



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 6SXG / pdb_00006sxg
Title : Crystal Structure of the Voltage-Gated Sodium Channel NavMs in complex with 4-hydroxytamoxifen (2.4 Angstrom resolution)
Authors : Sula, A.; Hollingworth, D.; Wallace, B.A.
Deposited on : 2019-09-25
Resolution : 2.40 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

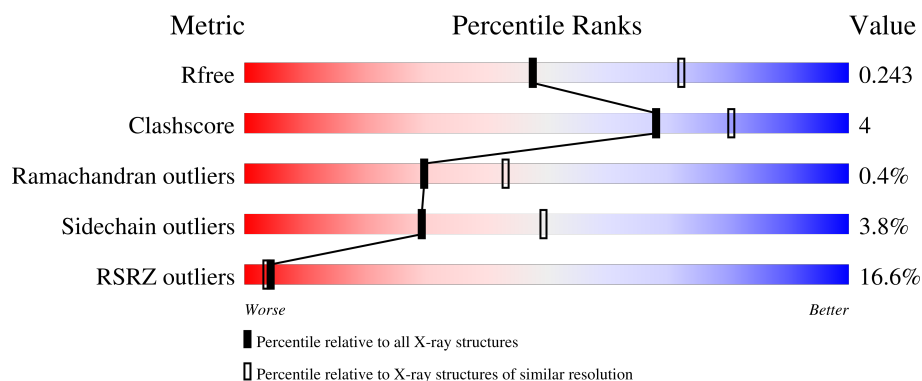
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	277	16% 88% 9% ..

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
2	NA	A	302	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2340 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2148	1399	363	374	12			

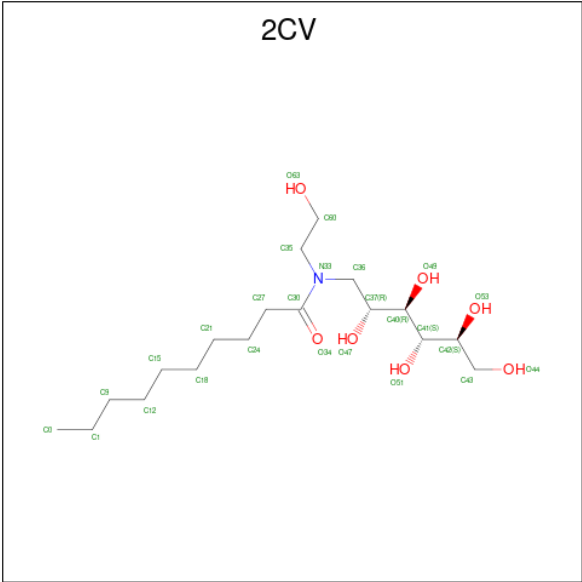
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0L5S6
A	-1	SER	-	expression tag	UNP A0L5S6
A	0	HIS	-	expression tag	UNP A0L5S6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

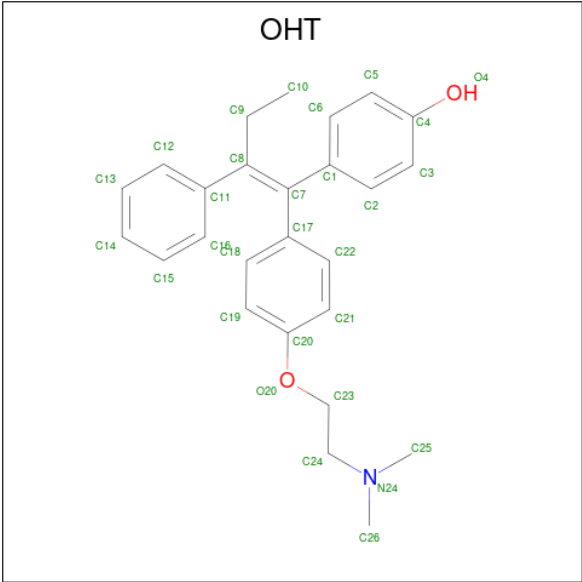
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		

- Molecule 3 is HEGA-10 (CCD ID: 2CV) (formula: C₁₈H₃₇NO₇).



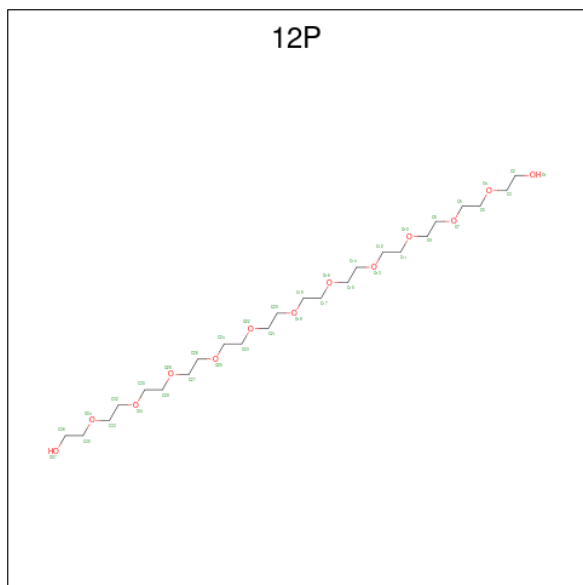
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	A	1	Total	C			0	0
			10	10				
3	A	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 4 is 4-HYDROXYTAMOXIFEN (CCD ID: OHT) (formula: C₂₆H₂₉NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	26	1	2		
4	A	1	Total	C	N	O	0	0
			29	26	1	2		

- Molecule 5 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



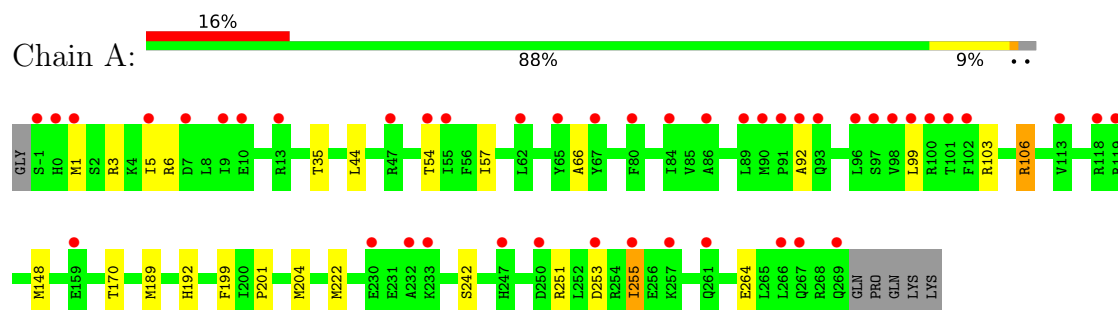
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			26	17	9		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		

i

- Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.91Å 108.91Å 211.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.76 – 2.40 27.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.76-2.40) 99.9 (27.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.221 , 0.261 (Not available) , 0.243	Depositor DCC
R_{free} test set	1265 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2340	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2CV, NA, 12P, 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	0.86	0/2190	1.41	2/2972 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	253	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	199	PHE	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2148	0	2236	13	0
2	A	3	0	0	0	0
3	A	56	0	85	4	0
4	A	58	0	58	4	0
5	A	26	0	33	3	0
6	A	49	0	0	0	0
All	All	2340	0	2412	17	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 4.

All (17) 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:A:192:HIS:HB3	5:A:306:12P:H141	1.36	1.05
1:A:189:MET:CE	3:A:304:2CV:O51	2.46	0.63
4:A:307:OHT:H2	4:A:307:OHT:H92	1.83	0.61
4:A:307:OHT:H92	4:A:307:OHT:C2	2.35	0.57
1:A:201:PRO:HA	1:A:204:MET:HE2	1.86	0.56
1:A:192:HIS:HB3	5:A:306:12P:C14	2.25	0.56
1:A:148:MET:HE1	5:A:306:12P:H232	1.90	0.53
1:A:222:MET:HE3	4:A:305:OHT:H242	1.92	0.51
1:A:251:ARG:O	1:A:255:ILE:HG23	2.11	0.50
1:A:1:MET:HE3	1:A:5:ILE:HD11	1.94	0.49
4:A:305:OHT:H262	4:A:307:OHT:H21	1.94	0.48
1:A:6:ARG:HG3	1:A:66:ALA:HB1	1.97	0.47
1:A:54:THR:HA	1:A:57:ILE:HD12	1.98	0.46
1:A:189:MET:HE1	3:A:304:2CV:O51	2.15	0.45
1:A:189:MET:HE3	3:A:304:2CV:O51	2.15	0.44
3:A:304:2CV:H272	3:A:304:2CV:H361	1.64	0.42
1:A:103:ARG:O	1:A:106:ARG:HB2	2.20	0.41

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	269/277 (97%)	263 (98%)	5 (2%)	1 (0%)	30	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ALA

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	237/242 (98%)	228 (96%)	9 (4%)	29 49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	35	THR
1	A	44	LEU
1	A	99	LEU
1	A	106	ARG
1	A	170	THR
1	A	242	SER
1	A	255	ILE
1	A	264	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	228	GLN
1	A	238	GLN
1	A	243	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](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
4	OHT	A	305	-	31,31,31	0.28	0	41,41,41	0.49	0
3	2CV	A	308	-	9,9,25	0.36	0	8,8,30	0.10	0
3	2CV	A	309	-	19,19,25	0.24	0	21,21,30	0.57	1 (4%)
4	OHT	A	307	-	31,31,31	0.28	0	41,41,41	0.45	0
3	2CV	A	304	-	25,25,25	0.22	0	29,30,30	0.75	1 (3%)
5	12P	A	306	-	25,25,36	0.20	0	24,24,35	0.18	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
4	OHT	A	305	-	-	4/24/24/24	0/3/3/3
3	2CV	A	308	-	-	3/7/7/34	-
3	2CV	A	309	-	-	6/22/22/34	-
4	OHT	A	307	-	-	8/24/24/24	0/3/3/3
3	2CV	A	304	-	-	9/34/34/34	-
5	12P	A	306	-	-	11/23/23/34	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	309	2CV	C37-C36-N33	2.20	115.50	113.10
3	A	304	2CV	C36-C37-C40	-2.12	103.91	109.66

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	2CV	C37-C40-C41-C42
3	A	304	2CV	O49-C40-C41-C42
3	A	309	2CV	N33-C36-C37-C40
3	A	304	2CV	C21-C24-C27-C30
3	A	304	2CV	C37-C40-C41-O51
3	A	304	2CV	O49-C40-C41-O51
4	A	307	OHT	C23-C24-N24-C26
5	A	306	12P	O28-C29-C30-O31
5	A	306	12P	O31-C32-C33-O34
3	A	304	2CV	C18-C21-C24-C27
3	A	304	2CV	O53-C42-C43-O44
3	A	309	2CV	N33-C36-C37-O47
4	A	305	OHT	C23-C24-N24-C25
4	A	307	OHT	C23-C24-N24-C25
3	A	308	2CV	C15-C12-C9-C1
4	A	305	OHT	C24-C23-O20-C20
3	A	309	2CV	O47-C37-C40-O49
4	A	305	OHT	C23-C24-N24-C26
3	A	308	2CV	C0-C1-C9-C12
5	A	306	12P	C15-C14-O13-C12
5	A	306	12P	C32-C33-O34-C35
5	A	306	12P	C33-C32-O31-C30
5	A	306	12P	C24-C23-O22-C21
5	A	306	12P	C18-C17-O16-C15
3	A	309	2CV	C15-C18-C21-C24
5	A	306	12P	C23-C24-O25-C26
4	A	307	OHT	C22-C17-C7-C8
4	A	307	OHT	C18-C17-C7-C8
5	A	306	12P	C21-C20-O19-C18
3	A	309	2CV	N33-C35-C60-O63
5	A	306	12P	C17-C18-O19-C20
4	A	307	OHT	C22-C17-C7-C1
4	A	307	OHT	C18-C17-C7-C1

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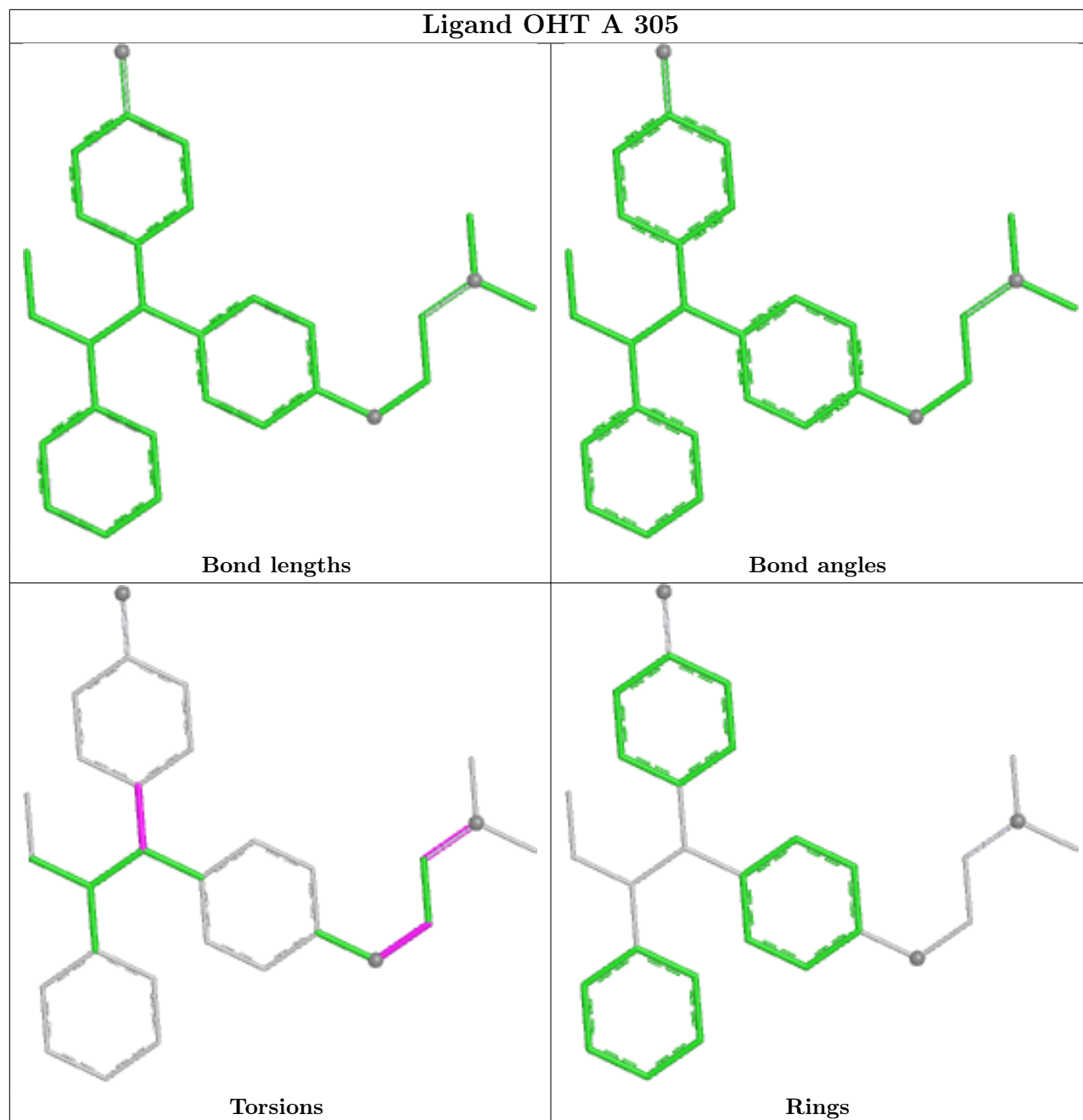
Mol	Chain	Res	Type	Atoms
3	A	304	2CV	C41-C42-C43-O44
4	A	307	OHT	C24-C23-O20-C20
5	A	306	12P	O16-C17-C18-O19
3	A	309	2CV	C36-C37-C40-O49
4	A	307	OHT	C16-C11-C8-C9
4	A	305	OHT	C2-C1-C7-C8
3	A	304	2CV	C15-C18-C21-C24
3	A	308	2CV	C9-C12-C15-C18

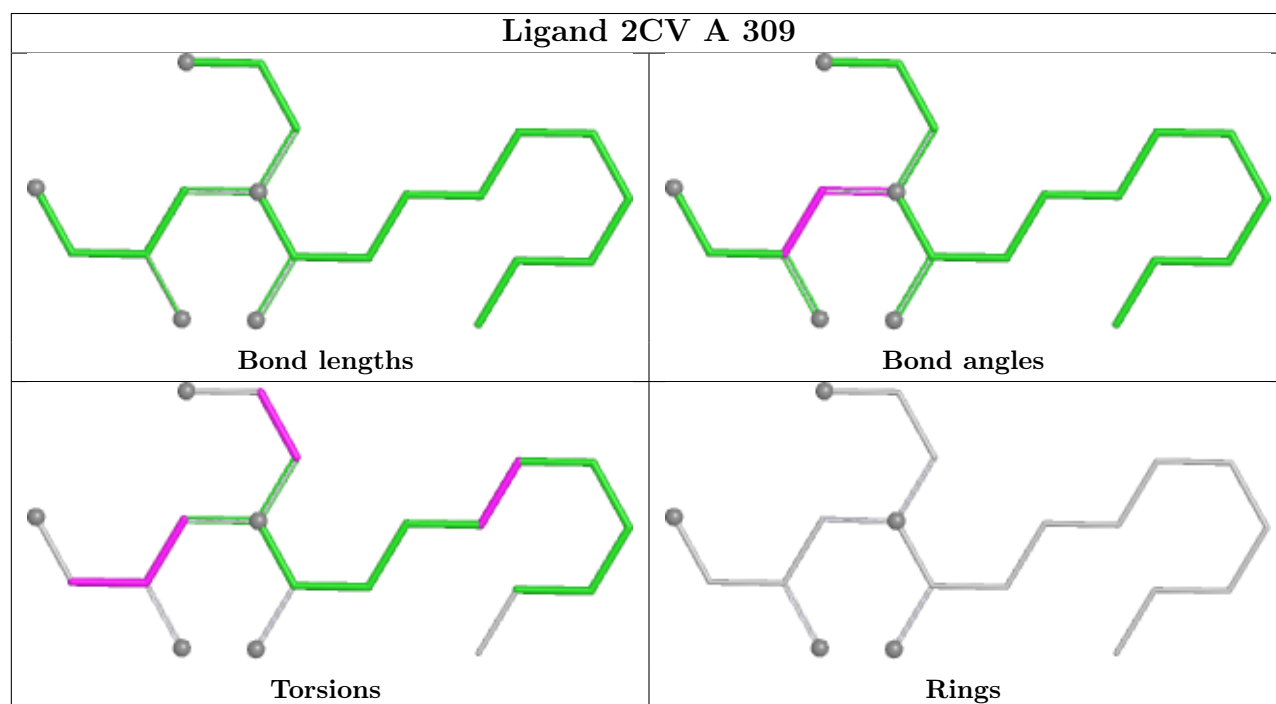
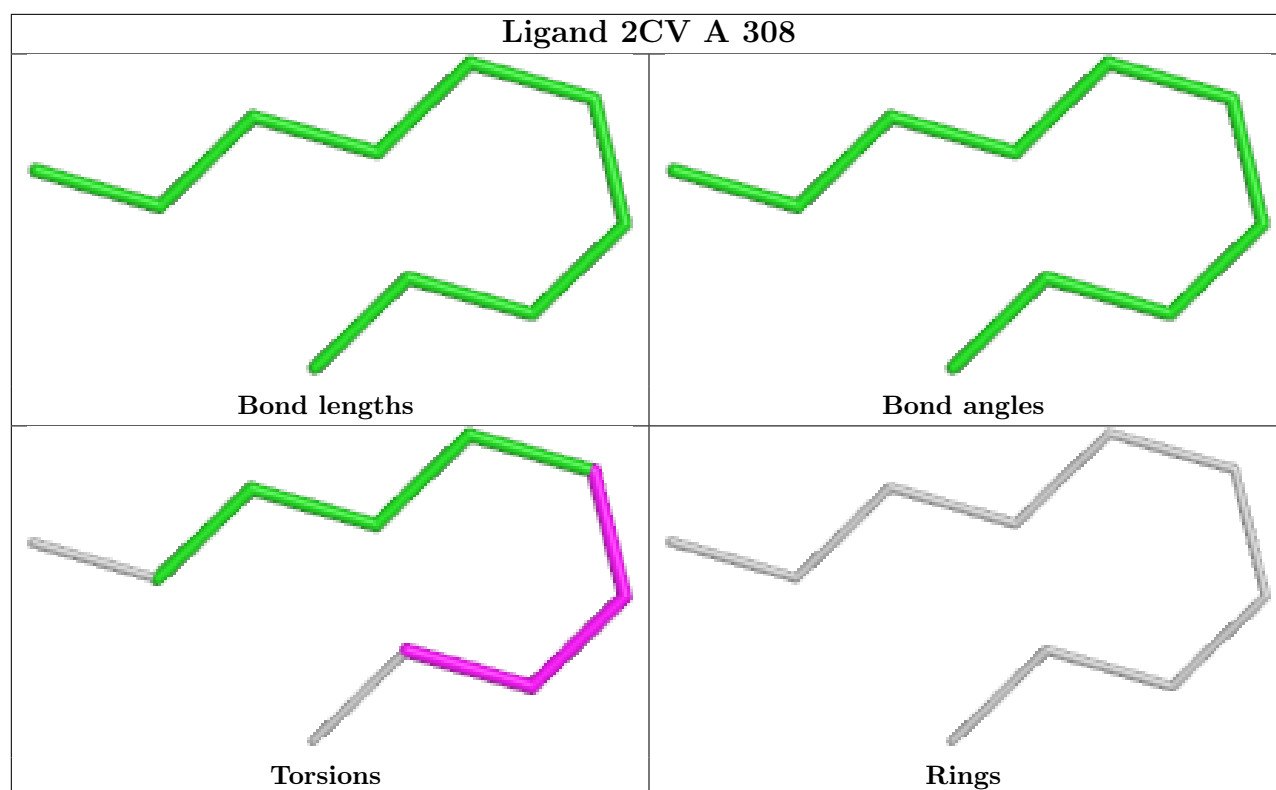
There are no ring outliers.

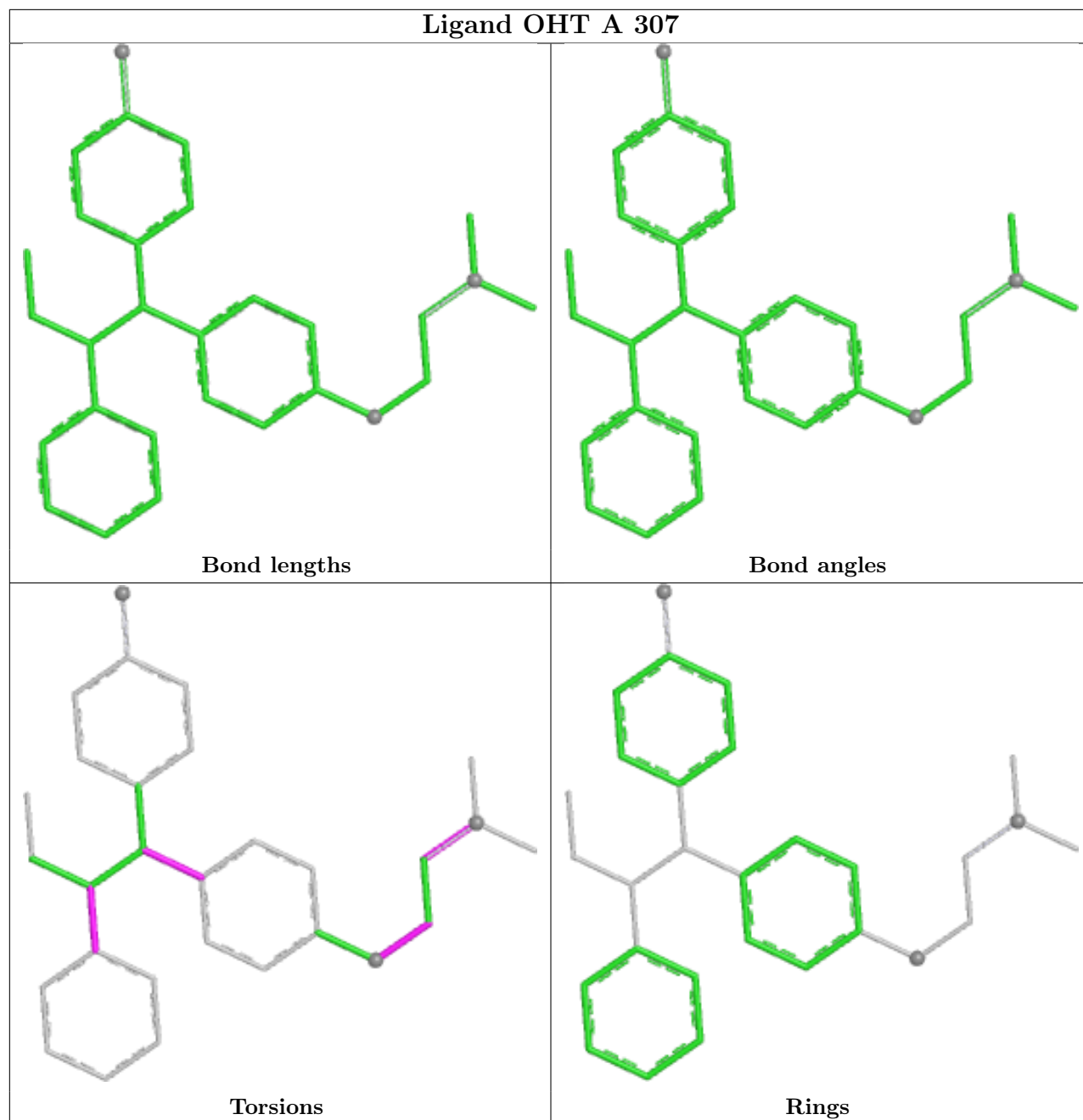
4 monomers are involved in 11 short contacts:

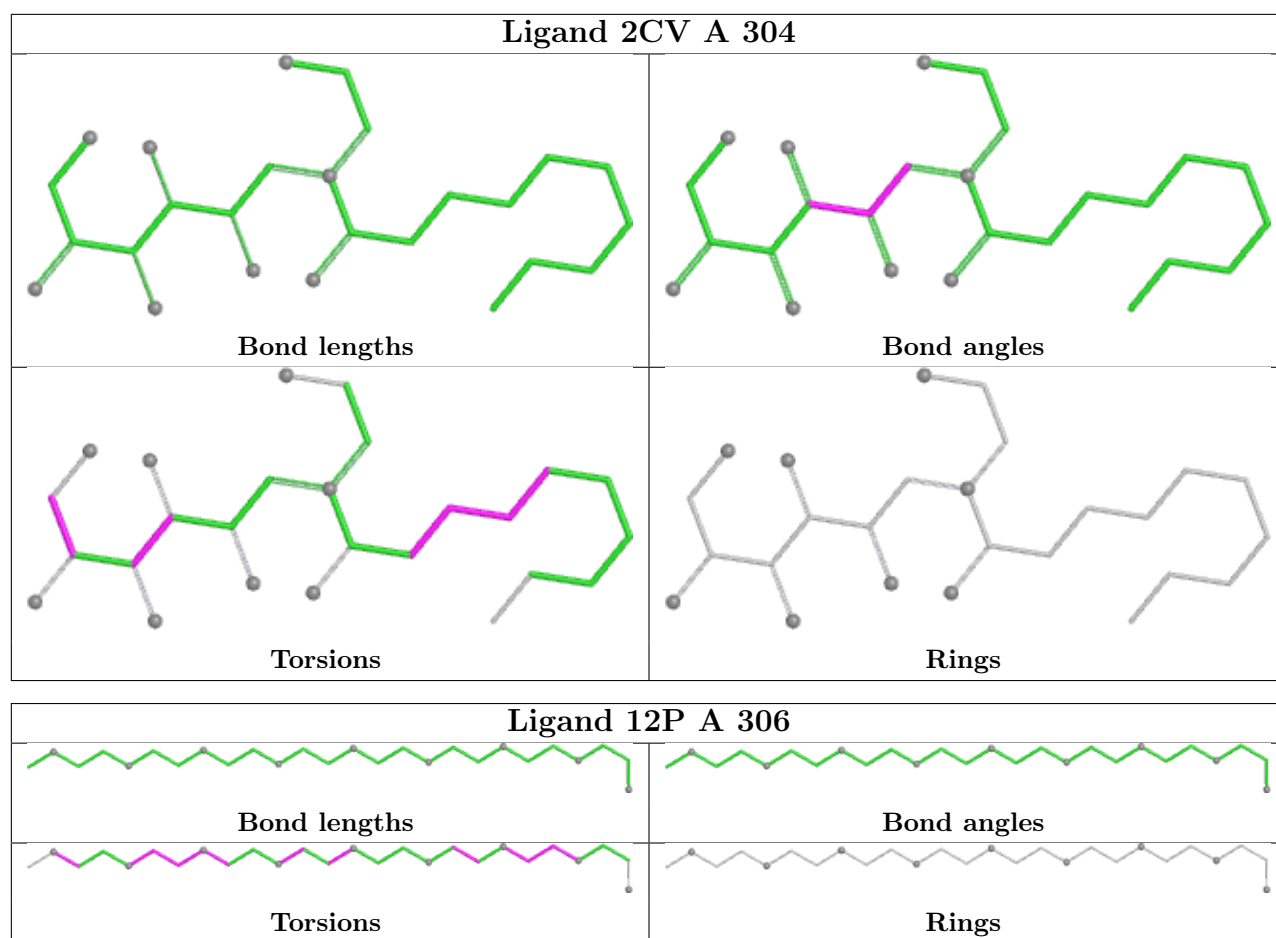
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	OHT	2	0
4	A	307	OHT	3	0
3	A	304	2CV	4	0
5	A	306	12P	3	0

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	271/277 (97%)	0.89	45 (16%) 4 3	37, 83, 161, 188	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	VAL	9.7
1	A	99	LEU	9.2
1	A	96	LEU	5.7
1	A	97	SER	4.9
1	A	89	LEU	4.9
1	A	269	GLN	4.7
1	A	91	PRO	4.2
1	A	253	ASP	4.1
1	A	232	ALA	3.9
1	A	102	PHE	3.9
1	A	0	HIS	3.9
1	A	266	LEU	3.5
1	A	7	ASP	3.4
1	A	100	ARG	3.4
1	A	92	ALA	3.3
1	A	101	THR	3.3
1	A	9	ILE	3.3
1	A	267	GLN	3.1
1	A	255	ILE	3.1
1	A	119	ARG	3.0
1	A	86	ALA	2.9
1	A	54	THR	2.9
1	A	250	ASP	2.9
1	A	159	GLU	2.8
1	A	-1	SER	2.7
1	A	84	ILE	2.6
1	A	257	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLU	2.5
1	A	55	ILE	2.4
1	A	62	LEU	2.4
1	A	233	LYS	2.4
1	A	65	TYR	2.4
1	A	90	MET	2.4
1	A	113	VAL	2.4
1	A	261	GLN	2.3
1	A	67	TYR	2.3
1	A	230	GLU	2.2
1	A	118	ARG	2.2
1	A	93	GLN	2.2
1	A	5	ILE	2.1
1	A	13	ARG	2.1
1	A	80	PHE	2.1
1	A	47	ARG	2.1
1	A	1	MET	2.1
1	A	247	HIS	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.

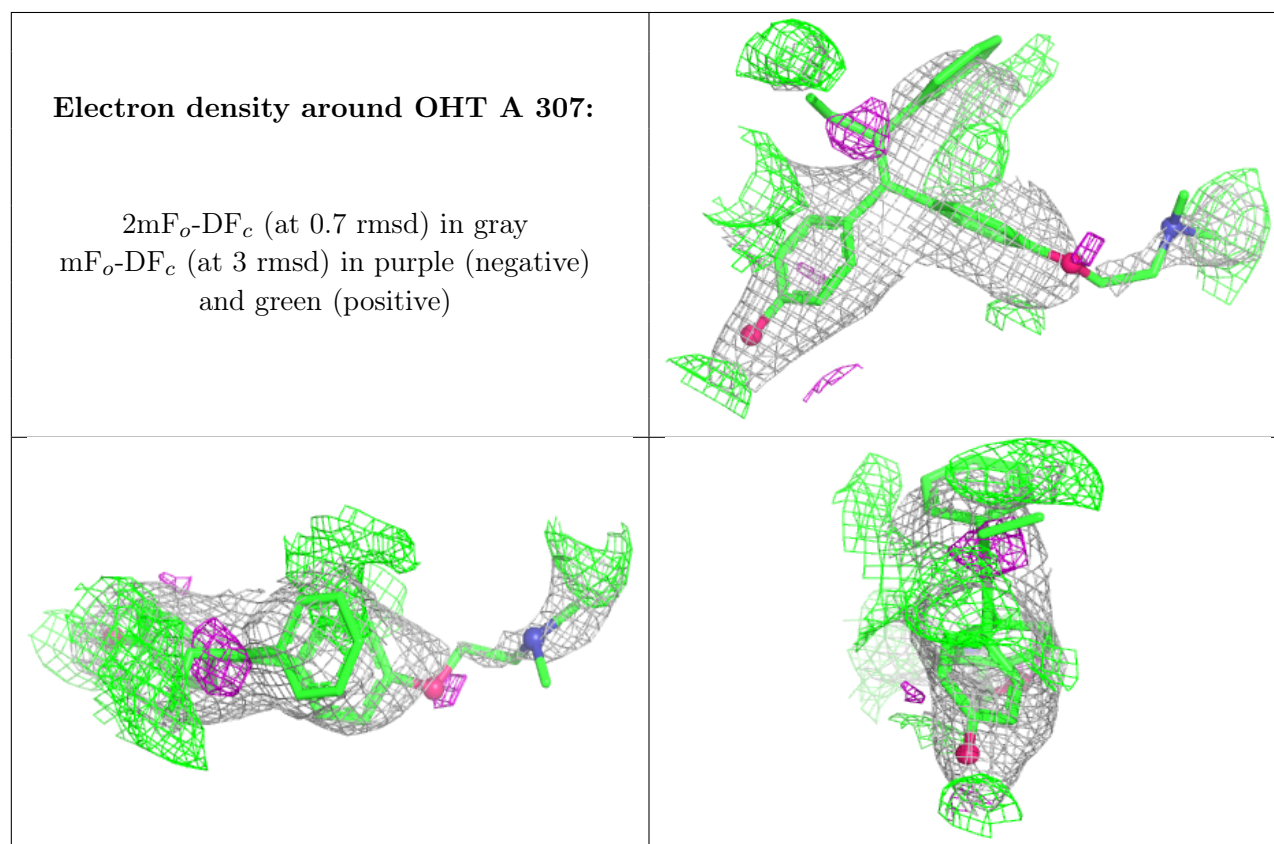
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	302	1/1	0.49	1.08	125,125,125,125	1
4	OHT	A	307	29/29	0.61	0.34	86,120,126,126	0
4	OHT	A	305	29/29	0.73	0.29	81,86,105,106	0
3	2CV	A	309	20/26	0.80	0.27	94,124,134,134	0
3	2CV	A	304	26/26	0.81	0.24	63,85,97,101	0

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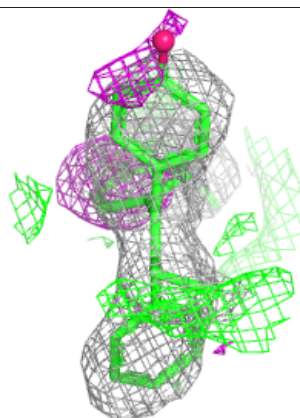
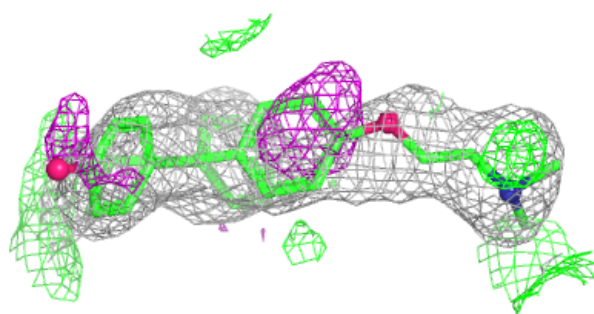
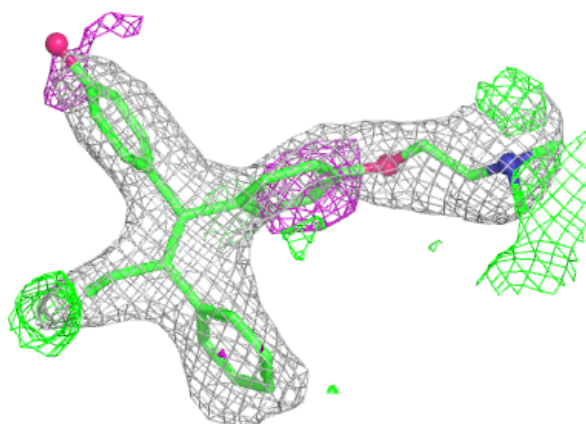
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	12P	A	306	26/37	0.81	0.25	58,96,107,108	0
2	NA	A	303	1/1	0.84	0.38	69,69,69,69	1
3	2CV	A	308	10/26	0.85	0.27	68,76,83,84	0
2	NA	A	301	1/1	0.89	0.39	83,83,83,83	1

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.

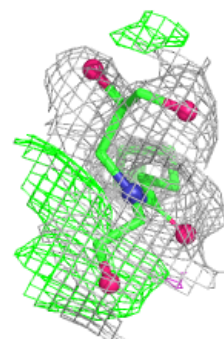
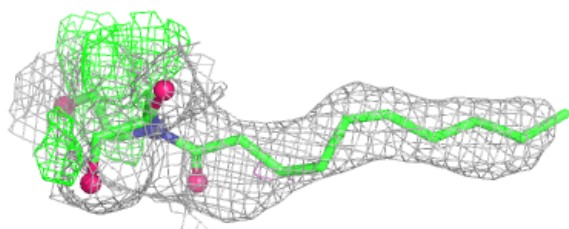
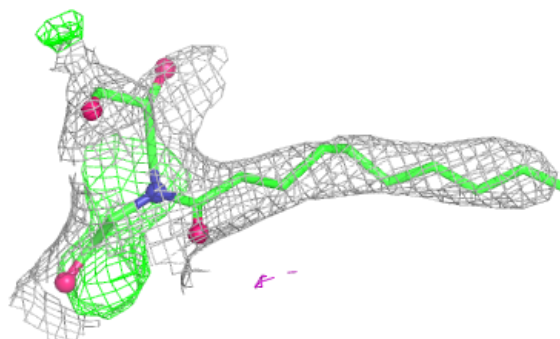


Electron density around OHT A 305:

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

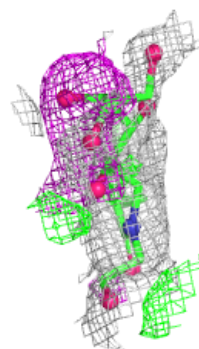
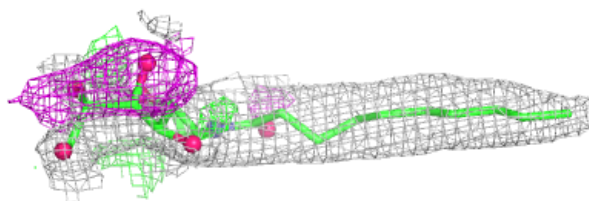
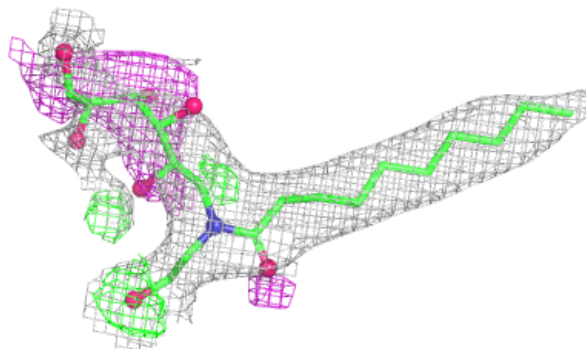
**Electron density around 2CV A 309:**

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

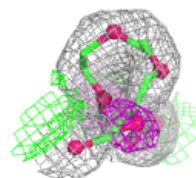
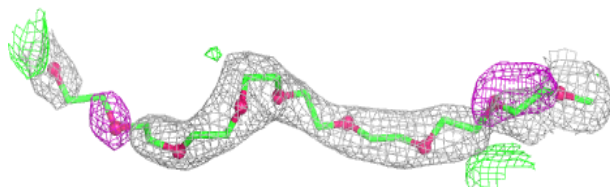
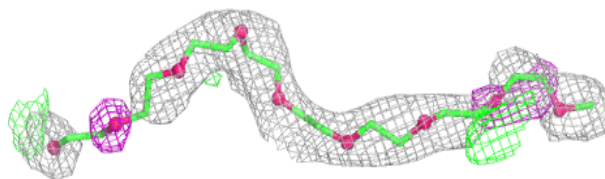


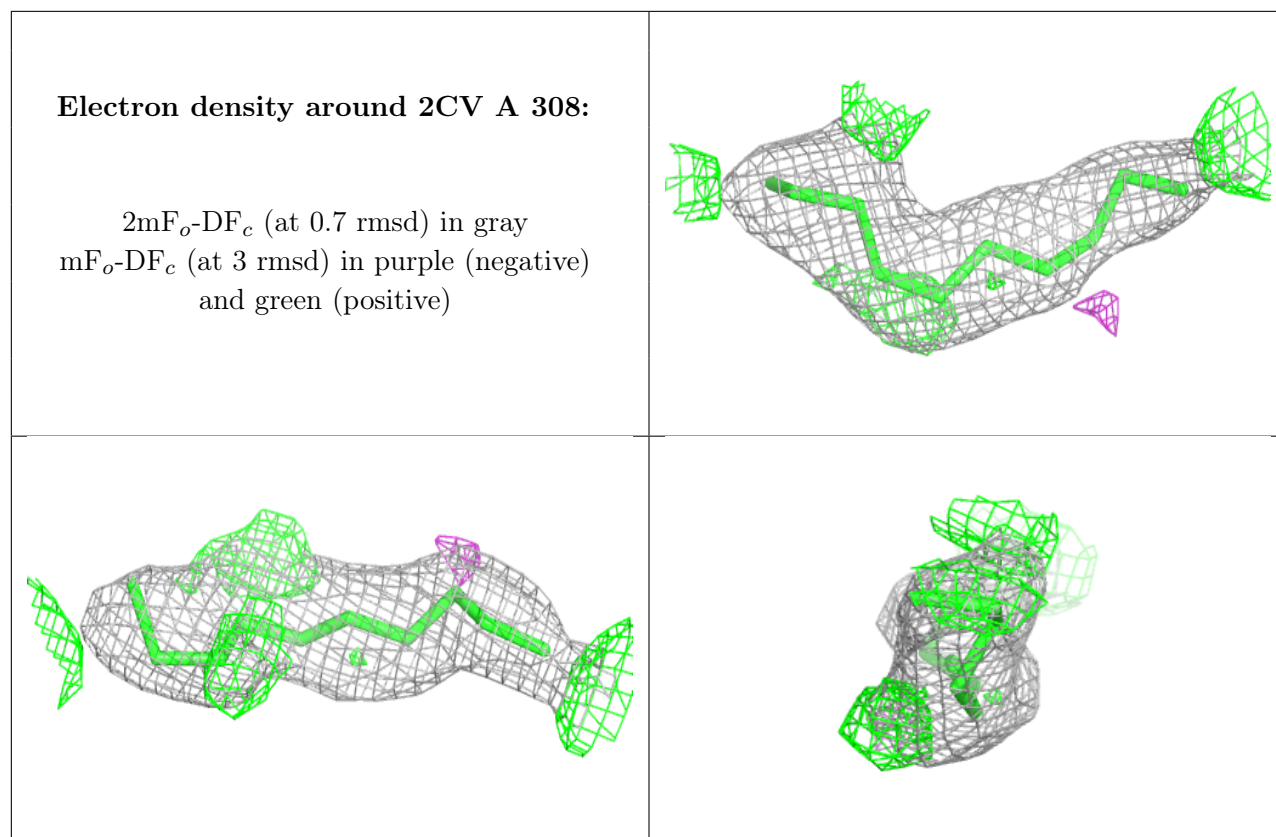
Electron density around 2CV A 304:

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

**Electron density around 12P A 306:**

$2mF_o-DF_c$ (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.