



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:08 AM UTC

PDB ID : 5HYA / pdb_00005hya
Title : Structural mechanisms of extracellular ion exchange and induced binding-site occlusion in the sodium-calcium exchanger NCX_Mj soaked with 150 mM Na⁺ and nominal Ca²⁺
Authors : Liao, J.; Jiang, Y.X.; Faraldo-Gomez, J.D.
Deposited on : 2016-02-01
Resolution : 1.90 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

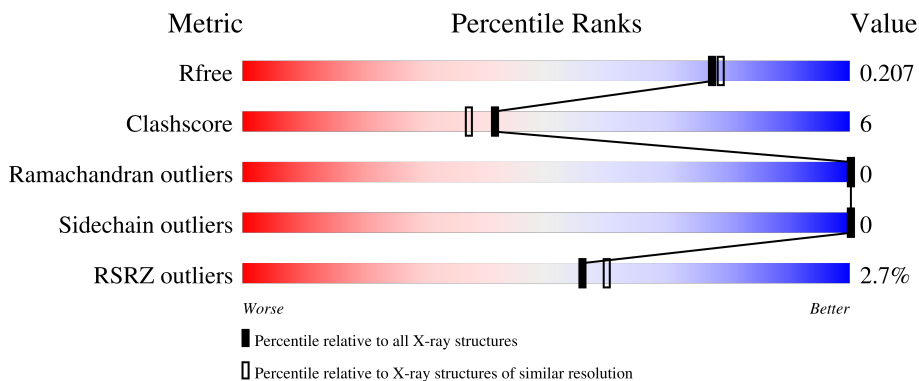
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	304	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2590 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 sodium,calcium exchanger.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2229	1489	352	377	11	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q57556
A	303	GLY	-	expression tag	UNP Q57556
A	304	GLY	-	expression tag	UNP Q57556

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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

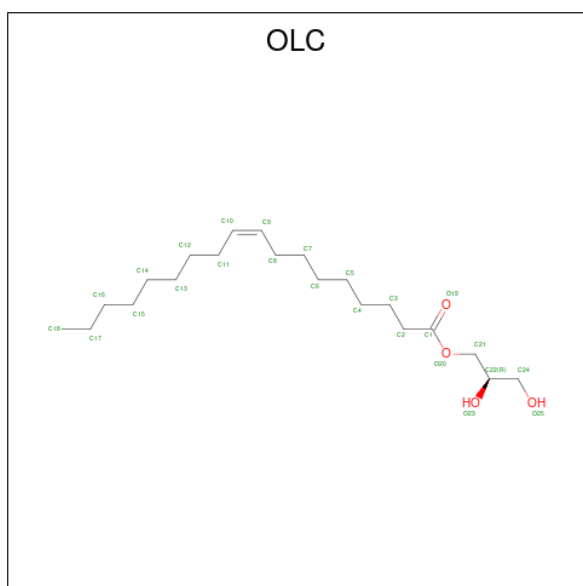
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



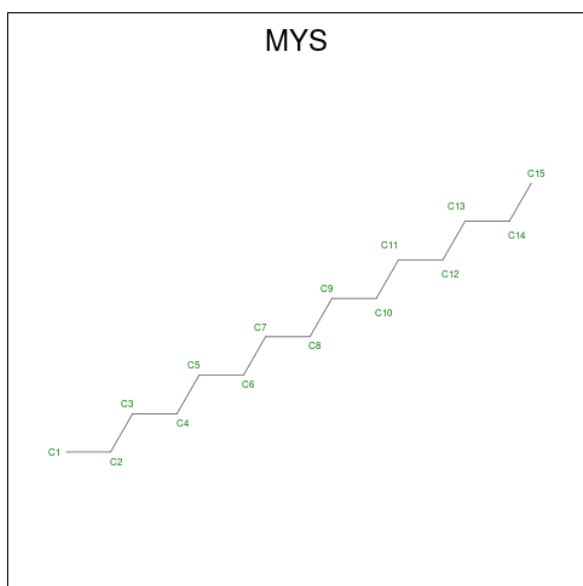
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- 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	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			20	16	4		
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



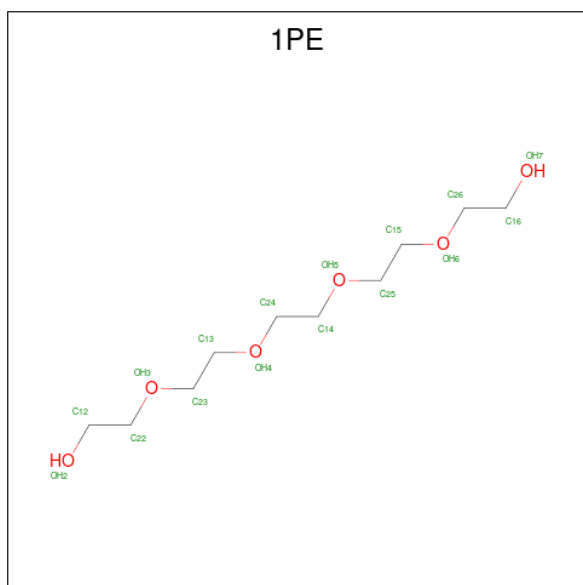
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C	0	0
			15	15		
6	A	1	Total	C	0	0
			12	12		
6	A	1	Total	C	0	0
			10	10		
6	A	1	Total	C	0	0
			5	5		
6	A	1	Total	C	0	0
			15	15		
6	A	1	Total	C	0	0
			15	15		
6	A	1	Total	C	0	0
			14	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 5 5	0	0
6	A	1	Total C 14 14	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0

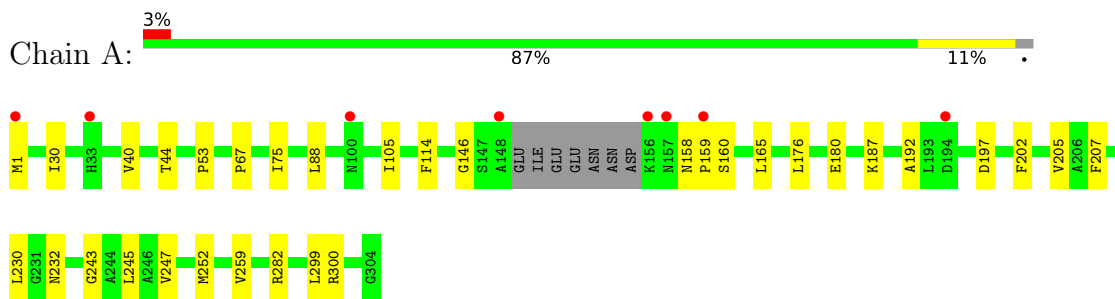
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	100	Total O 100 100	0	0

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: sodium,calcium exchanger



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.49Å 72.88Å 96.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.67 – 1.90 37.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.67-1.90) 93.9 (37.67-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.179 , 0.207 0.181 , 0.207	Depositor DCC
R_{free} test set	2000 reflections (7.16%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2590	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: ACT, NA, 1PE, CA, OLC, MYS

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	0.42	0/2274	0.71	0/3089

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	2229	0	2375	27	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	16	0	12	0	0
5	A	120	0	186	17	0
6	A	105	0	198	6	0
7	A	16	0	22	0	0
8	A	100	0	0	1	0
All	All	2590	0	2793	34	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 (34) 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:53:PRO:HB3	5:A:422:OLC:H22	1.69	0.74
1:A:197:ASP:H	5:A:411:OLC:H21A	1.51	0.74
1:A:299:LEU:HD23	6:A:419:MYS:H111	1.72	0.71
1:A:40:VAL:HG21	1:A:146:GLY:HA3	1.81	0.63
1:A:259:VAL:HG11	6:A:419:MYS:H112	1.82	0.60
1:A:114:PHE:CD1	5:A:410:OLC:H10	2.42	0.55
1:A:176:LEU:HD13	5:A:422:OLC:H7A	1.88	0.55
1:A:180:GLU:OE1	5:A:422:OLC:H21	2.07	0.55
1:A:67:PRO:HD3	1:A:252:MET:SD	2.48	0.54
1:A:282:ARG:HE	6:A:418:MYS:H52	1.74	0.52
1:A:158:ASN:OD1	1:A:160:SER:HB2	2.10	0.51
1:A:30:ILE:HD11	1:A:165:LEU:HG	1.95	0.49
1:A:53:PRO:HA	5:A:422:OLC:H2A	1.94	0.48
1:A:202:PHE:HA	1:A:205:VAL:HG23	1.95	0.48
1:A:105:ILE:HD11	1:A:230:LEU:HD21	1.95	0.48
1:A:300:ARG:H	6:A:419:MYS:H131	1.79	0.47
1:A:232:ASN:HB3	8:A:502:HOH:O	2.15	0.47
1:A:1:MET:HG3	1:A:192:ALA:HB2	1.97	0.47
5:A:423:OLC:H7	5:A:423:OLC:H4A	1.50	0.45
1:A:300:ARG:H	6:A:419:MYS:C13	2.29	0.45
1:A:88:LEU:HD11	5:A:423:OLC:H10	1.99	0.45
1:A:53:PRO:CB	5:A:422:OLC:H22	2.44	0.43
1:A:187:LYS:HD3	5:A:411:OLC:H6A	2.01	0.43
1:A:207:PHE:HB2	5:A:423:OLC:H24A	2.01	0.43
5:A:411:OLC:H6	5:A:411:OLC:H3A	1.90	0.43
5:A:409:OLC:H8	5:A:409:OLC:H11	1.52	0.42
1:A:243:GLY:O	1:A:247:VAL:HG23	2.20	0.41
5:A:411:OLC:H11	5:A:411:OLC:H8	1.49	0.41
5:A:409:OLC:H2	5:A:410:OLC:O19	2.20	0.41
1:A:44:THR:HB	6:A:413:MYS:H72	2.03	0.41
5:A:422:OLC:H11	5:A:422:OLC:H8A	1.97	0.41
1:A:75:ILE:HD11	1:A:245:LEU:HD12	2.03	0.41
1:A:158:ASN:HA	1:A:159:PRO:HD2	1.82	0.41
5:A:409:OLC:H12	5:A:410:OLC:H12A	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	294/304 (97%)	289 (98%)	5 (2%)	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	236/242 (98%)	236 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	73	ASN
1	A	104	ASN
1	A	253	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	406	-	3,3,3	0.82	0	3,3,3	1.36	0
4	ACT	A	408	-	3,3,3	0.80	0	3,3,3	1.38	0
6	MYS	A	416	-	4,4,14	0.14	0	3,3,13	0.29	0
7	1PE	A	415	-	15,15,15	0.65	0	14,14,14	0.33	0
6	MYS	A	421	-	13,13,14	0.08	0	12,12,13	0.37	0
6	MYS	A	420	-	4,4,14	0.16	0	3,3,13	0.27	0
4	ACT	A	405	-	3,3,3	0.82	0	3,3,3	1.36	0
6	MYS	A	412	-	14,14,14	0.10	0	13,13,13	0.45	0
6	MYS	A	418	-	14,14,14	0.10	0	13,13,13	0.56	0
6	MYS	A	419	-	13,13,14	0.08	0	12,12,13	0.46	0
6	MYS	A	414	-	9,9,14	0.10	0	8,8,13	0.56	0
6	MYS	A	417	-	14,14,14	0.09	0	13,13,13	0.35	0
5	OLC	A	411	-	24,24,24	1.37	2 (8%)	25,25,25	1.00	1 (4%)
5	OLC	A	409	3	24,24,24	1.37	2 (8%)	25,25,25	0.93	1 (4%)
5	OLC	A	422	-	19,19,24	1.50	2 (10%)	20,20,25	0.98	1 (5%)
5	OLC	A	423	-	24,24,24	1.35	2 (8%)	25,25,25	0.84	1 (4%)
6	MYS	A	413	-	11,11,14	0.10	0	10,10,13	0.35	0
4	ACT	A	407	-	3,3,3	0.80	0	3,3,3	1.37	0
5	OLC	A	410	-	24,24,24	1.35	2 (8%)	25,25,25	0.82	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MYS	A	412	-	-	7/12/12/12	-
5	OLC	A	411	-	-	9/24/24/24	-
6	MYS	A	418	-	-	6/12/12/12	-
6	MYS	A	416	-	-	0/2/2/12	-
6	MYS	A	419	-	-	0/11/11/12	-
5	OLC	A	409	3	-	6/24/24/24	-
7	1PE	A	415	-	-	2/13/13/13	-
5	OLC	A	422	-	-	13/19/19/24	-
6	MYS	A	414	-	-	3/7/7/12	-
5	OLC	A	423	-	-	12/24/24/24	-
6	MYS	A	417	-	-	1/12/12/12	-
6	MYS	A	421	-	-	2/11/11/12	-
6	MYS	A	420	-	-	0/2/2/12	-
6	MYS	A	413	-	-	2/9/9/12	-
5	OLC	A	410	-	-	13/24/24/24	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	422	OLC	C9-C10	4.19	1.55	1.31
5	A	411	OLC	C9-C10	4.18	1.55	1.31
5	A	409	OLC	C9-C10	4.18	1.55	1.31
5	A	423	OLC	C9-C10	4.16	1.55	1.31
5	A	410	OLC	C9-C10	4.08	1.54	1.31
5	A	410	OLC	O20-C1	3.66	1.44	1.33
5	A	409	OLC	O20-C1	3.66	1.44	1.33
5	A	422	OLC	O20-C1	3.61	1.43	1.33
5	A	423	OLC	O20-C1	3.58	1.43	1.33
5	A	411	OLC	O20-C1	3.57	1.43	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	409	OLC	O20-C1-C2	2.92	120.73	111.83
5	A	411	OLC	O20-C1-C2	2.92	120.73	111.83
5	A	423	OLC	O20-C1-C2	2.79	120.34	111.83
5	A	422	OLC	O20-C1-C2	2.72	120.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	410	OLC	O20-C1-C2	2.23	118.62	111.83

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	410	OLC	O20-C21-C22-C24
5	A	422	OLC	O19-C1-O20-C21
5	A	422	OLC	C2-C1-O20-C21
5	A	410	OLC	O20-C21-C22-O23
5	A	410	OLC	C13-C14-C15-C16
5	A	423	OLC	C4-C5-C6-C7
6	A	413	MYS	C6-C7-C8-C9
5	A	410	OLC	C11-C10-C9-C8
5	A	422	OLC	C1-C2-C3-C4
5	A	422	OLC	C21-C22-C24-O25
5	A	410	OLC	C4-C5-C6-C7
5	A	411	OLC	C6-C7-C8-C9
6	A	412	MYS	C4-C5-C6-C7
5	A	423	OLC	C2-C3-C4-C5
5	A	410	OLC	C15-C16-C17-C18
6	A	418	MYS	C4-C5-C6-C7
5	A	422	OLC	C3-C4-C5-C6
5	A	411	OLC	C12-C13-C14-C15
5	A	422	OLC	C11-C10-C9-C8
5	A	409	OLC	C4-C5-C6-C7
5	A	411	OLC	C13-C14-C15-C16
5	A	410	OLC	C11-C12-C13-C14
6	A	418	MYS	C5-C6-C7-C8
5	A	410	OLC	C22-C21-O20-C1
5	A	423	OLC	C6-C7-C8-C9
6	A	418	MYS	C3-C4-C5-C6
5	A	409	OLC	C5-C6-C7-C8
5	A	409	OLC	C3-C4-C5-C6
5	A	423	OLC	C10-C11-C12-C13
5	A	411	OLC	C3-C4-C5-C6
6	A	412	MYS	C2-C3-C4-C5
5	A	423	OLC	C3-C4-C5-C6
6	A	412	MYS	C7-C8-C9-C10
5	A	423	OLC	C11-C12-C13-C14
5	A	410	OLC	O20-C1-C2-C3
5	A	409	OLC	C6-C7-C8-C9

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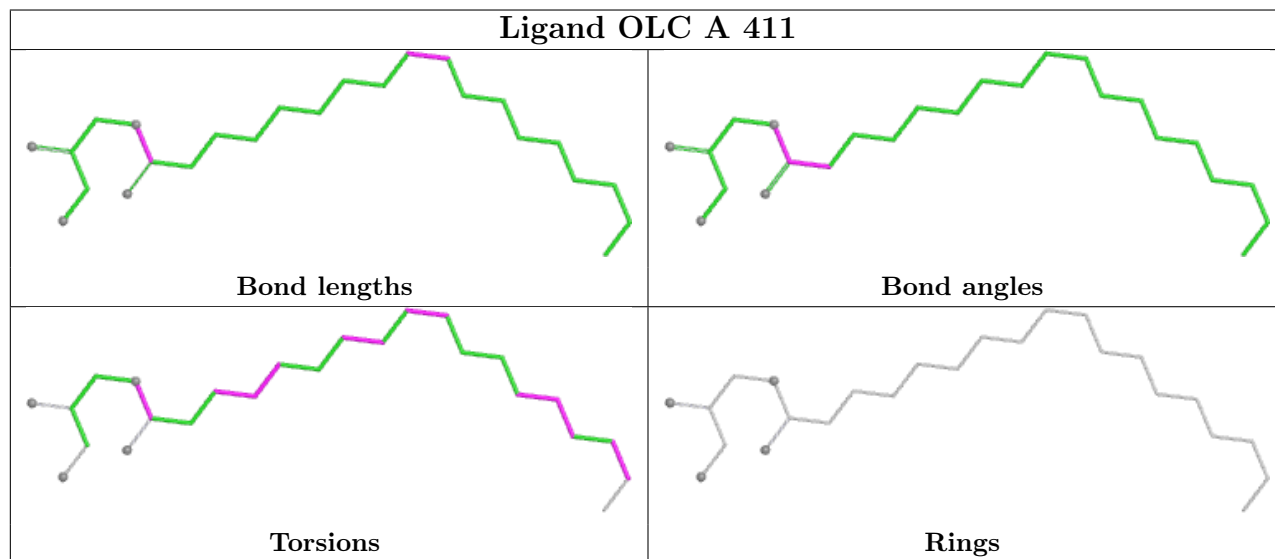
Mol	Chain	Res	Type	Atoms
5	A	410	OLC	C12-C13-C14-C15
6	A	421	MYS	C2-C3-C4-C5
7	A	415	1PE	OH7-C16-C26-OH6
5	A	423	OLC	C5-C6-C7-C8
7	A	415	1PE	C12-C22-OH3-C23
5	A	422	OLC	C5-C6-C7-C8
5	A	422	OLC	O23-C22-C24-O25
6	A	418	MYS	C2-C3-C4-C5
5	A	410	OLC	C7-C8-C9-C10
6	A	412	MYS	C6-C7-C8-C9
6	A	414	MYS	C11-C10-C9-C8
5	A	409	OLC	C11-C10-C9-C8
6	A	412	MYS	C5-C6-C7-C8
5	A	423	OLC	C7-C8-C9-C10
5	A	423	OLC	C12-C13-C14-C15
6	A	417	MYS	C10-C11-C12-C13
5	A	411	OLC	O19-C1-O20-C21
6	A	413	MYS	C11-C10-C9-C8
5	A	411	OLC	C2-C1-O20-C21
6	A	412	MYS	C11-C10-C9-C8
5	A	411	OLC	C11-C10-C9-C8
6	A	418	MYS	C11-C12-C13-C14
5	A	411	OLC	C2-C3-C4-C5
5	A	409	OLC	C2-C3-C4-C5
5	A	422	OLC	C10-C11-C12-C13
6	A	412	MYS	C3-C4-C5-C6
6	A	414	MYS	C6-C7-C8-C9
5	A	423	OLC	C9-C10-C11-C12
6	A	418	MYS	C10-C11-C12-C13
5	A	422	OLC	O20-C21-C22-O23
6	A	414	MYS	C2-C3-C4-C5
5	A	410	OLC	C5-C6-C7-C8
5	A	422	OLC	C9-C10-C11-C12
5	A	410	OLC	O19-C1-C2-C3
5	A	422	OLC	O20-C1-C2-C3
5	A	411	OLC	C15-C16-C17-C18
5	A	423	OLC	O20-C1-C2-C3
5	A	422	OLC	O19-C1-C2-C3
6	A	421	MYS	C7-C8-C9-C10
5	A	423	OLC	O19-C1-C2-C3

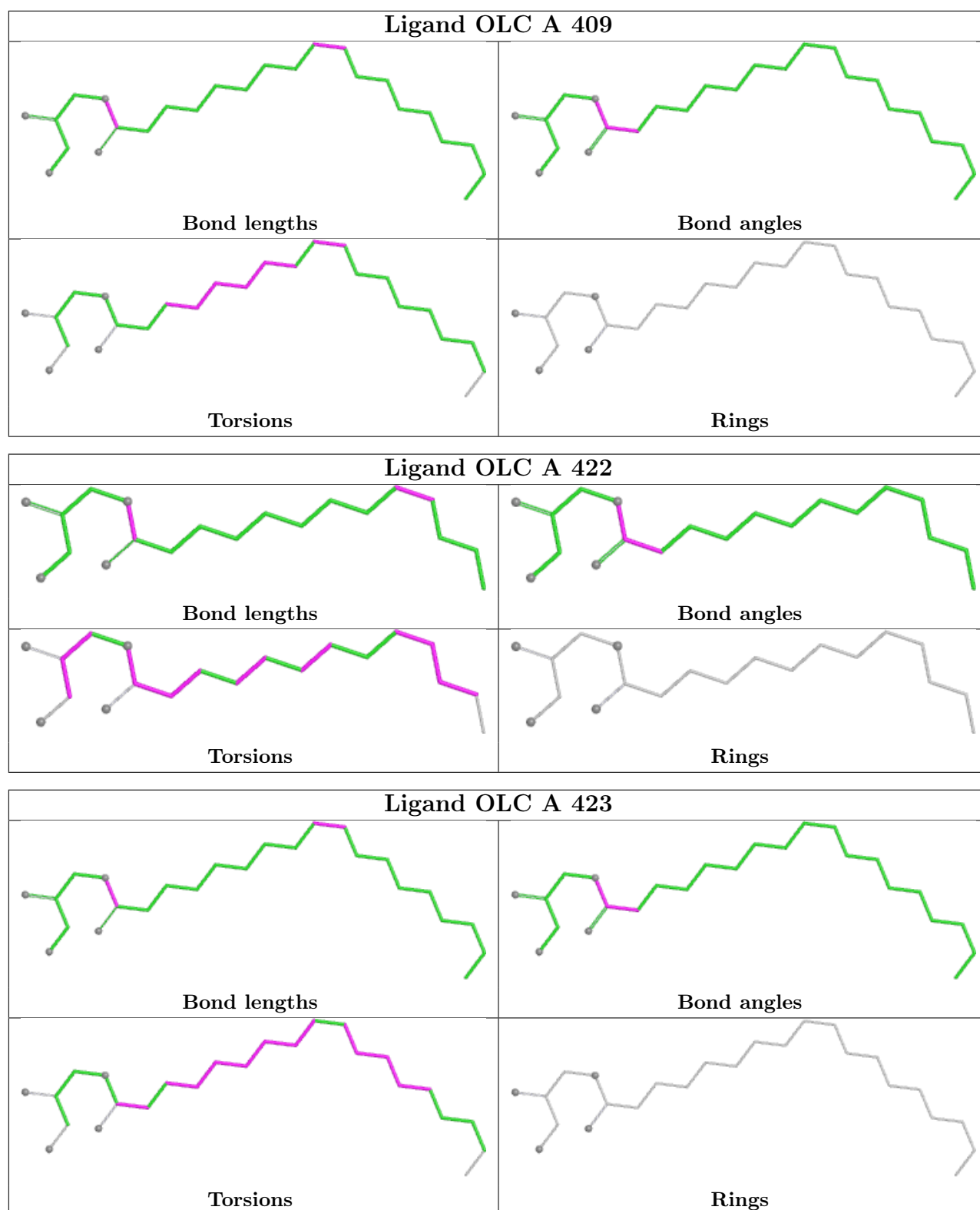
There are no ring outliers.

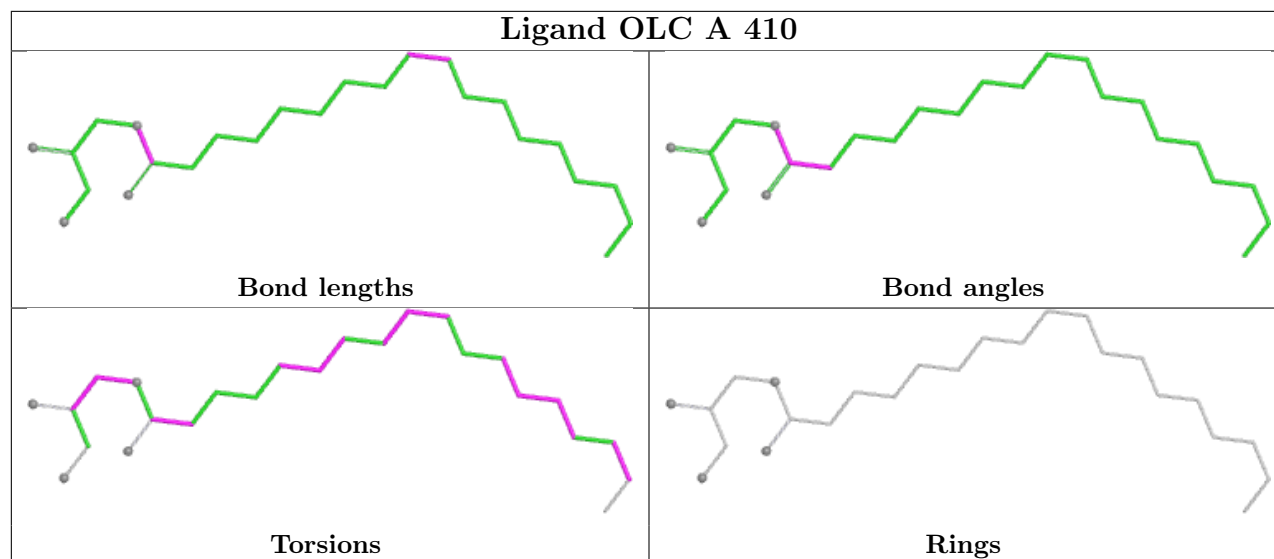
8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	418	MYS	1	0
6	A	419	MYS	4	0
5	A	411	OLC	4	0
5	A	409	OLC	3	0
5	A	422	OLC	6	0
5	A	423	OLC	3	0
6	A	413	MYS	1	0
5	A	410	OLC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	297/304 (97%)	0.04	8 (2%) 56 60	13, 23, 41, 66	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	ALA	4.2
1	A	157	ASN	3.3
1	A	100	ASN	2.6
1	A	194	ASP	2.5
1	A	33	HIS	2.1
1	A	1	MET	2.1
1	A	159	PRO	2.1
1	A	156	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

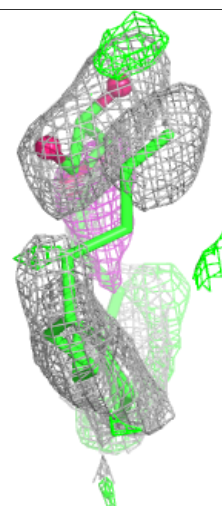
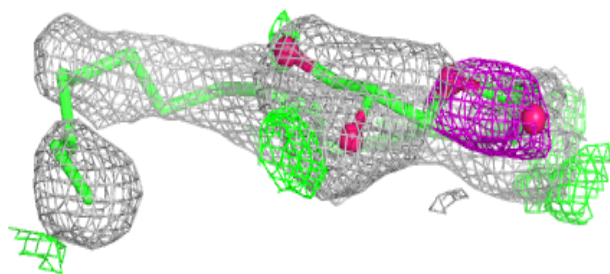
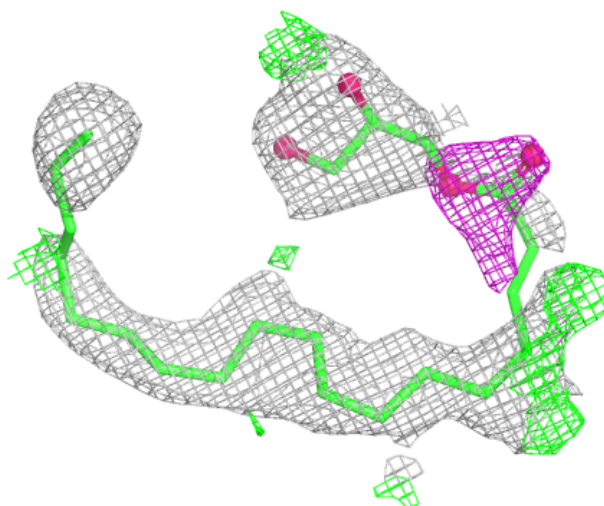
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	OLC	A	411	25/25	0.59	0.22	38,47,54,56	0
5	OLC	A	422	20/25	0.66	0.20	32,52,60,65	0
4	ACT	A	405	4/4	0.71	0.19	49,51,53,56	0
6	MYS	A	421	14/15	0.72	0.17	44,52,57,58	0
4	ACT	A	407	4/4	0.73	0.15	51,60,61,64	0
6	MYS	A	420	5/15	0.74	0.12	44,46,47,47	0
6	MYS	A	416	5/15	0.74	0.15	42,45,51,53	0
4	ACT	A	406	4/4	0.75	0.14	38,51,52,59	0
6	MYS	A	417	15/15	0.75	0.18	40,45,49,51	0
5	OLC	A	409	25/25	0.76	0.15	32,48,64,67	0
5	OLC	A	410	25/25	0.76	0.18	34,48,55,59	0
5	OLC	A	423	25/25	0.79	0.15	22,38,51,53	0
6	MYS	A	414	10/15	0.80	0.16	33,41,45,49	0
6	MYS	A	418	15/15	0.82	0.15	28,37,51,52	0
6	MYS	A	419	14/15	0.82	0.13	27,38,47,51	0
6	MYS	A	413	12/15	0.83	0.11	33,39,43,48	0
6	MYS	A	412	15/15	0.84	0.16	35,43,72,72	0
4	ACT	A	408	4/4	0.86	0.14	38,43,43,46	0
7	1PE	A	415	16/16	0.87	0.12	27,42,53,54	0
2	NA	A	403	1/1	0.98	0.10	20,20,20,20	0
2	NA	A	402	1/1	0.98	0.04	21,21,21,21	0
2	NA	A	401	1/1	0.99	0.04	18,18,18,18	0
3	CA	A	404	1/1	1.00	0.09	27,27,27,27	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.

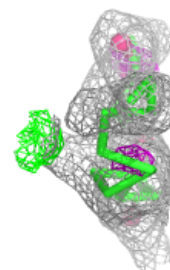
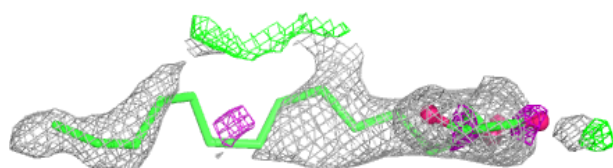
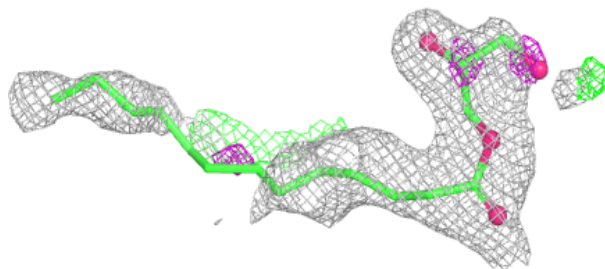
Electron density around OLC A 411:

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

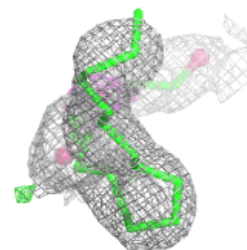
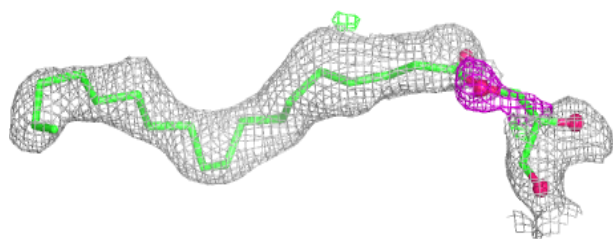
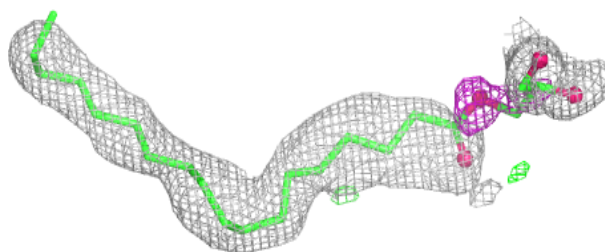


Electron density around OLC A 422:

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

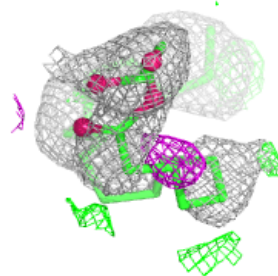
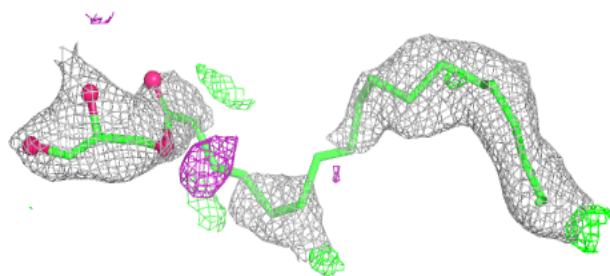
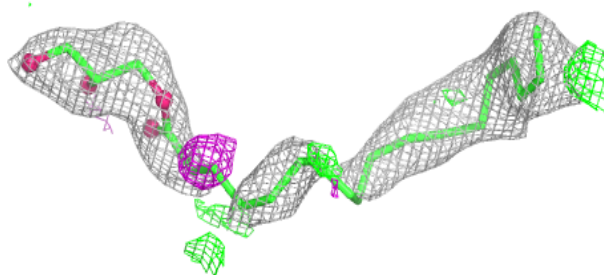
**Electron density around OLC A 409:**

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

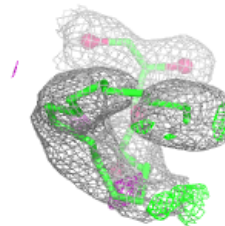
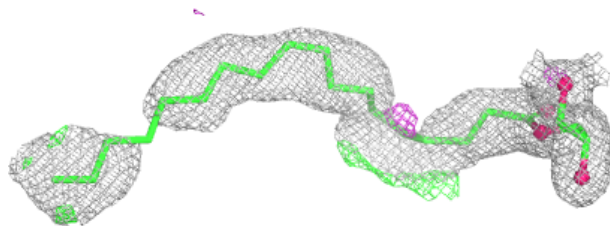
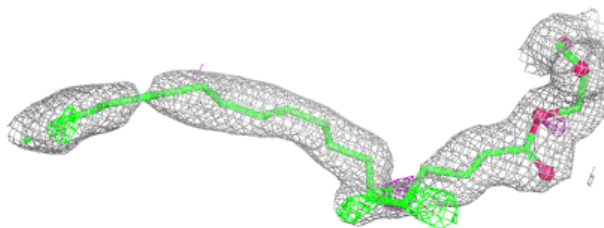


Electron density around OLC A 410:

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

**Electron density around OLC A 423:**

$2mF_o-DF_c$ (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.