:LEU:HD13	2.01	0.42
1:F:235:ASN:OD1	1:F:237:ILE:N	2.53	0.42
3:F:505:OHT:C22	3:F:505:OHT:C11	2.98	0.42
1:C:304:ALA:HB2	1:C:377:SER:HB3	2.02	0.41
1:E:275:GLU:O	1:E:278:VAL:HG22	2.20	0.41
1:C:280:ILE:HG21	2:I:1327:ALA:CB	2.50	0.41
3:B:501:OHT:C22	3:B:501:OHT:C11	2.99	0.41
1:C:254:ASP:OD1	1:C:256:THR:OG1	2.36	0.41
1:A:433:GLN:O	1:A:434:HIS:C	2.62	0.41
1:D:320:PHE:CE1	1:D:325:VAL:HG21	2.56	0.41
3:D:503:OHT:C22	3:D:503:OHT:C11	2.99	0.41
1:F:390:LYS:O	1:F:394:VAL:HG23	2.21	0.41
1:B:421:LEU:N	1:B:422:PRO:CD	2.84	0.41
1:B:447:HIS:CE1	1:D:298:MET:HE1	2.56	0.41
1:D:300:LEU:HD22	1:D:374:LEU:O	2.21	0.41
1:A:440:LEU:N	1:A:440:LEU:CD1	2.83	0.41
1:B:310:ILE:HD13	1:B:427:THR:HG22	2.03	0.41
1:C:359:MET:CE	1:C:417:MET:HE2	2.48	0.40
1:D:240:HIS:HB2	4:D:43:HOH:O	2.21	0.40
1:A:271:LEU:O	1:A:272:ALA:C	2.64	0.40
1:B:447:HIS:CE1	1:D:298:MET:CE	3.03	0.40
1:D:367:VAL:HG23	1:D:368:THR:N	2.35	0.40
1:C:369:LEU:HD23	1:C:369:LEU:HA	1.94	0.40
1:E:368:THR:O	1:E:371:ALA:HB3	2.22	0.40
1:C:429:THR:CG2	1:C:433:GLN:HE22	2.34	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	225/230 (98%)	209 (93%)	16 (7%)	0	100	100
1	B	223/230 (97%)	211 (95%)	11 (5%)	1 (0%)	30	48
1	C	222/230 (96%)	211 (95%)	11 (5%)	0	100	100
1	D	208/230 (90%)	197 (95%)	11 (5%)	0	100	100
1	E	206/230 (90%)	198 (96%)	8 (4%)	0	100	100
1	F	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
2	G	10/22 (46%)	8 (80%)	1 (10%)	1 (10%)	0	0
2	H	11/22 (50%)	9 (82%)	2 (18%)	0	100	100
2	I	10/22 (46%)	10 (100%)	0	0	100	100
All	All	1322/1446 (91%)	1251 (95%)	69 (5%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	GLY
2	G	1320	LEU

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	202/203 (100%)	194 (96%)	8 (4%)	28	53
1	B	200/203 (98%)	190 (95%)	10 (5%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	198/203 (98%)	192 (97%)	6 (3%)	36	61
1	D	185/203 (91%)	179 (97%)	6 (3%)	34	59
1	E	183/203 (90%)	180 (98%)	3 (2%)	55	76
1	F	185/203 (91%)	176 (95%)	9 (5%)	22	45
2	G	8/18 (44%)	8 (100%)	0	100	100
2	H	8/18 (44%)	8 (100%)	0	100	100
2	I	8/18 (44%)	8 (100%)	0	100	100
All	All	1177/1272 (92%)	1135 (96%)	42 (4%)	31	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	259	ASP
1	A	291	THR
1	A	313	VAL
1	A	358	SER
1	A	380	MET
1	A	433	GLN
1	A	440	LEU
1	B	243	VAL
1	B	247	GLU
1	B	261	ASP
1	B	276	LEU
1	B	319	SER
1	B	344	ASP
1	B	390	LYS
1	B	408	MET
1	B	429	THR
1	B	446	MET
1	C	234	TYR
1	C	243	VAL
1	C	269	CYS
1	C	433	GLN
1	C	439	LYS
1	C	453	MET
1	D	234	TYR
1	D	252	MET
1	D	261	ASP
1	D	380	MET

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Mol	Chain	Res	Type
1	D	390	LYS
1	D	433	GLN
1	E	234	TYR
1	E	256	THR
1	E	380	MET
1	F	234	TYR
1	F	235	ASN
1	F	243	VAL
1	F	321	GLU
1	F	345	LEU
1	F	358	SER
1	F	385	VAL
1	F	389	GLN
1	F	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	HIS
1	A	437	ASN
1	B	426	GLN
1	B	433	GLN
1	C	336	GLN
1	C	433	GLN
1	D	235	ASN
1	D	302	GLN
1	D	336	GLN
1	D	376	ASN
1	D	426	GLN
1	D	433	GLN
1	E	302	GLN
1	E	392	GLN
1	F	285	HIS
1	F	336	GLN
1	F	396	HIS
1	F	426	GLN
1	F	433	GLN

5.3.3 RNA ⓘ

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](#)

6 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	OHT	A	500	-	31,31,31	0.95	2 (6%)	41,41,41	1.35	5 (12%)
3	OHT	E	504	-	31,31,31	0.85	0	41,41,41	1.27	5 (12%)
3	OHT	D	503	-	31,31,31	0.84	0	41,41,41	1.03	3 (7%)
3	OHT	F	505	-	31,31,31	0.97	3 (9%)	41,41,41	1.32	5 (12%)
3	OHT	B	501	-	31,31,31	0.93	2 (6%)	41,41,41	1.17	4 (9%)
3	OHT	C	502	-	31,31,31	0.85	1 (3%)	41,41,41	1.18	2 (4%)

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	OHT	A	500	-	-	5/24/24/24	0/3/3/3
3	OHT	E	504	-	-	4/24/24/24	0/3/3/3
3	OHT	D	503	-	-	5/24/24/24	0/3/3/3
3	OHT	F	505	-	-	4/24/24/24	0/3/3/3
3	OHT	B	501	-	-	4/24/24/24	0/3/3/3
3	OHT	C	502	-	-	3/24/24/24	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	OHT	C17-C7	-3.03	1.44	1.49
3	B	501	OHT	C1-C7	-2.47	1.45	1.49
3	F	505	OHT	C11-C8	-2.46	1.44	1.49
3	B	501	OHT	C17-C7	-2.30	1.45	1.49
3	C	502	OHT	C17-C7	-2.16	1.45	1.49
3	F	505	OHT	C17-C7	-2.06	1.46	1.49
3	A	500	OHT	C1-C7	-2.06	1.46	1.49
3	F	505	OHT	C1-C7	-2.01	1.46	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	OHT	C9-C8-C7	4.27	127.71	123.46
3	F	505	OHT	C9-C8-C7	4.03	127.47	123.46
3	A	500	OHT	C17-C7-C8	-4.02	117.99	122.83
3	F	505	OHT	C23-O20-C20	-3.90	107.80	117.93
3	E	504	OHT	C23-O20-C20	-3.86	107.90	117.93
3	E	504	OHT	C11-C8-C7	-3.69	118.72	122.35
3	B	501	OHT	C9-C8-C7	3.51	126.96	123.46
3	D	503	OHT	C9-C8-C7	3.48	126.93	123.46
3	A	500	OHT	C23-C24-N24	-2.79	107.14	114.57
3	C	502	OHT	C17-C7-C8	-2.72	119.56	122.83
3	B	501	OHT	C23-O20-C20	-2.70	110.91	117.93
3	E	504	OHT	C9-C8-C7	2.68	126.13	123.46
3	E	504	OHT	C12-C11-C8	-2.44	117.86	121.00
3	D	503	OHT	C10-C9-C8	-2.40	109.44	112.87
3	B	501	OHT	C12-C11-C8	-2.36	117.96	121.00
3	A	500	OHT	C23-O20-C20	-2.28	112.00	117.93
3	E	504	OHT	C17-C7-C8	-2.25	120.12	122.83
3	F	505	OHT	C17-C7-C8	-2.20	120.18	122.83
3	D	503	OHT	C17-C7-C8	-2.19	120.20	122.83
3	A	500	OHT	C22-C17-C18	2.16	121.31	118.57
3	B	501	OHT	C18-C17-C7	-2.13	117.25	120.91
3	F	505	OHT	C10-C9-C8	-2.11	109.86	112.87
3	A	500	OHT	C9-C8-C7	2.10	125.56	123.46
3	F	505	OHT	C11-C8-C7	-2.04	120.34	122.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	OHT	O20-C23-C24-N24
3	D	503	OHT	O20-C23-C24-N24
3	B	501	OHT	C19-C20-O20-C23
3	B	501	OHT	C21-C20-O20-C23
3	E	504	OHT	C21-C20-O20-C23
3	F	505	OHT	O20-C23-C24-N24
3	F	505	OHT	C21-C20-O20-C23
3	E	504	OHT	C19-C20-O20-C23
3	F	505	OHT	C19-C20-O20-C23
3	D	503	OHT	C21-C20-O20-C23
3	D	503	OHT	C19-C20-O20-C23
3	E	504	OHT	O20-C23-C24-N24
3	D	503	OHT	C11-C8-C9-C10
3	A	500	OHT	O20-C23-C24-N24
3	A	500	OHT	C21-C20-O20-C23
3	A	500	OHT	C19-C20-O20-C23
3	A	500	OHT	C11-C8-C9-C10
3	E	504	OHT	C23-C24-N24-C25
3	C	502	OHT	O20-C23-C24-N24
3	A	500	OHT	C7-C8-C9-C10
3	D	503	OHT	C7-C8-C9-C10
3	B	501	OHT	C23-C24-N24-C26
3	C	502	OHT	C21-C20-O20-C23
3	C	502	OHT	C19-C20-O20-C23
3	F	505	OHT	C24-C23-O20-C20

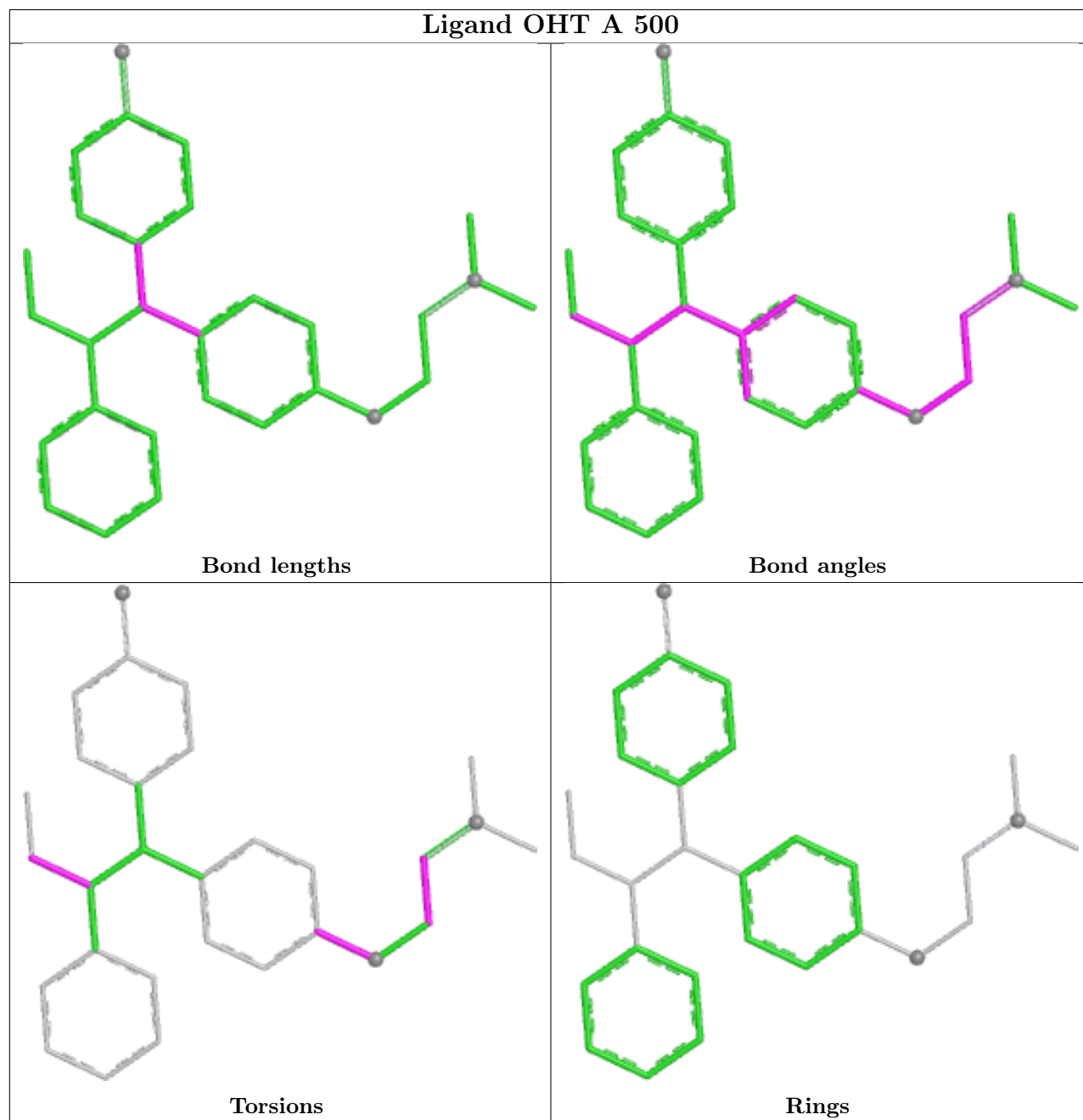
There are no ring outliers.

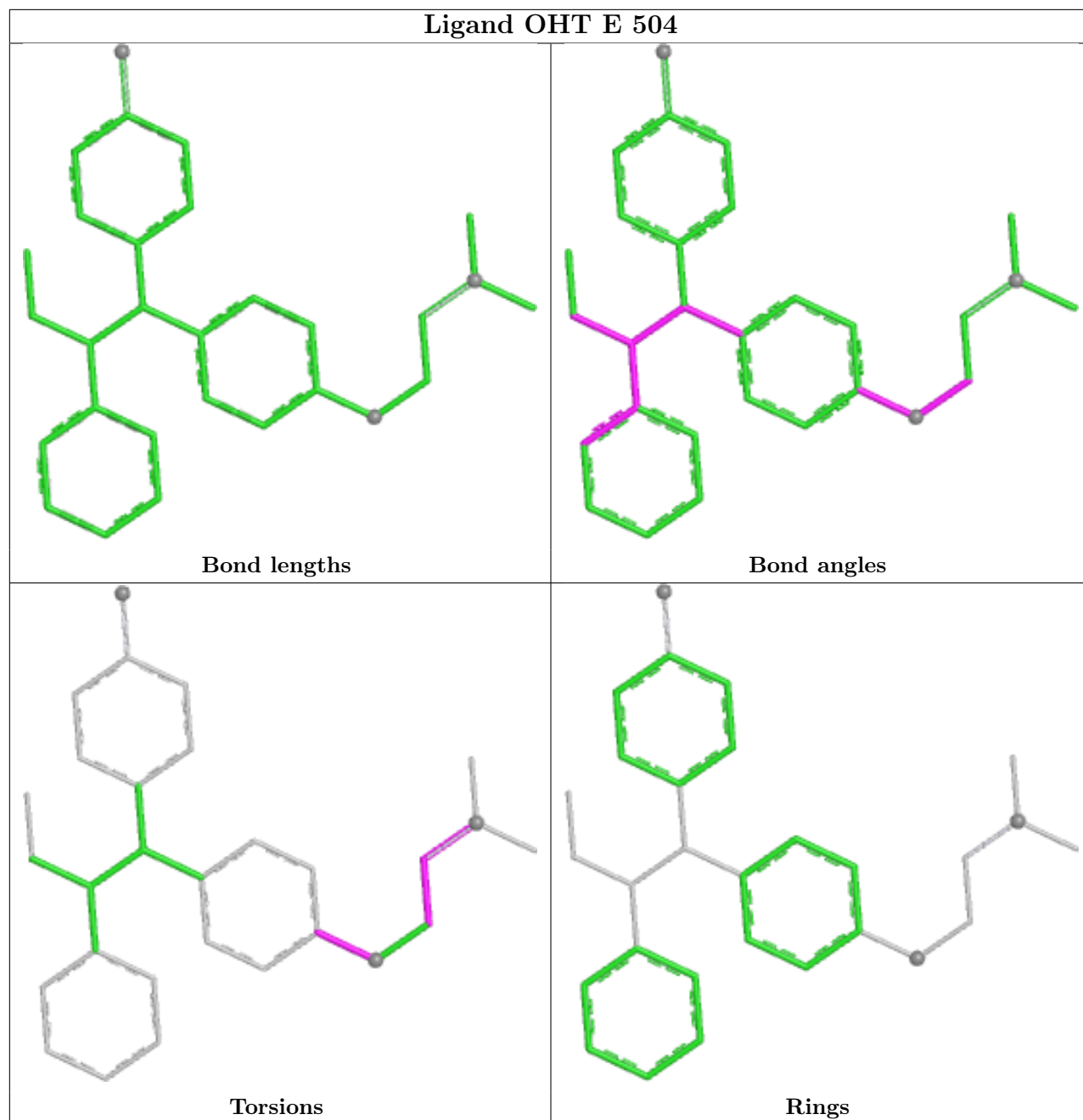
5 monomers are involved in 12 short contacts:

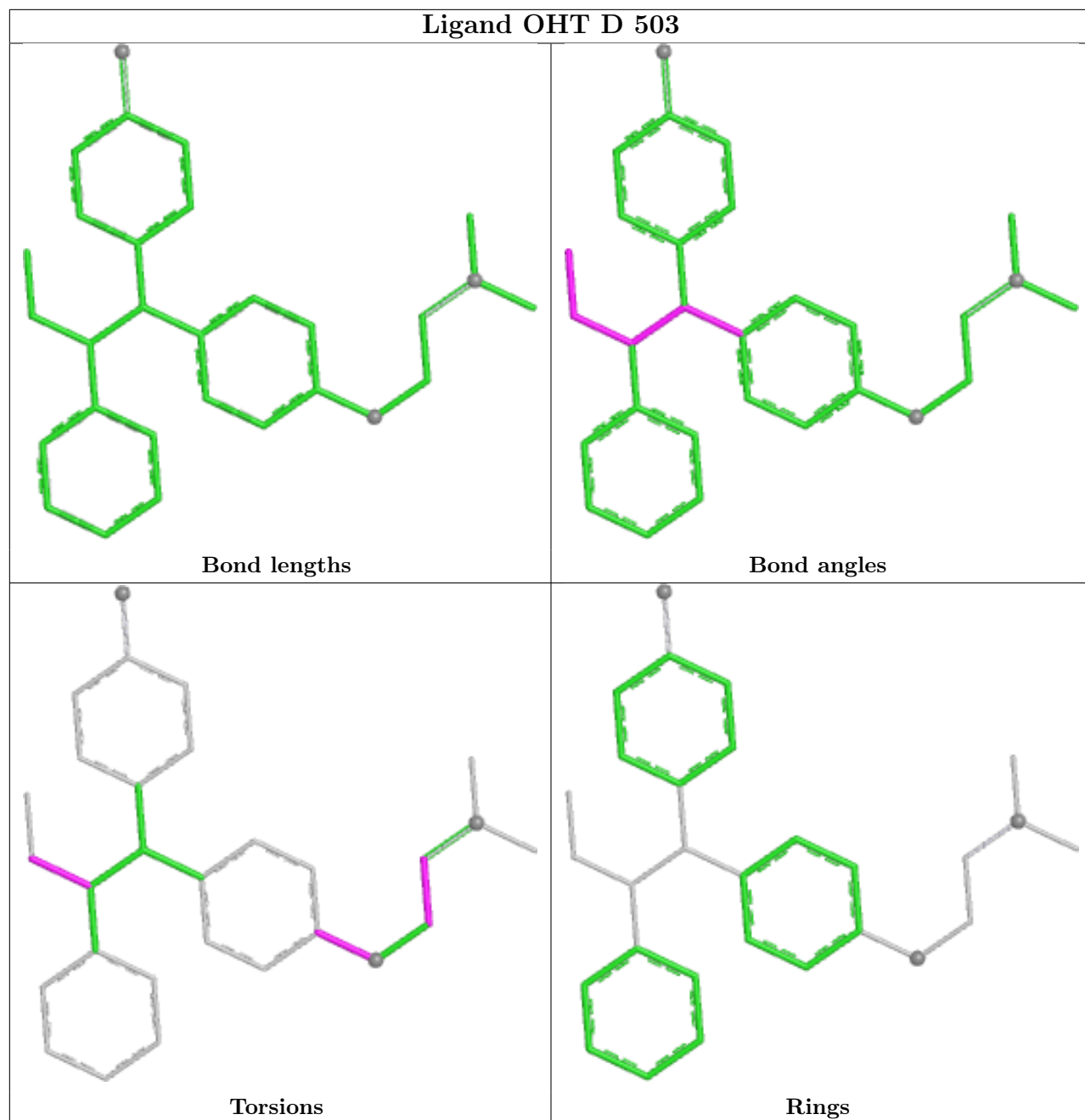
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	OHT	2	0
3	E	504	OHT	5	0
3	D	503	OHT	2	0
3	F	505	OHT	1	0
3	B	501	OHT	2	0

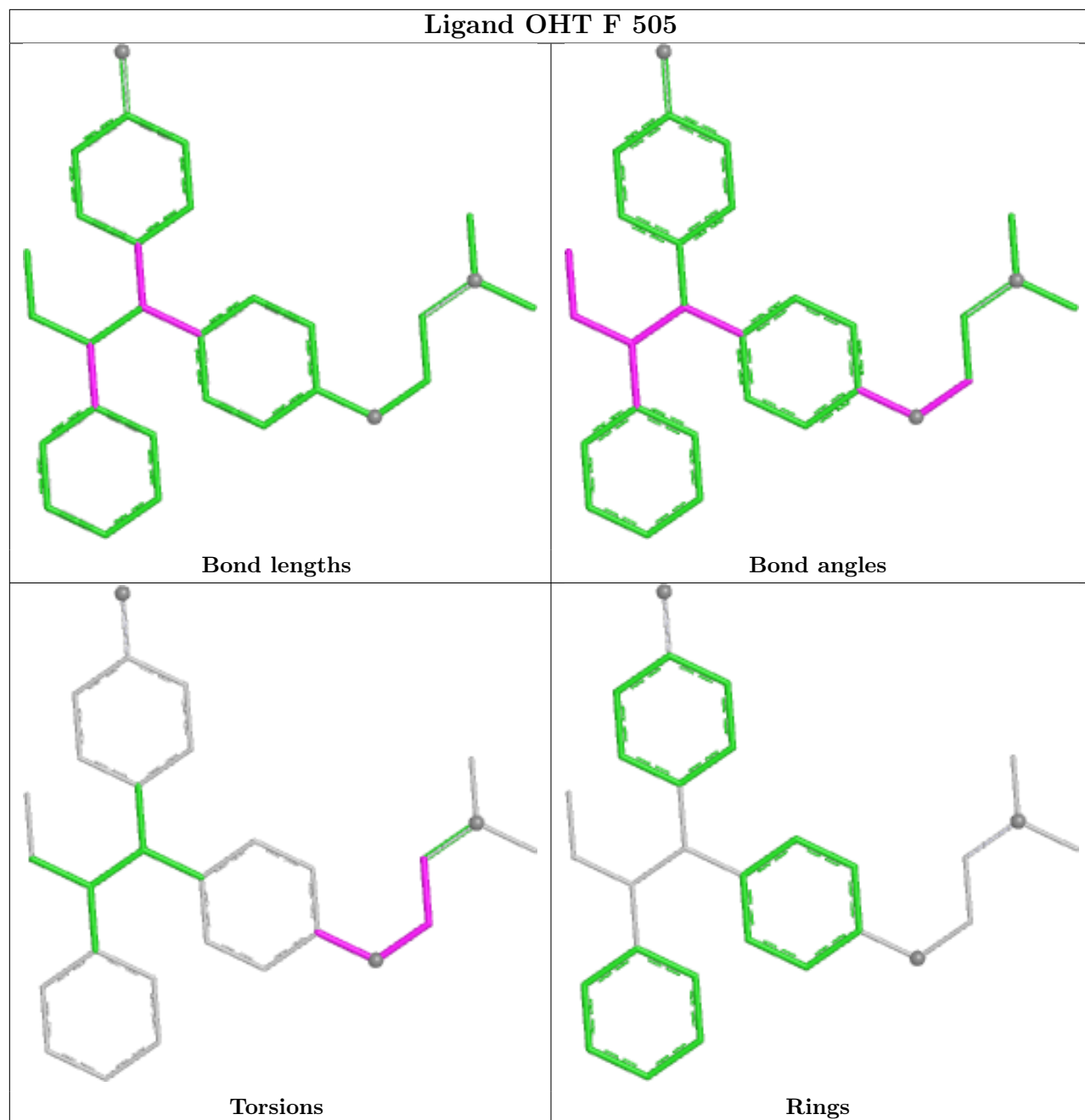
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

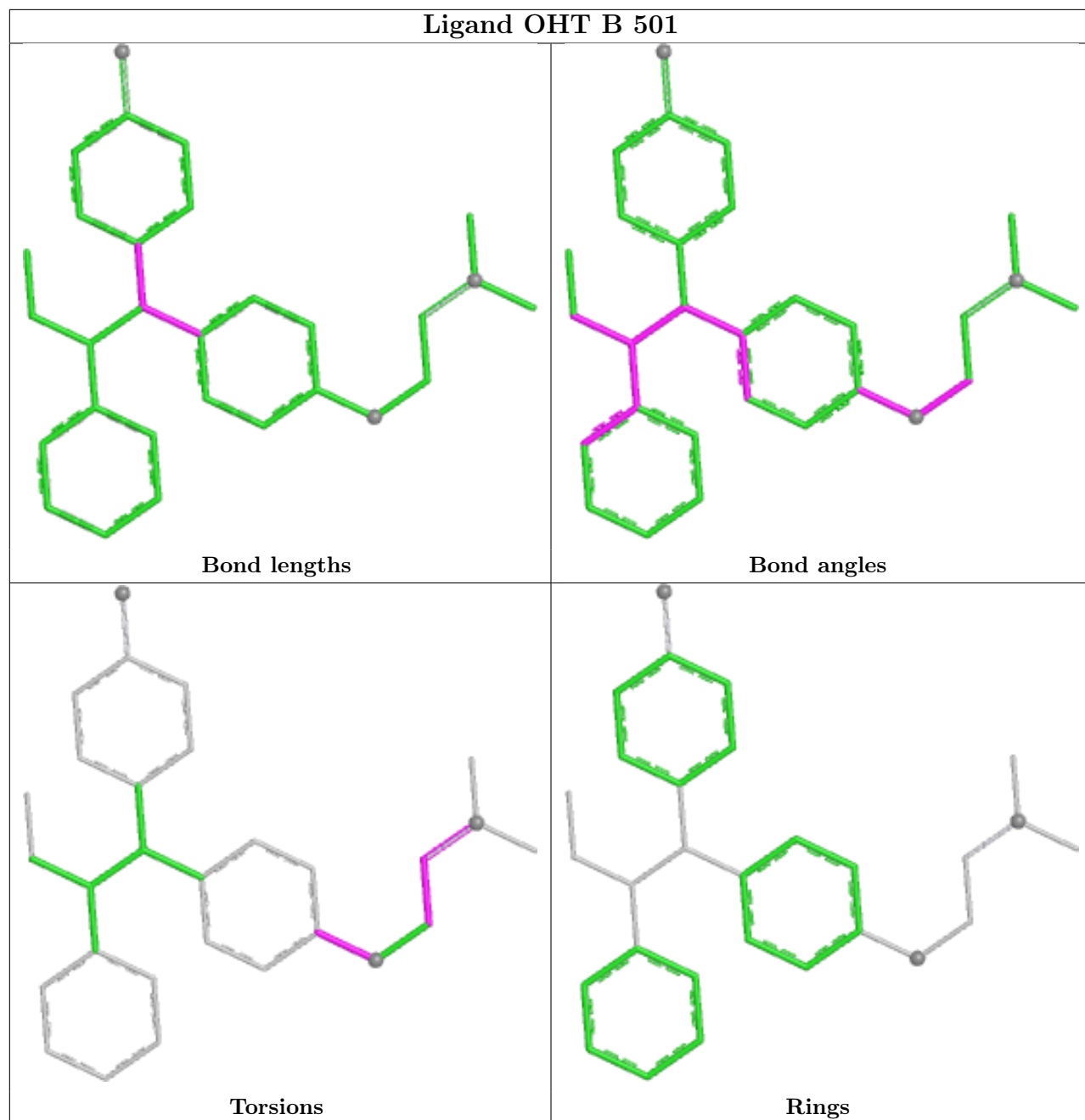
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

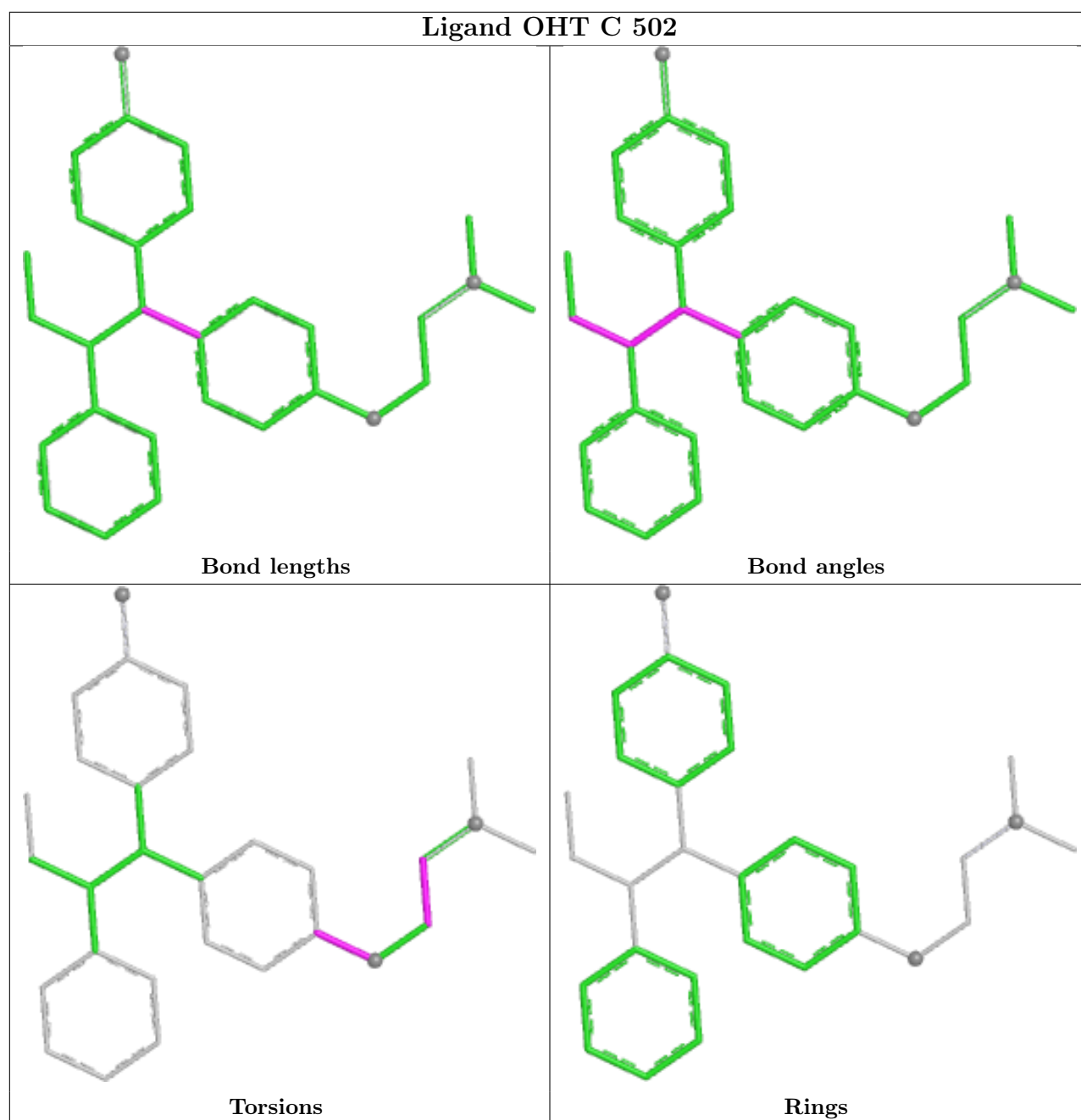












5.7 Other polymers [i](#)

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

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	224/230 (97%)	0.03	7 (3%)	51	43	6, 16, 27, 30	3 (1%)
1	B	223/230 (96%)	0.15	8 (3%)	46	36	6, 16, 27, 29	2 (0%)
1	C	223/230 (96%)	0.01	4 (1%)	67	61	7, 16, 27, 29	1 (0%)
1	D	209/230 (90%)	0.49	10 (4%)	35	28	9, 15, 21, 38	1 (0%)
1	E	208/230 (90%)	-0.05	3 (1%)	73	67	11, 16, 21, 38	0
1	F	208/230 (90%)	-0.13	1 (0%)	87	85	7, 15, 21, 31	1 (0%)
2	G	12/22 (54%)	0.56	0	100	100	24, 27, 30, 31	0
2	H	12/22 (54%)	0.65	0	100	100	13, 26, 29, 30	1 (8%)
2	I	12/22 (54%)	0.57	1 (8%)	17	13	24, 26, 30, 31	0
All	All	1331/1446 (92%)	0.09	34 (2%)	57	48	6, 16, 27, 38	9 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	THR	4.0
1	A	454	LEU	3.5
2	I	1329	MET	3.1
1	C	440	LEU	3.0
1	D	240	HIS	3.0
1	B	442	GLY	2.7
1	D	381[A]	HIS	2.7
1	E	234	TYR	2.7
1	E	436	TYR	2.7
1	D	254	ASP	2.6
1	A	451	LEU	2.5
1	A	436	TYR	2.5
1	B	437	ASN	2.5
1	B	234	TYR	2.4
1	F	234	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	344	ASP	2.3
1	B	270	ASP	2.3
1	B	408	MET	2.3
1	B	290	SER	2.2
1	B	233	PRO	2.2
1	A	455	GLU	2.2
1	C	436	TYR	2.1
1	A	440	LEU	2.1
1	B	452	GLU	2.1
1	C	453	MET	2.1
1	D	266	THR	2.1
1	D	267	THR	2.1
1	D	327	ALA	2.1
1	D	260	SER	2.1
1	D	257	VAL	2.1
1	E	240	HIS	2.0
1	A	449[A]	LEU	2.0
1	A	442	GLY	2.0
1	D	436	TYR	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
3	OHT	D	503	29/29	0.84	0.14	29,32,34,34	0
3	OHT	B	501	29/29	0.89	0.11	15,17,21,22	0
3	OHT	A	500	29/29	0.90	0.10	15,17,19,20	0
3	OHT	E	504	29/29	0.90	0.10	20,23,27,28	0

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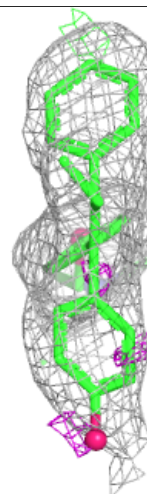
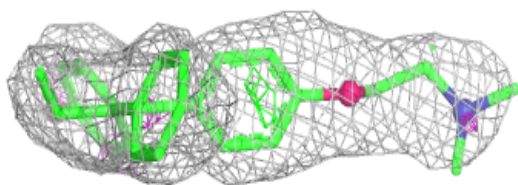
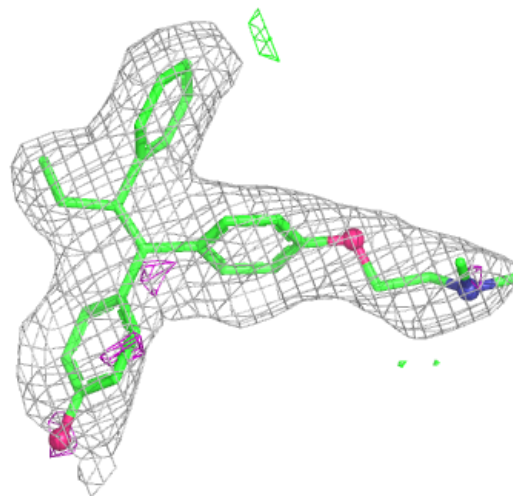
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OHT	C	502	29/29	0.92	0.09	20,25,30,30	0
3	OHT	F	505	29/29	0.92	0.09	19,21,25,25	0

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.

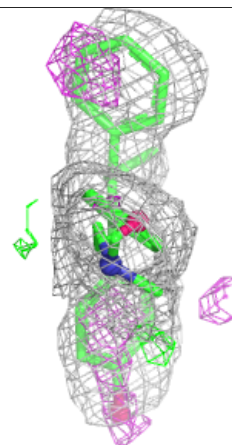
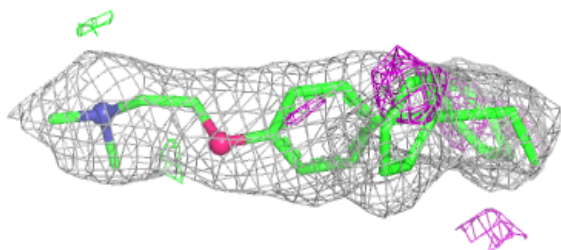
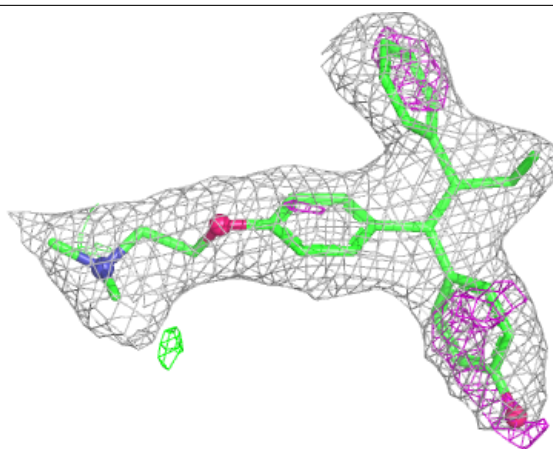
Electron density around OHT D 503:

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



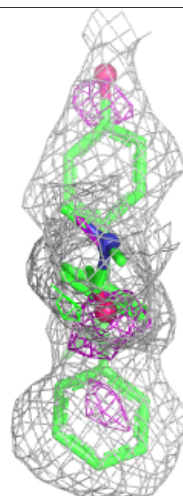
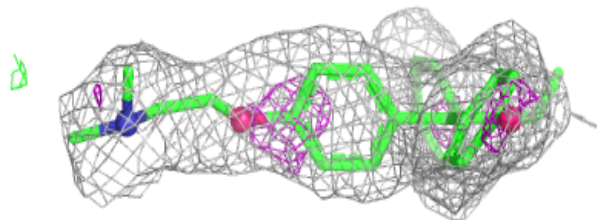
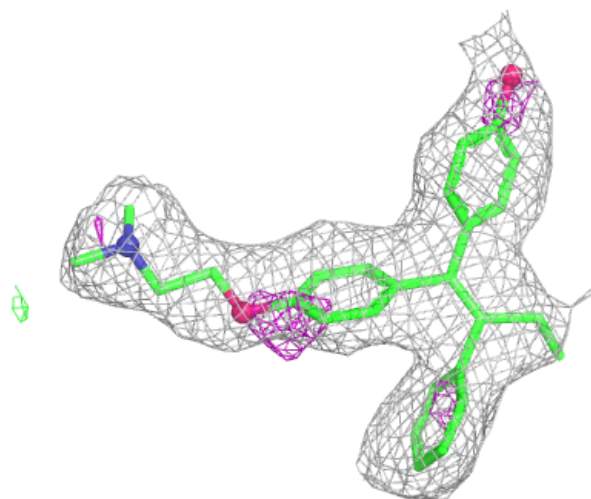
Electron density around OHT B 501:

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



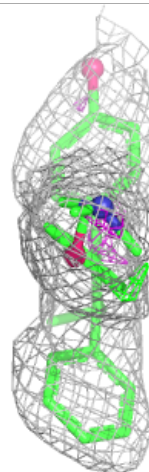
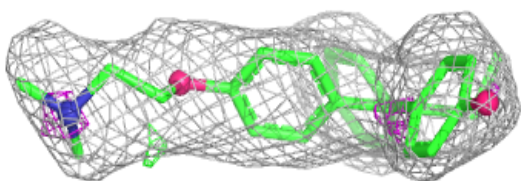
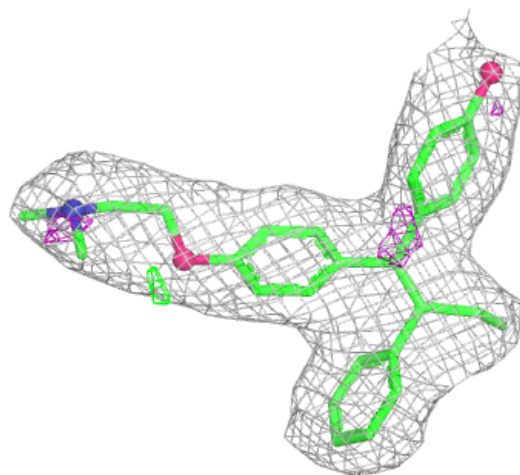
Electron density around OHT A 500:

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



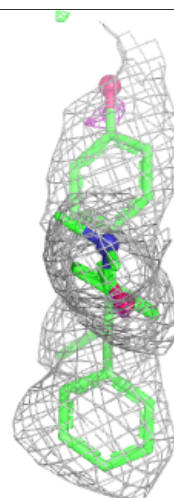
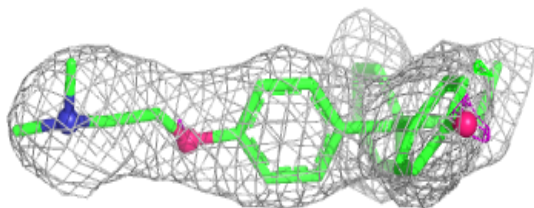
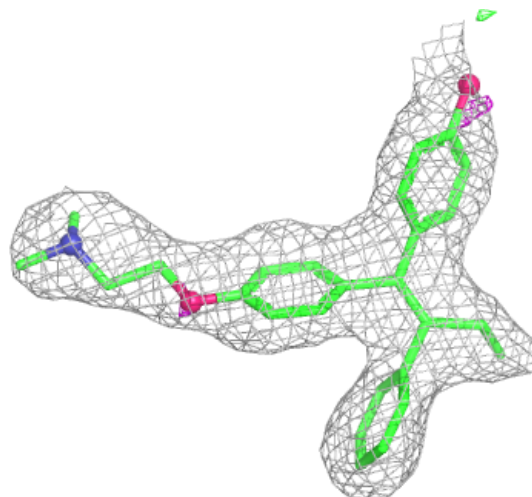
Electron density around OHT E 504:

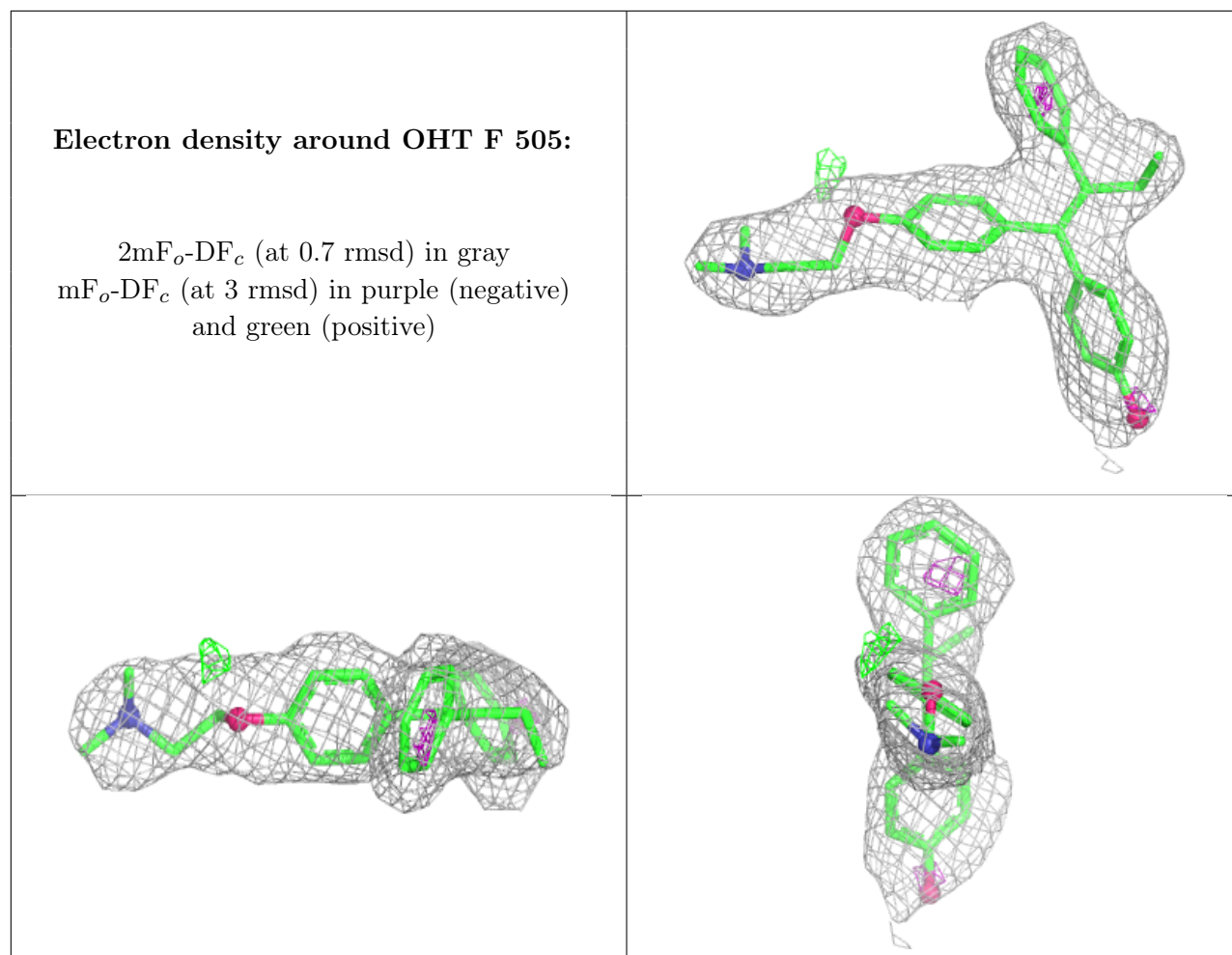
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHT C 502:

$2mF_o-DF_c$ (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.