



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 4U4W / pdb_00004u4w
Title : Structure of a nitrate/nitrite antiporter NarK in nitrate-bound occluded state
Authors : Fukuda, M.; Takeda, H.; Kato, H.E.; Doki, S.; Ito, K.; Maturana, A.D.; Ishitani, R.; Nureki, O.
Deposited on : 2014-07-24
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

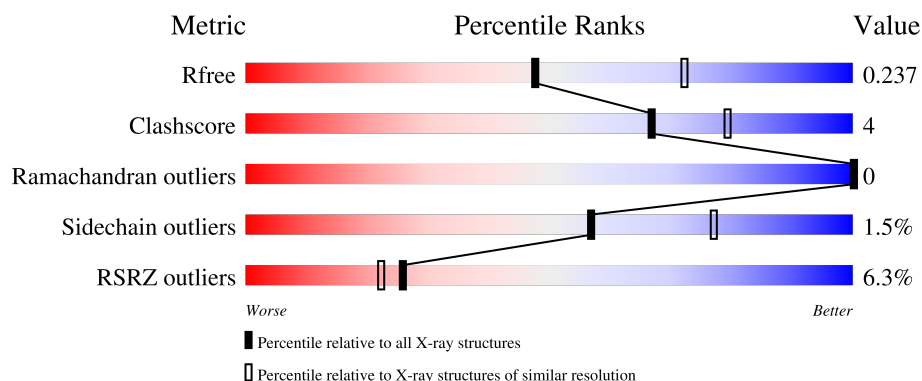
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	475	5% 80% 11% 8%
1	B	475	6% 84% 6% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6814 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.

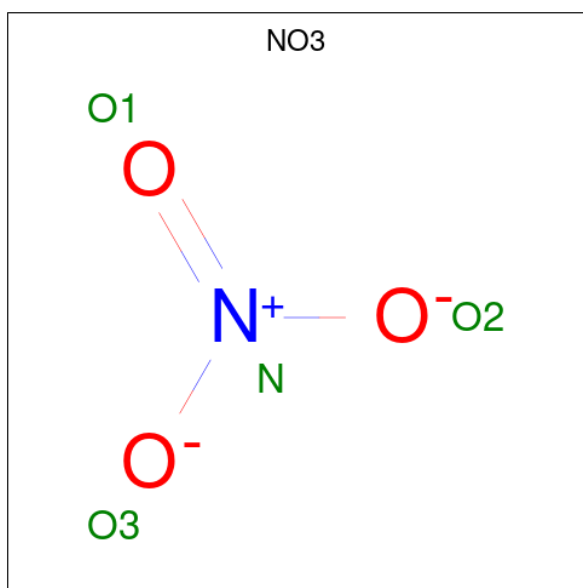
- Molecule 1 is a protein called Nitrate/nitrite transporter NarK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3268	2173	522	554	19			
1	B	430	Total	C	N	O	S	0	0	0
			3218	2142	512	544	20			

There are 24 discrepancies between the modelled and reference sequences:

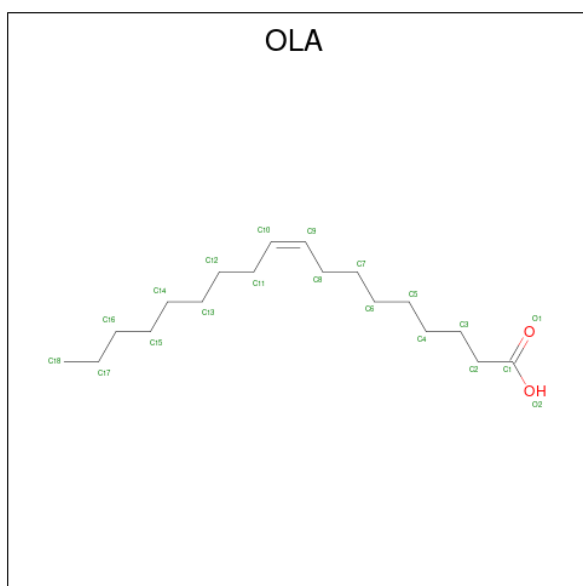
Chain	Residue	Modelled	Actual	Comment	Reference
A	464	LEU	-	expression tag	UNP P10903
A	465	GLU	-	expression tag	UNP P10903
A	466	SER	-	expression tag	UNP P10903
A	467	SER	-	expression tag	UNP P10903
A	468	GLY	-	expression tag	UNP P10903
A	469	GLU	-	expression tag	UNP P10903
A	470	ASN	-	expression tag	UNP P10903
A	471	LEU	-	expression tag	UNP P10903
A	472	TYR	-	expression tag	UNP P10903
A	473	PHE	-	expression tag	UNP P10903
A	474	GLN	-	expression tag	UNP P10903
A	475	GLY	-	expression tag	UNP P10903
B	464	LEU	-	expression tag	UNP P10903
B	465	GLU	-	expression tag	UNP P10903
B	466	SER	-	expression tag	UNP P10903
B	467	SER	-	expression tag	UNP P10903
B	468	GLY	-	expression tag	UNP P10903
B	469	GLU	-	expression tag	UNP P10903
B	470	ASN	-	expression tag	UNP P10903
B	471	LEU	-	expression tag	UNP P10903
B	472	TYR	-	expression tag	UNP P10903
B	473	PHE	-	expression tag	UNP P10903
B	474	GLN	-	expression tag	UNP P10903
B	475	GLY	-	expression tag	UNP P10903

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: $\text{C}_{18}\text{H}_{34}\text{O}_2$).



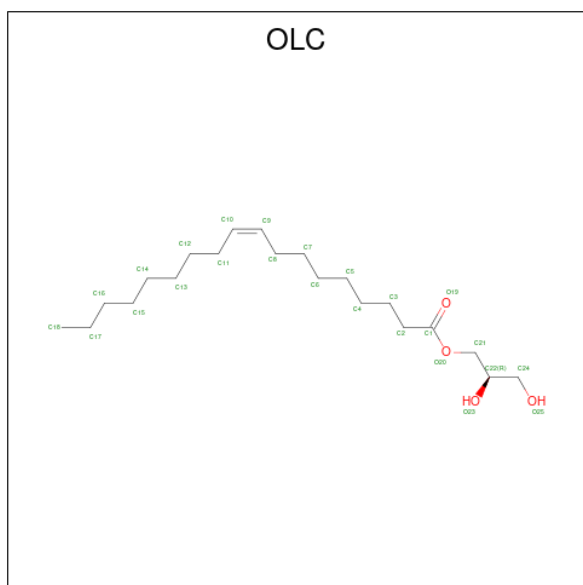
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 12 12	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C 13 13	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C O 17 15 2	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 7 7	0	0
4	A	1	Total C O 25 21 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 18 2	0	0
4	B	1	Total C O 25 21 4	0	0
4	B	1	Total C 17 17	0	0

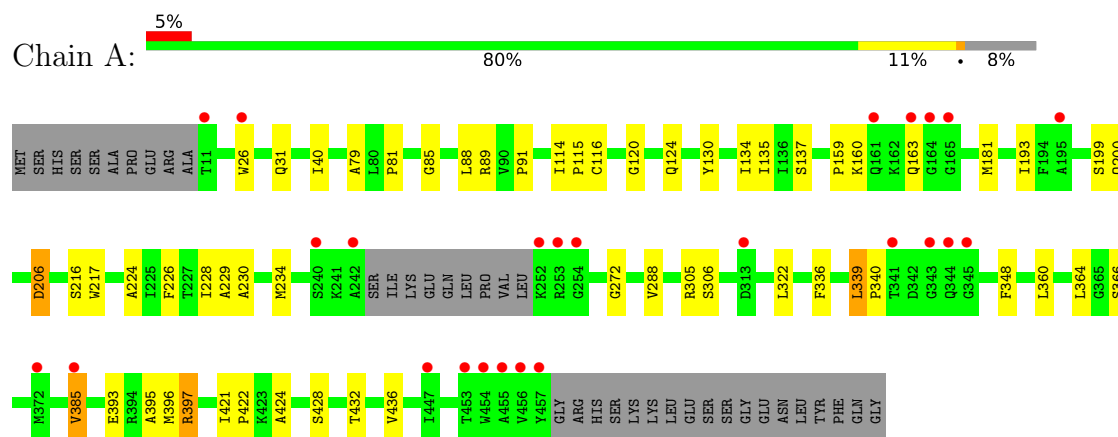
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	56	Total O 56 56	0	0

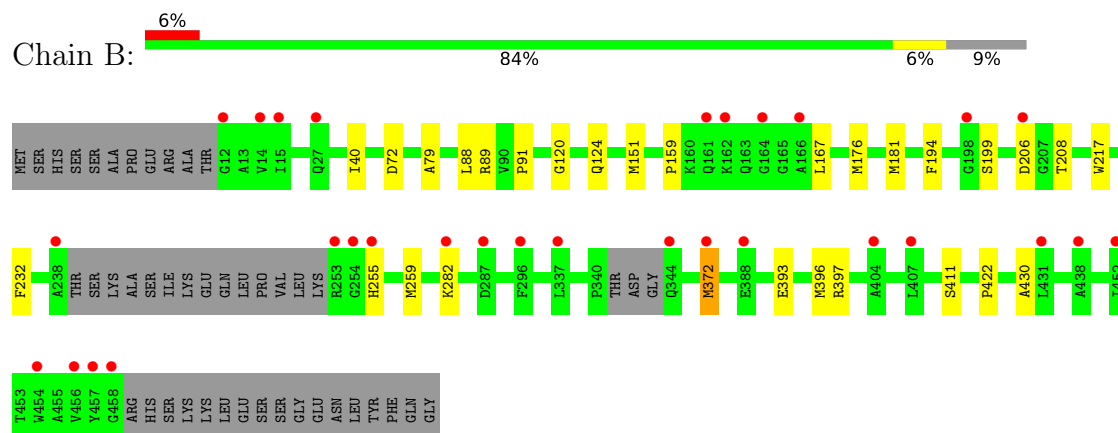
3 Residue-property plots

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: Nitrate/nitrite transporter NarK



• Molecule 1: Nitrate/nitrite transporter NarK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.78Å 86.10Å 221.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.35-2.40) 84.8 (48.35-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.219 , 0.237 0.222 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: OLC, NO3, OLA

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	0.31	0/3359	0.74	1/4572 (0.0%)
1	B	0.31	0/3307	0.73	1/4496 (0.0%)
All	All	0.31	0/6666	0.73	2/9068 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ILE	N-CA-C	-5.62	107.34	112.96
1	A	40	ILE	N-CA-C	-5.39	107.57	112.96

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	3268	0	3265	30	0
1	B	3218	0	3226	19	0
2	A	4	0	0	0	0
2	B	4	0	0	1	0
3	A	65	0	107	2	0
3	B	57	0	85	4	0
4	A	52	0	83	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	71	2	0
5	A	48	0	0	0	0
5	B	56	0	0	0	0
All	All	6814	0	6837	50	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 4.

All (50) 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:124:GLN:HE22	1:A:199:SER:HA	1.52	0.75
1:B:124:GLN:HE22	1:B:199:SER:HA	1.58	0.68
1:A:91:PRO:HB3	3:A:502:OLA:H171	1.77	0.66
1:A:159:PRO:HB2	1:A:396:MET:HB3	1.77	0.65
1:A:385:VAL:HG11	1:A:395:ALA:HA	1.87	0.57
1:A:305:ARG:NH1	1:A:366:SER:OG	2.38	0.56
1:B:89:ARG:NH2	2:B:501:NO3:O3	2.39	0.56
1:A:26:TRP:NE1	1:A:31:GLN:OE1	2.34	0.54
1:A:116:CYS:O	1:A:216:SER:OG	2.26	0.54
1:B:176:MET:HE2	4:B:508:OLC:H16	1.90	0.53
1:A:79:ALA:HB2	1:A:422:PRO:HB2	1.92	0.51
1:A:272:GLY:HA3	1:A:421:ILE:HD12	1.92	0.51
1:B:159:PRO:HB2	1:B:396:MET:HB3	1.93	0.50
1:B:393:GLU:OE2	1:B:397:ARG:NH2	2.42	0.50
1:A:160:LYS:HA	1:A:396:MET:HE2	1.94	0.49
1:A:135:ILE:HD11	3:B:502:OLA:H51	1.95	0.49
1:A:336:PHE:HE2	1:A:436:VAL:HG13	1.78	0.48
1:B:194:PHE:CE1	3:B:504:OLA:H10	2.48	0.48
1:A:26:TRP:HZ2	1:A:163:GLN:HE22	1.62	0.48
1:A:181:MET:HE3	1:A:181:MET:HB3	1.75	0.48
1:B:79:ALA:HB2	1:B:422:PRO:HB2	1.95	0.48
1:B:194:PHE:HE1	3:B:504:OLA:H10	1.80	0.47
1:B:72:ASP:HB2	1:B:430:ALA:HB2	1.98	0.45
1:A:428:SER:O	1:A:432:THR:OG1	2.33	0.45
1:A:85:GLY:O	1:A:89:ARG:HG3	2.18	0.44
1:A:114:ILE:HB	1:A:115:PRO:HD3	2.00	0.44
1:B:181:MET:HE3	1:B:181:MET:HB3	1.79	0.44
1:A:88:LEU:C	1:A:91:PRO:HD2	2.43	0.44
1:A:424:ALA:HA	3:A:506:OLA:H142	2.00	0.44
1:B:89:ARG:NH1	1:B:411:SER:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HD3	1:A:137:SER:OG	2.18	0.43
1:A:206:ASP:OD1	1:A:206:ASP:N	2.52	0.43
1:A:124:GLN:NE2	1:A:200:GLN:H	2.17	0.43
1:A:120:GLY:HA3	1:A:217:TRP:NE1	2.33	0.43
1:B:151:MET:HE1	1:B:167:LEU:O	2.19	0.42
4:A:508:OLC:H21A	1:B:232:PHE:HE1	1.84	0.42
1:B:372:MET:HE2	1:B:372:MET:HB2	1.90	0.42
1:A:393:GLU:OE2	1:A:397:ARG:NH1	2.53	0.42
1:A:130:TYR:CZ	1:A:134:ILE:HD11	2.55	0.42
1:A:339:LEU:HA	1:A:340:PRO:HD3	1.94	0.42
1:A:224:ALA:O	1:A:228:ILE:HG12	2.20	0.42
1:B:255:HIS:O	1:B:259:MET:HG2	2.19	0.41
1:A:226:PHE:HA	1:A:229:ALA:HB3	2.00	0.41
1:A:288:VAL:HG11	1:A:348:PHE:CZ	2.55	0.41
1:A:230:ALA:HA	1:A:234:MET:HG3	2.02	0.41
1:B:206:ASP:OD1	1:B:208:THR:OG1	2.38	0.41
1:B:282:LYS:HA	1:B:282:LYS:HD2	1.90	0.41
3:B:503:OLA:H183	4:B:508:OLC:H7A	2.02	0.41
1:B:120:GLY:HA3	1:B:217:TRP:NE1	2.36	0.40
1:B:88:LEU:C	1:B:91:PRO:HD2	2.46	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	434/475 (91%)	426 (98%)	8 (2%)	0	100	100
1	B	424/475 (89%)	414 (98%)	10 (2%)	0	100	100
All	All	858/950 (90%)	840 (98%)	18 (2%)	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	326/372 (88%)	317 (97%)	9 (3%)	38	60
1	B	322/372 (87%)	321 (100%)	1 (0%)	86	93
All	All	648/744 (87%)	638 (98%)	10 (2%)	57	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ILE
1	A	206	ASP
1	A	306	SER
1	A	322	LEU
1	A	339	LEU
1	A	360	LEU
1	A	364	LEU
1	A	385	VAL
1	A	397	ARG
1	B	372	MET

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	124	GLN
1	A	146	ASN
1	A	163	GLN
1	A	175	ASN
1	A	289	GLN
1	B	124	GLN
1	B	163	GLN
1	B	170	ASN
1	B	175	ASN
1	B	255	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	OLA	B	503	-	7,7,19	0.27	0	6,6,19	0.48	0
3	OLA	B	505	-	9,9,19	0.97	1 (11%)	8,8,19	0.50	0
3	OLA	B	504	-	10,10,19	0.92	1 (10%)	9,9,19	0.52	0
4	OLC	B	508	-	16,16,24	0.87	1 (6%)	15,15,25	0.75	0
3	OLA	A	506	-	12,12,19	0.83	1 (8%)	11,11,19	0.58	0
3	OLA	A	505	-	19,19,19	0.81	1 (5%)	19,19,19	0.93	1 (5%)
2	NO3	B	501	-	1,3,3	3.29	1 (100%)	0,3,3	-	-
2	NO3	A	501	-	1,3,3	3.30	1 (100%)	0,3,3	-	-
3	OLA	A	502	-	11,11,19	0.89	1 (9%)	10,10,19	0.62	0
4	OLC	A	509	-	19,19,24	0.97	2 (10%)	19,19,25	1.04	0
3	OLA	A	504	-	7,7,19	0.40	0	6,6,19	0.68	0
3	OLA	A	503	-	11,11,19	0.89	1 (9%)	10,10,19	0.68	0
3	OLA	B	506	-	16,16,19	0.88	1 (6%)	16,16,19	0.95	1 (6%)
4	OLC	A	508	-	24,24,24	1.11	2 (8%)	25,25,25	1.01	1 (4%)
4	OLC	A	507	-	6,6,24	0.33	0	5,5,25	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	B	507	-	24,24,24	1.11	2 (8%)	25,25,25	0.94	1 (4%)
3	OLA	B	502	-	10,10,19	0.93	1 (10%)	9,9,19	0.68	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
3	OLA	B	503	-	-	4/5/5/17	-
3	OLA	B	505	-	-	5/7/7/17	-
3	OLA	B	504	-	-	5/8/8/17	-
4	OLC	B	508	-	-	5/14/14/24	-
3	OLA	A	506	-	-	5/10/10/17	-
3	OLA	A	505	-	-	6/17/17/17	-
3	OLA	A	502	-	-	5/9/9/17	-
4	OLC	A	509	-	-	2/17/17/24	-
3	OLA	A	504	-	-	3/5/5/17	-
3	OLA	A	503	-	-	4/9/9/17	-
3	OLA	B	506	-	-	7/14/14/17	-
4	OLC	A	508	-	-	11/24/24/24	-
4	OLC	A	507	-	-	0/4/4/24	-
4	OLC	B	507	-	-	8/24/24/24	-
3	OLA	B	502	-	-	6/8/8/17	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NO3	O1-N	3.30	1.40	1.24
2	B	501	NO3	O1-N	3.29	1.40	1.24
4	B	507	OLC	C9-C10	3.17	1.49	1.31
4	B	508	OLC	C9-C10	3.15	1.49	1.31
4	A	509	OLC	C9-C10	3.15	1.49	1.31
4	A	508	OLC	C9-C10	3.14	1.49	1.31
4	B	507	OLC	O20-C21	-3.07	1.38	1.45
4	A	508	OLC	O20-C21	-3.02	1.38	1.45
3	B	505	OLA	C10-C9	2.81	1.47	1.31
3	A	502	OLA	C10-C9	2.81	1.47	1.31
3	A	503	OLA	C10-C9	2.80	1.47	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	OLA	C10-C9	2.80	1.47	1.31
3	B	504	OLA	C10-C9	2.80	1.47	1.31
3	B	506	OLA	C10-C9	2.79	1.47	1.31
3	A	505	OLA	C10-C9	2.76	1.47	1.31
3	A	506	OLA	C10-C9	2.76	1.47	1.31
4	A	509	OLC	O20-C1	2.16	1.38	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	508	OLC	O20-C1-C2	2.64	119.88	111.83
4	B	507	OLC	O20-C1-C2	2.49	119.43	111.83
3	B	506	OLA	O2-C1-C2	2.10	120.63	114.00
3	A	505	OLA	O2-C1-C2	2.00	120.33	114.00

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	508	OLC	C2-C1-O20-C21
4	A	508	OLC	O19-C1-O20-C21
4	B	507	OLC	O20-C21-C22-O23
4	B	507	OLC	O20-C21-C22-C24
4	A	508	OLC	O23-C22-C24-O25
4	B	507	OLC	C1-C2-C3-C4
3	B	506	OLA	C1-C2-C3-C4
4	A	508	OLC	O20-C21-C22-O23
3	A	504	OLA	C11-C12-C13-C14
4	A	508	OLC	C21-C22-C24-O25
3	A	506	OLA	C11-C12-C13-C14
4	B	508	OLC	C11-C12-C13-C14
3	A	505	OLA	C11-C12-C13-C14
3	A	505	OLA	C4-C5-C6-C7
3	B	504	OLA	C11-C10-C9-C8
3	B	503	OLA	C12-C13-C14-C15
3	A	503	OLA	C7-C8-C9-C10
3	B	504	OLA	C11-C12-C13-C14
4	A	508	OLC	C10-C11-C12-C13
3	B	506	OLA	C11-C10-C9-C8
4	A	509	OLC	C10-C11-C12-C13
4	A	508	OLC	C3-C4-C5-C6
4	B	507	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	506	OLA	C11-C10-C9-C8
3	A	502	OLA	C10-C11-C12-C13
3	A	502	OLA	C11-C10-C9-C8
3	A	503	OLA	C11-C10-C9-C8
3	A	505	OLA	C11-C10-C9-C8
3	B	505	OLA	C11-C10-C9-C8
4	B	508	OLC	C4-C5-C6-C7
3	B	502	OLA	C11-C10-C9-C8
4	A	508	OLC	C11-C12-C13-C14
4	B	508	OLC	C6-C7-C8-C9
4	A	508	OLC	C4-C5-C6-C7
3	B	506	OLA	C11-C12-C13-C14
3	B	503	OLA	C11-C12-C13-C14
3	B	502	OLA	C3-C4-C5-C6
3	B	505	OLA	C5-C6-C7-C8
3	A	503	OLA	C12-C13-C14-C15
4	B	507	OLC	C6-C7-C8-C9
3	A	502	OLA	C12-C13-C14-C15
3	A	506	OLA	C12-C13-C14-C15
3	B	502	OLA	C5-C6-C7-C8
3	B	505	OLA	C4-C5-C6-C7
3	A	506	OLA	C7-C8-C9-C10
3	B	502	OLA	C4-C5-C6-C7
3	B	504	OLA	C12-C13-C14-C15
3	A	502	OLA	C7-C8-C9-C10
3	B	502	OLA	C9-C10-C11-C12
3	A	505	OLA	C9-C10-C11-C12
4	B	507	OLC	C7-C8-C9-C10
4	A	509	OLC	C11-C10-C9-C8
3	B	506	OLA	O2-C1-C2-C3
3	A	504	OLA	C12-C13-C14-C15
3	B	506	OLA	O1-C1-C2-C3
3	B	505	OLA	C9-C10-C11-C12
3	B	506	OLA	C7-C8-C9-C10
3	B	504	OLA	C7-C8-C9-C10
3	B	505	OLA	C7-C8-C9-C10
3	A	503	OLA	C9-C10-C11-C12
3	B	504	OLA	C9-C10-C11-C12
4	B	508	OLC	C9-C10-C11-C12
3	B	503	OLA	C13-C14-C15-C16
3	A	505	OLA	C7-C8-C9-C10
3	B	502	OLA	C7-C8-C9-C10

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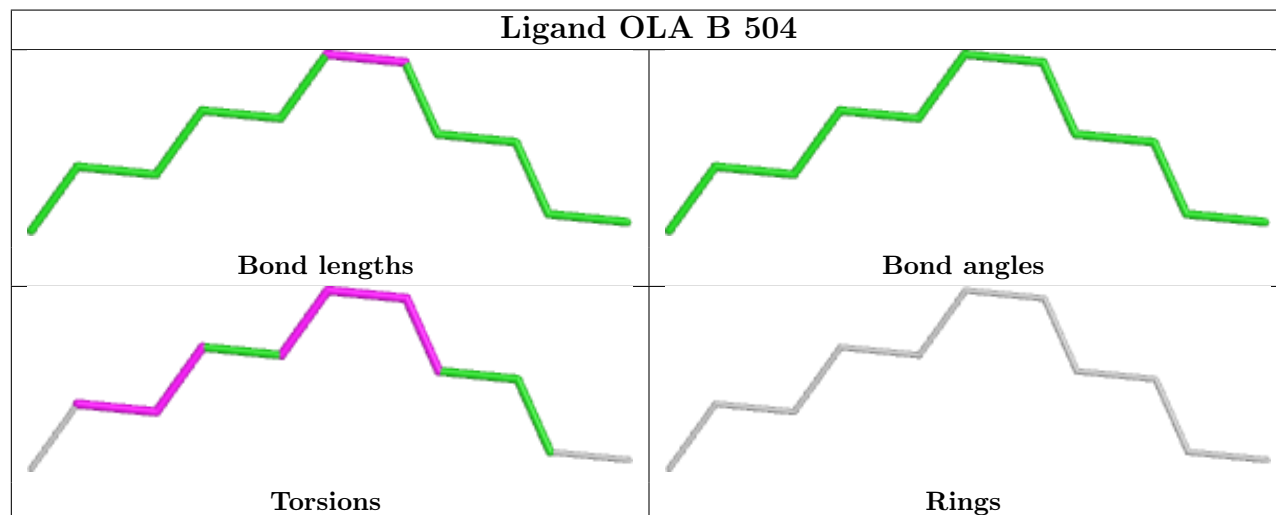
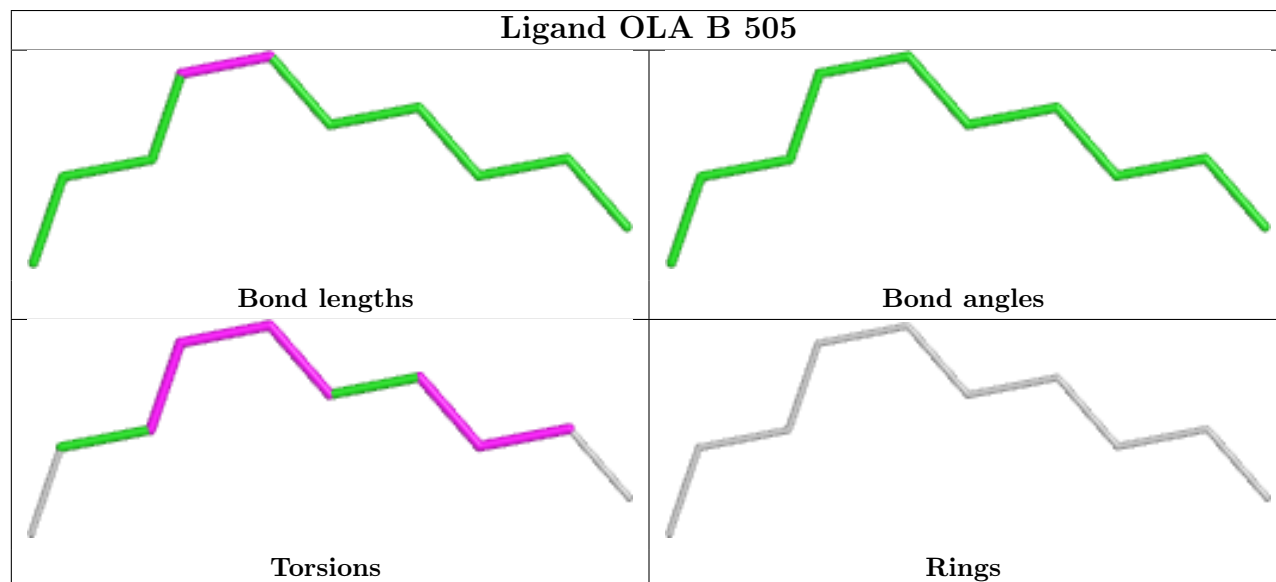
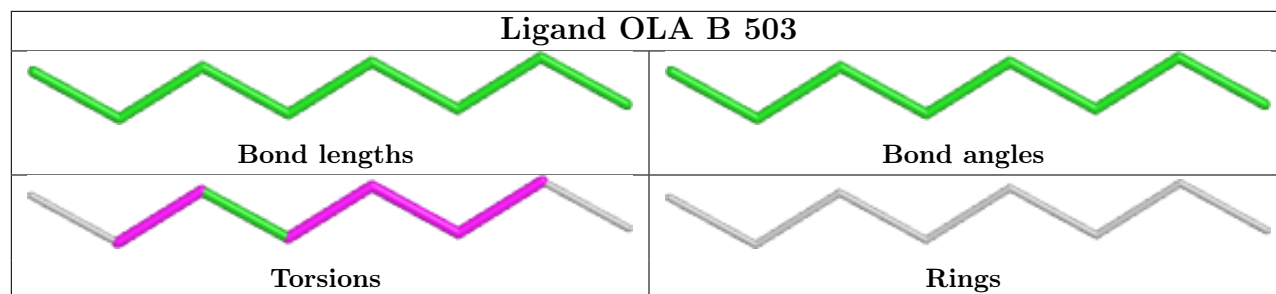
Mol	Chain	Res	Type	Atoms
3	A	504	OLA	C14-C15-C16-C17
3	A	502	OLA	C9-C10-C11-C12
4	A	508	OLC	C7-C8-C9-C10
4	A	508	OLC	O20-C21-C22-C24
4	B	507	OLC	O20-C1-C2-C3
3	A	505	OLA	C3-C4-C5-C6
4	B	507	OLC	O19-C1-C2-C3
4	B	508	OLC	C11-C10-C9-C8
3	B	503	OLA	C15-C16-C17-C18
3	A	506	OLA	C14-C15-C16-C17
3	B	506	OLA	C4-C5-C6-C7

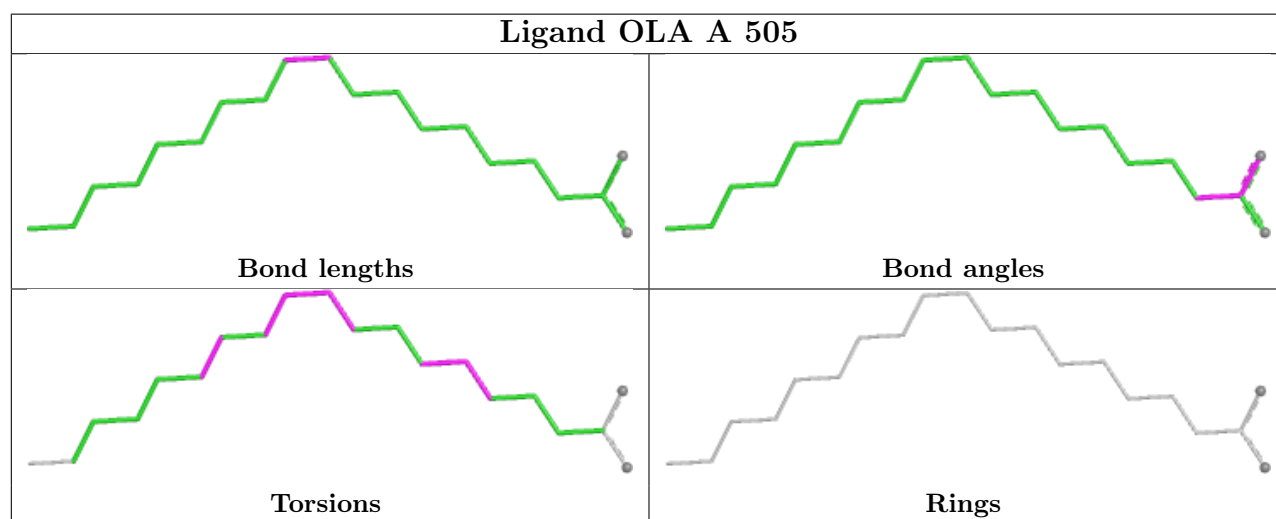
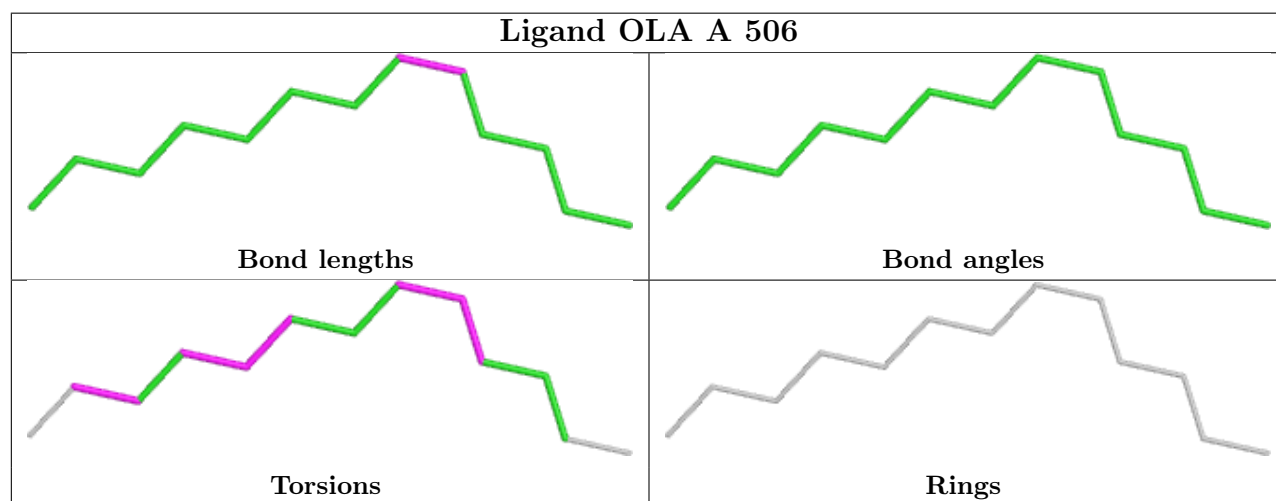
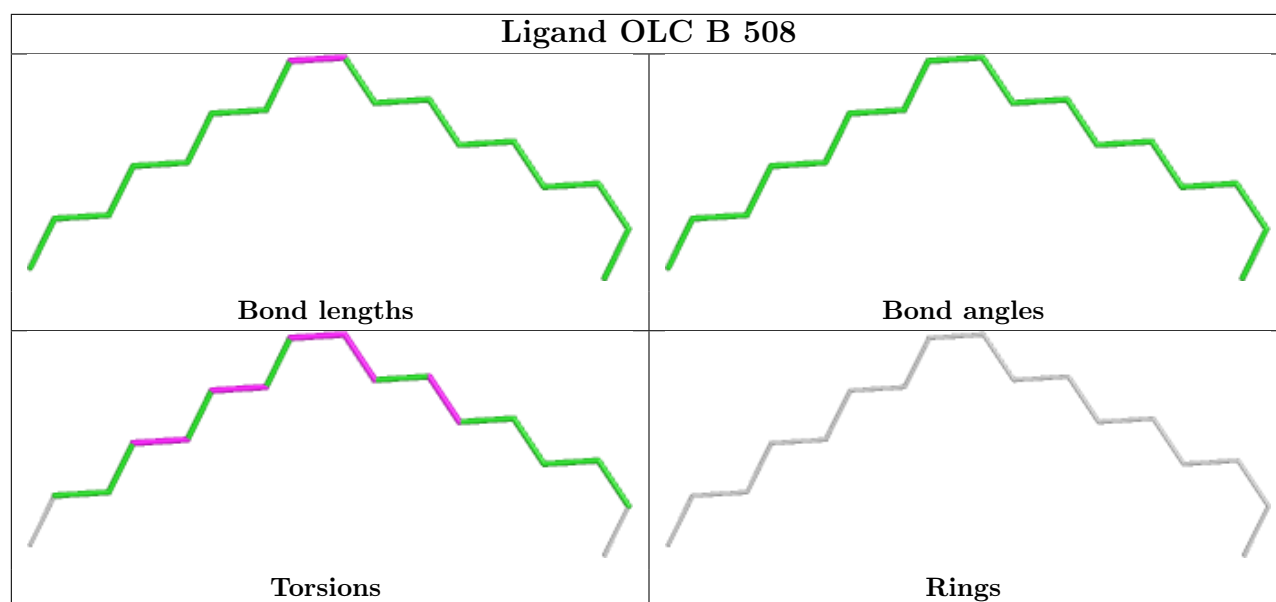
There are no ring outliers.

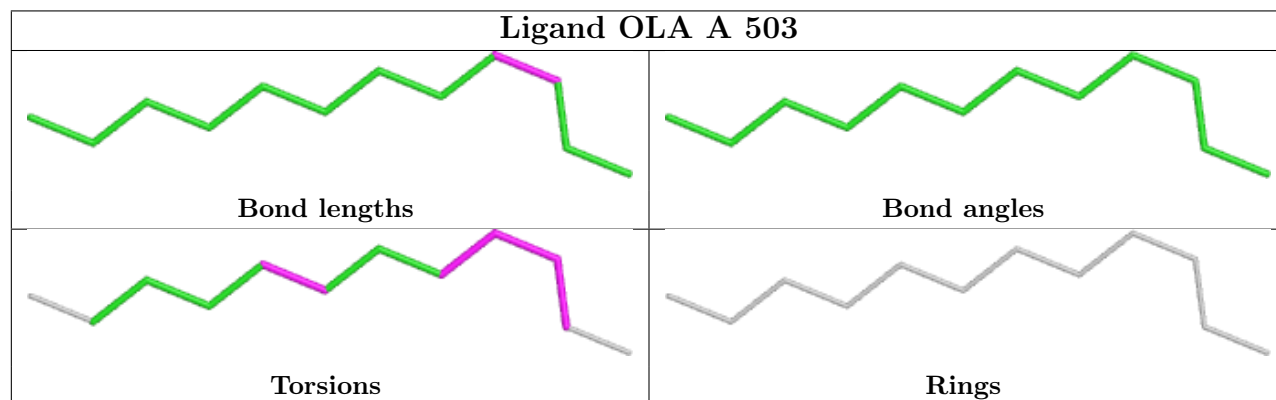
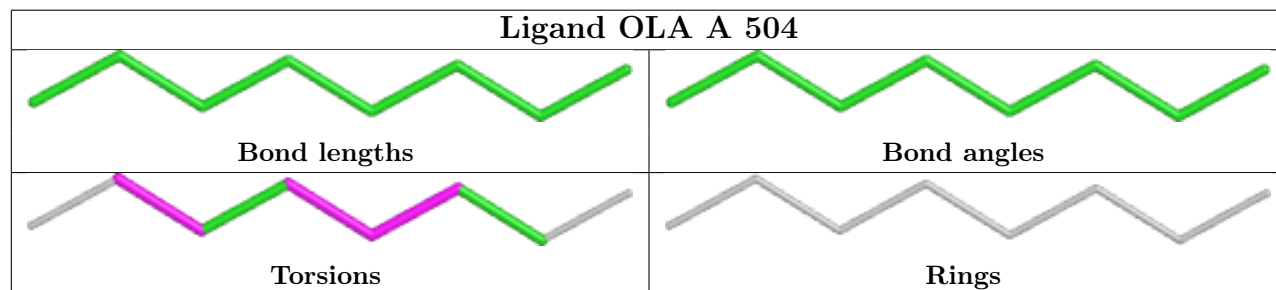
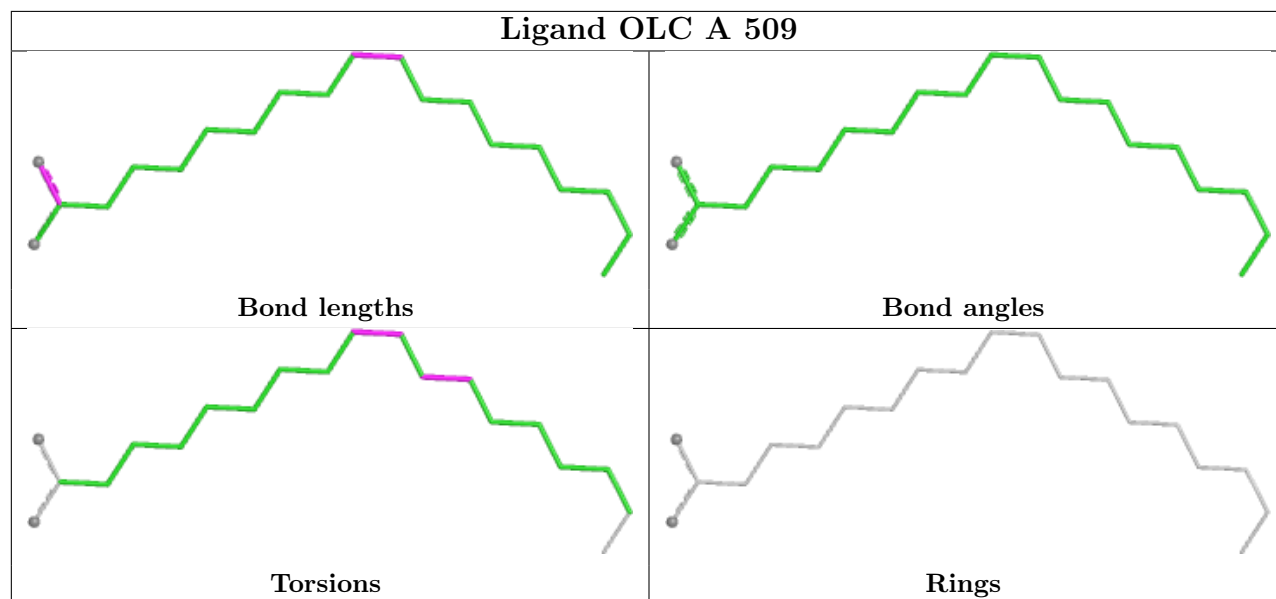
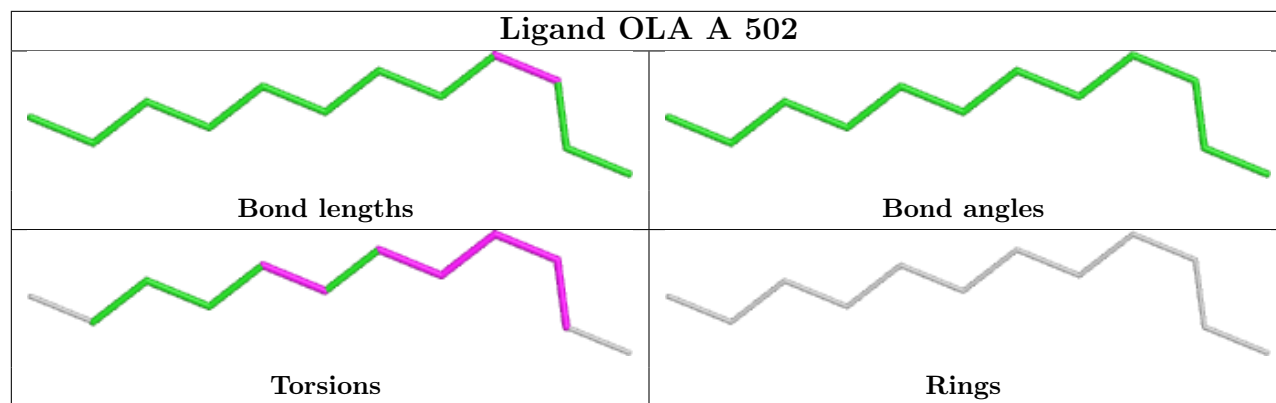
8 monomers are involved in 9 short contacts:

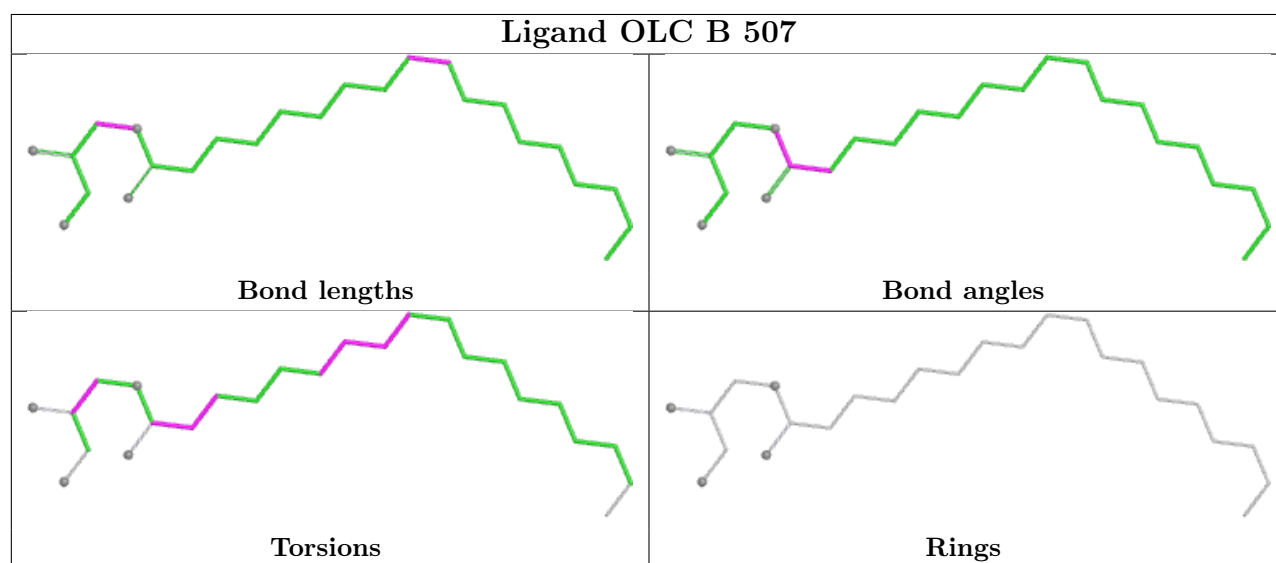
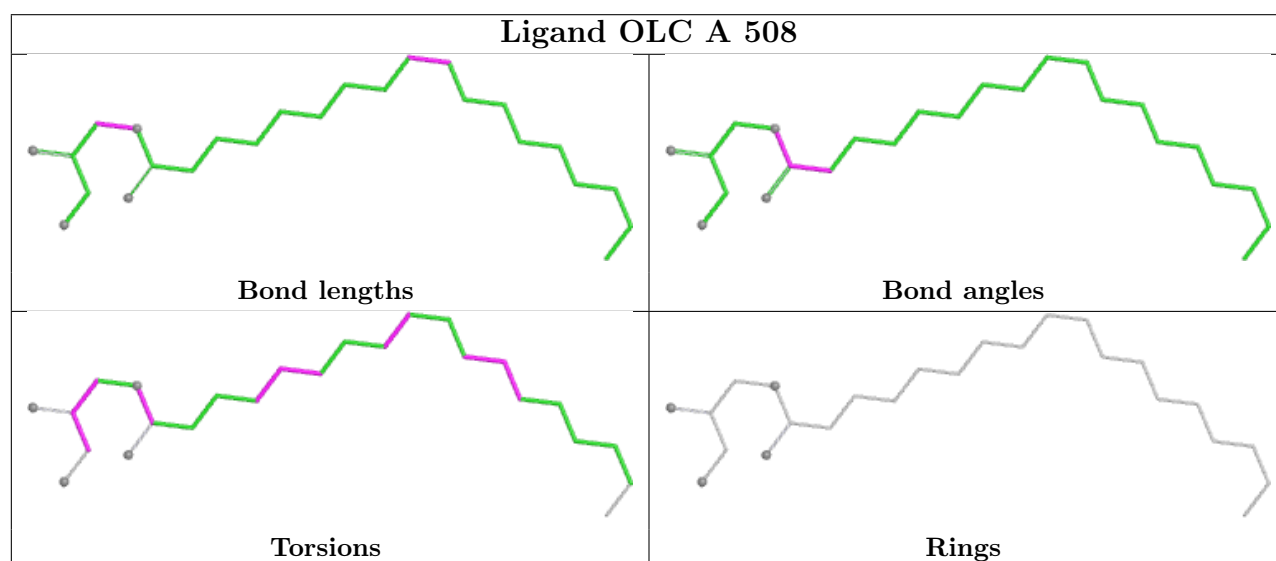
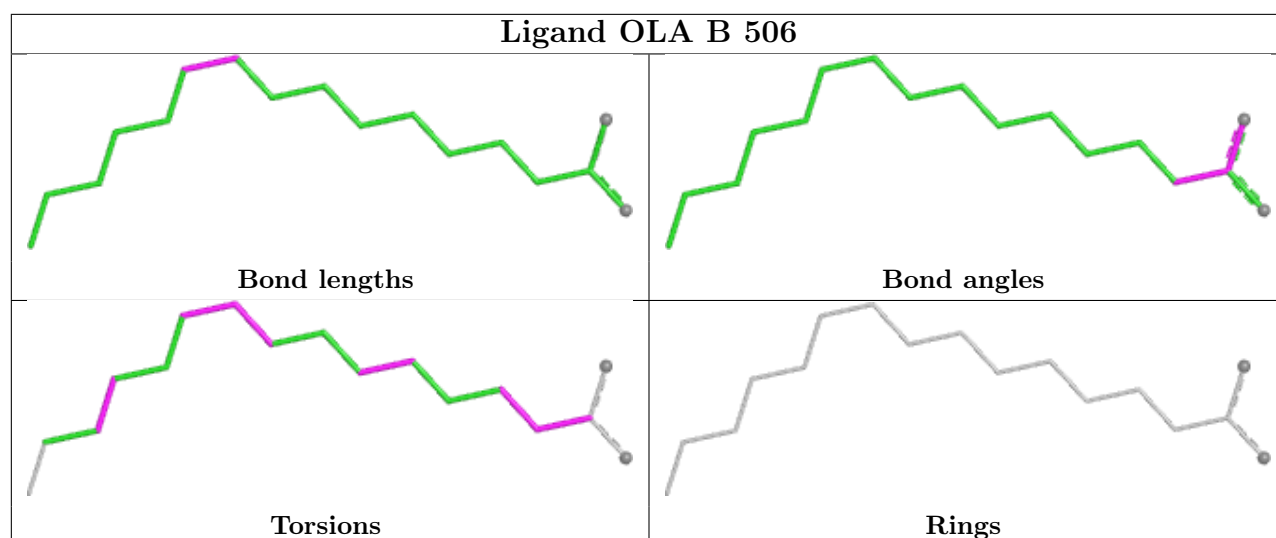
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	OLA	1	0
3	B	504	OLA	2	0
4	B	508	OLC	2	0
3	A	506	OLA	1	0
2	B	501	NO3	1	0
3	A	502	OLA	1	0
4	A	508	OLC	1	0
3	B	502	OLA	1	0

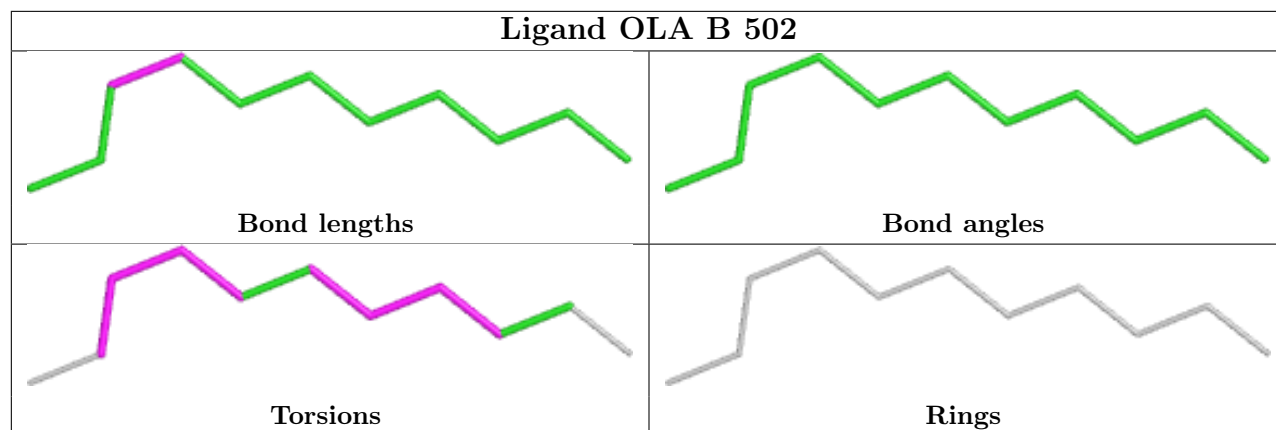
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/475 (92%)	0.51	25 (5%) 29 25	37, 47, 77, 115	0
1	B	430/475 (90%)	0.60	30 (6%) 22 19	36, 51, 75, 101	0
All	All	868/950 (91%)	0.55	55 (6%) 26 22	36, 49, 76, 115	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	GLY	6.2
1	A	11	THR	5.6
1	B	344	GLN	5.5
1	A	457	TYR	4.9
1	B	238	ALA	4.8
1	A	343	GLY	4.4
1	B	253	ARG	4.3
1	B	458	GLY	4.0
1	A	344	GLN	3.8
1	A	341	THR	3.7
1	A	456	VAL	3.7
1	A	161	GLN	3.6
1	A	240	SER	3.6
1	A	252	LYS	3.4
1	A	385	VAL	3.4
1	B	452	ILE	3.4
1	A	454	TRP	3.1
1	B	14	VAL	3.0
1	A	26	TRP	2.8
1	B	407	LEU	2.8
1	B	15	ILE	2.8
1	A	165	GLY	2.7
1	A	453	THR	2.7
1	B	454	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	313	ASP	2.6
1	A	372	MET	2.6
1	B	287	ASP	2.6
1	A	163	GLN	2.6
1	A	242	ALA	2.6
1	B	456	VAL	2.5
1	B	198	GLY	2.5
1	B	372	MET	2.4
1	A	345	GLY	2.4
1	A	455	ALA	2.3
1	B	388	GLU	2.3
1	A	254	GLY	2.3
1	B	161	GLN	2.3
1	B	337	LEU	2.3
1	B	457	TYR	2.3
1	A	447	ILE	2.2
1	B	162	LYS	2.2
1	B	438	ALA	2.2
1	B	12	GLY	2.2
1	B	206	ASP	2.2
1	B	27	GLN	2.2
1	A	253	ARG	2.2
1	A	195	ALA	2.1
1	B	404	ALA	2.1
1	B	296	PHE	2.1
1	B	255	HIS	2.1
1	B	254	GLY	2.1
1	B	166	ALA	2.1
1	B	164	GLY	2.1
1	B	431	LEU	2.1
1	B	282	LYS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

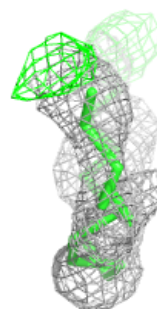
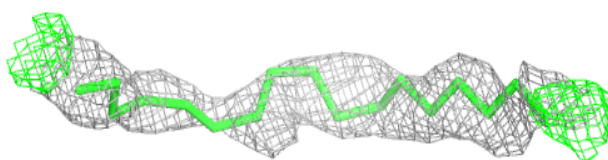
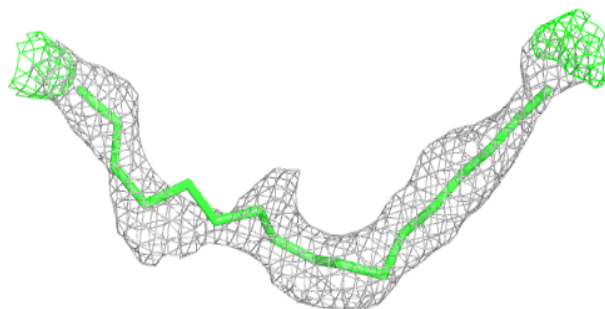
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	507	7/25	0.56	0.28	63,64,66,67	0
4	OLC	B	508	17/25	0.73	0.26	61,69,75,75	0
3	OLA	A	505	20/20	0.79	0.16	40,54,69,75	0
3	OLA	B	506	17/20	0.79	0.26	59,66,83,84	0
3	OLA	B	505	10/20	0.80	0.27	67,73,75,75	0
3	OLA	A	503	12/20	0.83	0.22	61,63,66,69	0
3	OLA	A	502	12/20	0.85	0.18	54,60,65,68	0
4	OLC	B	507	25/25	0.85	0.18	48,62,86,88	0
3	OLA	B	504	11/20	0.85	0.17	45,54,60,60	0
3	OLA	A	506	13/20	0.87	0.20	55,58,63,63	0
3	OLA	B	502	11/20	0.88	0.17	59,61,65,66	0
4	OLC	A	508	25/25	0.89	0.16	56,66,80,81	0
2	NO3	A	501	4/4	0.90	0.17	44,44,44,46	4
3	OLA	A	504	8/20	0.90	0.18	53,56,59,60	0
3	OLA	B	503	8/20	0.91	0.19	67,70,71,71	0
2	NO3	B	501	4/4	0.93	0.22	42,43,44,47	4
4	OLC	A	509	20/25	0.93	0.11	38,47,73,73	0

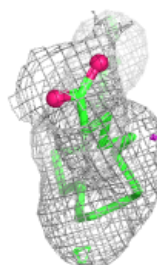
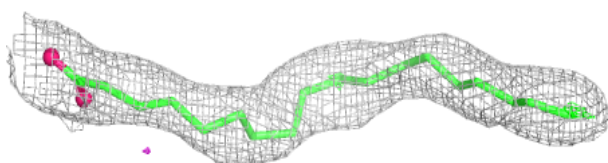
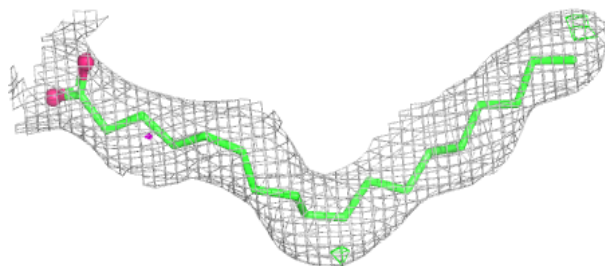
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLC B 508:

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

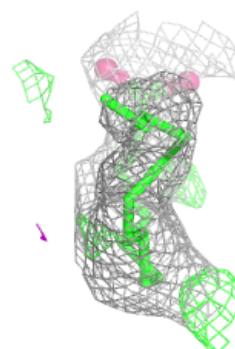
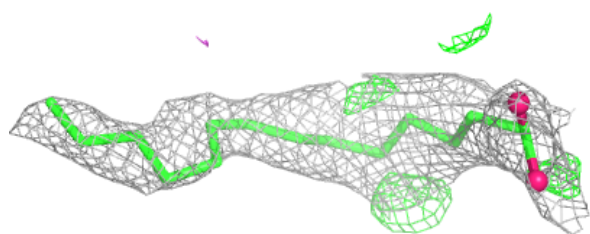
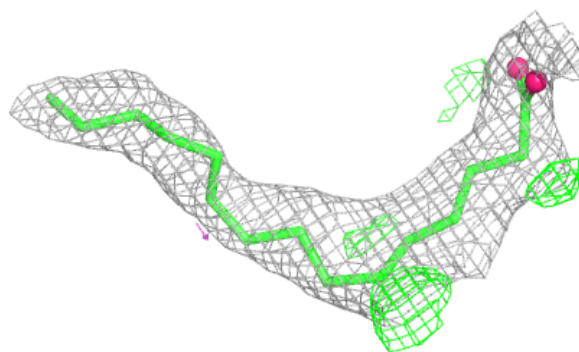
**Electron density around OLA A 505:**

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

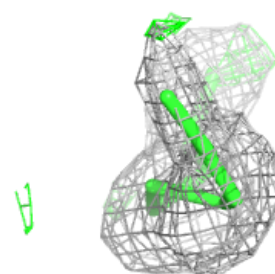
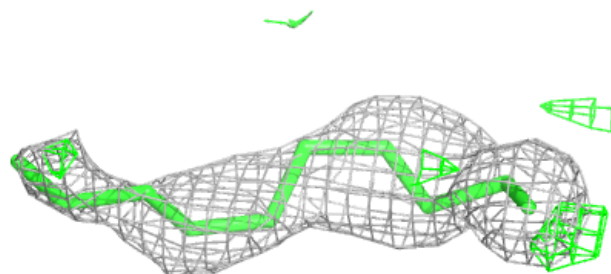
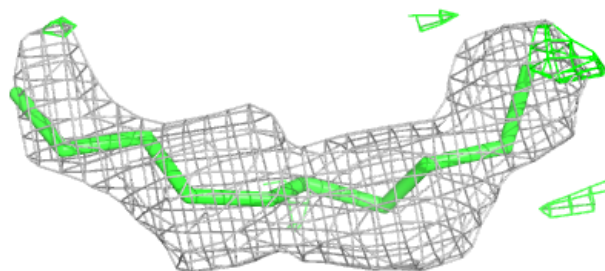


Electron density around OLA B 506:

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

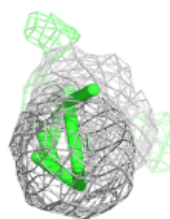
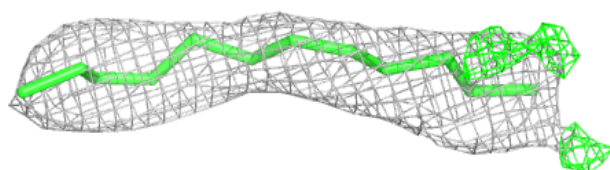
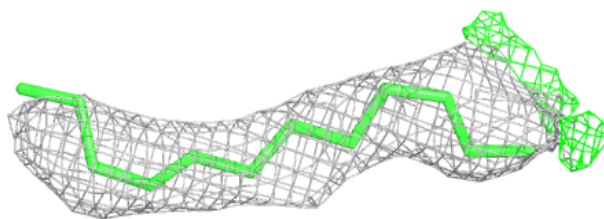
**Electron density around OLA B 505:**

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

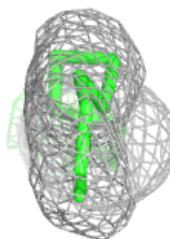
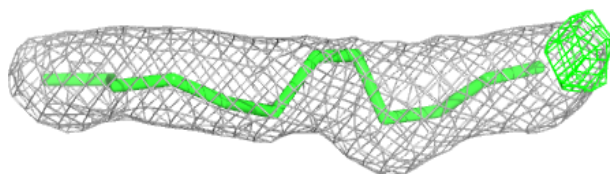
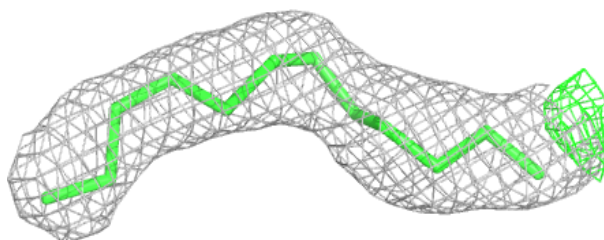


Electron density around OLA A 503:

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and green (positive)

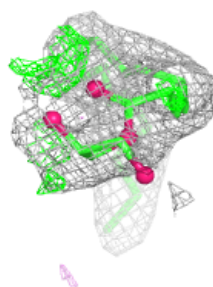
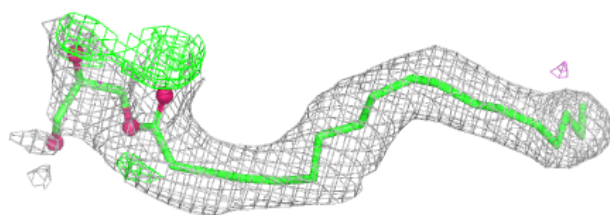
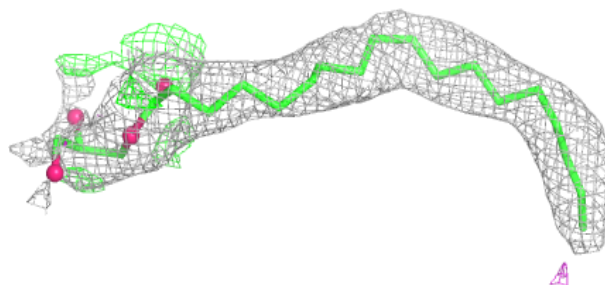
**Electron density around OLA A 502:**

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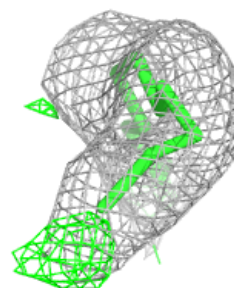
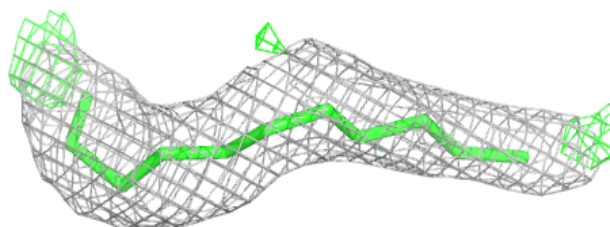
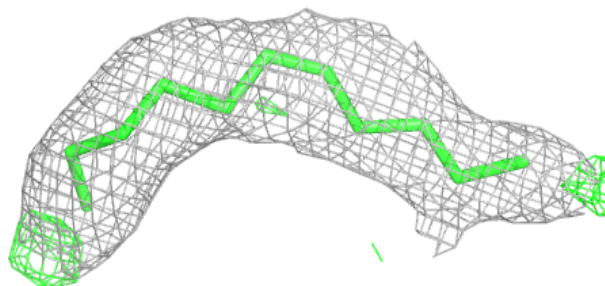


Electron density around OLC B 507:

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

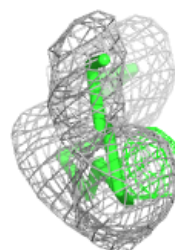
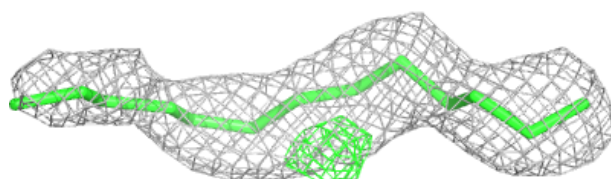
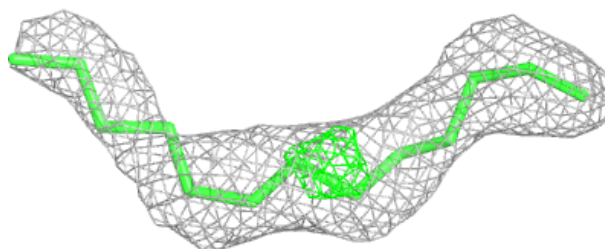
**Electron density around OLA B 504:**

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

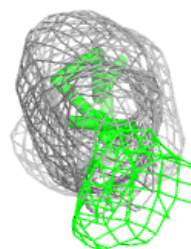
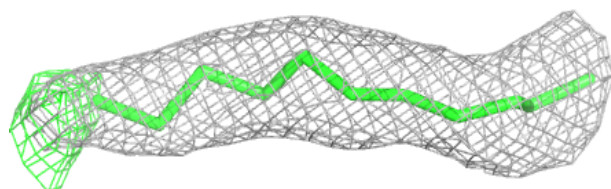
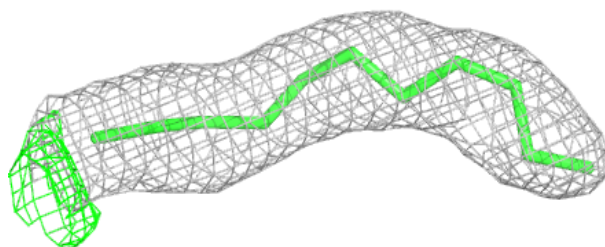


Electron density around OLA A 506:

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

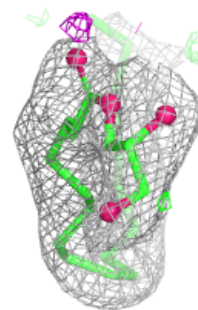
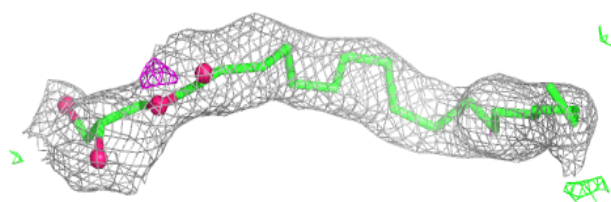
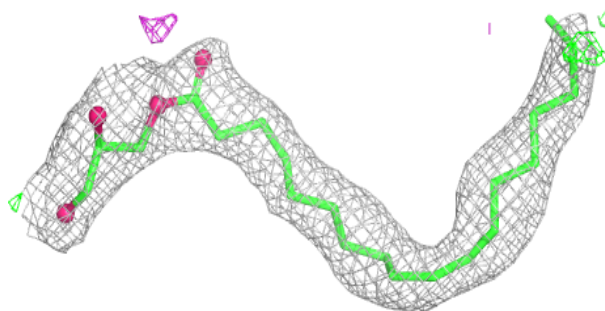
**Electron density around OLA B 502:**

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

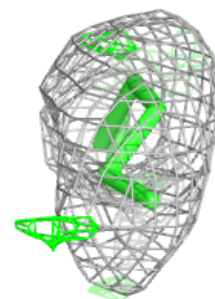
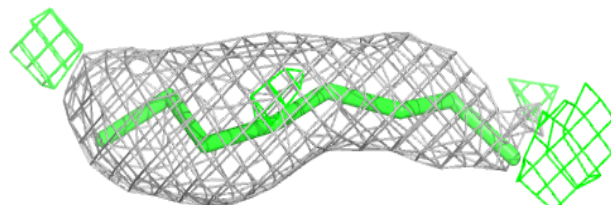
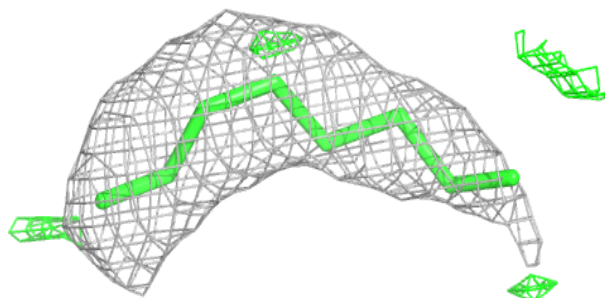


Electron density around OLC A 508:

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

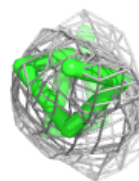
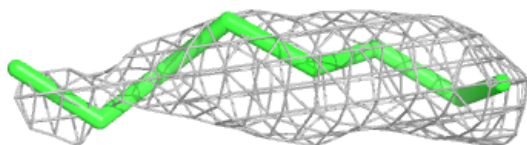
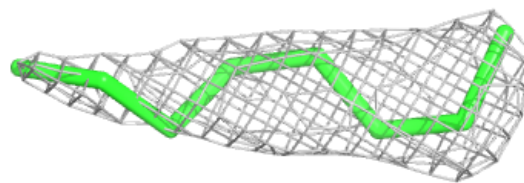
**Electron density around OLA A 504:**

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

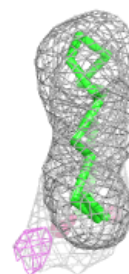
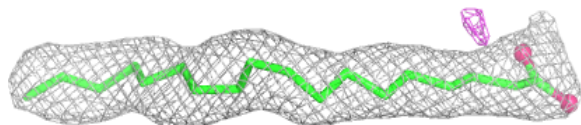
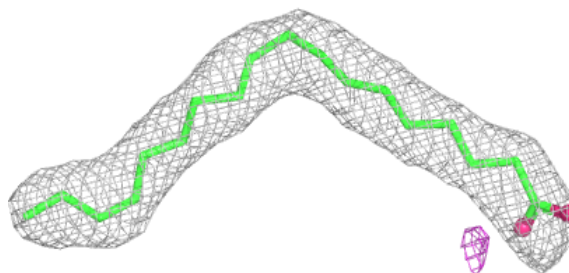


Electron density around OLA B 503:

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

**Electron density around OLC A 509:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.