Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2025 – 02:20 PM JST

PDB ID	:	9IN8
Title	:	True-atomic resolution crystal structure of the open state of the viral channel-rhodopsin OLPVR1
Authors	:	Bukhdruker, S.; Zabelskii, D.; Astashkin, R.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2024-07-05
Resolution	:	1.34 Å(reported)

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

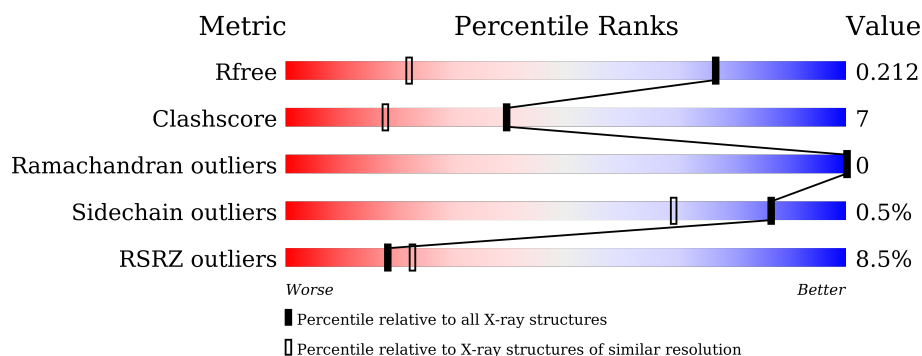|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 1.34 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		0.212
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		8.5%

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}	164625	1904 (1.36-1.32)
Clashscore	180529	2038 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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	231	8% 82% 15% •

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3031 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 Viral rhodopsin OLPVR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	2587	1771	367	432	17	0	78	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	LEU	-	expression tag	UNP F2Y337
A	225	GLU	-	expression tag	UNP F2Y337
A	226	HIS	-	expression tag	UNP F2Y337
A	227	HIS	-	expression tag	UNP F2Y337
A	228	HIS	-	expression tag	UNP F2Y337
A	229	HIS	-	expression tag	UNP F2Y337
A	230	HIS	-	expression tag	UNP F2Y337
A	231	HIS	-	expression tag	UNP F2Y337

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).
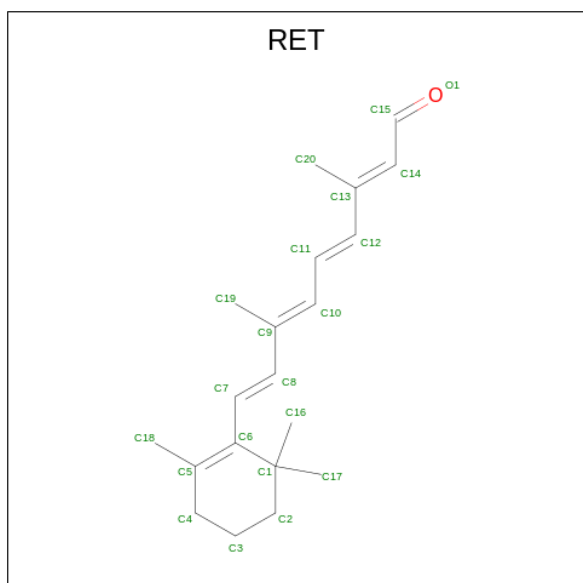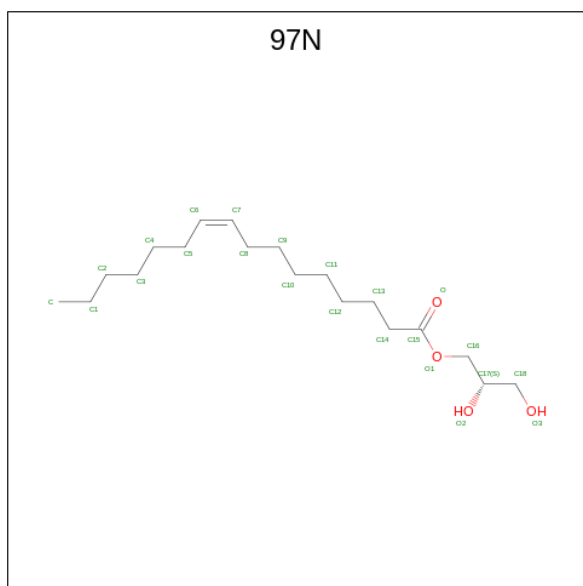
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total C 60 60		0	1

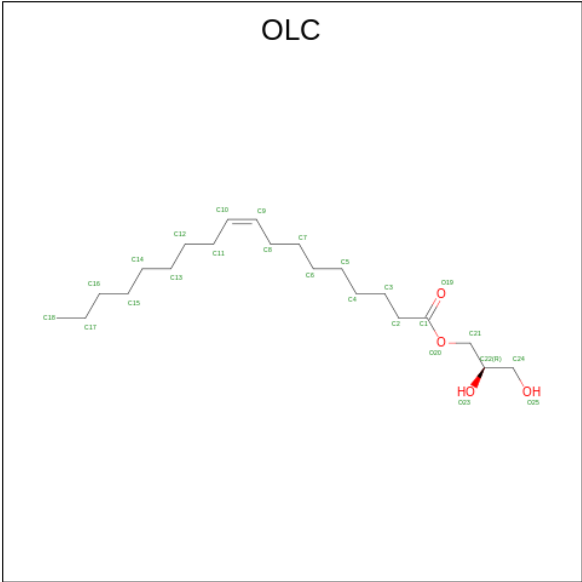- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

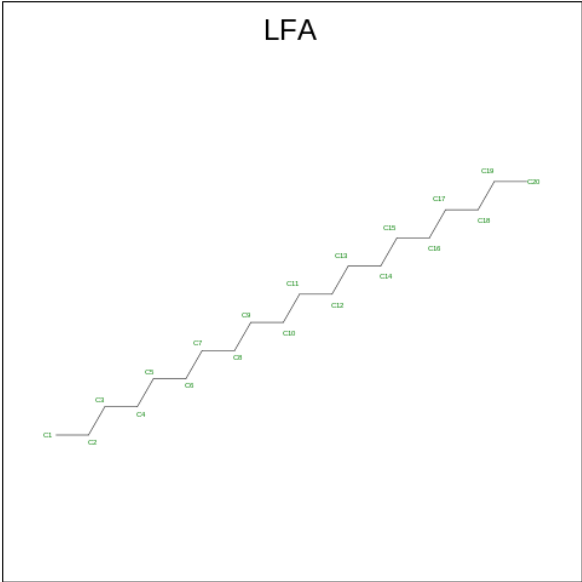- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-hexadec-9-enoate (three-letter code: 97N) (formula: $C_{19}H_{36}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total C O 23 19 4			0	1

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).

OLC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 16	C 14	O 2	0	0
5	A	1	Total 11	C 7	O 4	0	0
5	A	1	Total 18	C 14	O 4	0	0
5	A	1	Total 9	C 7	O 2	0	0
5	A	1	Total 16	C 14	O 2	0	0
5	A	1	Total 16	C 14	O 2	0	0

- Molecule 6 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).

LFA

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 10	C 10	0	0
6	A	1	Total 13	C 13	0	0
6	A	1	Total 12	C 12	0	0
6	A	1	Total 15	C 15	0	0
6	A	1	Total 16	C 16	0	0
6	A	1	Total 5	C 5	0	0
6	A	1	Total 3	C 3	0	0
6	A	1	Total 6	C 6	0	0
6	A	1	Total 20	C 20	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1　　C2

HO

O1

OH

O2

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	151	Total 156	O 156	0	22

WORLDWIDE

PDB

PROTEIN DATA BANK

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: Viral rhodopsin OLPVR1
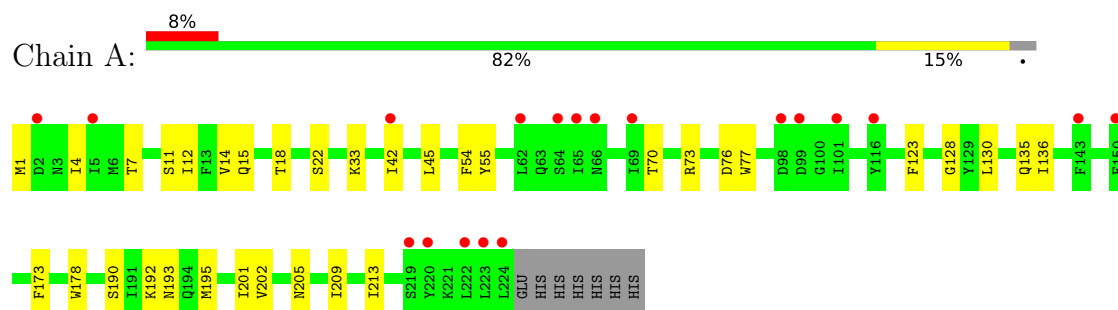
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	46.43Å 115.03Å 53.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 1.34 39.11 – 1.34	Depositor EDS
% Data completeness (in resolution range)	72.9 (39.11-1.34) 73.3 (39.11-1.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 1.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.212 0.184 , 0.212	Depositor DCC
R_{free} test set	4211 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, GOL, 97N, FME, RET, LFA

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	0.46	0/2650	0.61	2/3595 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76[A]	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	76[B]	ASP	CB-CG-OD1	5.22	123.00	118.30

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	2587	0	2577	29	0
2	A	60	0	81	9	0
3	A	1	0	0	0	0
4	A	23	0	0	0	0
5	A	86	0	108	2	0
6	A	100	0	191	12	0
7	A	18	0	24	2	0
8	A	156	0	0	3	0
All	All	3031	0	2981	39	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 7.

All (39) 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:18[B]:THR:HG21	1:A:205:ASN:HB3	1.68	0.76
1:A:70[B]:THR:HB	1:A:193[B]:ASN:HD21	1.53	0.73
1:A:54[B]:PHE:HB2	6:A:308:LFA:H111	1.80	0.63
1:A:70[B]:THR:HG21	1:A:192:LYS:HE3	1.80	0.63
1:A:135[B]:GLN:HG2	5:A:321:OLC:H2A	1.82	0.62
1:A:33:LYS:NZ	8:A:402:HOH:O	2.34	0.61
1:A:195[A]:MET:HG2	6:A:307:LFA:H72	1.82	0.61
2:A:301[B]:RET:H161	2:A:301[B]:RET:H8	1.83	0.60
2:A:301[A]:RET:H8	2:A:301[A]:RET:H161	1.86	0.55
1:A:202:VAL:HG22	6:A:313:LFA:H61	1.88	0.55
1:A:18[B]:THR:HG22	1:A:209:ILE:HD11	1.90	0.52
1:A:4[B]:ILE:HD11	1:A:190:SER:HA	1.92	0.52
1:A:213:ILE:HD12	6:A:305:LFA:H32	1.91	0.52
1:A:14[B]:VAL:HG11	1:A:201:ILE:HG23	1.93	0.51
1:A:135[A]:GLN:OE1	7:A:314[A]:GOL:H11	2.10	0.51
1:A:11[B]:SER:HB2	1:A:15:GLN:HE21	1.75	0.51
1:A:54[A]:PHE:HB2	6:A:308:LFA:H111	1.93	0.50
1:A:178[B]:TRP:CE2	2:A:301[B]:RET:H202	2.46	0.50
1:A:12[B]:ILE:HD11	1:A:55[B]:TYR:HB3	1.93	0.50
1:A:73[B]:ARG:HG2	1:A:77[B]:TRP:NE1	2.28	0.49
1:A:130:LEU:HD13	1:A:136[B]:ILE:HD11	1.95	0.48
7:A:315:GOL:H31	8:A:499:HOH:O	2.13	0.48
1:A:123:PHE:CE2	6:A:309:LFA:H122	2.50	0.46
2:A:301[C]:RET:H171	2:A:301[C]:RET:H8	1.97	0.45
1:A:7[A]:THR:HG22	6:A:313:LFA:H161	1.98	0.45
1:A:128:GLY:HA3	2:A:301[B]:RET:H162	1.99	0.44
1:A:4[A]:ILE:HD11	1:A:190:SER:HA	1.98	0.44
1:A:202:VAL:CG2	6:A:313:LFA:H61	2.47	0.43
1:A:123:PHE:CD2	6:A:309:LFA:H122	2.53	0.43
1:A:22:SER:HB2	1:A:45[A]:LEU:HD21	2.00	0.43
1:A:173[A]:PHE:CZ	6:A:313:LFA:H13	2.54	0.43
6:A:313:LFA:H32	6:A:313:LFA:H62	1.65	0.43
2:A:301[A]:RET:H7	2:A:301[A]:RET:H181	1.84	0.42
1:A:136[B]:ILE:HG22	8:A:405:HOH:O	2.20	0.42
2:A:301[A]:RET:H161	2:A:301[A]:RET:C8	2.50	0.42
5:A:321:OLC:H8A	5:A:321:OLC:H11A	1.83	0.41
1:A:123:PHE:CE2	6:A:309:LFA:H101	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301[B]:RET:H181	2:A:301[B]:RET:H7	1.87	0.40
2:A:301[A]:RET:H8	2:A:301[A]:RET:H171	2.02	0.40

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	301/231 (130%)	293 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/220 (127%)	278 (99%)	2 (1%)	81	59

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42[A]	ILE
1	A	42[B]	ILE

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	FME	A	1	1	8,9,10	0.90	0	7,9,11	1.23	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	C-CA-N	2.28	113.84	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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).

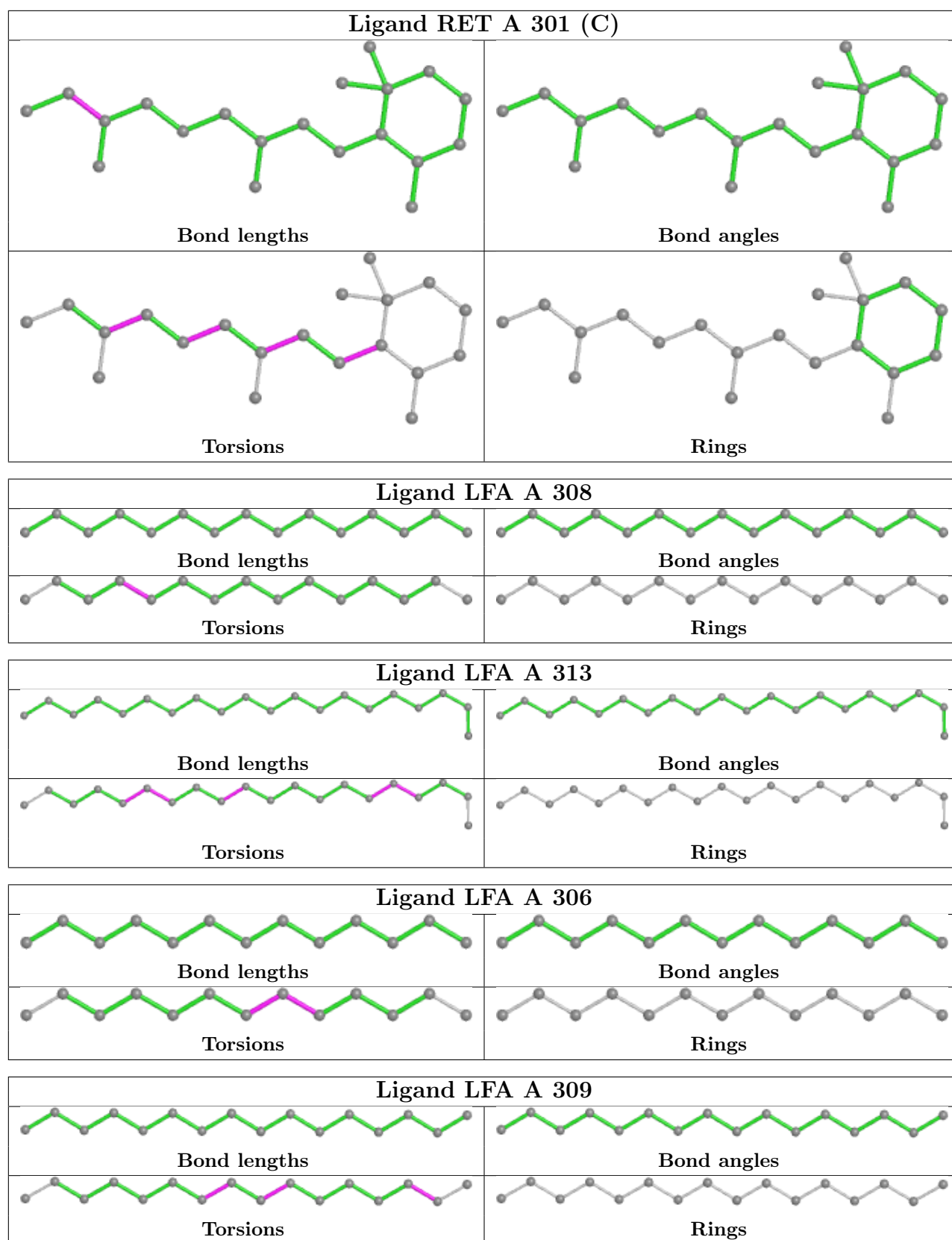| Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	OLC	A	304	-	15,15,24	0.35	0	15,15,25	0.38	0
2	RET	A	301[B]	1	20,20,21	0.85	1 (5%)	27,27,28	0.85	1 (3%)
5	OLC	A	318	-	17,17,24	0.26	0	18,18,25	0.39	0
5	OLC	A	319	-	8,8,24	0.39	0	8,8,25	0.40	0
2	RET	A	301[C]	1	20,20,21	0.74	1 (5%)	27,27,28	0.53	0
6	LFA	A	308	-	14,14,19	0.10	0	13,13,18	0.12	0
7	GOL	A	314[A]	-	5,5,5	0.82	0	5,5,5	0.93	0
6	LFA	A	313	-	19,19,19	0.12	0	18,18,18	0.19	0
6	LFA	A	306	-	12,12,19	0.09	0	11,11,18	0.11	0
6	LFA	A	312	-	5,5,19	0.11	0	4,4,18	0.25	0
6	LFA	A	309	-	15,15,19	0.08	0	14,14,18	0.21	0
7	GOL	A	316	-	5,5,5	0.90	0	5,5,5	0.95	0
7	GOL	A	315	-	5,5,5	0.95	0	5,5,5	0.89	0
6	LFA	A	311	-	2,2,19	0.05	0	0,1,18	-	-
6	LFA	A	307	-	11,11,19	0.08	0	10,10,18	0.09	0
5	OLC	A	317	-	10,10,24	0.25	0	11,11,25	0.31	0
5	OLC	A	320	-	15,15,24	0.32	0	14,15,25	0.21	0
2	RET	A	301[A]	1	20,20,21	0.68	1 (5%)	27,27,28	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
6	LFA	A	305	-	9,9,19	0.12	0	8,8,18	0.14	0
5	OLC	A	321	-	15,15,24	0.39	0	15,15,25	0.33	0
6	LFA	A	310	-	4,4,19	0.17	0	3,3,18	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	304	-	-	2/13/13/24	-
2	RET	A	301[B]	1	-	0/13/30/31	0/1/1/1
5	OLC	A	318	-	-	5/17/17/24	-
5	OLC	A	319	-	-	0/6/6/24	-
2	RET	A	301[C]	1	-	7/13/30/31	0/1/1/1
6	LFA	A	308	-	-	1/12/12/17	-
7	GOL	A	314[A]	-	-	2/4/4/4	-
6	LFA	A	313	-	-	5/17/17/17	-
6	LFA	A	306	-	-	2/10/10/17	-
6	LFA	A	312	-	-	0/3/3/17	-
6	LFA	A	309	-	-	3/13/13/17	-
7	GOL	A	316	-	-	4/4/4/4	-
7	GOL	A	315	-	-	2/4/4/4	-
6	LFA	A	307	-	-	2/9/9/17	-
5	OLC	A	317	-	-	1/10/10/24	-
5	OLC	A	320	-	-	2/14/14/24	-
2	RET	A	301[A]	1	-	0/13/30/31	0/1/1/1
6	LFA	A	305	-	-	0/7/7/17	-
5	OLC	A	321	-	-	3/13/13/24	-
6	LFA	A	310	-	-	0/2/2/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	RET	C14-C13	2.97	1.36	1.33
2	A	301[C]	RET	C14-C13	2.90	1.36	1.33
2	A	301[A]	RET	C14-C13	2.11	1.35	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301[B]	RET	C8-C7-C6	3.46	136.92	127.20

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[C]	RET	C1-C6-C7-C8
2	A	301[C]	RET	C5-C6-C7-C8
2	A	301[C]	RET	C7-C8-C9-C10
2	A	301[C]	RET	C7-C8-C9-C19
2	A	301[C]	RET	C11-C12-C13-C14
2	A	301[C]	RET	C11-C12-C13-C20
5	A	318	OLC	O20-C21-C22-C24
5	A	318	OLC	O20-C21-C22-O23
7	A	315	GOL	C1-C2-C3-O3
7	A	315	GOL	O2-C2-C3-O3
7	A	316	GOL	O1-C1-C2-C3
6	A	313	LFA	C3-C4-C5-C6
6	A	309	LFA	C12-C13-C14-C15
5	A	318	OLC	C5-C6-C7-C8
6	A	313	LFA	C4-C5-C6-C7
7	A	314[A]	GOL	C1-C2-C3-O3
7	A	316	GOL	C1-C2-C3-O3
5	A	318	OLC	C2-C3-C4-C5
7	A	314[A]	GOL	O2-C2-C3-O3
7	A	316	GOL	O1-C1-C2-O2
5	A	317	OLC	C1-C2-C3-C4
5	A	320	OLC	C9-C10-C11-C12
6	A	309	LFA	C10-C11-C12-C13
5	A	304	OLC	C11-C12-C13-C14
6	A	309	LFA	C5-C6-C7-C8
6	A	307	LFA	C11-C10-C9-C8
6	A	306	LFA	C11-C12-C13-C14
5	A	320	OLC	C6-C7-C8-C9
6	A	313	LFA	C14-C15-C16-C17
6	A	307	LFA	C9-C10-C11-C12
6	A	313	LFA	C10-C11-C12-C13
6	A	306	LFA	C12-C13-C14-C15
2	A	301[C]	RET	C9-C10-C11-C12
5	A	304	OLC	C9-C10-C11-C12
5	A	318	OLC	C7-C8-C9-C10
5	A	321	OLC	C2-C3-C4-C5
7	A	316	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	313	LFA	C13-C14-C15-C16
5	A	321	OLC	O20-C1-C2-C3
5	A	321	OLC	O19-C1-C2-C3
6	A	308	LFA	C15-C16-C17-C18

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301[B]	RET	4	0
2	A	301[C]	RET	1	0
6	A	308	LFA	2	0
7	A	314[A]	GOL	1	0
6	A	313	LFA	5	0
6	A	309	LFA	3	0
7	A	315	GOL	1	0
6	A	307	LFA	1	0
2	A	301[A]	RET	4	0
6	A	305	LFA	1	0
5	A	321	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 A 304

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 301 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 318

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 301 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 308

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 313

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 306

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 309

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 307

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 317

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 320

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 321

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	223/231 (96%)	0.69	19 (8%)	18	22	6, 21, 31, 94	78 (34%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	LEU	8.6
1	A	224	LEU	8.5
1	A	220[A]	TYR	7.3
1	A	66[A]	ASN	4.7
1	A	222	LEU	4.6
1	A	65[A]	ILE	4.1
1	A	143[A]	PHE	4.0
1	A	62[A]	LEU	3.1
1	A	98[A]	ASP	3.1
1	A	219	SER	2.9
1	A	99[A]	ASP	2.8
1	A	150[A]	PHE	2.6
1	A	42[A]	ILE	2.4
1	A	69[A]	ILE	2.4
1	A	101[A]	ILE	2.4
1	A	5[A]	ILE	2.3
1	A	2[A]	ASP	2.3
1	A	64[A]	SER	2.2
1	A	116	TYR	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.71	0.23	36,53,90,134	0

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
7	GOL	A	314[A]	6/6	0.60	0.25	48,51,52,56	6
7	GOL	A	316	6/6	0.64	0.17	48,64,69,75	0
5	OLC	A	320	16/25	0.66	0.16	48,56,80,86	0
5	OLC	A	317	11/25	0.70	0.28	33,42,62,62	11
5	OLC	A	321	16/25	0.71	0.19	33,57,83,84	0
7	GOL	A	315	6/6	0.72	0.14	37,58,62,72	0
6	LFA	A	313	20/20	0.74	0.18	43,51,66,66	0
6	LFA	A	311	3/20	0.74	0.16	50,50,52,57	0
5	OLC	A	318	18/25	0.76	0.14	40,58,77,77	0
5	OLC	A	319	9/25	0.79	0.13	42,46,75,93	0
6	LFA	A	306	13/20	0.79	0.17	42,50,68,75	0
6	LFA	A	310	5/20	0.79	0.17	36,39,45,49	0
4	97N	A	303[A]	23/23	0.79	0.20	30,42,51,58	8
6	LFA	A	309	16/20	0.80	0.15	36,54,75,82	0
6	LFA	A	307	12/20	0.84	0.19	33,43,48,49	0
6	LFA	A	305	10/20	0.84	0.15	32,40,46,47	0
5	OLC	A	304	16/25	0.85	0.16	32,45,60,73	0
6	LFA	A	312	6/20	0.85	0.11	36,40,42,49	0
6	LFA	A	308	15/20	0.85	0.11	33,40,55,59	0
3	NA	A	302[A]	1/1	0.90	0.27	28,28,28,28	1
2	RET	A	301[C]	20/21	0.94	0.08	12,17,21,21	20
2	RET	A	301[A]	20/21	0.94	0.08	11,16,21,21	20
2	RET	A	301[B]	20/21	0.94	0.08	13,18,22,24	20

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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Electron density around OLC A 320:

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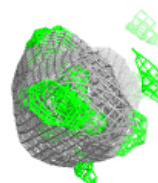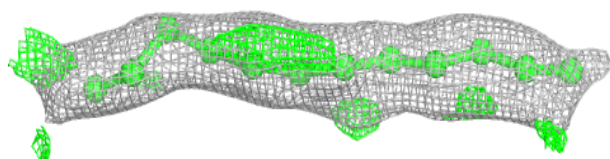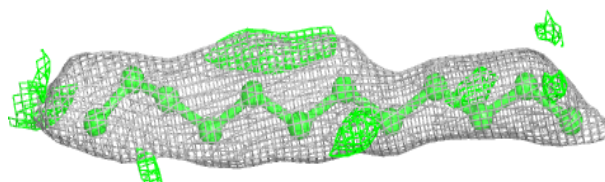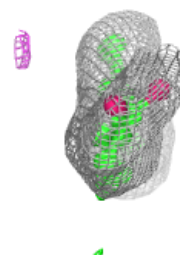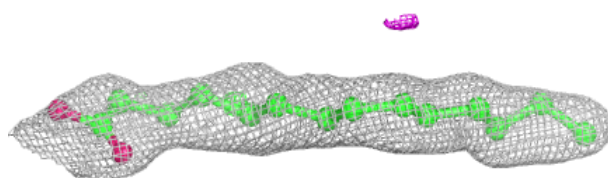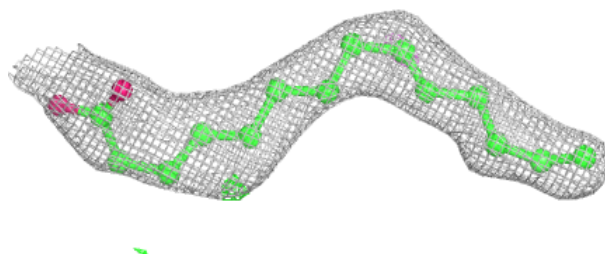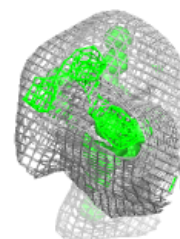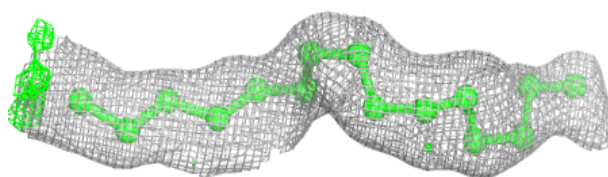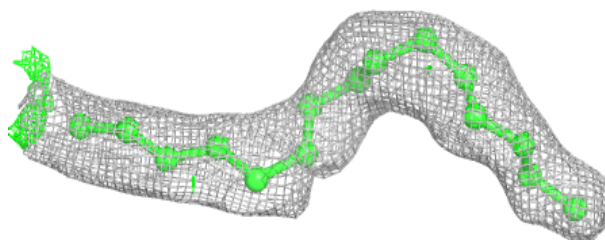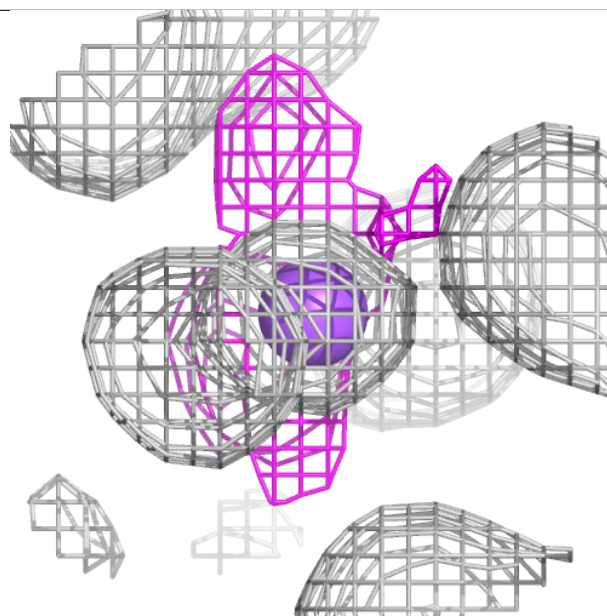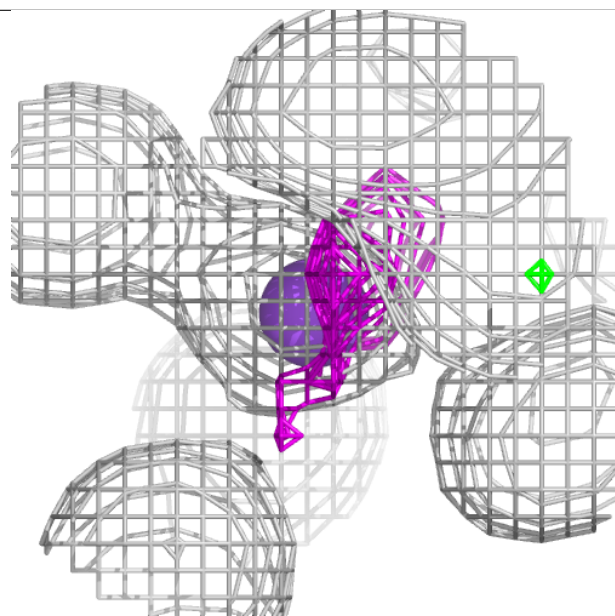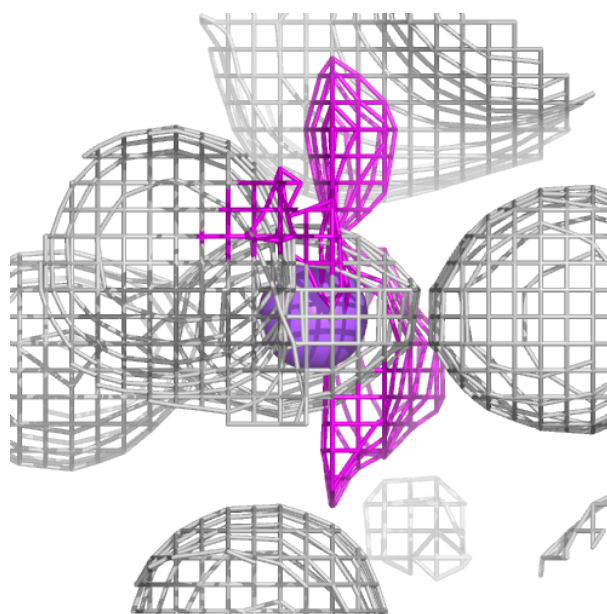$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
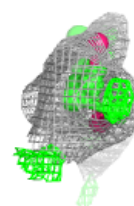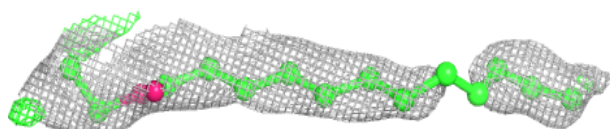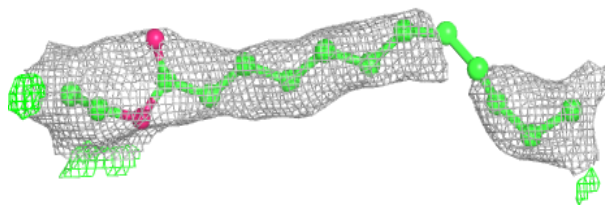
Electron density around OLC A 317:

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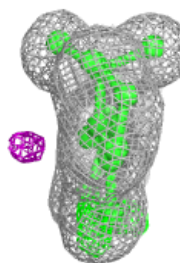$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
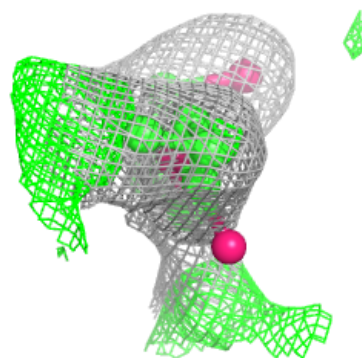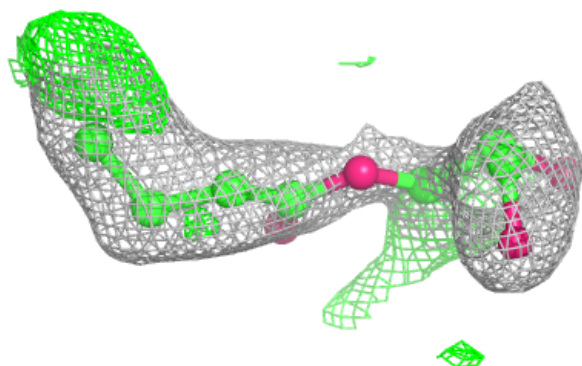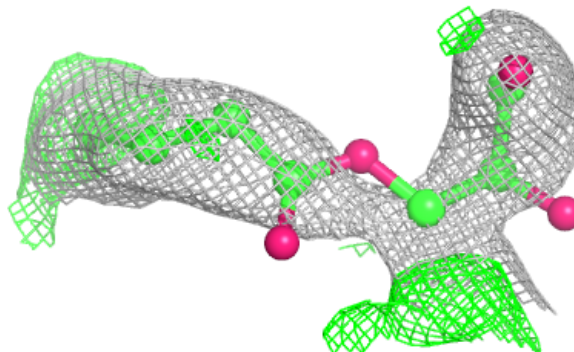
Electron density around OLC A 321:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
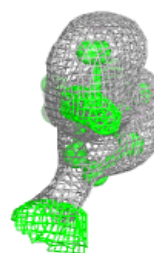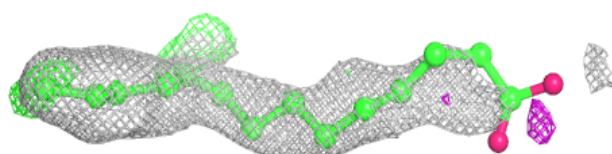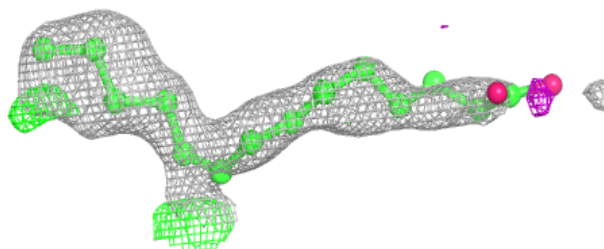
Electron density around LFA A 313:

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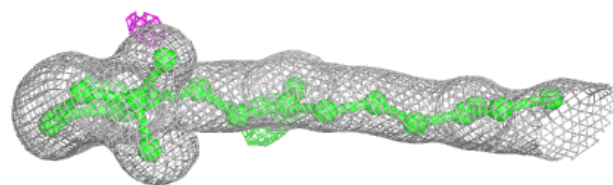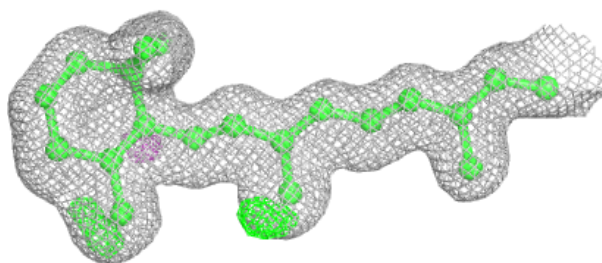mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
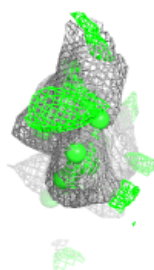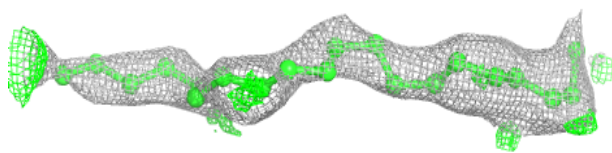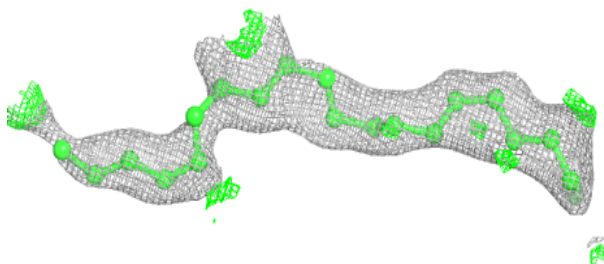
Electron density around OLC A 318:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
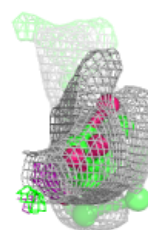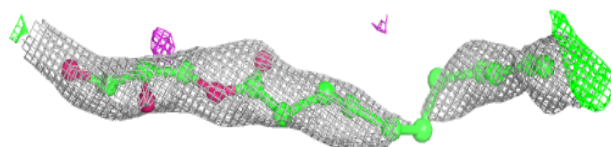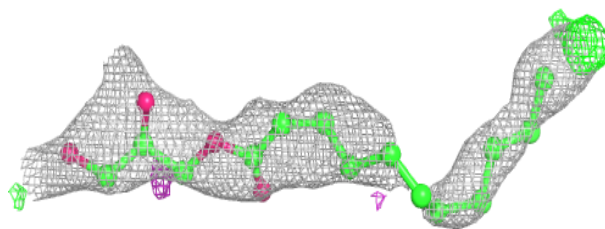
Electron density around LFA A 306:

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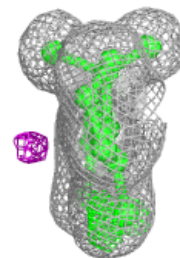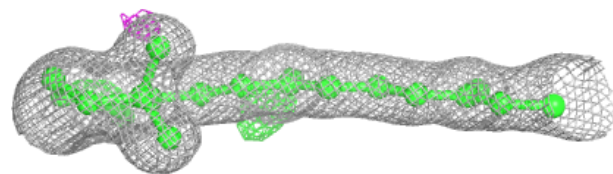and green (positive)
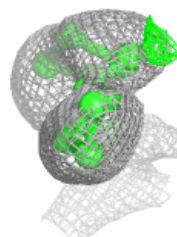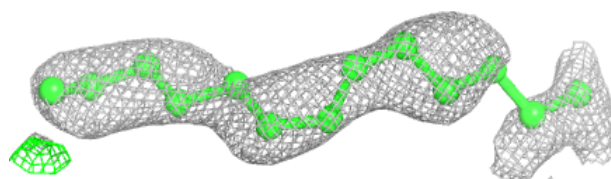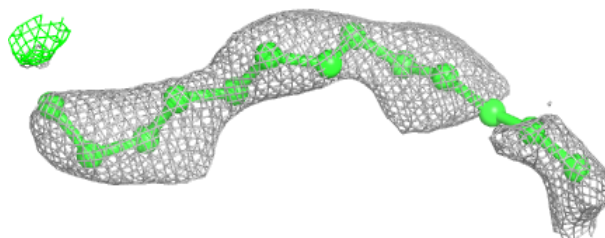
Electron density around LFA A 309:

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mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
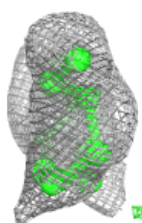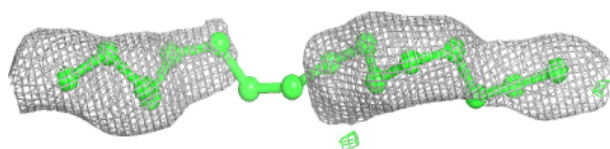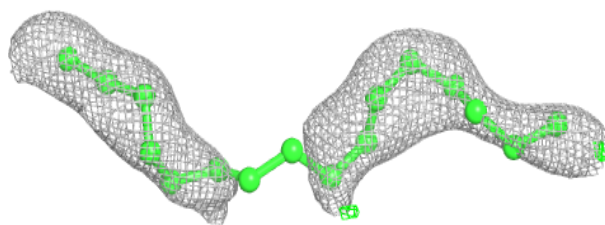
Electron density around LFA A 307:

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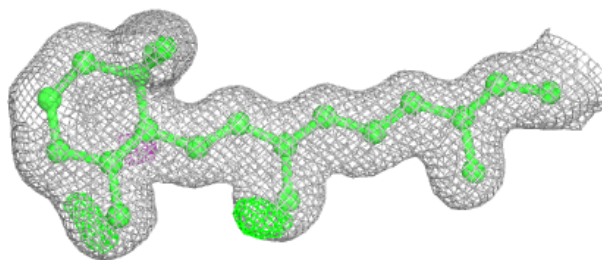and green (positive)

Electron density around OLC A 304:

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

Electron density around LFA A 308:

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

Electron density around NA A 302 (A):

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

Electron density around RET A 301 (C):

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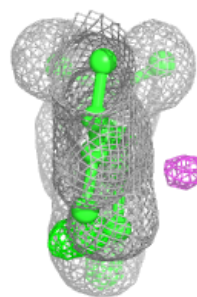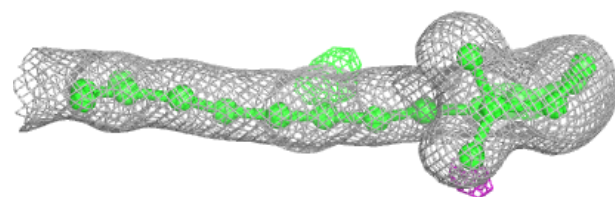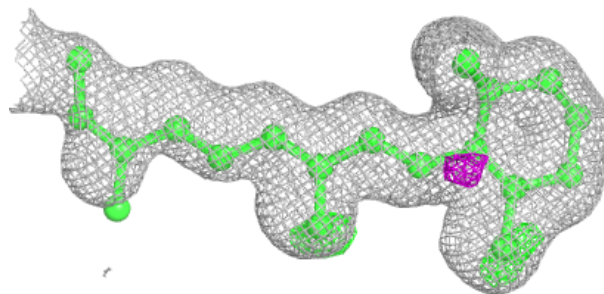mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around RET A 301 (A):

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

Electron density around RET A 301 (B):

$2mF_o$-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.