



## Full wwPDB EM Validation Report ⓘ

Mar 15, 2023 – 02:18 PM EDT

PDB ID : 8FYN  
EMDB ID : EMD-29586  
Title : MicroED structure of A2A from plasma milled lamellae  
Authors : Martynowycz, M.W.; Shiriaeva, A.; Clabbers, M.T.B.; Nicolas, W.J.; Weaver, S.J.; Hattne, J.; Gonen, T.  
Deposited on : 2023-01-26  
Resolution : 2.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

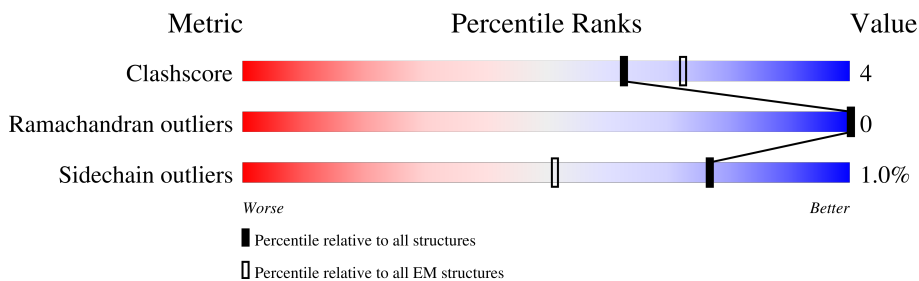
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 2.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7345 atoms, of which 3723 are hydrogens and 0 are deuteriums.

In the tables below, 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 Adenosine receptor A2a,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	390	6104	1965	3092	507	519	21	0	0

There are 39 discrepancies between the modelled and reference sequences:

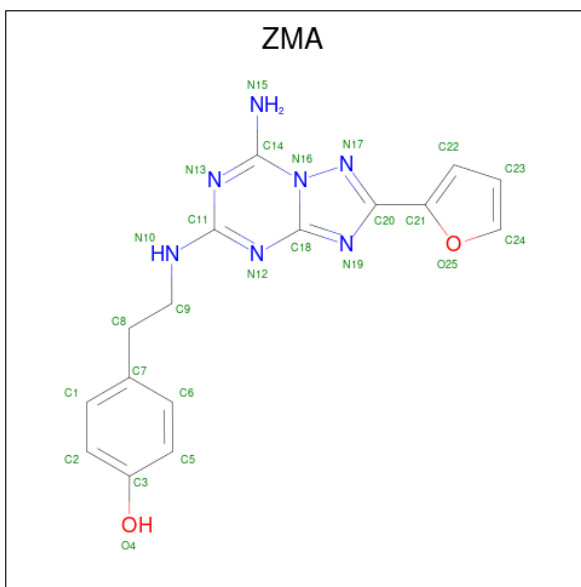
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	LEU	GLY	conflict	UNP P29274
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl}phenol (three-letter code: ZMA) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).



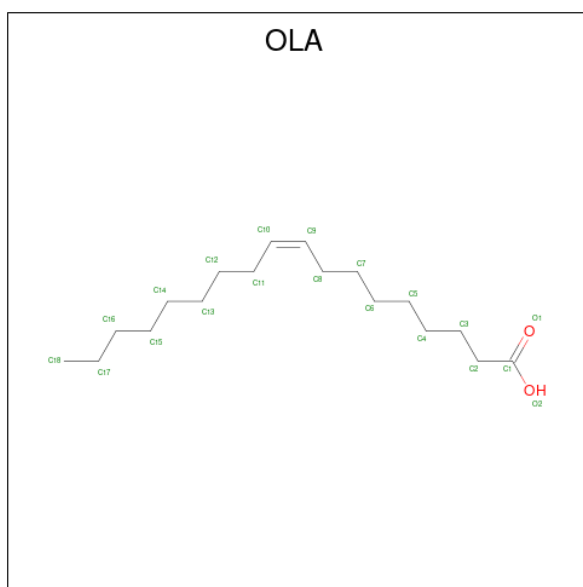
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
2	A	1	40	16	15	7	2	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			74	27	46	1	
3	A	1	Total	C	H	O	0
			74	27	46	1	
3	A	1	Total	C	H	O	0
			74	27	46	1	

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



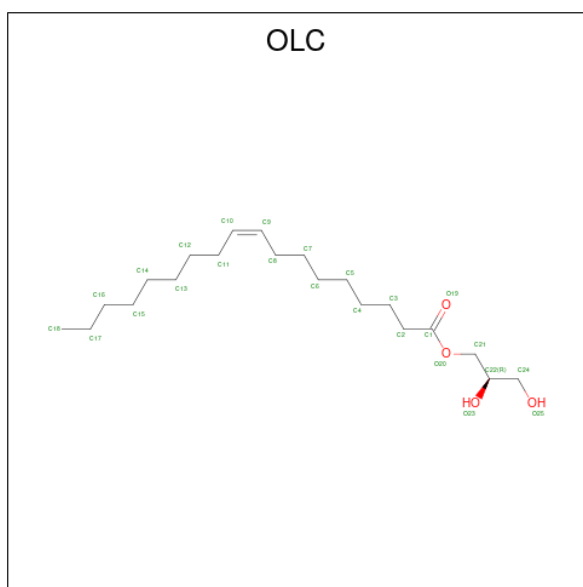
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			53	18	33	2	

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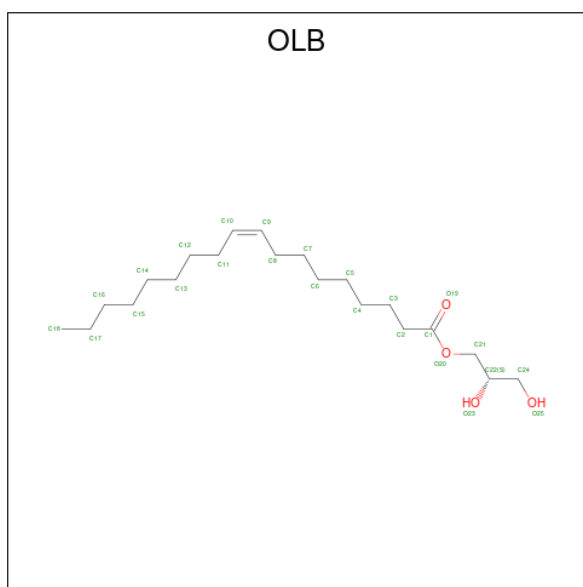
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	37	13	22	2	0
4	A	1	26	9	15	2	0
4	A	1	49	17	30	2	0
4	A	1	26	9	15	2	0
4	A	1	21	7	12	2	0
4	A	1	18	6	10	2	0
4	A	1	24	8	14	2	0
4	A	1	21	7	12	2	0
4	A	1	28	10	16	2	0
4	A	1	46	16	28	2	0
4	A	1	53	18	33	2	0
4	A	1	53	18	33	2	0
4	A	1	37	13	22	2	0
4	A	1	49	17	30	2	0

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
5	A	1	39	13	22	4	0
5	A	1	55	18	33	4	0
5	A	1	39	13	22	4	0
5	A	1	36	11	21	4	0
5	A	1	52	17	31	4	0

- Molecule 6 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		O
6	A	1	42	14	24	4	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
7	A	1	1	1	0

- Molecule 8 is water.

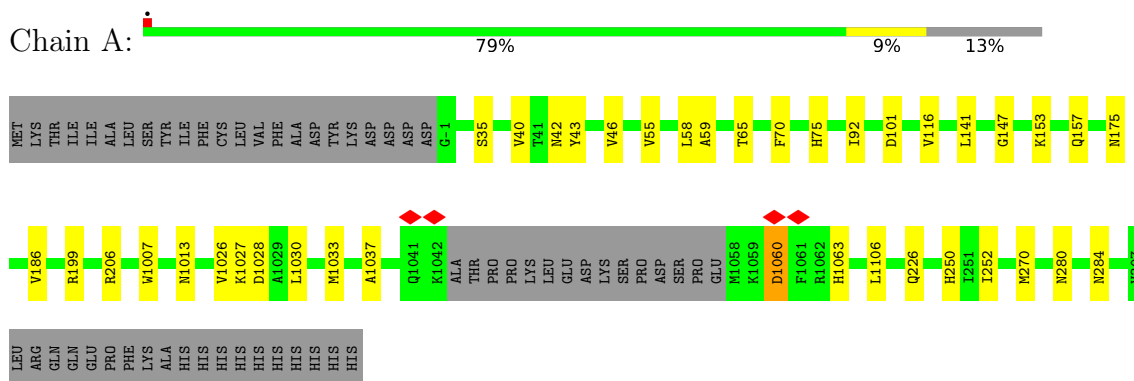
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	A	174	174	174	0



### 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Adenosine receptor A2a,Soluble cytochrome b562



## 4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a=39.08 \text{ \AA}$ , $b=177.51 \text{ \AA}$ , $c=139.29 \text{ \AA}$ , $\alpha=90^\circ$ , $\beta=90^\circ$ , $\gamma=90^\circ$ , space group=20	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	0.001	Depositor
Minimum defocus (nm)	0	Depositor
Maximum defocus (nm)	0	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.347	Depositor
Minimum map value	-4.061	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.932	Depositor
Recommended contour level	1.0	Depositor
Map size ( $\text{\AA}$ )	39.08, 175.86002, 139.29	wwPDB
Map dimensions	118, 221, 145	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.48850003, 0.48850006, 0.4836458	Depositor

## 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, CLR, NA, OLA, OLB, ZMA

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	0.24	0/3075	0.45	2/4181 (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	A	157	GLN	CB-CA-C	5.68	121.77	110.40
1	A	1060	ASP	CB-CA-C	5.66	121.72	110.40

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	3012	3092	3064	30	1
2	A	25	15	15	1	0
3	A	84	138	138	1	0
4	A	216	325	304	1	0
5	A	92	129	114	1	0
6	A	18	24	23	0	0
7	A	1	0	0	0	0
8	A	174	0	0	13	2
All	All	3622	3723	3658	31	2

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 (31) 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:141:LEU:O	8:A:2501:HOH:O	1.82	0.96
1:A:280:ASN:O	8:A:2504:HOH:O	1.99	0.81
4:A:2419:OLA:O2	8:A:2505:HOH:O	2.02	0.77
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.71	0.73
1:A:199:ARG:NH2	8:A:2511:HOH:O	2.28	0.66
1:A:1106:LEU:HD21	8:A:2517:HOH:O	1.99	0.62
1:A:147:GLY:N	8:A:2506:HOH:O	2.19	0.60
1:A:75:HIS:HB3	8:A:2522:HOH:O	2.02	0.58
1:A:92:ILE:CD1	1:A:186:VAL:HG22	2.38	0.53
1:A:101:ASP:OD1	1:A:116:VAL:HG11	2.08	0.53
1:A:284:ASN:ND2	8:A:2515:HOH:O	2.34	0.52
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.45	0.52
1:A:250:HIS:CE1	2:A:2401:ZMA:H24	2.46	0.50
1:A:1060:ASP:HA	1:A:1063:HIS:HB3	1.94	0.50
1:A:65:THR:HG22	1:A:70:PHE:CE1	2.48	0.48
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.41	0.48
1:A:199:ARG:CZ	8:A:2511:HOH:O	2.61	0.46
1:A:58:LEU:HD21	3:A:2402:CLR:H272	1.99	0.45
1:A:1026:VAL:HG12	1:A:1030:LEU:HD12	2.00	0.43
1:A:252:ILE:HG21	1:A:270:MET:SD	2.58	0.43
1:A:1007:TRP:CD2	1:A:1106:LEU:HD22	2.53	0.43
1:A:1013:ASN:N	1:A:1013:ASN:HD22	2.16	0.42
1:A:199:ARG:NE	8:A:2511:HOH:O	2.53	0.41
1:A:226:GLN:HB3	8:A:2534:HOH:O	2.19	0.41
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.01	0.41
1:A:40:VAL:N	8:A:2512:HOH:O	2.54	0.41
1:A:42:ASN:O	1:A:46:VAL:HG23	2.20	0.41
1:A:65:THR:HG21	5:A:2421:OLC:H5	2.01	0.41
1:A:1033:MET:O	1:A:1037:ALA:N	2.49	0.40
1:A:153:LYS:HD2	1:A:153:LYS:O	2.21	0.40
1:A:206:ARG:NE	8:A:2509:HOH:O	2.23	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2592:HOH:O	8:A:2626:HOH:O[5_545]	1.97	0.23
1:A:175:ASN:O	8:A:2501:HOH:O[3_555]	2.15	0.05

### 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 PDB entries followed by that with respect to all EM entries.

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	382/447 (86%)	374 (98%)	8 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

#### 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 PDB entries followed by that with respect to all EM entries.

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	314/374 (84%)	311 (99%)	3 (1%)	<a href="#">76</a> <a href="#">81</a>

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

Mol	Chain	Res	Type
1	A	35	SER
1	A	1027	LYS
1	A	1028	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	157	GLN
1	A	1011	ASN
1	A	1013	ASN
1	A	1025	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	OLA	A	2417	-	19,19,19	0.79	1 (5%)	19,19,19	0.91	1 (5%)
3	CLR	A	2403	-	31,31,31	0.34	0	48,48,48	0.52	0
5	OLC	A	2424	-	14,14,24	1.17	1 (7%)	15,15,25	1.06	1 (6%)
4	OLA	A	2406	-	14,14,19	0.92	1 (7%)	14,14,19	1.01	1 (7%)
6	OLB	A	2423	-	17,17,24	0.38	0	18,18,25	0.41	0
3	CLR	A	2402	-	31,31,31	0.35	0	48,48,48	0.48	0
4	OLA	A	2410	-	8,8,19	0.69	0	8,8,19	1.27	1 (12%)
4	OLA	A	2415	-	17,17,19	0.83	1 (5%)	17,17,19	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ZMA	A	2401	-	21,28,28	2.14	2 (9%)	20,39,39	1.58	4 (20%)
4	OLA	A	2407	-	10,10,19	0.63	0	10,10,19	1.12	1 (10%)
4	OLA	A	2414	-	11,11,19	1.04	1 (9%)	11,11,19	1.12	0
4	OLA	A	2411	-	7,7,19	0.75	0	7,7,19	1.30	1 (14%)
4	OLA	A	2409	-	10,10,19	0.63	0	10,10,19	1.16	1 (10%)
4	OLA	A	2419	-	18,18,19	0.80	1 (5%)	18,18,19	0.92	1 (5%)
5	OLC	A	2420	-	15,15,24	1.43	2 (13%)	15,15,25	1.00	1 (6%)
4	OLA	A	2408	-	18,18,19	0.82	1 (5%)	18,18,19	0.86	0
4	OLA	A	2418	-	14,14,19	0.91	1 (7%)	14,14,19	1.00	1 (7%)
4	OLA	A	2405	-	19,19,19	0.79	1 (5%)	19,19,19	0.94	0
5	OLC	A	2421	-	21,21,24	1.08	1 (4%)	22,22,25	1.48	2 (9%)
4	OLA	A	2416	-	19,19,19	0.79	1 (5%)	19,19,19	0.91	1 (5%)
5	OLC	A	2422	-	15,15,24	1.42	2 (13%)	15,15,25	0.97	1 (6%)
4	OLA	A	2412	-	9,9,19	0.66	0	9,9,19	1.16	0
5	OLC	A	2425	-	19,19,24	1.15	1 (5%)	19,19,25	0.99	1 (5%)
4	OLA	A	2413	-	8,8,19	0.70	0	8,8,19	1.23	0
3	CLR	A	2404	-	31,31,31	0.35	0	48,48,48	0.49	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
4	OLA	A	2417	-	-	9/17/17/17	-
3	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	OLC	A	2424	-	-	5/14/14/24	-
4	OLA	A	2406	-	-	7/12/12/17	-
6	OLB	A	2423	-	-	7/17/17/24	-
3	CLR	A	2402	-	-	3/10/68/68	0/4/4/4
4	OLA	A	2410	-	-	1/6/6/17	-
4	OLA	A	2415	-	-	7/15/15/17	-
2	ZMA	A	2401	-	-	0/6/10/10	0/4/4/4
4	OLA	A	2407	-	-	6/8/8/17	-
4	OLA	A	2414	-	-	5/9/9/17	-
4	OLA	A	2411	-	-	1/5/5/17	-
4	OLA	A	2409	-	-	2/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2419	-	-	8/16/16/17	-
5	OLC	A	2420	-	-	7/14/14/24	-
4	OLA	A	2408	-	-	11/16/16/17	-
4	OLA	A	2418	-	-	5/12/12/17	-
4	OLA	A	2405	-	-	8/17/17/17	-
5	OLC	A	2421	-	-	12/21/21/24	-
4	OLA	A	2416	-	-	9/17/17/17	-
5	OLC	A	2422	-	-	7/14/14/24	-
4	OLA	A	2412	-	-	4/7/7/17	-
5	OLC	A	2425	-	-	5/17/17/24	-
4	OLA	A	2413	-	-	5/6/6/17	-
3	CLR	A	2404	-	-	1/10/68/68	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	ZMA	C11-N10	7.33	1.45	1.34
2	A	2401	ZMA	C14-N15	5.52	1.45	1.34
5	A	2420	OLC	C11-C10	-3.27	1.34	1.50
5	A	2422	OLC	C11-C10	-3.27	1.34	1.50
5	A	2425	OLC	O20-C1	2.91	1.41	1.33
5	A	2422	OLC	O20-C1	2.90	1.41	1.33
5	A	2421	OLC	O20-C1	2.88	1.41	1.33
5	A	2420	OLC	O20-C1	2.87	1.41	1.33
5	A	2424	OLC	O20-C1	2.85	1.41	1.33
4	A	2405	OLA	C10-C9	2.78	1.47	1.31
4	A	2414	OLA	C10-C9	2.78	1.47	1.28
4	A	2406	OLA	C10-C9	2.75	1.47	1.31
4	A	2408	OLA	C10-C9	2.74	1.47	1.31
4	A	2417	OLA	C10-C9	2.71	1.47	1.31
4	A	2416	OLA	C10-C9	2.71	1.47	1.31
4	A	2418	OLA	C10-C9	2.71	1.47	1.31
4	A	2415	OLA	C10-C9	2.70	1.47	1.31
4	A	2419	OLA	C10-C9	2.69	1.47	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2421	OLC	C8-C9-C10	5.06	163.53	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ZMA	N12-C11-N13	-3.77	120.27	126.23
2	A	2401	ZMA	N15-C14-N16	2.73	119.81	117.97
5	A	2424	OLC	O20-C1-C2	2.63	120.17	111.91
2	A	2401	ZMA	N15-C14-N13	2.61	120.47	117.03
5	A	2420	OLC	O20-C1-C2	2.54	119.86	111.91
5	A	2421	OLC	O20-C1-C2	2.53	119.83	111.91
5	A	2422	OLC	O20-C1-C2	2.46	119.62	111.91
5	A	2425	OLC	O20-C1-C2	2.45	119.58	111.91
2	A	2401	ZMA	C9-N10-C11	-2.25	119.85	123.75
4	A	2419	OLA	O2-C1-C2	2.08	120.71	114.03
4	A	2410	OLA	O2-C1-C2	2.07	120.67	114.03
4	A	2409	OLA	O2-C1-C2	2.05	120.61	114.03
4	A	2416	OLA	O2-C1-C2	2.05	120.61	114.03
4	A	2417	OLA	O2-C1-C2	2.04	120.59	114.03
4	A	2418	OLA	O2-C1-C2	2.04	120.59	114.03
4	A	2406	OLA	O2-C1-C2	2.03	120.57	114.03
4	A	2411	OLA	O2-C1-C2	2.03	120.55	114.03
4	A	2407	OLA	O2-C1-C2	2.02	120.53	114.03

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2420	OLC	C21-C22-C24-O25
5	A	2421	OLC	O20-C21-C22-C24
5	A	2421	OLC	O20-C21-C22-O23
5	A	2422	OLC	O20-C21-C22-C24
5	A	2422	OLC	O20-C21-C22-O23
5	A	2424	OLC	C21-C22-C24-O25
5	A	2425	OLC	C21-C22-C24-O25
6	A	2423	OLB	O20-C21-C22-O23
6	A	2423	OLB	C2-C1-O20-C21
4	A	2419	OLA	C11-C10-C9-C8
5	A	2421	OLC	C2-C1-O20-C21
5	A	2421	OLC	O19-C1-O20-C21
6	A	2423	OLB	O19-C1-O20-C21
5	A	2425	OLC	C2-C1-O20-C21
5	A	2425	OLC	O19-C1-O20-C21
5	A	2420	OLC	C2-C1-O20-C21
5	A	2424	OLC	C2-C1-O20-C21
3	A	2404	CLR	C22-C23-C24-C25
4	A	2406	OLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	2408	OLA	C1-C2-C3-C4
5	A	2424	OLC	O23-C22-C24-O25
5	A	2425	OLC	O23-C22-C24-O25
4	A	2405	OLA	C1-C2-C3-C4
4	A	2413	OLA	C1-C2-C3-C4
4	A	2407	OLA	C1-C2-C3-C4
3	A	2402	CLR	C22-C23-C24-C25
5	A	2424	OLC	O19-C1-O20-C21
5	A	2420	OLC	O19-C1-O20-C21
4	A	2415	OLA	C11-C10-C9-C8
4	A	2415	OLA	C11-C12-C13-C14
4	A	2408	OLA	C2-C3-C4-C5
5	A	2420	OLC	C1-C2-C3-C4
6	A	2423	OLB	C5-C6-C7-C8
4	A	2405	OLA	C3-C4-C5-C6
4	A	2417	OLA	C11-C12-C13-C14
3	A	2402	CLR	C21-C20-C22-C23
4	A	2410	OLA	C1-C2-C3-C4
4	A	2412	OLA	C1-C2-C3-C4
5	A	2420	OLC	O23-C22-C24-O25
4	A	2415	OLA	C3-C4-C5-C6
5	A	2421	OLC	C1-C2-C3-C4
4	A	2408	OLA	C11-C12-C13-C14
4	A	2419	OLA	C3-C4-C5-C6
4	A	2408	OLA	C6-C7-C8-C9
5	A	2421	OLC	C6-C7-C8-C9
4	A	2417	OLA	C1-C2-C3-C4
5	A	2422	OLC	C2-C1-O20-C21
4	A	2414	OLA	C3-C4-C5-C6
5	A	2422	OLC	C4-C5-C6-C7
4	A	2409	OLA	C1-C2-C3-C4
4	A	2406	OLA	C3-C4-C5-C6
4	A	2419	OLA	C6-C7-C8-C9
4	A	2419	OLA	C10-C11-C12-C13
4	A	2407	OLA	C4-C5-C6-C7
4	A	2414	OLA	C6-C7-C8-C9
5	A	2422	OLC	O19-C1-O20-C21
4	A	2417	OLA	C11-C10-C9-C8
6	A	2423	OLB	C2-C3-C4-C5
4	A	2416	OLA	C5-C6-C7-C8
4	A	2412	OLA	C4-C5-C6-C7
4	A	2416	OLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	A	2420	OLC	C3-C4-C5-C6
4	A	2407	OLA	C6-C7-C8-C9
4	A	2408	OLA	C11-C10-C9-C8
4	A	2418	OLA	C11-C10-C9-C8
5	A	2421	OLC	C5-C6-C7-C8
5	A	2425	OLC	C15-C16-C17-C18
5	A	2421	OLC	C3-C4-C5-C6
4	A	2414	OLA	C1-C2-C3-C4
4	A	2411	OLA	C3-C4-C5-C6
4	A	2408	OLA	C13-C14-C15-C16
4	A	2417	OLA	C5-C6-C7-C8
6	A	2423	OLB	O20-C21-C22-C24
4	A	2408	OLA	C12-C13-C14-C15
5	A	2421	OLC	C7-C8-C9-C10
4	A	2413	OLA	C2-C3-C4-C5
5	A	2422	OLC	C3-C4-C5-C6
4	A	2415	OLA	C1-C2-C3-C4
4	A	2409	OLA	C4-C5-C6-C7
4	A	2407	OLA	C3-C4-C5-C6
4	A	2416	OLA	C11-C12-C13-C14
5	A	2421	OLC	C11-C12-C13-C14
5	A	2420	OLC	C2-C3-C4-C5
4	A	2416	OLA	C13-C14-C15-C16
4	A	2416	OLA	C10-C11-C12-C13
4	A	2406	OLA	C7-C8-C9-C10
4	A	2405	OLA	C11-C10-C9-C8
4	A	2407	OLA	O1-C1-C2-C3
4	A	2406	OLA	C11-C10-C9-C8
4	A	2418	OLA	O1-C1-C2-C3
4	A	2408	OLA	C7-C8-C9-C10
4	A	2405	OLA	O1-C1-C2-C3
4	A	2408	OLA	C4-C5-C6-C7
4	A	2417	OLA	C3-C4-C5-C6
4	A	2406	OLA	O1-C1-C2-C3
4	A	2405	OLA	O2-C1-C2-C3
4	A	2414	OLA	C4-C5-C6-C7
4	A	2418	OLA	O2-C1-C2-C3
4	A	2418	OLA	C1-C2-C3-C4
5	A	2422	OLC	C2-C3-C4-C5
4	A	2407	OLA	O2-C1-C2-C3
4	A	2412	OLA	O2-C1-C2-C3
4	A	2406	OLA	O2-C1-C2-C3

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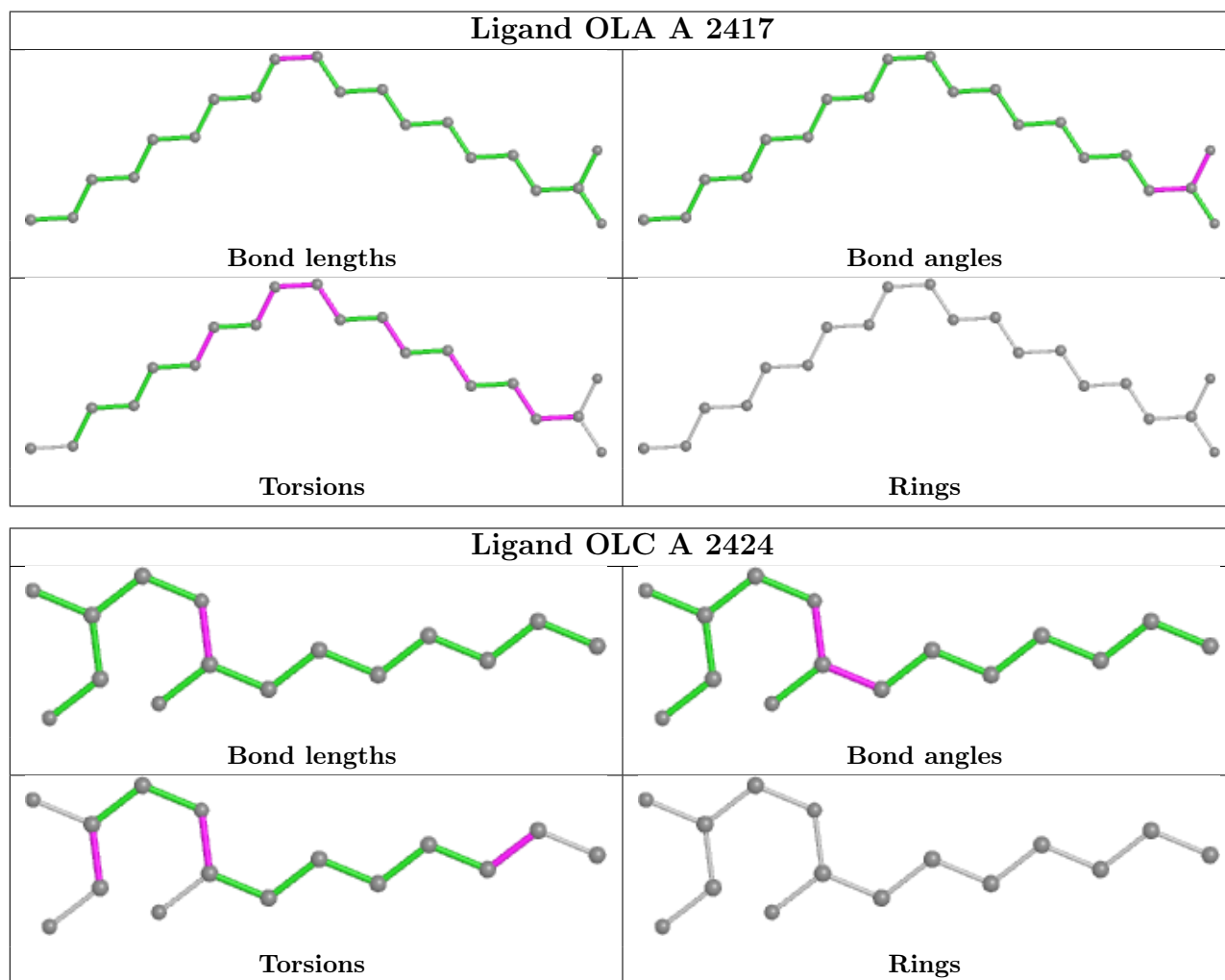
Mol	Chain	Res	Type	Atoms
4	A	2406	OLA	C4-C5-C6-C7
4	A	2417	OLA	O2-C1-C2-C3
5	A	2421	OLC	C21-C22-C24-O25
4	A	2417	OLA	C9-C10-C11-C12
4	A	2412	OLA	O1-C1-C2-C3
4	A	2416	OLA	C9-C10-C11-C12
5	A	2421	OLC	O23-C22-C24-O25
4	A	2416	OLA	O1-C1-C2-C3
4	A	2405	OLA	C10-C11-C12-C13
4	A	2413	OLA	C4-C5-C6-C7
4	A	2415	OLA	C7-C8-C9-C10
4	A	2415	OLA	C2-C3-C4-C5
4	A	2413	OLA	O2-C1-C2-C3
4	A	2416	OLA	C12-C13-C14-C15
4	A	2415	OLA	C9-C10-C11-C12
4	A	2417	OLA	C7-C8-C9-C10
4	A	2418	OLA	C7-C8-C9-C10
4	A	2419	OLA	O1-C1-C2-C3
4	A	2419	OLA	O2-C1-C2-C3
4	A	2417	OLA	O1-C1-C2-C3
4	A	2405	OLA	C14-C15-C16-C17
5	A	2424	OLC	C5-C6-C7-C8
4	A	2413	OLA	O1-C1-C2-C3
3	A	2402	CLR	C23-C24-C25-C26
4	A	2416	OLA	O2-C1-C2-C3
4	A	2419	OLA	C7-C8-C9-C10
6	A	2423	OLB	C21-C22-C24-O25
4	A	2405	OLA	C4-C5-C6-C7
4	A	2408	OLA	O2-C1-C2-C3
4	A	2419	OLA	C2-C3-C4-C5
4	A	2414	OLA	C7-C8-C9-C10
4	A	2408	OLA	O1-C1-C2-C3

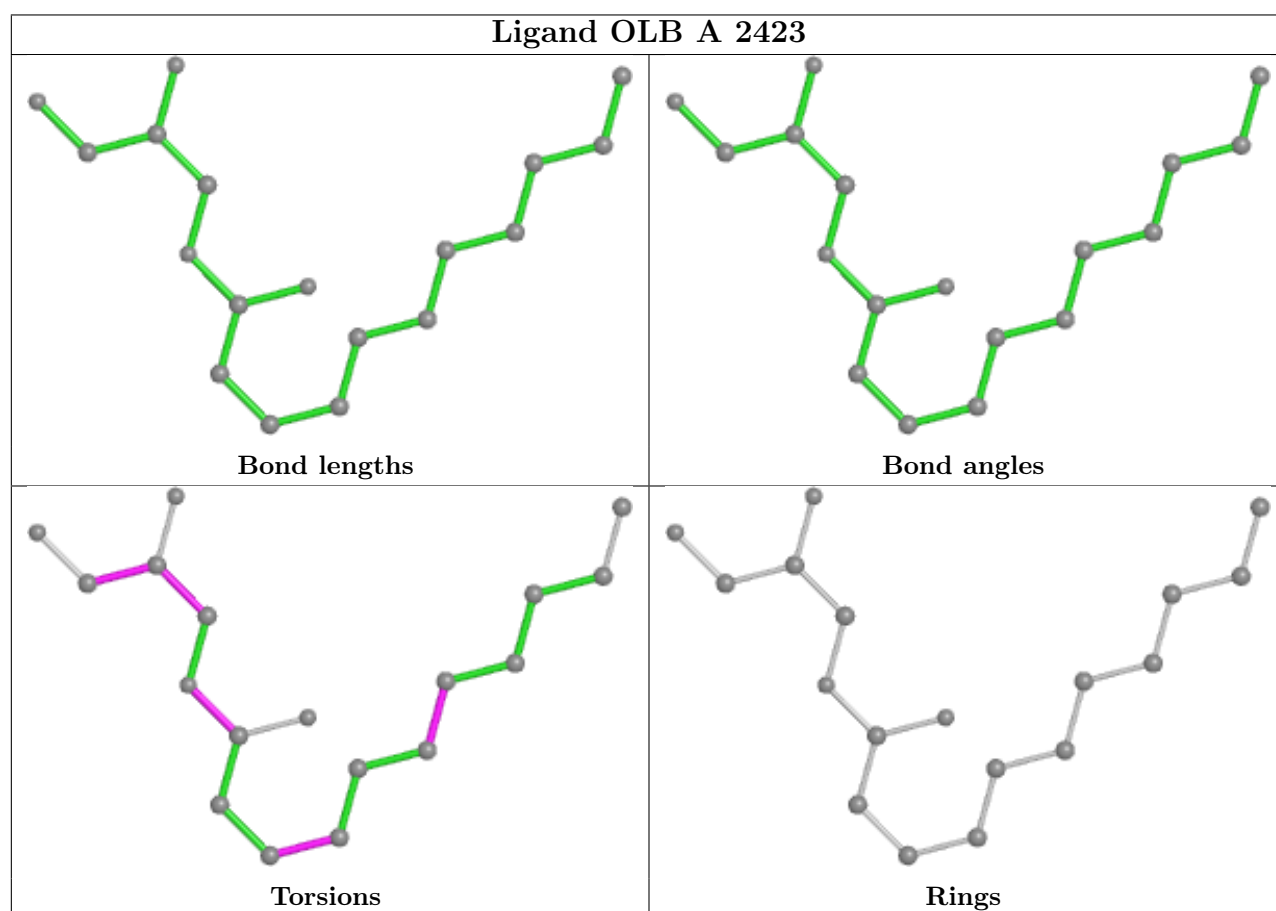
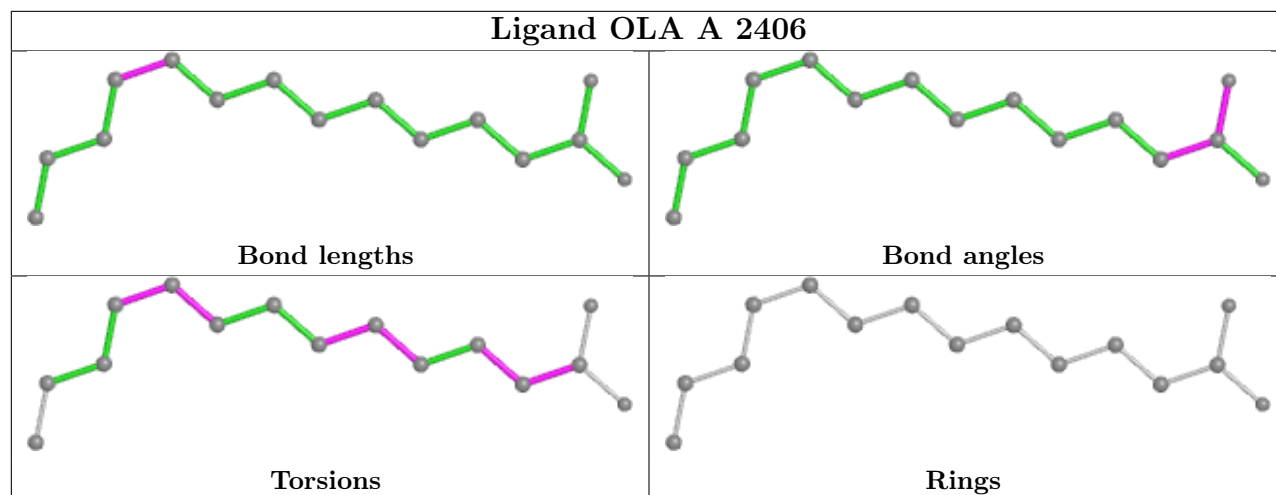
There are no ring outliers.

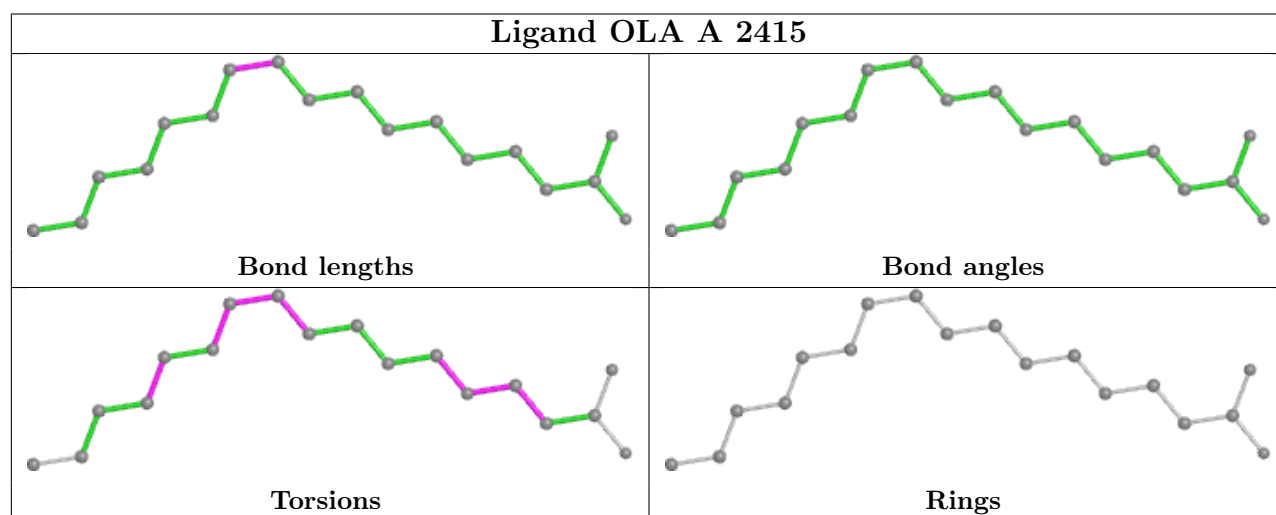
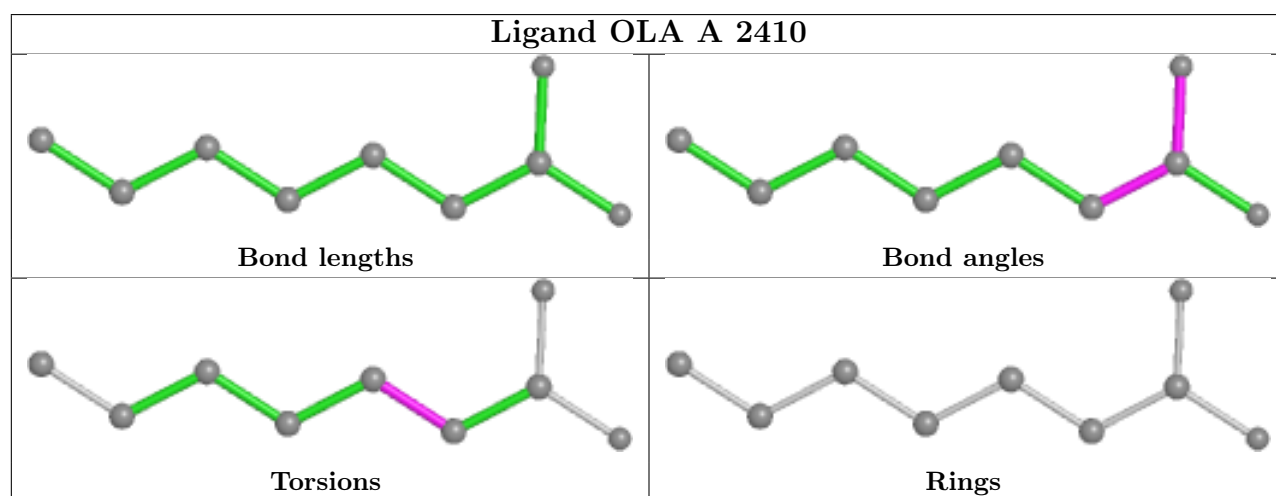
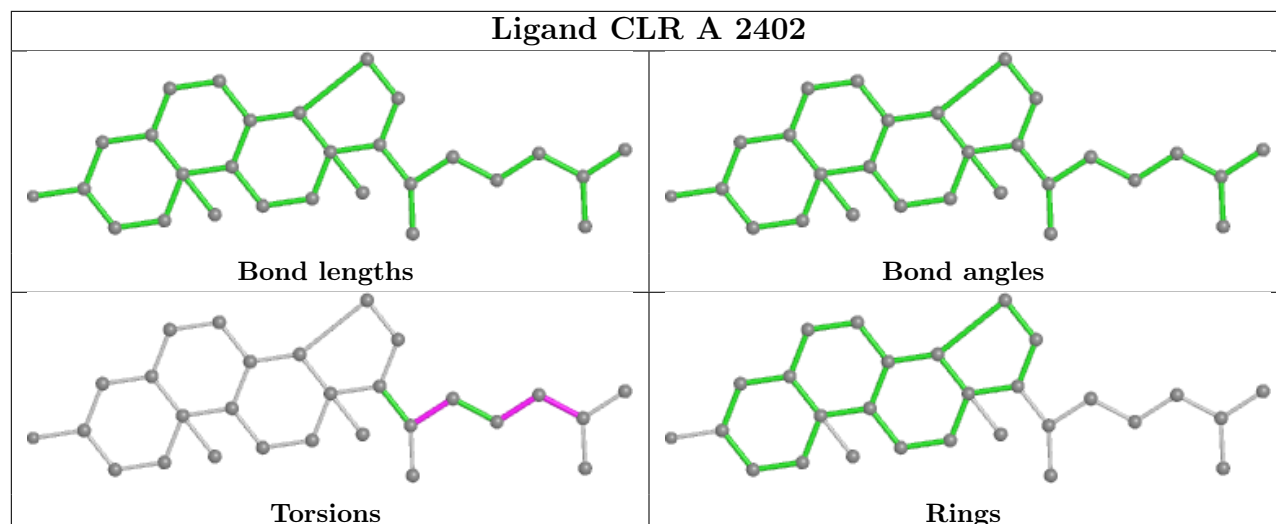
4 monomers are involved in 4 short contacts:

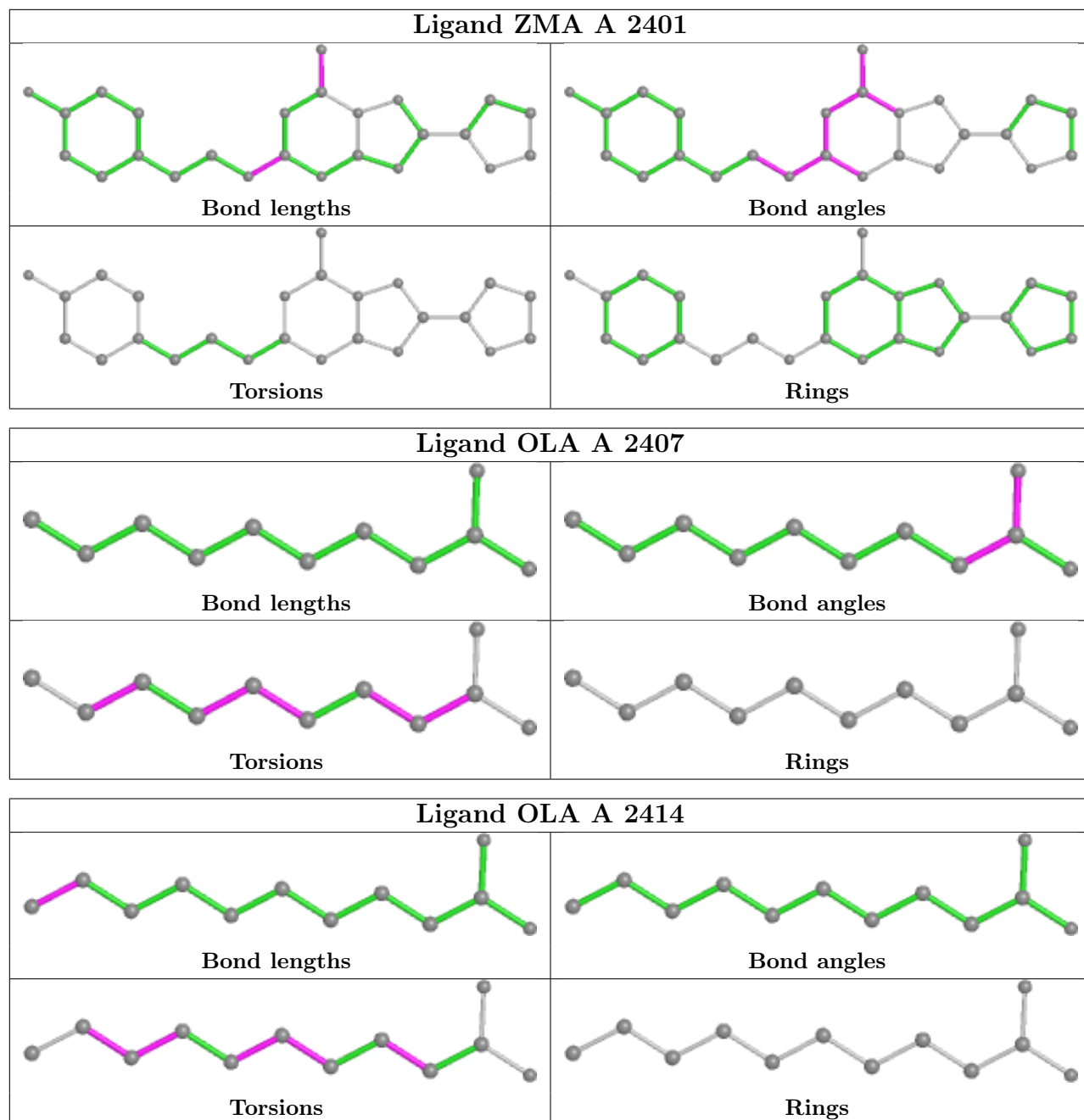
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2402	CLR	1	0
2	A	2401	ZMA	1	0
4	A	2419	OLA	1	0
5	A	2421	OLC	1	0

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.

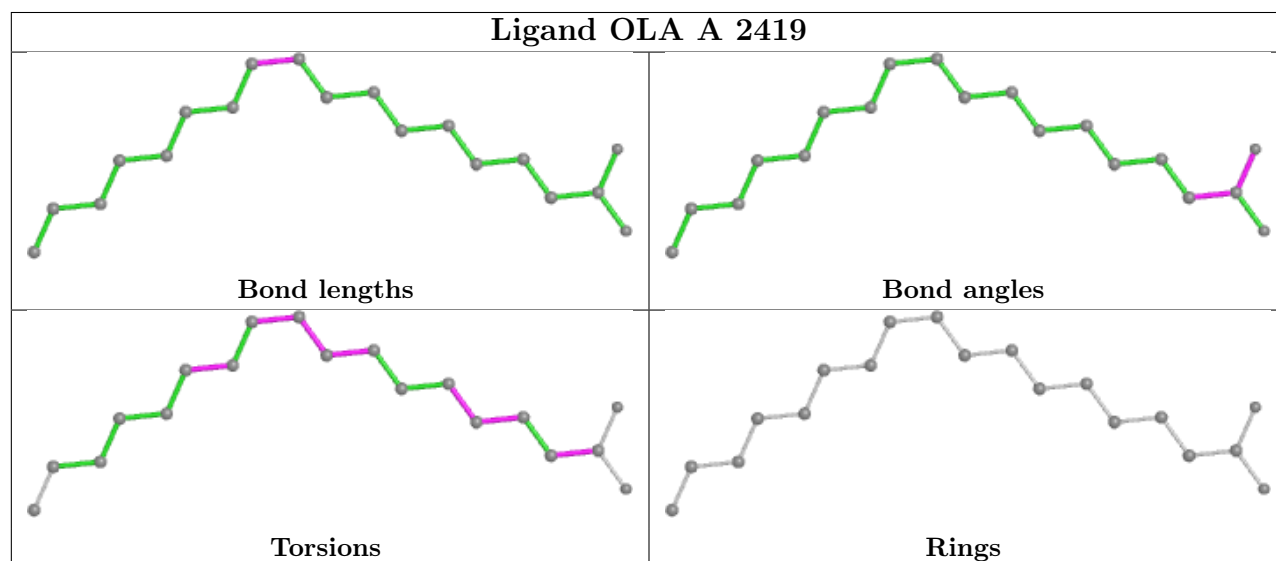
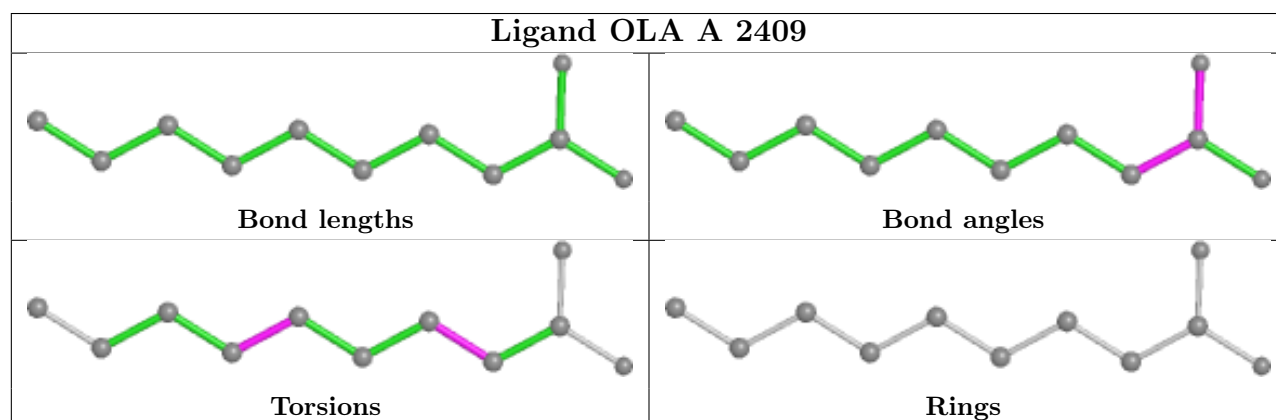
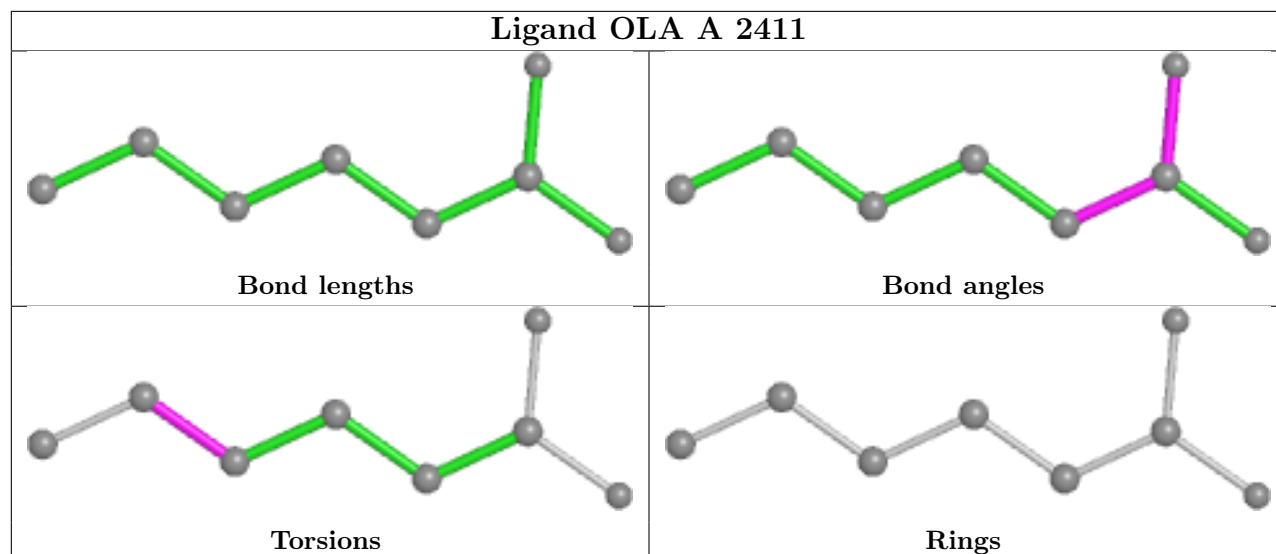


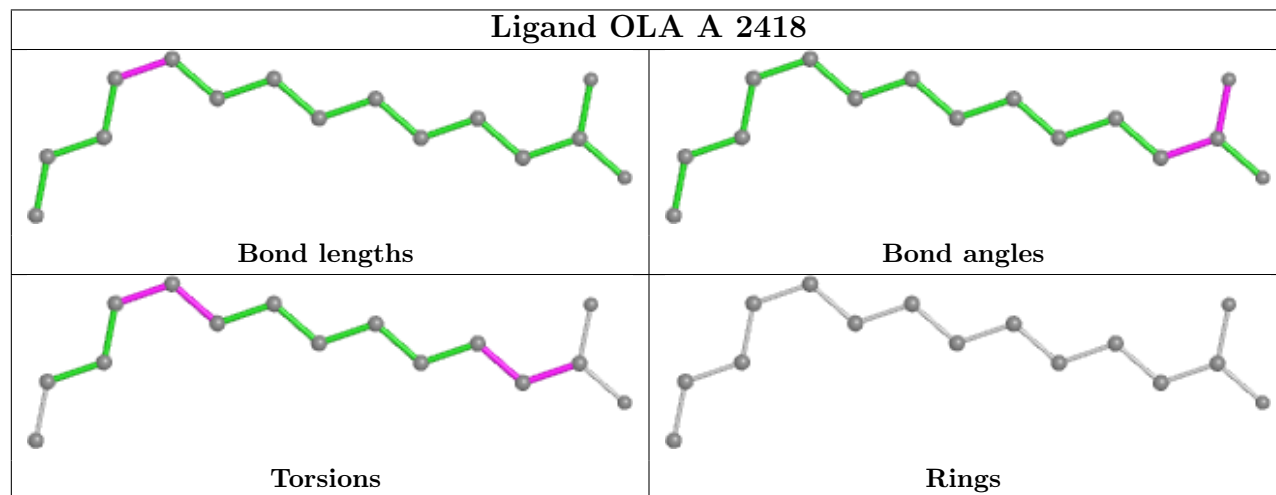
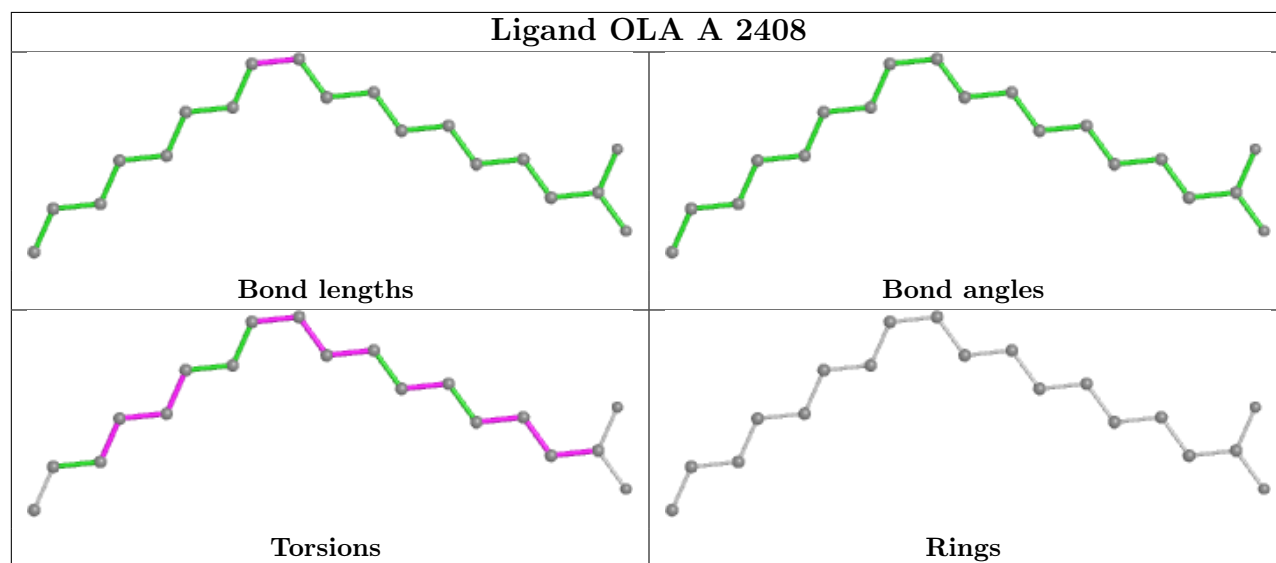
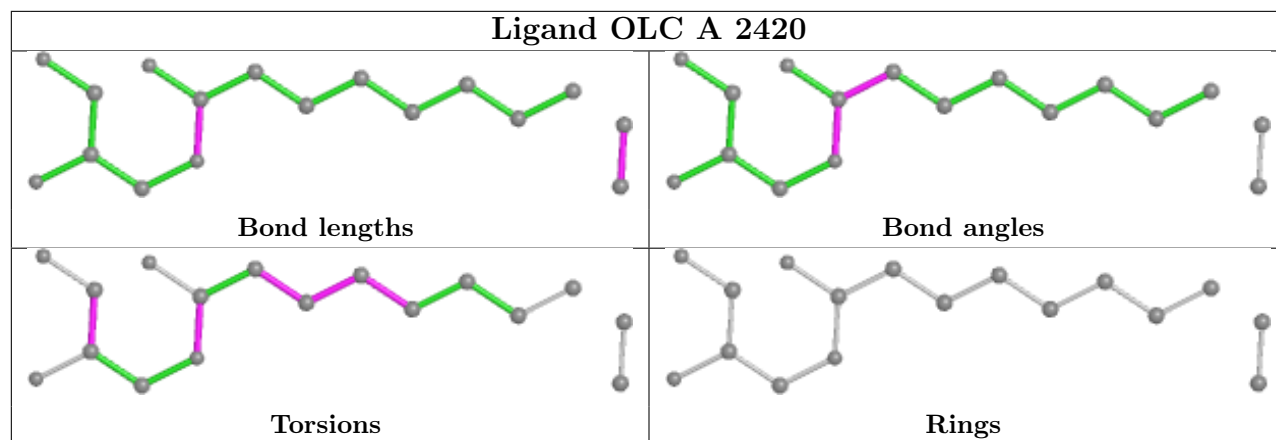


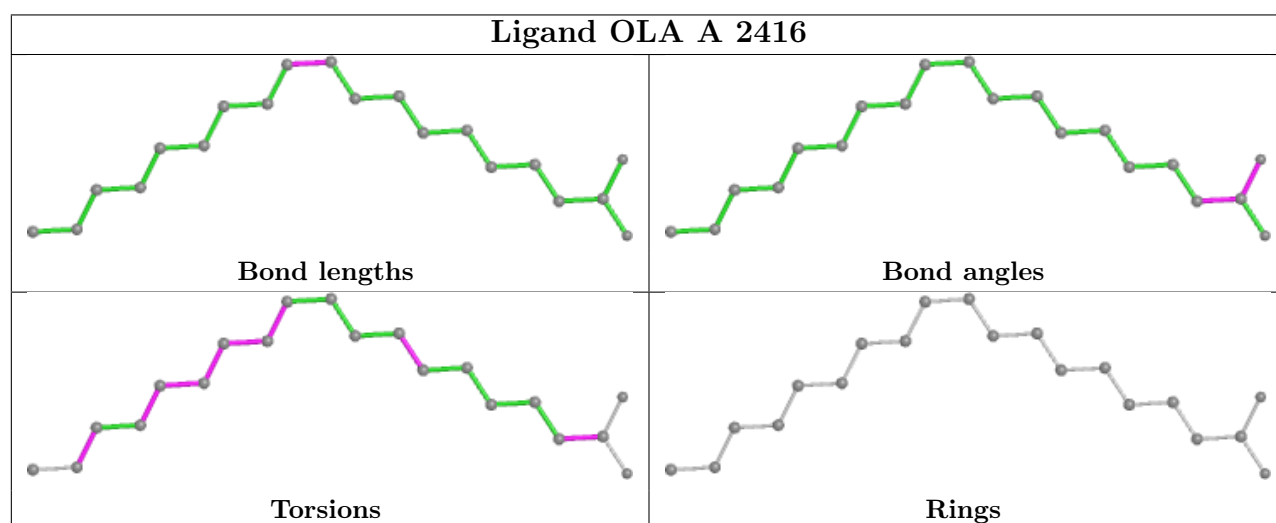
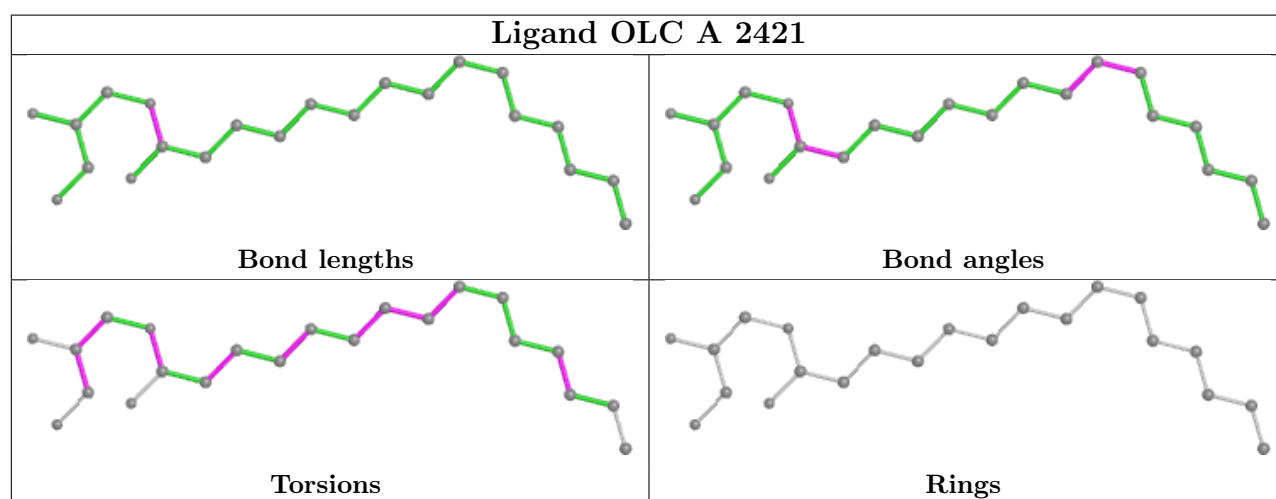
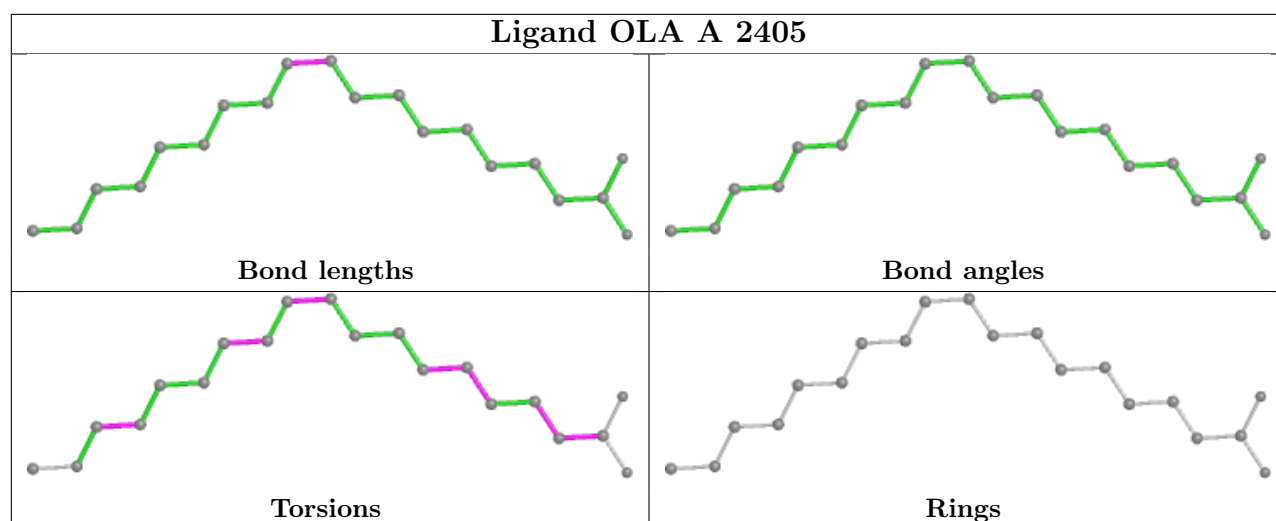


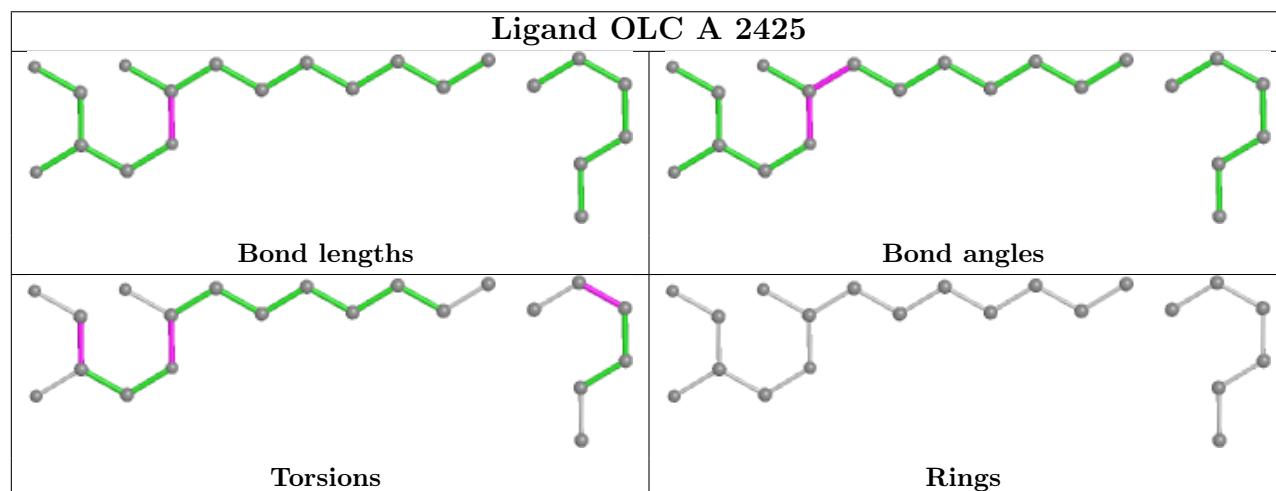
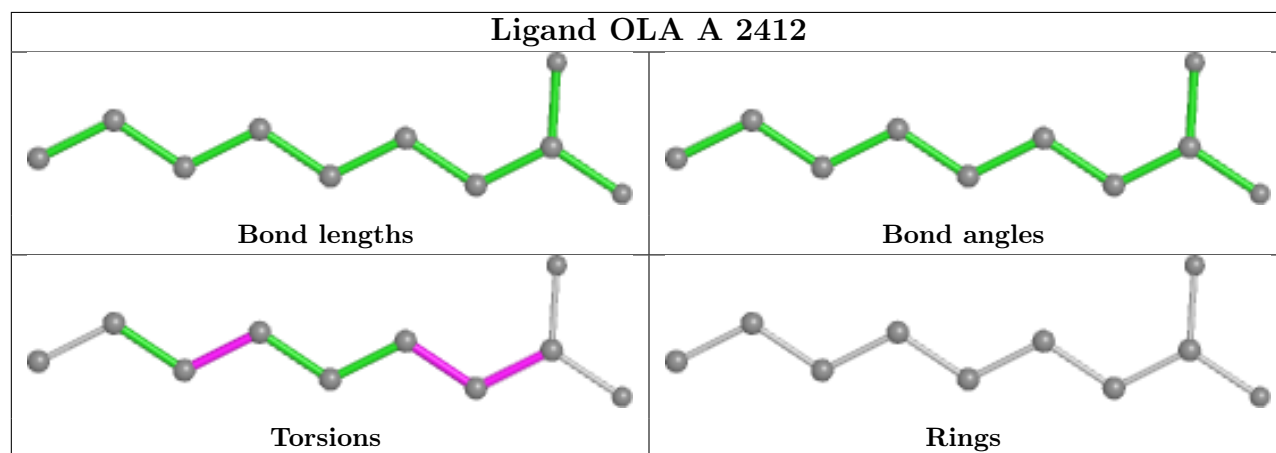
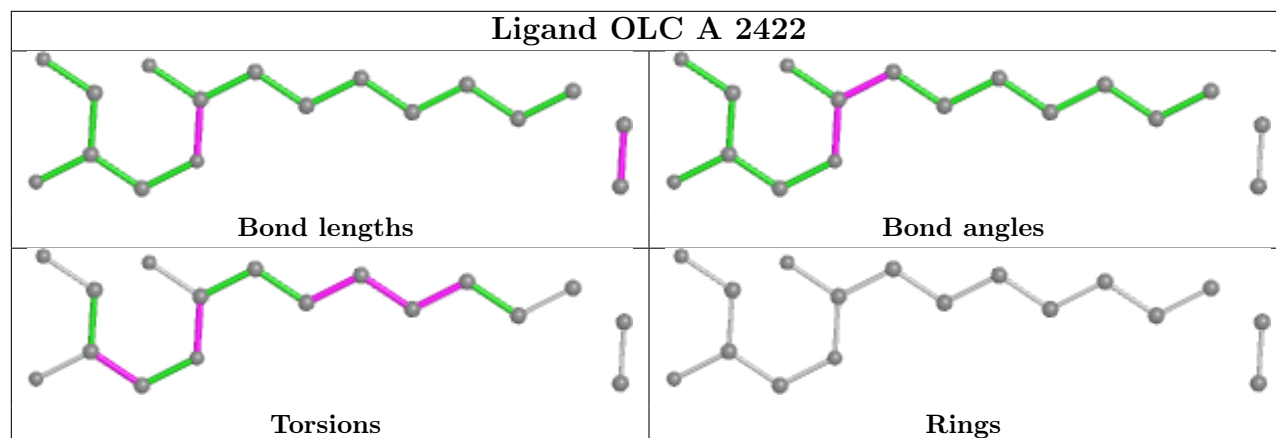


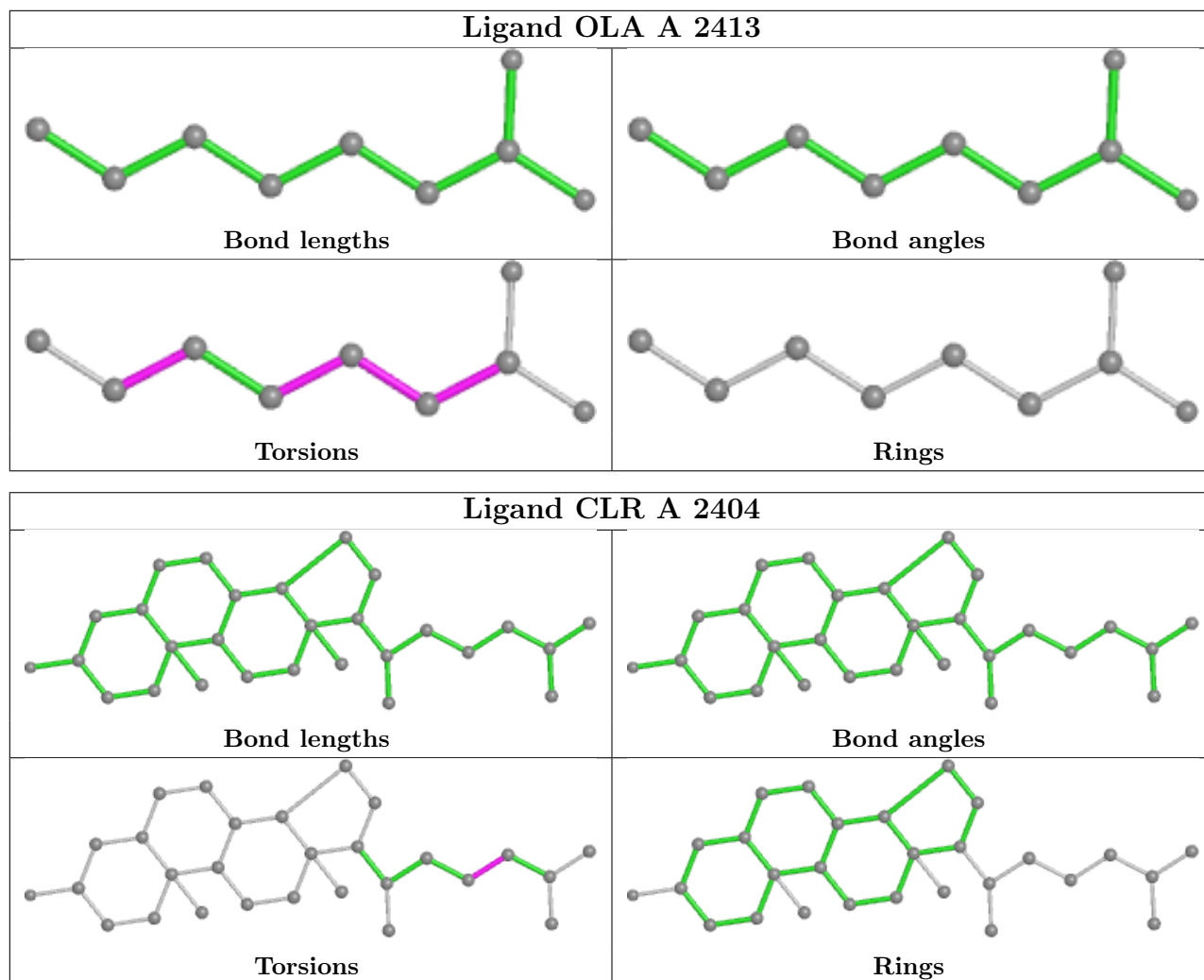












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1106:LEU	C	219:GLU	N	3.13
1	A	208:LEU	C	1001:ALA	N	2.91

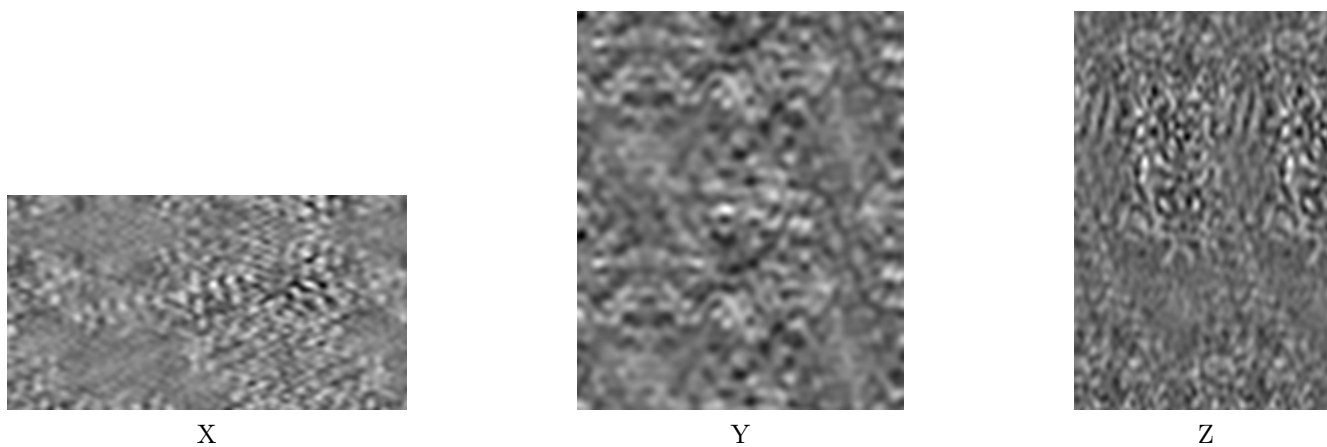
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29586. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

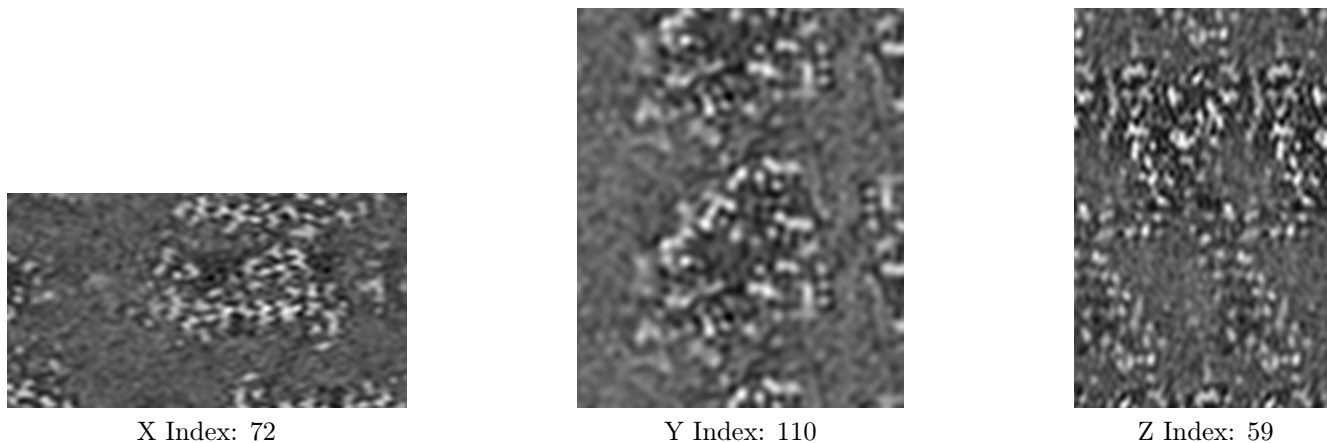
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

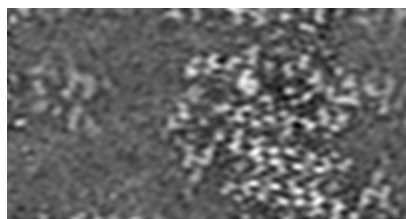
#### 6.2.1 Primary map



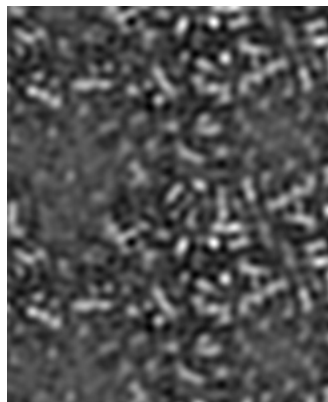
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

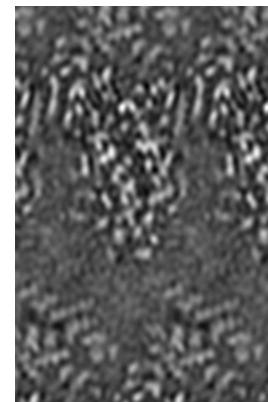
### 6.3.1 Primary map



X Index: 38



Y Index: 164

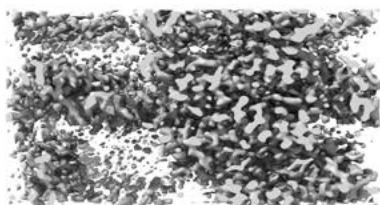


Z Index: 75

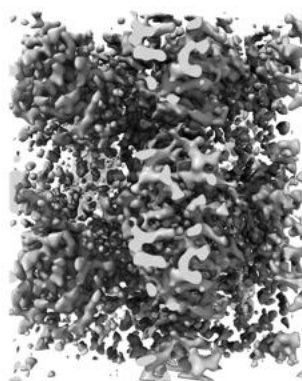
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

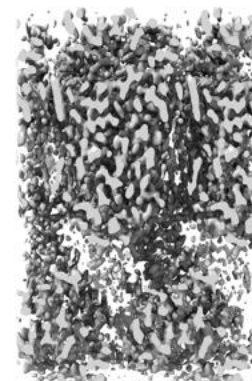
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

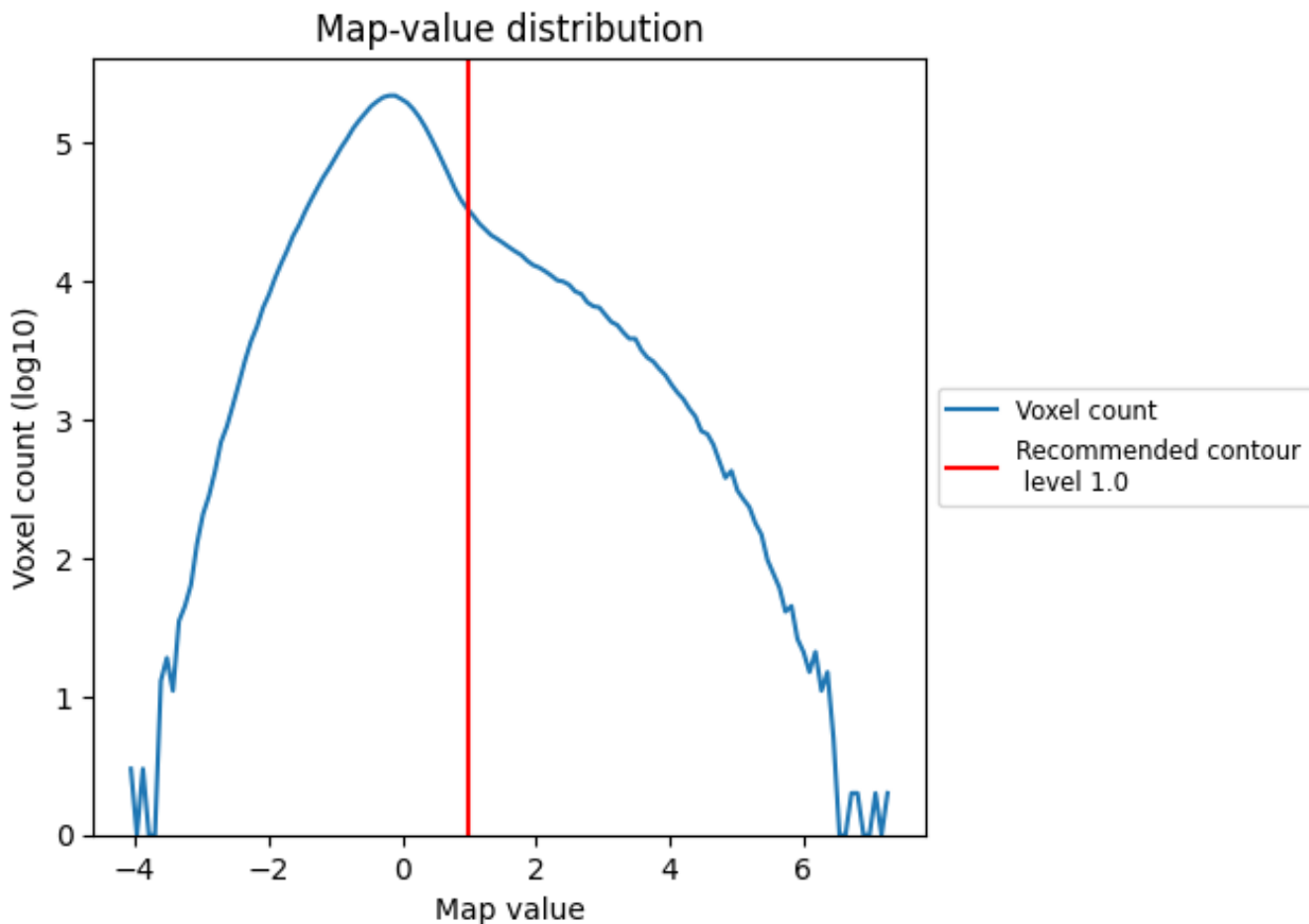
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

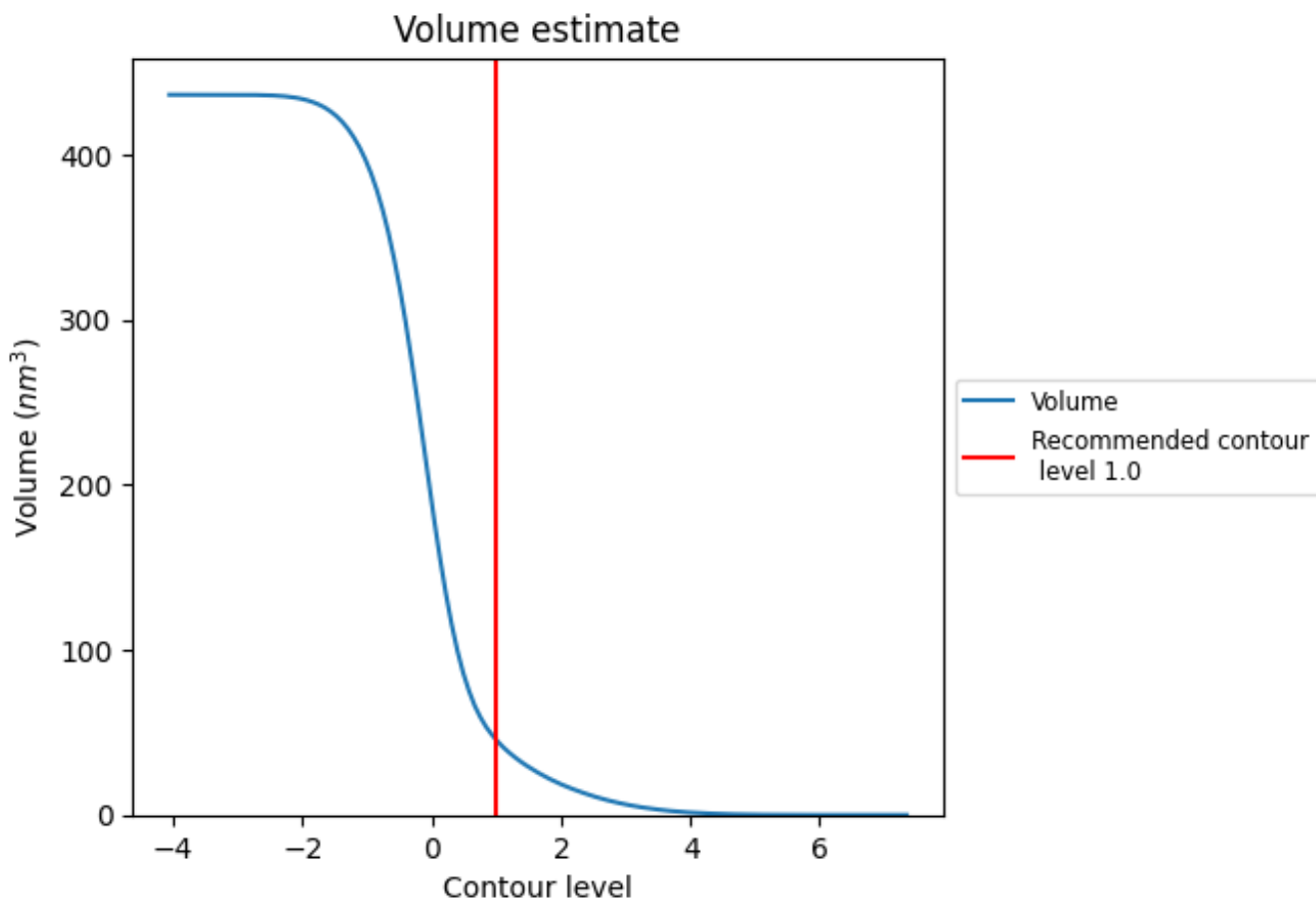
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm<sup>3</sup>; this corresponds to an approximate mass of 41 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

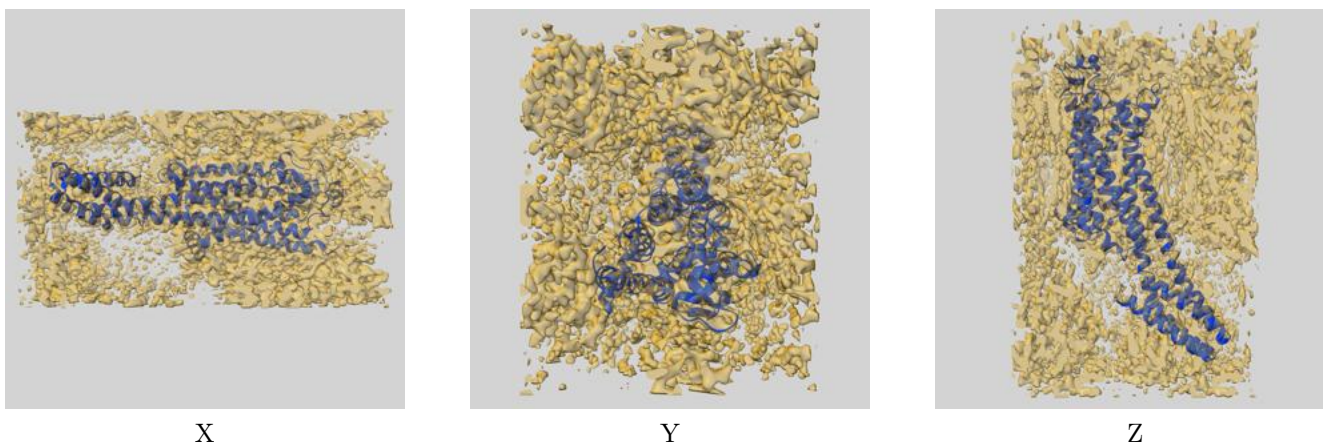
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

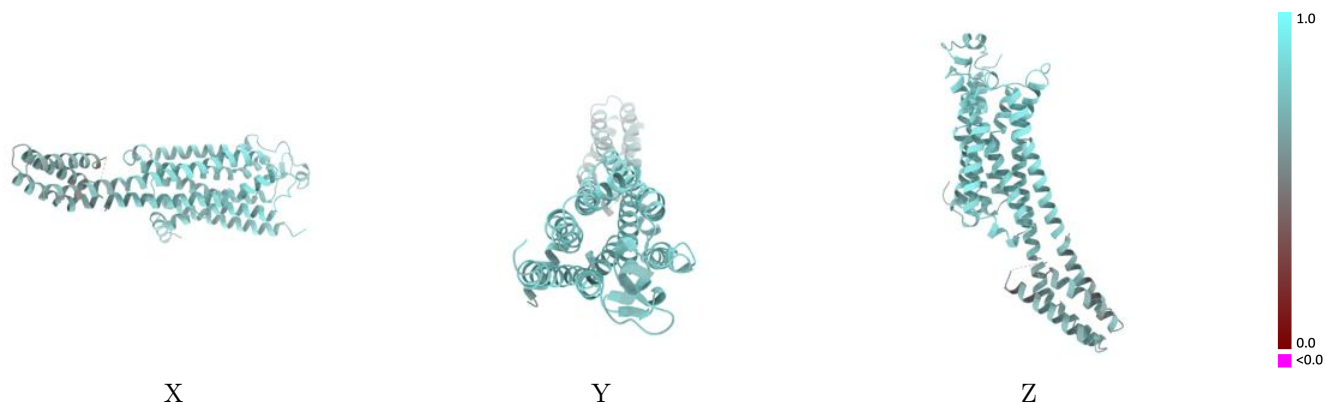
This section contains information regarding the fit between EMDB map EMD-29586 and PDB model 8FYN. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



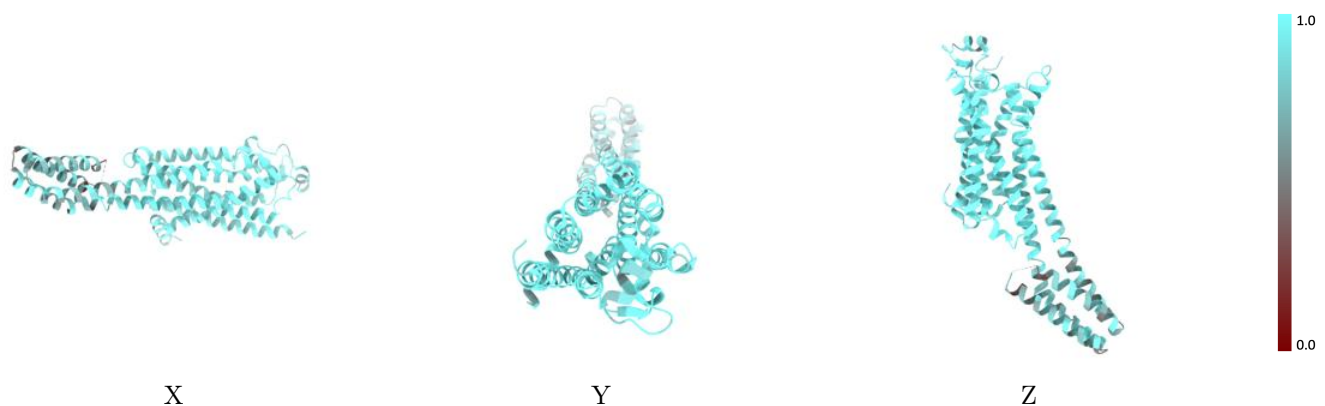
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



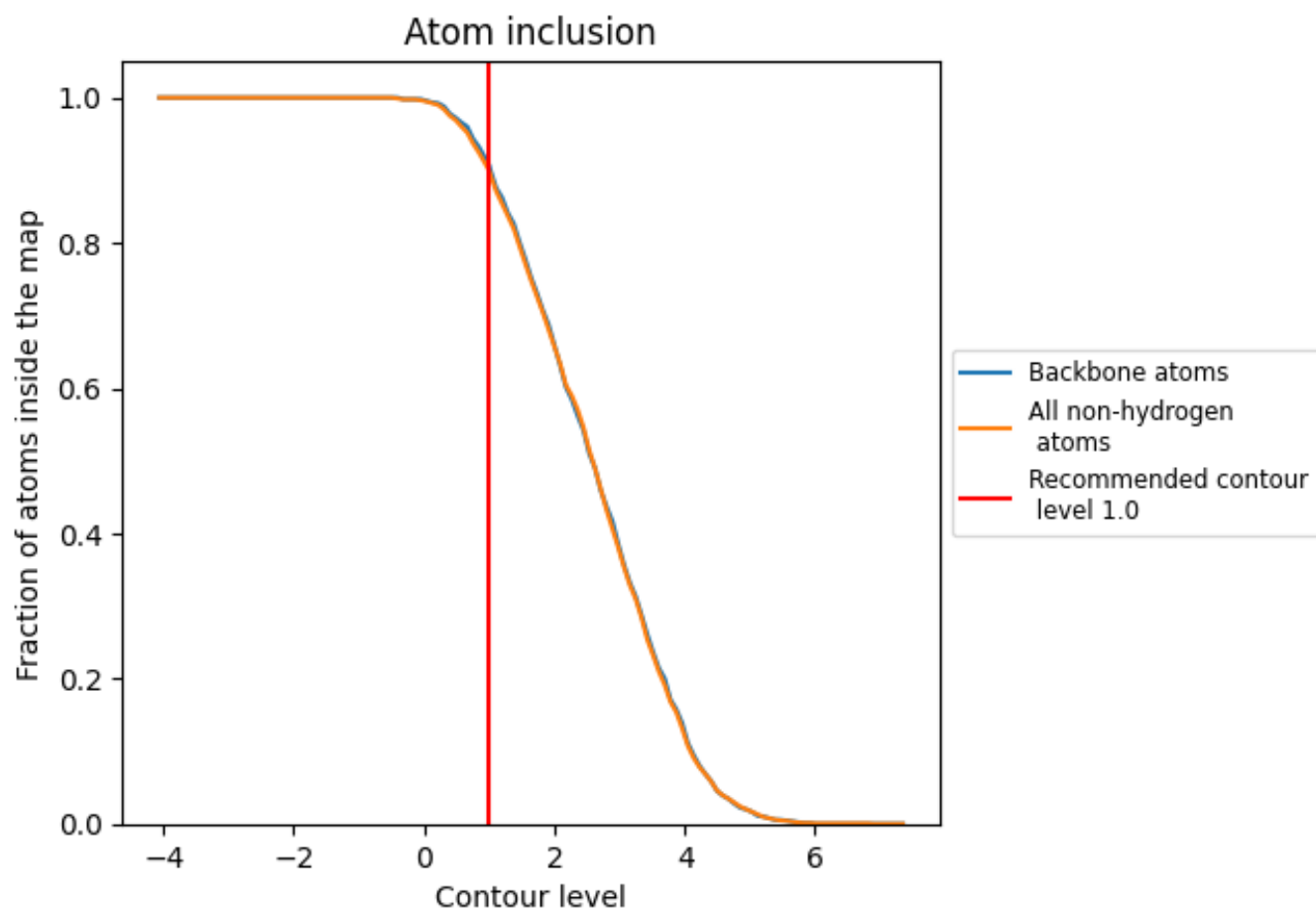
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8993	 0.7110
A	 0.9017	 0.7110

