WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 10:03 PM EDT

PDB ID	:	5I20
Title	:	Crystal structure of protein
Authors	:	Ishitani, R.; Nureki, O.
Deposited on	:	2016-02-08
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

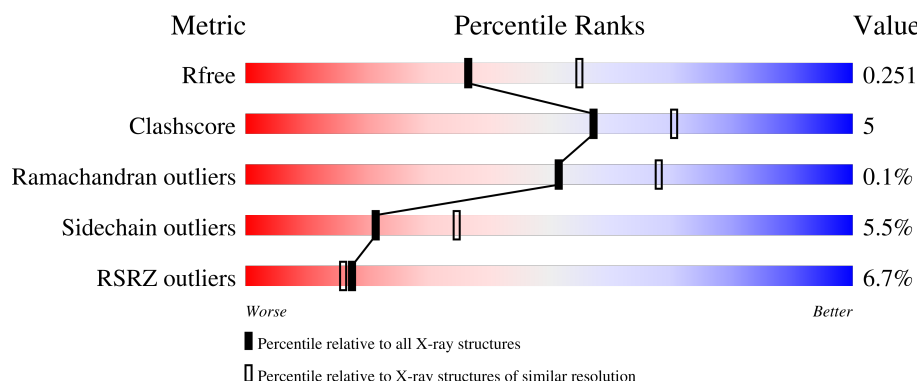|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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		0.251
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		5.5%
RSRZ outliers		6.7%

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	298	5% — 82% — 14% · ·
1	B	298	3% — 85% — 8% · 6%
1	C	298	5% — 81% — 13% · 5%
1	D	298	6% — 83% — 10% · 6%
1	E	298	2% — 85% — 12% ·

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Mol	Chain	Length	Quality of chain
1	F	298	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11923 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2060	1377	333	344	6			
1	B	279	Total	C	N	O	S	0	1	0
			2005	1339	322	338	6			
1	C	282	Total	C	N	O	S	0	0	0
			1993	1332	318	337	6			
1	D	280	Total	C	N	O	S	0	0	0
			1954	1313	303	332	6			
1	E	291	Total	C	N	O	S	0	0	0
			2071	1386	331	348	6			
1	F	219	Total	C	N	O	S	0	0	0
			1480	981	237	257	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	LEU	-	expression tag	UNP D7A5Q8
A	289	GLU	-	expression tag	UNP D7A5Q8
A	290	SER	-	expression tag	UNP D7A5Q8
A	291	SER	-	expression tag	UNP D7A5Q8
A	292	GLY	-	expression tag	UNP D7A5Q8
A	293	GLU	-	expression tag	UNP D7A5Q8
A	294	ASN	-	expression tag	UNP D7A5Q8
A	295	LEU	-	expression tag	UNP D7A5Q8
A	296	TYR	-	expression tag	UNP D7A5Q8
A	297	PHE	-	expression tag	UNP D7A5Q8
A	298	GLN	-	expression tag	UNP D7A5Q8
B	288	LEU	-	expression tag	UNP D7A5Q8
B	289	GLU	-	expression tag	UNP D7A5Q8
B	290	SER	-	expression tag	UNP D7A5Q8
B	291	SER	-	expression tag	UNP D7A5Q8
B	292	GLY	-	expression tag	UNP D7A5Q8
B	293	GLU	-	expression tag	UNP D7A5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ASN	-	expression tag	UNP D7A5Q8
B	295	LEU	-	expression tag	UNP D7A5Q8
B	296	TYR	-	expression tag	UNP D7A5Q8
B	297	PHE	-	expression tag	UNP D7A5Q8
B	298	GLN	-	expression tag	UNP D7A5Q8
C	288	LEU	-	expression tag	UNP D7A5Q8
C	289	GLU	-	expression tag	UNP D7A5Q8
C	290	SER	-	expression tag	UNP D7A5Q8
C	291	SER	-	expression tag	UNP D7A5Q8
C	292	GLY	-	expression tag	UNP D7A5Q8
C	293	GLU	-	expression tag	UNP D7A5Q8
C	294	ASN	-	expression tag	UNP D7A5Q8
C	295	LEU	-	expression tag	UNP D7A5Q8
C	296	TYR	-	expression tag	UNP D7A5Q8
C	297	PHE	-	expression tag	UNP D7A5Q8
C	298	GLN	-	expression tag	UNP D7A5Q8
D	288	LEU	-	expression tag	UNP D7A5Q8
D	289	GLU	-	expression tag	UNP D7A5Q8
D	290	SER	-	expression tag	UNP D7A5Q8
D	291	SER	-	expression tag	UNP D7A5Q8
D	292	GLY	-	expression tag	UNP D7A5Q8
D	293	GLU	-	expression tag	UNP D7A5Q8
D	294	ASN	-	expression tag	UNP D7A5Q8
D	295	LEU	-	expression tag	UNP D7A5Q8
D	296	TYR	-	expression tag	UNP D7A5Q8
D	297	PHE	-	expression tag	UNP D7A5Q8
D	298	GLN	-	expression tag	UNP D7A5Q8
E	288	LEU	-	expression tag	UNP D7A5Q8
E	289	GLU	-	expression tag	UNP D7A5Q8
E	290	SER	-	expression tag	UNP D7A5Q8
E	291	SER	-	expression tag	UNP D7A5Q8
E	292	GLY	-	expression tag	UNP D7A5Q8
E	293	GLU	-	expression tag	UNP D7A5Q8
E	294	ASN	-	expression tag	UNP D7A5Q8
E	295	LEU	-	expression tag	UNP D7A5Q8
E	296	TYR	-	expression tag	UNP D7A5Q8
E	297	PHE	-	expression tag	UNP D7A5Q8
E	298	GLN	-	expression tag	UNP D7A5Q8
F	288	LEU	-	expression tag	UNP D7A5Q8
F	289	GLU	-	expression tag	UNP D7A5Q8
F	290	SER	-	expression tag	UNP D7A5Q8
F	291	SER	-	expression tag	UNP D7A5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	292	GLY	-	expression tag	UNP D7A5Q8
F	293	GLU	-	expression tag	UNP D7A5Q8
F	294	ASN	-	expression tag	UNP D7A5Q8
F	295	LEU	-	expression tag	UNP D7A5Q8
F	296	TYR	-	expression tag	UNP D7A5Q8
F	297	PHE	-	expression tag	UNP D7A5Q8
F	298	GLN	-	expression tag	UNP D7A5Q8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).
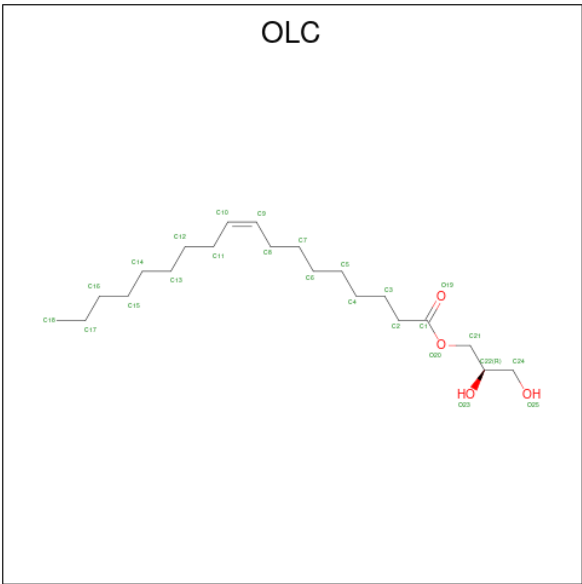
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 15	C 15		0	0
2	A	1	Total 10	C 8	O 2	0	0
2	A	1	Total 8	C 8		0	0
2	A	1	Total 13	C 11	O 2	0	0
2	B	1	Total 25	C 21	O 4	0	0
2	B	1	Total 13	C 11	O 2	0	0
2	B	1	Total 17	C 13	O 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 13 13	0	0
2	B	1	Total C O 17 15 2	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C O 24 21 3	0	0
2	C	1	Total C O 13 11 2	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 7 5 2	0	0
2	D	1	Total C 11 11	0	0
2	D	1	Total C O 16 14 2	0	0
2	D	1	Total C O 13 9 4	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C O 14 10 4	0	0
2	E	1	Total C O 14 10 4	0	0
2	E	1	Total C O 14 12 2	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2
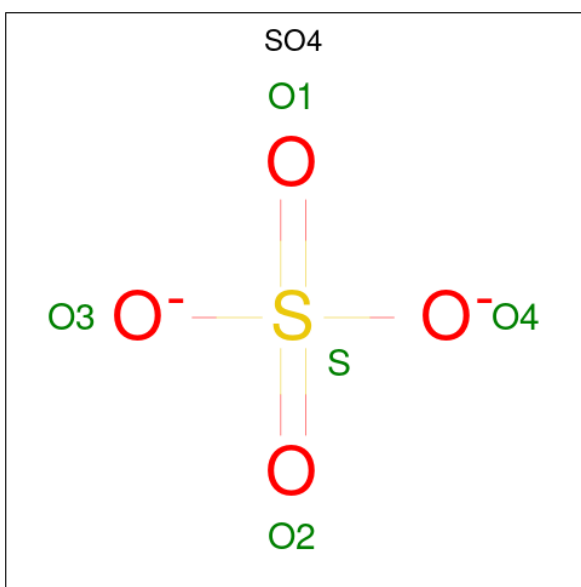
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total 4	O 4	0	0
4	C	3	Total 3	O 3	0	0
4	D	2	Total 2	O 2	0	0
4	E	2	Total 2	O 2	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: Uncharacterized protein
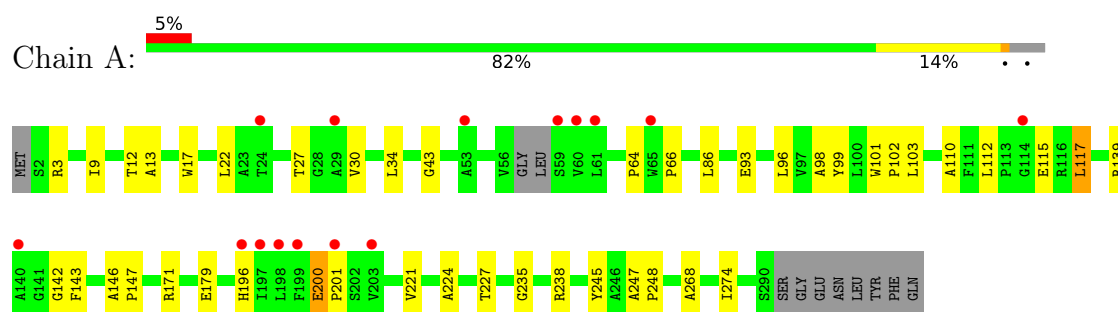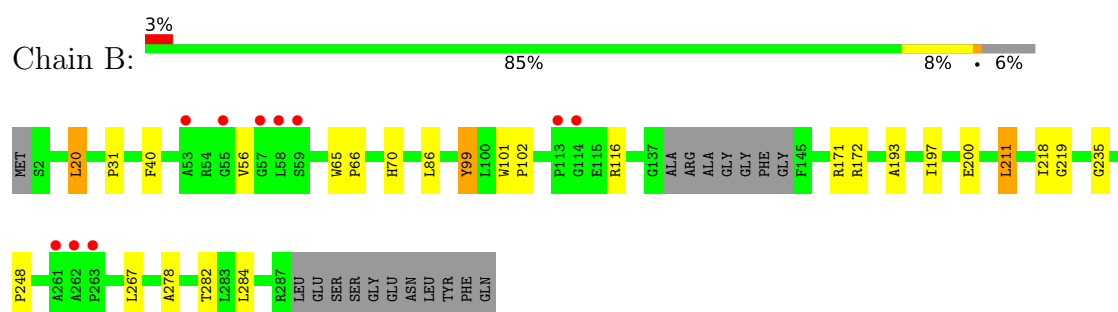
Chain A:

- Molecule 1: Uncharacterized protein

Chain B:

- Molecule 1: Uncharacterized protein

Chain C:

- Molecule 1: Uncharacterized protein

Chain D:

• Molecule 1: Uncharacterized protein

Chain E:

• Molecule 1: Uncharacterized protein

Chain F:
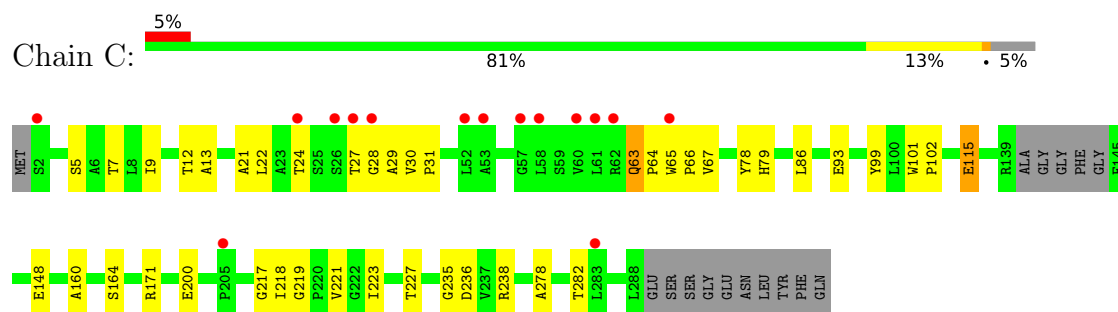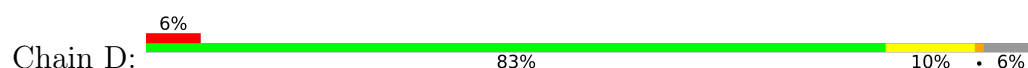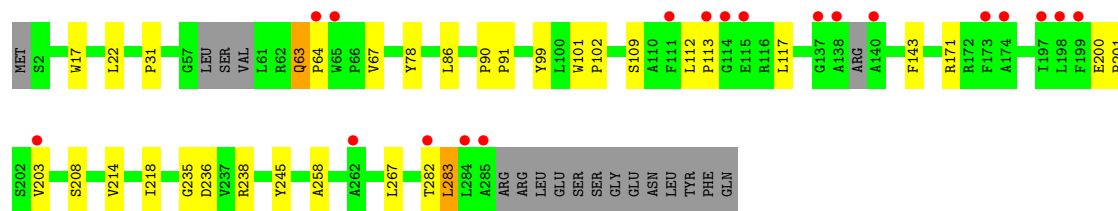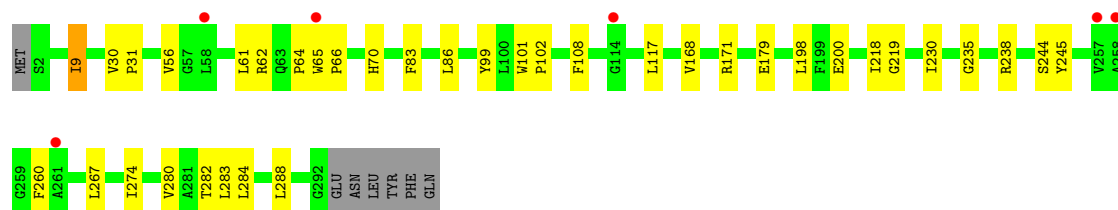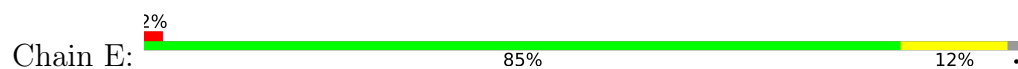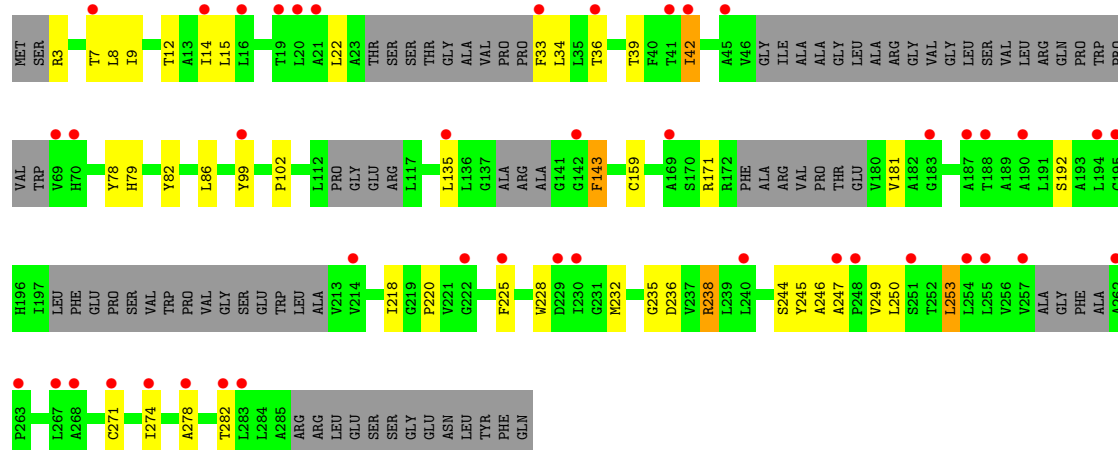
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.84Å 84.65Å 112.25Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	45.97 – 2.40 45.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.97-2.40) 93.9 (45.97-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.226 , 0.249 0.228 , 0.251	Depositor DCC
R_{free} test set	3642 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.5	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	0.93	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: OLC, SO4

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	0.23	0/2119	0.39	0/2912
1	B	0.23	0/2062	0.40	0/2838
1	C	0.22	0/2050	0.39	0/2825
1	D	0.23	0/2012	0.40	0/2775
1	E	0.23	0/2131	0.41	0/2931
1	F	0.21	0/1512	0.39	0/2071
All	All	0.23	0/11886	0.40	0/16352

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	2060	0	2105	24	0
1	B	2005	0	2047	16	0
1	C	1993	0	2010	23	0
1	D	1954	0	1956	16	0
1	E	2071	0	2116	16	0
1	F	1480	0	1413	23	0
2	A	46	0	64	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	85	0	122	6	0
2	C	48	0	69	3	0
2	D	72	0	99	3	0
2	E	93	0	135	5	0
3	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	11923	0	12136	118	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 5.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:O	1:C:238:ARG:NH2	2.22	0.73
1:E:9:ILE:HD11	1:E:230:ILE:HB	1.70	0.72
1:E:56:VAL:HG21	1:E:179:GLU:HG2	1.71	0.72
1:C:9:ILE:O	1:C:227:THR:OG1	2.08	0.71
1:D:282:THR:HG23	1:D:283:LEU:HD13	1.74	0.69

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	283/298 (95%)	275 (97%)	8 (3%)	0	100	100
1	B	276/298 (93%)	271 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	278/298 (93%)	275 (99%)	3 (1%)	0	100	100
1	D	274/298 (92%)	270 (98%)	4 (2%)	0	100	100
1	E	289/298 (97%)	286 (99%)	3 (1%)	0	100	100
1	F	203/298 (68%)	195 (96%)	7 (3%)	1 (0%)	29	41
All	All	1603/1788 (90%)	1572 (98%)	30 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	220	PRO

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	195/212 (92%)	186 (95%)	9 (5%)	27	43
1	B	192/212 (91%)	184 (96%)	8 (4%)	30	47
1	C	186/212 (88%)	177 (95%)	9 (5%)	25	41
1	D	181/212 (85%)	172 (95%)	9 (5%)	24	40
1	E	196/212 (92%)	182 (93%)	14 (7%)	14	23
1	F	124/212 (58%)	114 (92%)	10 (8%)	11	18
All	All	1074/1272 (84%)	1015 (94%)	59 (6%)	21	35

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	TYR
1	F	99	TYR
1	E	9	ILE
1	F	79	HIS
1	F	8	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	63	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.06	0
2	OLC	D	304	-	15,15,24	1.04	2 (13%)	15,15,25	1.10	1 (6%)
2	OLC	A	301	-	14,14,24	0.88	1 (7%)	13,13,25	0.73	0
2	OLC	B	304	-	12,12,24	0.95	1 (8%)	11,11,25	0.67	0
2	OLC	D	305	-	12,12,24	1.18	1 (8%)	13,13,25	1.02	1 (7%)
2	OLC	D	302	-	6,6,24	0.95	1 (16%)	6,6,25	1.29	0
2	OLC	E	304	-	13,13,24	1.13	1 (7%)	14,14,25	1.11	1 (7%)
2	OLC	A	302	-	9,9,24	0.81	1 (11%)	9,9,25	1.23	1 (11%)
2	OLC	B	305	-	16,16,24	1.00	2 (12%)	16,16,25	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	OLC	A	304	-	12,12,24	1.76	3 (25%)	12,12,25	1.22	0
2	OLC	A	303	-	7,7,24	0.28	0	6,6,25	0.70	0
2	OLC	B	302	-	12,12,24	1.76	3 (25%)	12,12,25	1.29	1 (8%)
2	OLC	D	301	-	24,24,24	1.07	2 (8%)	25,25,25	0.96	1 (4%)
2	OLC	E	301	-	15,15,24	0.86	1 (6%)	14,14,25	0.69	0
2	OLC	B	303	-	16,16,24	1.31	2 (12%)	17,17,25	1.06	1 (5%)
2	OLC	E	306	-	13,13,24	1.11	2 (15%)	12,13,25	1.14	0
2	OLC	B	301	-	24,24,24	1.08	2 (8%)	25,25,25	0.98	1 (4%)
2	OLC	D	303	-	10,10,24	1.02	1 (10%)	9,9,25	0.70	0
2	OLC	E	303	-	9,9,24	1.07	1 (11%)	7,8,25	0.74	0
2	OLC	E	305	-	13,13,24	1.13	1 (7%)	14,14,25	1.06	1 (7%)
2	OLC	C	301	-	10,10,24	1.03	1 (10%)	8,9,25	0.72	0
2	OLC	C	302	-	22,23,24	1.06	2 (9%)	22,24,25	1.01	1 (4%)
2	OLC	E	302	-	24,24,24	1.04	2 (8%)	25,25,25	0.95	1 (4%)
2	OLC	C	303	-	12,12,24	1.06	2 (16%)	12,12,25	1.26	1 (8%)

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
2	OLC	D	304	-	-	6/13/13/24	-
2	OLC	A	301	-	-	5/12/12/24	-
2	OLC	B	304	-	-	5/10/10/24	-
2	OLC	D	305	-	-	5/12/12/24	-
2	OLC	D	302	-	-	1/4/4/24	-
2	OLC	E	304	-	-	6/13/13/24	-
2	OLC	A	302	-	-	3/7/7/24	-
2	OLC	B	305	-	-	3/14/14/24	-
2	OLC	A	304	-	-	3/10/10/24	-
2	OLC	A	303	-	-	3/5/5/24	-
2	OLC	B	302	-	-	5/10/10/24	-
2	OLC	D	301	-	-	12/24/24/24	-
2	OLC	E	301	-	-	9/13/13/24	-
2	OLC	B	303	-	-	5/16/16/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	E	306	-	-	3/11/11/24	-
2	OLC	B	301	-	-	13/24/24/24	-
2	OLC	D	303	-	-	1/8/8/24	-
2	OLC	E	303	-	-	3/7/7/24	-
2	OLC	E	305	-	-	3/13/13/24	-
2	OLC	C	301	-	-	4/8/8/24	-
2	OLC	C	302	-	-	10/22/22/24	-
2	OLC	E	302	-	-	12/24/24/24	-
2	OLC	C	303	-	-	2/10/10/24	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	OLC	O19-C1	4.76	1.37	1.22
2	B	302	OLC	O19-C1	4.75	1.37	1.22
2	B	303	OLC	C10-C9	3.11	1.49	1.28
2	C	301	OLC	C9-C10	3.10	1.49	1.31
2	E	302	OLC	C9-C10	3.08	1.49	1.31

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	302	OLC	O20-C1-C2	2.75	120.54	111.91
2	C	302	OLC	O20-C1-C2	2.69	120.33	111.91
2	E	304	OLC	O20-C1-C2	2.55	119.90	111.91
2	D	301	OLC	O20-C1-C2	2.46	119.64	111.91
2	E	305	OLC	O20-C1-C2	2.44	119.57	111.91

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	OLC	C9-C10-C11-C12
2	C	302	OLC	O20-C21-C22-C24
2	C	302	OLC	O20-C21-C22-O23
2	C	302	OLC	O19-C1-O20-C21
2	D	301	OLC	O20-C21-C22-C24

There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	OLC	2	0
2	B	305	OLC	3	0
2	A	304	OLC	1	0
2	A	303	OLC	1	0
2	D	301	OLC	3	0
2	E	301	OLC	1	0
2	B	303	OLC	1	0
2	B	301	OLC	2	0
2	E	305	OLC	2	0
2	C	301	OLC	1	0
2	C	302	OLC	2	0
2	E	302	OLC	2	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 OLC D 304

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 304

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC D 305

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 304

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 305

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 304

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 306

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC D 303

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 303

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 305

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC C 303

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	287/298 (96%)	0.20	15 (5%)	27	26	35, 54, 96, 123	0
1	B	279/298 (93%)	0.06	10 (3%)	42	42	39, 54, 95, 135	0
1	C	282/298 (94%)	0.16	15 (5%)	26	25	42, 61, 100, 123	0
1	D	280/298 (93%)	0.28	19 (6%)	17	15	40, 60, 107, 131	0
1	E	291/298 (97%)	-0.00	6 (2%)	63	61	34, 51, 95, 118	0
1	F	219/298 (73%)	1.09	44 (20%)	1	0	62, 107, 152, 201	0
All	All	1638/1788 (91%)	0.27	109 (6%)	17	16	34, 60, 118, 201	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	254	LEU	7.8
1	F	257	VAL	6.1
1	D	113	PRO	5.6
1	A	203	VAL	5.4
1	F	195	CYS	5.2

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
2	OLC	E	305	14/25	0.66	0.27	62,74,85,91	0
2	OLC	E	304	14/25	0.69	0.22	54,81,94,97	0
2	OLC	B	303	17/25	0.71	0.31	64,71,86,89	0
2	OLC	D	304	16/25	0.72	0.22	62,70,83,85	0
2	OLC	B	305	17/25	0.75	0.22	64,72,82,82	0
2	OLC	D	303	11/25	0.78	0.22	65,72,76,77	0
2	OLC	A	304	13/25	0.80	0.27	64,68,78,79	0
2	OLC	B	304	13/25	0.81	0.24	60,63,66,68	0
2	OLC	E	306	14/25	0.81	0.19	71,73,88,88	0
2	OLC	D	305	13/25	0.82	0.22	62,78,92,93	0
2	OLC	D	301	25/25	0.82	0.30	45,63,106,110	0
2	OLC	E	302	25/25	0.83	0.20	34,60,76,80	0
2	OLC	B	301	25/25	0.83	0.21	37,62,81,84	0
2	OLC	C	302	24/25	0.84	0.23	40,69,92,94	0
2	OLC	E	301	16/25	0.84	0.27	58,63,71,71	0
2	OLC	C	301	11/25	0.84	0.20	60,62,70,70	0
2	OLC	A	302	10/25	0.85	0.17	60,68,76,77	0
2	OLC	A	303	8/25	0.88	0.23	61,61,63,65	0
2	OLC	B	302	13/25	0.89	0.16	55,62,81,83	0
2	OLC	C	303	13/25	0.89	0.23	62,64,72,72	0
2	OLC	E	303	10/25	0.89	0.16	64,67,72,72	0
2	OLC	A	301	15/25	0.90	0.20	36,50,66,70	0
2	OLC	D	302	7/25	0.93	0.11	61,64,67,68	0
3	SO4	A	305	5/5	0.97	0.13	84,84,85,91	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 E 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
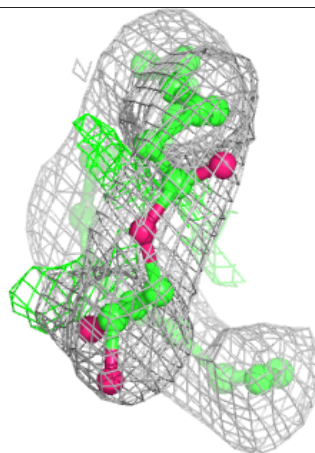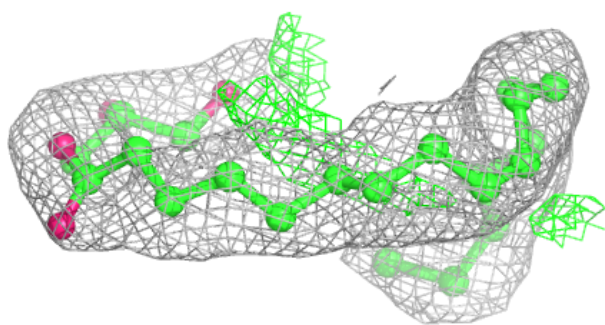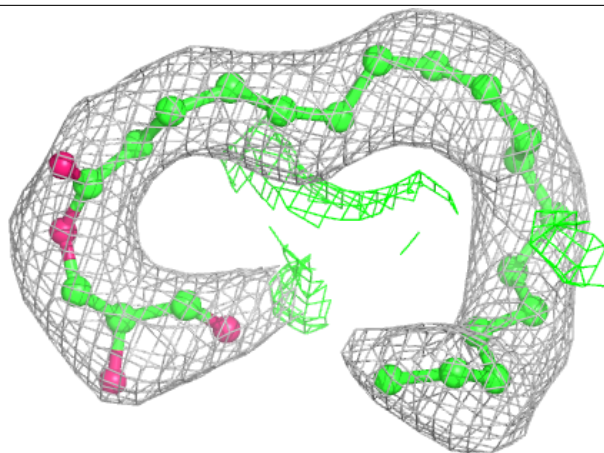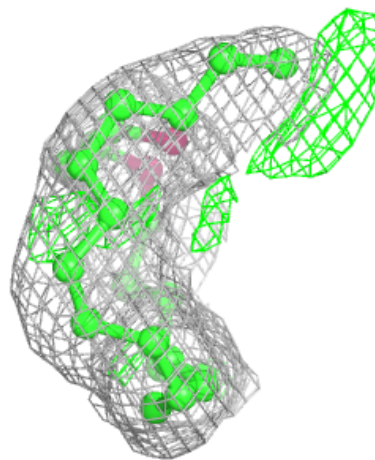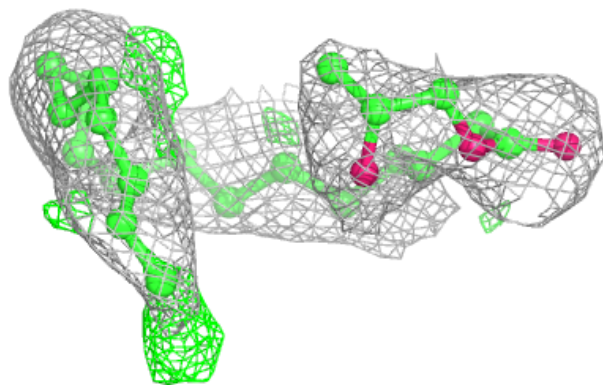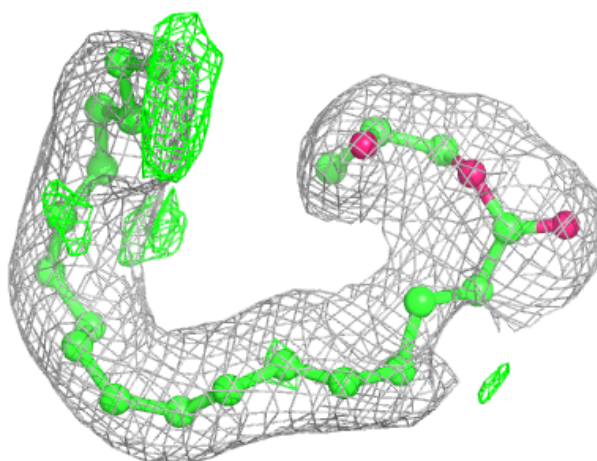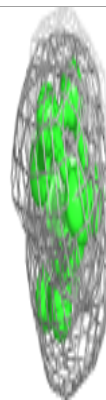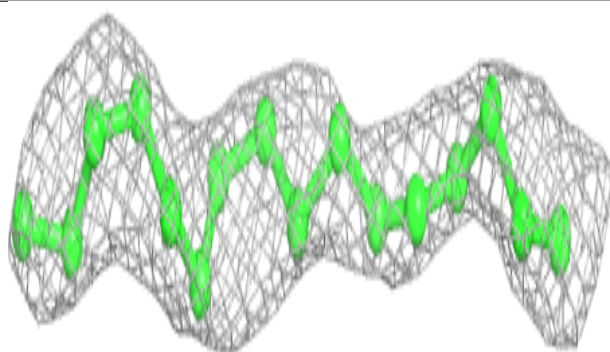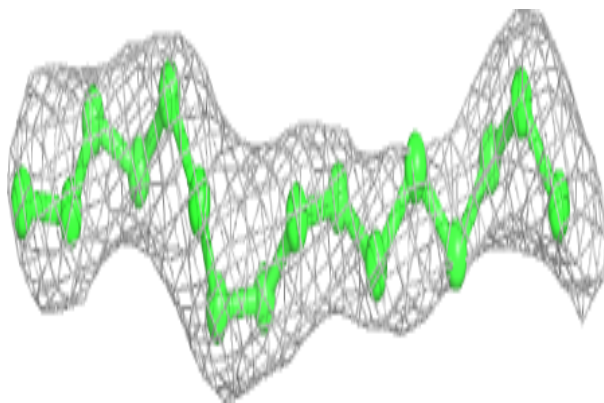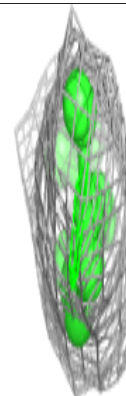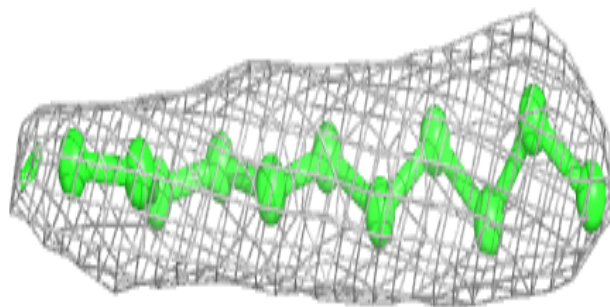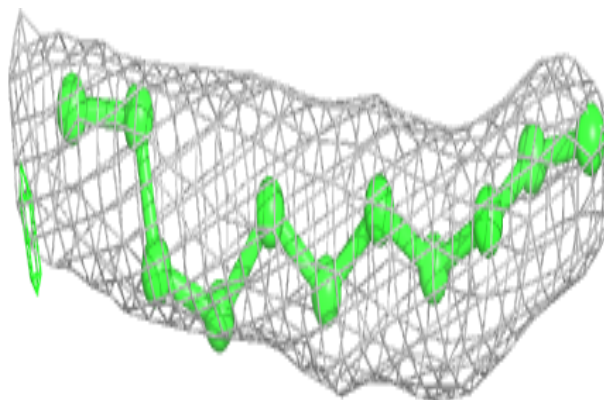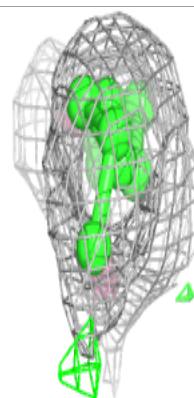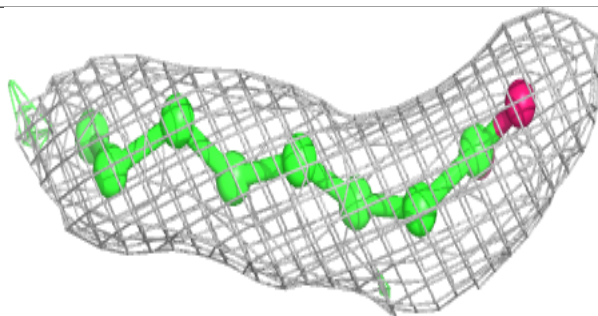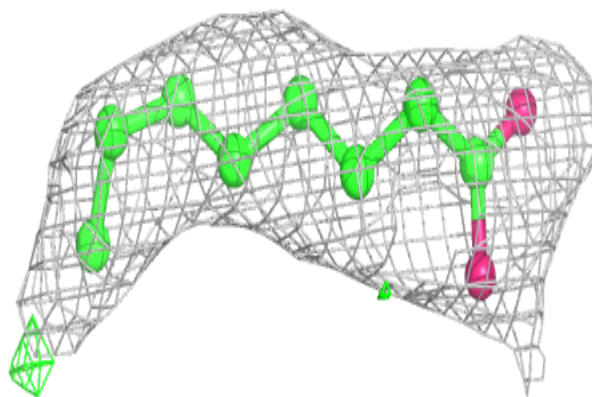and green (positive)
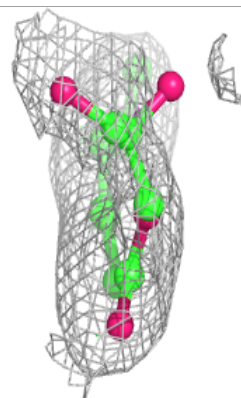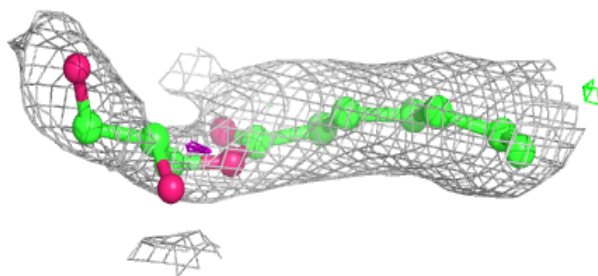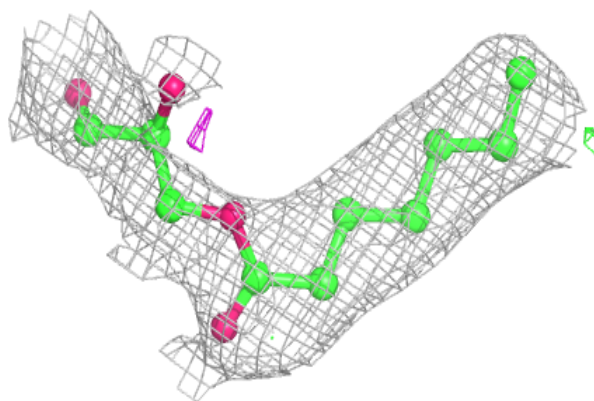
Electron density around OLC E 304:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
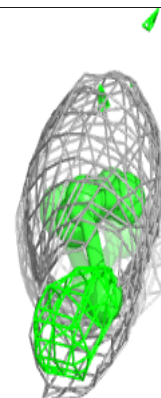and green (positive)
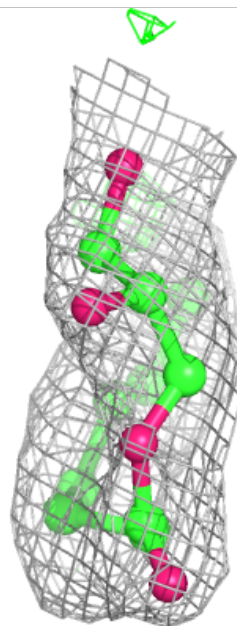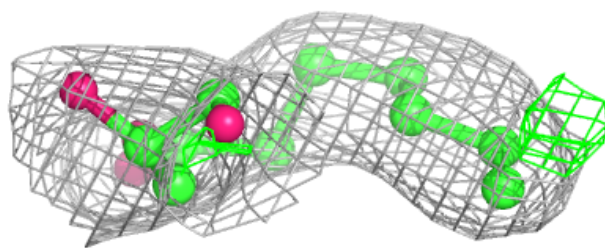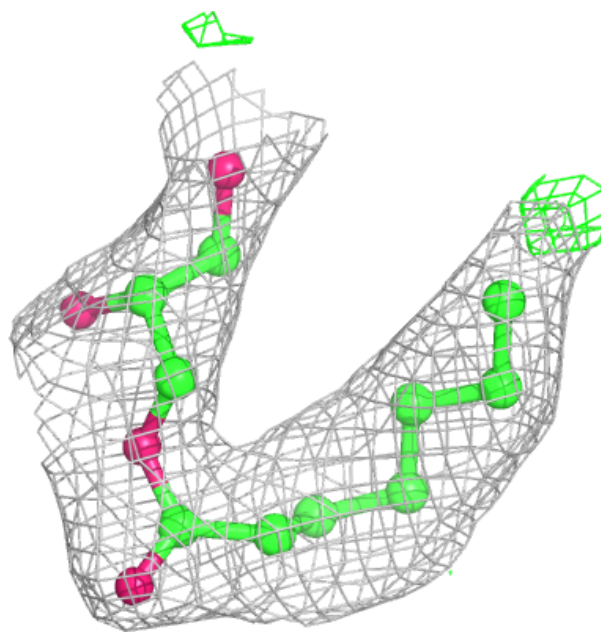
Electron density around OLC B 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
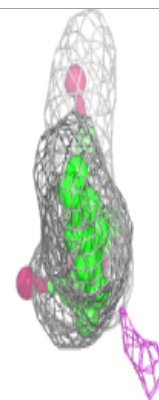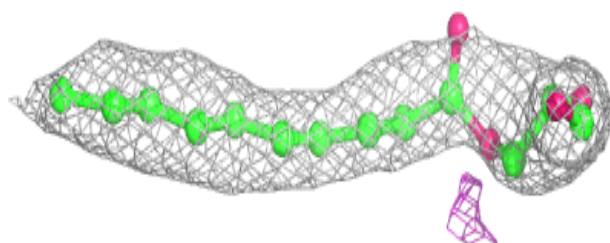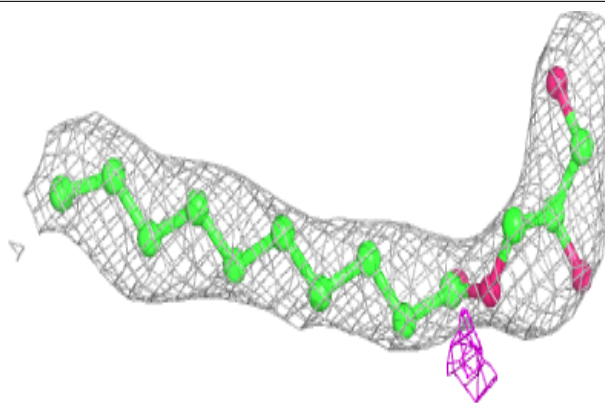
Electron density around OLC D 304:

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and green (positive)
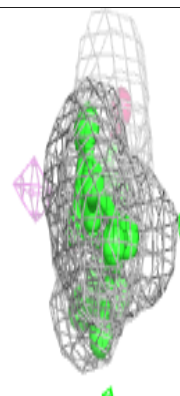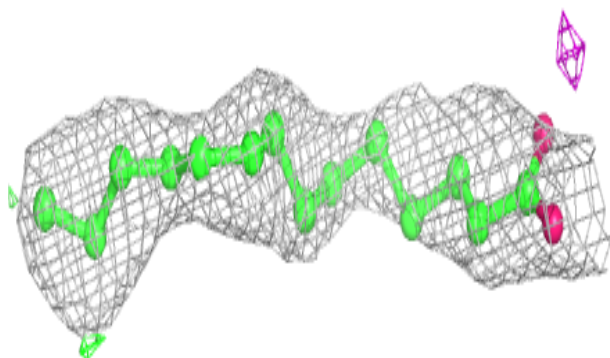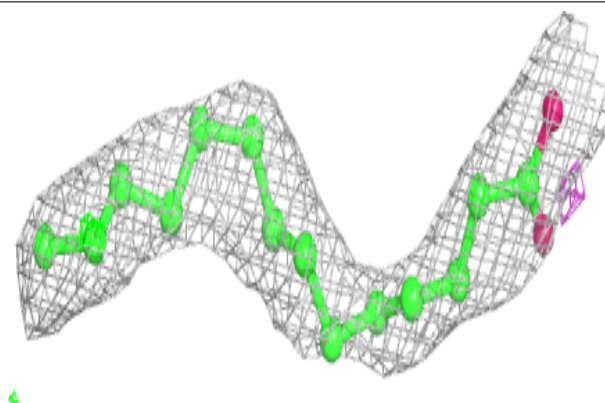
Electron density around OLC B 305:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
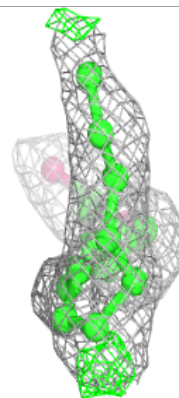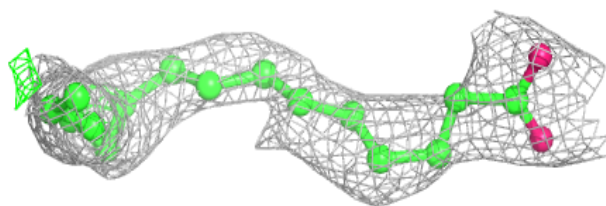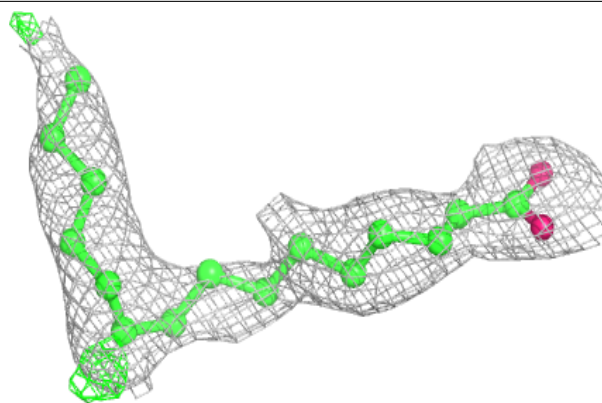
Electron density around OLC D 303:

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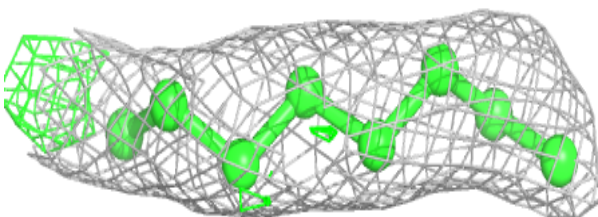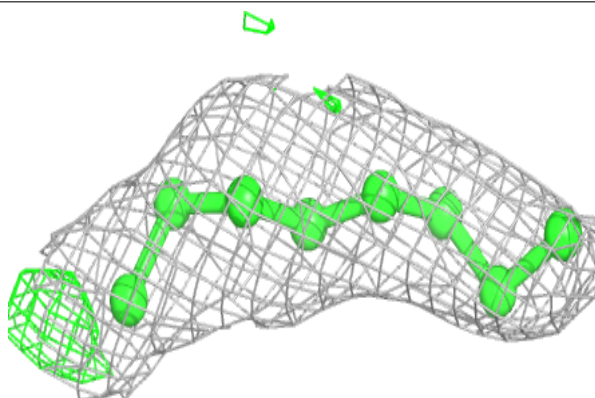$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
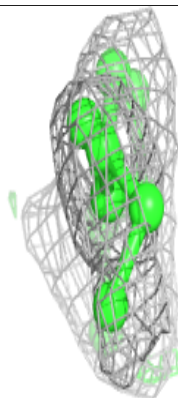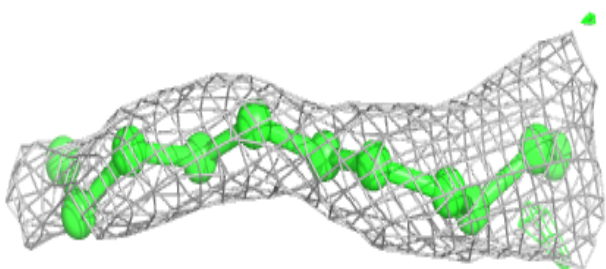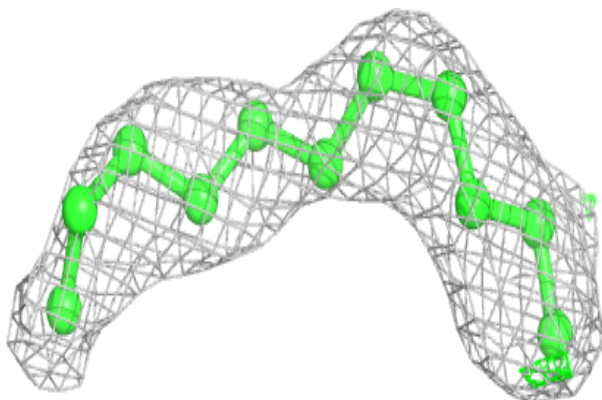
Electron density around OLC A 304:

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and green (positive)
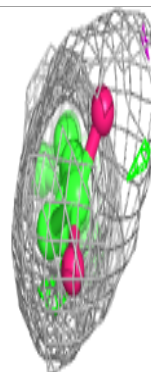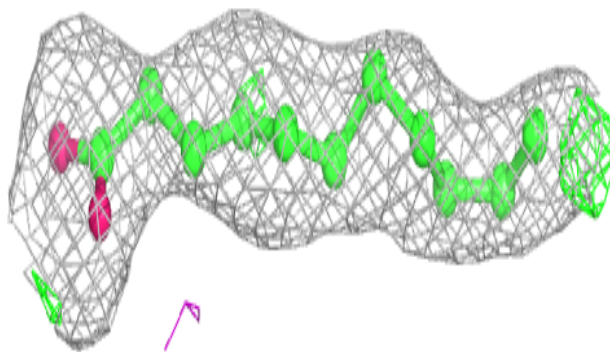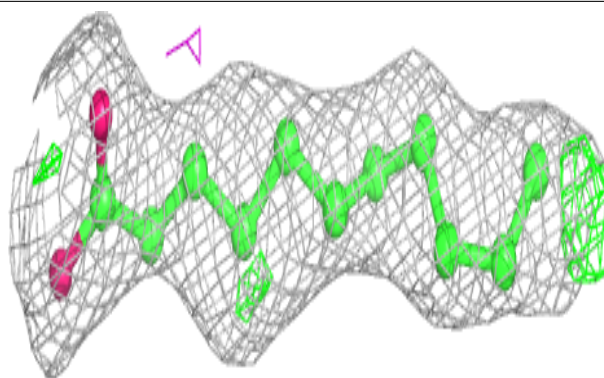
Electron density around OLC B 304:

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mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
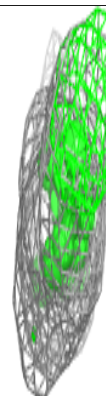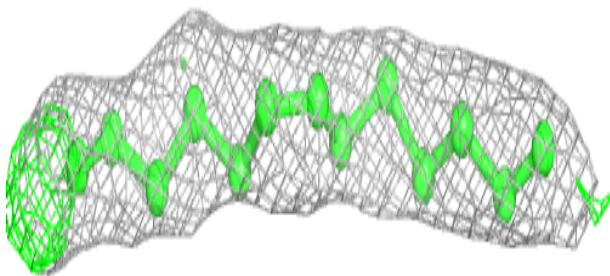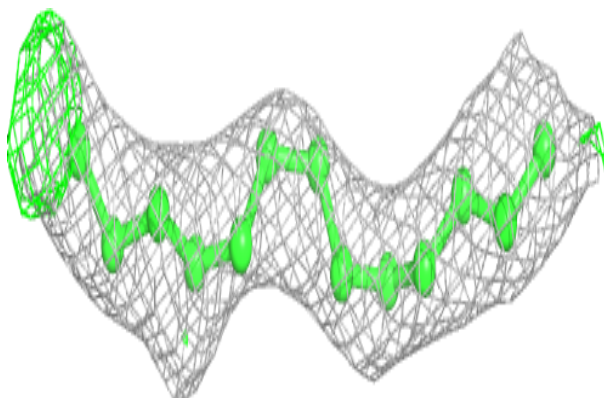
Electron density around OLC E 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
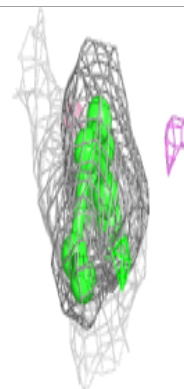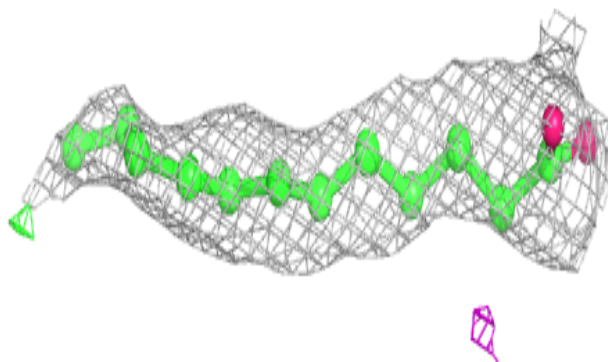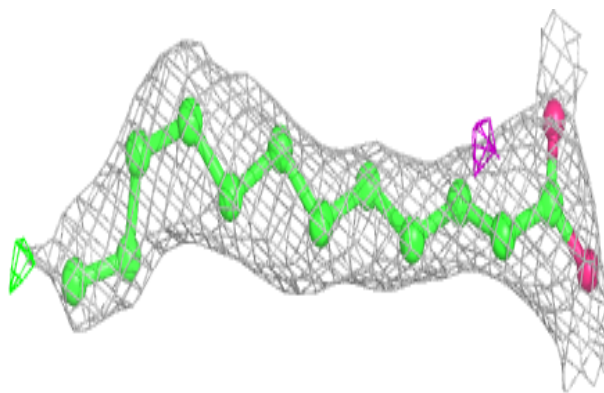
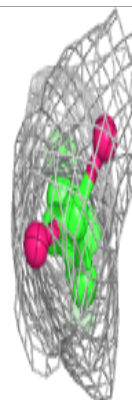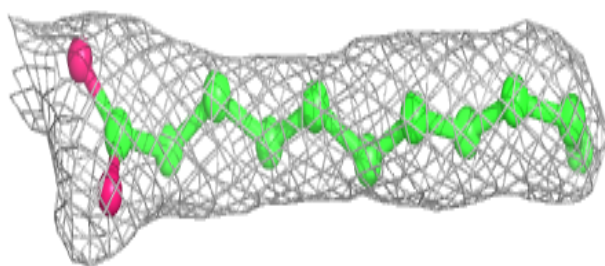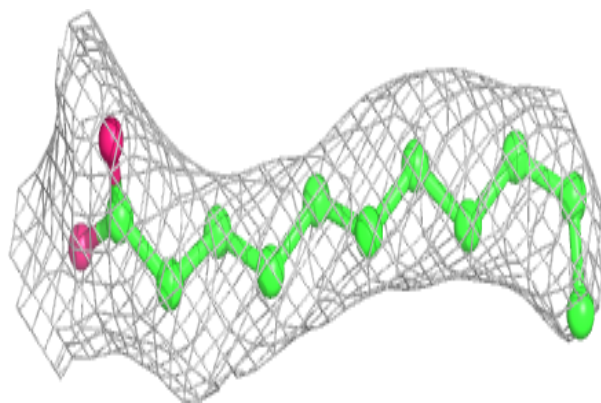
Electron density around OLC D 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
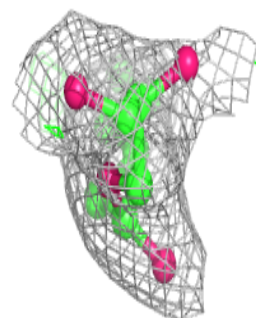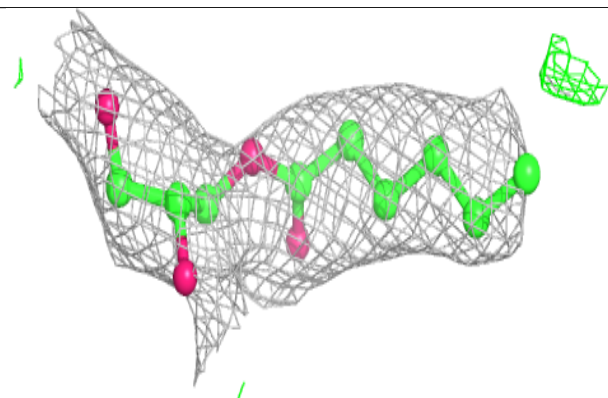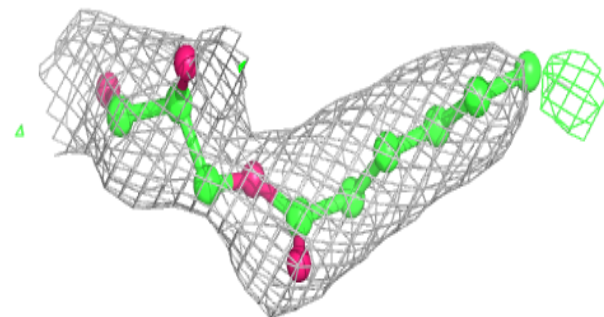
Electron density around OLC D 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
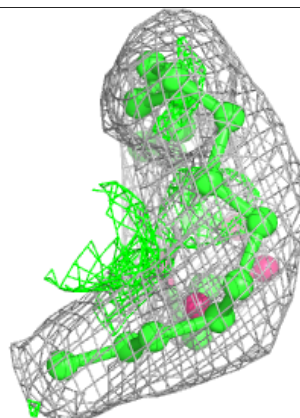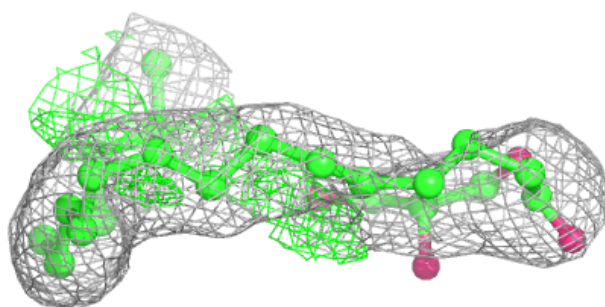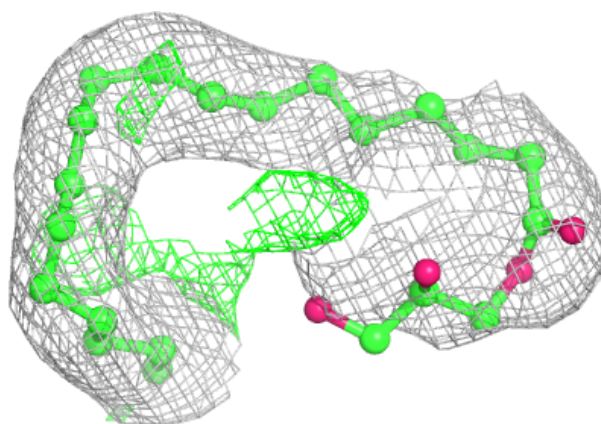
Electron density around OLC E 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
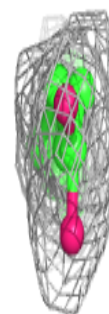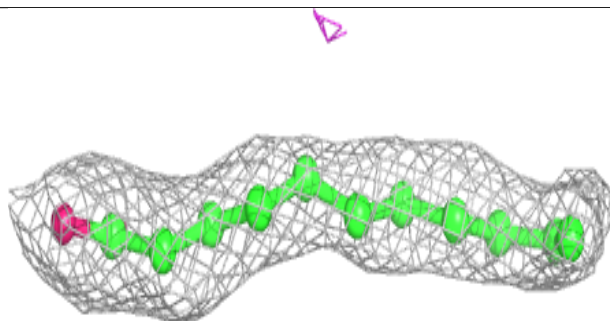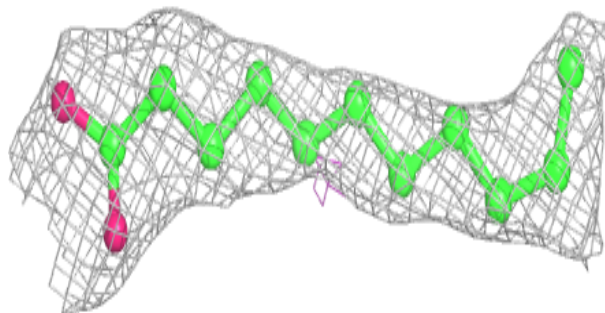and green (positive)
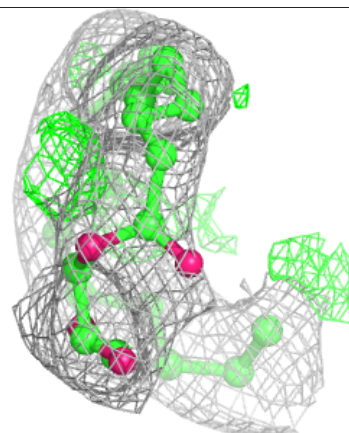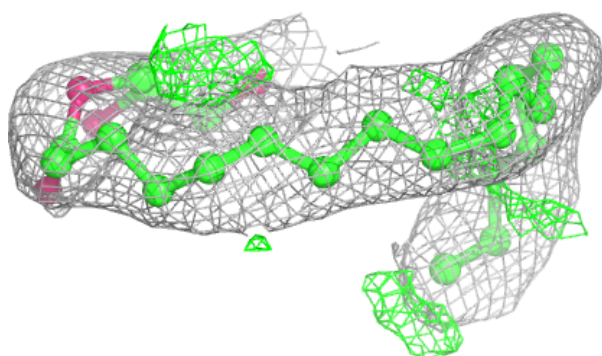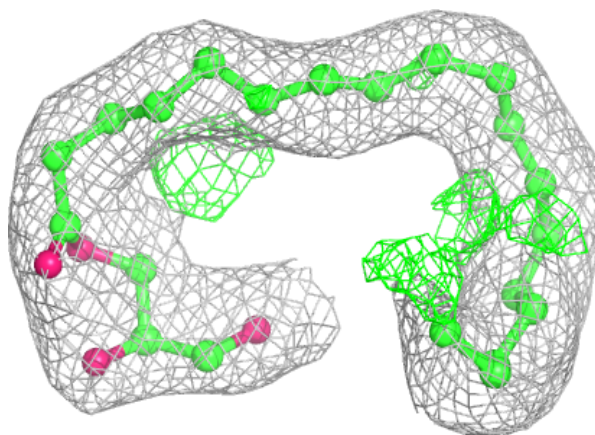
Electron density around OLC B 301:

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

Electron density around OLC C 302:

$2mF_o$-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 E 301:

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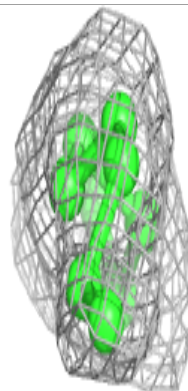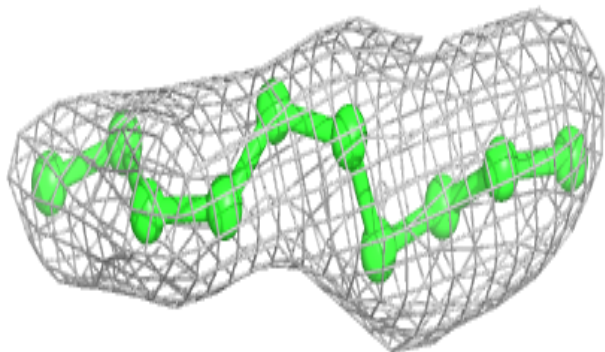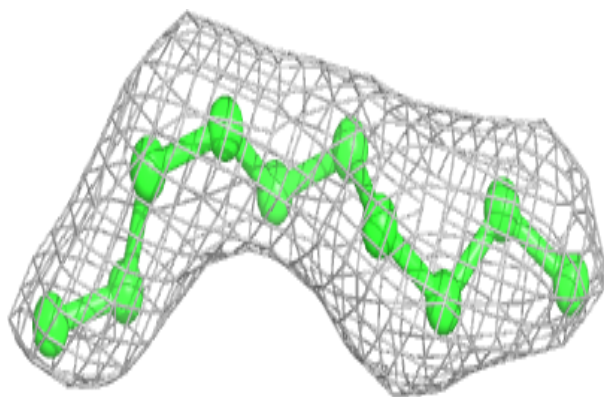and green (positive)

Electron density around OLC C 301:

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

Electron density around OLC A 302:

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

Electron density around OLC A 303:

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

Electron density around OLC B 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around OLC C 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
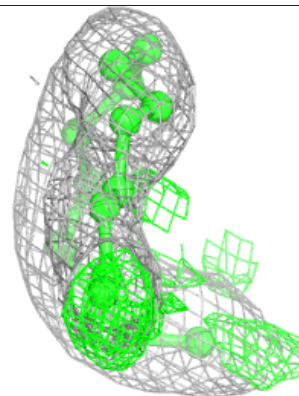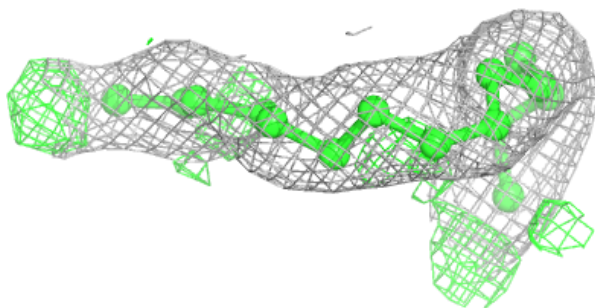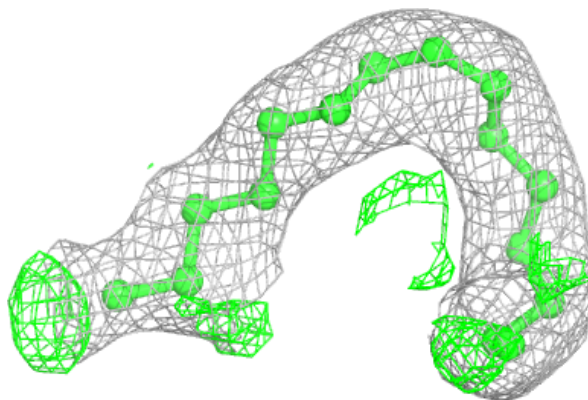and green (positive)

Electron density around OLC E 303:

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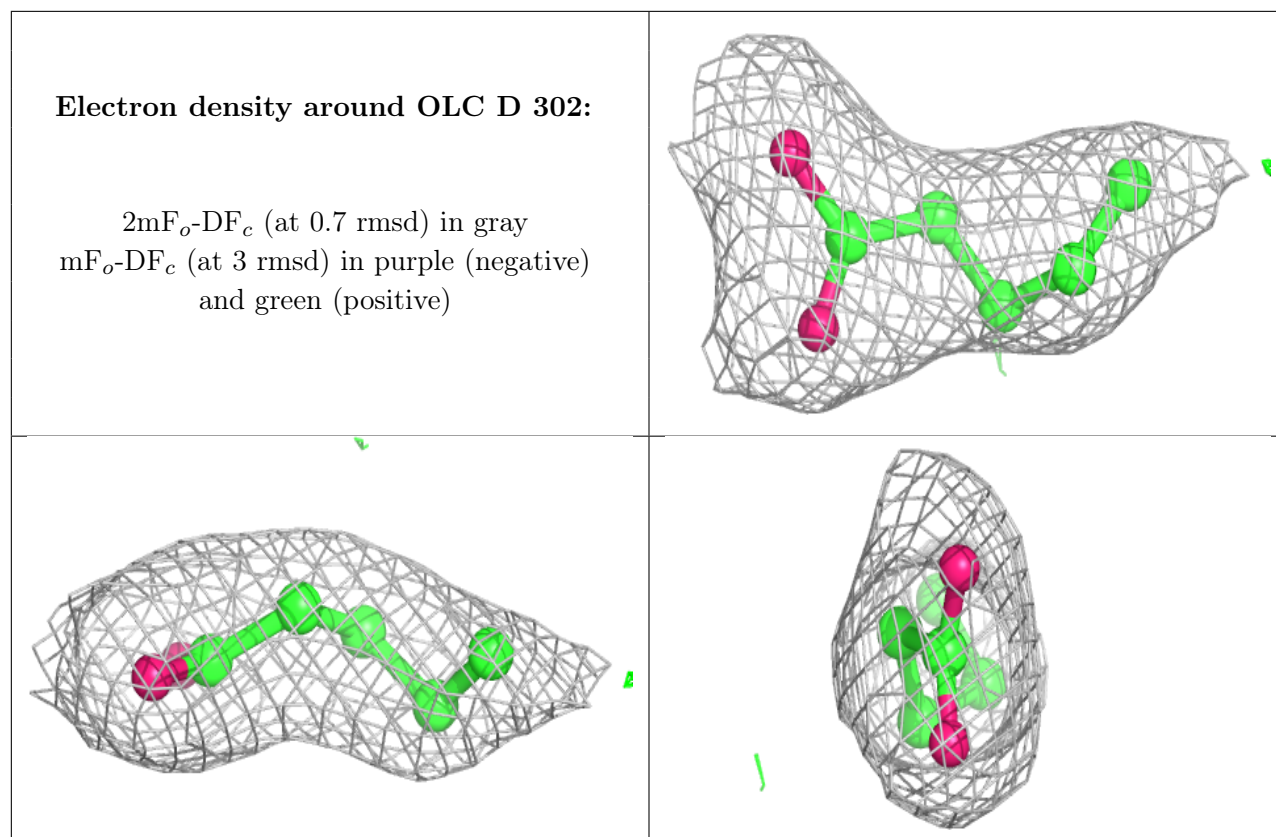mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around OLC A 301:

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

Electron density around OLC D 302:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.