Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 02:32 pm GMT

PDB ID	:	5LWY
Title	:	Revised crystal structure of the human adiponectin receptor 2 in complex with a C18 free fatty acid
Authors	:	Leyrat, C.; Vasiliauskaite-Brooks, I.; Granier, S.
Deposited on	:	2016-09-19
Resolution	:	2.40 Å(reported)

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

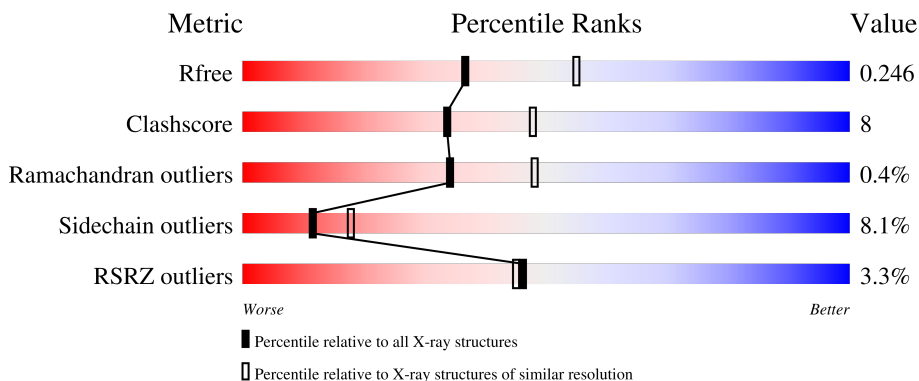|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
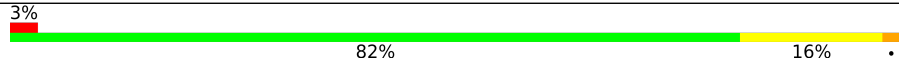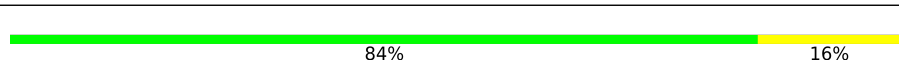*X-RAY DIFFRACTION*

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		0.246
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		8.1%
RSRZ outliers		3.3%

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	292	5% / 76% / 18% / · ·
2	H	119	3% / 82% / 16% / ·
3	L	107	84% / 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OLB	A	405	-	-	-	X
5	OLB	A	406	-	-	-	X
5	OLB	A	407	-	-	-	X
5	OLB	A	409	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 4613 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 Adiponectin receptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total 2325	C 1563	N 377	O 368	S 17	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q86V24
A	-3	GLY	-	expression tag	UNP Q86V24
A	-2	SER	-	expression tag	UNP Q86V24
A	-1	GLU	-	expression tag	UNP Q86V24
A	0	PHE	-	expression tag	UNP Q86V24

- Molecule 2 is a protein called V REGION HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total 927	C 592	N 149	O 182	S 4	0	0	0

- Molecule 3 is a protein called V REGION LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	107	Total 820	C 517	N 137	O 163	S 3	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0

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

OLB
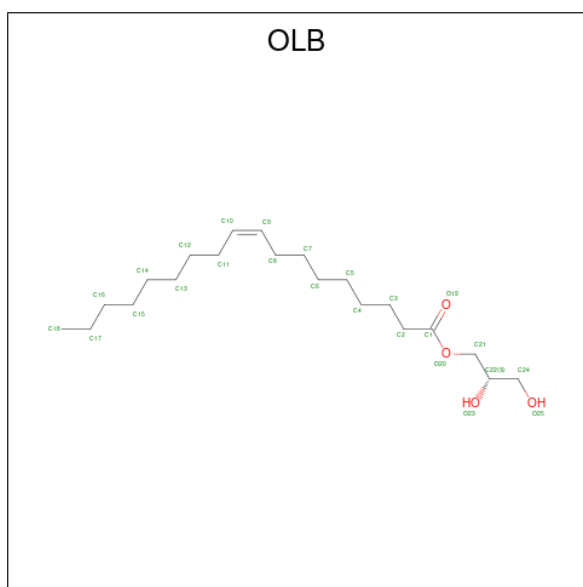
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	6	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

OLA
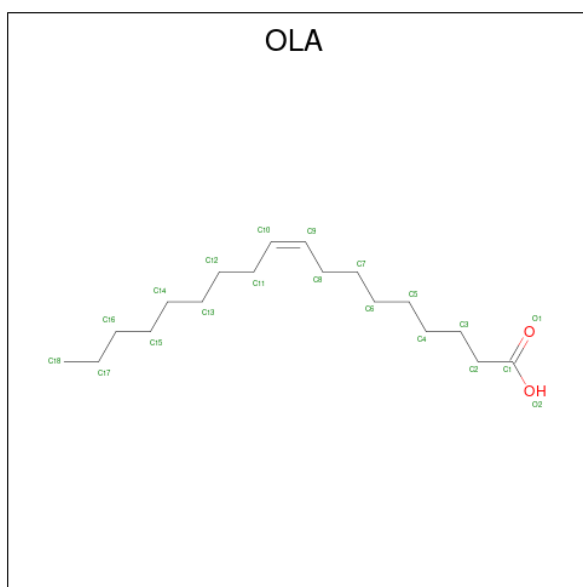
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 20	C 18	O 2	0	0

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

GOL

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

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	153	Total O 153 153	0	0
8	H	89	Total O 89 89	0	0
8	L	72	Total O 72 72	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.
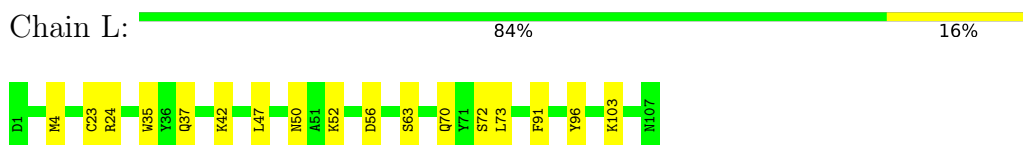
• Molecule 1: Adiponectin receptor protein 2
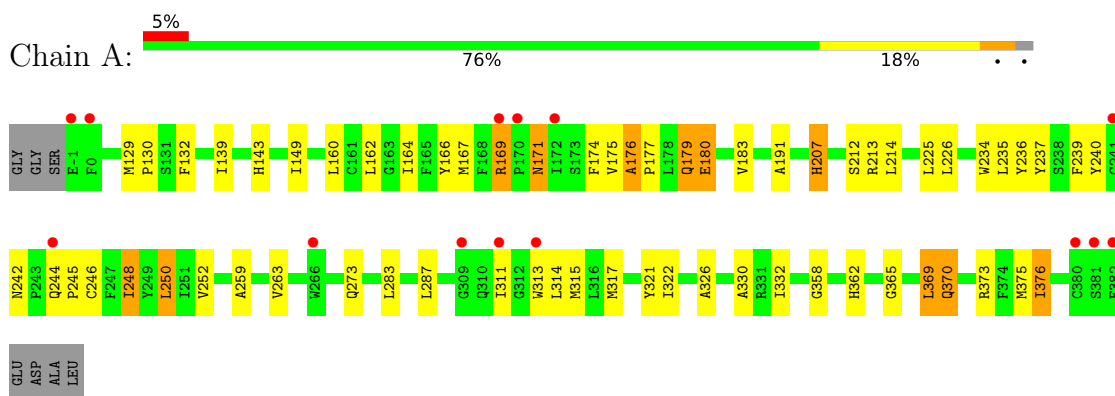
Chain A:

• Molecule 2: V REGION HEAVY CHAIN
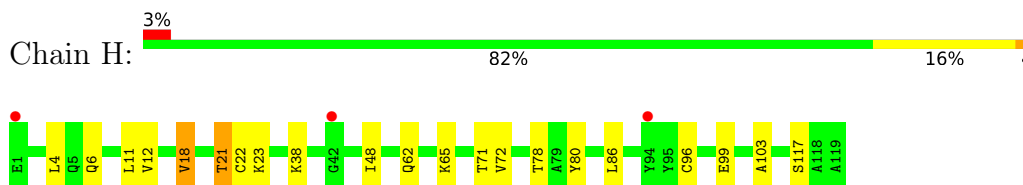
Chain H:

• Molecule 3: V REGION LIGHT CHAIN

Chain L:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	74.58Å 101.03Å 108.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.52 – 2.40 19.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.52-2.40) 98.3 (19.52-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.198 , 0.224 0.222 , 0.246	Depositor DCC
R_{free} test set	1609 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4613	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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: OLA, OLB, ZN, GOL

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	0.44	0/2413	0.64	0/3282
2	H	0.36	0/951	0.64	0/1291
3	L	0.37	0/840	0.59	0/1140
All	All	0.41	0/4204	0.63	0/5713

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	2325	0	2289	56	0
2	H	927	0	888	10	0
3	L	820	0	786	6	0
4	A	1	0	0	0	0
5	A	200	0	320	8	0
6	A	20	0	33	2	0
7	L	6	0	8	0	0
8	A	153	0	0	4	0
8	H	89	0	0	0	0
8	L	72	0	0	0	0
All	All	4613	0	4324	72	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 8.

All (72) 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:183:VAL:HG13	8:A:501:HOH:O	1.45	1.15
1:A:179:GLN:NE2	8:A:501:HOH:O	1.84	1.09
1:A:171:ASN:HB3	1:A:177:PRO:HG2	1.29	1.07
1:A:171:ASN:HB3	1:A:177:PRO:CG	1.90	1.00
1:A:237:TYR:CE2	1:A:370:GLN:HA	2.08	0.88
1:A:174:PHE:HB2	1:A:177:PRO:HG3	1.59	0.85
1:A:176:ALA:O	1:A:180:GLU:HB2	1.76	0.84
1:A:166:TYR:CE1	1:A:169:ARG:NH2	2.51	0.79
1:A:237:TYR:HE2	1:A:370:GLN:HA	1.47	0.77
1:A:245:PRO:HA	1:A:248:ILE:HD11	1.69	0.75
1:A:321:TYR:HA	6:A:410:OLA:H111	1.73	0.70
1:A:183:VAL:CG1	8:A:501:HOH:O	2.20	0.70
1:A:245:PRO:HA	1:A:248:ILE:CD1	2.23	0.69
1:A:322:ILE:HD12	5:A:408:OLB:H5	1.77	0.67
2:H:12:VAL:HG11	2:H:18:VAL:HG13	1.83	0.61
1:A:234[B]:TRP:CZ3	1:A:369:LEU:HD11	2.37	0.60
1:A:143:HIS:HB2	8:A:505:HOH:O	2.04	0.57
1:A:171:ASN:HD22	1:A:177:PRO:HB2	1.70	0.57
2:H:22:CYS:HG	2:H:96:CYS:HG	1.39	0.56
5:A:404:OLB:O23	5:A:409:OLB:H19	2.05	0.56
1:A:287:LEU:HD12	5:A:408:OLB:H21	1.89	0.55
1:A:330:ALA:HB3	1:A:332:ILE:HD12	1.88	0.55
1:A:175:VAL:O	1:A:176:ALA:HB2	2.06	0.54
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.89	0.54
1:A:160:LEU:O	1:A:164:ILE:HG12	2.08	0.53
1:A:373:ARG:NH2	1:A:376:ILE:HD11	2.24	0.53
1:A:166:TYR:CD1	1:A:169:ARG:NH2	2.77	0.53
1:A:248:ILE:O	1:A:252:VAL:HG23	2.09	0.53
1:A:283:LEU:HD11	1:A:322:ILE:HD13	1.89	0.52
1:A:171:ASN:ND2	1:A:177:PRO:CB	2.72	0.52
1:A:175:VAL:O	1:A:175:VAL:HG12	2.09	0.52
1:A:225:LEU:HD11	5:A:405:OLB:H241	1.91	0.52
1:A:171:ASN:ND2	1:A:177:PRO:HB2	2.24	0.51
2:H:6:GLN:HA	2:H:21:THR:O	2.11	0.51
1:A:139:ILE:HG12	1:A:149:ILE:HG21	1.93	0.49
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.93	0.49
1:A:259:ALA:O	1:A:263:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.95	0.48
1:A:171:ASN:OD1	1:A:171:ASN:N	2.47	0.48
1:A:365:GLY:O	1:A:369:LEU:HD12	2.14	0.47
3:L:4:MET:CE	3:L:23:CYS:SG	3.02	0.47
1:A:240:TYR:CE2	1:A:373:ARG:HD2	2.49	0.47
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.14	0.46
1:A:166:TYR:HE1	1:A:169:ARG:HH22	1.62	0.46
1:A:174:PHE:N	1:A:174:PHE:CD1	2.84	0.46
1:A:236:TYR:HD2	1:A:237:TYR:CE1	2.33	0.46
1:A:166:TYR:HE1	1:A:169:ARG:NH2	2.05	0.46
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.50	0.46
2:H:12:VAL:HG11	2:H:18:VAL:CG1	2.44	0.45
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.00	0.44
1:A:130:PRO:HG3	3:L:50:ASN:HB3	1.99	0.44
1:A:237:TYR:CE2	1:A:370:GLN:CA	2.93	0.44
1:A:287:LEU:CD1	5:A:408:OLB:H21	2.47	0.44
1:A:358:GLY:HA3	6:A:410:OLA:H162	1.98	0.44
2:H:23:LYS:HA	2:H:78:THR:HG22	1.99	0.43
2:H:99:GLU:HG2	2:H:103:ALA:HA	2.00	0.43
1:A:129:MET:O	1:A:207:HIS:HA	2.18	0.43
1:A:313[B]:TRP:CZ2	1:A:362:HIS:HA	2.54	0.43
1:A:317:MET:HE2	5:A:409:OLB:C18	2.48	0.43
1:A:239:PHE:CB	1:A:246:CYS:HB2	2.49	0.43
1:A:313[B]:TRP:CE3	1:A:314:LEU:HG	2.54	0.43
1:A:326:ALA:HA	5:A:408:OLB:H20	2.01	0.43
3:L:4:MET:HE3	3:L:23:CYS:SG	2.59	0.43
1:A:132:PHE:HB2	5:A:402:OLB:H4A	2.01	0.42
1:A:171:ASN:HD22	1:A:177:PRO:CB	2.32	0.42
1:A:242:ASN:O	1:A:245:PRO:HD2	2.21	0.41
1:A:235:LEU:HD12	1:A:250:LEU:HD12	2.02	0.41
1:A:171:ASN:HB3	1:A:177:PRO:CB	2.48	0.41
1:A:175:VAL:O	1:A:175:VAL:CG1	2.69	0.41
1:A:248:ILE:H	1:A:248:ILE:HG13	1.66	0.41
3:L:91:PHE:HA	3:L:96:TYR:CD1	2.55	0.40
1:A:191:ALA:HA	1:A:226:LEU:HD13	2.03	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	285/292 (98%)	275 (96%)	8 (3%)	2 (1%)	22	32
2	H	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
3	L	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
All	All	507/518 (98%)	492 (97%)	13 (3%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ALA
1	A	207	HIS

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	244/246 (99%)	225 (92%)	19 (8%)	12	19
2	H	99/99 (100%)	91 (92%)	8 (8%)	11	18
3	L	90/90 (100%)	82 (91%)	8 (9%)	9	14
All	All	433/435 (100%)	398 (92%)	35 (8%)	11	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	LEU

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W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

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Mol	Chain	Res	Type
1	A	167	MET
1	A	169	ARG
1	A	171	ASN
1	A	179	GLN
1	A	180	GLU
1	A	212	SER
1	A	213	ARG
1	A	214	LEU
1	A	244	GLN
1	A	248	ILE
1	A	250	LEU
1	A	273	GLN
1	A	311	ILE
1	A	315	MET
1	A	369	LEU
1	A	370	GLN
1	A	375	MET
1	A	376	ILE
2	H	4	LEU
2	H	11	LEU
2	H	18	VAL
2	H	21	THR
2	H	62	GLN
2	H	65	LYS
2	H	72	VAL
2	H	117	SER
3	L	24	ARG
3	L	42	LYS
3	L	52	LYS
3	L	56	ASP
3	L	63	SER
3	L	70	GLN
3	L	72	SER
3	L	103	LYS

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	244	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#|Z| > 2$
7	GOL	L	201	-	5,5,5	0.08	0	5,5,5	0.30	0
5	OLB	A	405	-	24,24,24	0.20	0	25,25,25	0.29	0
5	OLB	A	404	-	24,24,24	0.23	0	25,25,25	0.49	0
5	OLB	A	408	-	24,24,24	0.28	0	25,25,25	0.45	0
6	OLA	A	410	-	19,19,19	0.21	0	19,19,19	0.36	0
5	OLB	A	406	-	24,24,24	0.29	0	25,25,25	0.26	0
5	OLB	A	403	-	24,24,24	0.20	0	25,25,25	0.32	0
5	OLB	A	402	-	24,24,24	0.18	0	25,25,25	0.23	0
5	OLB	A	409	-	24,24,24	0.17	0	25,25,25	0.41	0
5	OLB	A	407	-	24,24,24	0.24	0	25,25,25	0.23	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
7	GOL	L	201	-	-	3/4/4/4	-
5	OLB	A	405	-	-	12/24/24/24	-
5	OLB	A	404	-	-	11/24/24/24	-
5	OLB	A	408	-	-	8/24/24/24	-
6	OLA	A	410	-	-	10/17/17/17	-
5	OLB	A	406	-	-	7/24/24/24	-
5	OLB	A	403	-	-	10/24/24/24	-
5	OLB	A	402	-	-	9/24/24/24	-
5	OLB	A	409	-	-	11/24/24/24	-
5	OLB	A	407	-	-	4/24/24/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	OLB	C21-C22-C24-O25
5	A	409	OLB	O20-C21-C22-C24
5	A	404	OLB	C2-C1-O20-C21
5	A	409	OLB	C2-C1-O20-C21
5	A	409	OLB	O20-C21-C22-O23
5	A	404	OLB	O19-C1-O20-C21
5	A	409	OLB	O19-C1-O20-C21
5	A	405	OLB	O20-C21-C22-C24
5	A	405	OLB	O20-C21-C22-O23
5	A	402	OLB	C1-C2-C3-C4
5	A	405	OLB	O23-C22-C24-O25
5	A	408	OLB	C1-C2-C3-C4
6	A	410	OLA	C1-C2-C3-C4
5	A	407	OLB	C12-C13-C14-C15
6	A	410	OLA	C12-C13-C14-C15
5	A	406	OLB	C4-C5-C6-C7
5	A	406	OLB	C3-C4-C5-C6
7	L	201	GOL	O1-C1-C2-C3
6	A	410	OLA	C5-C6-C7-C8
6	A	410	OLA	C13-C14-C15-C16
5	A	409	OLB	C4-C5-C6-C7
5	A	402	OLB	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	403	OLB	C2-C3-C4-C5
5	A	404	OLB	C5-C6-C7-C8
5	A	405	OLB	C4-C5-C6-C7
5	A	408	OLB	C2-C3-C4-C5
5	A	407	OLB	C6-C7-C8-C9
6	A	410	OLA	C6-C7-C8-C9
5	A	409	OLB	C11-C12-C13-C14
6	A	410	OLA	C14-C15-C16-C17
5	A	405	OLB	C5-C6-C7-C8
5	A	403	OLB	C11-C12-C13-C14
5	A	408	OLB	C5-C6-C7-C8
6	A	410	OLA	C2-C3-C4-C5
5	A	404	OLB	C3-C4-C5-C6
5	A	403	OLB	C10-C11-C12-C13
5	A	405	OLB	C6-C7-C8-C9
5	A	408	OLB	C10-C11-C12-C13
5	A	404	OLB	O20-C21-C22-C24
5	A	402	OLB	C4-C5-C6-C7
5	A	407	OLB	O20-C21-C22-O23
5	A	404	OLB	C11-C12-C13-C14
5	A	404	OLB	O20-C21-C22-O23
5	A	406	OLB	C15-C16-C17-C18
5	A	403	OLB	C14-C15-C16-C17
5	A	409	OLB	C15-C16-C17-C18
5	A	408	OLB	C2-C1-O20-C21
5	A	405	OLB	C13-C14-C15-C16
6	A	410	OLA	C3-C4-C5-C6
5	A	403	OLB	O23-C22-C24-O25
7	L	201	GOL	O1-C1-C2-O2
7	L	201	GOL	C1-C2-C3-O3
5	A	402	OLB	O20-C21-C22-O23
5	A	404	OLB	C4-C5-C6-C7
5	A	408	OLB	C4-C5-C6-C7
5	A	408	OLB	O19-C1-O20-C21
6	A	410	OLA	C15-C16-C17-C18
5	A	402	OLB	C7-C8-C9-C10
5	A	406	OLB	C7-C8-C9-C10
5	A	409	OLB	C7-C8-C9-C10
5	A	406	OLB	C9-C10-C11-C12
5	A	406	OLB	C2-C3-C4-C5
5	A	406	OLB	C11-C12-C13-C14
5	A	403	OLB	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
5	A	403	OLB	C7-C8-C9-C10
5	A	402	OLB	C11-C12-C13-C14
5	A	402	OLB	C12-C13-C14-C15
6	A	410	OLA	C9-C10-C11-C12
5	A	402	OLB	O20-C1-C2-C3
5	A	403	OLB	O20-C1-C2-C3
5	A	404	OLB	C9-C10-C11-C12
5	A	409	OLB	O20-C1-C2-C3
5	A	403	OLB	O20-C21-C22-O23
5	A	405	OLB	C9-C10-C11-C12
5	A	402	OLB	O19-C1-C2-C3
5	A	404	OLB	O19-C1-C2-C3
5	A	407	OLB	C13-C14-C15-C16
5	A	405	OLB	C7-C8-C9-C10
5	A	409	OLB	O19-C1-C2-C3
5	A	404	OLB	O20-C1-C2-C3
5	A	403	OLB	O19-C1-C2-C3
5	A	408	OLB	C7-C8-C9-C10
5	A	409	OLB	C13-C14-C15-C16
5	A	405	OLB	O19-C1-C2-C3
5	A	405	OLB	O20-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	OLB	1	0
5	A	404	OLB	1	0
5	A	408	OLB	4	0
6	A	410	OLA	2	0
5	A	402	OLB	1	0
5	A	409	OLB	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 OLB A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLB A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLB A 408

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 410

Bond lengths

Bond angles

Torsions

Rings

Ligand OLB A 406

Bond lengths

Bond angles

Torsions

Rings

Ligand OLB A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand OLB A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand OLB A 409

Bond lengths

Bond angles

Torsions

Rings

Ligand OLB A 407

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	285/292 (97%)	0.07	14 (4%)	29	28	53, 81, 151, 176	2 (0%)
2	H	119/119 (100%)	-0.16	3 (2%)	57	55	56, 70, 86, 100	0
3	L	107/107 (100%)	-0.28	0	100	100	50, 65, 79, 92	0
All	All	511/518 (98%)	-0.06	17 (3%)	46	45	50, 73, 138, 176	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ILE	6.2
1	A	170	PRO	3.9
1	A	311	ILE	3.9
1	A	382	GLU	3.2
1	A	381	SER	3.1
2	H	42	GLY	3.1
1	A	380	CYS	3.0
1	A	169	ARG	2.9
1	A	266	TRP	2.7
1	A	309	GLY	2.6
1	A	244	GLN	2.6
1	A	241	CYS	2.5
2	H	94	TYR	2.5
1	A	313[A]	TRP	2.5
1	A	0	PHE	2.1
2	H	1	GLU	2.1
1	A	-1	GLU	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	OLB	A	403	25/25	0.52	0.30	81,94,116,121	0
5	OLB	A	406	25/25	0.57	0.46	85,93,118,122	0
5	OLB	A	409	25/25	0.57	0.40	85,111,146,152	0
5	OLB	A	404	25/25	0.61	0.30	120,131,140,142	0
5	OLB	A	408	25/25	0.68	0.31	100,106,112,114	0
5	OLB	A	405	25/25	0.72	0.46	83,86,99,103	6
5	OLB	A	407	25/25	0.76	0.49	88,94,104,105	0
5	OLB	A	402	25/25	0.78	0.23	85,88,115,124	0
7	GOL	L	201	6/6	0.83	0.22	76,78,81,82	0
6	OLA	A	410	20/20	0.85	0.25	72,76,78,78	0
4	ZN	A	401	1/1	0.99	0.12	61,61,61,61	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.
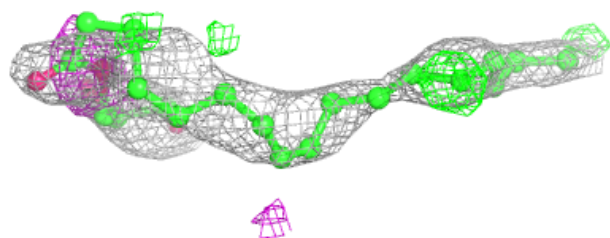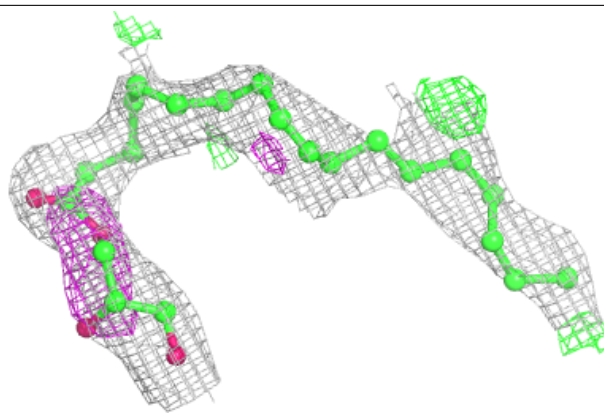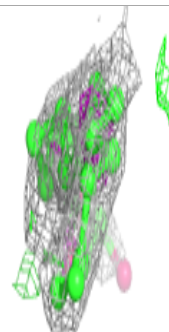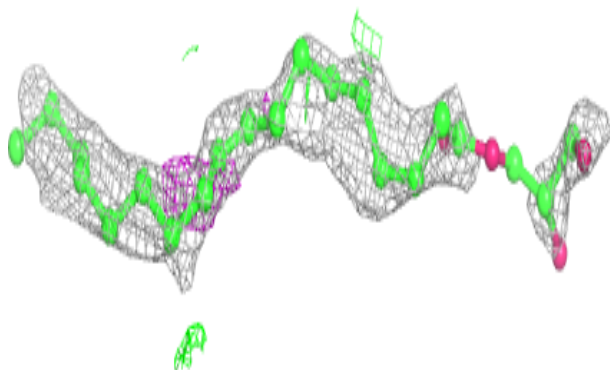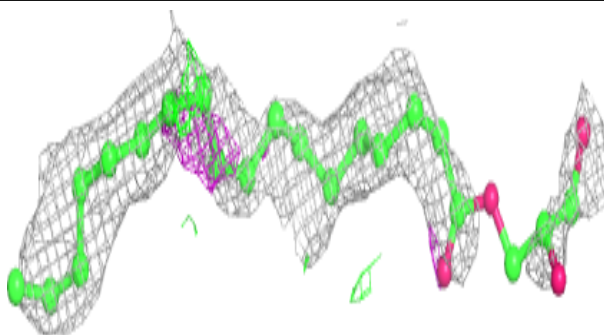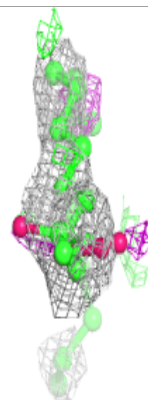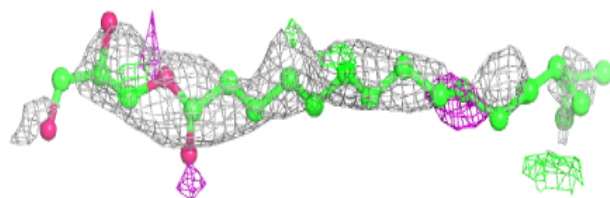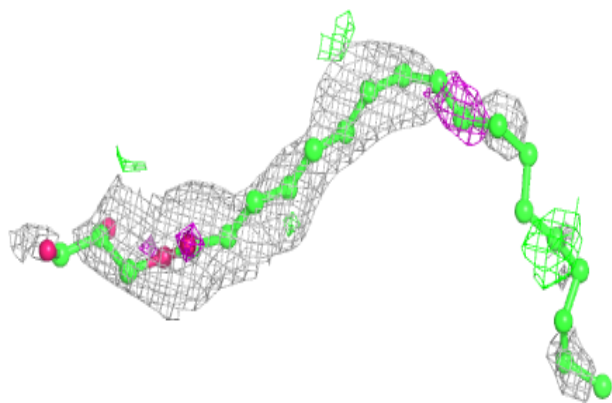
Electron density around OLB A 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
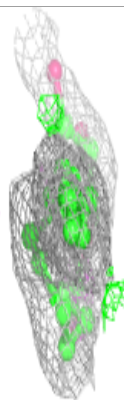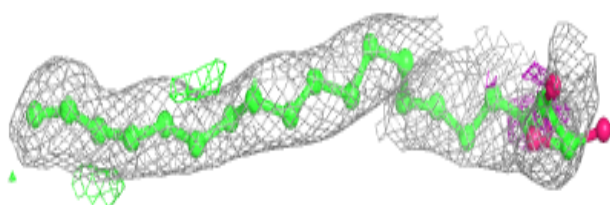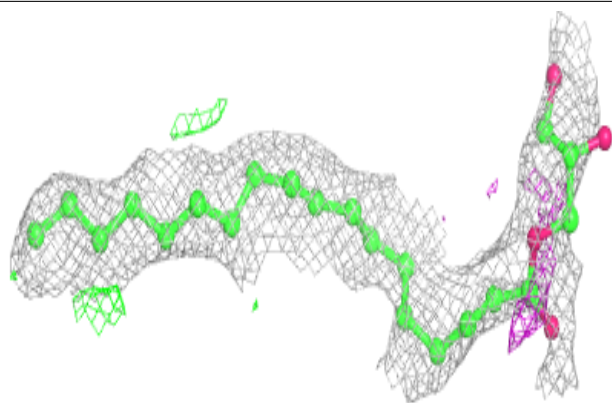
Electron density around OLB A 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
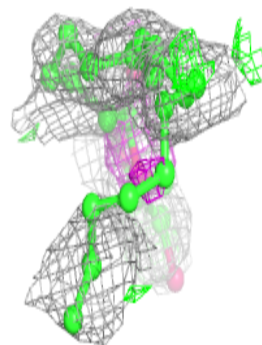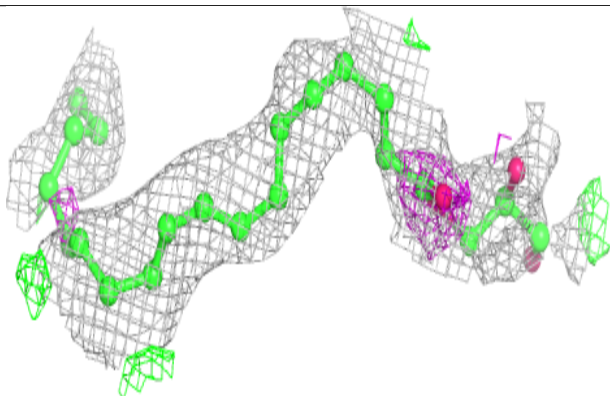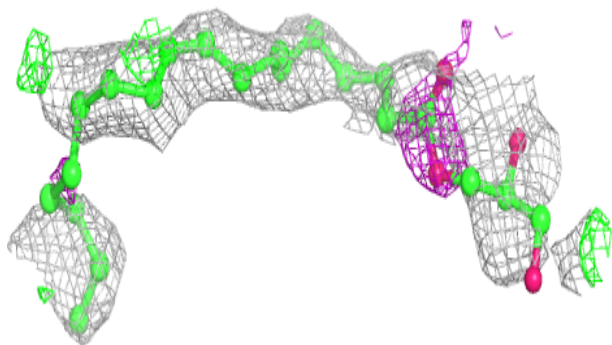
Electron density around OLB A 409:

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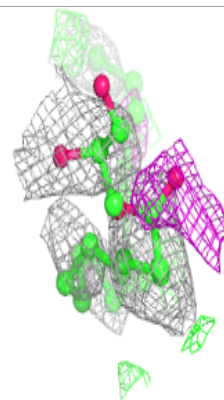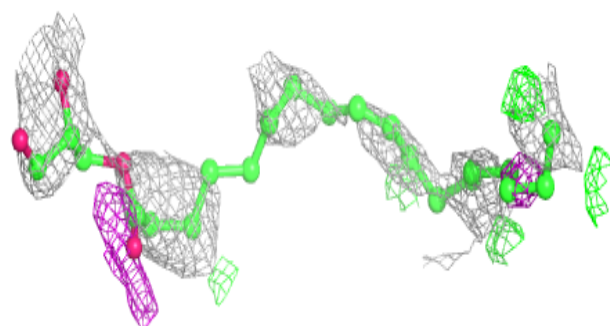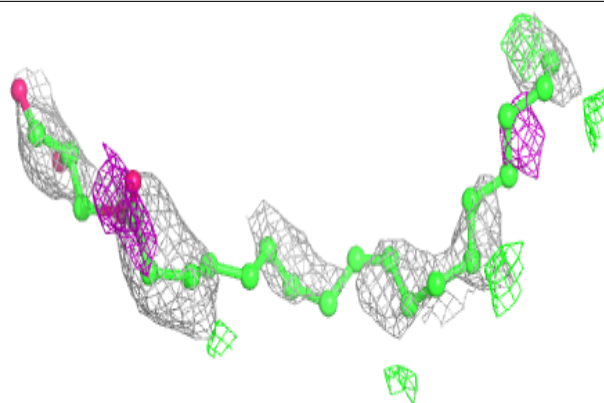

Electron density around OLB A 404:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
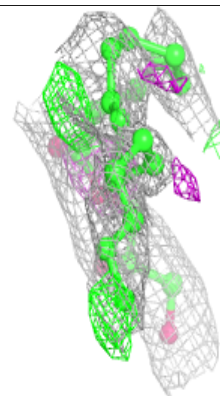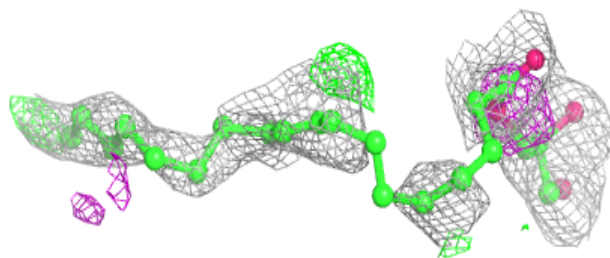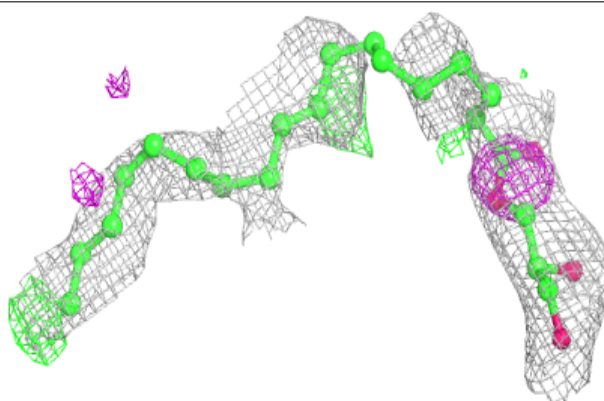
Electron density around OLB A 408:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
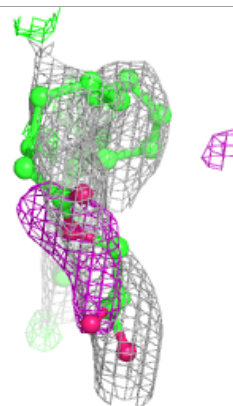
Electron density around OLB A 405:

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

Electron density around OLB A 407:

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

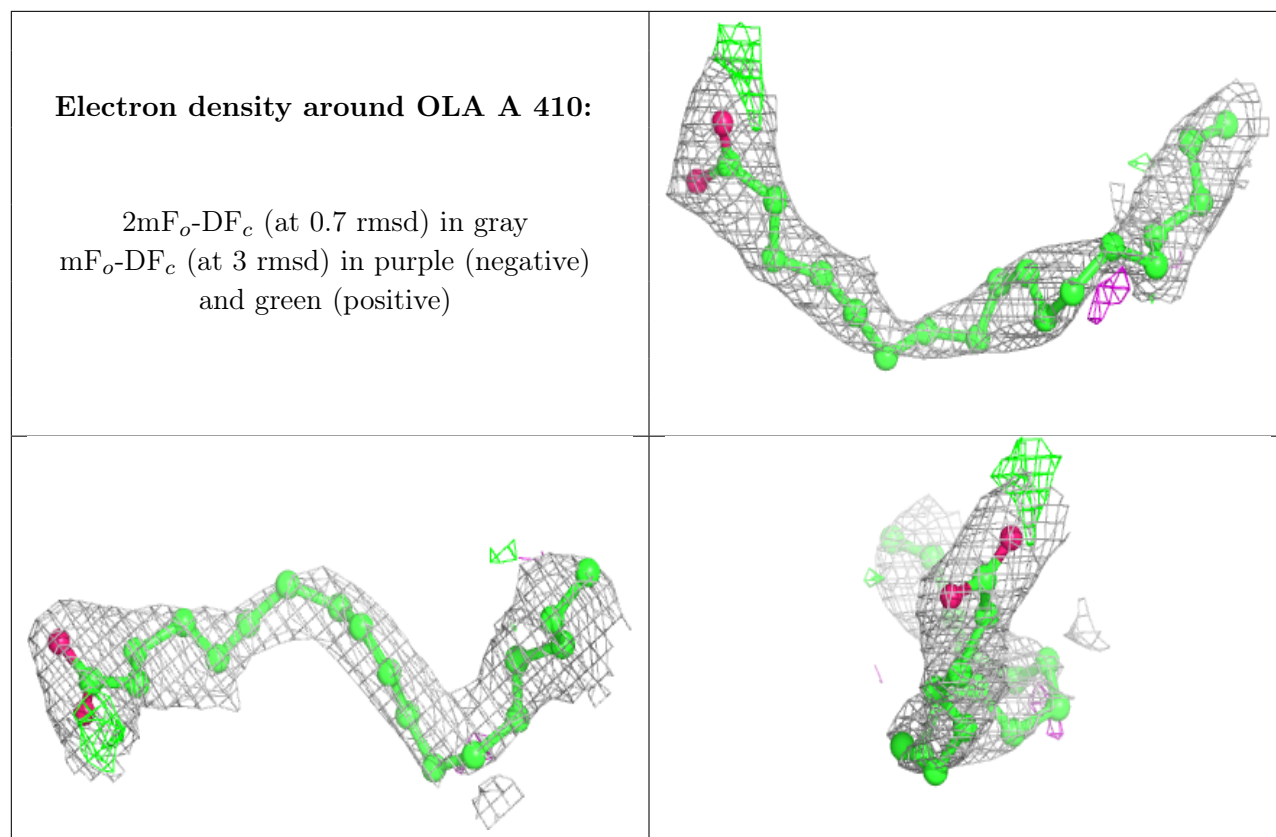**Electron density around OLB A 402:**

$2mF_o\text{-}DF_c$ (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 410:

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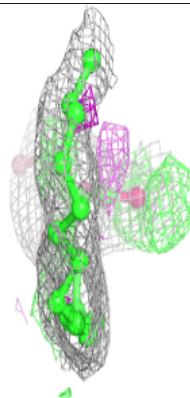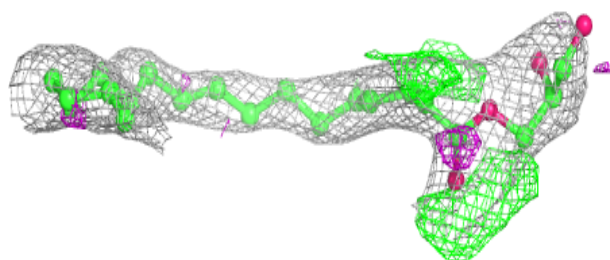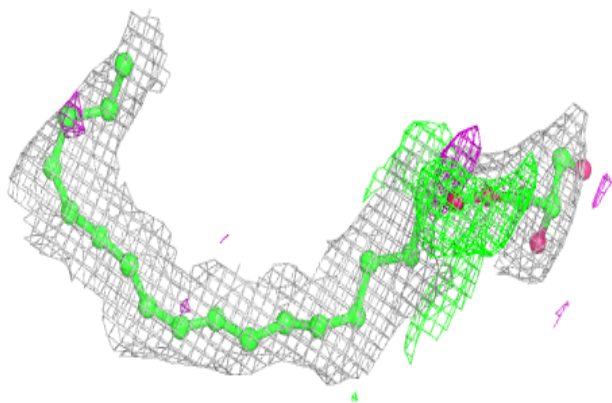
6.5 Other polymers (i)

There are no such residues in this entry.