Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:49 PM EDT

PDB ID	:	3CWD
Title	:	Molecular recognition of nitro-fatty acids by PPAR gamma
Authors	:	Martynowski, D.; Li, Y.
Deposited on	:	2008-04-21
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

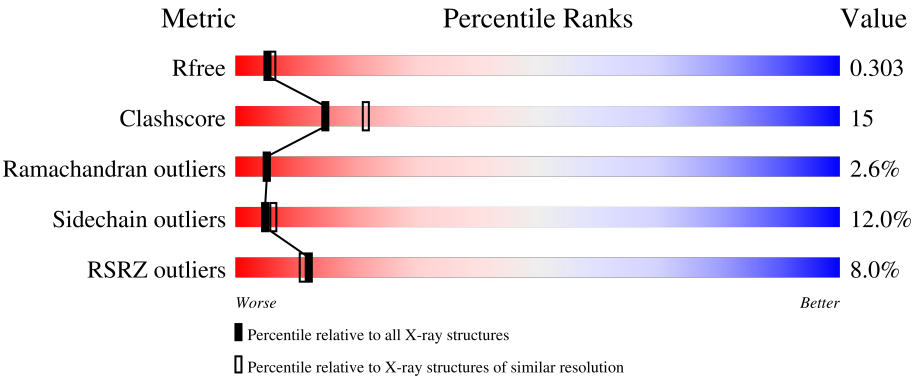
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	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	270	7% 70% 21% • • 5%
1	B	270	6% 68% 22% 5% • •
2	C	16	12% 56% 25% 6% 12%
2	D	16	44% 56% 31% 12%

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
3	LNA	B	1[A]	-	-	X	-
4	LNB	B	478[B]	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4798 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.

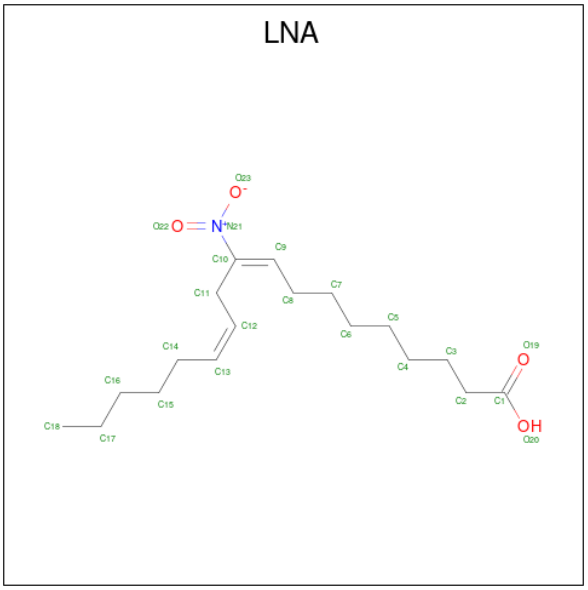
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			2067	1333	334	390	10			
1	B	260	Total	C	N	O	S	0	6	0
			2103	1355	345	392	11			

- Molecule 2 is a protein called SRC1-2 PEPTIDE.

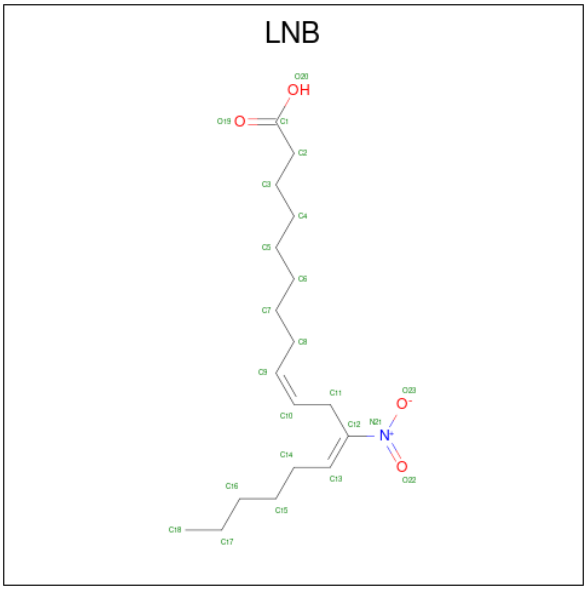
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	0	1	0
			139	84	31	24			
2	D	16	Total	C	N	O	0	0	0
			134	82	28	24			

- Molecule 3 is (9E,12Z)-10-nitrooctadeca-9,12-dienoic acid (three-letter code: LNA) (formula: $C_{18}H_{31}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 23 18 1 4	0	1
3	B	1	Total C N O 23 18 1 4	0	1

- Molecule 4 is (9Z,12E)-12-nitrooctadeca-9,12-dienoic acid (three-letter code: LNB) (formula: $C_{18}H_{31}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 23 18 1 4	0	1
4	B	1	Total C N O 23 18 1 4	0	1

- Molecule 5 is water.

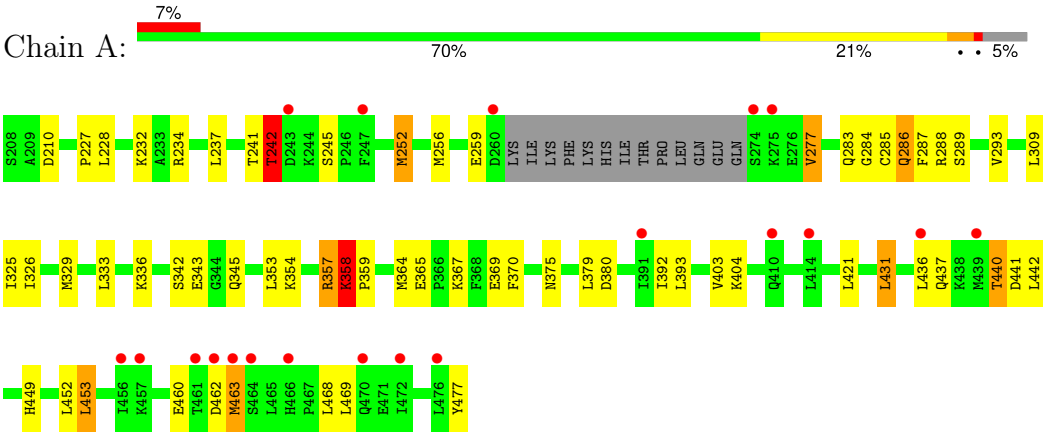
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0
5	B	141	Total O 141 141	0	0
5	C	13	Total O 13 13	0	0
5	D	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

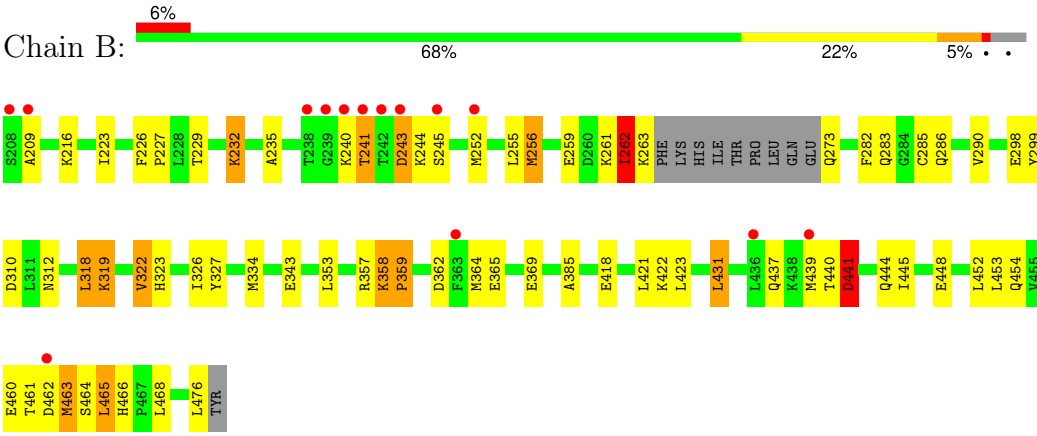
• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:

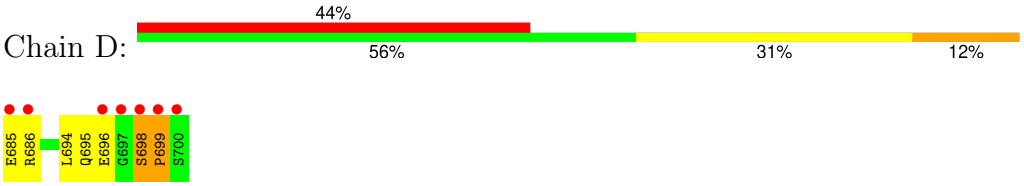


• Molecule 2: SRC1-2 PEPTIDE

Chain C:

• Molecule 2: SRC1-2 PEPTIDE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.04Å 86.20Å 97.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.11 – 2.40 43.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.11-2.40) 96.5 (43.10-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.290 0.248 , 0.303	Depositor DCC
R_{free} test set	1346 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4798	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: LNA, LNB

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	0.72	0/2108	0.77	0/2839
1	B	0.77	0/2164	0.82	1/2914 (0.0%)
2	C	0.65	0/147	1.20	2/193 (1.0%)
2	D	0.79	0/136	0.96	0/179
All	All	0.75	0/4555	0.81	3/6125 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	698	SER	C-N-CD	-8.87	101.10	120.60
2	C	698	SER	C-N-CA	6.77	150.43	122.00
1	B	441	ASP	CB-CG-OD1	5.46	123.21	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	334	MET	Peptide

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Mol	Chain	Res	Type	Group
2	C	698	SER	Peptide

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	2067	0	2118	49	0
1	B	2103	0	2162	73	0
2	C	139	0	141	5	0
2	D	134	0	136	5	0
3	A	23	0	30	7	0
3	B	23	0	30	14	0
4	A	23	0	30	5	0
4	B	23	0	30	10	0
5	A	100	0	0	7	0
5	B	141	0	0	5	0
5	C	13	0	0	2	0
5	D	9	0	0	0	0
All	All	4798	0	4677	140	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 15.

All (140) 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:B:285:CYS:SG	3:B:1[A]:LNA:H16	1.59	1.42
1:A:286:GLN:NE2	3:A:1[A]:LNA:O20	1.69	1.25
1:B:285:CYS:SG	3:B:1[A]:LNA:C16	2.33	1.17
1:A:358:LYS:HB3	1:A:359:PRO:HD3	1.18	1.12
2:D:698:SER:HB3	2:D:699:PRO:HA	1.31	1.07
1:A:286:GLN:NE2	4:A:478[B]:LNB:O19	1.92	1.02
1:A:358:LYS:HB3	1:A:359:PRO:CD	1.95	0.97
1:A:357:ARG:HE	1:A:358:LYS:HG2	1.29	0.94
1:B:261:LYS:O	1:B:262:ILE:HB	1.68	0.93
1:B:358:LYS:CB	1:B:359:PRO:HD3	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:478[B]:LNB:O23	4:B:478[B]:LNB:H10	1.71	0.90
4:A:478[B]:LNB:H10	4:A:478[B]:LNB:O23	1.71	0.87
1:B:285:CYS:SG	4:B:478[B]:LNB:H15A	2.16	0.86
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.04	0.85
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.60	0.84
1:B:286:GLN:HB3	1:B:466[B]:HIS:CD2	2.13	0.84
1:B:252:MET:HE1	1:B:256:MET:SD	2.19	0.83
1:B:323[A]:HIS:CD2	3:B:1[A]:LNA:H4A	2.14	0.83
1:B:252:MET:CE	1:B:256:MET:SD	2.67	0.82
3:A:1[A]:LNA:O23	3:A:1[A]:LNA:H12	1.78	0.81
3:B:1[A]:LNA:H12	3:B:1[A]:LNA:O23	1.79	0.81
1:B:323[A]:HIS:NE2	3:B:1[A]:LNA:H4A	1.95	0.81
1:B:235:ALA:HB1	1:B:240:LYS:HB2	1.64	0.80
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.65	0.79
1:A:358:LYS:CB	1:A:359:PRO:CD	2.59	0.77
1:B:323[A]:HIS:CD2	3:B:1[A]:LNA:C4	2.68	0.76
2:D:698:SER:HB3	2:D:699:PRO:CA	2.12	0.76
1:A:284:GLY:O	1:A:287:PHE:CD2	2.42	0.73
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.69	0.73
3:B:1[A]:LNA:O23	3:B:1[A]:LNA:C12	2.35	0.73
2:C:699:PRO:HD3	5:C:121:HOH:O	1.89	0.73
3:A:1[A]:LNA:O23	3:A:1[A]:LNA:C12	2.35	0.72
1:B:285:CYS:SG	3:B:1[A]:LNA:H16A	2.28	0.72
1:B:285:CYS:SG	4:B:478[B]:LNB:C17	2.77	0.72
1:B:358:LYS:CB	1:B:359:PRO:CD	2.67	0.71
4:A:478[B]:LNB:O23	4:A:478[B]:LNB:C10	2.39	0.70
1:B:323[A]:HIS:NE2	3:B:1[A]:LNA:C4	2.53	0.70
1:B:285:CYS:SG	4:B:478[B]:LNB:C15	2.80	0.70
1:A:357:ARG:HE	1:A:358:LYS:CG	2.04	0.70
1:A:284:GLY:O	1:A:287:PHE:HD2	1.73	0.70
1:A:437:GLN:O	1:A:440:THR:HG22	1.93	0.68
1:B:353:LEU:HD13	1:B:364:MET:HG3	1.78	0.65
1:B:456:ILE:HG22	1:B:463[A]:MET:CE	2.26	0.65
1:B:285:CYS:SG	4:B:478[B]:LNB:H17	2.36	0.65
1:A:227:PRO:HD2	5:A:533:HOH:O	2.00	0.62
1:B:362:ASP:HB2	5:B:500:HOH:O	2.00	0.61
1:A:421:LEU:HD22	1:A:431:LEU:HD13	1.83	0.60
4:B:478[B]:LNB:O23	4:B:478[B]:LNB:C10	2.39	0.60
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.84	0.59
1:A:285:CYS:SG	4:A:478[B]:LNB:H8	2.43	0.59
1:B:318:LEU:HD21	2:D:694:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:O	1:B:322:VAL:HB	2.03	0.58
1:A:289:SER:O	1:A:293:VAL:HG23	2.04	0.57
1:B:460:GLU:HB2	1:B:463[A]:MET:HG2	1.85	0.57
1:B:456:ILE:CG2	1:B:463[B]:MET:HG2	2.34	0.57
1:B:358:LYS:HB2	1:B:359:PRO:CD	2.33	0.56
1:B:273:GLN:HG3	5:B:511:HOH:O	2.05	0.56
1:B:318:LEU:HD23	2:D:694:LEU:HD11	1.87	0.56
1:A:441:ASP:O	1:A:445:ILE:HG13	2.06	0.56
1:B:244:LYS:HG3	1:B:245:SER:N	2.20	0.56
1:A:375:ASN:O	5:A:511:HOH:O	2.18	0.55
1:B:456:ILE:HG22	1:B:463[A]:MET:HE3	1.89	0.54
1:A:326:ILE:HG21	3:A:1[A]:LNA:H5	1.89	0.53
1:A:342:SER:HB2	1:A:345:GLN:HB2	1.89	0.53
1:A:228:LEU:HD23	1:A:333:LEU:CD2	2.38	0.53
1:A:392:ILE:HG22	1:A:393:LEU:HD22	1.89	0.53
1:B:319:LYS:HD3	1:B:476:LEU:HD12	1.90	0.53
1:B:323[A]:HIS:HD2	3:B:1[A]:LNA:H5A	1.73	0.53
1:B:357:ARG:HD2	1:B:358:LYS:HB2	1.90	0.52
1:B:244:LYS:HG3	1:B:245:SER:H	1.72	0.52
1:B:421:LEU:HD22	1:B:431:LEU:HD13	1.92	0.52
1:B:357:ARG:HH11	1:B:358:LYS:HB2	1.74	0.52
1:B:444:GLN:HE21	1:B:448:GLU:HG3	1.75	0.51
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.11	0.50
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.41	0.50
1:B:255:LEU:O	1:B:259:GLU:HG3	2.11	0.50
1:B:306:PHE:O	1:B:309:LEU:HB2	2.11	0.50
1:B:326:ILE:HG21	3:B:1[A]:LNA:H5	1.93	0.50
1:B:441:ASP:OD1	1:B:441:ASP:N	2.45	0.50
1:A:232:LYS:HG2	5:A:521:HOH:O	2.11	0.50
1:B:285:CYS:SG	4:B:478[B]:LNB:H17A	2.51	0.49
1:A:286:GLN:HG3	1:A:469:LEU:HD12	1.93	0.49
1:B:418:GLU:O	1:B:422:LYS:HG3	2.12	0.49
1:A:285:CYS:HB2	3:A:1[A]:LNA:H16	1.95	0.48
1:B:273:GLN:HA	5:B:609:HOH:O	2.11	0.48
1:A:285:CYS:SG	3:A:1[A]:LNA:H8A	2.54	0.48
1:B:323[A]:HIS:HD2	3:B:1[A]:LNA:C5	2.26	0.48
1:B:261:LYS:O	1:B:262:ILE:CB	2.53	0.48
2:C:697:GLY:O	2:C:698:SER:O	2.32	0.48
1:A:228:LEU:HA	5:A:501:HOH:O	2.13	0.47
1:B:244:LYS:CG	1:B:245:SER:H	2.27	0.47
1:A:256:MET:O	1:A:259:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HG2	5:A:502:HOH:O	2.14	0.47
1:B:323[A]:HIS:NE2	3:B:1[A]:LNA:H4	2.28	0.46
1:A:325:ILE:O	1:A:329:MET:HG3	2.16	0.46
3:B:1[A]:LNA:H6A	3:B:1[A]:LNA:H3	1.13	0.46
1:B:365:GLU:O	1:B:369:GLU:HG3	2.14	0.46
1:B:286:GLN:HB3	1:B:466[B]:HIS:HD2	1.74	0.46
1:A:286:GLN:HG3	1:A:469:LEU:CD1	2.46	0.46
1:B:262:ILE:HG12	1:B:263:LYS:HB3	1.97	0.46
2:C:698:SER:HB3	2:C:699:PRO:HB2	1.98	0.46
1:A:353:LEU:HD13	1:A:364:MET:HG3	1.96	0.46
1:B:456:ILE:HG21	1:B:463[B]:MET:HG2	1.98	0.46
4:B:478[B]:LNB:H6A	4:B:478[B]:LNB:H3	1.53	0.46
1:A:365:GLU:O	1:A:369:GLU:HG3	2.15	0.45
1:A:449:HIS:O	1:A:453:LEU:HD22	2.17	0.45
1:B:458:LYS:HA	1:B:458:LYS:HD2	1.75	0.45
1:B:299:TYR:OH	1:B:385:ALA:O	2.29	0.45
1:A:357:ARG:HH21	1:A:358:LYS:HG3	1.83	0.44
1:B:298:GLU:HG2	5:B:494:HOH:O	2.18	0.44
1:A:442:LEU:O	1:A:446:VAL:HG23	2.18	0.43
1:A:286:GLN:HE21	1:A:286:GLN:HA	1.83	0.43
1:B:456:ILE:HG22	1:B:463[A]:MET:HE2	1.99	0.43
1:A:460[A]:GLU:HB3	1:A:463:MET:HG3	2.01	0.43
1:A:252:MET:CE	1:A:277:VAL:HG13	2.48	0.43
1:B:318:LEU:CD2	2:D:694:LEU:HD21	2.48	0.43
4:A:478[B]:LNB:H3	4:A:478[B]:LNB:H6A	1.46	0.43
1:B:229:THR:OG1	1:B:232:LYS:CG	2.67	0.43
1:A:228:LEU:HD23	1:A:333:LEU:HD22	2.01	0.43
1:B:445:ILE:HD11	5:B:568:HOH:O	2.18	0.43
1:B:226:PHE:HA	1:B:227:PRO:HD2	1.94	0.42
1:B:310:ASP:OD1	1:B:312:ASN:HB2	2.20	0.42
1:B:327:TYR:HE1	4:B:478[B]:LNB:C5	2.33	0.42
3:A:1[A]:LNA:H3	3:A:1[A]:LNA:H6A	1.13	0.42
1:A:460[B]:GLU:HB3	1:A:463:MET:HG3	2.01	0.42
1:B:282:PHE:HD2	1:B:283[B]:GLN:HE22	1.67	0.42
1:B:243:ASP:N	1:B:243:ASP:OD1	2.52	0.41
2:C:686:ARG:CZ	5:C:219:HOH:O	2.68	0.41
1:A:468:LEU:HD11	2:C:690:LEU:HD13	2.02	0.41
1:B:290:VAL:HG13	1:B:468:LEU:HD23	2.01	0.41
1:A:364:MET:O	1:A:367:LYS:HB2	2.21	0.41
1:A:367:LYS:NZ	5:A:572:HOH:O	2.47	0.40
1:B:327:TYR:CE1	4:B:478[B]:LNB:H5	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.38	0.40
1:A:241:THR:O	1:A:242:THR:HB	2.21	0.40
1:B:454:GLN:NE2	1:B:457:LYS:NZ	2.69	0.40
1:B:445:ILE:HD13	1:B:445:ILE:HA	1.91	0.40
1:B:463[A]:MET:HE1	1:B:465:LEU:HD21	2.03	0.40
1:A:380:ASP:HB2	5:A:488:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/270 (94%)	238 (93%)	12 (5%)	5 (2%)	7	9
1	B	262/270 (97%)	244 (93%)	12 (5%)	6 (2%)	6	7
2	C	15/16 (94%)	12 (80%)	1 (7%)	2 (13%)	0	0
2	D	14/16 (88%)	9 (64%)	3 (21%)	2 (14%)	0	0
All	All	546/572 (96%)	503 (92%)	28 (5%)	15 (3%)	5	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	VAL
1	A	358	LYS
1	B	262	ILE
1	B	358	LYS
2	C	698	SER
2	C	699	PRO
1	B	209	ALA
2	D	698	SER
1	A	343[A]	GLU

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Mol	Chain	Res	Type
1	A	343[B]	GLU
1	B	241	THR
1	A	242	THR
1	B	464	SER
1	B	359	PRO
2	D	699	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/243 (96%)	206 (89%)	26 (11%)	6	8
1	B	239/243 (98%)	213 (89%)	26 (11%)	6	8
2	C	16/15 (107%)	12 (75%)	4 (25%)	0	0
2	D	15/15 (100%)	11 (73%)	4 (27%)	0	0
All	All	502/516 (97%)	442 (88%)	60 (12%)	5	6

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	A	234	ARG
1	A	237	LEU
1	A	242	THR
1	A	245	SER
1	A	252	MET
1	A	283	GLN
1	A	286	GLN
1	A	288	ARG
1	A	309	LEU
1	A	322	VAL
1	A	336	LYS
1	A	354	LYS
1	A	357	ARG
1	A	358	LYS

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	403	VAL
1	A	404	LYS
1	A	431	LEU
1	A	436	LEU
1	A	440	THR
1	A	452	LEU
1	A	453	LEU
1	A	462	ASP
1	A	463	MET
1	A	477	TYR
1	B	216	LYS
1	B	223	ILE
1	B	232	LYS
1	B	241	THR
1	B	243	ASP
1	B	256	MET
1	B	262	ILE
1	B	309	LEU
1	B	318	LEU
1	B	319	LYS
1	B	322	VAL
1	B	343	GLU
1	B	423	LEU
1	B	431	LEU
1	B	437	GLN
1	B	439	MET
1	B	440	THR
1	B	441	ASP
1	B	452	LEU
1	B	453	LEU
1	B	458	LYS
1	B	461	THR
1	B	462	ASP
1	B	463[A]	MET
1	B	463[B]	MET
1	B	465	LEU
2	C	688	LYS
2	C	690	LEU
2	C	695	GLN
2	C	699	PRO
2	D	685	GLU

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Mol	Chain	Res	Type
2	D	686	ARG
2	D	695	GLN
2	D	696	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	A	454	GLN
1	A	470	GLN
1	B	308	ASN
1	B	424	ASN
1	B	437	GLN
1	B	444	GLN
1	B	454	GLN
2	C	691	HIS
2	D	695	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)

4 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	LNA	B	1[A]	-	20,22,22	1.00	2 (10%)	17,24,24	2.36	3 (17%)
4	LNB	B	478[B]	-	20,22,22	1.11	4 (20%)	17,24,24	1.09	1 (5%)
3	LNA	A	1[A]	-	20,22,22	0.95	2 (10%)	17,24,24	2.39	3 (17%)
4	LNB	A	478[B]	-	20,22,22	1.10	4 (20%)	17,24,24	1.10	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LNA	B	1[A]	-	-	11/19/23/23	-
4	LNB	B	478[B]	-	-	11/19/23/23	-
3	LNA	A	1[A]	-	-	11/19/23/23	-
4	LNB	A	478[B]	-	-	11/19/23/23	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	478[B]	LNB	O22-N21	-2.83	1.17	1.22
4	B	478[B]	LNB	O22-N21	-2.82	1.17	1.22
3	B	1[A]	LNA	O23-N21	-2.37	1.19	1.35
3	A	1[A]	LNA	O23-N21	-2.36	1.19	1.35
4	B	478[B]	LNB	O23-N21	-2.35	1.19	1.35
4	A	478[B]	LNB	O23-N21	-2.34	1.19	1.35
4	B	478[B]	LNB	C13-C12	2.23	1.34	1.32
4	A	478[B]	LNB	C13-C12	2.22	1.34	1.32
3	A	1[A]	LNA	O22-N21	-2.15	1.19	1.22
3	B	1[A]	LNA	O22-N21	-2.11	1.19	1.22
4	B	478[B]	LNB	O20-C1	-2.08	1.23	1.30
4	A	478[B]	LNB	O20-C1	-2.05	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1[A]	LNA	C11-C12-C13	-7.28	108.73	125.14
3	B	1[A]	LNA	C11-C12-C13	-7.11	109.11	125.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1[A]	LNA	C7-C8-C9	-4.54	103.77	112.79
3	A	1[A]	LNA	C7-C8-C9	-4.52	103.80	112.79
4	A	478[B]	LNB	C11-C10-C9	-2.80	118.82	125.14
4	B	478[B]	LNB	C11-C10-C9	-2.77	118.90	125.14
3	A	1[A]	LNA	C3-C2-C1	-2.58	107.78	114.51
3	B	1[A]	LNA	C3-C2-C1	-2.57	107.79	114.51

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1[A]	LNA	C9-C10-C11-C12
3	A	1[A]	LNA	C10-C11-C12-C13
3	B	1[A]	LNA	C9-C10-C11-C12
3	B	1[A]	LNA	C10-C11-C12-C13
4	A	478[B]	LNB	C10-C11-C12-C13
4	B	478[B]	LNB	C10-C11-C12-C13
4	A	478[B]	LNB	C3-C4-C5-C6
3	A	1[A]	LNA	C3-C4-C5-C6
3	B	1[A]	LNA	C3-C4-C5-C6
4	B	478[B]	LNB	C3-C4-C5-C6
4	B	478[B]	LNB	C1-C2-C3-C4
4	A	478[B]	LNB	C1-C2-C3-C4
4	A	478[B]	LNB	C4-C5-C6-C7
4	B	478[B]	LNB	C4-C5-C6-C7
4	B	478[B]	LNB	C5-C6-C7-C8
4	A	478[B]	LNB	C5-C6-C7-C8
3	A	1[A]	LNA	C5-C6-C7-C8
3	B	1[A]	LNA	C5-C6-C7-C8
4	B	478[B]	LNB	C14-C15-C16-C17
4	A	478[B]	LNB	C14-C15-C16-C17
3	A	1[A]	LNA	C14-C15-C16-C17
3	B	1[A]	LNA	C14-C15-C16-C17
3	A	1[A]	LNA	C6-C7-C8-C9
3	B	1[A]	LNA	C6-C7-C8-C9
3	A	1[A]	LNA	C15-C16-C17-C18
3	B	1[A]	LNA	C15-C16-C17-C18
3	B	1[A]	LNA	C4-C5-C6-C7
3	A	1[A]	LNA	C4-C5-C6-C7
3	A	1[A]	LNA	C1-C2-C3-C4
3	B	1[A]	LNA	C1-C2-C3-C4
4	A	478[B]	LNB	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	B	478[B]	LNB	C2-C3-C4-C5
4	A	478[B]	LNB	C9-C10-C11-C12
4	B	478[B]	LNB	C9-C10-C11-C12
3	A	1[A]	LNA	O20-C1-C2-C3
3	B	1[A]	LNA	O20-C1-C2-C3
4	A	478[B]	LNB	O20-C1-C2-C3
4	B	478[B]	LNB	O20-C1-C2-C3
3	A	1[A]	LNA	O19-C1-C2-C3
3	B	1[A]	LNA	O19-C1-C2-C3
4	A	478[B]	LNB	O19-C1-C2-C3
4	B	478[B]	LNB	O19-C1-C2-C3
4	A	478[B]	LNB	C15-C16-C17-C18
4	B	478[B]	LNB	C15-C16-C17-C18

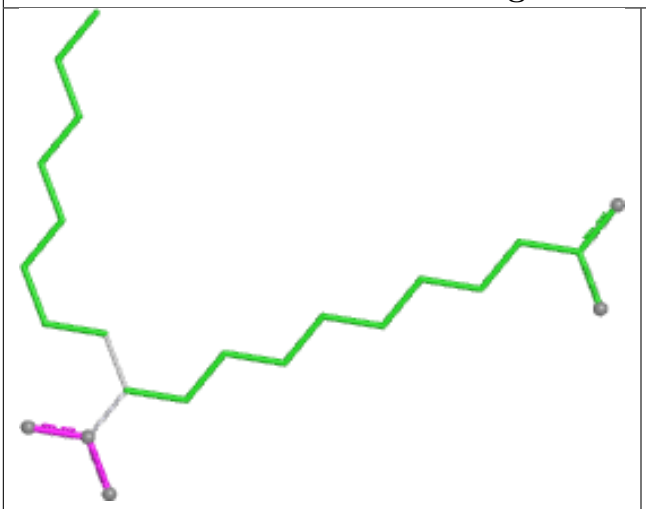
There are no ring outliers.

4 monomers are involved in 36 short contacts:

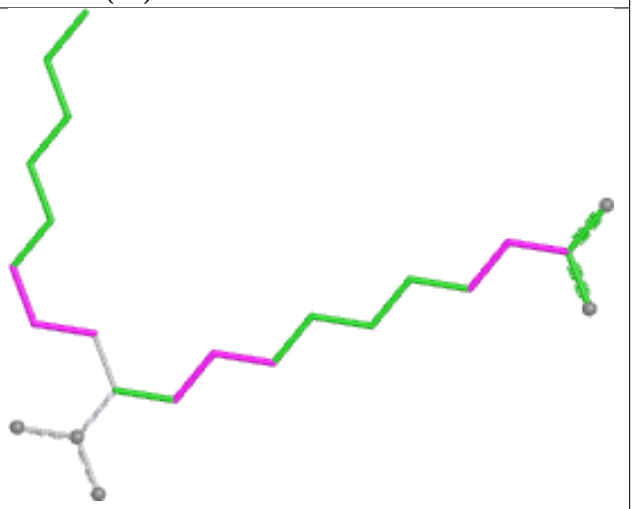
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1[A]	LNA	14	0
4	B	478[B]	LNB	10	0
3	A	1[A]	LNA	7	0
4	A	478[B]	LNB	5	0

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.

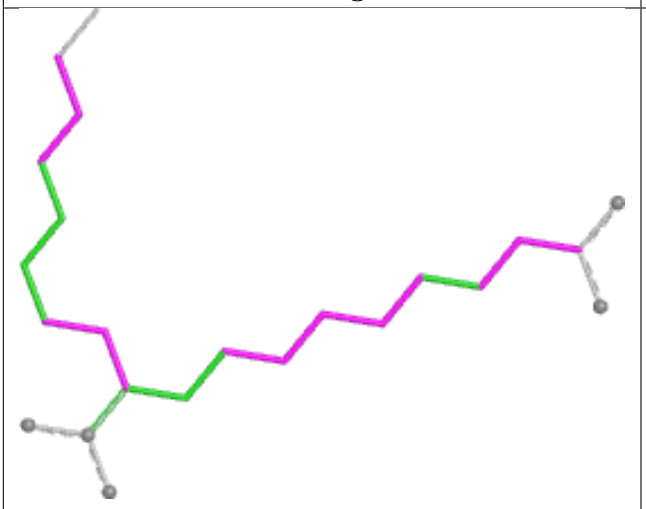
Ligand LNA B 1 (A)



Bond lengths



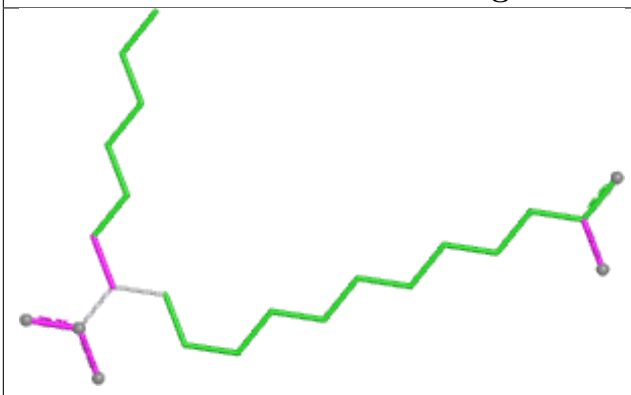
Bond angles



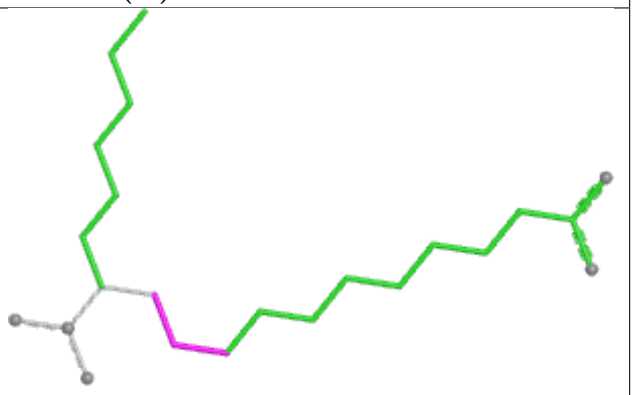
Torsions

Rings

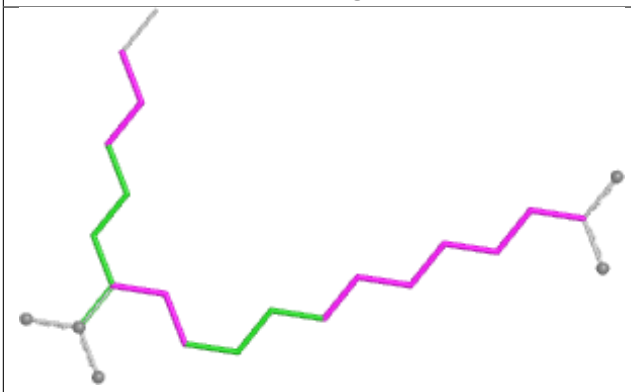
Ligand LNB B 478 (B)



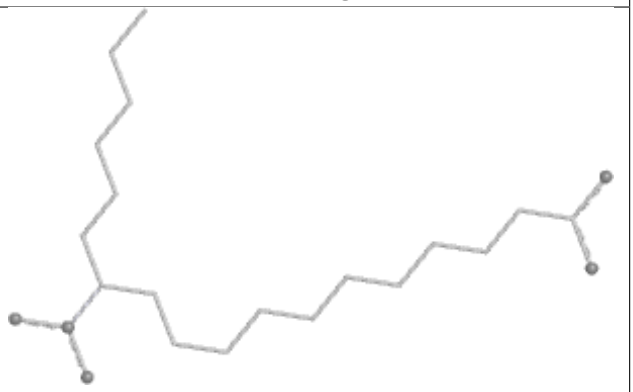
Bond lengths



Bond angles

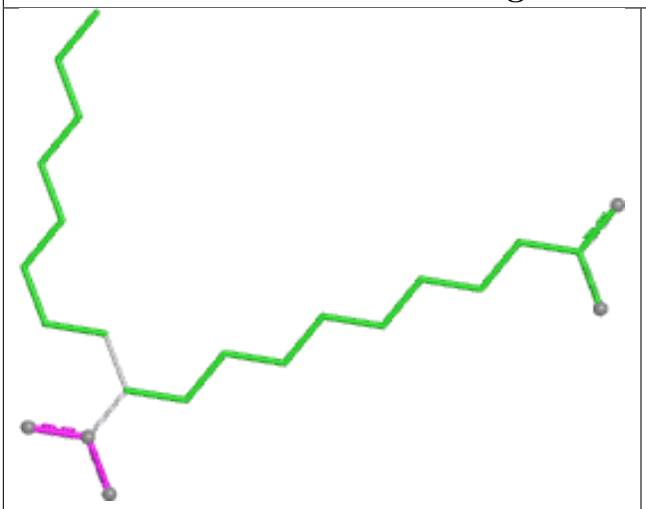


Torsions

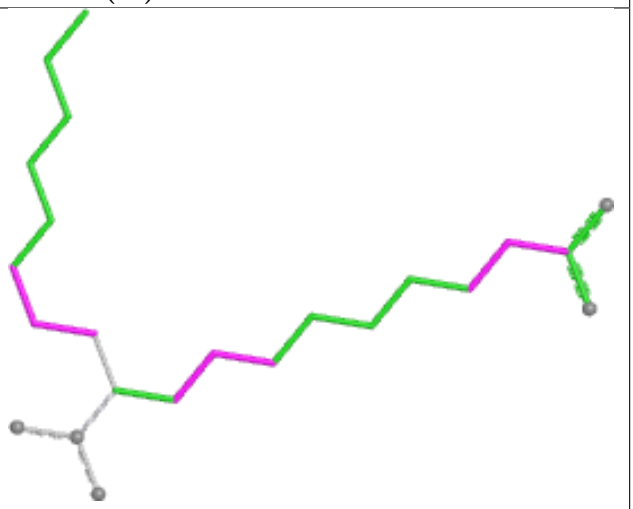


Rings

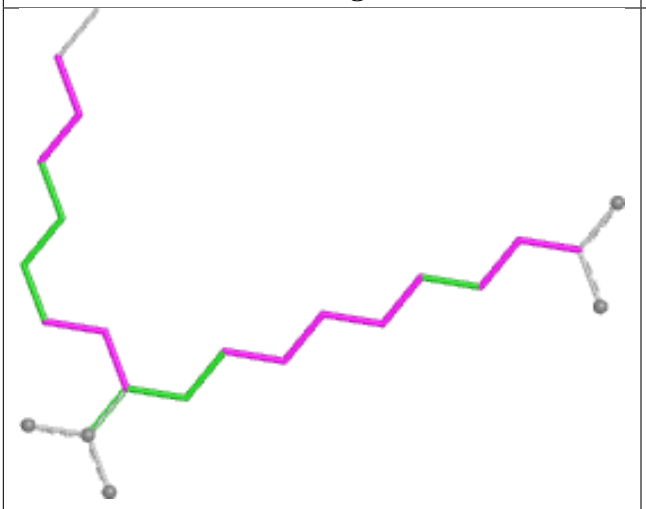
Ligand LNA A 1 (A)



Bond lengths



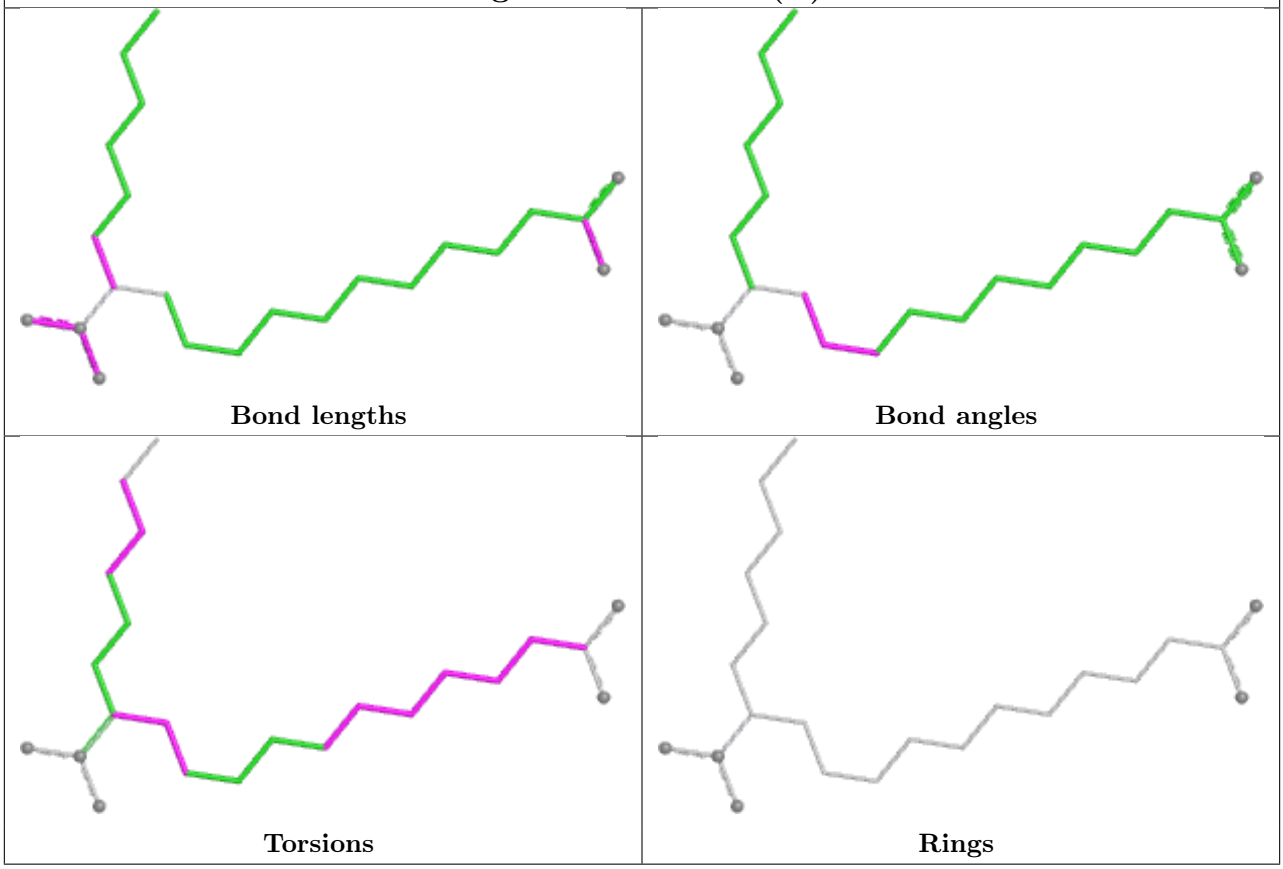
Bond angles



Torsions

Rings

Ligand LNB A 478 (B)



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, 95^{th} 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	257/270 (95%)	0.45	20 (7%)	13 11	23, 35, 55, 60	0
1	B	260/270 (96%)	0.32	15 (5%)	23 22	22, 31, 54, 62	0
2	C	16/16 (100%)	0.48	2 (12%)	3 3	45, 56, 73, 74	0
2	D	16/16 (100%)	1.37	7 (43%)	0 0	37, 53, 80, 81	0
All	All	549/572 (95%)	0.42	44 (8%)	12 11	22, 34, 57, 81	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	8.3
1	A	463	MET	7.2
1	B	241	THR	6.0
1	B	208	SER	5.4
1	B	209	ALA	5.3
1	B	243	ASP	4.7
1	A	464	SER	4.6
2	D	698	SER	4.4
1	A	461	THR	4.2
1	B	245	SER	4.1
1	A	462	ASP	3.8
2	D	700	SER	3.5
1	A	457	LYS	3.5
1	B	239	GLY	3.1
2	D	697	GLY	3.0
1	A	247	PHE	3.0
1	A	476	LEU	3.0
2	C	685	GLU	2.9
2	D	696	GLU	2.9
1	B	240	LYS	2.8
1	A	274	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	470	GLN	2.7
1	B	238	THR	2.7
2	D	685	GLU	2.6
2	D	699	PRO	2.6
1	A	439	MET	2.6
2	C	700	SER	2.5
1	A	414	LEU	2.5
1	A	456	ILE	2.5
1	A	275	LYS	2.5
1	B	252	MET	2.3
2	D	686	ARG	2.3
1	A	391	ILE	2.3
1	B	457	LYS	2.2
1	A	260	ASP	2.2
1	A	243	ASP	2.2
1	B	439	MET	2.1
1	B	363	PHE	2.1
1	A	466	HIS	2.1
1	A	436	LEU	2.0
1	B	462	ASP	2.0
1	A	410	GLN	2.0
1	A	472	ILE	2.0
1	B	436	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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.

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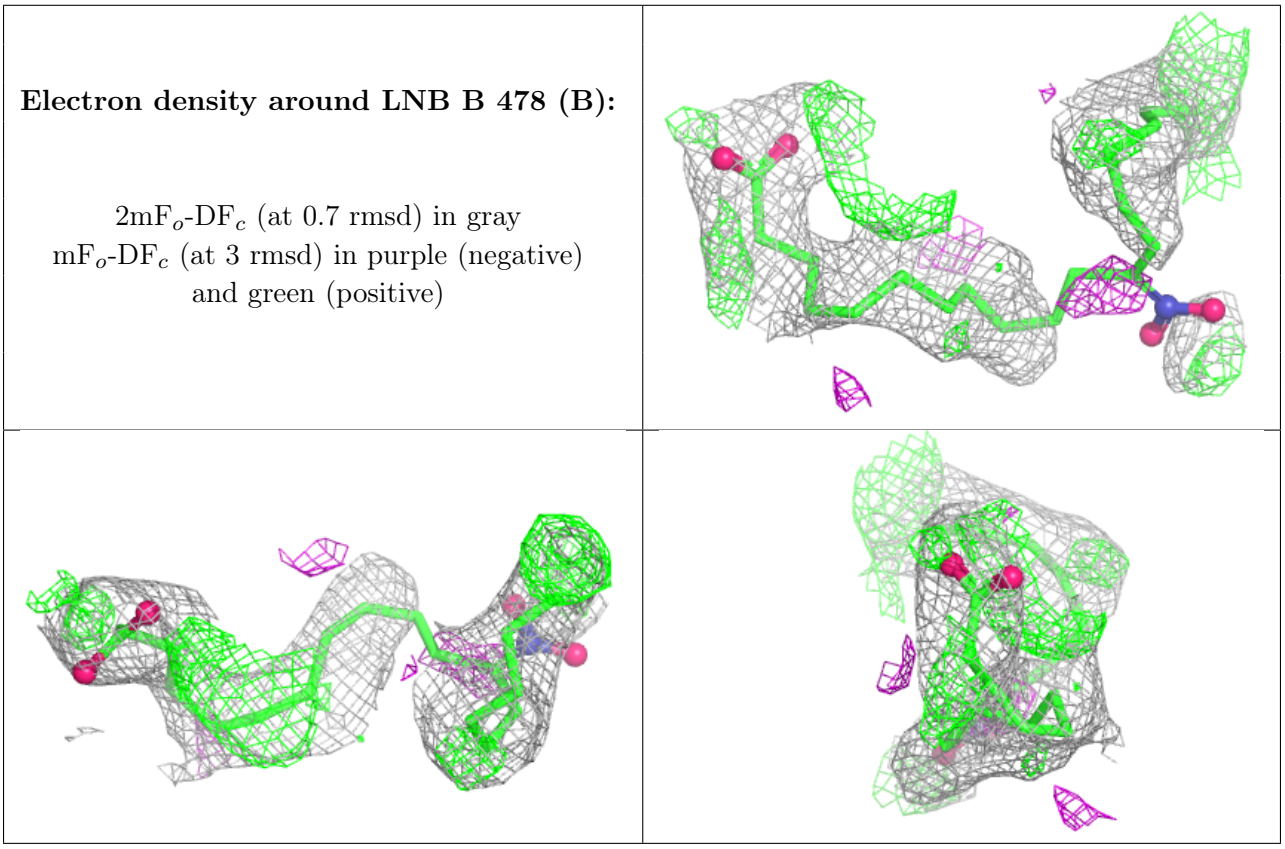
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LNB	B	478[B]	23/23	0.48	0.37	47,55,65,65	23
3	LNA	B	1[A]	23/23	0.52	0.38	54,58,61,61	23
3	LNA	A	1[A]	23/23	0.55	0.31	54,58,61,61	23
4	LNB	A	478[B]	23/23	0.63	0.29	47,54,65,66	23

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.

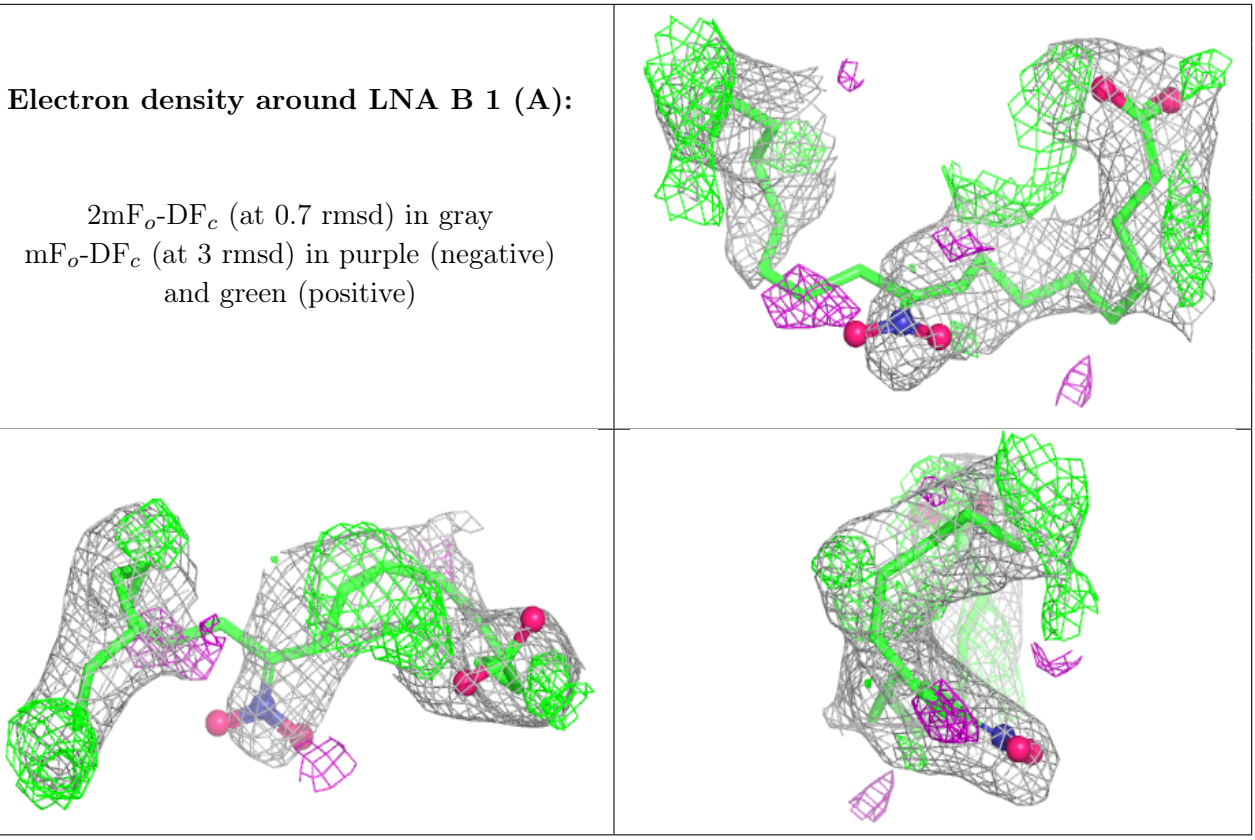
Electron density around LNB B 478 (B):

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



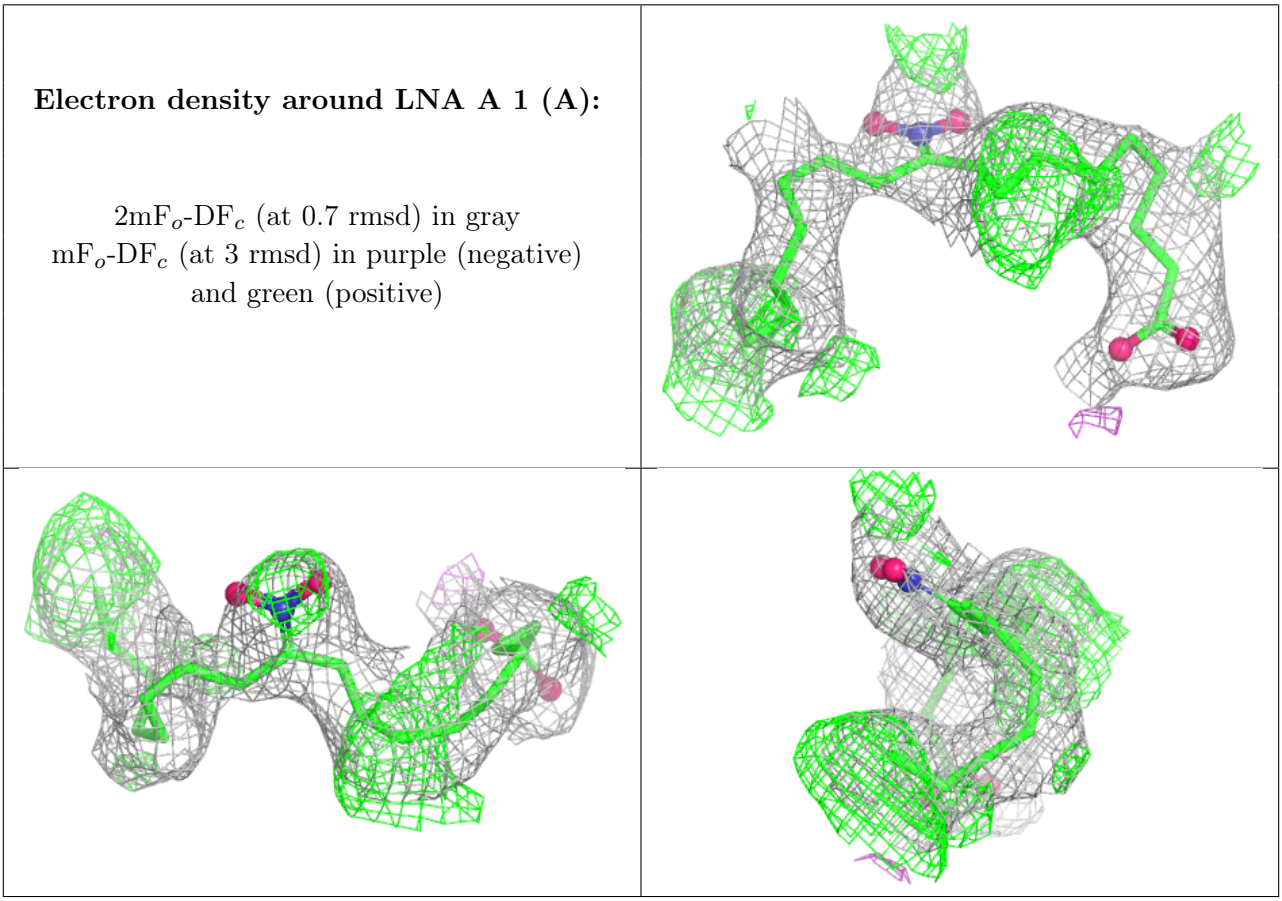
Electron density around LNA B 1 (A):

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



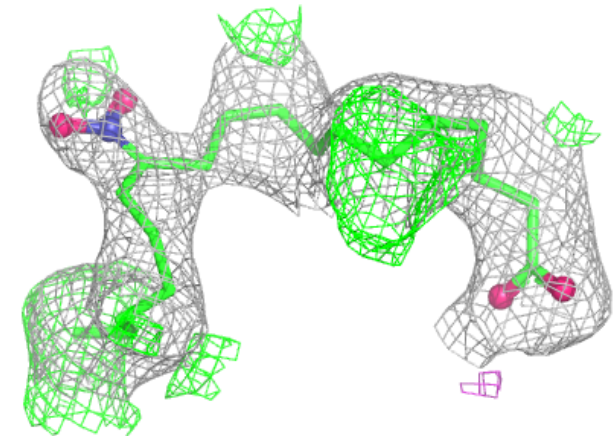
Electron density around LNA A 1 (A):

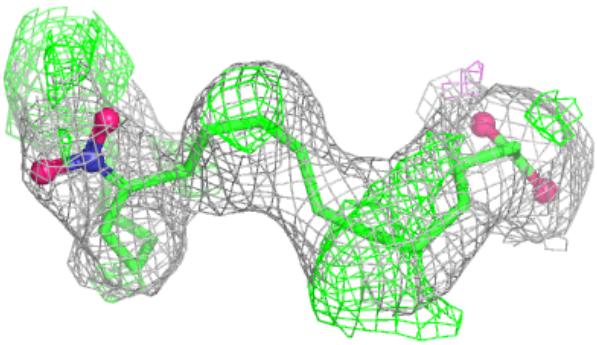
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

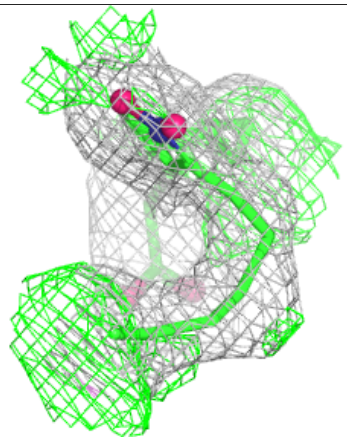


Electron density around LNB A 478 (B):

$2mF_o$-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.