



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:03 PM UTC

PDB ID : 5HK1 / pdb_00005hk1
Title : Human sigma-1 receptor bound to PD144418
Authors : Schmidt, H.R.; Zheng, S.; Gurpinar, E.; Koehl, A.; Manglik, A.; Kruse, A.C.
Deposited on : 2016-01-13
Resolution : 2.51 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

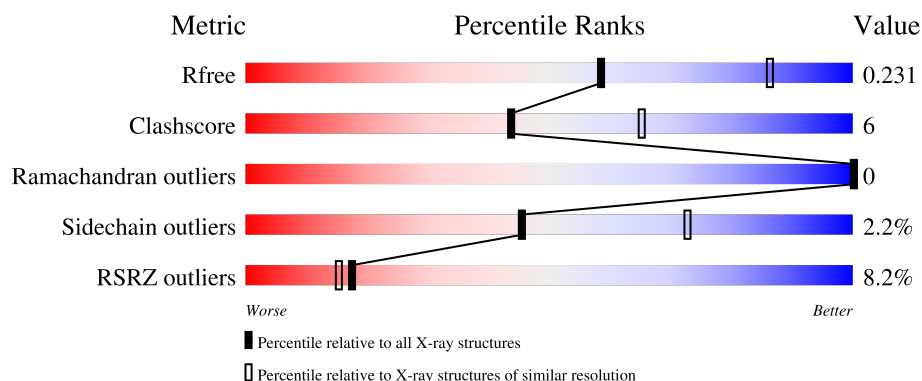
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	227	7% 73% 20% • 7%
1	B	227	10% 85% 11% •
1	C	227	7% 81% 15% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5470 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.

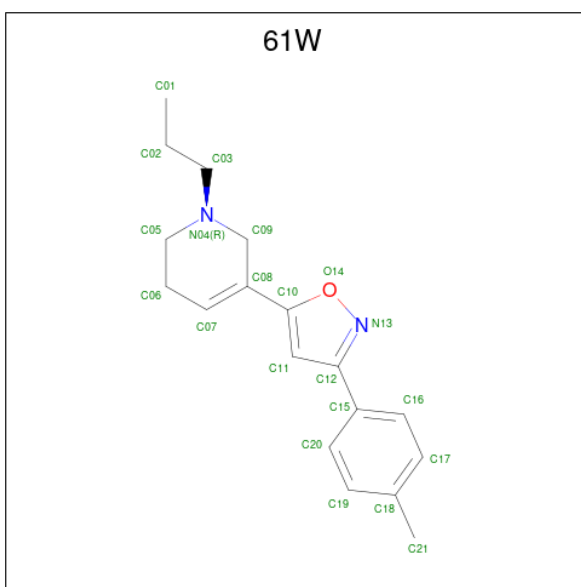
- Molecule 1 is a protein called Sigma non-opioid intracellular receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1668	1086	280	298	4			
1	B	219	Total	C	N	O	S	0	0	0
			1714	1117	292	301	4			
1	C	219	Total	C	N	O	S	0	0	0
			1715	1116	289	306	4			

There are 12 discrepancies between the modelled and reference sequences:

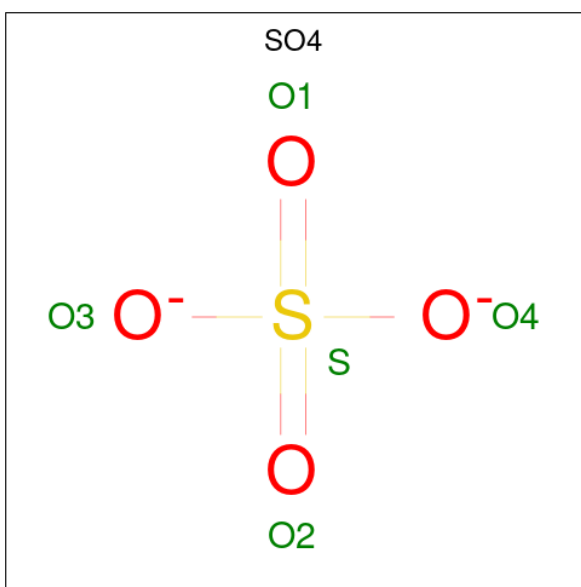
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q99720
A	-2	PRO	-	expression tag	UNP Q99720
A	-1	GLY	-	expression tag	UNP Q99720
A	0	SER	-	expression tag	UNP Q99720
B	-3	GLY	-	expression tag	UNP Q99720
B	-2	PRO	-	expression tag	UNP Q99720
B	-1	GLY	-	expression tag	UNP Q99720
B	0	SER	-	expression tag	UNP Q99720
C	-3	GLY	-	expression tag	UNP Q99720
C	-2	PRO	-	expression tag	UNP Q99720
C	-1	GLY	-	expression tag	UNP Q99720
C	0	SER	-	expression tag	UNP Q99720

- Molecule 2 is 3-(4-methylphenyl)-5-(1-propyl-3,6-dihydro-2H-pyridin-5-yl)-1,2-oxazole (CCD ID: 61W) (formula: C₁₈H₂₂N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	18	2	1		
2	B	1	Total	C	N	O	0	0
			21	18	2	1		
2	C	1	Total	C	N	O	0	0
			21	18	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



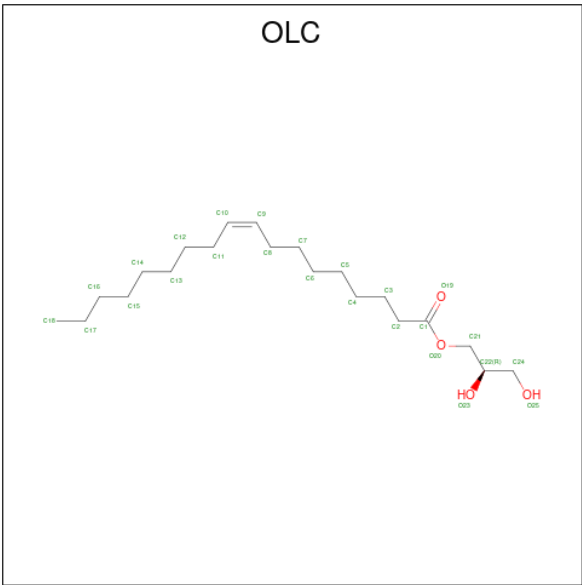
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		
4	A	1	Total	C	O	0	0
			12	8	4		
4	C	1	Total	C	O	0	0
			11	7	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			12	8	4		
4	C	1	Total	C	O	0	0
			12	8	4		
4	C	1	Total	C	O	0	0
			10	6	4		

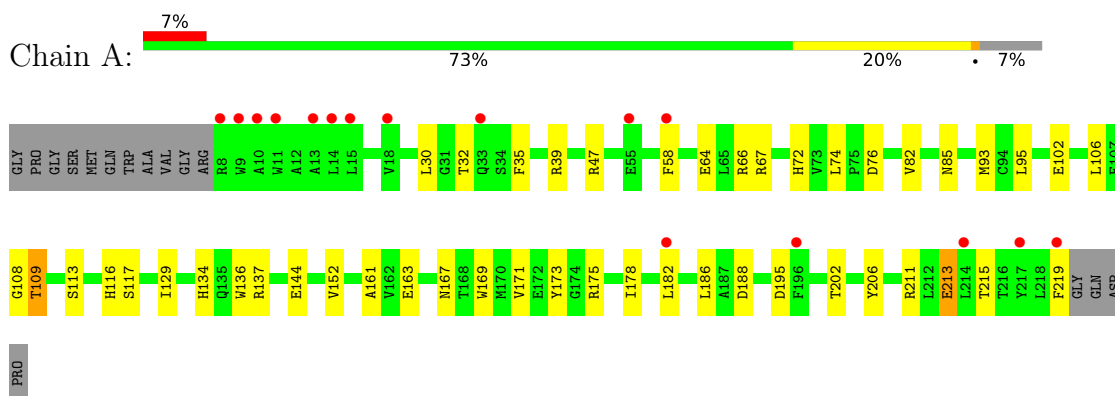
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	B	35	Total	O	0	0
			35	35		
5	C	67	Total	O	0	0
			67	67		

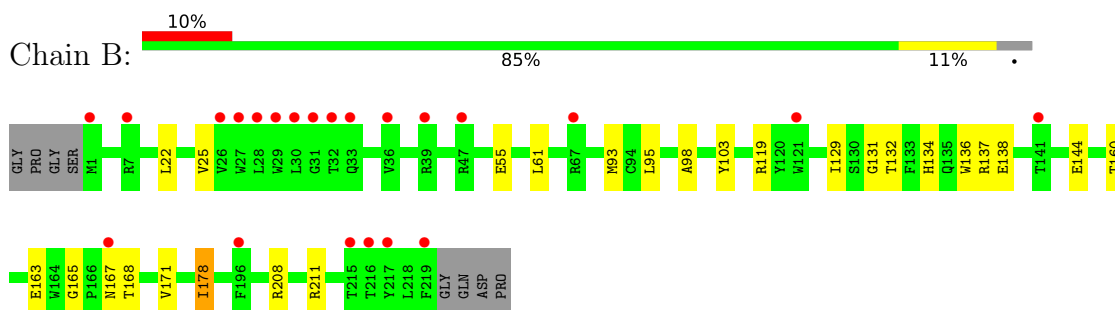
3 Residue-property plots [i](#)

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.

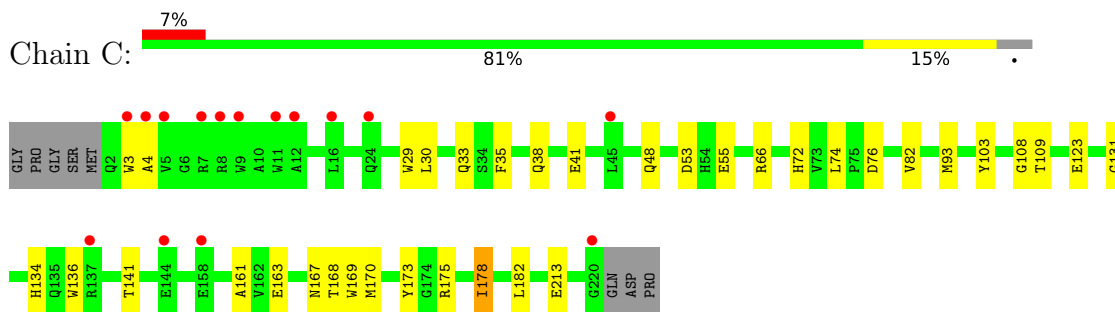
- Molecule 1: Sigma non-opioid intracellular receptor 1



- Molecule 1: Sigma non-opioid intracellular receptor 1



- Molecule 1: Sigma non-opioid intracellular receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 126.06Å 109.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.51 40.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.51) 98.8 (40.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.233 0.200 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5470	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: SO4, OLC, 61W

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	0.37	1/1716 (0.1%)	0.72	1/2343 (0.0%)
1	B	0.28	0/1765	0.67	1/2413 (0.0%)
1	C	0.27	0/1767	0.68	1/2416 (0.0%)
All	All	0.31	1/5248 (0.0%)	0.69	3/7172 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SER	C-N	-6.76	1.23	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ILE	CB-CA-C	-5.42	108.61	114.35
1	B	178	ILE	CB-CA-C	-5.26	108.77	114.35
1	C	178	ILE	CB-CA-C	-5.02	109.03	114.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	HIS	Mainchain

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	1668	0	1616	27	0
1	B	1714	0	1656	17	0
1	C	1715	0	1635	23	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
3	A	35	0	0	2	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
4	A	25	0	28	1	0
4	C	55	0	55	3	0
5	A	58	0	0	2	0
5	B	35	0	0	0	0
5	C	67	0	0	4	0
All	All	5470	0	4990	63	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 6.

All (63) 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:C:66:ARG:NH1	1:C:76:ASP:OD1	2.01	0.91
1:A:66:ARG:NH1	1:A:76:ASP:OD1	2.08	0.86
1:B:55:GLU:OE2	1:C:141:THR:OG1	2.08	0.71
1:A:195:ASP:OD1	1:B:119:ARG:NH1	2.26	0.67
1:A:137:ARG:NH1	1:A:144:GLU:OE2	2.28	0.66
1:A:167:ASN:ND2	5:A:401:HOH:O	2.28	0.66
1:A:93:MET:HE1	1:A:95:LEU:HB2	1.81	0.63
1:A:47:ARG:NH2	5:A:403:HOH:O	2.33	0.62
1:C:29:TRP:HE3	1:C:30:LEU:HD12	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE1	1:A:67:ARG:NH1	2.36	0.57
1:C:123:GLU:HB2	4:C:308:OLC:H24A	1.87	0.56
1:A:72:HIS:ND1	1:A:213:GLU:OE2	2.25	0.56
1:A:134:HIS:HB2	1:A:163:GLU:HB3	1.89	0.55
1:B:134:HIS:HB2	1:B:163:GLU:HB3	1.88	0.55
1:C:141:THR:O	5:C:401:HOH:O	2.18	0.55
1:C:103:TYR:HD2	1:C:178:ILE:HD12	1.71	0.55
1:C:33:GLN:NE2	4:C:307:OLC:O23	2.40	0.55
1:B:129:ILE:HD11	1:B:171:VAL:HG13	1.89	0.54
1:A:66:ARG:NH2	1:A:74:LEU:O	2.42	0.52
1:B:137:ARG:NH1	1:B:144:GLU:OE2	2.42	0.52
1:C:72:HIS:ND1	1:C:213:GLU:OE1	2.34	0.52
1:A:39:ARG:HD3	3:A:303:SO4:O1	2.09	0.51
1:A:30:LEU:HD22	4:A:310:OLC:H21	1.92	0.51
1:C:134:HIS:HB2	1:C:163:GLU:HB3	1.93	0.51
1:B:22:LEU:HA	1:B:25:VAL:HG22	1.94	0.50
1:C:3:TRP:HE3	1:C:4:ALA:H	1.60	0.50
1:C:167:ASN:OD1	5:C:402:HOH:O	2.19	0.50
1:A:215:THR:O	1:A:219:PHE:N	2.44	0.49
1:B:103:TYR:HD2	1:B:178:ILE:HD12	1.77	0.49
1:A:129:ILE:HD11	1:A:171:VAL:HG23	1.95	0.49
1:B:167:ASN:ND2	5:C:401:HOH:O	2.41	0.49
1:A:211:ARG:NH2	3:A:302:SO4:O2	2.44	0.48
1:A:136:TRP:HB3	1:A:161:ALA:HB3	1.94	0.48
1:B:208:ARG:HG2	1:B:211:ARG:NH1	2.29	0.48
1:B:132:THR:H	1:B:168:THR:HG22	1.79	0.48
1:B:119:ARG:NH2	1:B:138:GLU:OE1	2.47	0.47
1:B:131:GLY:HA3	1:B:168:THR:HG22	1.97	0.47
1:C:53:ASP:OD2	1:C:55:GLU:HB2	2.15	0.47
1:B:165:GLY:O	1:B:168:THR:HG23	2.15	0.47
1:C:66:ARG:NH2	1:C:74:LEU:O	2.48	0.46
1:A:182:LEU:HD11	1:A:206:TYR:CD2	2.51	0.46
1:C:35:PHE:CE1	1:C:175:ARG:HD2	2.50	0.46
1:A:102:GLU:OE2	1:A:173:TYR:OH	2.31	0.45
1:C:131:GLY:HA3	1:C:168:THR:HA	1.99	0.45
1:A:108:GLY:HA3	1:A:169:TRP:CE3	2.53	0.44
1:A:39:ARG:HH21	1:A:175:ARG:NH2	2.16	0.44
1:C:136:TRP:HB3	1:C:161:ALA:HB3	2.00	0.44
1:A:35:PHE:CD1	1:A:175:ARG:HD2	2.53	0.43
1:A:136:TRP:CH2	1:C:109:THR:HA	2.53	0.43
1:C:48:GLN:NE2	5:C:410:HOH:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:THR:H	1:B:168:THR:CG2	2.32	0.43
1:C:170:MET:HE2	1:C:170:MET:HB3	1.86	0.42
1:C:38:GLN:HB2	1:C:41:GLU:HB2	2.02	0.42
1:A:109:THR:HA	1:B:136:TRP:CH2	2.55	0.41
1:A:186:LEU:HD21	1:A:202:THR:HG21	2.02	0.41
1:B:137:ARG:HA	1:B:160:THR:HG22	2.01	0.41
1:A:64:GLU:OE2	1:A:67:ARG:HD3	2.19	0.41
1:C:108:GLY:HA3	1:C:169:TRP:CE3	2.56	0.41
1:A:58:PHE:CD1	1:A:106:LEU:HD13	2.55	0.41
1:C:173:TYR:OH	1:C:175:ARG:HD3	2.21	0.41
1:A:85:ASN:O	1:A:188:ASP:HB2	2.21	0.41
1:B:95:LEU:HD21	1:B:98:ALA:HB2	2.04	0.40
1:C:29:TRP:HH2	4:C:307:OLC:H21A	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/227 (92%)	209 (100%)	1 (0%)	0	100	100
1	B	217/227 (96%)	213 (98%)	4 (2%)	0	100	100
1	C	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
All	All	644/681 (95%)	636 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	168/182 (92%)	162 (96%)	6 (4%)	31	58
1	B	169/182 (93%)	167 (99%)	2 (1%)	63	83
1	C	169/182 (93%)	166 (98%)	3 (2%)	51	77
All	All	506/546 (93%)	495 (98%)	11 (2%)	45	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	82	VAL
1	A	109	THR
1	A	113	SER
1	A	152	VAL
1	A	213	GLU
1	B	61	LEU
1	B	93	MET
1	C	82	VAL
1	C	93	MET
1	C	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	B	24	GLN
1	B	85	ASN
1	C	24	GLN
1	C	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

24 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	$\# Z > 2$
4	OLC	C	306	-	9,9,24	1.10	1 (11%)	10,10,25	1.13	1 (10%)
3	SO4	A	306	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.06	0
2	61W	B	301	-	22,23,23	2.36	9 (40%)	26,31,31	4.43	15 (57%)
3	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.07	0
4	OLC	C	309	-	9,9,24	1.07	1 (11%)	10,10,25	1.18	1 (10%)
3	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.08	0
2	61W	A	301	-	22,23,23	2.32	9 (40%)	26,31,31	4.39	15 (57%)
3	SO4	B	305	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	303	-	4,4,4	0.23	0	6,6,6	0.07	0
2	61W	C	301	-	22,23,23	2.15	7 (31%)	26,31,31	4.32	16 (61%)
3	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	307	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.07	0
4	OLC	C	307	-	11,11,24	0.99	1 (9%)	12,12,25	0.98	1 (8%)
3	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.07	0
4	OLC	C	305	-	10,10,24	1.04	1 (10%)	11,11,25	1.15	1 (9%)
3	SO4	A	308	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.12	0
4	OLC	A	310	-	11,11,24	0.98	1 (9%)	12,12,25	1.03	1 (8%)
4	OLC	C	308	-	11,11,24	1.00	1 (9%)	12,12,25	1.01	1 (8%)
4	OLC	A	309	-	12,12,24	0.94	1 (8%)	13,13,25	1.00	1 (7%)
3	SO4	C	304	-	4,4,4	0.24	0	6,6,6	0.21	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	OLC	C	306	-	-	6/9/9/24	-
4	OLC	C	305	-	-	4/10/10/24	-
4	OLC	C	308	-	-	6/11/11/24	-
4	OLC	A	310	-	-	6/11/11/24	-
2	61W	C	301	-	-	2/8/21/21	0/3/3/3
4	OLC	A	309	-	-	1/12/12/24	-
4	OLC	C	307	-	-	6/11/11/24	-
4	OLC	C	309	-	-	4/9/9/24	-
2	61W	B	301	-	-	1/8/21/21	0/3/3/3
2	61W	A	301	-	-	1/8/21/21	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	61W	C15-C12	4.80	1.54	1.47
2	A	301	61W	C11-C12	4.57	1.48	1.40
2	B	301	61W	C11-C12	4.54	1.48	1.40
2	A	301	61W	C15-C12	4.40	1.54	1.47
2	C	301	61W	C11-C12	4.33	1.47	1.40
2	C	301	61W	C15-C12	3.70	1.53	1.47
2	C	301	61W	O14-N13	-3.62	1.35	1.42
2	B	301	61W	C12-N13	3.59	1.37	1.31
2	A	301	61W	O14-N13	-3.54	1.35	1.42
2	B	301	61W	O14-N13	-3.52	1.36	1.42
2	A	301	61W	C12-N13	3.48	1.36	1.31
2	A	301	61W	C07-C08	3.34	1.43	1.34
2	B	301	61W	C07-C08	3.33	1.43	1.34
2	C	301	61W	C07-C08	3.29	1.43	1.34
2	C	301	61W	C12-N13	3.22	1.36	1.31
2	B	301	61W	C11-C10	2.96	1.40	1.35
2	A	301	61W	C11-C10	2.94	1.40	1.35
2	C	301	61W	C11-C10	2.75	1.40	1.35
4	C	306	OLC	O20-C1	2.67	1.41	1.33
4	C	308	OLC	O20-C1	2.64	1.41	1.33
4	C	305	OLC	O20-C1	2.63	1.41	1.33
4	C	307	OLC	O20-C1	2.63	1.41	1.33
4	A	310	OLC	O20-C1	2.63	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	309	OLC	O20-C1	2.63	1.41	1.33
2	B	301	61W	O14-C10	2.62	1.40	1.35
4	C	309	OLC	O20-C1	2.59	1.40	1.33
2	A	301	61W	O14-C10	2.57	1.40	1.35
2	A	301	61W	C09-N04	2.55	1.48	1.46
2	B	301	61W	C09-N04	2.48	1.48	1.46
2	C	301	61W	O14-C10	2.47	1.40	1.35
2	A	301	61W	C17-C16	2.01	1.42	1.38
2	B	301	61W	C17-C16	2.00	1.42	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	61W	C10-C11-C12	11.79	110.34	105.06
2	A	301	61W	C10-C11-C12	11.61	110.26	105.06
2	C	301	61W	C10-C11-C12	11.45	110.19	105.06
2	A	301	61W	O14-C10-C11	-10.32	103.05	109.86
2	C	301	61W	O14-C10-C11	-10.30	103.06	109.86
2	B	301	61W	O14-C10-C11	-10.27	103.08	109.86
2	B	301	61W	C11-C12-N13	-7.80	103.99	111.17
2	A	301	61W	C11-C12-N13	-7.69	104.10	111.17
2	C	301	61W	C11-C12-N13	-7.48	104.29	111.17
2	B	301	61W	O14-N13-C12	5.72	110.22	105.65
2	A	301	61W	O14-N13-C12	5.57	110.10	105.65
2	C	301	61W	O14-N13-C12	5.40	109.96	105.65
2	A	301	61W	C05-C06-C07	5.03	116.54	111.51
2	B	301	61W	C20-C15-C16	-4.93	112.29	118.57
2	B	301	61W	C05-C06-C07	4.91	116.42	111.51
2	C	301	61W	C05-C06-C07	4.87	116.38	111.51
2	A	301	61W	C20-C15-C16	-4.82	112.44	118.57
2	B	301	61W	C03-N04-C05	-4.77	98.52	111.24
2	A	301	61W	C03-N04-C05	-4.73	98.64	111.24
2	C	301	61W	C03-N04-C05	-4.71	98.68	111.24
2	C	301	61W	C15-C12-N13	4.59	127.87	120.04
2	C	301	61W	C20-C15-C16	-4.58	112.74	118.57
2	B	301	61W	C15-C12-N13	4.53	127.76	120.04
2	A	301	61W	C15-C12-N13	4.50	127.72	120.04
2	C	301	61W	C10-O14-N13	3.71	112.50	108.38
2	A	301	61W	C10-O14-N13	3.70	112.49	108.38
2	B	301	61W	C10-O14-N13	3.59	112.37	108.38
2	A	301	61W	C16-C15-C12	3.55	124.85	120.87
2	B	301	61W	C16-C15-C12	3.52	124.81	120.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	61W	C09-C08-C10	3.25	125.38	117.34
2	C	301	61W	C09-C08-C10	3.19	125.23	117.34
2	B	301	61W	C19-C20-C15	3.17	124.18	120.80
2	A	301	61W	C09-C08-C10	3.06	124.92	117.34
2	A	301	61W	C19-C20-C15	3.04	124.05	120.80
4	C	309	OLC	O20-C1-C2	3.00	120.26	111.15
2	B	301	61W	C08-C09-N04	2.95	115.38	110.96
2	C	301	61W	C16-C15-C12	2.94	124.16	120.87
2	A	301	61W	C08-C09-N04	2.93	115.35	110.96
4	C	306	OLC	O20-C1-C2	2.93	120.03	111.15
2	C	301	61W	C08-C09-N04	2.89	115.29	110.96
4	C	305	OLC	O20-C1-C2	2.88	120.61	111.83
2	C	301	61W	C19-C20-C15	2.82	123.81	120.80
2	A	301	61W	C17-C16-C15	2.81	123.81	120.80
2	B	301	61W	C17-C16-C15	2.81	123.80	120.80
4	A	309	OLC	O20-C1-C2	2.81	120.39	111.83
2	C	301	61W	C17-C16-C15	2.77	123.76	120.80
4	A	310	OLC	O20-C1-C2	2.77	120.27	111.83
4	C	308	OLC	O20-C1-C2	2.65	119.91	111.83
4	C	307	OLC	O20-C1-C2	2.64	119.89	111.83
2	B	301	61W	C19-C18-C17	-2.24	113.76	118.11
2	A	301	61W	C19-C18-C17	-2.19	113.87	118.11
2	C	301	61W	C19-C18-C17	-2.06	114.12	118.11
2	C	301	61W	C02-C03-N04	-2.01	107.36	114.44

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	61W	C07-C08-C10-C11
4	A	310	OLC	O20-C21-C22-O23
4	C	305	OLC	C21-C22-C24-O25
4	C	307	OLC	C21-C22-C24-O25
4	C	308	OLC	C21-C22-C24-O25
4	C	309	OLC	C21-C22-C24-O25
4	C	309	OLC	O20-C21-C22-O23
4	C	308	OLC	O19-C1-O20-C21
4	C	308	OLC	C2-C1-O20-C21
4	C	305	OLC	C2-C1-O20-C21
4	A	310	OLC	O20-C21-C22-C24
4	C	307	OLC	O20-C21-C22-C24
4	C	305	OLC	O23-C22-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	305	OLC	O19-C1-O20-C21
4	C	306	OLC	C2-C1-O20-C21
4	C	307	OLC	O20-C21-C22-O23
4	A	310	OLC	C2-C1-O20-C21
4	C	307	OLC	C2-C1-O20-C21
4	C	306	OLC	C21-C22-C24-O25
4	A	310	OLC	O19-C1-O20-C21
4	C	306	OLC	O19-C1-O20-C21
4	C	308	OLC	O23-C22-C24-O25
4	C	309	OLC	O23-C22-C24-O25
4	C	307	OLC	O19-C1-O20-C21
4	C	309	OLC	O20-C21-C22-C24
4	C	307	OLC	O23-C22-C24-O25
2	C	301	61W	C02-C03-N04-C05
4	C	306	OLC	O20-C21-C22-C24
4	C	306	OLC	O23-C22-C24-O25
4	C	306	OLC	O20-C21-C22-O23
2	C	301	61W	C02-C03-N04-C09
4	C	308	OLC	O20-C1-C2-C3
4	A	310	OLC	C1-C2-C3-C4
2	B	301	61W	C02-C03-N04-C05
4	C	308	OLC	O19-C1-C2-C3
4	A	309	OLC	O23-C22-C24-O25
4	A	310	OLC	O20-C1-C2-C3

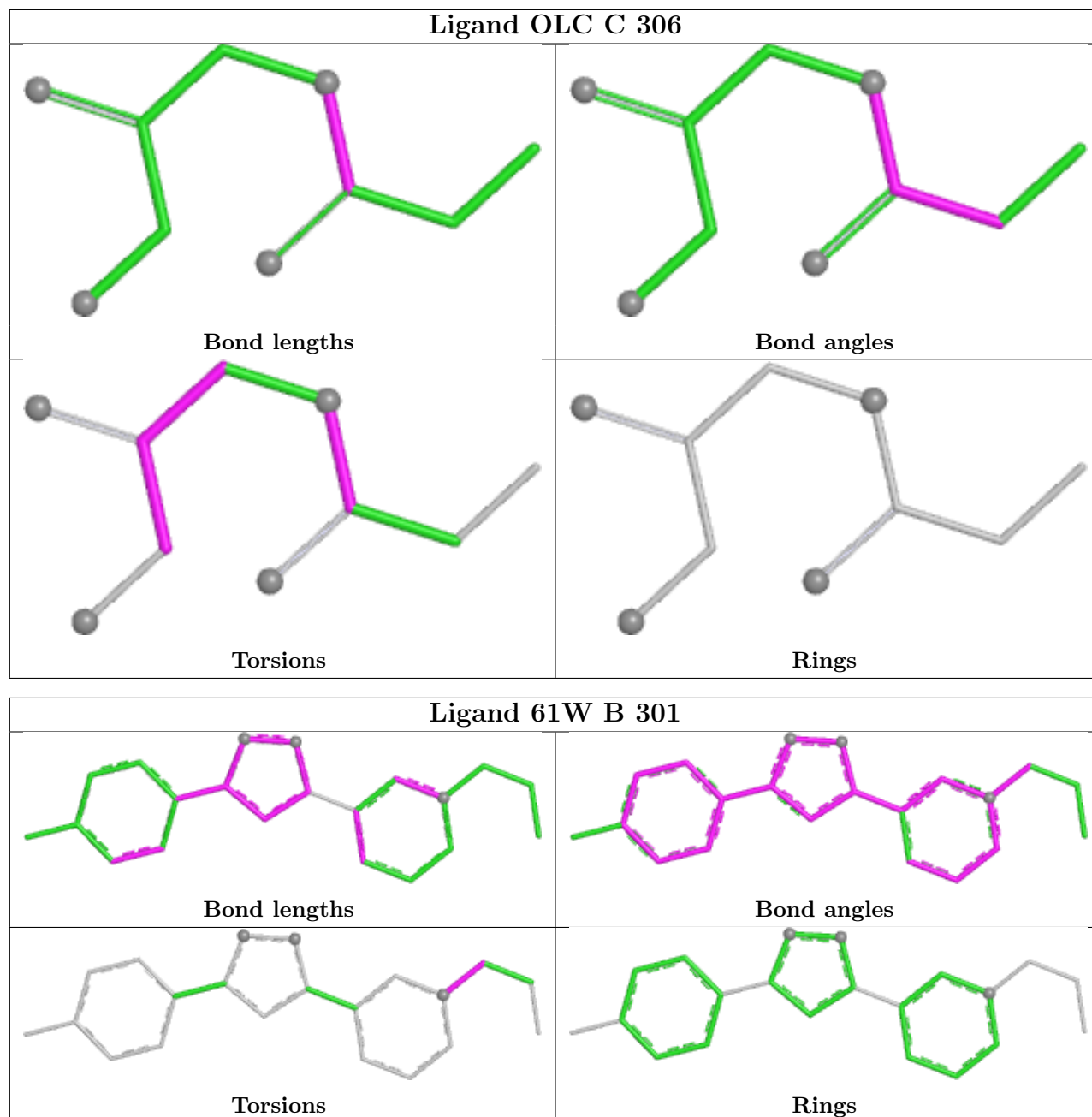
There are no ring outliers.

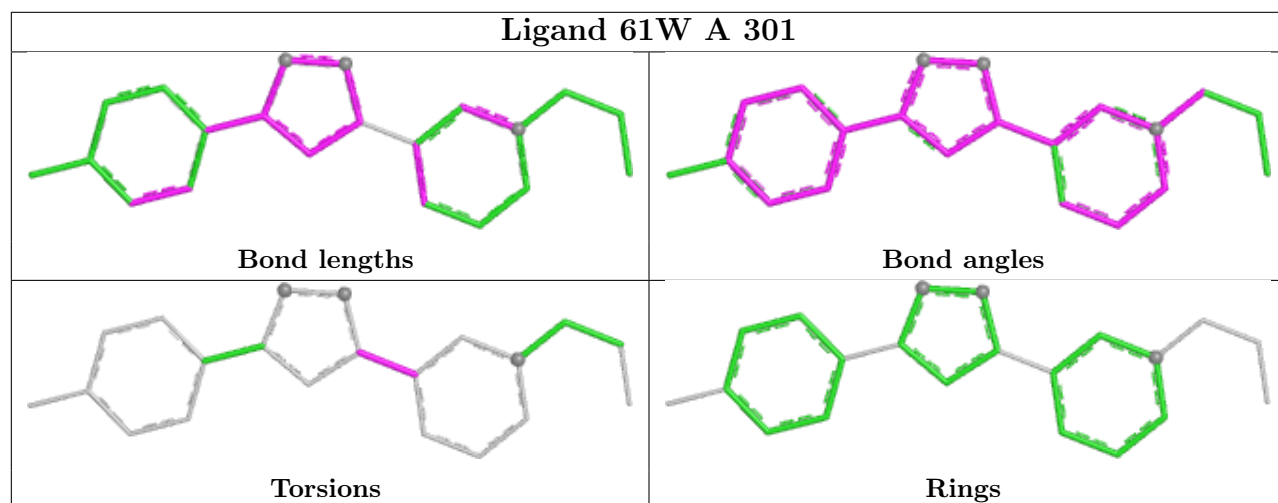
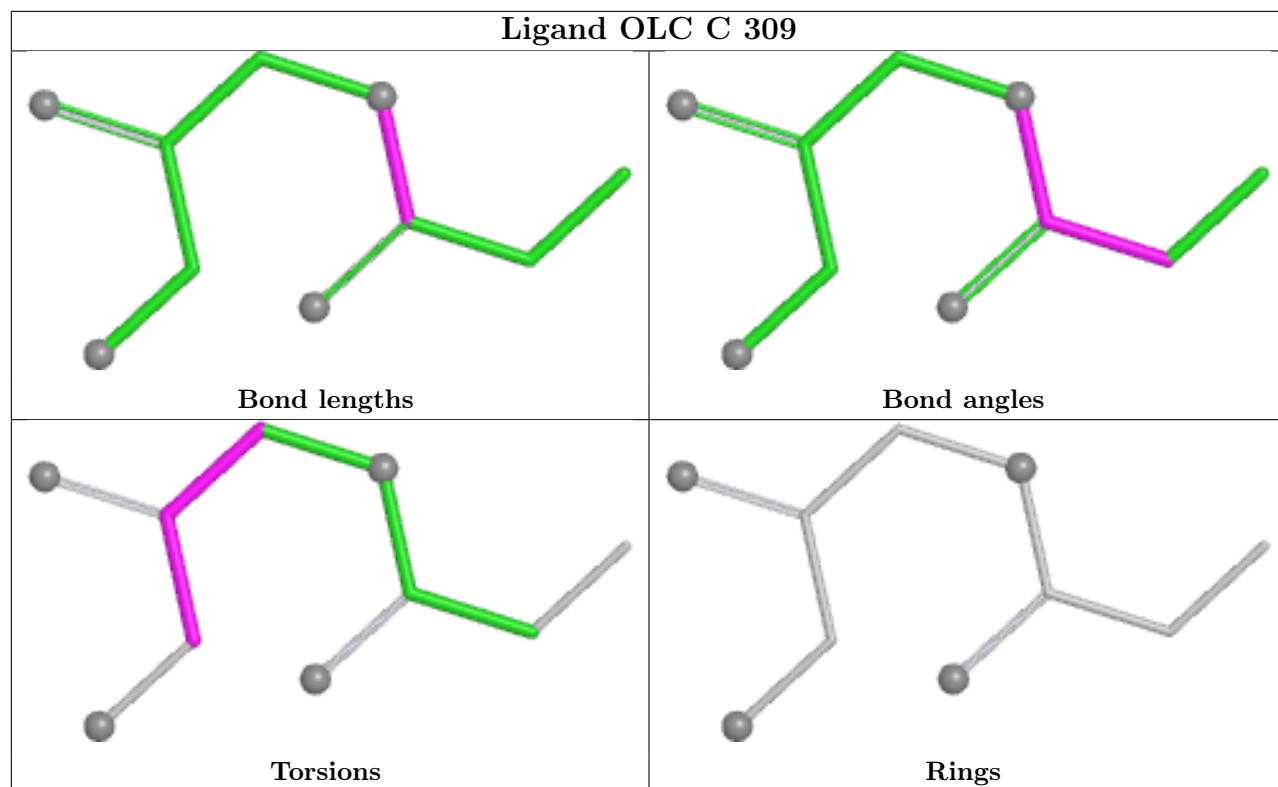
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SO4	1	0
3	A	303	SO4	1	0
4	C	307	OLC	2	0
4	A	310	OLC	1	0
4	C	308	OLC	1	0

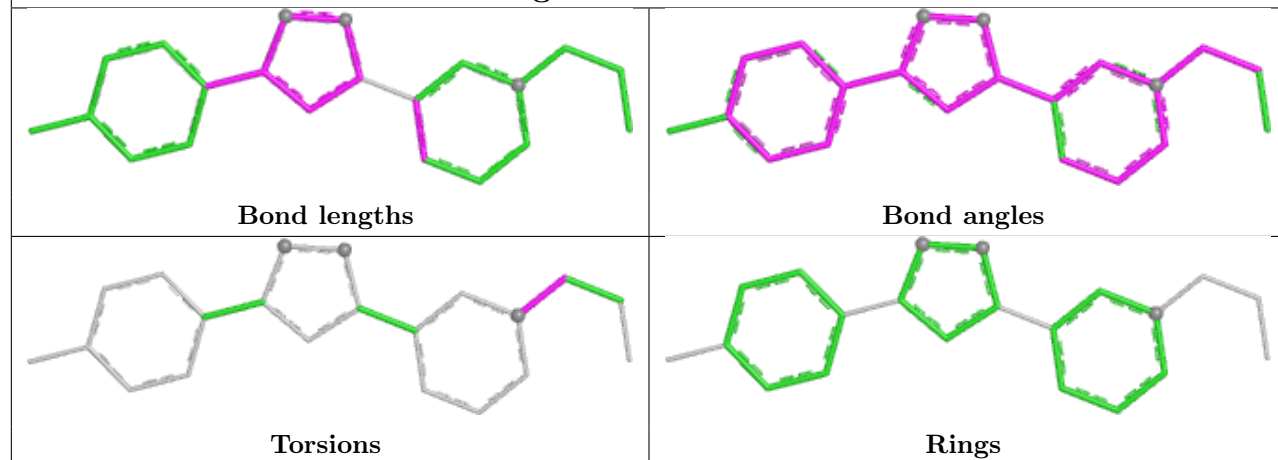
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

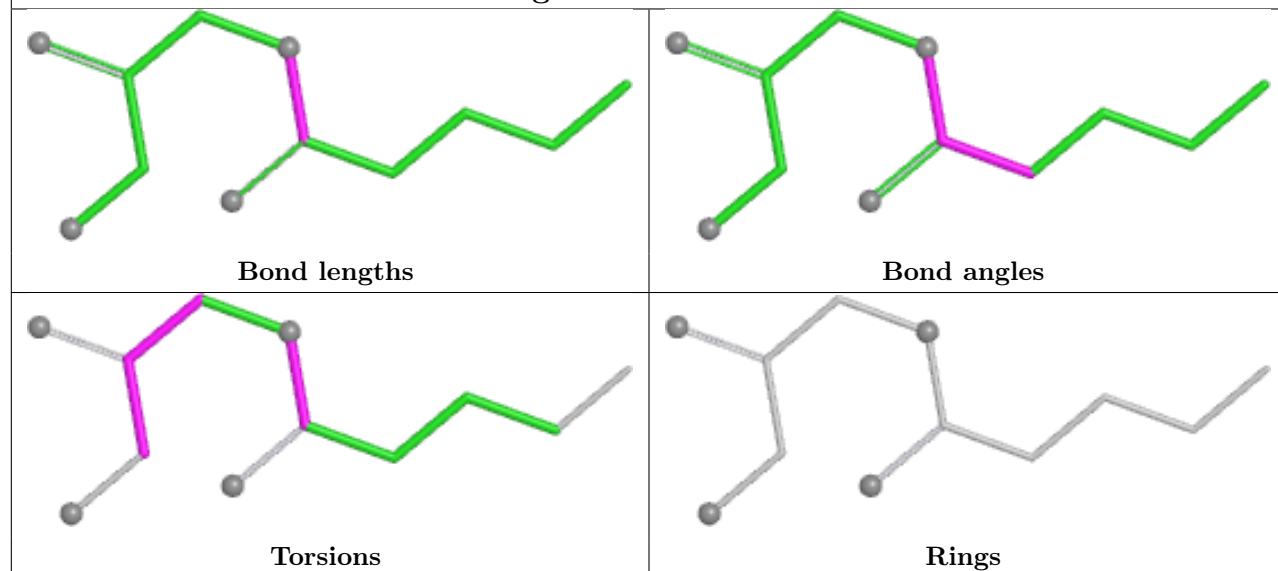


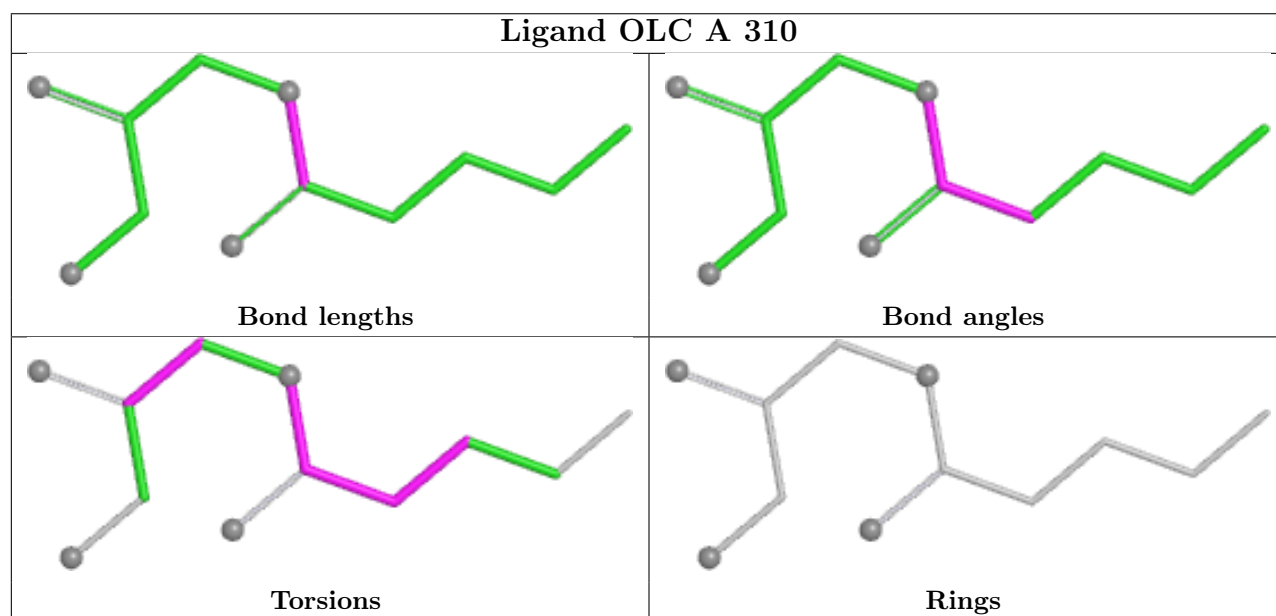
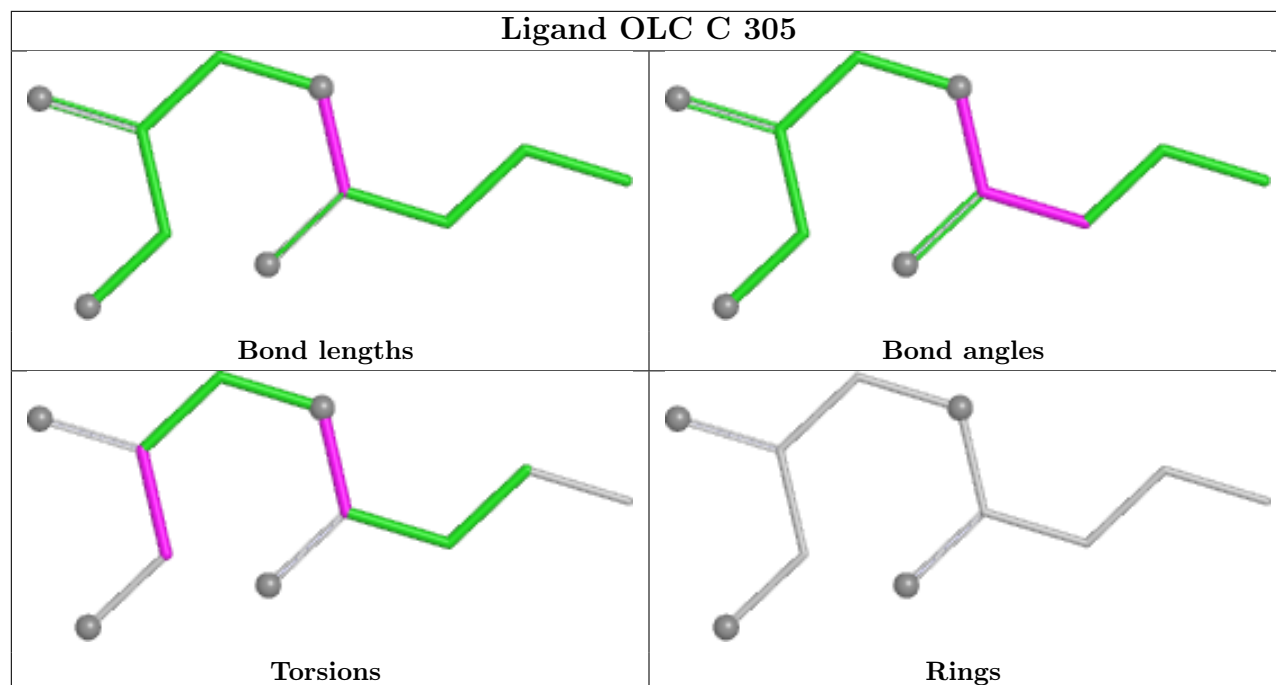


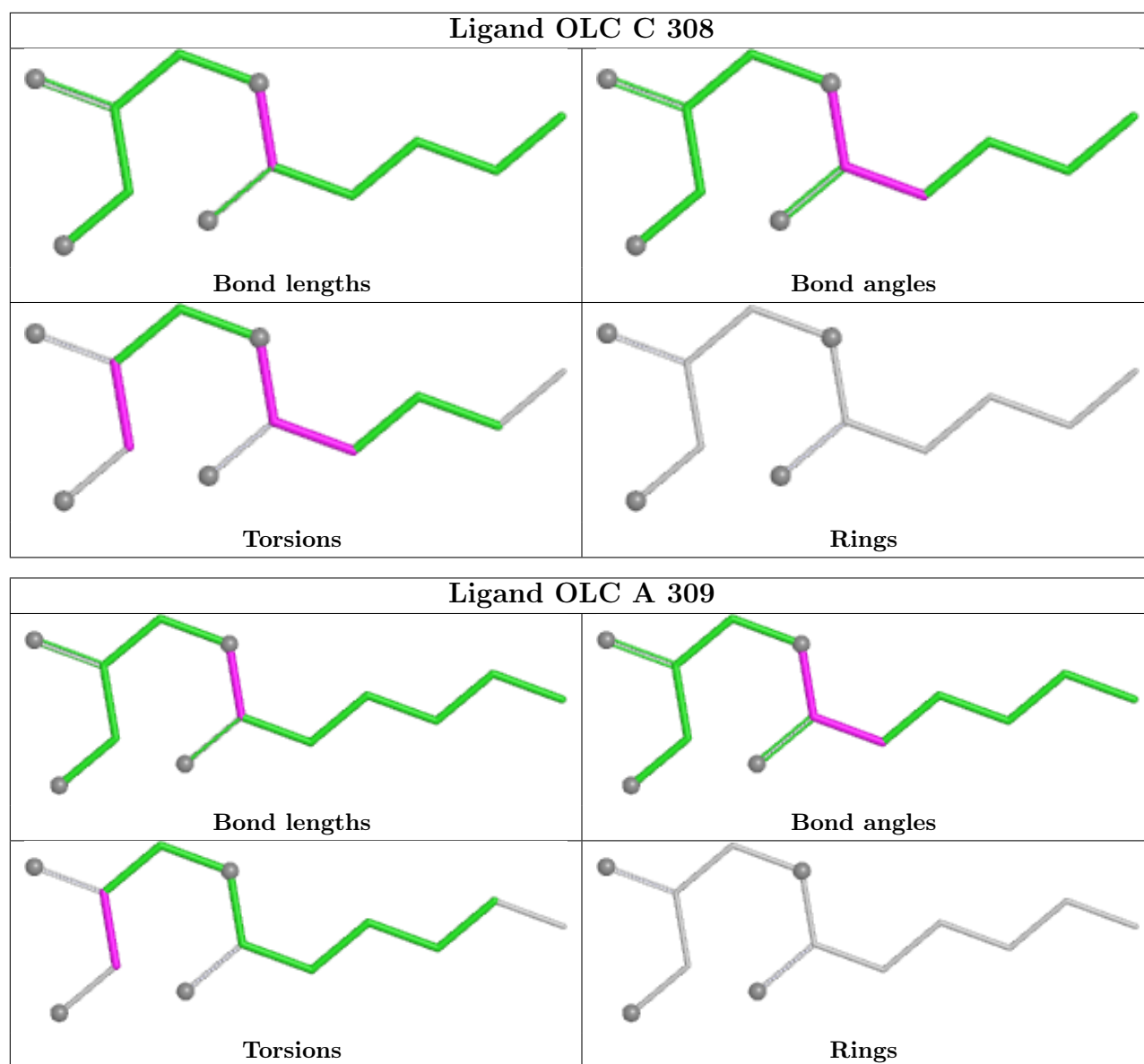
Ligand 61W C 301



Ligand OLC C 307







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	212/227 (93%)	0.45	16 (7%) 20 18	49, 67, 125, 162	0
1	B	219/227 (96%)	0.68	22 (10%) 12 10	47, 84, 137, 172	0
1	C	219/227 (96%)	0.42	15 (6%) 23 20	48, 64, 141, 185	0
All	All	650/681 (95%)	0.52	53 (8%) 17 15	47, 71, 137, 185	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.1
1	B	30	LEU	5.4
1	B	33	GLN	5.2
1	C	220	GLY	4.4
1	C	7	ARG	4.3
1	B	28	LEU	4.3
1	A	8	ARG	4.0
1	B	29	TRP	3.9
1	A	9	TRP	3.8
1	A	15	LEU	3.7
1	A	10	ALA	3.6
1	B	215	THR	3.5
1	B	27	TRP	3.5
1	B	31	GLY	3.4
1	A	33	GLN	3.2
1	A	11	TRP	3.2
1	C	3	TRP	3.2
1	A	55	GLU	3.2
1	A	196	PHE	3.2
1	B	121	TRP	3.0
1	C	9	TRP	3.0
1	A	219	PHE	3.0
1	B	167	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	36	VAL	2.9
1	C	4	ALA	2.9
1	C	158	GLU	2.9
1	B	141	THR	2.9
1	B	32	THR	2.8
1	C	137	ARG	2.8
1	A	217	TYR	2.6
1	B	39	ARG	2.6
1	A	214	LEU	2.6
1	B	217	TYR	2.5
1	C	11	TRP	2.4
1	C	12	ALA	2.4
1	B	47	ARG	2.4
1	C	16	LEU	2.3
1	C	5	VAL	2.3
1	B	196	PHE	2.3
1	B	67	ARG	2.3
1	B	7	ARG	2.3
1	C	24	GLN	2.2
1	C	8	ARG	2.2
1	A	18	VAL	2.2
1	A	182	LEU	2.2
1	C	144	GLU	2.2
1	B	26	VAL	2.1
1	A	58	PHE	2.1
1	A	14	LEU	2.1
1	A	13	ALA	2.1
1	B	219	PHE	2.0
1	C	45	LEU	2.0
1	B	216	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

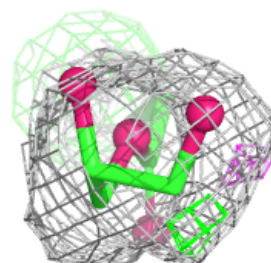
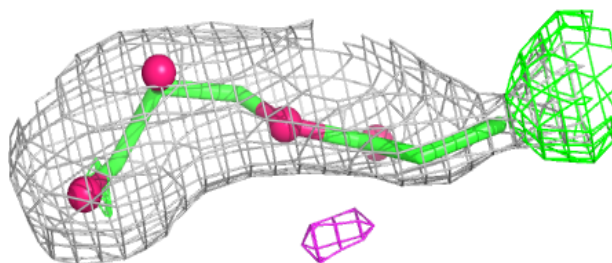
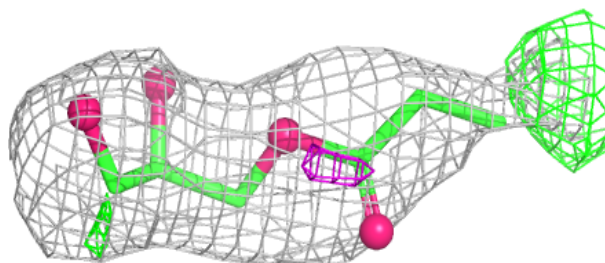
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	305	5/5	0.67	0.14	139,157,160,161	0
3	SO4	A	308	5/5	0.73	0.15	166,181,200,202	0
4	OLC	C	309	10/25	0.75	0.26	119,131,144,144	0
3	SO4	B	305	5/5	0.76	0.12	120,131,137,140	0
3	SO4	B	303	5/5	0.78	0.07	143,145,147,148	0
3	SO4	C	304	5/5	0.79	0.17	113,114,117,118	5
3	SO4	B	304	5/5	0.82	0.10	120,130,131,143	0
3	SO4	A	307	5/5	0.83	0.13	123,129,135,139	0
4	OLC	C	307	12/25	0.85	0.21	86,113,120,126	0
4	OLC	C	308	12/25	0.85	0.19	83,102,116,121	0
4	OLC	C	306	10/25	0.85	0.19	107,122,130,140	0
3	SO4	A	303	5/5	0.86	0.09	98,103,119,136	0
4	OLC	A	310	12/25	0.87	0.22	84,115,124,126	0
4	OLC	A	309	13/25	0.89	0.17	60,80,109,124	0
3	SO4	C	302	5/5	0.89	0.10	120,129,134,136	0
3	SO4	B	302	5/5	0.90	0.09	120,120,124,132	0
3	SO4	C	303	5/5	0.92	0.07	81,92,107,120	0
2	61W	A	301	21/21	0.92	0.18	66,89,98,102	0
2	61W	B	301	21/21	0.93	0.17	70,83,100,103	0
2	61W	C	301	21/21	0.94	0.16	65,73,88,100	0
4	OLC	C	305	11/25	0.94	0.16	75,96,108,120	0
3	SO4	A	304	5/5	0.95	0.07	88,95,102,104	0
3	SO4	A	302	5/5	0.95	0.06	107,109,110,123	0
3	SO4	A	306	5/5	0.97	0.09	91,91,100,114	0

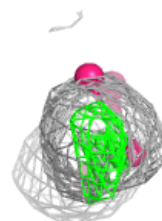
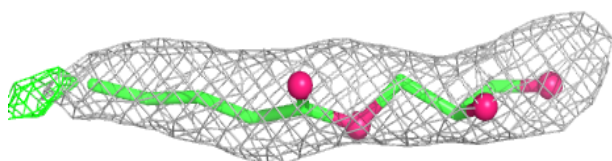
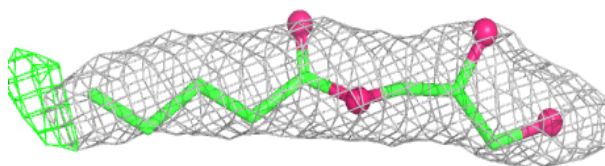
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLC C 309:

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

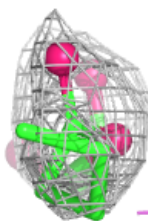
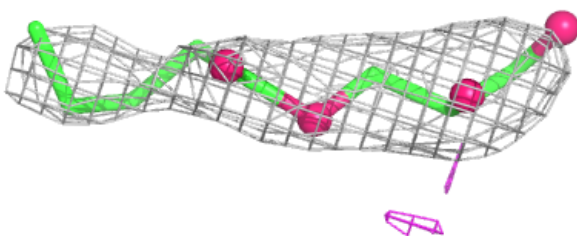
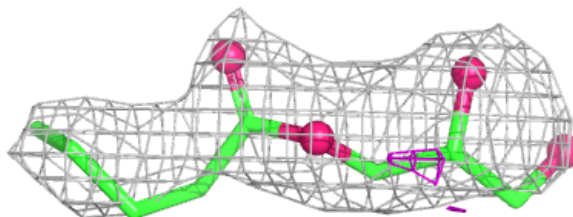
**Electron density around OLC C 307:**

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

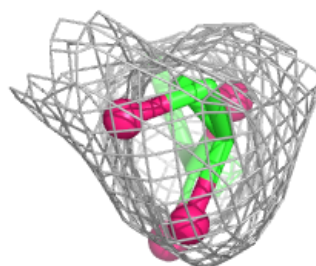
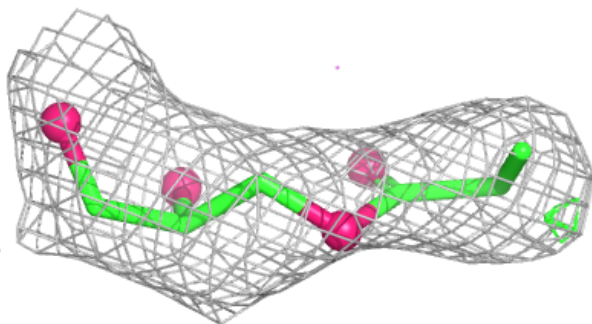
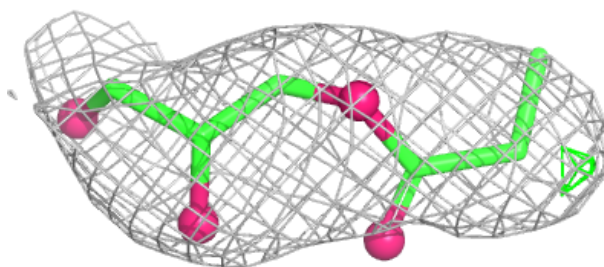


Electron density around OLC C 308:

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

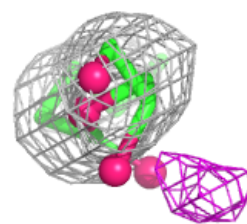
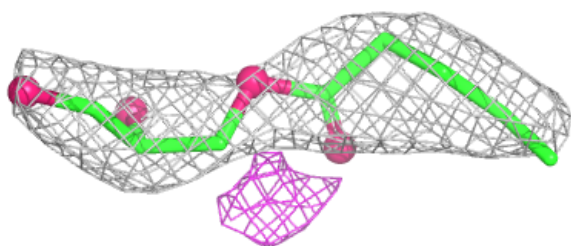
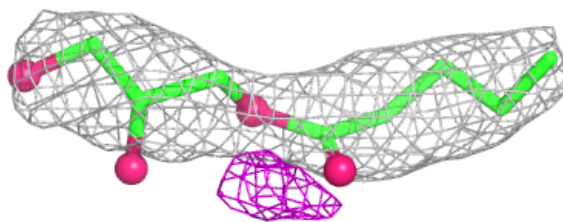
**Electron density around OLC C 306:**

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

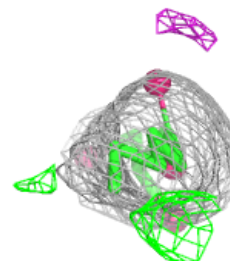
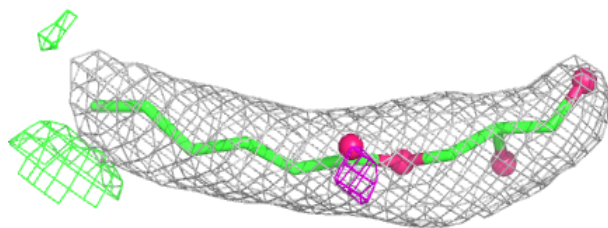
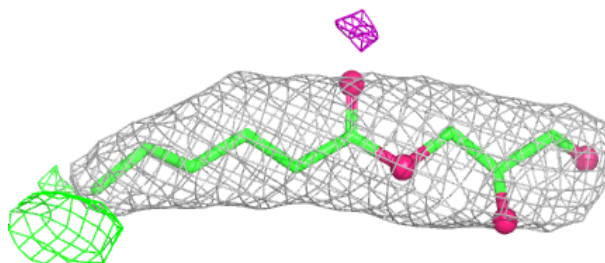


Electron density around OLC A 310:

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

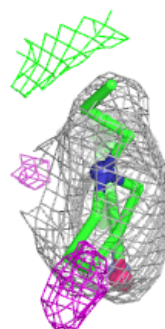
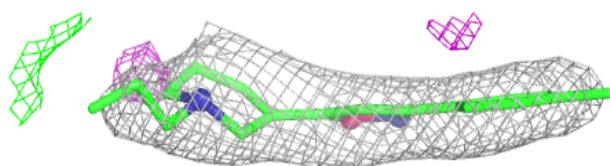
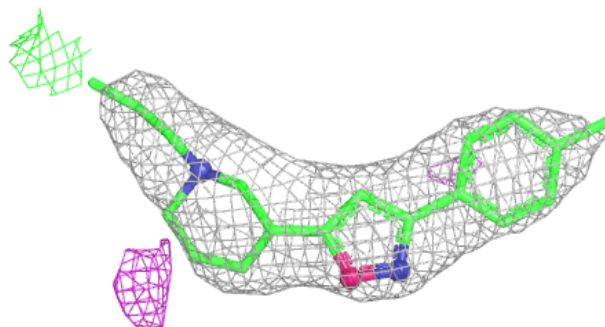
**Electron density around OLC A 309:**

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

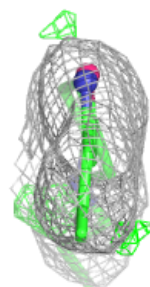
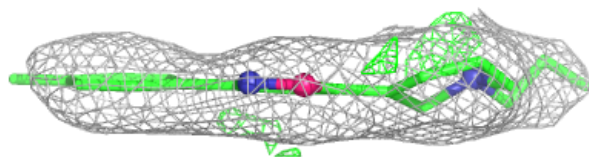
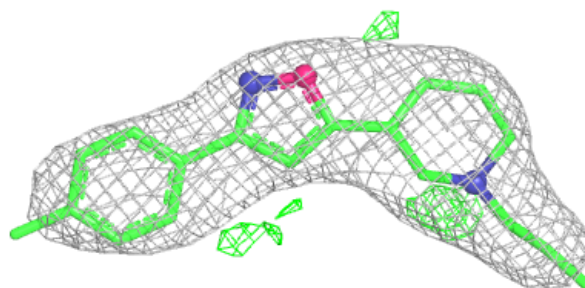


Electron density around 61W A 301:

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

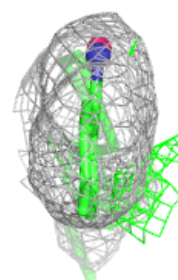
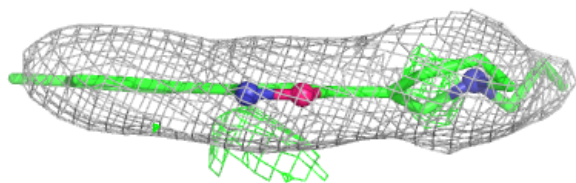
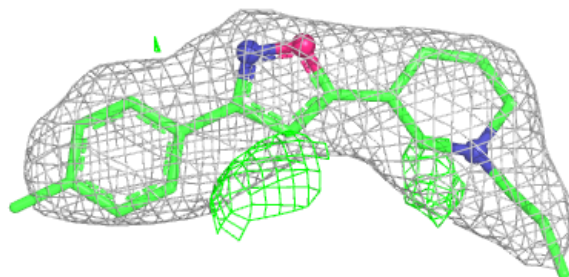
**Electron density around 61W B 301:**

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

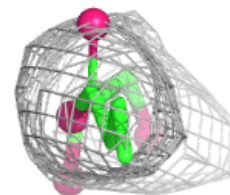
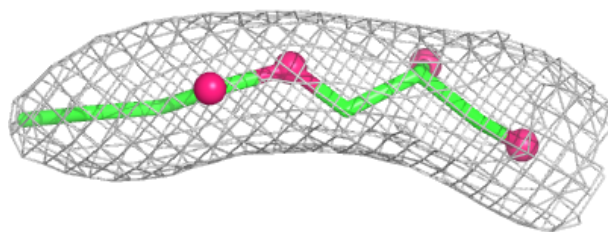
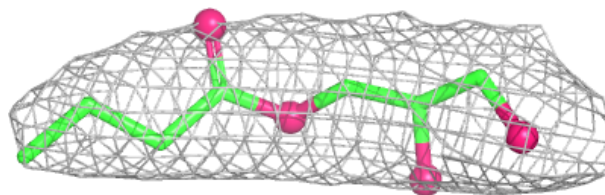


Electron density around 61W C 301:

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

**Electron density around OLC C 305:**

$2mF_o-DF_c$ (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.