Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:53 PM EDT

PDB ID	:	5WIV
Title	:	Structure of the sodium-bound human D4 Dopamine receptor in complex with Nemonapride
Authors	:	Wacker, D.; Wang, S.; Levit, A.; Che, T.; Betz, R.M.; McCorvy, J.D.; Venkatakrishnan, A.J.; Huang, X.-P.; Dror, R.O.; Shoichet, B.K.; Roth, B.L.
Deposited on	:	2017-07-20
Resolution	:	2.14 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

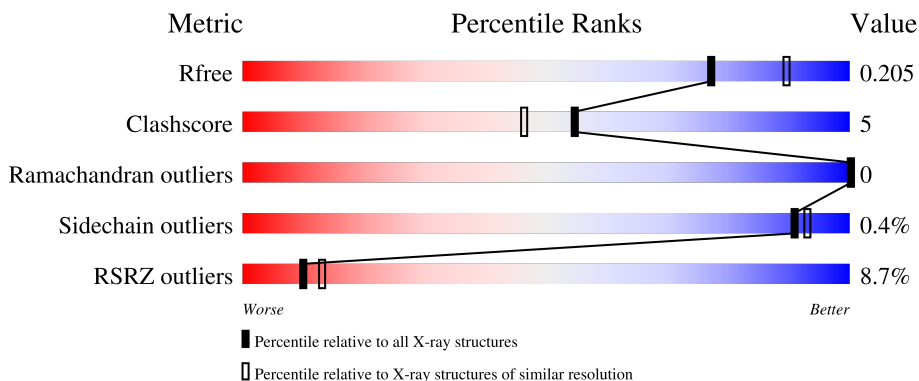|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.14 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	Percentile Ranks	Value
Rfree		0.205
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.4%
RSRZ outliers		8.7%

Worse	*Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	422	8% / 80% / 10% / 10%

2 Entity composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3149 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 D(4) dopamine receptor, soluble cytochrome b562 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total 2819	C 1827	N 470	O 503	S 19	0	9	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P21917
A	-2	GLY	-	expression tag	UNP P21917
A	-1	THR	-	expression tag	UNP P21917
A	0	THR	-	expression tag	UNP P21917
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7

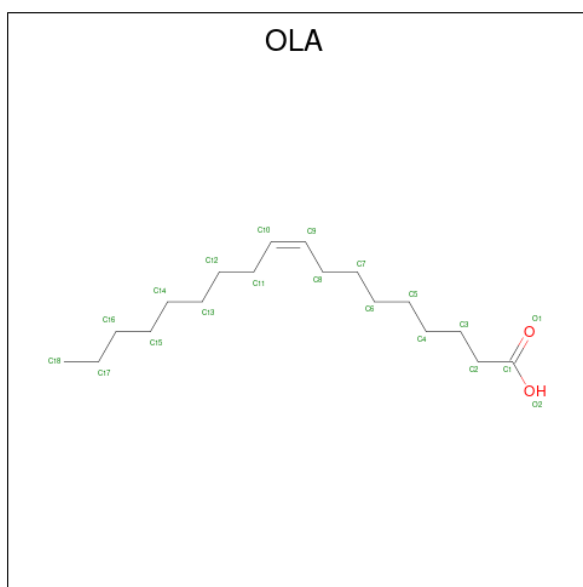- Molecule 2 is Nemonapride (three-letter code: AQD) (formula: $C_{21}H_{26}ClN_3O_2$).
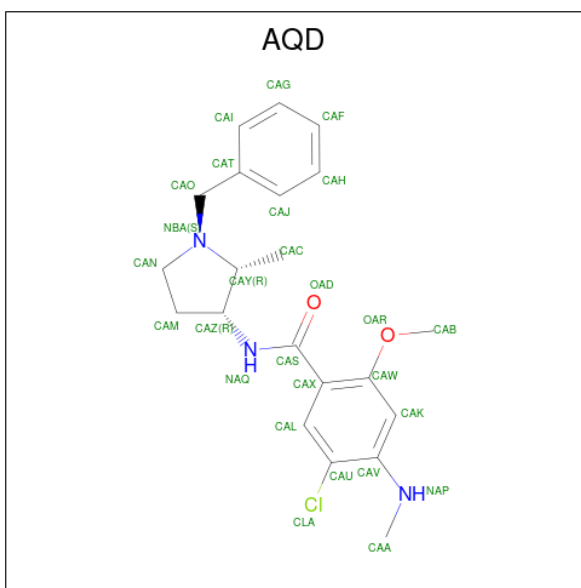
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 21	Cl 1	N 3	O 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

OLA

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 17	C 15	O 2	0	0
4	A	1	Total 17	C 15	O 2	0	0
4	A	1	Total 17	C 15	O 2	0	0
4	A	1	Total 20	C 18	O 2	0	0
4	A	1	Total 20	C 18	O 2	0	0
4	A	1	Total 16	C 14	O 2	0	0
4	A	1	Total 20	C 18	O 2	0	0
4	A	1	Total 20	C 18	O 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0
5	A	1	Total 7	C 4	O 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	67	Total O 67 67		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: D(4) dopamine receptor, soluble cytochrome b562 chimera
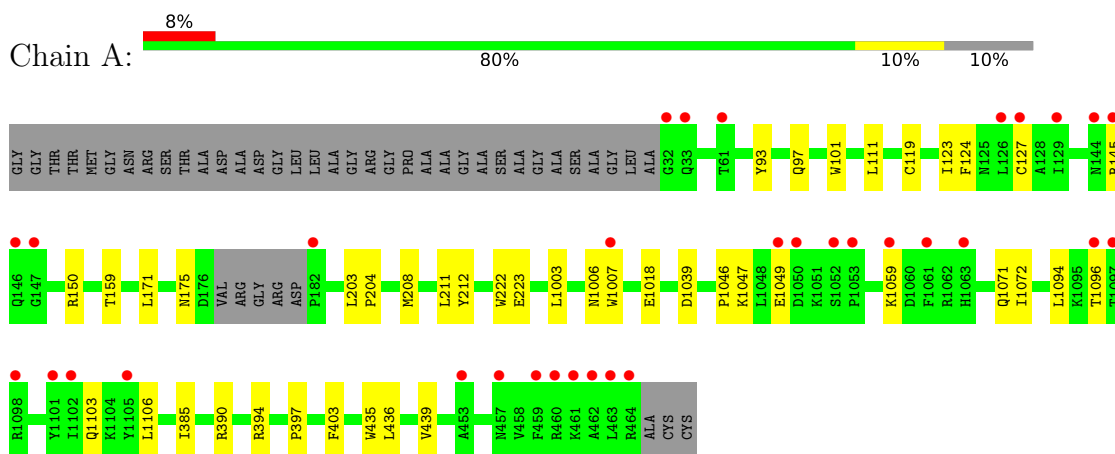
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	67.86Å 162.84Å 83.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.14 29.69 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.69-2.14) 96.8 (29.69-2.14)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.227 0.200 , 0.205	Depositor DCC
R_{free} test set	1256 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3149	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, OLA, PO4, AQD, PEG

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	0.41	0/2900	0.53	0/3969

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 ⓘ

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	2819	0	2821	30	1
2	A	27	0	0	0	0
3	A	25	0	0	0	0
4	A	147	0	226	1	0
5	A	63	0	81	1	0
6	A	1	0	0	0	0
7	A	67	0	0	4	0
All	All	3149	0	3128	32	1

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 5.

All (32) 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:1018:GLU:OE1	7:A:1301:HOH:O	2.09	0.71
1:A:1007:TRP:HH2	1:A:1103:GLN:HE21	1.40	0.69
1:A:123:ILE:HG12	1:A:403:PHE:CZ	2.31	0.65
1:A:1106:LEU:HD23	1:A:385:ILE:HD11	1.79	0.65
1:A:1007:TRP:CH2	1:A:1103:GLN:HG3	2.32	0.65
1:A:93:TYR:O	1:A:97:GLN:HG2	2.03	0.58
5:A:1215:PEG:O4	7:A:1302:HOH:O	2.17	0.56
1:A:127[B]:CYS:HA	1:A:208:MET:HG3	1.88	0.55
1:A:127[A]:CYS:SG	1:A:204:PRO:HB3	2.51	0.51
1:A:127[A]:CYS:HA	1:A:208:MET:HG3	1.92	0.51
1:A:394:ARG:O	1:A:397:PRO:HD2	2.12	0.50
1:A:101:TRP:CH2	1:A:111:LEU:HD12	2.47	0.50
1:A:435:TRP:O	1:A:439:VAL:HG13	2.12	0.50
1:A:436:LEU:O	1:A:439:VAL:HG22	2.13	0.49
1:A:150:ARG:HA	7:A:1362:HOH:O	2.13	0.49
1:A:123:ILE:HG12	1:A:403:PHE:CE1	2.48	0.48
1:A:1003:LEU:HD21	1:A:385:ILE:HG13	1.95	0.48
4:A:1210:OLA:H41	4:A:1210:OLA:H71	1.52	0.47
1:A:223:GLU:OE2	1:A:390:ARG:HD3	2.15	0.47
1:A:1046:PRO:HA	1:A:1049:GLU:CD	2.35	0.46
1:A:222:TRP:CZ2	1:A:1047:LYS:HG2	2.51	0.46
1:A:203:LEU:HB3	1:A:204:PRO:HD3	1.98	0.45
1:A:175:ASN:ND2	7:A:1305:HOH:O	2.41	0.44
1:A:1072:ILE:HG13	1:A:1094:LEU:HD11	2.00	0.44
1:A:124:PHE:HB3	1:A:159:THR:HG23	2.00	0.44
1:A:1003:LEU:CD2	1:A:385:ILE:HG13	2.49	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.84	0.42
1:A:208:MET:HG2	1:A:212:TYR:CE2	2.55	0.42
1:A:1006:ASN:HD21	1:A:1039:ASP:HB3	1.85	0.42
1:A:1059:LYS:HB3	1:A:1059:LYS:HE3	1.81	0.41
1:A:1071:GLN:HB3	1:A:1094:LEU:HD12	2.01	0.41
1:A:119:CYS:O	1:A:123:ILE:HG13	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:NH1	1:A:171:LEU:O[4_555]	2.14	0.06

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	384/422 (91%)	379 (99%)	5 (1%)	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	286/330 (87%)	285 (100%)	1 (0%)	92	94

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

Mol	Chain	Res	Type
1	A	1096	THR

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	1103	GLN
1	A	414	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	#$|Z| > 2$
5	PEG	A	1218	-	6,6,6	1.46	1 (16%)	5,5,5	1.56	0
3	PO4	A	1206	-	4,4,4	0.84	0	6,6,6	0.41	0
4	OLA	A	1207	-	16,16,19	0.53	0	16,16,19	1.01	1 (6%)
5	PEG	A	1216	-	6,6,6	1.48	1 (16%)	5,5,5	1.59	1 (20%)
3	PO4	A	1205	-	4,4,4	0.81	0	6,6,6	0.50	0
5	PEG	A	1219	-	6,6,6	1.47	1 (16%)	5,5,5	1.48	0
4	OLA	A	1211	-	19,19,19	0.48	0	19,19,19	0.94	1 (5%)
3	PO4	A	1203	-	4,4,4	0.82	0	6,6,6	0.54	0
5	PEG	A	1222	-	6,6,6	1.45	1 (16%)	5,5,5	1.49	0
5	PEG	A	1223	-	6,6,6	1.48	1 (16%)	5,5,5	1.48	0
4	OLA	A	1209	-	16,16,19	0.50	0	16,16,19	1.05	1 (6%)
5	PEG	A	1217	-	6,6,6	1.46	1 (16%)	5,5,5	1.59	0
4	OLA	A	1210	-	19,19,19	0.49	0	19,19,19	0.95	1 (5%)
5	PEG	A	1221	-	6,6,6	1.49	1 (16%)	5,5,5	1.46	0
4	OLA	A	1212	-	15,15,19	0.55	0	15,15,19	1.10	2 (13%)
4	OLA	A	1208	-	16,16,19	0.52	0	16,16,19	0.88	0
2	AQD	A	1201	-	29,29,29	2.11	8 (27%)	39,40,40	1.90	10 (25%)
3	PO4	A	1204	-	4,4,4	0.91	0	6,6,6	0.46	0
4	OLA	A	1213	-	19,19,19	0.52	0	19,19,19	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	PEG	A	1220	-	6,6,6	1.46	1 (16%)	5,5,5	1.53	1 (20%)
5	PEG	A	1215	-	6,6,6	1.46	1 (16%)	5,5,5	1.57	0
3	PO4	A	1202	-	4,4,4	0.82	0	6,6,6	0.48	0
4	OLA	A	1214	-	19,19,19	0.50	0	19,19,19	0.83	1 (5%)

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	OLA	A	1209	-	-	7/14/14/17	-
4	OLA	A	1208	-	-	8/14/14/17	-
5	PEG	A	1218	-	-	2/4/4/4	-
2	AQD	A	1201	-	-	1/16/29/29	0/3/3/3
4	OLA	A	1207	-	-	9/14/14/17	-
4	OLA	A	1213	-	-	4/17/17/17	-
5	PEG	A	1217	-	-	1/4/4/4	-
5	PEG	A	1215	-	-	2/4/4/4	-
5	PEG	A	1216	-	-	0/4/4/4	-
5	PEG	A	1220	-	-	1/4/4/4	-
4	OLA	A	1212	-	-	7/13/13/17	-
4	OLA	A	1210	-	-	6/17/17/17	-
5	PEG	A	1219	-	-	1/4/4/4	-
5	PEG	A	1221	-	-	1/4/4/4	-
5	PEG	A	1222	-	-	2/4/4/4	-
4	OLA	A	1211	-	-	7/17/17/17	-
5	PEG	A	1223	-	-	4/4/4/4	-
4	OLA	A	1214	-	-	7/17/17/17	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	AQD	CAM-CAN	5.35	1.63	1.52
2	A	1201	AQD	CAS-NAQ	4.34	1.43	1.34
2	A	1201	AQD	CAV-NAP	4.26	1.45	1.37
2	A	1201	AQD	CAY-NBA	-4.24	1.40	1.47
2	A	1201	AQD	CAY-CAZ	-3.30	1.46	1.53
2	A	1201	AQD	OAR-CAW	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1221	PEG	O2-C2	-2.85	1.29	1.42
5	A	1216	PEG	O2-C2	-2.82	1.29	1.42
5	A	1223	PEG	O2-C2	-2.80	1.29	1.42
5	A	1217	PEG	O2-C2	-2.79	1.29	1.42
5	A	1220	PEG	O2-C2	-2.79	1.29	1.42
5	A	1219	PEG	O2-C2	-2.76	1.30	1.42
5	A	1215	PEG	O2-C2	-2.75	1.30	1.42
5	A	1222	PEG	O2-C2	-2.75	1.30	1.42
5	A	1218	PEG	O2-C2	-2.73	1.30	1.42
2	A	1201	AQD	CAO-CAT	2.57	1.56	1.51
2	A	1201	AQD	CAO-NBA	-2.53	1.43	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	AQD	CAZ-CAY-NBA	5.73	106.27	101.46
2	A	1201	AQD	CAM-CAZ-NAQ	-4.27	105.84	112.73
2	A	1201	AQD	CAO-NBA-CAY	-3.78	108.27	113.51
2	A	1201	AQD	CAZ-NAQ-CAS	-3.70	116.28	123.01
2	A	1201	AQD	CAX-CAS-NAQ	2.89	122.15	116.80
2	A	1201	AQD	CAW-CAX-CAS	-2.62	121.39	126.16
2	A	1201	AQD	CAK-CAV-CAU	2.44	120.71	118.17
2	A	1201	AQD	CAM-CAZ-CAY	2.30	107.94	104.07
2	A	1201	AQD	CAL-CAX-CAW	2.30	121.51	118.29
4	A	1212	OLA	O2-C1-C2	2.25	121.26	114.03
4	A	1210	OLA	O2-C1-C2	2.23	121.20	114.03
4	A	1211	OLA	C3-C2-C1	-2.16	109.04	114.47
4	A	1207	OLA	C3-C2-C1	-2.11	109.15	114.47
4	A	1214	OLA	O2-C1-C2	2.09	120.73	114.03
5	A	1216	PEG	O2-C3-C4	2.06	119.14	110.07
2	A	1201	AQD	OAR-CAW-CAK	-2.05	120.59	124.12
5	A	1220	PEG	O2-C3-C4	2.01	118.91	110.07
4	A	1209	OLA	O2-C1-C2	2.01	120.50	114.03
4	A	1212	OLA	O2-C1-O1	-2.01	118.29	123.30

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1213	OLA	C11-C10-C9-C8
4	A	1208	OLA	C11-C10-C9-C8
4	A	1210	OLA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	1214	OLA	C11-C10-C9-C8
4	A	1210	OLA	C4-C5-C6-C7
2	A	1201	AQD	CAT-CAO-NBA-CAN
4	A	1211	OLA	C1-C2-C3-C4
5	A	1217	PEG	O1-C1-C2-O2
4	A	1210	OLA	C1-C2-C3-C4
5	A	1219	PEG	O1-C1-C2-O2
5	A	1223	PEG	O1-C1-C2-O2
5	A	1223	PEG	O2-C3-C4-O4
4	A	1208	OLA	C3-C4-C5-C6
4	A	1212	OLA	C3-C4-C5-C6
4	A	1212	OLA	C1-C2-C3-C4
5	A	1215	PEG	O1-C1-C2-O2
4	A	1207	OLA	C3-C4-C5-C6
4	A	1211	OLA	C4-C5-C6-C7
4	A	1214	OLA	C11-C12-C13-C14
4	A	1207	OLA	C5-C6-C7-C8
5	A	1221	PEG	C4-C3-O2-C2
4	A	1209	OLA	C11-C12-C13-C14
5	A	1215	PEG	O2-C3-C4-O4
4	A	1208	OLA	C4-C5-C6-C7
4	A	1208	OLA	C2-C3-C4-C5
4	A	1207	OLA	C6-C7-C8-C9
4	A	1212	OLA	C11-C12-C13-C14
4	A	1207	OLA	C1-C2-C3-C4
4	A	1213	OLA	C4-C5-C6-C7
4	A	1214	OLA	C1-C2-C3-C4
4	A	1210	OLA	C5-C6-C7-C8
4	A	1211	OLA	C6-C7-C8-C9
4	A	1214	OLA	C10-C11-C12-C13
4	A	1208	OLA	C1-C2-C3-C4
4	A	1209	OLA	C1-C2-C3-C4
4	A	1209	OLA	C5-C6-C7-C8
4	A	1214	OLA	C3-C4-C5-C6
5	A	1220	PEG	O1-C1-C2-O2
4	A	1211	OLA	C10-C11-C12-C13
4	A	1213	OLA	C11-C12-C13-C14
4	A	1214	OLA	C5-C6-C7-C8
4	A	1209	OLA	C4-C5-C6-C7
4	A	1213	OLA	C12-C13-C14-C15
4	A	1214	OLA	C12-C13-C14-C15
4	A	1211	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	1210	OLA	C12-C13-C14-C15
5	A	1222	PEG	O2-C3-C4-O4
4	A	1207	OLA	C11-C12-C13-C14
5	A	1218	PEG	O2-C3-C4-O4
4	A	1212	OLA	C5-C6-C7-C8
5	A	1223	PEG	C1-C2-O2-C3
5	A	1223	PEG	C4-C3-O2-C2
5	A	1222	PEG	C4-C3-O2-C2
4	A	1210	OLA	C11-C12-C13-C14
4	A	1207	OLA	O1-C1-C2-C3
4	A	1207	OLA	O2-C1-C2-C3
4	A	1207	OLA	C11-C10-C9-C8
4	A	1209	OLA	C11-C10-C9-C8
4	A	1212	OLA	C7-C8-C9-C10
4	A	1209	OLA	O2-C1-C2-C3
4	A	1212	OLA	O2-C1-C2-C3
5	A	1218	PEG	C4-C3-O2-C2
4	A	1208	OLA	O2-C1-C2-C3
4	A	1209	OLA	O1-C1-C2-C3
4	A	1211	OLA	C15-C16-C17-C18
4	A	1207	OLA	C2-C3-C4-C5
4	A	1212	OLA	O1-C1-C2-C3
4	A	1208	OLA	O1-C1-C2-C3
4	A	1208	OLA	C7-C8-C9-C10
4	A	1211	OLA	C9-C10-C11-C12

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1210	OLA	1	0
5	A	1215	PEG	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 then 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 OLA A 1207

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1211

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1209

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1210

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1212

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1208

Bond lengths

Bond angles

Torsions

Rings

Ligand AQD A 1201

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1213

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1214

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	379/422 (89%)	0.41	33 (8%)	10	13	37, 54, 93, 116	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	6.8
1	A	32	GLY	5.4
1	A	453	ALA	4.8
1	A	1096	THR	4.4
1	A	1105	TYR	4.2
1	A	457	ASN	4.0
1	A	459	PHE	3.9
1	A	144	ASN	3.9
1	A	61	THR	3.7
1	A	146	GLN	3.7
1	A	464	ARG	3.6
1	A	1101	TYR	3.6
1	A	1097	THR	3.6
1	A	147	GLY	3.6
1	A	33	GLN	3.5
1	A	462	ALA	3.5
1	A	129	ILE	3.2
1	A	461	LYS	3.2
1	A	1050	ASP	3.2
1	A	1061	PHE	3.0
1	A	145	ARG	2.9
1	A	1098	ARG	2.8
1	A	1102	ILE	2.5
1	A	182	PRO	2.5
1	A	1053	PRO	2.4
1	A	1049	GLU	2.3
1	A	1063	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	2.3
1	A	1052	SER	2.2
1	A	127[A]	CYS	2.1
1	A	1007	TRP	2.1
1	A	1059	LYS	2.0
1	A	460	ARG	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides 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
4	OLA	A	1213	20/20	0.43	0.39	65,79,101,102	0
5	PEG	A	1220	7/7	0.67	0.16	76,82,93,93	0
5	PEG	A	1219	7/7	0.68	0.21	78,84,87,89	0
4	OLA	A	1210	20/20	0.69	0.29	67,79,89,95	0
4	OLA	A	1209	17/20	0.73	0.27	52,66,72,72	0
5	PEG	A	1221	7/7	0.75	0.17	65,81,95,100	0
3	PO4	A	1204	5/5	0.78	0.40	54,55,57,61	5
4	OLA	A	1214	20/20	0.79	0.21	59,71,77,78	0
5	PEG	A	1222	7/7	0.79	0.28	72,77,83,84	0
5	PEG	A	1218	7/7	0.81	0.15	68,70,75,78	0
4	OLA	A	1211	20/20	0.82	0.16	54,71,93,99	0
5	PEG	A	1217	7/7	0.84	0.19	62,64,78,82	0
4	OLA	A	1212	16/20	0.84	0.18	57,67,83,97	0
4	OLA	A	1207	17/20	0.86	0.13	56,70,80,86	0
5	PEG	A	1215	7/7	0.86	0.16	65,73,78,79	0
3	PO4	A	1203	5/5	0.88	0.39	80,94,101,119	5
5	PEG	A	1216	7/7	0.88	0.14	67,70,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	1206	5/5	0.89	0.21	93,98,106,110	5
4	OLA	A	1208	17/20	0.90	0.14	53,64,98,107	0
3	PO4	A	1205	5/5	0.91	0.22	69,95,97,98	0
5	PEG	A	1223	7/7	0.91	0.10	67,68,72,73	0
6	NA	A	1224	1/1	0.93	0.14	67,67,67,67	0
2	AQD	A	1201	27/27	0.95	0.16	36,45,62,67	0
3	PO4	A	1202	5/5	0.98	0.07	60,74,76,81	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 OLA A 1213:

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

Electron density around OLA A 1210:

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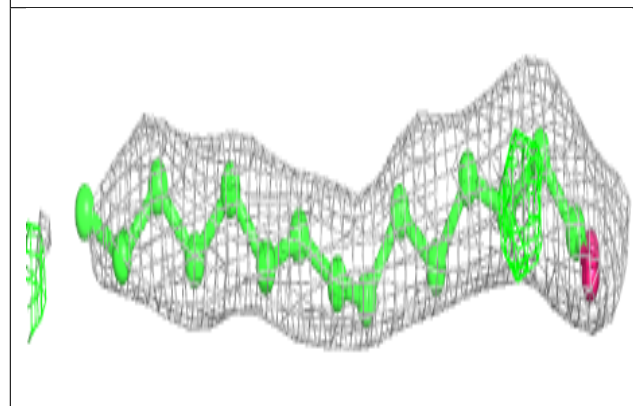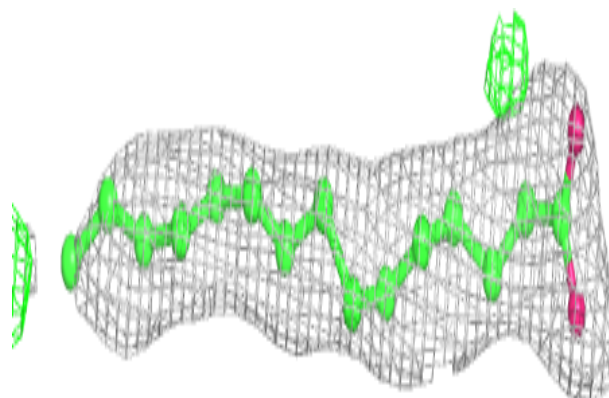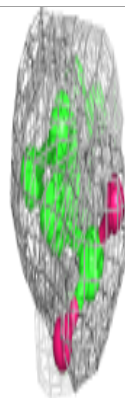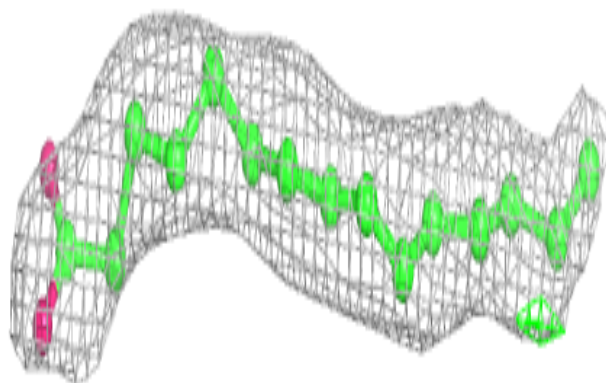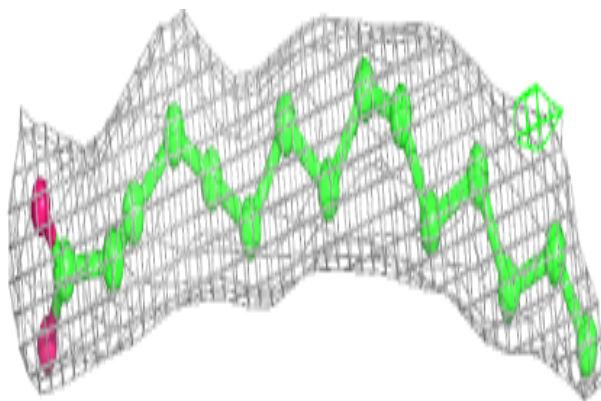mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
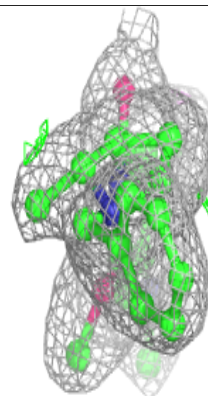

Electron density around OLA A 1209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
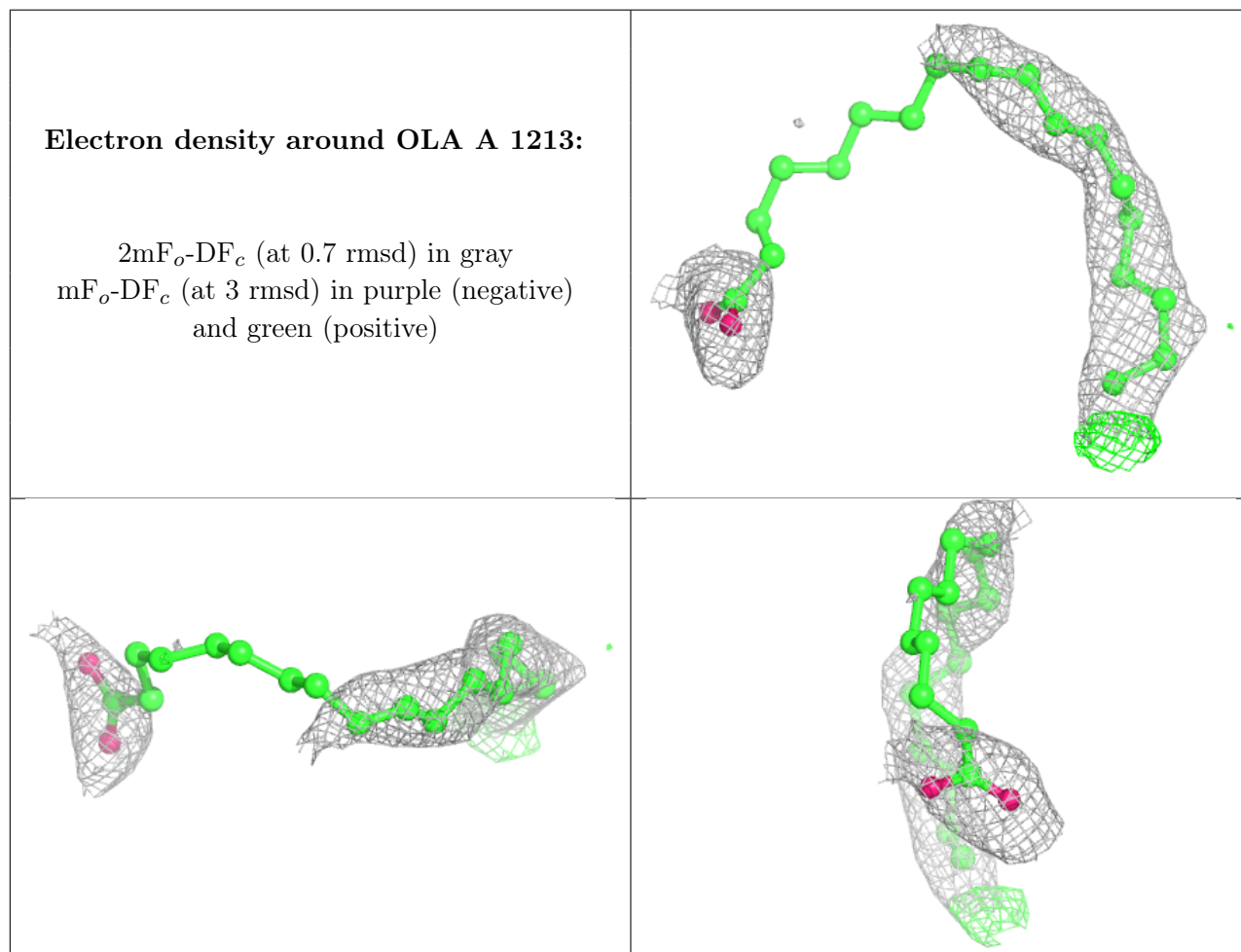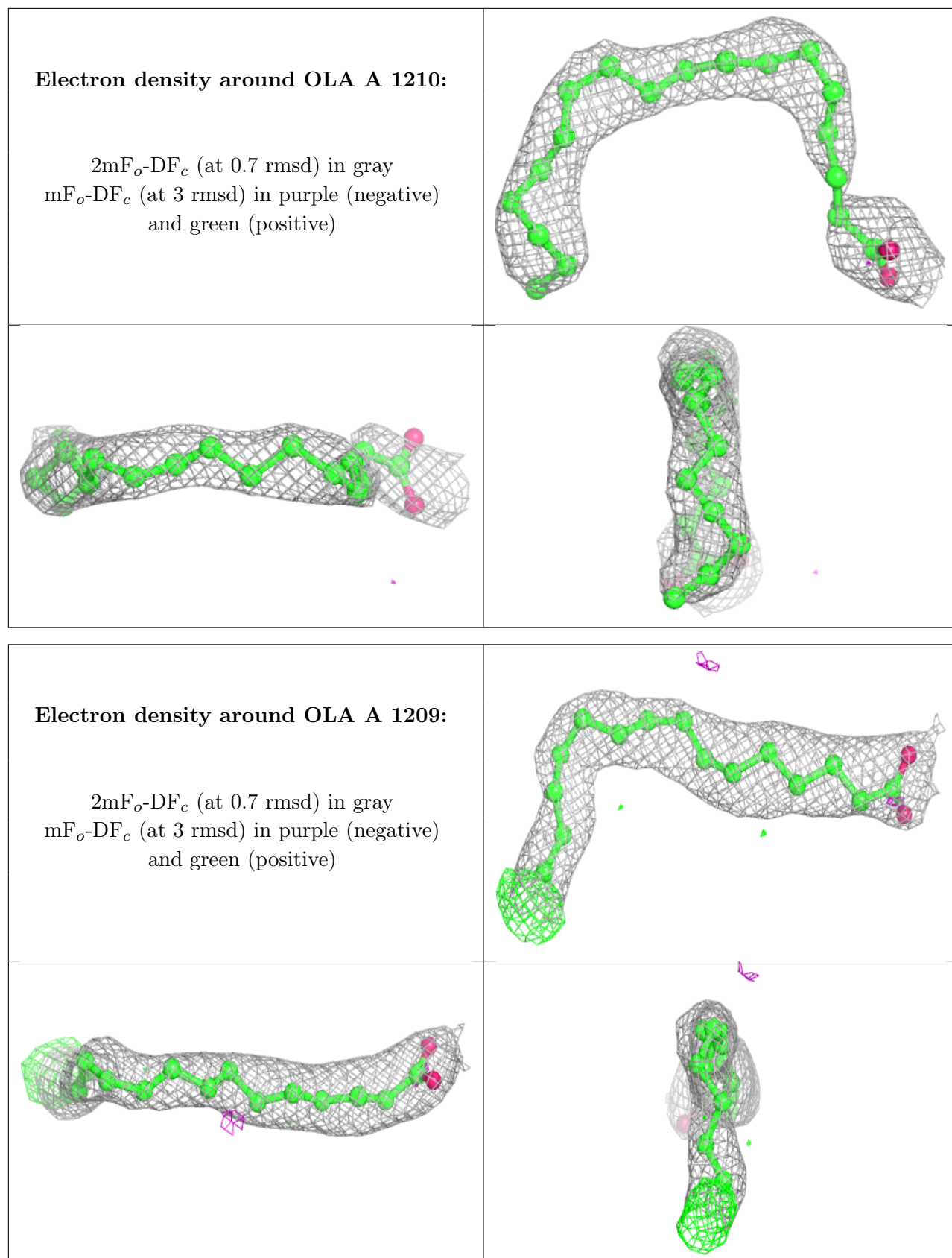
Electron density around OLA A 1214:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
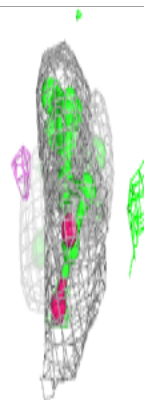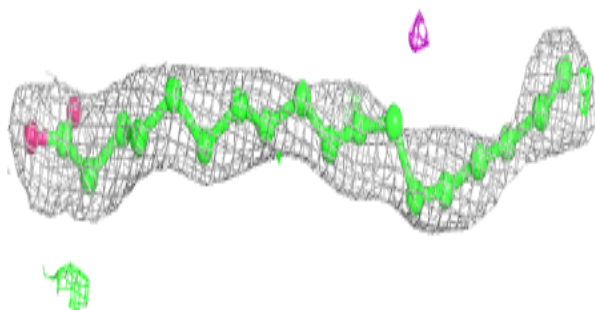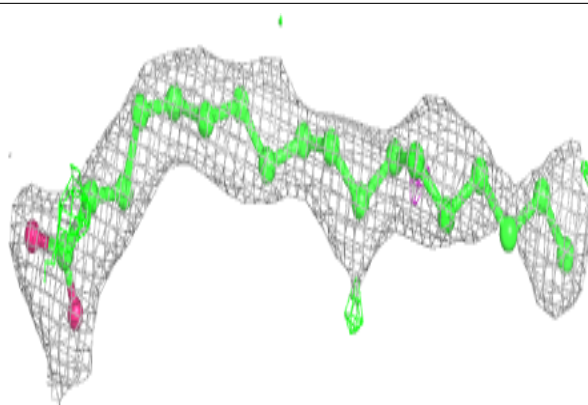
Electron density around OLA A 1211:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
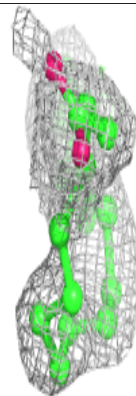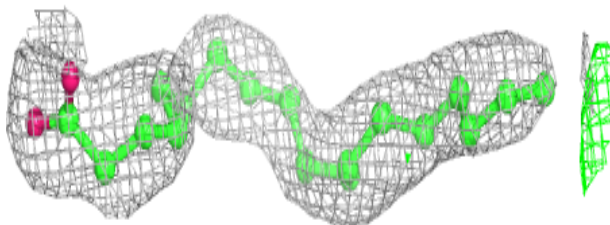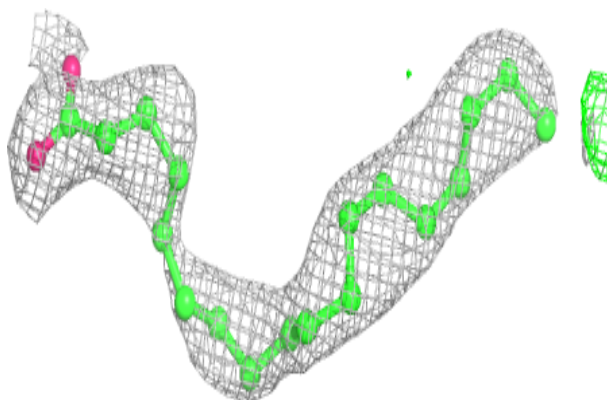
Electron density around OLA A 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
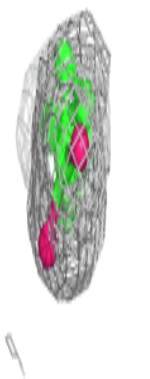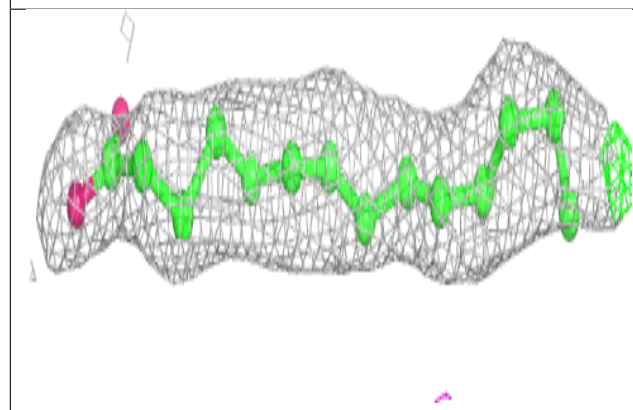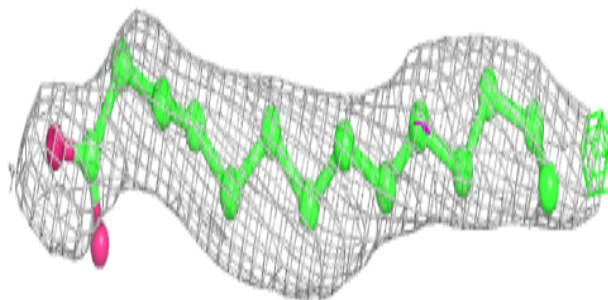
Electron density around OLA A 1207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
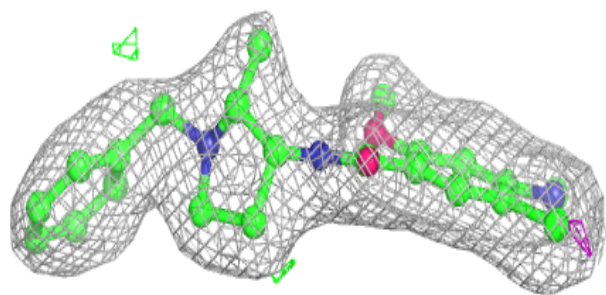mF_o-DF_c (at 3 rmsd) in purple (negative)
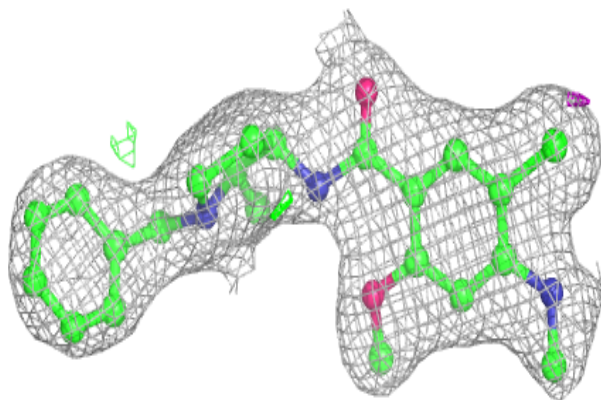and green (positive)
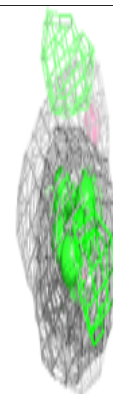
Electron density around OLA A 1208:

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

Electron density around AQD A 1201:

$2mF_o$-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 ⓘ

There are no such residues in this entry.