



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 10:12 am BST

PDB ID : 9RKF / pdb_00009rkf
Title : Dark structure of beta-2 Adrenergic receptor with photoazolol in Dark state recorded at SwissFEL
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 : 2.45 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

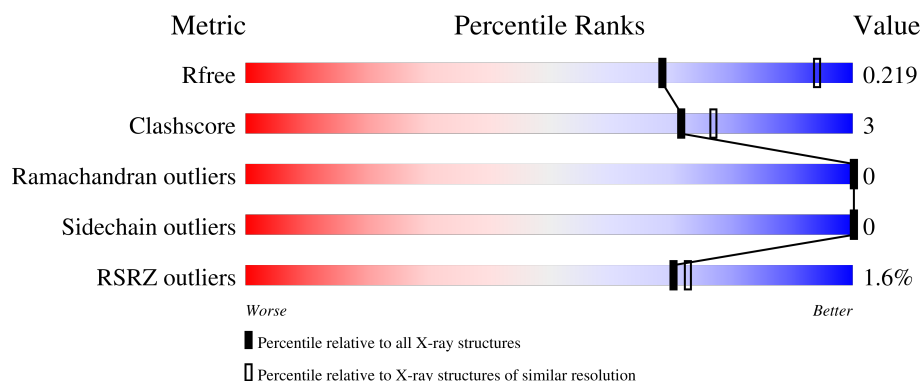
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

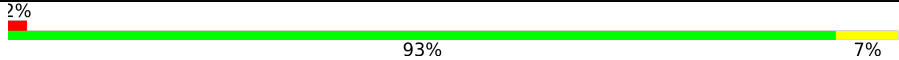
The reported resolution of this entry is 2.45 Å.

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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	443	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7669 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	443	7175	2327	3615	593	616	24	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

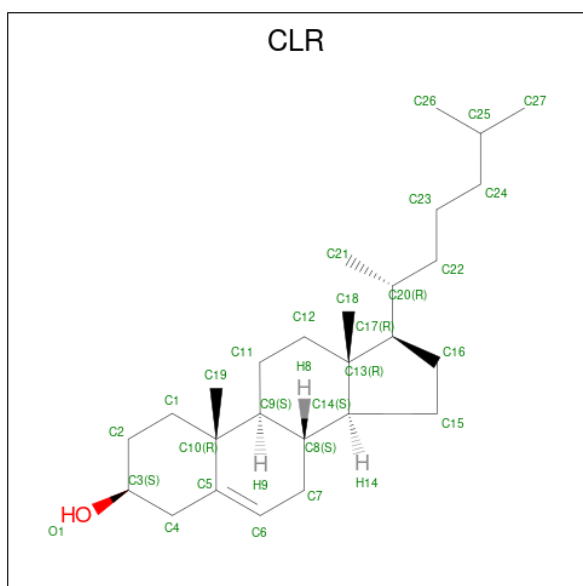
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	ARG	conflict	UNP P07550
A	122	TRP	GLU	conflict	UNP P07550
A	187	GLU	ASN	conflict	UNP P07550
A	241	GLY	ARG	conflict	UNP P00720
A	283	THR	CYS	conflict	UNP P00720
A	326	ALA	CYS	conflict	UNP P00720
A	366	ARG	ILE	conflict	UNP P00720

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



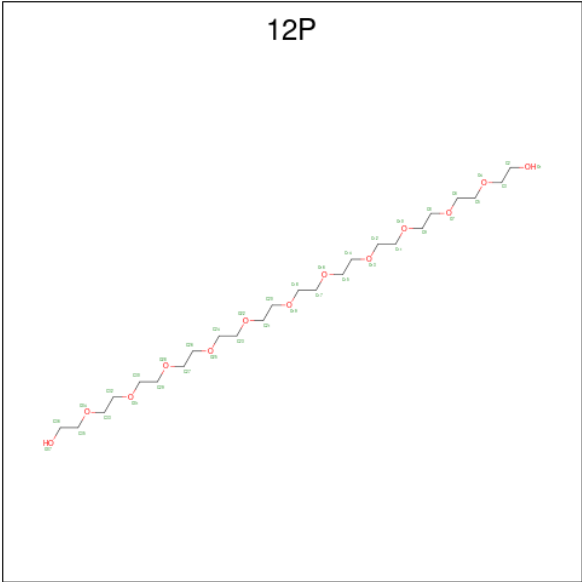
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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



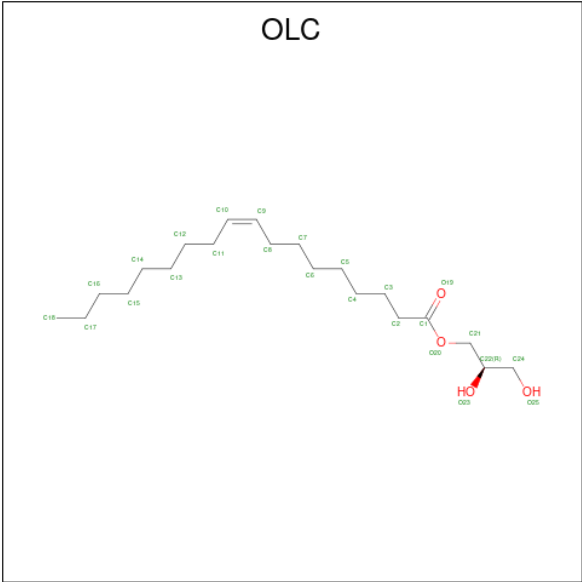
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0

- Molecule 4 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



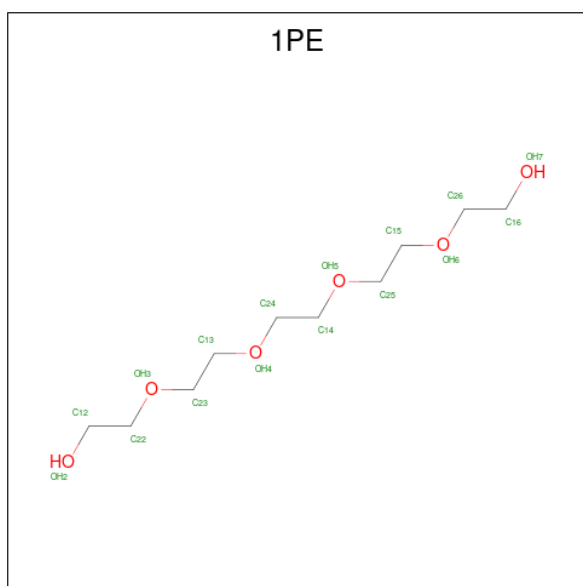
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	11	6		
4	A	1	Total	C	O	0	0
			20	13	7		
4	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



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

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			23	6	13	4		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



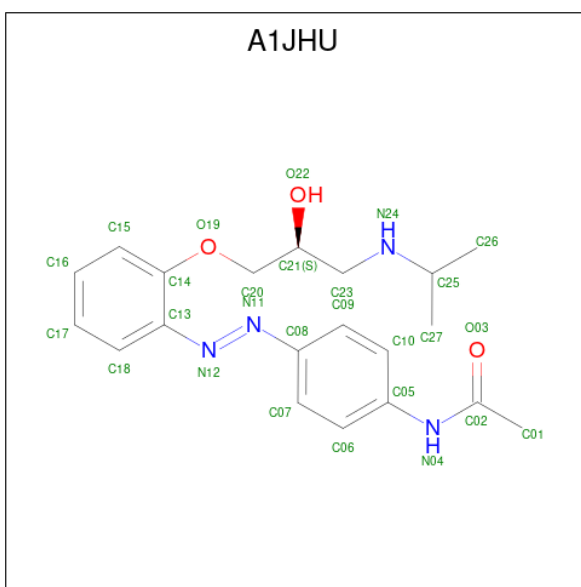
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



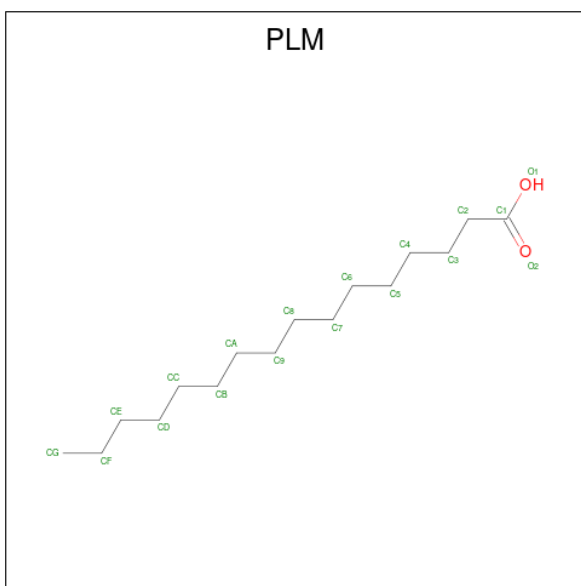
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is {N}-[4-[({E})-2-[(2 {S})-2-oxidanyl-3-(propan-2-ylamino)propoxy]phenyl]diazanyl]phenyl]ethanamide (CCD ID: A1JHU) (formula: $C_{20}H_{26}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



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

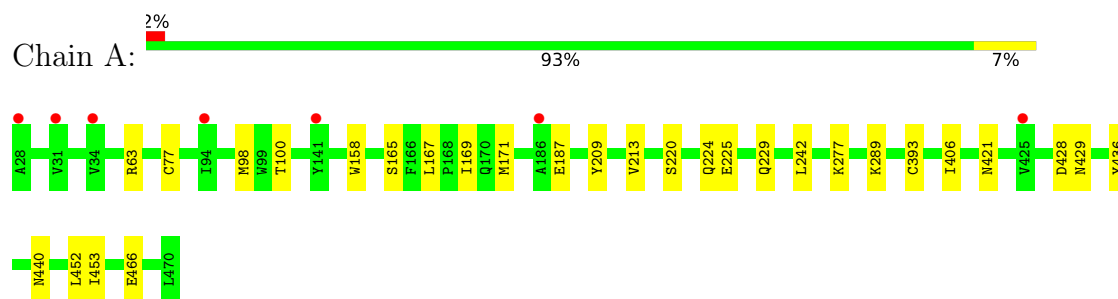
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	31	Total 31	O 31	0	0

3 Residue-property plots

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

- Molecule 1: Beta-2 adrenergic receptor, Endolysin



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)	45.60 – 2.45 45.60 – 2.45	Depositor EDS
% Data completeness (in resolution range)	86.3 (45.60-2.45) 86.3 (45.60-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20_4459)	Depositor
R, R_{free}	0.181 , 0.219 0.181 , 0.219	Depositor DCC
R_{free} test set	2007 reflections (7.26%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 100.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: CLR, PLM, 12P, GOL, EDO, 1PE, A1JHU, SO4, YCM, OLC

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	0.49	0/3632	0.36	0/4931

There are no bond length outliers.

There are no bond angle outliers.

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	3560	3615	3624	19	0
2	A	30	0	0	0	0
3	A	84	0	138	4	0
4	A	53	0	66	2	0
5	A	107	80	163	4	0
6	A	10	13	13	0	0
7	A	4	6	6	0	0
8	A	6	0	8	0	0
9	A	27	26	0	1	0
10	A	17	0	31	2	0
11	A	31	0	0	1	0
All	All	3929	3740	4049	26	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 3.

All (26) 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)
3:A:507:CLR:H242	10:A:521:PLM:HG2	1.67	0.77
1:A:187:GLU:OE2	11:A:601:HOH:O	2.10	0.69
1:A:466:GLU:C	1:A:466:GLU:OE1	2.39	0.65
1:A:277:LYS:HD2	1:A:277:LYS:O	1.99	0.63
1:A:209:TYR:O	1:A:213:VAL:HG23	2.01	0.61
3:A:507:CLR:H242	10:A:521:PLM:CG	2.36	0.55
1:A:421:ASN:OD1	1:A:436:TYR:OH	2.23	0.53
4:A:510:12P:H362	4:A:514:12P:H322	1.91	0.53
5:A:517:OLC:H11	5:A:517:OLC:H7A	1.91	0.52
1:A:158:TRP:CZ3	3:A:506:CLR:H213	2.45	0.51
1:A:406:ILE:HD13	1:A:453:ILE:HD13	1.96	0.48
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.79	0.47
1:A:428:ASP:OD1	1:A:429:ASN:N	2.48	0.47
1:A:220:SER:O	1:A:224:GLN:HG3	2.15	0.46
1:A:77:CYS:SG	3:A:508:CLR:H122	2.57	0.45
1:A:452:LEU:CD1	5:A:519:OLC:H8A	2.47	0.45
1:A:167:LEU:HD11	1:A:171:MET:HE2	1.99	0.45
1:A:225:GLU:O	1:A:229:GLN:HG3	2.17	0.44
4:A:514:12P:H242	4:A:514:12P:H271	1.82	0.44
1:A:165:SER:O	1:A:169:ILE:HD13	2.18	0.43
1:A:242:LEU:HD21	1:A:289:LYS:HG2	2.00	0.42
1:A:98:MET:HE2	1:A:100:THR:HG22	2.01	0.42
1:A:277:LYS:HD2	1:A:277:LYS:C	2.45	0.41
5:A:517:OLC:H7A	5:A:517:OLC:C11	2.50	0.41
5:A:517:OLC:H8	5:A:517:OLC:H5A	1.37	0.41
1:A:440:ASN:OD1	9:A:520:A1JHU:N24	2.53	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	440/443 (99%)	428 (97%)	12 (3%)	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	382/382 (100%)	382 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	224	GLN

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	1.00	0	4,10,12	3.26	1 (25%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	YCM	CE-CD-SG	-6.49	94.50	113.59

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	504	-	4,4,4	0.34	0	6,6,6	0.17	0
5	OLC	A	513	-	12,12,24	0.81	0	11,11,25	1.34	1 (9%)
5	OLC	A	517	-	24,24,24	1.07	1 (4%)	25,25,25	1.26	2 (8%)
6	1PE	A	515	-	9,9,15	0.18	0	8,8,14	0.12	0
9	A1JHU	A	520	-	28,28,28	1.41	4 (14%)	36,36,36	1.17	4 (11%)
10	PLM	A	521	1	16,16,17	0.54	0	15,15,17	0.44	0
5	OLC	A	519	-	18,18,24	1.13	1 (5%)	18,19,25	1.38	2 (11%)
4	12P	A	509	-	16,16,36	0.54	0	15,15,35	0.20	0
8	GOL	A	518	-	5,5,5	1.01	0	5,5,5	0.74	0
5	OLC	A	512	-	24,24,24	1.11	2 (8%)	25,25,25	1.22	2 (8%)
3	CLR	A	508	-	31,31,31	0.34	0	48,48,48	0.52	0
2	SO4	A	502[B]	-	4,4,4	0.11	0	6,6,6	0.07	0
5	OLC	A	511	-	24,24,24	1.13	2 (8%)	25,25,25	1.22	2 (8%)
3	CLR	A	507	-	31,31,31	0.40	0	48,48,48	0.48	0
2	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.24	0
4	12P	A	510	-	19,19,36	0.51	0	18,18,35	0.26	0
7	EDO	A	516	-	3,3,3	0.61	0	2,2,2	0.23	0
2	SO4	A	503	-	4,4,4	0.19	0	6,6,6	0.26	0
4	12P	A	514	-	15,15,36	0.55	0	14,14,35	0.29	0
3	CLR	A	506	-	31,31,31	0.45	0	48,48,48	0.72	0
2	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	502[A]	-	4,4,4	0.12	0	6,6,6	0.08	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	12P	A	514	-	-	6/13/13/34	-
9	A1JHU	A	520	-	-	2/19/19/19	0/2/2/2
10	PLM	A	521	1	-	2/13/14/15	-
5	OLC	A	513	-	-	5/10/10/24	-
5	OLC	A	519	-	-	7/18/18/24	-
4	12P	A	509	-	-	6/14/14/34	-
5	OLC	A	517	-	-	17/24/24/24	-
6	1PE	A	515	-	-	4/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	518	-	-	0/4/4/4	-
5	OLC	A	512	-	-	12/24/24/24	-
4	12P	A	510	-	-	9/17/17/34	-
3	CLR	A	508	-	-	4/10/68/68	0/4/4/4
3	CLR	A	506	-	-	5/10/68/68	0/4/4/4
7	EDO	A	516	-	-	0/1/1/1	-
5	OLC	A	511	-	-	8/24/24/24	-
3	CLR	A	507	-	-	0/10/68/68	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	520	A1JHU	C02-N04	5.52	1.46	1.36
5	A	517	OLC	O20-C1	3.21	1.42	1.33
5	A	512	OLC	O20-C1	3.15	1.42	1.33
5	A	511	OLC	O20-C1	3.05	1.42	1.33
5	A	519	OLC	O20-C1	2.92	1.41	1.33
5	A	511	OLC	C12-C11	2.51	1.62	1.52
9	A	520	A1JHU	O19-C14	2.23	1.42	1.37
9	A	520	A1JHU	C05-N04	2.16	1.46	1.41
5	A	512	OLC	C12-C11	2.09	1.60	1.52
9	A	520	A1JHU	O03-C02	-2.05	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	511	OLC	C8-C9-C10	4.34	158.02	124.73
5	A	512	OLC	C8-C9-C10	4.26	157.45	124.73
5	A	519	OLC	C8-C9-C10	3.67	152.91	124.73
5	A	517	OLC	C8-C9-C10	3.65	152.77	124.73
9	A	520	A1JHU	C01-C02-N04	3.65	120.34	114.98
5	A	513	OLC	C8-C9-C10	3.57	152.10	124.73
9	A	520	A1JHU	C13-N12-N11	3.40	122.41	114.56
9	A	520	A1JHU	C05-N04-C02	-3.01	122.52	127.99
5	A	519	OLC	O20-C1-C2	2.81	120.73	111.91
5	A	517	OLC	O20-C1-C2	2.63	120.15	111.91
5	A	511	OLC	O20-C1-C2	2.43	119.55	111.91
5	A	512	OLC	O20-C1-C2	2.41	119.48	111.91
9	A	520	A1JHU	O03-C02-C01	-2.03	118.28	122.06

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	517	OLC	O20-C21-C22-O23
5	A	519	OLC	C9-C10-C11-C12
5	A	519	OLC	C21-C22-C24-O25
5	A	511	OLC	O19-C1-O20-C21
3	A	506	CLR	C16-C17-C20-C21
3	A	506	CLR	C13-C17-C20-C21
5	A	511	OLC	C2-C1-O20-C21
3	A	506	CLR	C13-C17-C20-C22
3	A	506	CLR	C16-C17-C20-C22
5	A	517	OLC	C3-C4-C5-C6
4	A	510	12P	O28-C29-C30-O31
5	A	517	OLC	C5-C6-C7-C8
5	A	517	OLC	C2-C1-O20-C21
4	A	510	12P	O22-C23-C24-O25
5	A	512	OLC	C2-C1-O20-C21
4	A	510	12P	O25-C26-C27-O28
4	A	514	12P	C36-C35-O34-C33
6	A	515	1PE	OH5-C14-C24-OH4
5	A	517	OLC	O19-C1-O20-C21
4	A	514	12P	O31-C32-C33-O34
5	A	519	OLC	C1-C2-C3-C4
4	A	509	12P	O22-C23-C24-O25
5	A	512	OLC	O19-C1-O20-C21
5	A	512	OLC	C1-C2-C3-C4
4	A	514	12P	O22-C23-C24-O25
6	A	515	1PE	OH7-C16-C26-OH6
5	A	517	OLC	O20-C21-C22-C24
5	A	519	OLC	C3-C4-C5-C6
5	A	517	OLC	C12-C13-C14-C15
5	A	517	OLC	C14-C15-C16-C17
5	A	512	OLC	C3-C4-C5-C6
5	A	512	OLC	C21-C22-C24-O25
5	A	511	OLC	O20-C21-C22-O23
5	A	511	OLC	C11-C12-C13-C14
5	A	512	OLC	C12-C13-C14-C15
5	A	519	OLC	O23-C22-C24-O25
5	A	517	OLC	C11-C12-C13-C14
5	A	519	OLC	C6-C7-C8-C9
5	A	513	OLC	C11-C12-C13-C14
5	A	513	OLC	C12-C13-C14-C15
5	A	512	OLC	C2-C3-C4-C5
5	A	511	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	A	520	A1JHU	C26-C25-N24-C23
9	A	520	A1JHU	C27-C25-N24-C23
5	A	512	OLC	C11-C12-C13-C14
5	A	512	OLC	O23-C22-C24-O25
4	A	510	12P	O31-C32-C33-O34
5	A	511	OLC	O20-C21-C22-C24
4	A	509	12P	O25-C26-C27-O28
5	A	517	OLC	O20-C1-C2-C3
3	A	506	CLR	C20-C22-C23-C24
5	A	511	OLC	C3-C4-C5-C6
5	A	513	OLC	C3-C4-C5-C6
5	A	512	OLC	C13-C14-C15-C16
4	A	510	12P	C23-C24-O25-C26
10	A	521	PLM	C7-C8-C9-CA
5	A	519	OLC	C4-C5-C6-C7
5	A	517	OLC	O23-C22-C24-O25
4	A	509	12P	O16-C17-C18-O19
4	A	509	12P	C26-C27-O28-C29
4	A	510	12P	O34-C35-C36-O37
3	A	508	CLR	C13-C17-C20-C21
3	A	508	CLR	C13-C17-C20-C22
4	A	514	12P	C29-C30-O31-C32
4	A	510	12P	O19-C20-C21-O22
3	A	508	CLR	C16-C17-C20-C22
4	A	510	12P	C24-C23-O22-C21
5	A	517	OLC	C13-C14-C15-C16
5	A	517	OLC	C6-C7-C8-C9
5	A	517	OLC	C4-C5-C6-C7
5	A	513	OLC	C7-C8-C9-C10
4	A	510	12P	C29-C30-O31-C32
3	A	508	CLR	C16-C17-C20-C21
5	A	517	OLC	O19-C1-C2-C3
5	A	512	OLC	C4-C5-C6-C7
4	A	509	12P	C20-C21-O22-C23
4	A	514	12P	C23-C24-O25-C26
10	A	521	PLM	C8-C9-CA-CB
4	A	514	12P	C27-C26-O25-C24
4	A	509	12P	C24-C23-O22-C21
5	A	517	OLC	C9-C10-C11-C12
6	A	515	1PE	OH6-C15-C25-OH5
6	A	515	1PE	C25-C15-OH6-C26
5	A	513	OLC	C9-C10-C11-C12

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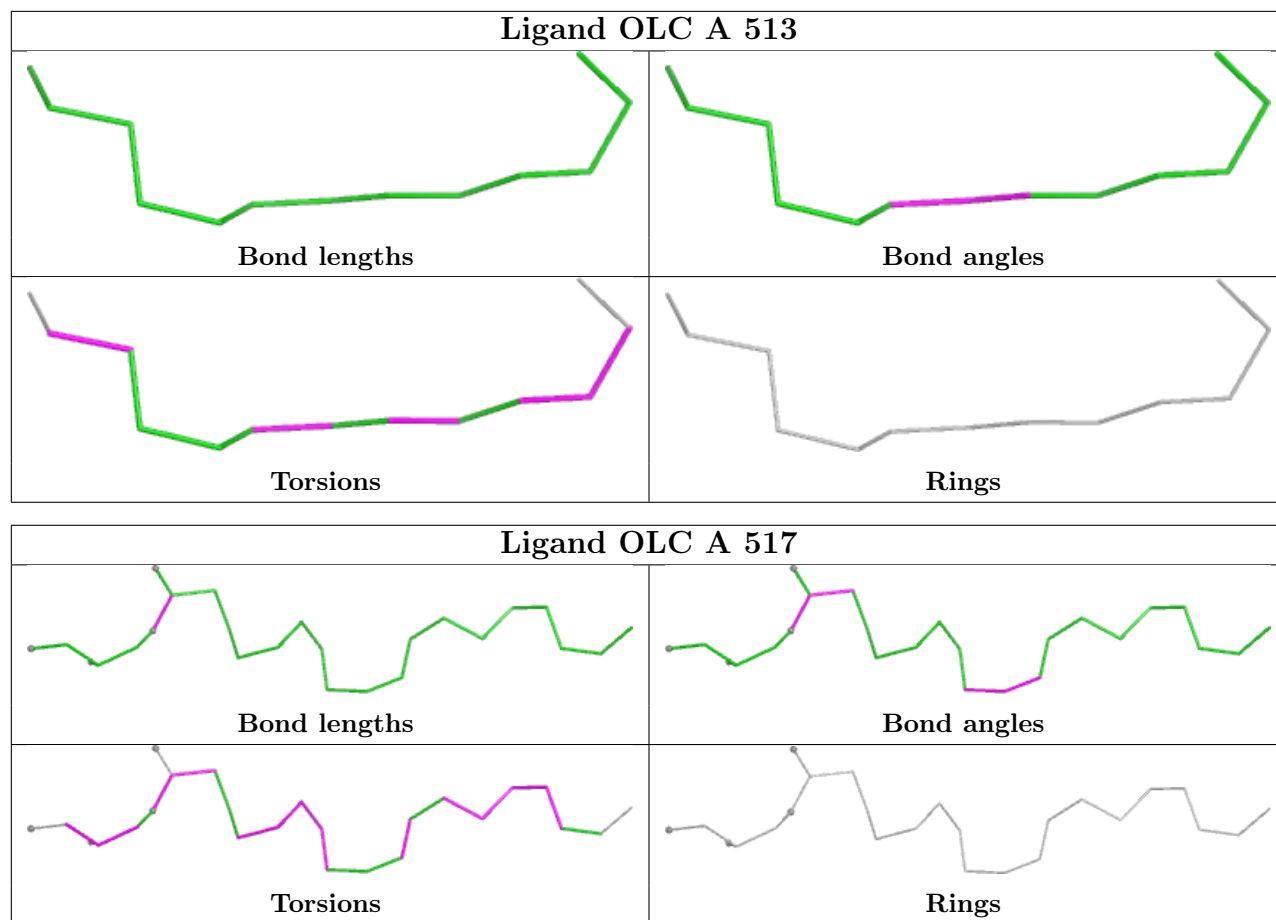
Mol	Chain	Res	Type	Atoms
5	A	517	OLC	C21-C22-C24-O25
5	A	511	OLC	C2-C3-C4-C5
5	A	512	OLC	C7-C8-C9-C10

There are no ring outliers.

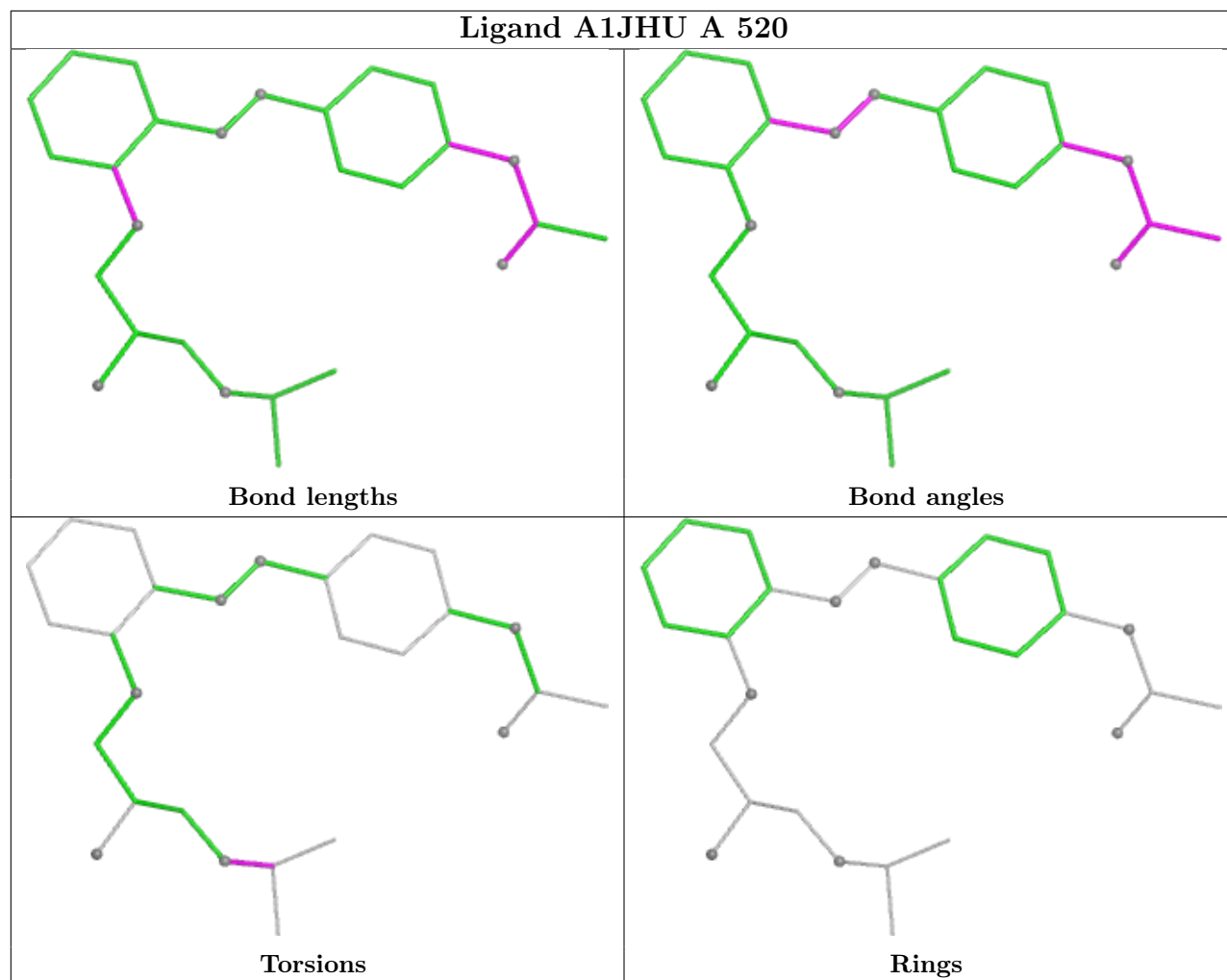
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	517	OLC	3	0
9	A	520	A1JHU	1	0
10	A	521	PLM	2	0
5	A	519	OLC	1	0
3	A	508	CLR	1	0
3	A	507	CLR	2	0
4	A	510	12P	1	0
4	A	514	12P	2	0
3	A	506	CLR	1	0

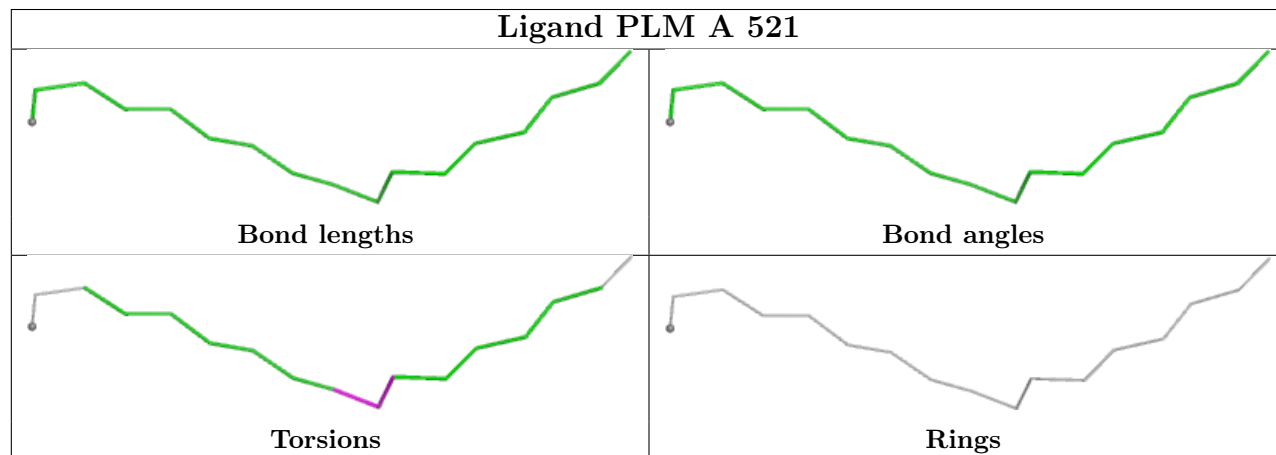
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

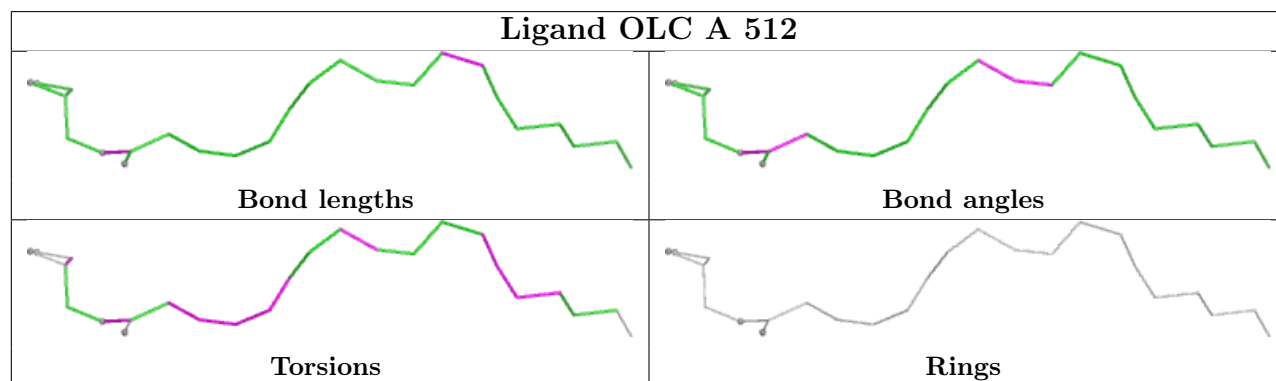
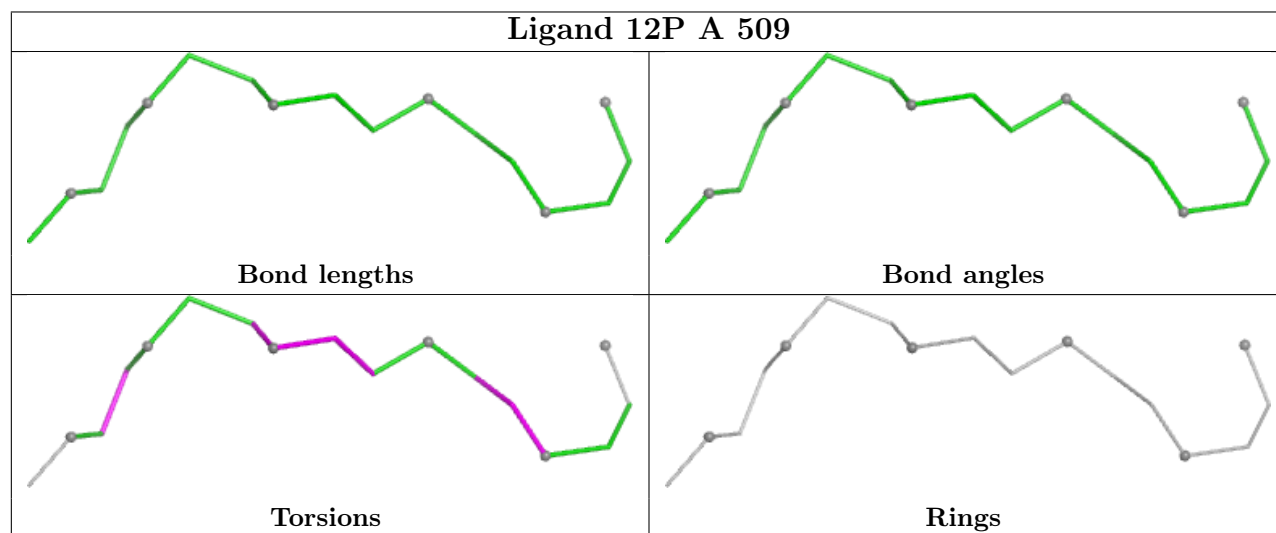
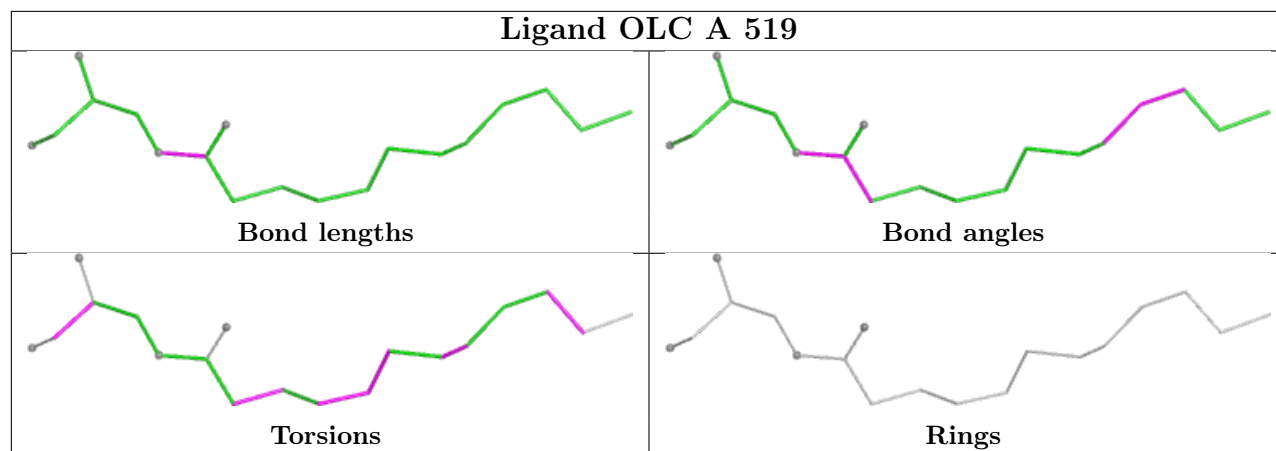


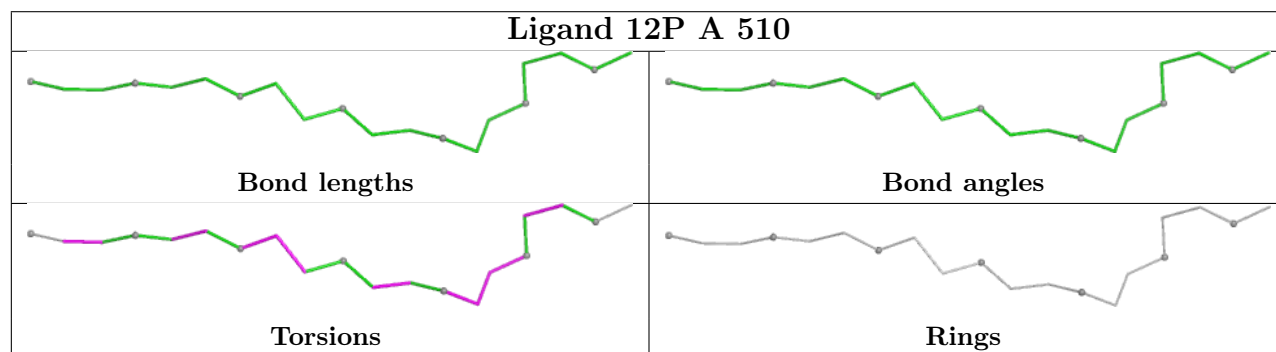
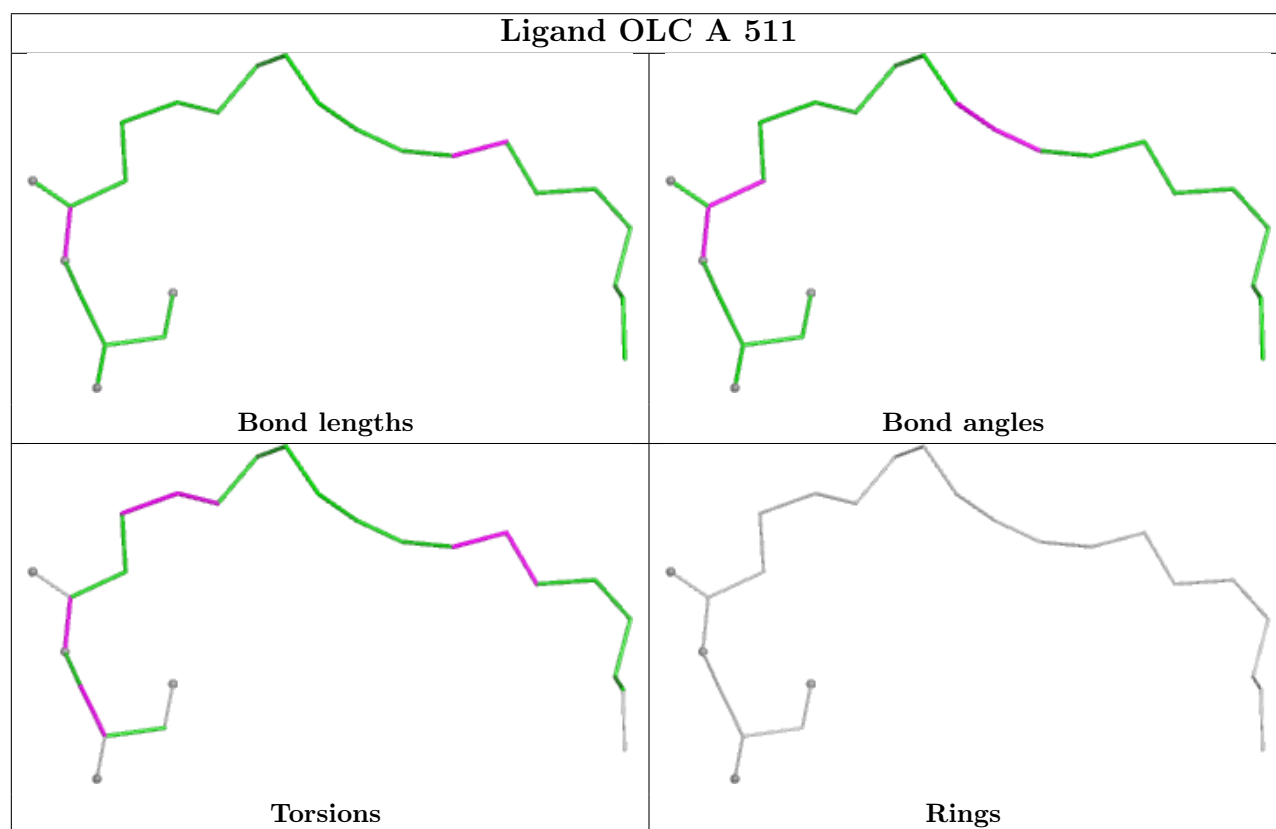
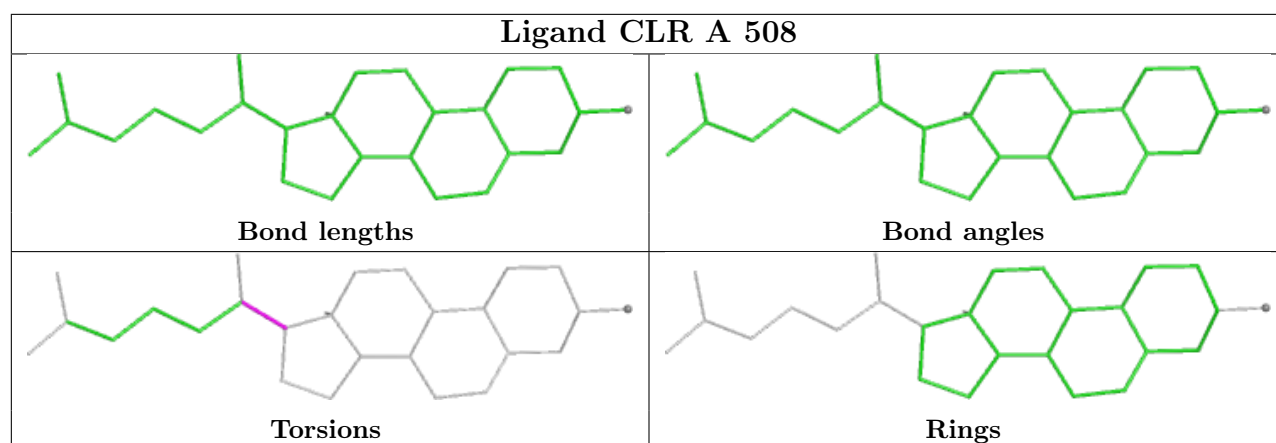
Ligand A1JHU A 520

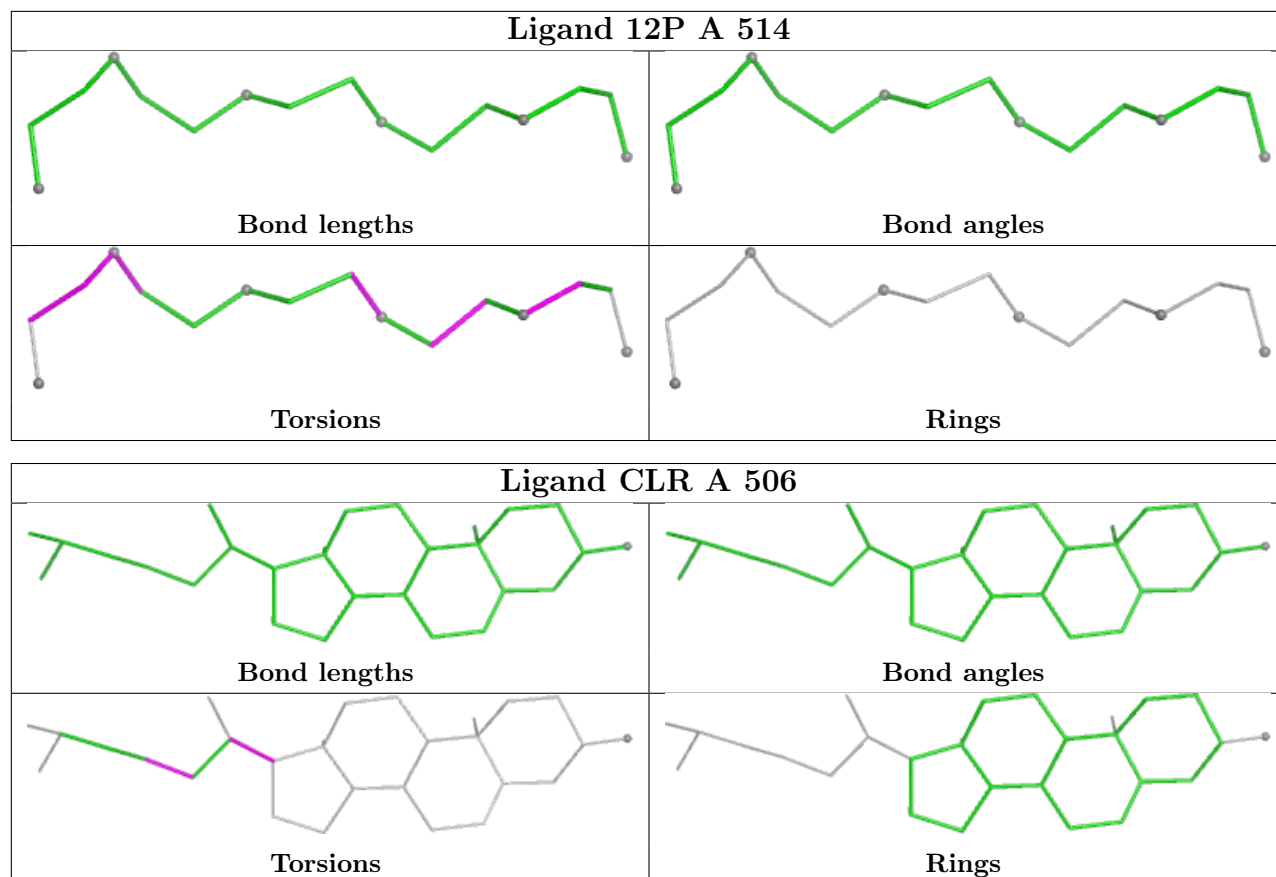


Ligand PLM A 521









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	442/443 (99%)	-0.07	7 (1%) 70 73	45, 79, 131, 212	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	ALA	4.8
1	A	31	VAL	3.3
1	A	34	VAL	2.8
1	A	186	ALA	2.6
1	A	425	VAL	2.4
1	A	141	TYR	2.3
1	A	94	ILE	2.0

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	0.98	0.07	50,59,77,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

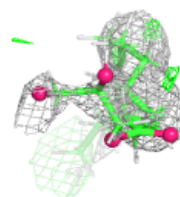
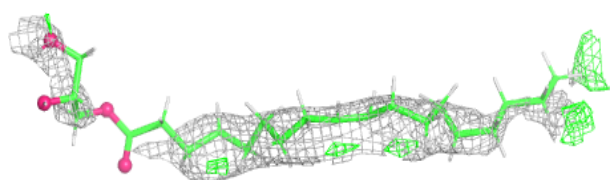
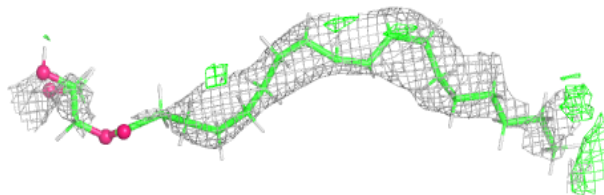
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OLC	A	512	25/25	0.77	0.22	95,126,169,173	0
2	SO4	A	502[B]	5/5	0.78	0.09	71,71,78,78	5
2	SO4	A	502[A]	5/5	0.78	0.09	76,82,84,95	5
8	GOL	A	518	6/6	0.79	0.20	83,87,91,91	0
2	SO4	A	505	5/5	0.80	0.09	89,96,124,138	0
5	OLC	A	511	25/25	0.80	0.16	95,129,175,179	0
5	OLC	A	517	25/25	0.81	0.25	91,99,112,113	0
4	12P	A	510	20/37	0.81	0.19	77,91,103,107	0
5	OLC	A	519	19/25	0.85	0.23	64,94,108,110	0
3	CLR	A	508	28/28	0.85	0.21	98,117,129,133	0
7	EDO	A	516	4/4	0.86	0.16	83,101,122,122	0
10	PLM	A	521	17/18	0.86	0.18	80,92,103,115	0
4	12P	A	514	16/37	0.90	0.14	72,82,92,94	0
6	1PE	A	515	10/16	0.91	0.15	73,96,114,116	0
4	12P	A	509	17/37	0.91	0.15	60,78,98,101	0
3	CLR	A	506	28/28	0.93	0.18	86,99,106,116	0
5	OLC	A	513	13/25	0.93	0.17	62,69,87,90	0
3	CLR	A	507	28/28	0.94	0.10	77,88,97,101	0
2	SO4	A	503	5/5	0.95	0.10	58,72,78,83	0
9	A1JHU	A	520	27/27	0.95	0.10	61,80,106,110	0
2	SO4	A	504	5/5	0.95	0.14	71,77,88,91	0
2	SO4	A	501	5/5	0.99	0.05	62,64,72,84	0

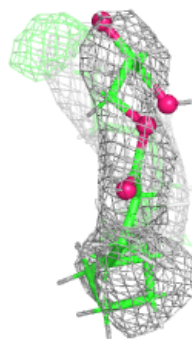
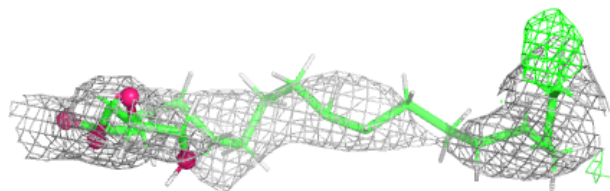
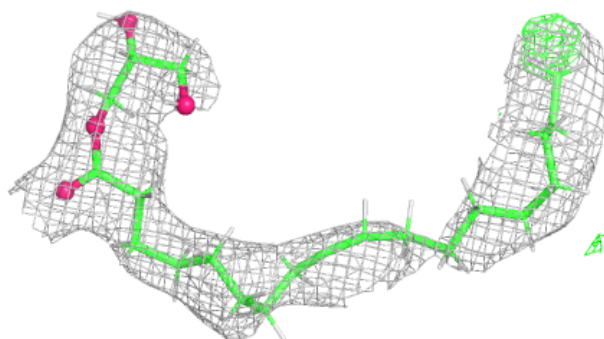
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 512:

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

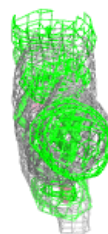
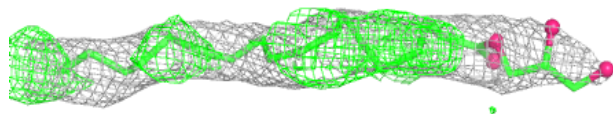
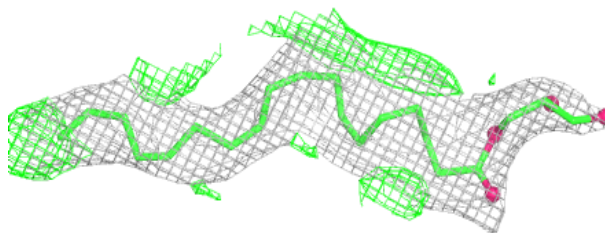
**Electron density around OLC A 511:**

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

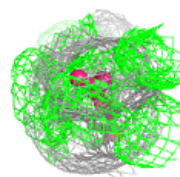
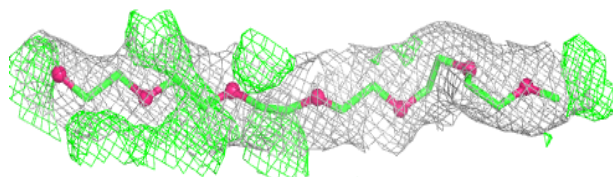
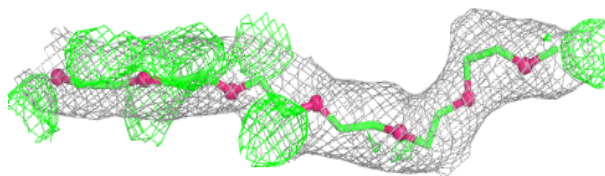


Electron density around OLC A 517:

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

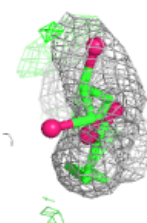
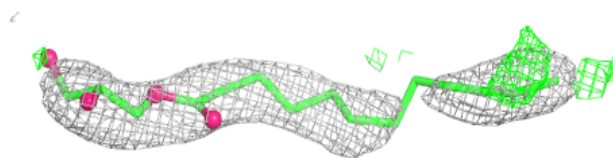
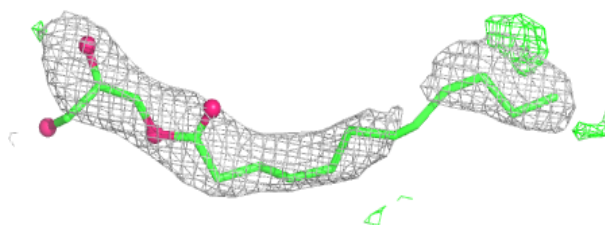
**Electron density around 12P A 510:**

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

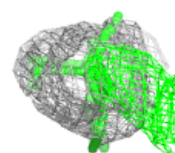
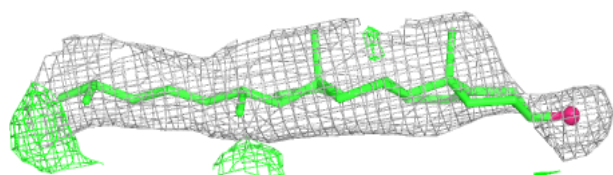
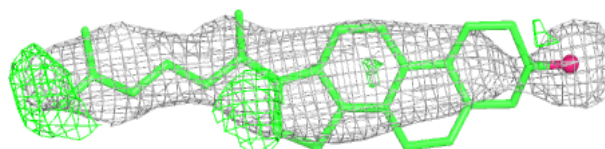


Electron density around OLC A 519:

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

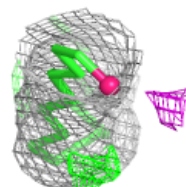
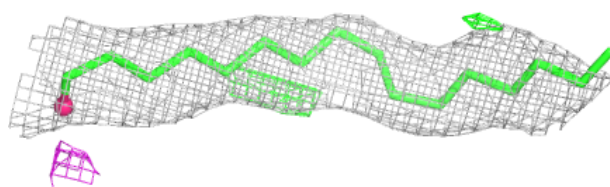
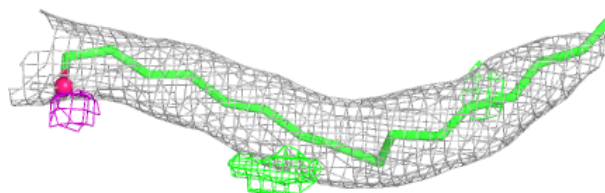
**Electron density around CLR A 508:**

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

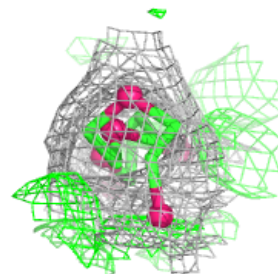
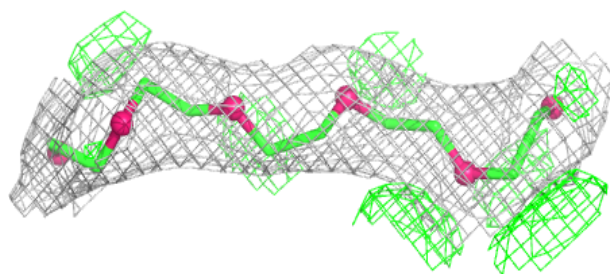
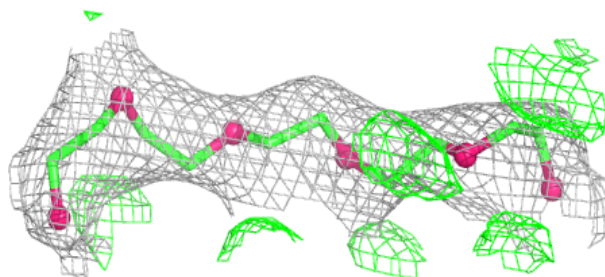


Electron density around PLM A 521:

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

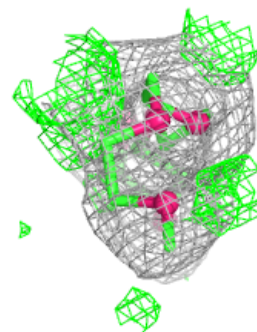
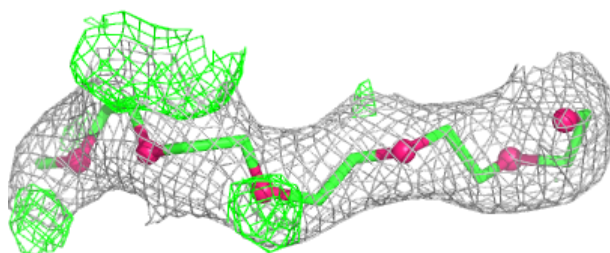
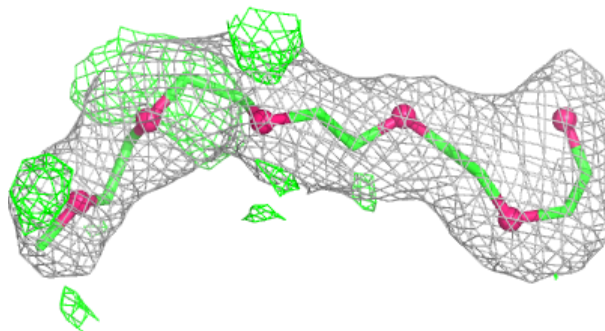
**Electron density around 12P A 514:**

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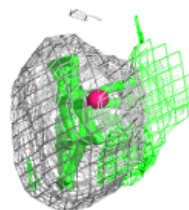
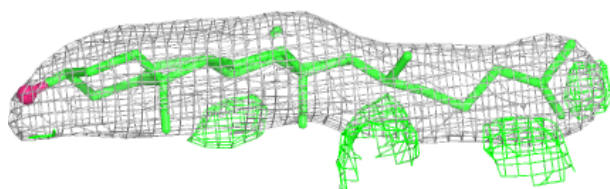
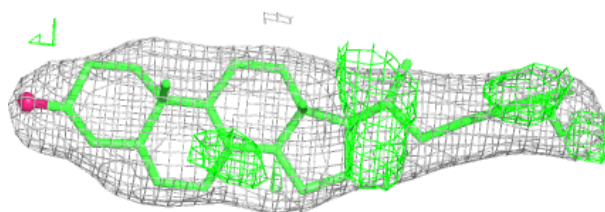


Electron density around 12P A 509:

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

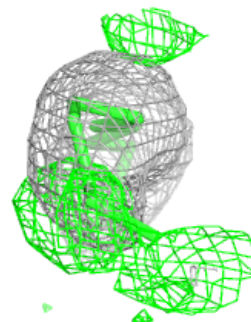
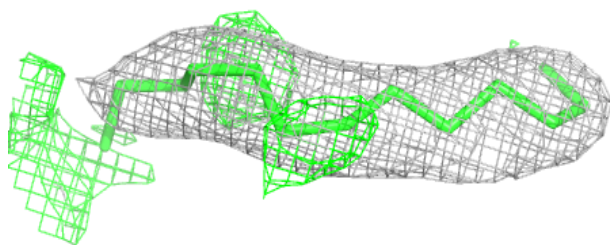
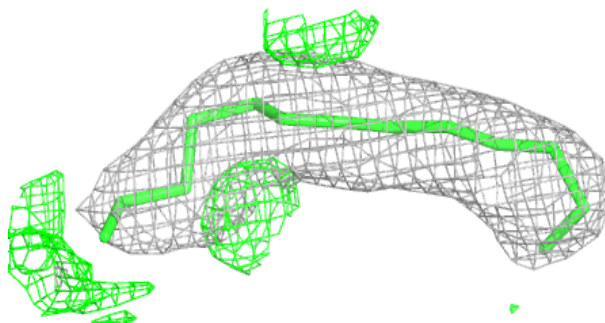
**Electron density around CLR A 506:**

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

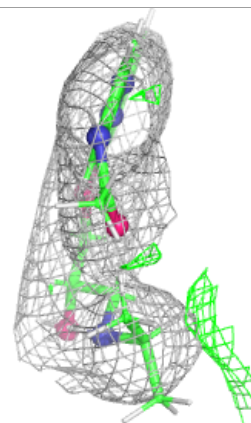
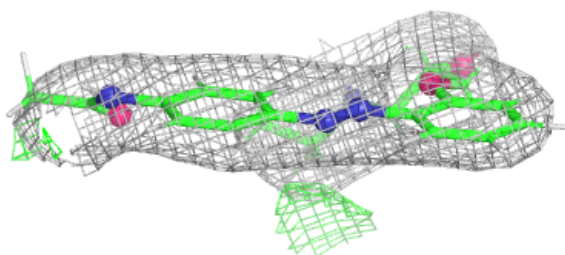
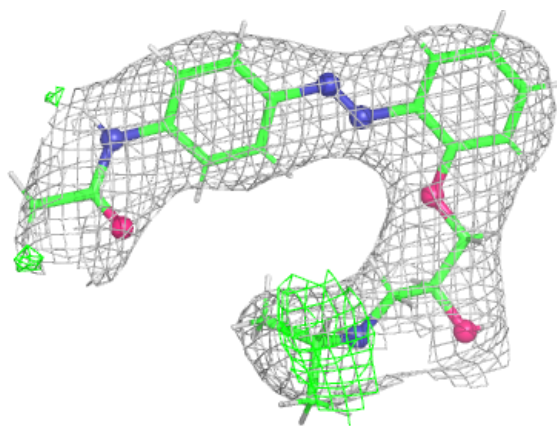


Electron density around OLC A 513:

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

**Electron density around A1JHU A 520:**

$2mF_o-DF_c$ (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.