



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:52 AM UTC

PDB ID : 4EA3 / pdb\_00004ea3  
Title : Structure of the N/OFQ Opioid Receptor in Complex with a Peptide Mimetic  
Authors : Thompson, A.A.; Liu, W.; Chun, E.; Katritch, V.; Wu, H.; Vardy, E.; Huang, X.P.; Trapella, C.; Guerrini, R.; Calo, G.; Roth, B.L.; Cherezov, V.; Stevens, R.C.; GPCR Network (GPCR)  
Deposited on : 2012-03-22  
Resolution : 3.01 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](mailto: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>.

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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

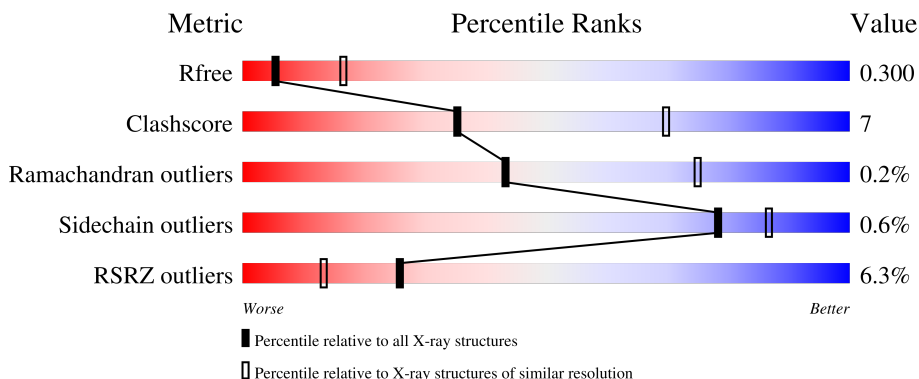
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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  $\geq 3$ , 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	434	 6% 55% 9% 36%
1	B	434	 4% 76% 11% 13%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5130 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 Fusion protein of Nociceptin receptor and cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	2113	1391	343	362	17	0	0	0
1	B	376	2894	1887	475	513	19	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	991	ASP	-	expression tag	UNP P0ABE7
A	992	TYR	-	expression tag	UNP P0ABE7
A	993	LYS	-	expression tag	UNP P0ABE7
A	994	ASP	-	expression tag	UNP P0ABE7
A	995	ASP	-	expression tag	UNP P0ABE7
A	996	ASP	-	expression tag	UNP P0ABE7
A	997	ASP	-	expression tag	UNP P0ABE7
A	998	GLY	-	expression tag	UNP P0ABE7
A	999	ALA	-	expression tag	UNP P0ABE7
A	1000	PRO	-	expression tag	UNP P0ABE7
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	340	GLY	-	expression tag	UNP P41146
A	341	ARG	-	expression tag	UNP P41146
A	342	PRO	-	expression tag	UNP P41146
A	343	LEU	-	expression tag	UNP P41146
A	344	GLU	-	expression tag	UNP P41146
A	345	VAL	-	expression tag	UNP P41146
A	346	LEU	-	expression tag	UNP P41146
A	347	PHE	-	expression tag	UNP P41146
A	348	GLN	-	expression tag	UNP P41146
A	349	GLY	-	expression tag	UNP P41146
A	350	PRO	-	expression tag	UNP P41146
A	351	HIS	-	expression tag	UNP P41146

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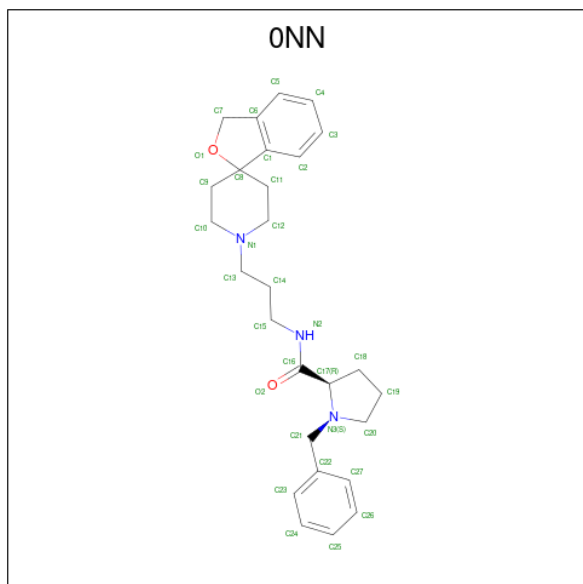
Chain	Residue	Modelled	Actual	Comment	Reference
A	352	HIS	-	expression tag	UNP P41146
A	353	HIS	-	expression tag	UNP P41146
A	354	HIS	-	expression tag	UNP P41146
A	355	HIS	-	expression tag	UNP P41146
A	356	HIS	-	expression tag	UNP P41146
A	357	HIS	-	expression tag	UNP P41146
A	358	HIS	-	expression tag	UNP P41146
A	359	HIS	-	expression tag	UNP P41146
A	360	HIS	-	expression tag	UNP P41146
B	991	ASP	-	expression tag	UNP P0ABE7
B	992	TYR	-	expression tag	UNP P0ABE7
B	993	LYS	-	expression tag	UNP P0ABE7
B	994	ASP	-	expression tag	UNP P0ABE7
B	995	ASP	-	expression tag	UNP P0ABE7
B	996	ASP	-	expression tag	UNP P0ABE7
B	997	ASP	-	expression tag	UNP P0ABE7
B	998	GLY	-	expression tag	UNP P0ABE7
B	999	ALA	-	expression tag	UNP P0ABE7
B	1000	PRO	-	expression tag	UNP P0ABE7
B	1007	TRP	MET	engineered mutation	UNP P0ABE7
B	1102	ILE	HIS	engineered mutation	UNP P0ABE7
B	1106	LEU	ARG	engineered mutation	UNP P0ABE7
B	340	GLY	-	expression tag	UNP P41146
B	341	ARG	-	expression tag	UNP P41146
B	342	PRO	-	expression tag	UNP P41146
B	343	LEU	-	expression tag	UNP P41146
B	344	GLU	-	expression tag	UNP P41146
B	345	VAL	-	expression tag	UNP P41146
B	346	LEU	-	expression tag	UNP P41146
B	347	PHE	-	expression tag	UNP P41146
B	348	GLN	-	expression tag	UNP P41146
B	349	GLY	-	expression tag	UNP P41146
B	350	PRO	-	expression tag	UNP P41146
B	351	HIS	-	expression tag	UNP P41146
B	352	HIS	-	expression tag	UNP P41146
B	353	HIS	-	expression tag	UNP P41146
B	354	HIS	-	expression tag	UNP P41146
B	355	HIS	-	expression tag	UNP P41146
B	356	HIS	-	expression tag	UNP P41146
B	357	HIS	-	expression tag	UNP P41146
B	358	HIS	-	expression tag	UNP P41146
B	359	HIS	-	expression tag	UNP P41146

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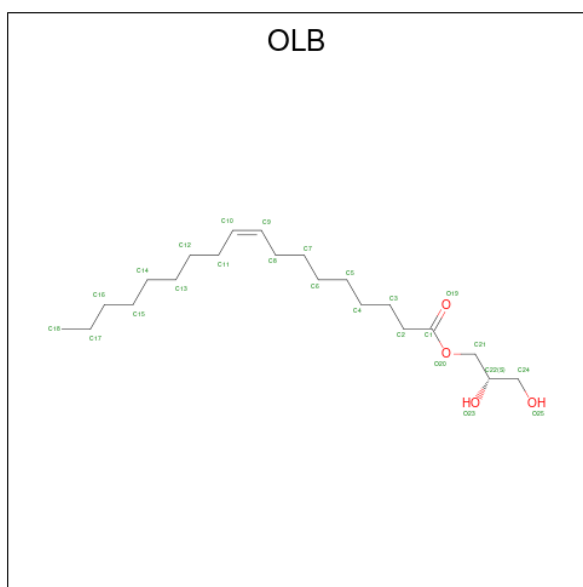
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	HIS	-	expression tag	UNP P41146

- Molecule 2 is 1-benzyl-N-[3-(1'H,3H-spiro[2-benzofuran-1,4'-piperidin]-1'-yl)propyl]-D-prolin amide (CCD ID: 0NN) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>).



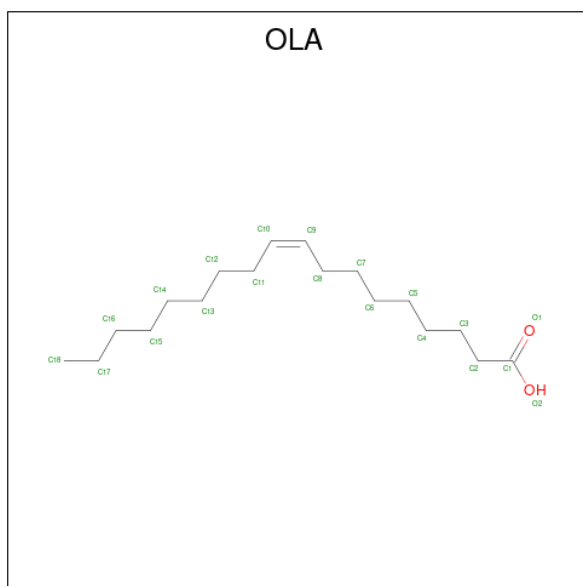
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	27	3	2	0	0
2	B	1	32	27	3	2	0	0

- Molecule 3 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



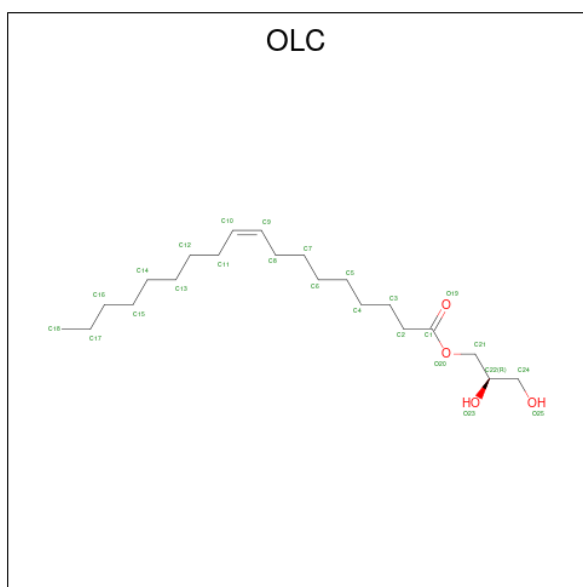
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula:  $C_{18}H_{34}O_2$ ).



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

- Molecule 5 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
5	B	1	Total	C O	0	0
			16	12 4		

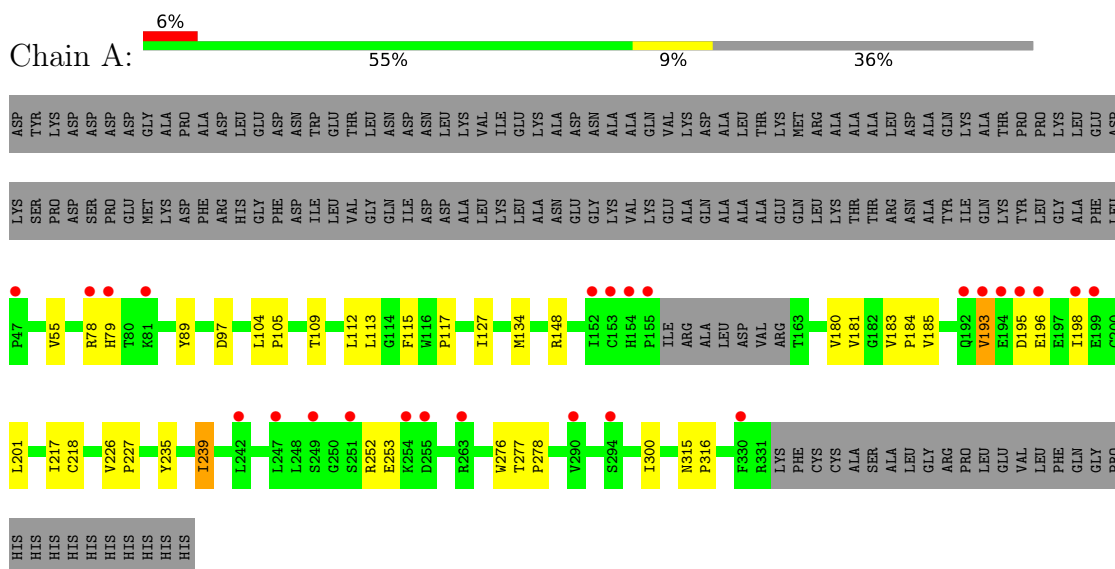
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	2	Total	O	0	0
			2	2		

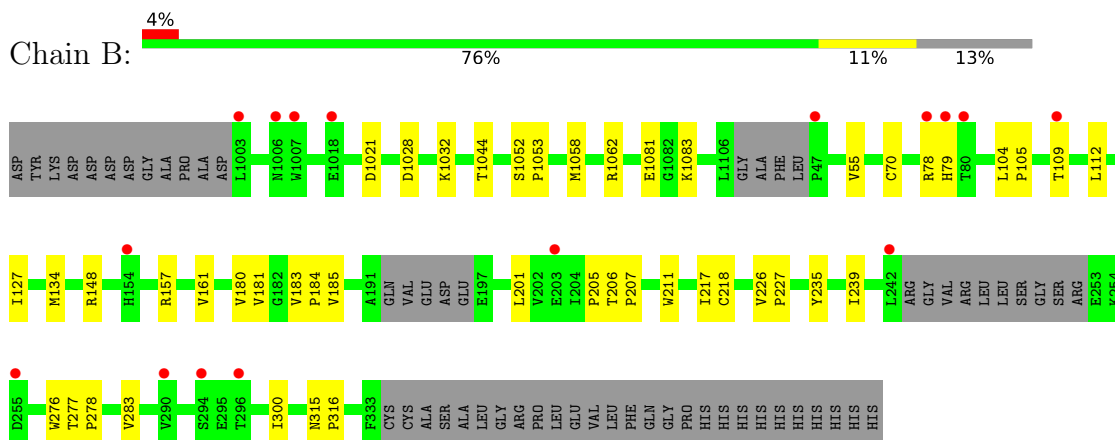
### 3 Residue-property plots

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: Fusion protein of Nociceptin receptor and cytochrome b562



- Molecule 1: Fusion protein of Nociceptin receptor and cytochrome b562



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.11Å 170.94Å 65.35Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	32.02 – 3.01 32.02 – 3.01	Depositor EDS
% Data completeness (in resolution range)	93.1 (32.02-3.01) 93.1 (32.02-3.01)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.248 , 0.288 (Not available) , 0.300	Depositor DCC
$R_{free}$ test set	847 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, ONN, OLB

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	0.30	0/2159	0.72	0/2950
1	B	0.29	0/2950	0.70	0/4015
All	All	0.30	0/5109	0.71	0/6965

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	2113	0	2167	37	0
1	B	2894	0	2978	34	0
2	A	32	0	35	4	0
2	B	32	0	35	5	0
3	A	15	0	19	1	0
4	A	20	0	33	8	0
5	B	16	0	21	0	0
6	A	6	0	0	1	0
6	B	2	0	0	0	0
All	All	5130	0	5288	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (77) 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:157:ARG:O	1:B:161:VAL:HG23	1.77	0.83
1:A:193:VAL:O	1:A:193:VAL:HG13	1.87	0.74
1:B:1028:ASP:OD2	1:B:1032:LYS:NZ	2.31	0.63
1:A:201:LEU:HA	2:A:1501:0NN:H30	1.81	0.62
1:A:113:LEU:HD12	1:A:117:PRO:HG3	1.86	0.58
1:B:180:VAL:O	1:B:184:PRO:HG2	2.06	0.56
1:A:193:VAL:HA	1:A:198:ILE:HA	1.87	0.56
1:A:180:VAL:O	1:A:184:PRO:HG2	2.06	0.56
1:A:183:VAL:HB	1:A:184:PRO:HD3	1.89	0.55
1:B:157:ARG:O	1:B:161:VAL:CG2	2.50	0.54
1:B:183:VAL:HB	1:B:184:PRO:HD3	1.89	0.54
1:A:235:TYR:O	1:A:239:ILE:HG13	2.09	0.53
1:A:113:LEU:HD11	4:A:1503:OLA:H112	1.91	0.52
1:B:205:PRO:HG2	1:B:211:TRP:CG	2.44	0.52
4:A:1503:OLA:H122	1:B:70:CYS:CB	2.40	0.52
1:A:55:VAL:HG11	4:A:1503:OLA:H183	1.92	0.51
1:A:193:VAL:O	1:A:193:VAL:CG1	2.58	0.51
1:A:115:PHE:CE1	1:A:117:PRO:HB3	2.46	0.50
1:A:105:PRO:O	1:A:109:THR:HG23	2.10	0.50
2:A:1501:0NN:H26	2:A:1501:0NN:N2	2.25	0.50
1:B:1053:PRO:O	1:B:1062:ARG:NH1	2.44	0.50
1:B:104:LEU:N	1:B:105:PRO:CD	2.74	0.49
1:B:1081:GLU:OE1	1:B:1083:LYS:NZ	2.46	0.49
1:A:104:LEU:N	1:A:105:PRO:CD	2.75	0.49
1:B:283:VAL:HG11	2:B:1501:0NN:H34	1.95	0.48
1:A:183:VAL:N	1:A:184:PRO:CD	2.76	0.48
1:A:315:ASN:HB2	1:A:316:PRO:HD3	1.95	0.48
1:A:217:ILE:HG23	1:A:218:CYS:N	2.28	0.48
1:B:226:VAL:HB	1:B:227:PRO:HD3	1.95	0.48
2:B:1501:0NN:H17	2:B:1501:0NN:C27	2.44	0.48
1:B:105:PRO:O	1:B:109:THR:HG23	2.13	0.48
1:A:113:LEU:CD1	1:A:117:PRO:HG3	2.43	0.47
1:A:148:ARG:NE	1:A:148:ARG:HA	2.29	0.47
1:B:183:VAL:N	1:B:184:PRO:CD	2.77	0.47
1:A:113:LEU:HD21	4:A:1503:OLA:H112	1.97	0.46
1:B:217:ILE:HG23	1:B:218:CYS:N	2.30	0.46
1:B:235:TYR:O	1:B:239:ILE:HG12	2.16	0.46
1:A:201:LEU:HD12	1:A:201:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:MET:HE1	1:B:276:TRP:CD2	2.51	0.45
1:B:226:VAL:N	1:B:227:PRO:CD	2.80	0.45
1:A:181:VAL:C	1:A:184:PRO:HD2	2.41	0.45
2:A:1501:0NN:C22	2:A:1501:0NN:C16	2.95	0.45
1:A:226:VAL:HB	1:A:227:PRO:HD3	1.97	0.45
1:B:1021:ASP:N	1:B:1021:ASP:OD1	2.49	0.45
1:A:195:ASP:O	1:A:196:GLU:CB	2.65	0.44
1:B:181:VAL:C	1:B:184:PRO:HD2	2.43	0.44
2:B:1501:0NN:C22	2:B:1501:0NN:C16	2.95	0.44
1:A:55:VAL:CG1	4:A:1503:OLA:H183	2.48	0.43
1:B:148:ARG:HA	1:B:148:ARG:NE	2.33	0.43
1:A:252:ARG:HG3	1:A:253:GLU:N	2.33	0.43
1:B:134:MET:HE1	1:B:276:TRP:CE3	2.53	0.43
1:A:112:LEU:HD12	4:A:1503:OLA:H161	2.01	0.43
1:A:134:MET:HE3	2:A:1501:0NN:H7	2.00	0.43
2:B:1501:0NN:H17	2:B:1501:0NN:H31	2.01	0.43
1:A:117:PRO:HA	4:A:1503:OLA:O2	2.18	0.43
1:A:217:ILE:CG2	1:A:218:CYS:N	2.82	0.43
1:A:115:PHE:O	1:A:117:PRO:HD3	2.19	0.42
1:A:277:THR:HB	1:A:278:PRO:HD3	2.00	0.42
1:B:277:THR:HB	1:B:278:PRO:HD3	2.00	0.42
1:B:55:VAL:HG21	1:B:112:LEU:HG	2.02	0.42
1:B:205:PRO:HG2	1:B:211:TRP:CD1	2.53	0.42
1:A:55:VAL:HG21	1:A:112:LEU:HG	2.01	0.42
1:A:127:ILE:HG22	1:A:185:VAL:HG12	2.02	0.41
1:A:134:MET:HE1	1:A:276:TRP:CD2	2.55	0.41
1:B:315:ASN:HB2	1:B:316:PRO:HD3	2.01	0.41
1:A:89:TYR:OH	3:A:1502:OLB:O25	2.37	0.41
1:A:97:ASP:OD1	6:A:1601:HOH:O	2.22	0.41
4:A:1503:OLA:H122	1:B:70:CYS:HB2	2.02	0.41
1:B:1052:SER:OG	1:B:1053:PRO:HD2	2.21	0.41
1:B:201:LEU:HD12	1:B:201:LEU:C	2.46	0.41
1:B:127:ILE:HG22	1:B:185:VAL:HG12	2.03	0.41
1:B:217:ILE:CG2	1:B:218:CYS:N	2.84	0.41
1:A:78:ARG:O	1:A:79:HIS:C	2.64	0.41
1:B:78:ARG:O	1:B:79:HIS:C	2.64	0.40
2:B:1501:0NN:C27	2:B:1501:0NN:C17	2.99	0.40
1:B:1044:THR:HG22	1:B:1058:MET:CE	2.51	0.40
1:B:206:THR:HG23	1:B:207:PRO:HA	2.04	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	274/434 (63%)	261 (95%)	12 (4%)	1 (0%)	30	63
1	B	368/434 (85%)	354 (96%)	14 (4%)	0	100	100
All	All	642/868 (74%)	615 (96%)	26 (4%)	1 (0%)	43	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL

### 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	228/365 (62%)	226 (99%)	2 (1%)	70	84
1	B	312/365 (86%)	311 (100%)	1 (0%)	86	90
All	All	540/730 (74%)	537 (99%)	3 (1%)	78	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ILE
1	A	300	ILE
1	B	300	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	192	GLN
1	B	1025	GLN
1	B	171	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	OLB	A	1502	-	14,14,24	1.23	1 (7%)	15,15,25	0.99	1 (6%)
4	OLA	A	1503	-	19,19,19	1.79	2 (10%)	19,19,19	0.91	1 (5%)
2	0NN	A	1501	-	36,36,36	3.23	13 (36%)	45,50,50	1.13	5 (11%)
5	OLC	B	1502	-	15,15,24	1.16	1 (6%)	16,16,25	1.01	1 (6%)
2	0NN	B	1501	-	36,36,36	3.25	13 (36%)	45,50,50	1.11	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLB	A	1502	-	-	7/14/14/24	-
4	OLA	A	1503	-	-	5/17/17/17	-
2	0NN	A	1501	-	-	3/15/49/49	0/5/5/5
5	OLC	B	1502	-	-	6/15/15/24	-
2	0NN	B	1501	-	-	3/15/49/49	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	0NN	C2-C1	9.24	1.51	1.39
2	A	1501	0NN	C2-C1	9.12	1.51	1.39
2	B	1501	0NN	C5-C6	7.56	1.51	1.39
2	A	1501	0NN	C5-C6	7.48	1.51	1.39
2	A	1501	0NN	C24-C23	7.36	1.51	1.38
2	B	1501	0NN	C24-C23	7.33	1.51	1.38
4	A	1503	OLA	O1-C1	7.31	1.46	1.22
2	B	1501	0NN	C27-C22	6.11	1.51	1.38
2	A	1501	0NN	C27-C22	6.06	1.50	1.38
2	B	1501	0NN	C16-N2	5.96	1.47	1.33
2	A	1501	0NN	C16-N2	5.95	1.47	1.33
2	A	1501	0NN	C26-C25	5.87	1.51	1.38
2	B	1501	0NN	C26-C25	5.84	1.51	1.38
2	A	1501	0NN	C3-C4	5.31	1.49	1.38
2	B	1501	0NN	C3-C4	5.25	1.49	1.38
3	A	1502	OLB	O20-C1	4.40	1.46	1.33
5	B	1502	OLC	O20-C1	4.31	1.45	1.33
2	B	1501	0NN	C8-C1	2.74	1.53	1.51
2	A	1501	0NN	C8-C1	2.72	1.53	1.51
2	B	1501	0NN	C11-C8	-2.60	1.50	1.53
4	A	1503	OLA	O2-C1	-2.60	1.22	1.30
2	B	1501	0NN	O1-C7	-2.59	1.39	1.44
2	A	1501	0NN	O1-C7	-2.52	1.40	1.44
2	B	1501	0NN	C6-C1	-2.35	1.36	1.39
2	A	1501	0NN	C18-C17	-2.32	1.48	1.53
2	B	1501	0NN	O1-C8	-2.29	1.40	1.45
2	A	1501	0NN	C6-C1	-2.21	1.36	1.39
2	B	1501	0NN	C18-C17	-2.18	1.48	1.53
2	A	1501	0NN	O1-C8	-2.14	1.40	1.45
2	A	1501	0NN	C9-C8	-2.06	1.51	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	0NN	C9-C8-C1	3.17	118.62	112.43
2	B	1501	0NN	C16-C17-N3	3.08	116.33	112.38
2	B	1501	0NN	C9-C8-C1	2.94	118.18	112.43
5	B	1502	OLC	O20-C1-C2	2.73	120.16	111.83
3	A	1502	OLB	O20-C1-C2	2.73	120.16	111.83
2	B	1501	0NN	C17-C16-N2	2.57	121.54	115.99
2	A	1501	0NN	C17-C16-N2	2.38	121.12	115.99
2	A	1501	0NN	C16-C17-N3	2.33	115.37	112.38
2	A	1501	0NN	C7-C6-C1	-2.27	107.64	108.83
4	A	1503	OLA	O2-C1-C2	2.13	120.72	114.00
2	A	1501	0NN	C12-C11-C8	2.10	113.64	111.79
2	B	1501	0NN	C10-C9-C8	2.08	113.62	111.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

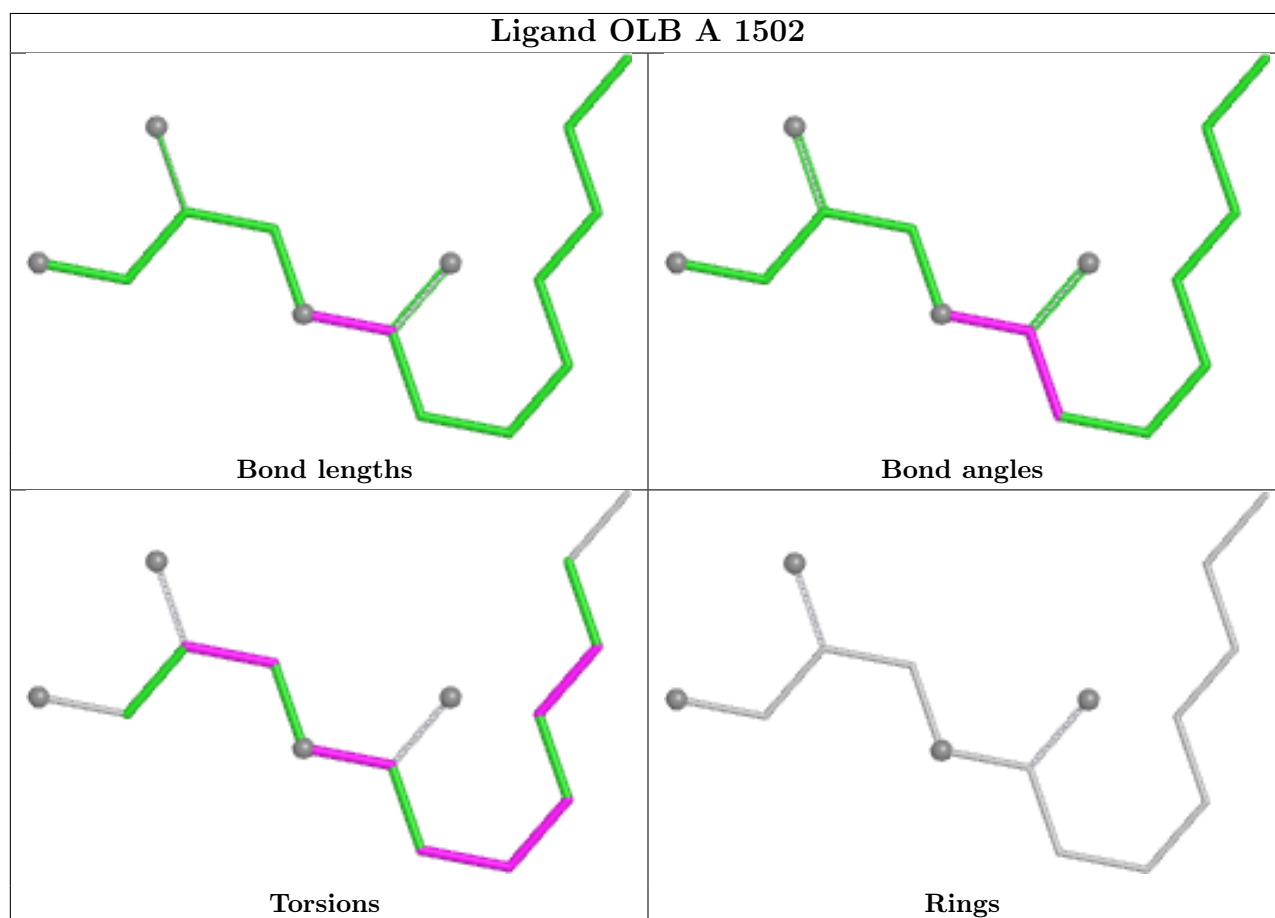
Mol	Chain	Res	Type	Atoms
2	B	1501	0NN	C22-C21-N3-C17
2	B	1501	0NN	C14-C13-N1-C10
3	A	1502	OLB	C1-C2-C3-C4
2	B	1501	0NN	C14-C13-N1-C12
5	B	1502	OLC	O20-C21-C22-O23
4	A	1503	OLA	C3-C4-C5-C6
3	A	1502	OLB	O20-C21-C22-O23
3	A	1502	OLB	O20-C21-C22-C24
4	A	1503	OLA	C13-C14-C15-C16
5	B	1502	OLC	C3-C4-C5-C6
4	A	1503	OLA	C12-C13-C14-C15
3	A	1502	OLB	C4-C5-C6-C7
5	B	1502	OLC	C1-C2-C3-C4
5	B	1502	OLC	O20-C21-C22-C24
5	B	1502	OLC	C5-C6-C7-C8
2	A	1501	0NN	O2-C16-C17-N3
3	A	1502	OLB	C2-C3-C4-C5
5	B	1502	OLC	C6-C7-C8-C9
4	A	1503	OLA	C11-C12-C13-C14
4	A	1503	OLA	C9-C10-C11-C12
2	A	1501	0NN	N2-C16-C17-N3
3	A	1502	OLB	O19-C1-O20-C21
3	A	1502	OLB	C2-C1-O20-C21
2	A	1501	0NN	C22-C21-N3-C17

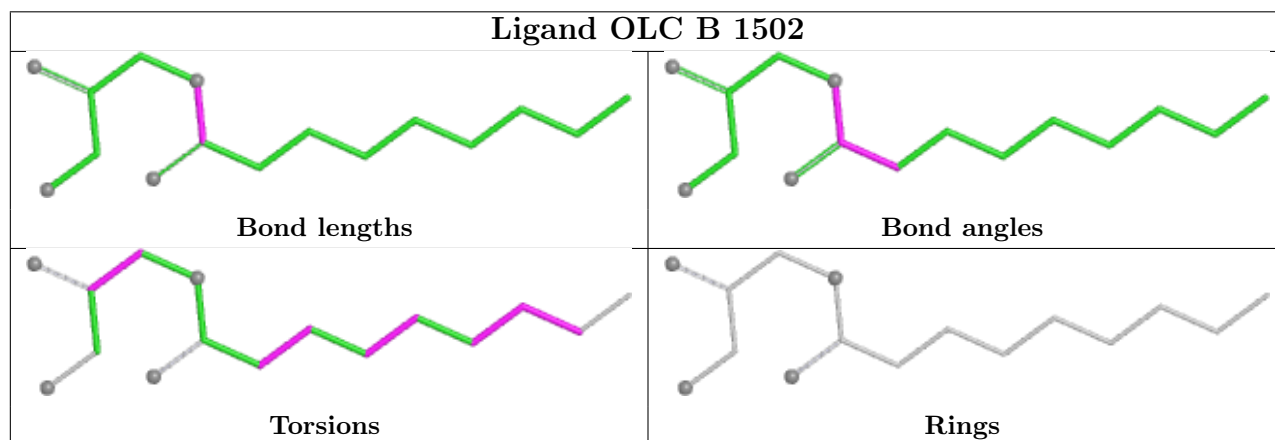
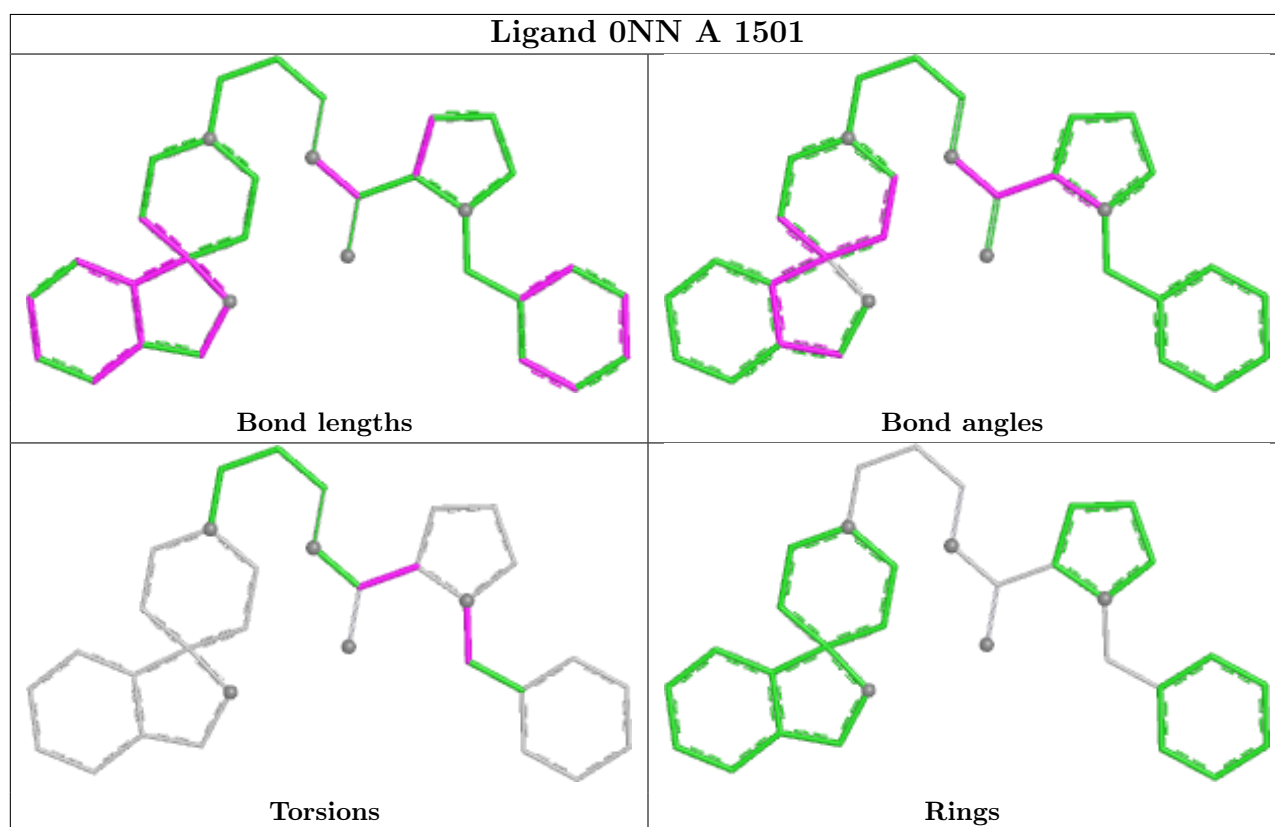
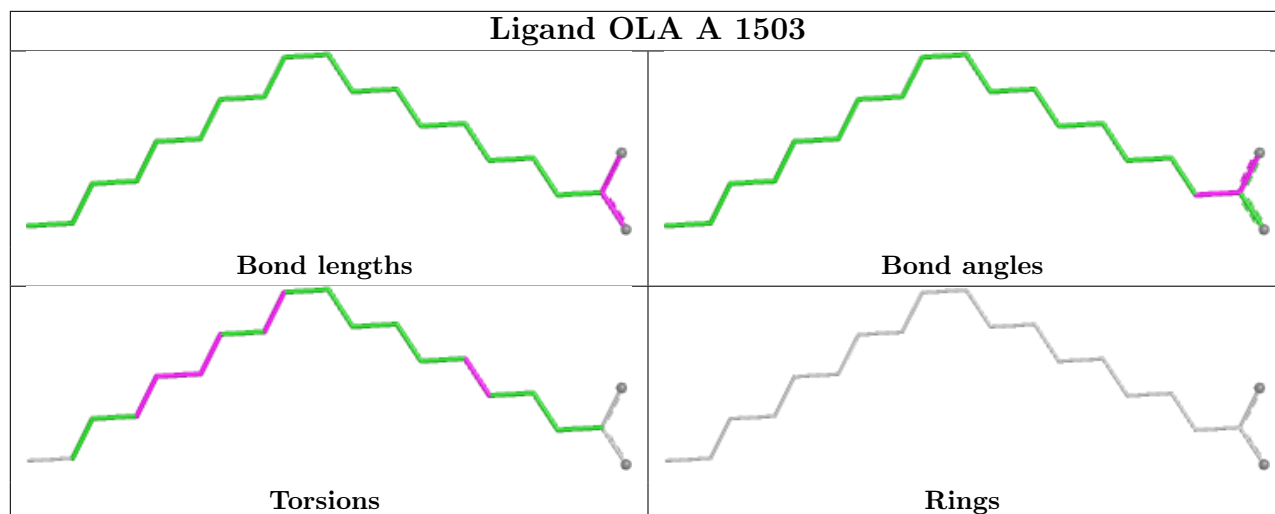
There are no ring outliers.

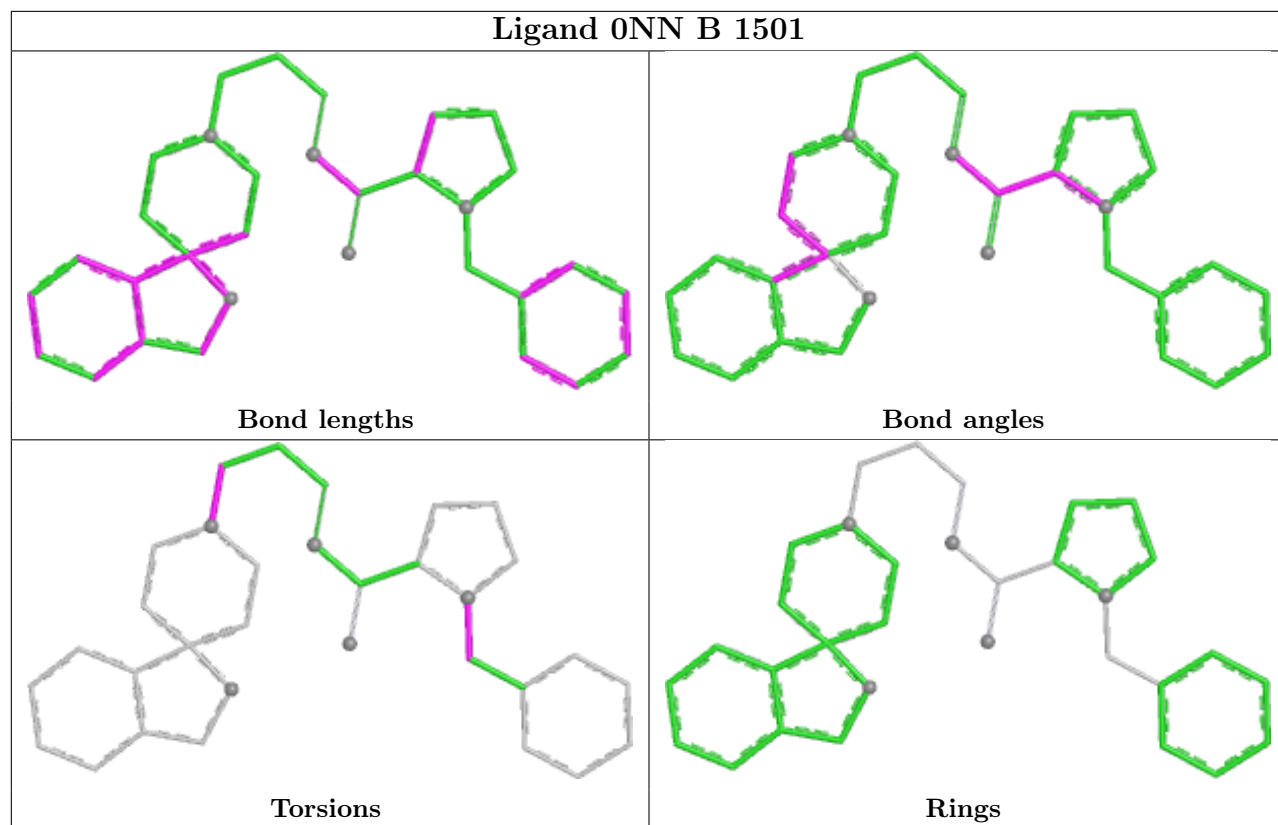
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	OLB	1	0
4	A	1503	OLA	8	0
2	A	1501	0NN	4	0
2	B	1501	0NN	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/434 (64%)	0.44	25 (8%) 15 8	39, 59, 141, 174	0
1	B	376/434 (86%)	0.43	16 (4%) 40 21	31, 69, 113, 156	0
All	All	654/868 (75%)	0.44	41 (6%) 26 13	31, 63, 124, 174	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	HIS	4.9
1	A	193	VAL	4.2
1	B	242	LEU	4.2
1	A	47	PRO	3.6
1	A	330	PHE	3.5
1	A	249	SER	3.5
1	A	290	VAL	3.3
1	B	255	ASP	3.2
1	A	194	GLU	3.2
1	A	263	ARG	3.1
1	A	153	CYS	3.0
1	B	78	ARG	3.0
1	B	80	THR	2.9
1	B	47	PRO	2.8
1	A	247	LEU	2.6
1	A	196	GLU	2.6
1	B	154	HIS	2.5
1	A	242	LEU	2.4
1	A	198	ILE	2.4
1	B	1018	GLU	2.4
1	B	290	VAL	2.4
1	A	81	LYS	2.4
1	A	154	HIS	2.3
1	B	1007	TRP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	296	THR	2.3
1	B	1003	LEU	2.3
1	A	195	ASP	2.3
1	A	152	ILE	2.2
1	A	78	ARG	2.2
1	A	79	HIS	2.2
1	A	251	SER	2.2
1	B	109	THR	2.2
1	A	155	PRO	2.2
1	B	203	GLU	2.1
1	B	1006	ASN	2.1
1	A	199	GLU	2.1
1	A	294	SER	2.1
1	A	254	LYS	2.1
1	A	255	ASP	2.1
1	B	294	SER	2.0
1	A	192	GLN	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](#)

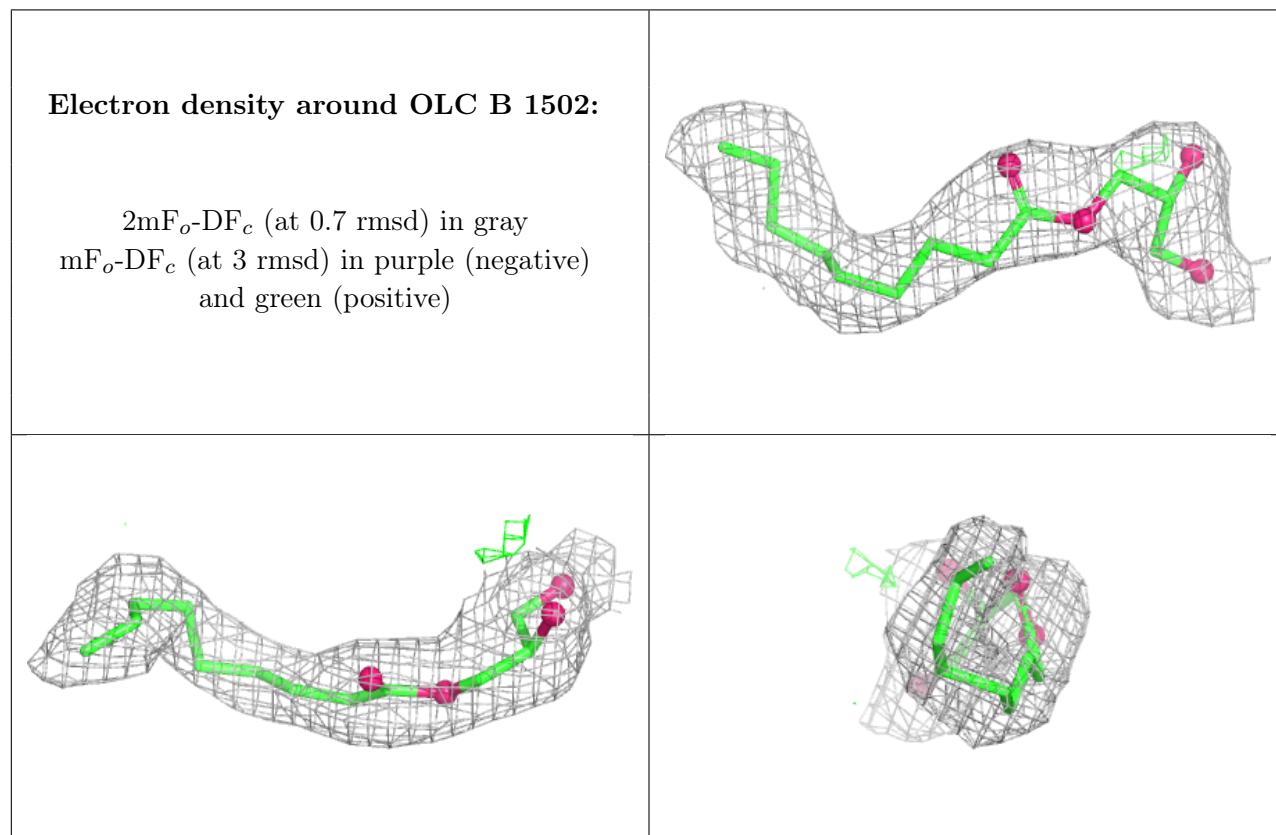
There are no oligosaccharides in this entry.

## 6.4 Ligands [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<sup>th</sup> 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.

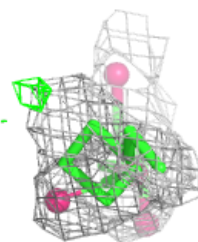
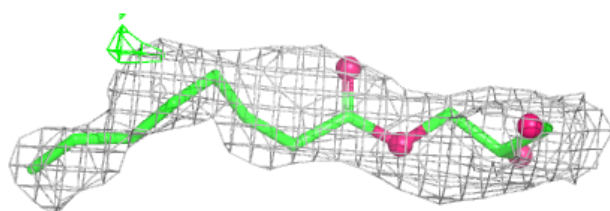
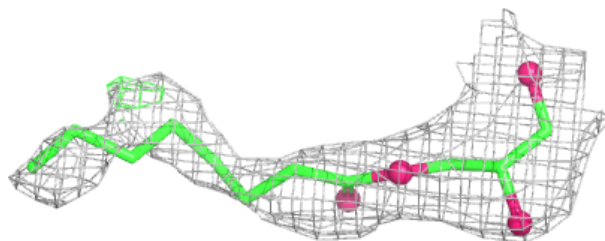
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OLC	B	1502	16/25	0.87	0.15	48,59,62,63	0
3	OLB	A	1502	15/25	0.88	0.21	76,91,96,96	0
4	OLA	A	1503	20/20	0.89	0.15	46,69,91,94	0
2	0NN	B	1501	32/32	0.92	0.13	50,60,70,71	0
2	0NN	A	1501	32/32	0.92	0.15	50,61,79,81	0

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.

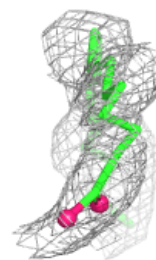
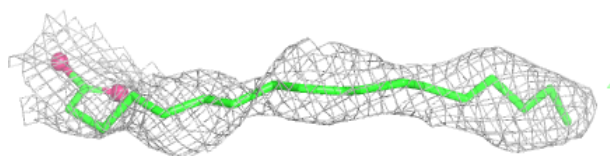
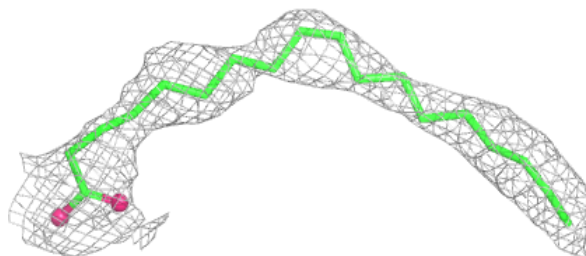


**Electron density around OLB A 1502:**

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

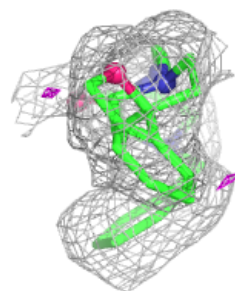
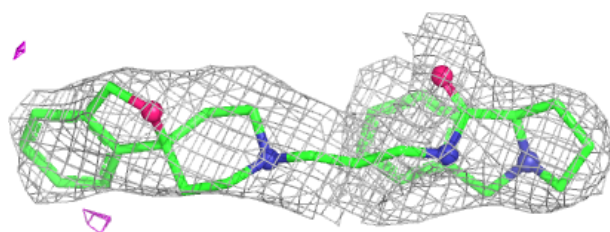
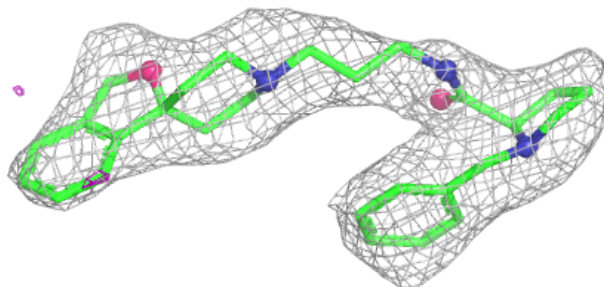
**Electron density around OLA A 1503:**

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

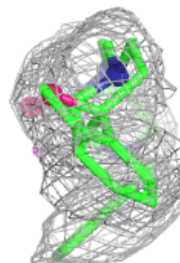
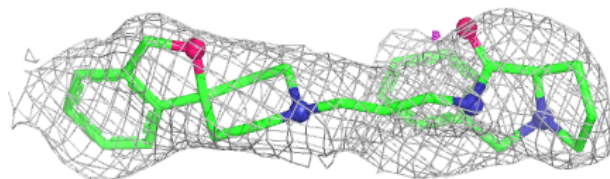
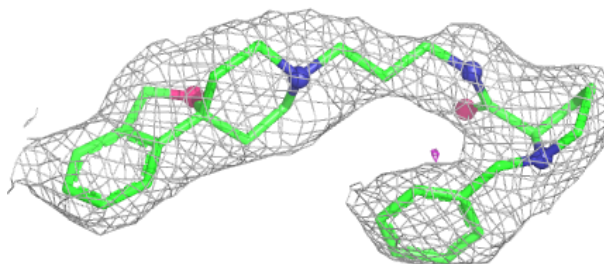


**Electron density around 0NN B 1501:**

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

**Electron density around 0NN A 1501:**

$2mF_o-DF_c$  (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.