



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 10:13 am BST

PDB ID : 9RKH / pdb_00009rkh
Title : Dark structure of beta-2 Adrenergic receptor with photoazolol in Dark state recorded at LCLS
Authors : Bertrand, Q.; Stipp, R.; Glover, H.; Stierli, F.; Siedel, H.P.; Mous, S.; Kepa, M.; Weinert, T.; Standfuss, J.
Deposited on : 2025-06-13
Resolution : 2.50 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	:	1.8.4, CSD as541be (2020)
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

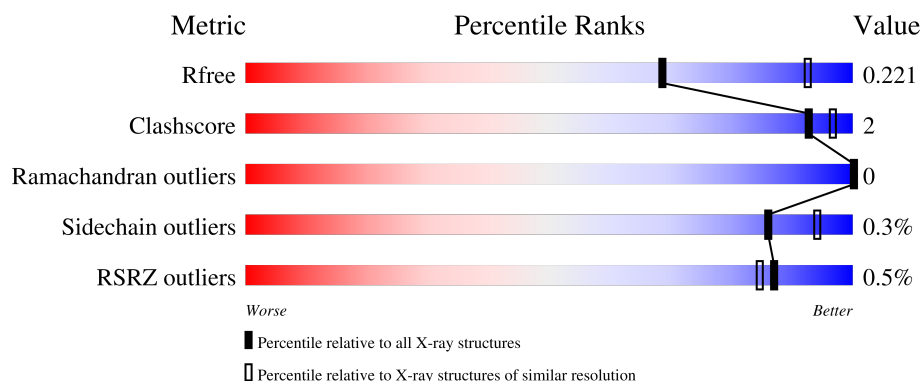
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

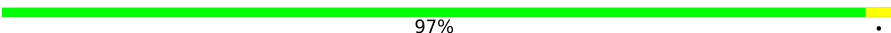
The reported resolution of this entry is 2.50 Å.

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	442	 97%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7649 atoms, of which 3740 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 Beta-2 adrenergic receptor,Endolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	442	7192	2330	3628	594	616	24	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

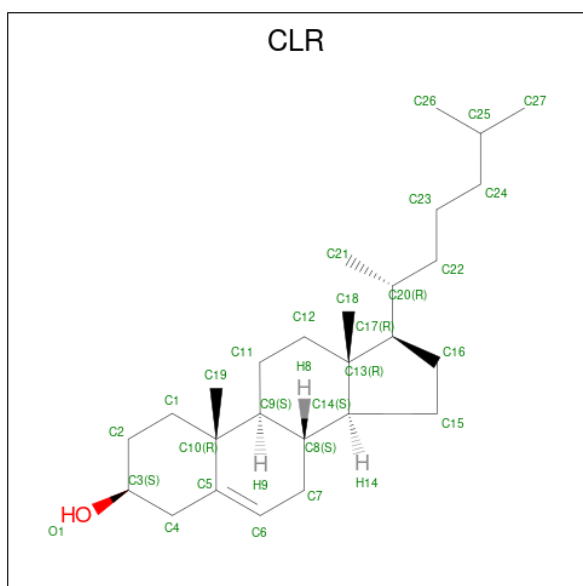
Chain	Residue	Modelled	Actual	Comment	Reference
A	122	TRP	GLU	conflict	UNP P07550
A	187	GLU	ASN	conflict	UNP P07550
A	241	GLY	ARG	conflict	UNP P00720
A	283	THR	CYS	conflict	UNP P00720
A	326	ALA	CYS	conflict	UNP P00720
A	366	ARG	ILE	conflict	UNP P00720

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



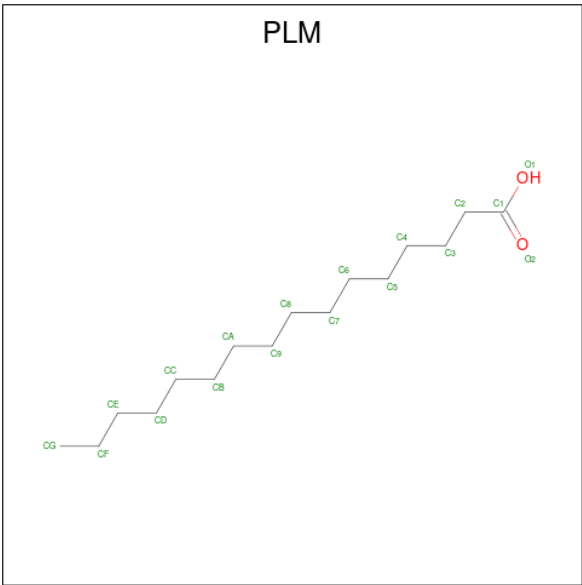
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



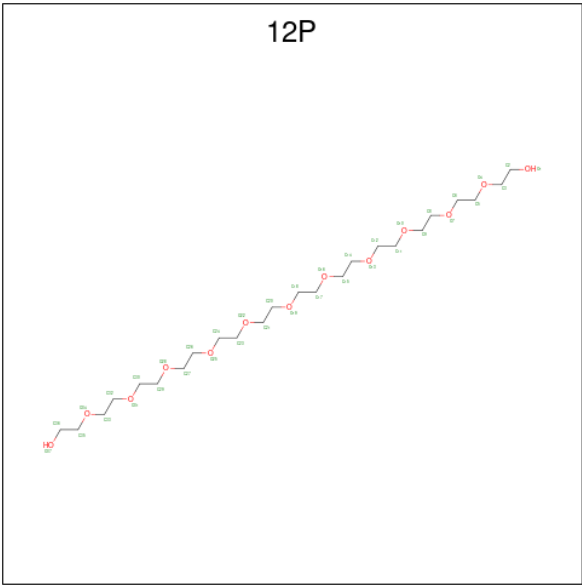
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



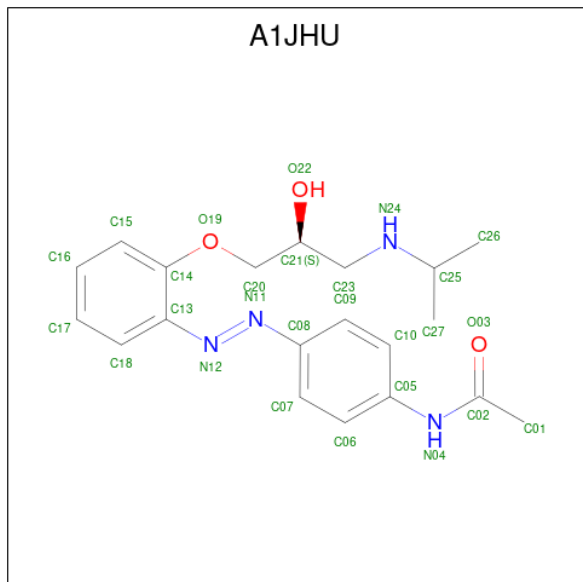
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 5 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



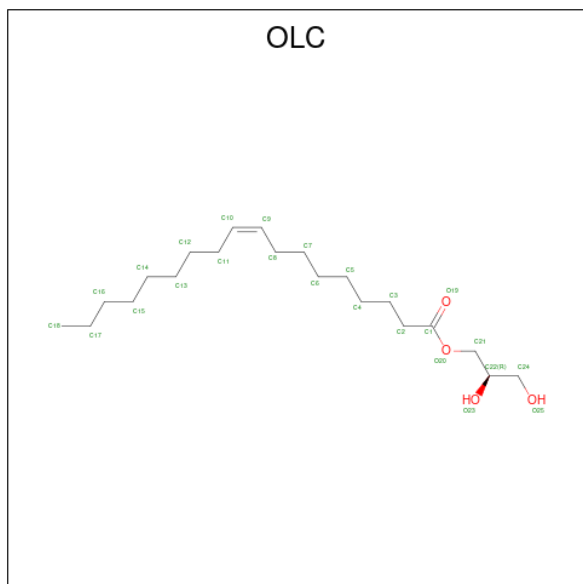
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	11	6		
5	A	1	Total	C	O	0	0
			20	13	7		
5	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is {N}-[4-[({E})]-2-[(2 {S})-2-oxidanyl-3-(propan-2-ylamino)propoxy]phenyl]diazanyl]phenyl]ethanamide (CCD ID: A1JHU) (formula: C₂₀H₂₆N₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			53	20	26	4	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



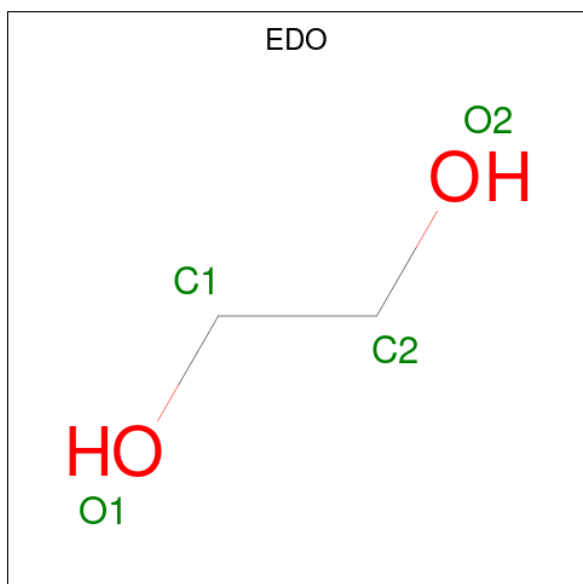
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			65	21	40	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 65 21 40 4	0	0
7	A	1	Total C 13 13	0	0
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C O 19 15 4	0	0
7	A	1	Total C 10 10	0	0
7	A	1	Total C 9 9	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 10 2 6 2	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	26	Total	O	0	0
			26	26		

3 Residue-property plots

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

- Molecule 1: Beta-2 adrenergic receptor,Endolysin

Chain A:  97% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.94Å 172.23Å 41.23Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	28.33 – 2.50 28.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.33-2.50) 99.7 (28.33-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.193 , 0.218 0.195 , 0.221	Depositor DCC
R_{free} test set	2010 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, PLM, OLC, EDO, 12P, YCM, GOL, CLR, A1JHU

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	0.18	0/3636	0.32	0/4935

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	348	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3564	3628	3631	8	0
2	A	30	0	0	0	0
3	A	56	0	92	1	0
4	A	17	0	31	0	0
5	A	53	0	65	2	0
6	A	27	26	0	0	0
7	A	126	80	191	4	0
8	A	4	6	6	0	0
9	A	6	0	8	0	0
10	A	26	0	0	0	0
All	All	3909	3740	4024	12	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 2.

All (12) 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:36:MET:HE2	1:A:36:MET:N	2.28	0.49
1:A:258:ILE:O	1:A:258:ILE:HG22	2.14	0.47
5:A:514:12P:H361	5:A:514:12P:H331	1.72	0.46
1:A:209:TYR:O	1:A:213:VAL:HG23	2.18	0.44
1:A:158:TRP:CZ2	3:A:505:CLR:H213	2.53	0.43
1:A:216:VAL:HG22	7:A:521:OLC:H12	2.00	0.43
7:A:516:OLC:H8A	7:A:516:OLC:H5A	1.35	0.43
1:A:35:GLY:C	1:A:36:MET:HE2	2.43	0.42
1:A:225:GLU:OE2	1:A:228:ARG:NH1	2.54	0.41
5:A:509:12P:H231	5:A:509:12P:H201	1.92	0.41
7:A:513:OLC:H8A	7:A:513:OLC:H5	1.73	0.41
1:A:464:PHE:HB2	7:A:518:OLC:H24A	2.02	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	440/442 (100%)	430 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	383/382 (100%)	382 (100%)	1 (0%)	86	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	179	GLN
1	A	224	GLN
1	A	229	GLN
1	A	369	ASN
1	A	440	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	YCM	A	393	1	7,9,10	0.86	0	4,10,12	4.53	2 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	A	393	1	-	2/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	YCM	CE-CD-SG	-8.83	87.61	113.59
1	A	393	YCM	CB-SG-CD	2.07	123.64	104.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	393	YCM	SG-CD-CE-OZ1
1	A	393	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.07	0
6	A1JHU	A	510	-	28,28,28	1.33	2 (7%)	36,36,36	1.13	3 (8%)
3	CLR	A	505	-	31,31,31	0.37	0	48,48,48	0.75	0
7	OLC	A	520	-	9,9,24	0.79	0	8,8,25	1.51	1 (12%)
7	OLC	A	511	-	24,24,24	1.06	1 (4%)	25,25,25	1.12	2 (8%)
7	OLC	A	516	-	24,24,24	1.05	1 (4%)	25,25,25	1.24	2 (8%)
5	12P	A	508	-	16,16,36	0.53	0	15,15,35	0.19	0
5	12P	A	509	-	19,19,36	0.54	0	18,18,35	0.23	0
4	PLM	A	507	1	16,16,17	0.55	0	15,15,17	0.43	0
7	OLC	A	518	-	18,18,24	0.27	0	18,19,25	0.29	0
9	GOL	A	517	-	5,5,5	0.94	0	5,5,5	0.94	0
7	OLC	A	513	-	12,12,24	0.79	0	11,11,25	1.31	1 (9%)
8	EDO	A	515	-	3,3,3	0.48	0	2,2,2	0.27	0
3	CLR	A	506	-	31,31,31	0.35	0	48,48,48	0.53	0
2	SO4	A	502[B]	-	4,4,4	0.14	0	6,6,6	0.05	0
7	OLC	A	512	-	24,24,24	1.06	1 (4%)	25,25,25	1.16	2 (8%)
7	OLC	A	521	-	8,8,24	0.28	0	7,7,25	0.19	0
2	SO4	A	519	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	0
5	12P	A	514	-	15,15,36	0.54	0	14,14,35	0.21	0
2	SO4	A	502[A]	-	4,4,4	0.42	0	6,6,6	0.05	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
3	CLR	A	505	-	-	1/10/68/68	0/4/4/4
3	CLR	A	506	-	-	0/10/68/68	0/4/4/4
7	OLC	A	518	-	-	3/18/18/24	-
7	OLC	A	512	-	-	13/24/24/24	-
7	OLC	A	520	-	-	1/7/7/24	-
7	OLC	A	521	-	-	1/6/6/24	-
7	OLC	A	511	-	-	8/24/24/24	-
9	GOL	A	517	-	-	0/4/4/4	-
7	OLC	A	516	-	-	14/24/24/24	-
5	12P	A	508	-	-	8/14/14/34	-
5	12P	A	514	-	-	6/13/13/34	-
5	12P	A	509	-	-	8/17/17/34	-
8	EDO	A	515	-	-	0/1/1/1	-
7	OLC	A	513	-	-	7/10/10/24	-
6	A1JHU	A	510	-	-	2/19/19/19	0/2/2/2
4	PLM	A	507	1	-	2/13/14/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	510	A1JHU	C02-N04	5.33	1.45	1.36
7	A	516	OLC	O20-C1	2.94	1.41	1.33
7	A	511	OLC	O20-C1	2.93	1.41	1.33
7	A	512	OLC	O20-C1	2.91	1.41	1.33
6	A	510	A1JHU	C05-N04	2.10	1.45	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	511	OLC	C8-C9-C10	3.83	154.10	124.73
7	A	512	OLC	C8-C9-C10	3.81	153.93	124.73
7	A	516	OLC	C8-C9-C10	3.72	153.30	124.73
7	A	520	OLC	C8-C9-C10	3.60	152.33	124.73
6	A	510	A1JHU	C05-N04-C02	-3.59	121.47	127.99
7	A	513	OLC	C8-C9-C10	3.52	151.71	124.73
6	A	510	A1JHU	C01-C02-N04	3.17	119.63	114.98
6	A	510	A1JHU	C13-N12-N11	2.85	121.13	114.56
7	A	516	OLC	O20-C1-C2	2.62	120.14	111.91
7	A	512	OLC	O20-C1-C2	2.41	119.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	511	OLC	O20-C1-C2	2.37	119.33	111.91

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	516	OLC	O20-C21-C22-C24
7	A	516	OLC	O20-C21-C22-O23
7	A	511	OLC	O19-C1-O20-C21
7	A	511	OLC	C2-C1-O20-C21
7	A	512	OLC	C2-C1-O20-C21
5	A	509	12P	O25-C26-C27-O28
7	A	512	OLC	O19-C1-O20-C21
5	A	509	12P	O19-C20-C21-O22
7	A	516	OLC	C5-C6-C7-C8
5	A	509	12P	C20-C21-O22-C23
7	A	516	OLC	C2-C1-O20-C21
5	A	509	12P	O22-C23-C24-O25
7	A	512	OLC	C1-C2-C3-C4
5	A	514	12P	O22-C23-C24-O25
7	A	516	OLC	C10-C11-C12-C13
7	A	516	OLC	C2-C3-C4-C5
5	A	508	12P	O22-C23-C24-O25
7	A	516	OLC	C3-C4-C5-C6
7	A	516	OLC	O19-C1-O20-C21
7	A	516	OLC	C11-C12-C13-C14
7	A	516	OLC	C13-C14-C15-C16
7	A	512	OLC	C21-C22-C24-O25
7	A	511	OLC	C11-C12-C13-C14
7	A	512	OLC	C11-C12-C13-C14
7	A	512	OLC	C12-C13-C14-C15
7	A	513	OLC	C12-C13-C14-C15
7	A	516	OLC	C12-C13-C14-C15
5	A	509	12P	O31-C32-C33-O34
7	A	511	OLC	C10-C11-C12-C13
7	A	512	OLC	C6-C7-C8-C9
6	A	510	A1JHU	C26-C25-N24-C23
6	A	510	A1JHU	C27-C25-N24-C23
7	A	513	OLC	C5-C6-C7-C8
7	A	520	OLC	C6-C7-C8-C9
7	A	516	OLC	C1-C2-C3-C4
5	A	514	12P	O25-C26-C27-O28

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Mol	Chain	Res	Type	Atoms
5	A	514	12P	C36-C35-O34-C33
7	A	512	OLC	C2-C3-C4-C5
7	A	513	OLC	C3-C4-C5-C6
4	A	507	PLM	C7-C8-C9-CA
7	A	511	OLC	C3-C4-C5-C6
7	A	511	OLC	O20-C21-C22-O23
3	A	505	CLR	C21-C20-C22-C23
7	A	516	OLC	C4-C5-C6-C7
7	A	518	OLC	C9-C10-C11-C12
7	A	512	OLC	C4-C5-C6-C7
5	A	514	12P	O31-C32-C33-O34
5	A	509	12P	C21-C20-O19-C18
7	A	511	OLC	O20-C21-C22-C24
5	A	508	12P	O16-C17-C18-O19
5	A	509	12P	O28-C29-C30-O31
5	A	508	12P	C26-C27-O28-C29
5	A	509	12P	C26-C27-O28-C29
7	A	516	OLC	C6-C7-C8-C9
4	A	507	PLM	C8-C9-CA-CB
5	A	508	12P	C27-C26-O25-C24
7	A	512	OLC	C13-C14-C15-C16
7	A	513	OLC	C11-C12-C13-C14
5	A	508	12P	C21-C20-O19-C18
5	A	508	12P	C24-C23-O22-C21
7	A	512	OLC	C3-C4-C5-C6
5	A	508	12P	O25-C26-C27-O28
7	A	513	OLC	C6-C7-C8-C9
5	A	514	12P	C29-C30-O31-C32
7	A	511	OLC	C2-C3-C4-C5
7	A	518	OLC	C6-C7-C8-C9
5	A	514	12P	C27-C26-O25-C24
7	A	512	OLC	C9-C10-C11-C12
7	A	512	OLC	C7-C8-C9-C10
7	A	513	OLC	C9-C10-C11-C12
5	A	508	12P	C20-C21-O22-C23
7	A	513	OLC	C7-C8-C9-C10
7	A	518	OLC	C5-C6-C7-C8
7	A	521	OLC	C5-C6-C7-C8

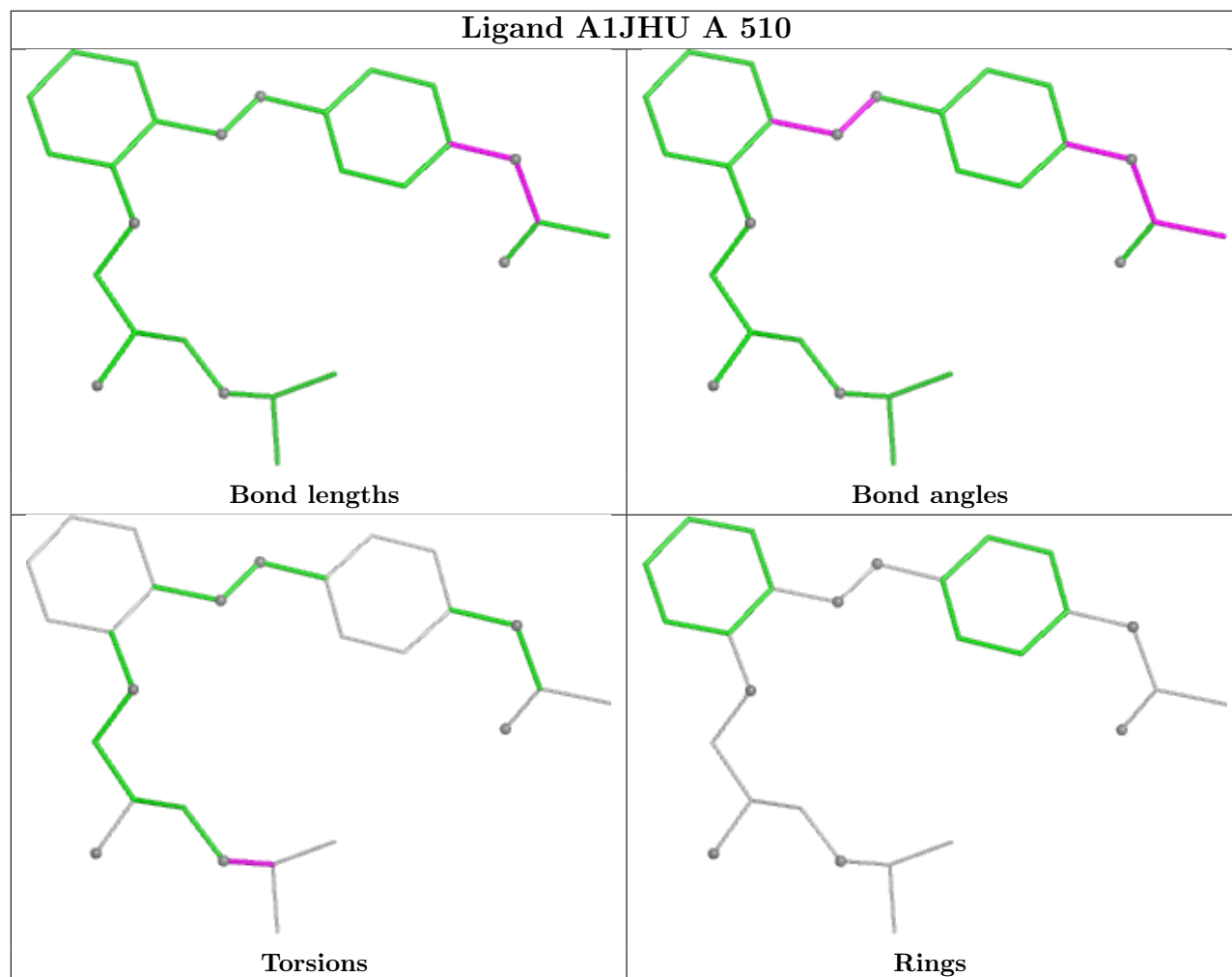
There are no ring outliers.

7 monomers are involved in 7 short contacts:

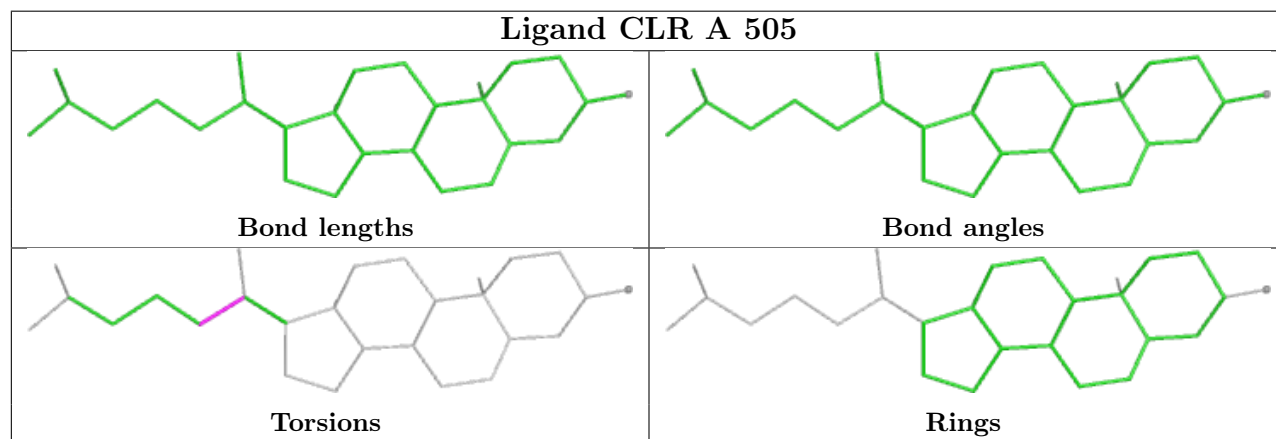
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	CLR	1	0
7	A	516	OLC	1	0
5	A	509	12P	1	0
7	A	518	OLC	1	0
7	A	513	OLC	1	0
7	A	521	OLC	1	0
5	A	514	12P	1	0

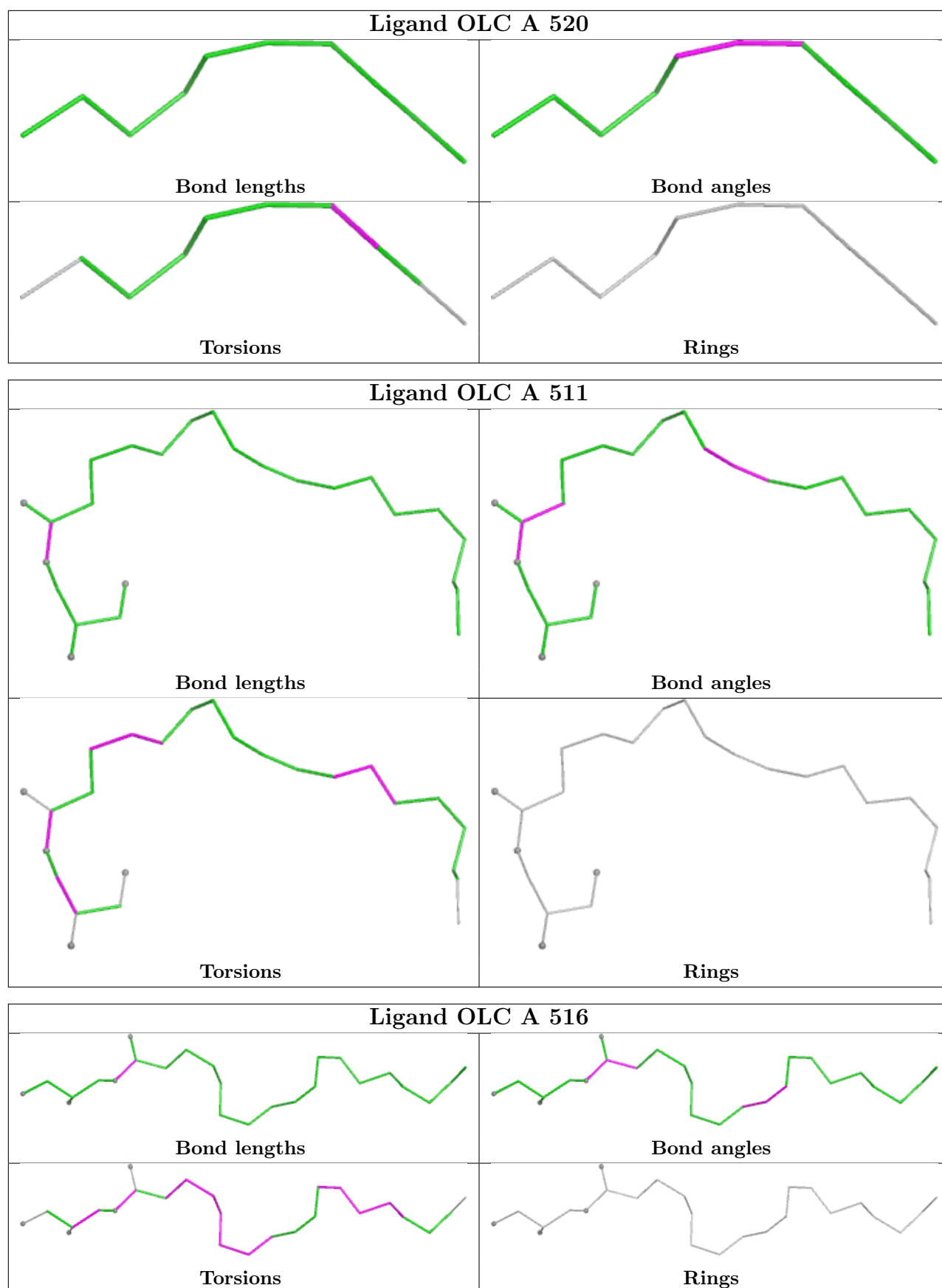
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

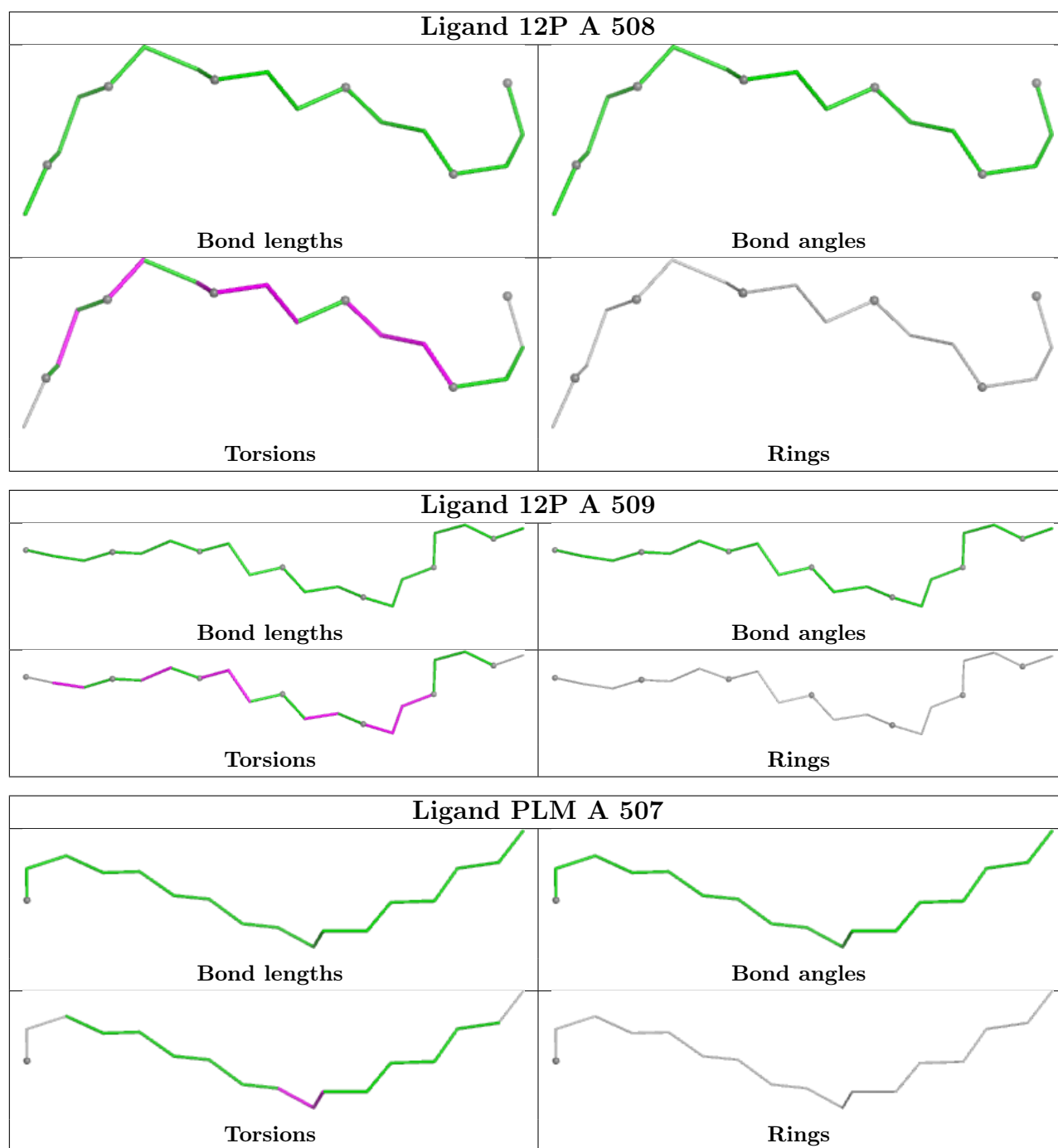
Ligand A1JHU A 510

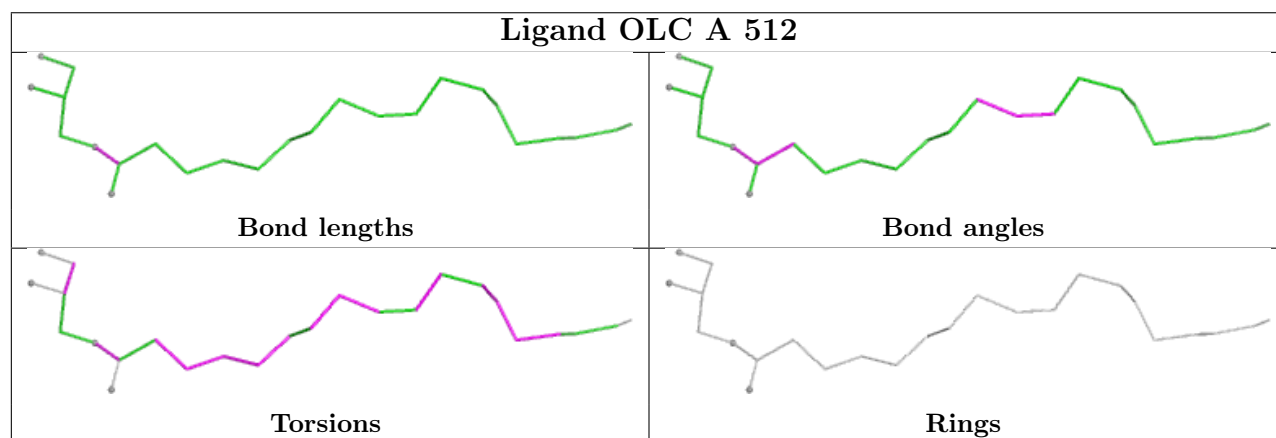
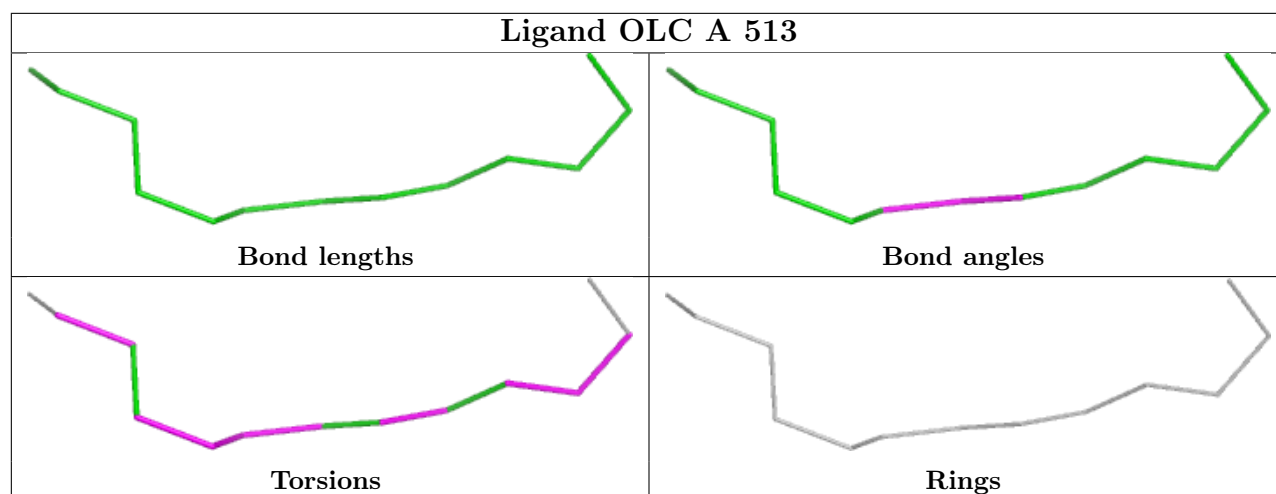
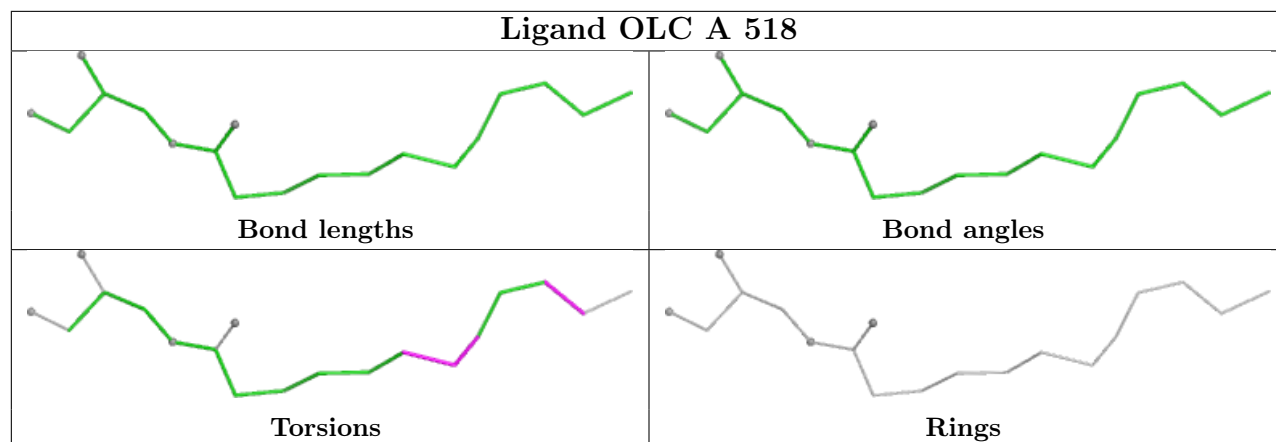


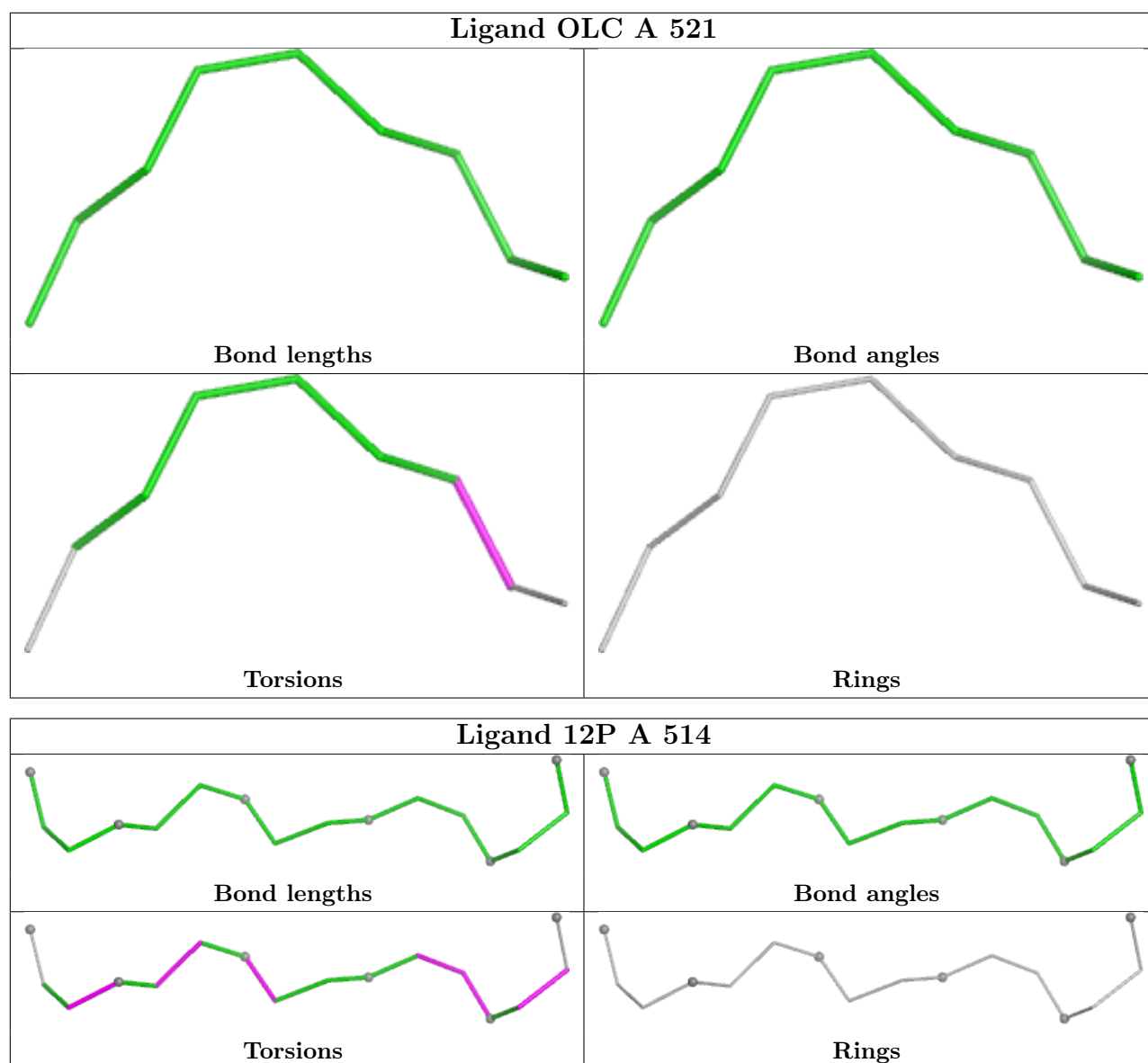
Ligand CLR A 505











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/442 (99%)	-0.31	2 (0%) 87 85	33, 83, 132, 195	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	PHE	2.9
1	A	31	VAL	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	YCM	A	393	10/11	0.97	0.07	55,66,78,86	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

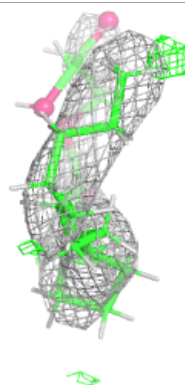
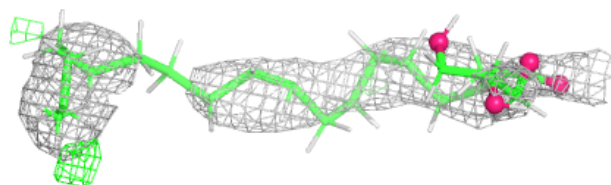
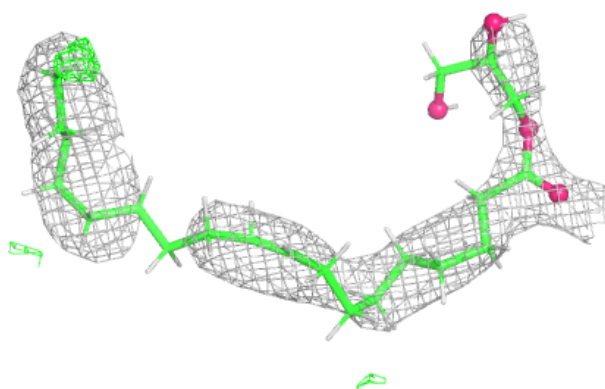
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	OLC	A	511	25/25	0.74	0.15	91,131,168,172	0
2	SO4	A	519	5/5	0.75	0.10	111,116,132,142	0
2	SO4	A	502[A]	5/5	0.78	0.09	80,85,91,98	5
2	SO4	A	502[B]	5/5	0.78	0.09	73,75,82,87	5
7	OLC	A	512	25/25	0.79	0.18	84,123,161,167	0
5	12P	A	509	20/37	0.82	0.16	70,91,110,116	0
7	OLC	A	516	25/25	0.82	0.19	83,103,118,122	0
7	OLC	A	518	19/25	0.84	0.17	84,100,122,127	0
8	EDO	A	515	4/4	0.84	0.17	78,100,120,120	0
9	GOL	A	517	6/6	0.85	0.17	91,103,107,111	0
7	OLC	A	520	10/25	0.86	0.24	76,86,95,95	0
4	PLM	A	507	17/18	0.89	0.18	90,102,128,130	0
5	12P	A	514	16/37	0.90	0.12	78,90,102,103	0
3	CLR	A	506	28/28	0.90	0.15	97,108,117,118	0
7	OLC	A	521	9/25	0.92	0.21	71,82,88,101	0
5	12P	A	508	17/37	0.92	0.13	60,81,97,104	0
3	CLR	A	505	28/28	0.92	0.15	91,104,109,117	0
2	SO4	A	504	5/5	0.94	0.11	67,86,99,103	0
7	OLC	A	513	13/25	0.94	0.17	73,79,92,97	0
6	A1JHU	A	510	27/27	0.95	0.12	60,86,114,118	0
2	SO4	A	503	5/5	0.97	0.08	67,78,82,93	0
2	SO4	A	501	5/5	0.99	0.04	64,70,78,89	0

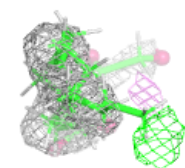
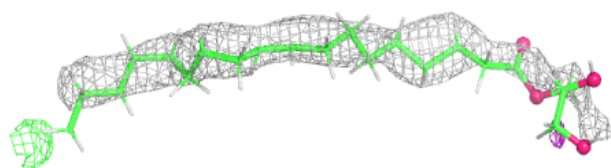
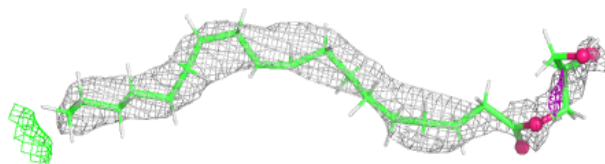
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 511:

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

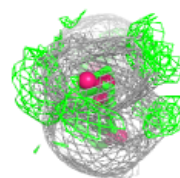
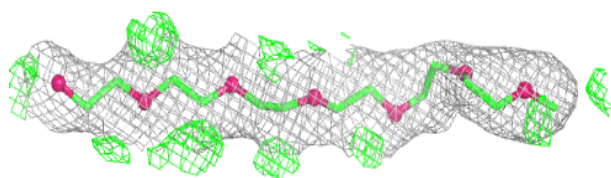
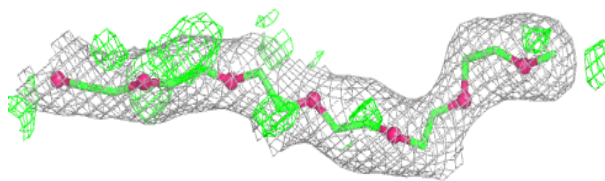
**Electron density around OLC A 512:**

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

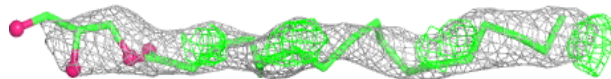
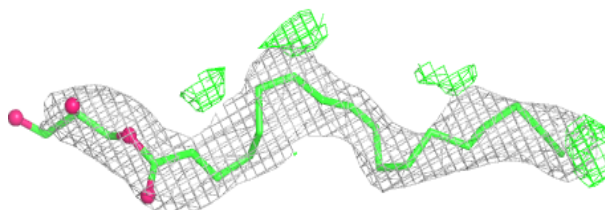


Electron density around 12P A 509:

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

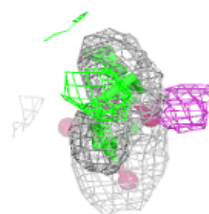
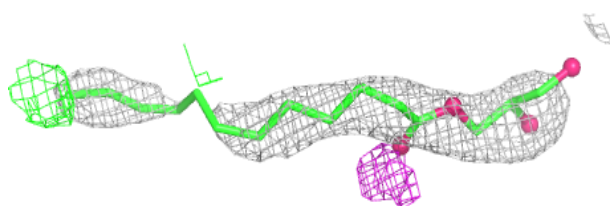
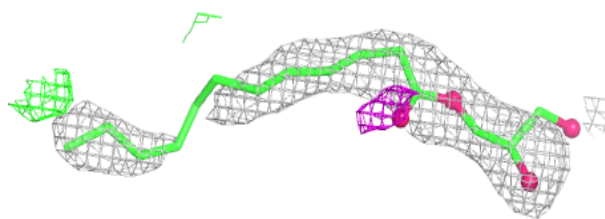
**Electron density around OLC A 516:**

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

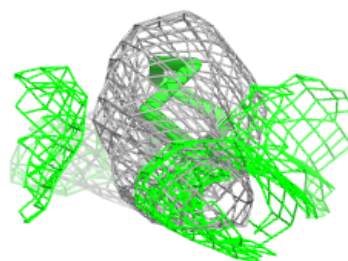
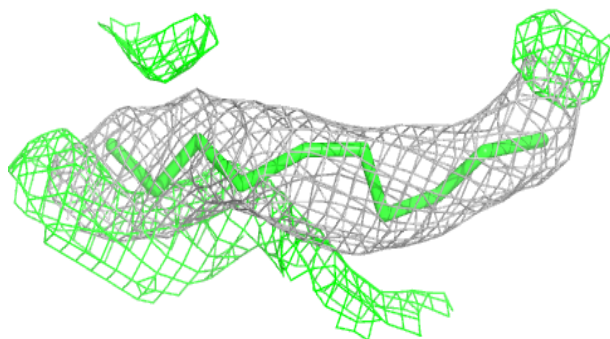
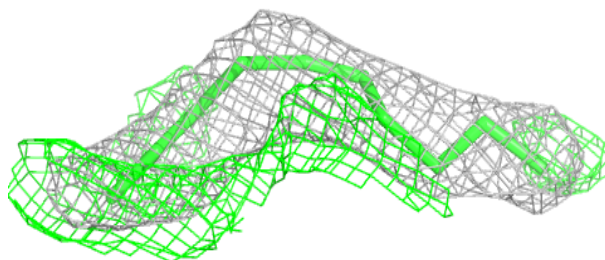


Electron density around OLC A 518:

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

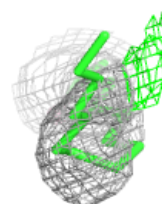
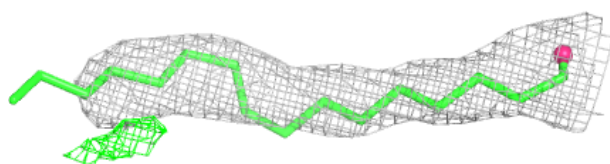
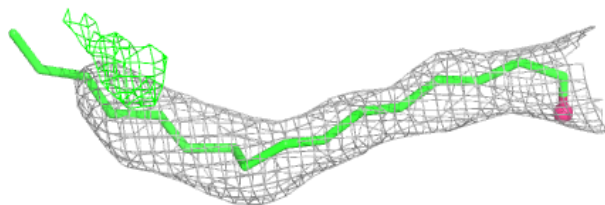
**Electron density around OLC A 520:**

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

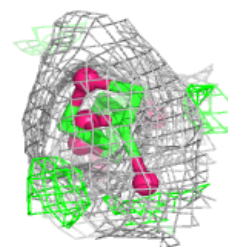
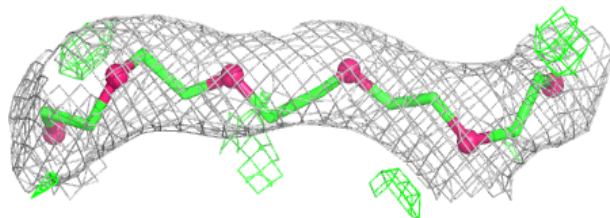
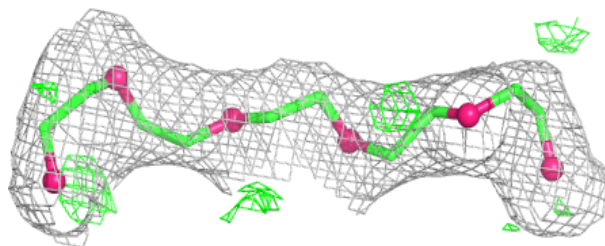


Electron density around PLM A 507:

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

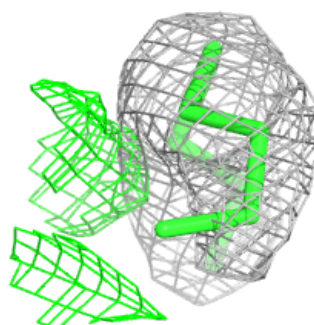
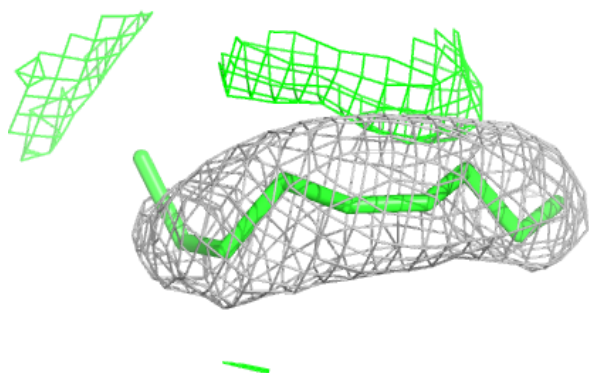
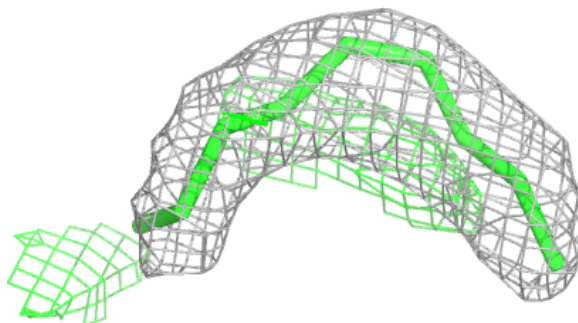
**Electron density around 12P A 514:**

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

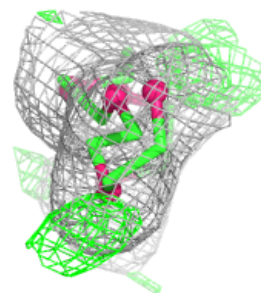
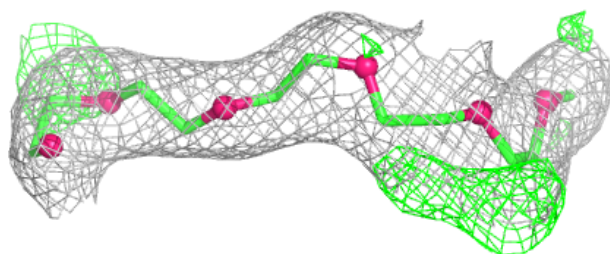
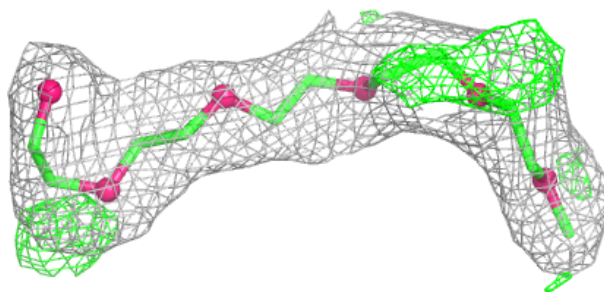


Electron density around OLC A 521:

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

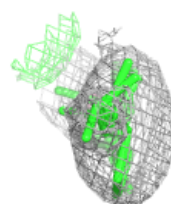
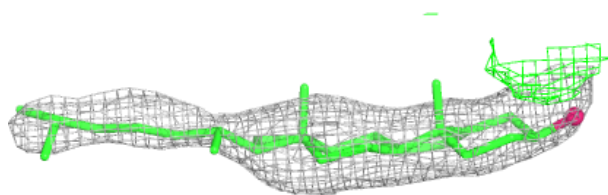
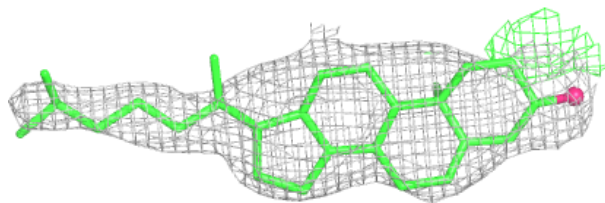
**Electron density around 12P A 508:**

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

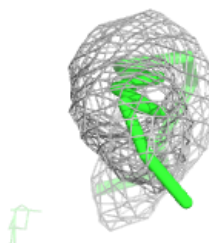
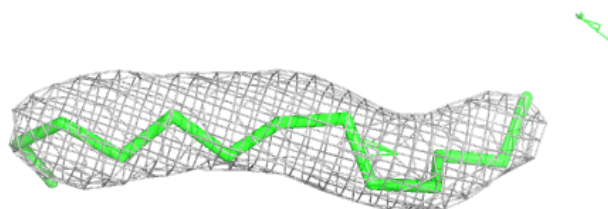
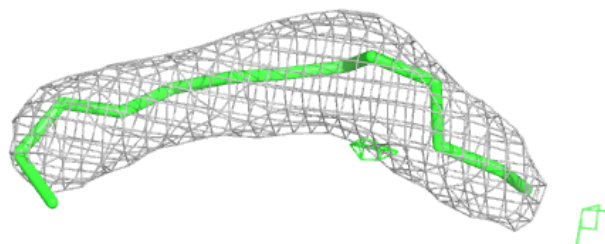


Electron density around CLR A 505:

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

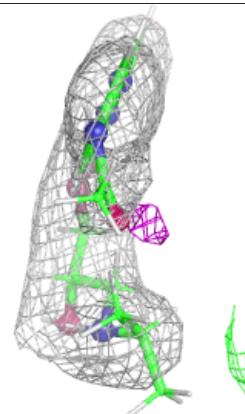
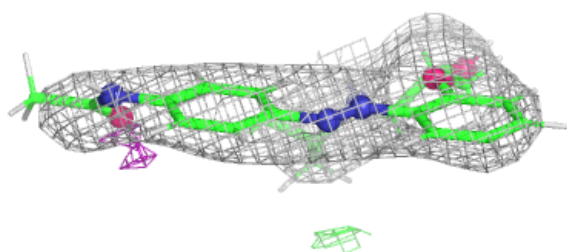
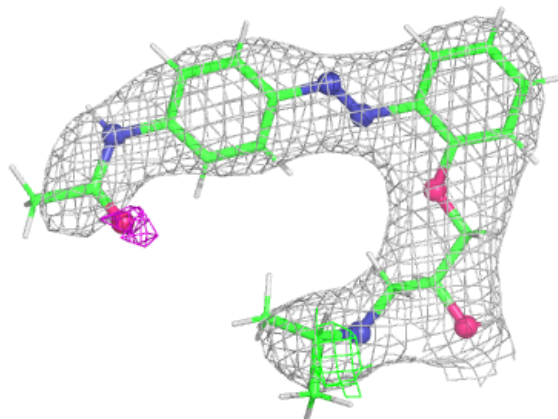
**Electron density around OLC A 513:**

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



Electron density around A1JHU A 510:

$2mF_o - DF_c$ (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.