



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 09:42 AM EST

PDB ID : 3HB3
Title : High resolution crystal structure of Paracoccus denitrificans cytochrome c oxidase
Authors : Koepke, J.; Angerer, H.; Peng, G.
Deposited on : 2009-05-04
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

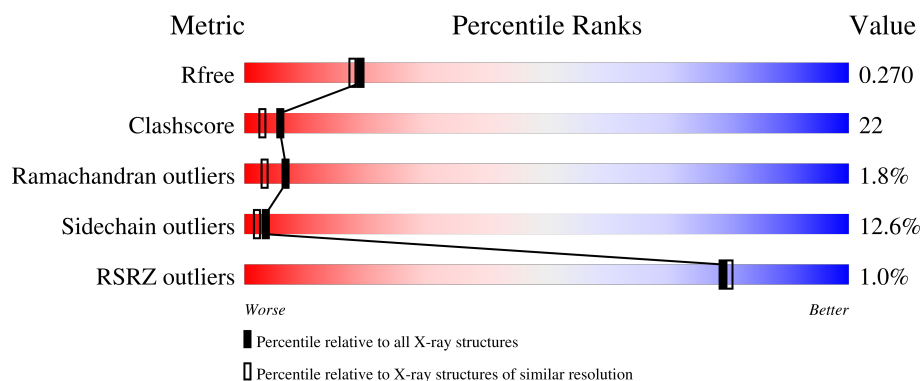
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	558	<div> <div>2%</div> <div>55% 32% 8% 5%</div> </div>
2	B	298	<div> <div>45% 29% 11% 15%</div> </div>
3	C	127	<div> <div>2%</div> <div>49% 31% 13% 7%</div> </div>
4	D	120	<div> <div>55% 28% 7% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEA	A	559	X	-	-	-
5	HEA	A	560	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9393 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 Cytochrome c oxidase subunit 1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	3	0
			4200	2819	659	689	33			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	2	0
			1985	1300	320	357	8			

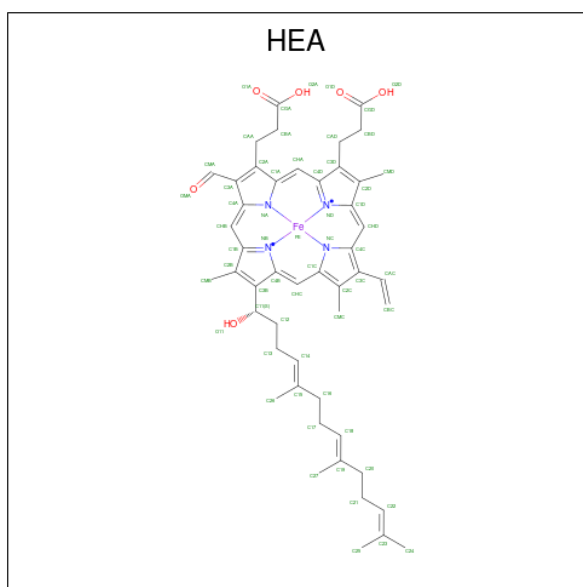
- Molecule 3 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	2	0
			940	591	158	185	6			

- Molecule 4 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	108	Total	C	N	O	S	0	0	0
			831	530	135	164	2			

- Molecule 5 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
5	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 6 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		
6	B	2	Total	Cu	0	0
			2	2		

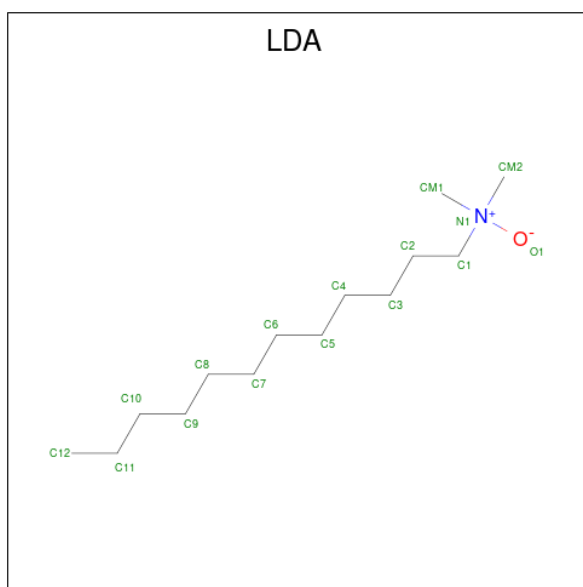
- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mn	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

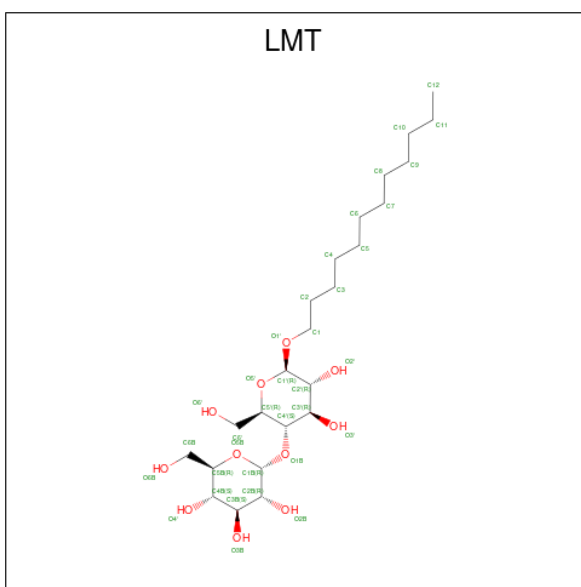
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



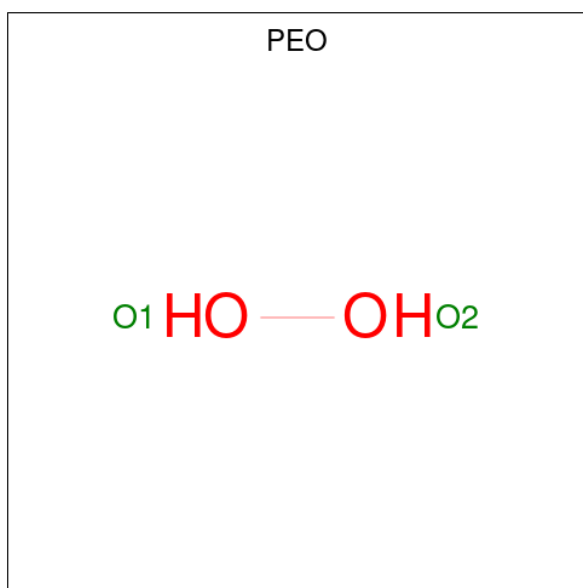
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 35	C 24	O 11	0	0
10	A	1	Total 35	C 24	O 11	0	0
10	A	1	Total 35	C 24	O 11	0	0
10	A	1	Total 47	C 30	O 17	0	1
10	A	1	Total 58	C 36	O 22	0	1
10	A	1	Total 47	C 30	O 17	0	1
10	A	1	Total 47	C 30	O 17	0	1
10	A	1	Total 47	C 30	O 17	0	1
10	B	1	Total 35	C 24	O 11	0	0
10	B	1	Total 35	C 24	O 11	0	0
10	B	1	Total 35	C 24	O 11	0	0
10	B	1	Total 35	C 24	O 11	0	0
10	B	1	Total 47	C 30	O 17	0	1
10	B	1	Total 58	C 36	O 22	0	1

- Molecule 11 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			2	2		

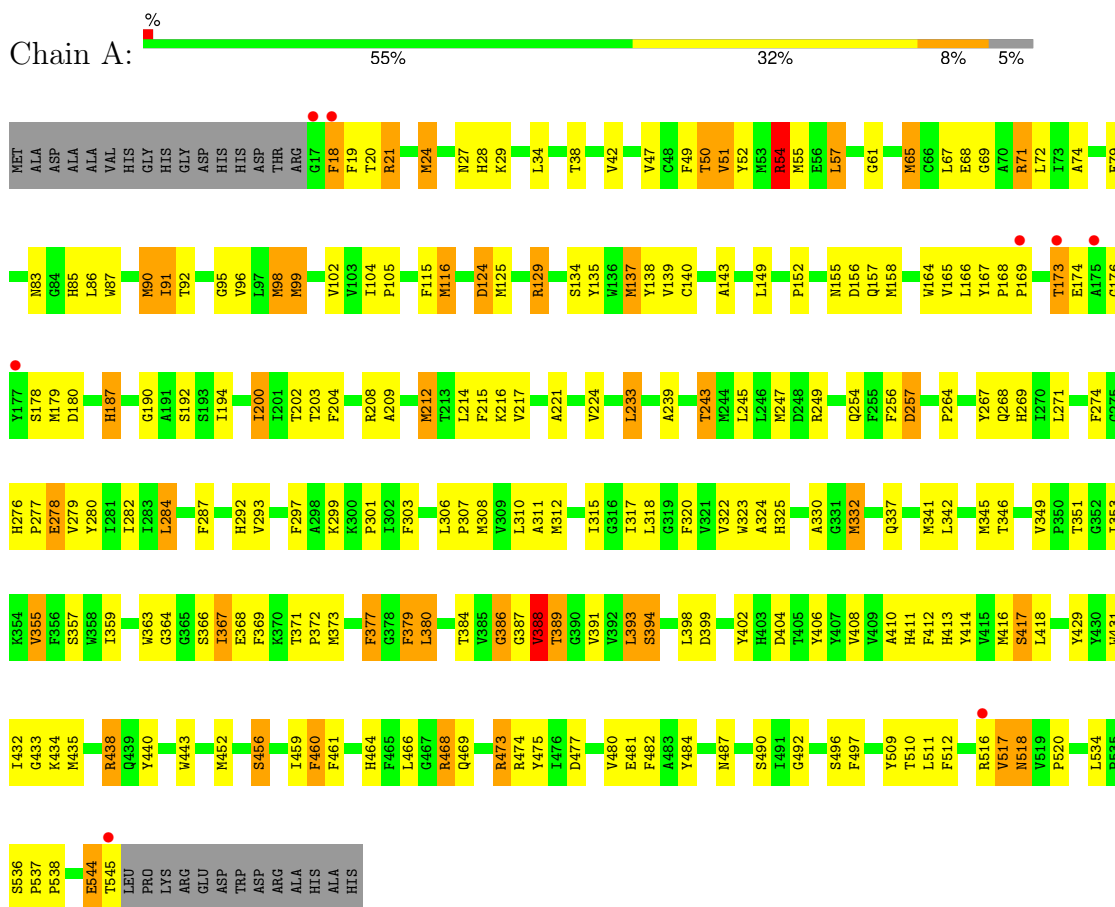
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	158	Total	O	0	0
			158	158		
12	B	228	Total	O	0	0
			228	228		
12	C	87	Total	O	0	0
			87	87		
12	D	81	Total	O	0	0
			81	81		

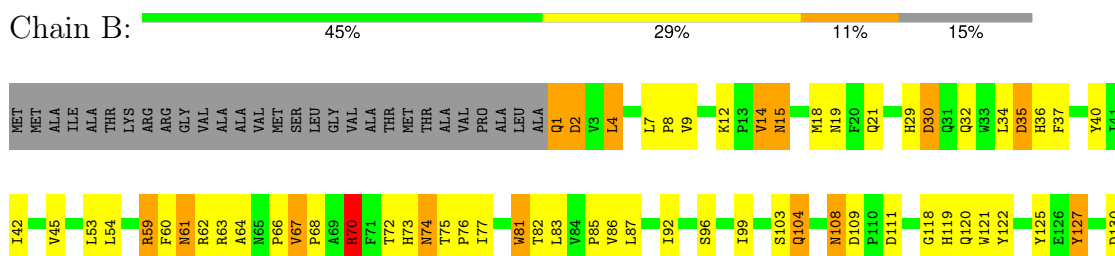
3 Residue-property plots

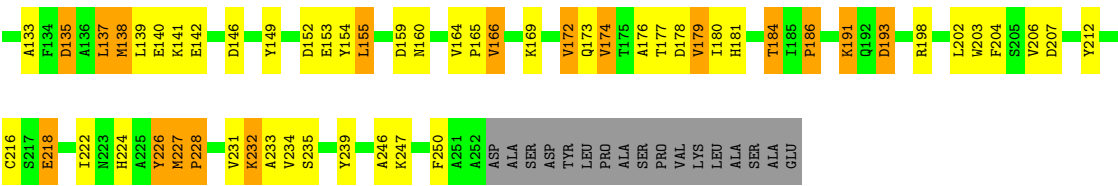
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome c oxidase subunit 1-beta

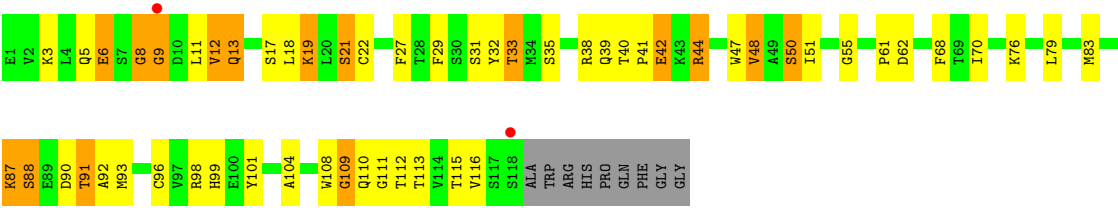


• Molecule 2: Cytochrome c oxidase subunit 2

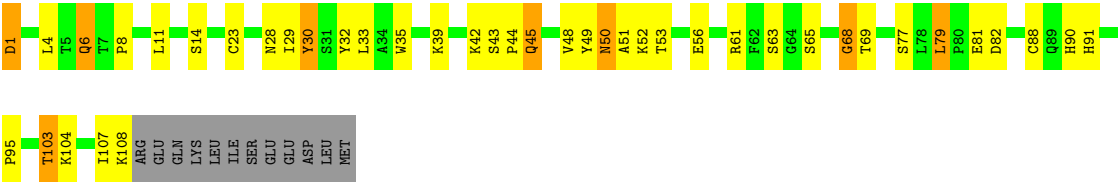




• Molecule 3: ANTIBODY FV FRAGMENT



• Molecule 4: ANTIBODY FV FRAGMENT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.40Å 150.47Å 157.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.25 19.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.98-2.25) 99.0 (19.98-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.280 0.211 , 0.270	Depositor DCC
R_{free} test set	2819 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9393	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, MN, PEO, LMT, CA, CU1, LDA

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	1.40	19/4368 (0.4%)	1.23	29/5959 (0.5%)
2	B	1.65	18/2050 (0.9%)	1.48	34/2810 (1.2%)
3	C	1.27	0/972	1.20	3/1314 (0.2%)
4	D	1.35	4/852 (0.5%)	1.19	2/1156 (0.2%)
All	All	1.45	41/8242 (0.5%)	1.29	68/11239 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
3	C	0	1
All	All	1	1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GLU	C-O	9.95	1.42	1.23
2	B	122	TYR	CD1-CE1	7.83	1.51	1.39
2	B	9	VAL	CB-CG2	-7.66	1.36	1.52
2	B	203	TRP	CB-CG	6.61	1.62	1.50
1	A	481	GLU	CD-OE2	-6.59	1.18	1.25

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH2	-14.55	113.02	120.30
1	A	477	ASP	CB-CG-OD2	9.46	126.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	71	ARG	NE-CZ-NH1	9.33	124.97	120.30
2	B	154	TYR	C-N-CA	-9.11	98.93	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	389	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	8	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4124	231	0
2	B	1985	0	1967	99	0
3	C	940	0	898	47	0
4	D	831	0	807	24	0
5	A	120	0	104	32	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	64	0	124	5	0
9	B	96	0	186	8	0
10	A	351	0	234	19	0
10	B	245	0	221	9	0
11	A	2	0	0	0	0
12	A	158	0	0	11	0
12	B	228	0	0	13	0
12	C	87	0	0	10	0
12	D	81	0	0	2	0
All	All	9393	0	8665	398	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 22.

The worst 5 of 398 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)
2:B:222:ILE:CD1	2:B:222:ILE:CG1	1.80	1.53
1:A:312:MET:SD	1:A:312:MET:CE	2.01	1.47
1:A:65:MET:SD	1:A:65:MET:CE	2.04	1.46
1:A:373:MET:SD	1:A:373:MET:CE	2.03	1.45
1:A:254:GLN:HB3	1:A:257:ASP:HB3	1.27	1.12

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	530/558 (95%)	462 (87%)	61 (12%)	7 (1%)	10	6
2	B	252/298 (85%)	216 (86%)	31 (12%)	5 (2%)	6	3
3	C	118/127 (93%)	105 (89%)	11 (9%)	2 (2%)	7	4
4	D	106/120 (88%)	99 (93%)	3 (3%)	4 (4%)	2	1
All	All	1006/1103 (91%)	882 (88%)	106 (10%)	18 (2%)	7	3

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PHE
1	A	544	GLU
2	B	74	ASN
3	C	12	VAL
2	B	235	SER

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	435/454 (96%)	390 (90%)	45 (10%)	6	4
2	B	213/243 (88%)	184 (86%)	29 (14%)	3	1
3	C	103/107 (96%)	85 (82%)	18 (18%)	1	0
4	D	92/104 (88%)	77 (84%)	15 (16%)	2	0
All	All	843/908 (93%)	736 (87%)	107 (13%)	3	2

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	83	LEU
2	B	191	LYS
4	D	63	SER
2	B	87	LEU
2	B	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	61	ASN
2	B	192	GLN
2	B	108	ASN
2	B	208	GLN
1	A	268	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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
10	LMT	A	571[B]	-	36,36,36	4.33	13 (36%)	47,47,47	1.65	7 (14%)
11	PEO	A	576	6,5	1,1,1	0.45	0	-		
5	HEA	A	560	1,11	58,67,67	3.70	27 (46%)	63,103,103	4.26	39 (61%)
9	LDA	B	275	-	13,15,15	2.40	2 (15%)	14,17,17	0.45	0
10	LMT	A	575[A]	-	36,36,36	4.37	13 (36%)	47,47,47	1.43	8 (17%)
10	LMT	A	574[B]	-	36,36,36	4.42	13 (36%)	47,47,47	1.07	2 (4%)
10	LMT	A	569	-	36,36,36	4.39	13 (36%)	47,47,47	1.35	5 (10%)
10	LMT	A	570	-	36,36,36	4.38	13 (36%)	47,47,47	1.24	4 (8%)
10	LMT	B	282[B]	-	36,36,36	4.38	13 (36%)	47,47,47	1.27	6 (12%)
10	LMT	B	283[A]	-	36,36,36	4.46	13 (36%)	47,47,47	1.21	2 (4%)
10	LMT	B	280	-	36,36,36	4.40	13 (36%)	47,47,47	1.16	3 (6%)
10	LMT	B	281	-	36,36,36	4.35	13 (36%)	47,47,47	1.19	5 (10%)
9	LDA	A	567	-	13,15,15	2.31	2 (15%)	14,17,17	0.50	0
10	LMT	B	279	-	36,36,36	4.36	13 (36%)	47,47,47	1.47	5 (10%)
10	LMT	A	575[B]	-	36,36,36	4.36	13 (36%)	47,47,47	1.49	8 (17%)
5	HEA	A	559	1	58,67,67	3.02	19 (32%)	63,103,103	4.67	44 (69%)
9	LDA	B	273	-	13,15,15	2.37	2 (15%)	14,17,17	0.42	0
10	LMT	A	573[A]	-	36,36,36	4.36	13 (36%)	47,47,47	1.43	6 (12%)
9	LDA	A	565	-	13,15,15	2.36	2 (15%)	14,17,17	0.43	0
10	LMT	A	572[A]	-	36,36,36	4.44	13 (36%)	47,47,47	1.23	2 (4%)
9	LDA	B	272	-	13,15,15	2.25	2 (15%)	14,17,17	0.62	0
10	LMT	A	571[A]	-	36,36,36	4.33	13 (36%)	47,47,47	1.64	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LDA	A	566	-	13,15,15	2.39	2 (15%)	14,17,17	0.41	0
9	LDA	B	276	-	13,15,15	2.34	2 (15%)	14,17,17	0.42	0
10	LMT	A	574[A]	-	36,36,36	4.40	13 (36%)	47,47,47	1.34	5 (10%)
9	LDA	A	564	-	13,15,15	2.29	2 (15%)	14,17,17	0.47	0
10	LMT	B	278	-	36,36,36	4.33	13 (36%)	47,47,47	1.30	6 (12%)
10	LMT	B	283[B]	-	36,36,36	4.47	13 (36%)	47,47,47	1.12	3 (6%)
9	LDA	B	277	-	13,15,15	2.39	2 (15%)	14,17,17	0.44	0
10	LMT	B	282[A]	-	36,36,36	4.38	13 (36%)	47,47,47	1.30	7 (14%)
9	LDA	B	274	-	13,15,15	2.32	2 (15%)	14,17,17	0.41	0
10	LMT	A	568	-	36,36,36	4.36	13 (36%)	47,47,47	1.00	3 (6%)
10	LMT	A	573[B]	-	36,36,36	4.38	14 (38%)	47,47,47	1.35	5 (10%)
10	LMT	A	572[B]	-	36,36,36	4.41	13 (36%)	47,47,47	1.28	6 (12%)

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
10	LMT	A	571[B]	-	-	15/21/61/61	0/2/2/2
5	HEA	A	560	1,11	1/1/7/16	18/32/76/76	-
9	LDA	B	275	-	-	6/13/13/13	-
10	LMT	A	575[A]	-	-	14/21/61/61	0/2/2/2
10	LMT	A	574[B]	-	-	12/21/61/61	0/2/2/2
10	LMT	A	569	-	-	10/21/61/61	0/2/2/2
10	LMT	A	570	-	-	11/21/61/61	0/2/2/2
10	LMT	B	282[B]	-	-	6/21/61/61	0/2/2/2
10	LMT	B	283[A]	-	-	11/21/61/61	0/2/2/2
10	LMT	B	280	-	-	14/21/61/61	0/2/2/2
10	LMT	B	281	-	-	17/21/61/61	0/2/2/2
9	LDA	A	567	-	-	9/13/13/13	-
10	LMT	B	279	-	-	7/21/61/61	0/2/2/2
10	LMT	A	575[B]	-	-	14/21/61/61	0/2/2/2
5	HEA	A	559	1	1/1/7/16	12/32/76/76	-
9	LDA	B	273	-	-	12/13/13/13	-
10	LMT	A	573[A]	-	-	17/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LDA	A	565	-	-	8/13/13/13	-
10	LMT	A	572[A]	-	-	15/21/61/61	0/2/2/2
9	LDA	B	272	-	-	8/13/13/13	-
10	LMT	A	571[A]	-	-	14/21/61/61	0/2/2/2
9	LDA	A	566	-	-	6/13/13/13	-
9	LDA	B	276	-	-	7/13/13/13	-
10	LMT	A	574[A]	-	-	12/21/61/61	0/2/2/2
9	LDA	A	564	-	-	9/13/13/13	-
10	LMT	B	278	-	-	11/21/61/61	0/2/2/2
10	LMT	B	283[B]	-	-	13/21/61/61	0/2/2/2
9	LDA	B	277	-	-	12/13/13/13	-
10	LMT	B	282[A]	-	-	6/21/61/61	0/2/2/2
9	LDA	B	274	-	-	8/13/13/13	-
10	LMT	A	568	-	-	14/21/61/61	0/2/2/2
10	LMT	A	573[B]	-	-	18/21/61/61	0/2/2/2
10	LMT	A	572[B]	-	-	10/21/61/61	0/2/2/2

The worst 5 of 340 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	O11-C11	-12.32	1.16	1.42
5	A	560	HEA	C14-C15	10.30	1.56	1.33
10	A	573[B]	LMT	C4B-C5B	-9.30	1.33	1.53
10	B	283[A]	LMT	C4B-C5B	-9.17	1.33	1.53
10	A	571[A]	LMT	C4B-C5B	-9.09	1.33	1.53

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	560	HEA	C13-C12-C11	-13.88	92.22	114.39
5	A	560	HEA	C12-C11-C3B	13.30	132.91	112.12
5	A	559	HEA	C4A-CHB-C1B	-11.99	106.74	122.56
5	A	559	HEA	CHB-C1B-NB	10.40	135.63	124.44
5	A	560	HEA	OMA-CMA-C3A	-9.20	102.99	124.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	559	HEA	C11
5	A	560	HEA	C11

5 of 376 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	559	HEA	O11-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C4B
5	A	559	HEA	O11-C11-C12-C13
5	A	559	HEA	C13-C14-C15-C26

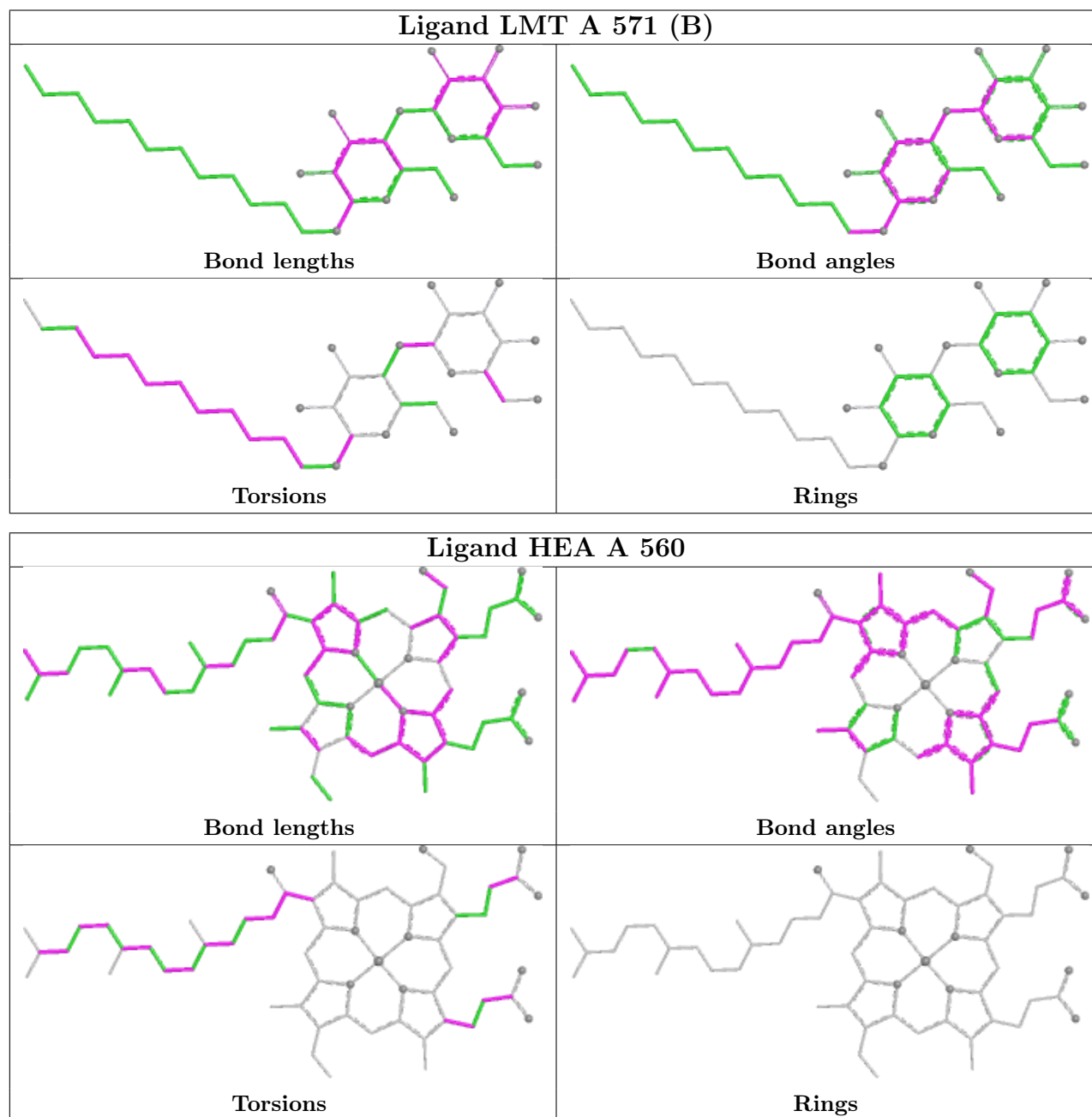
There are no ring outliers.

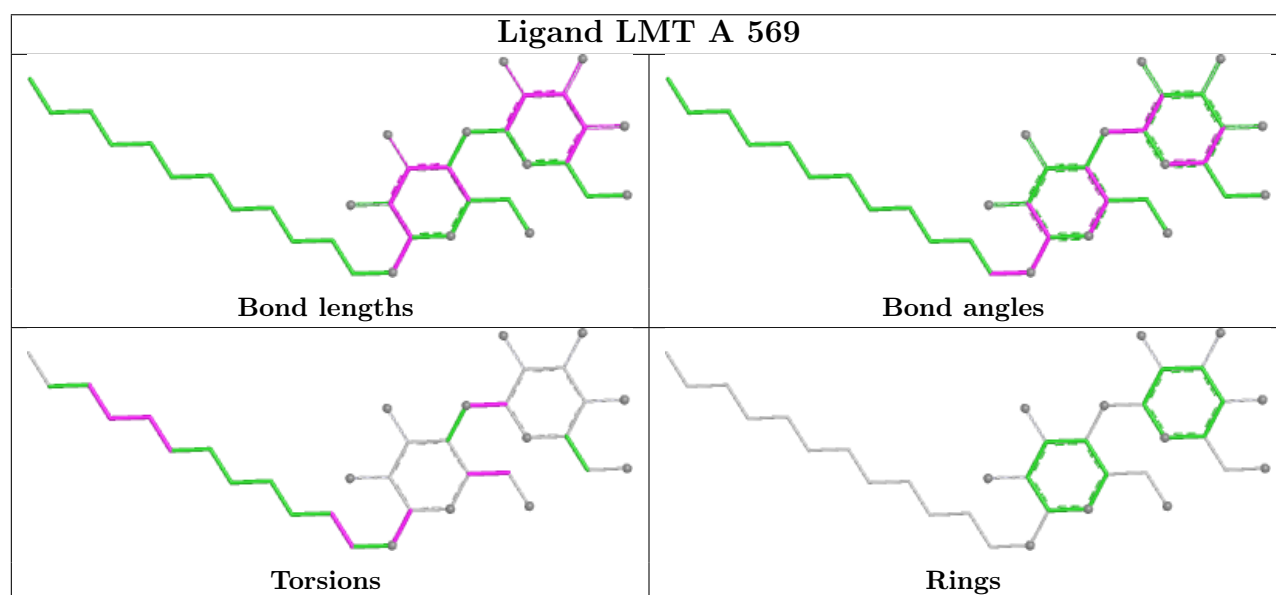
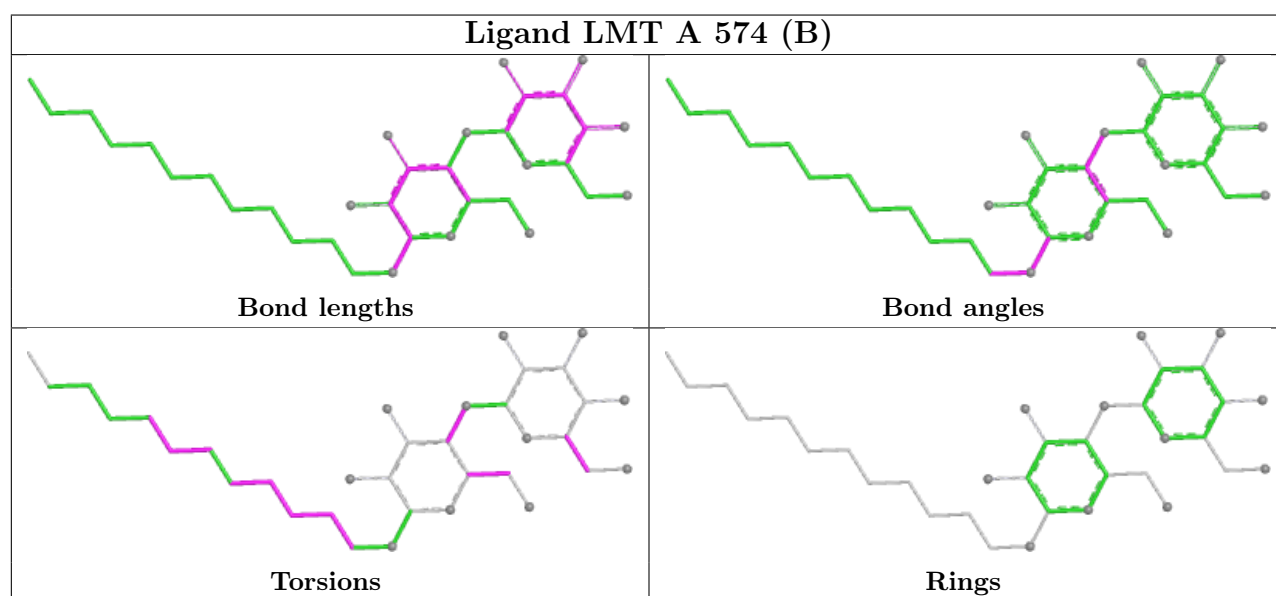
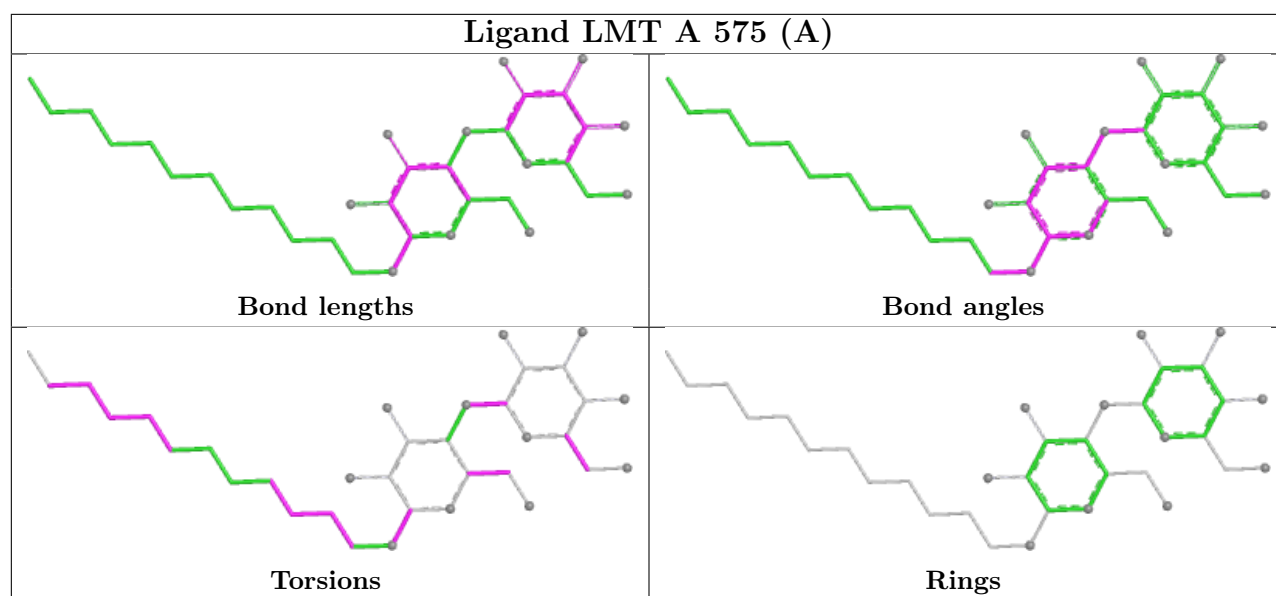
22 monomers are involved in 71 short contacts:

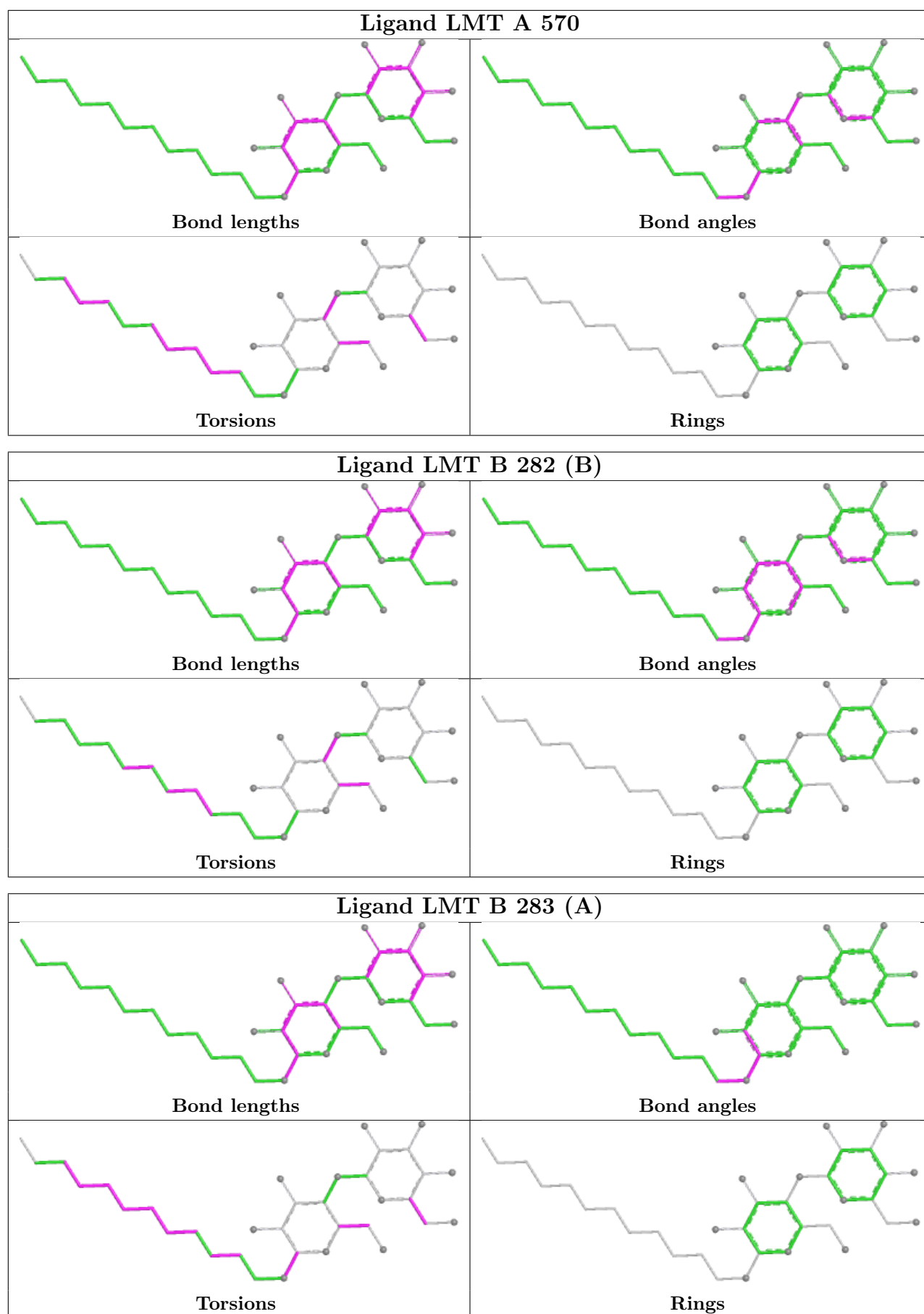
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	571[B]	LMT	1	0
5	A	560	HEA	18	0
10	A	574[B]	LMT	2	0
10	A	569	LMT	1	0
10	A	570	LMT	4	0
10	B	280	LMT	1	0
10	B	281	LMT	7	0
9	A	567	LDA	2	0
10	B	279	LMT	1	0
10	A	575[B]	LMT	2	0
5	A	559	HEA	14	0
9	B	273	LDA	4	0
9	A	565	LDA	1	0
10	A	572[A]	LMT	2	0
9	B	272	LDA	2	0
10	A	571[A]	LMT	1	0
9	B	276	LDA	1	0
10	A	574[A]	LMT	1	0
9	A	564	LDA	2	0
9	B	274	LDA	2	0
10	A	573[B]	LMT	3	0
10	A	572[B]	LMT	2	0

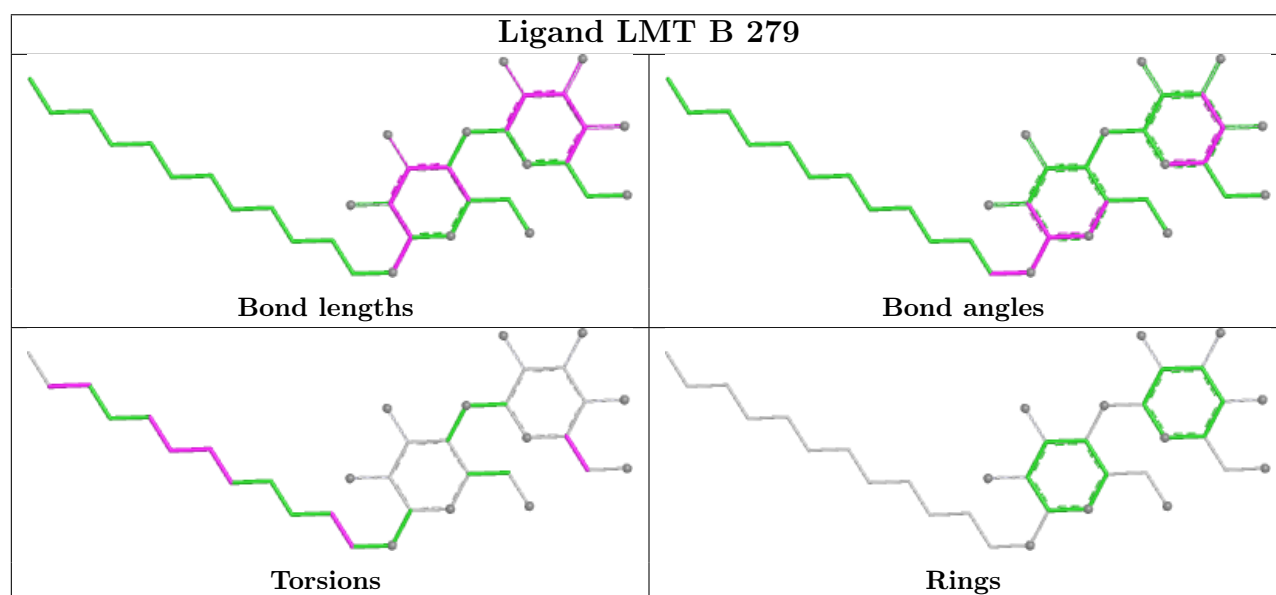
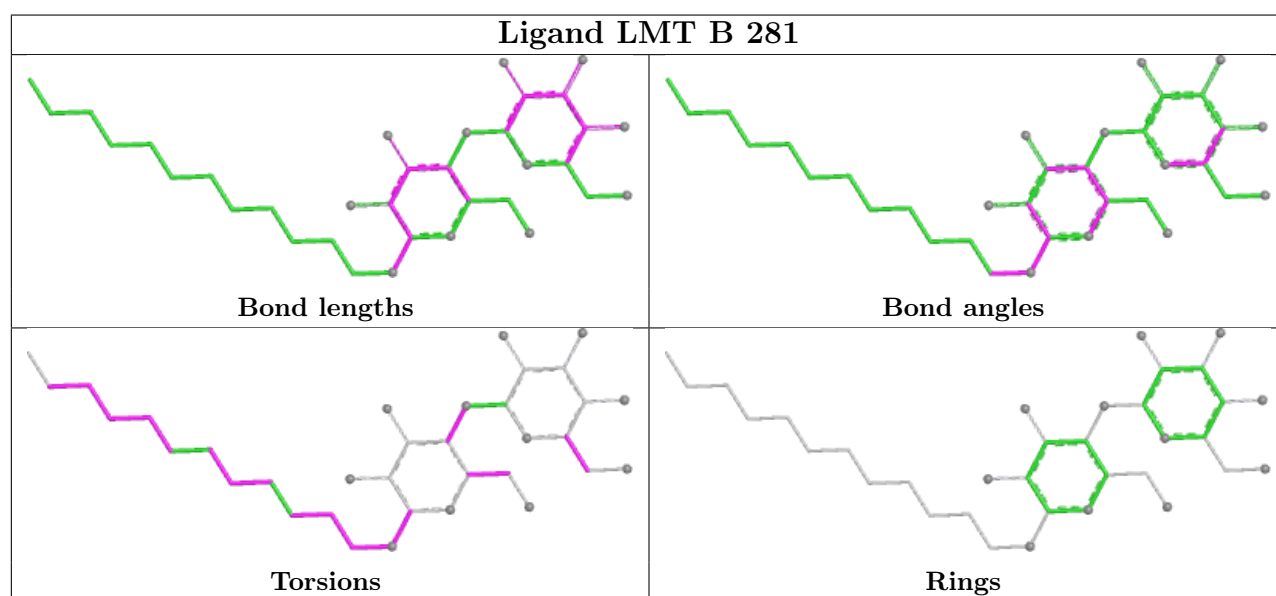
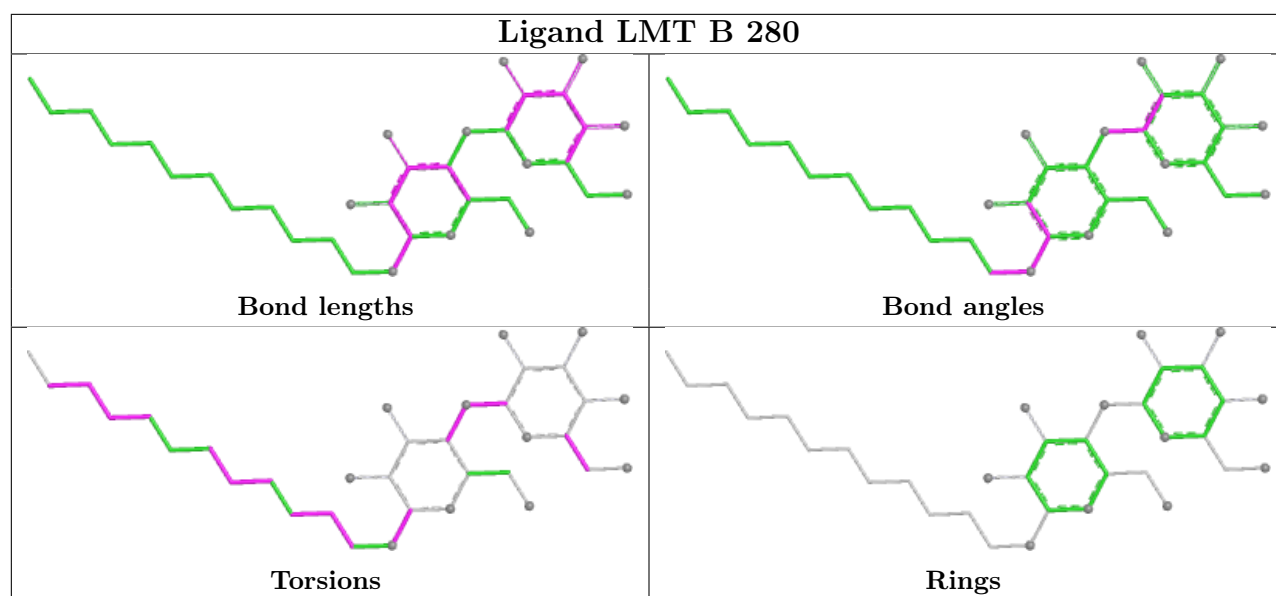
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

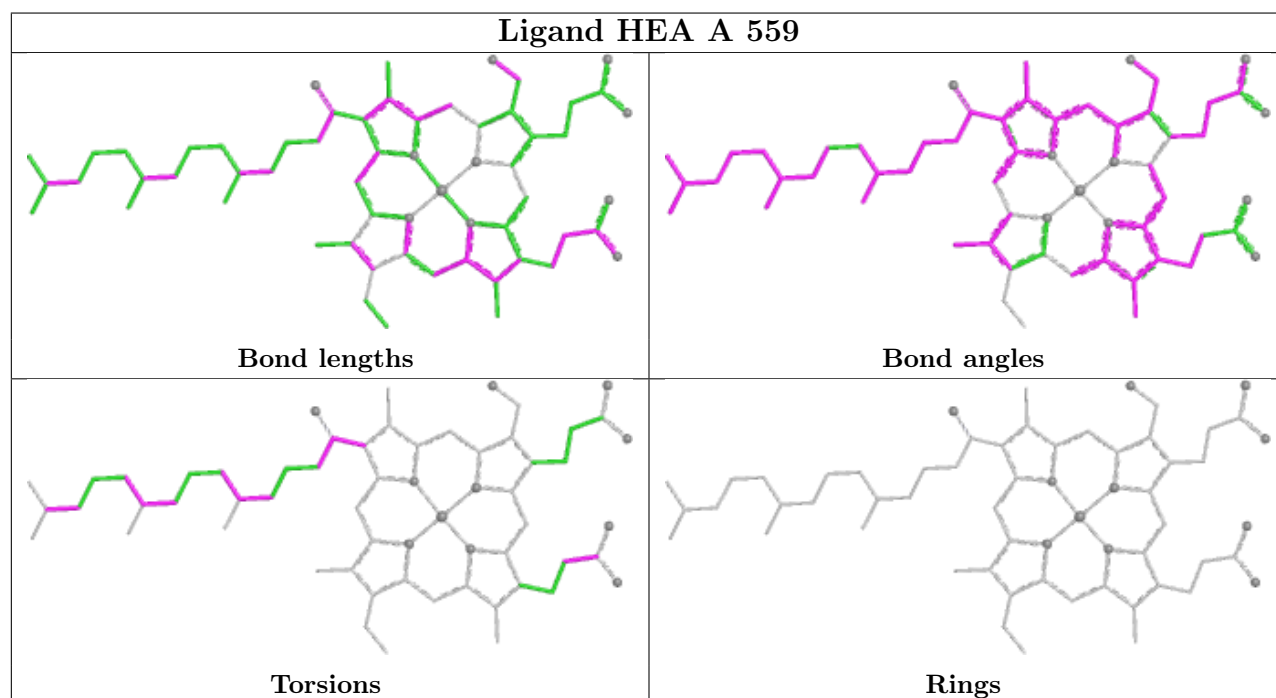
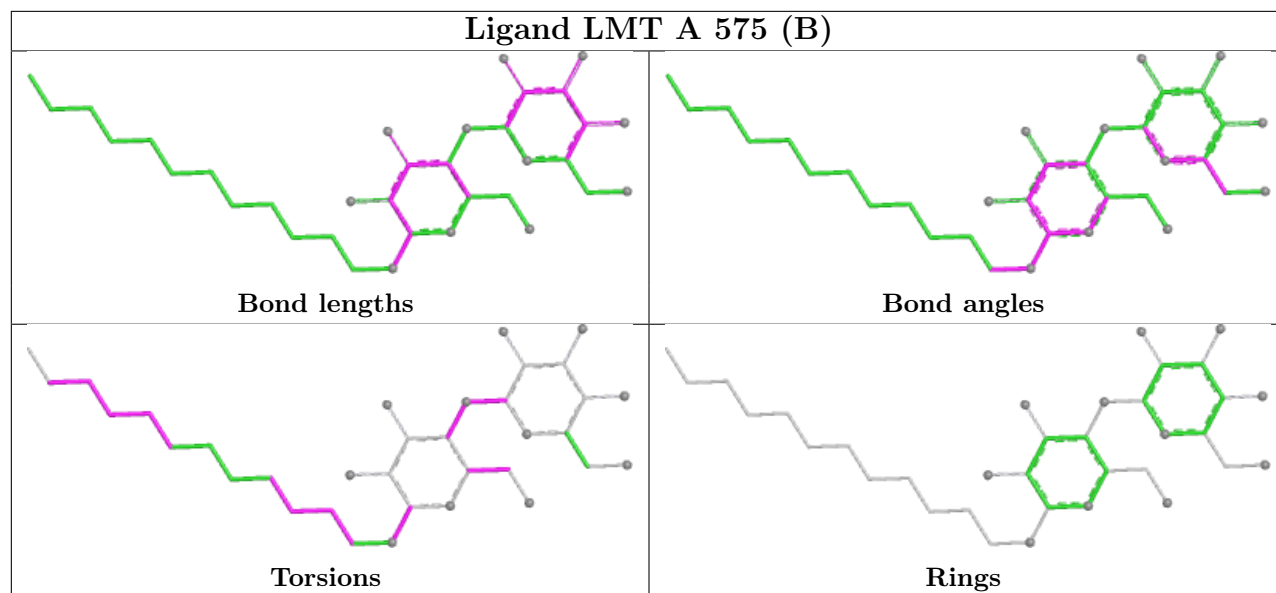
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

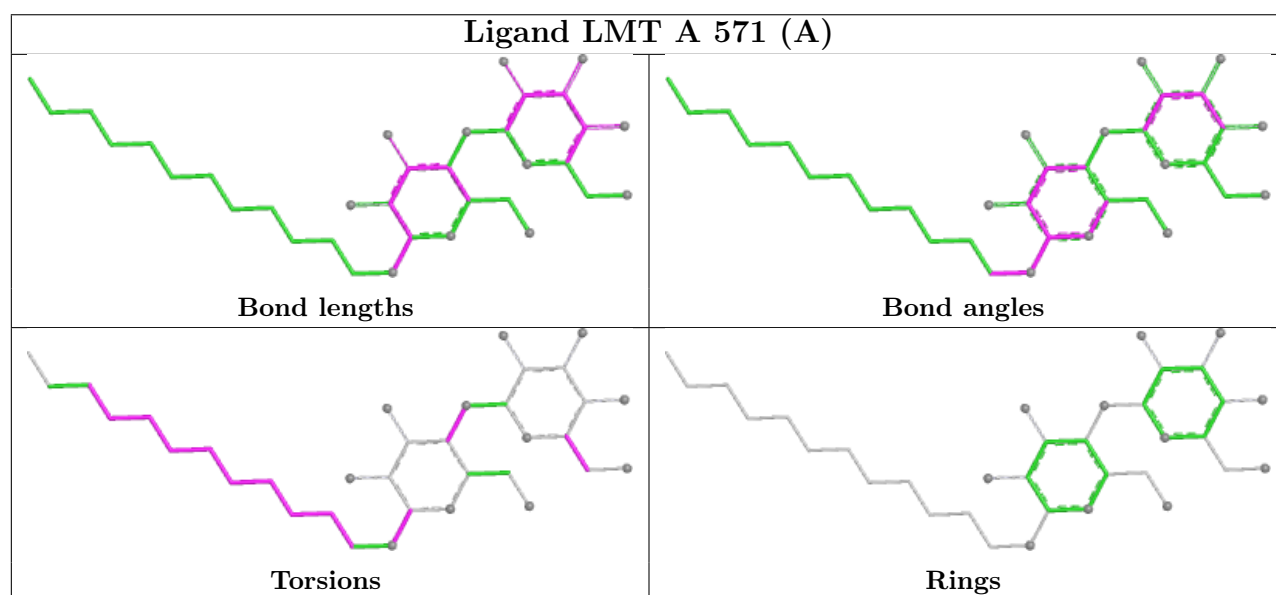
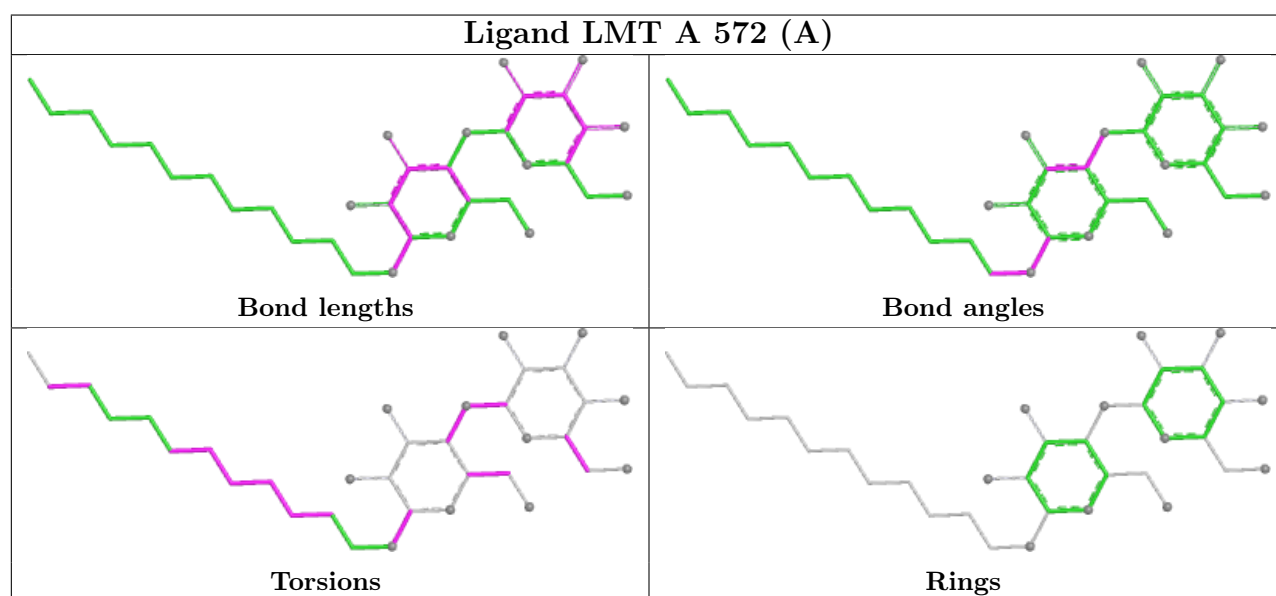
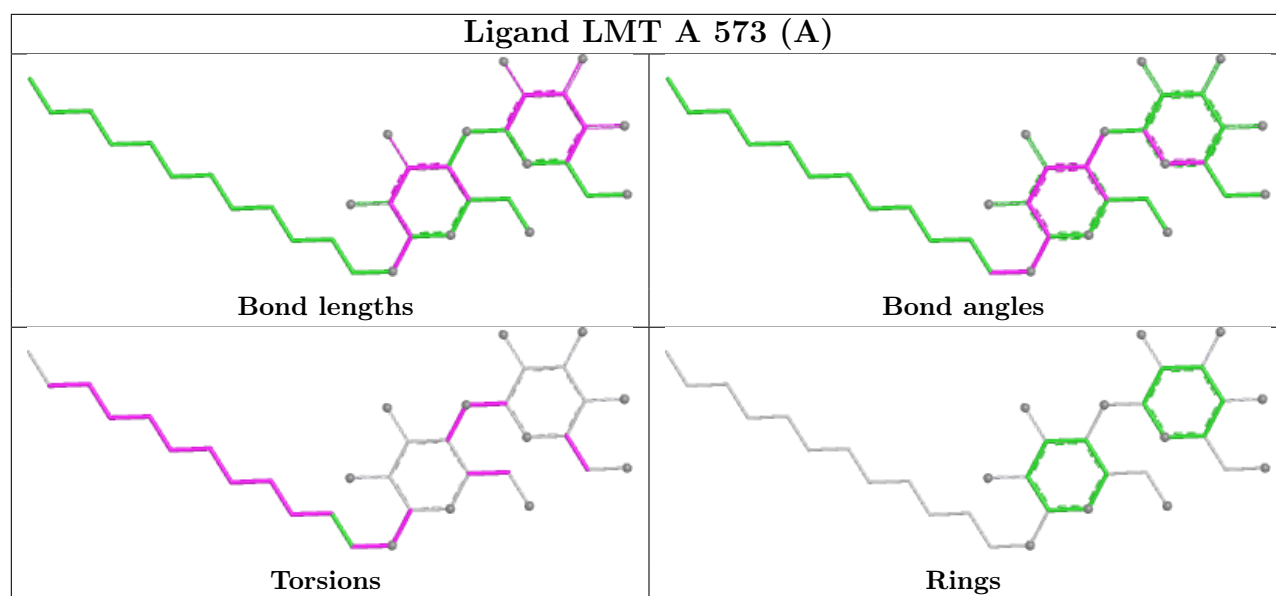


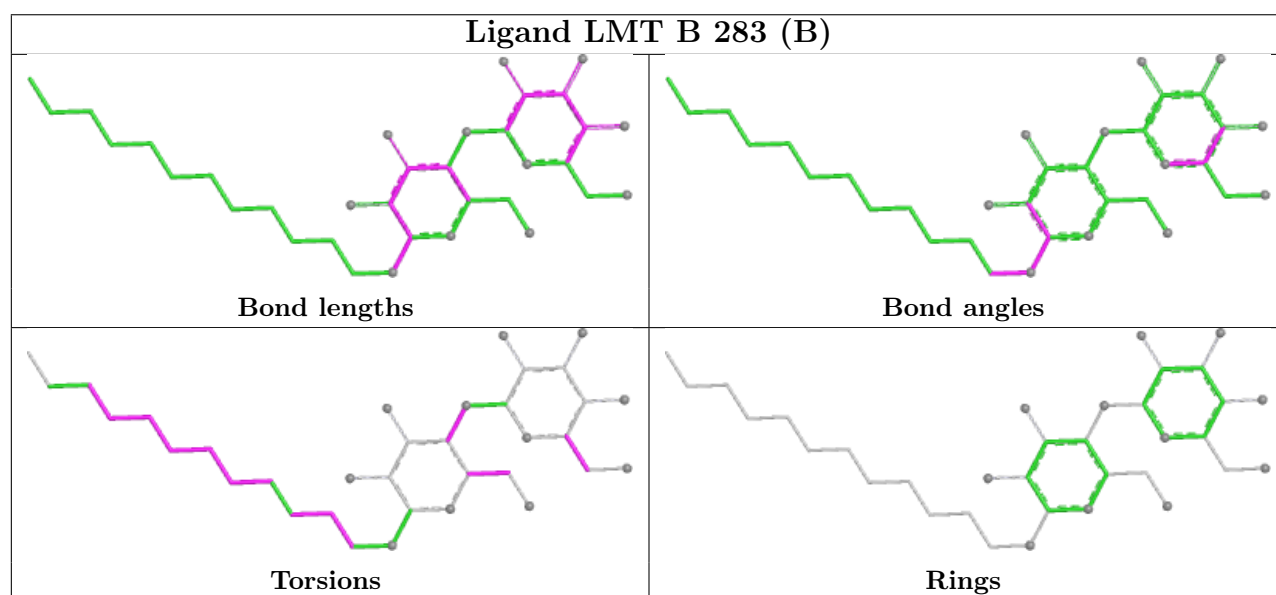
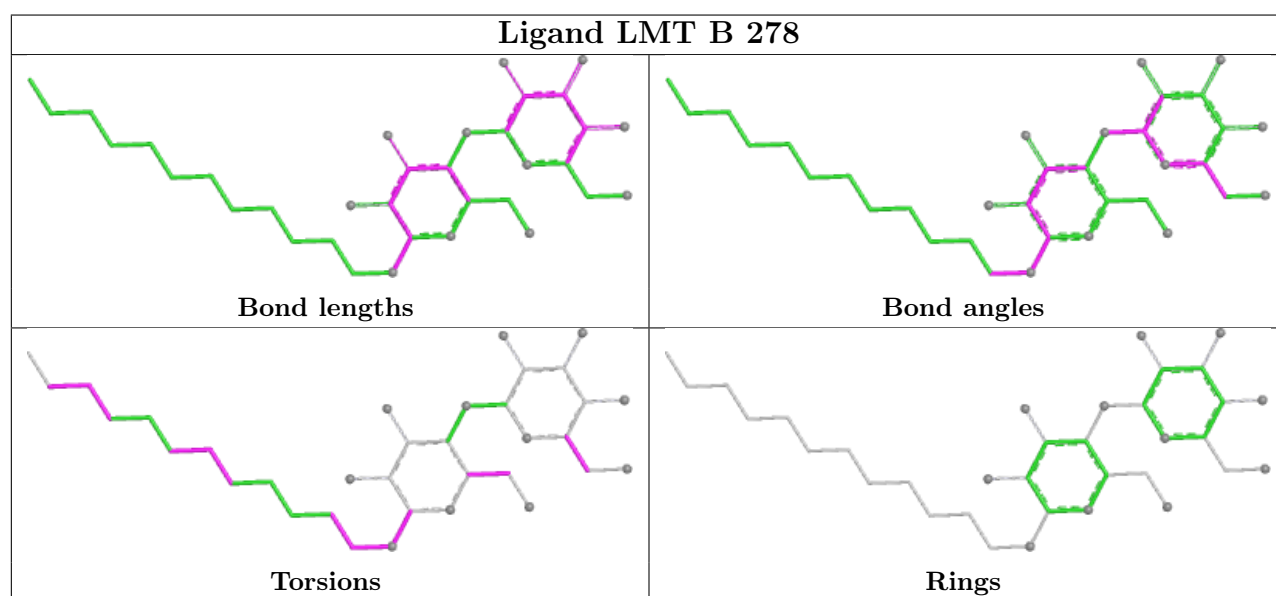
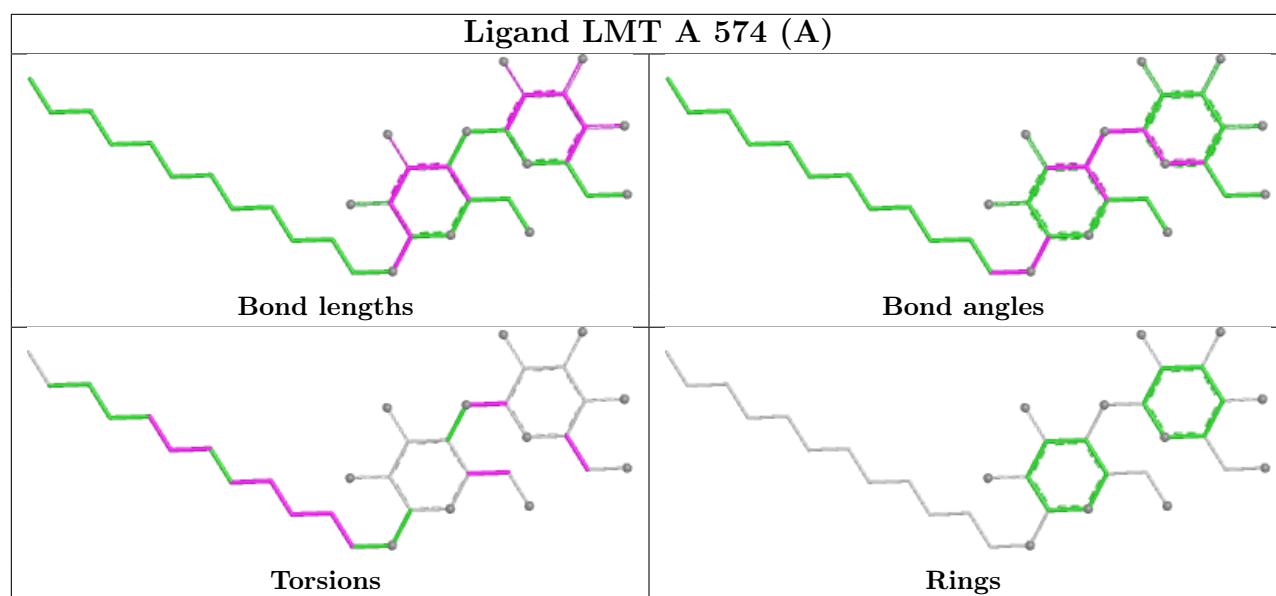


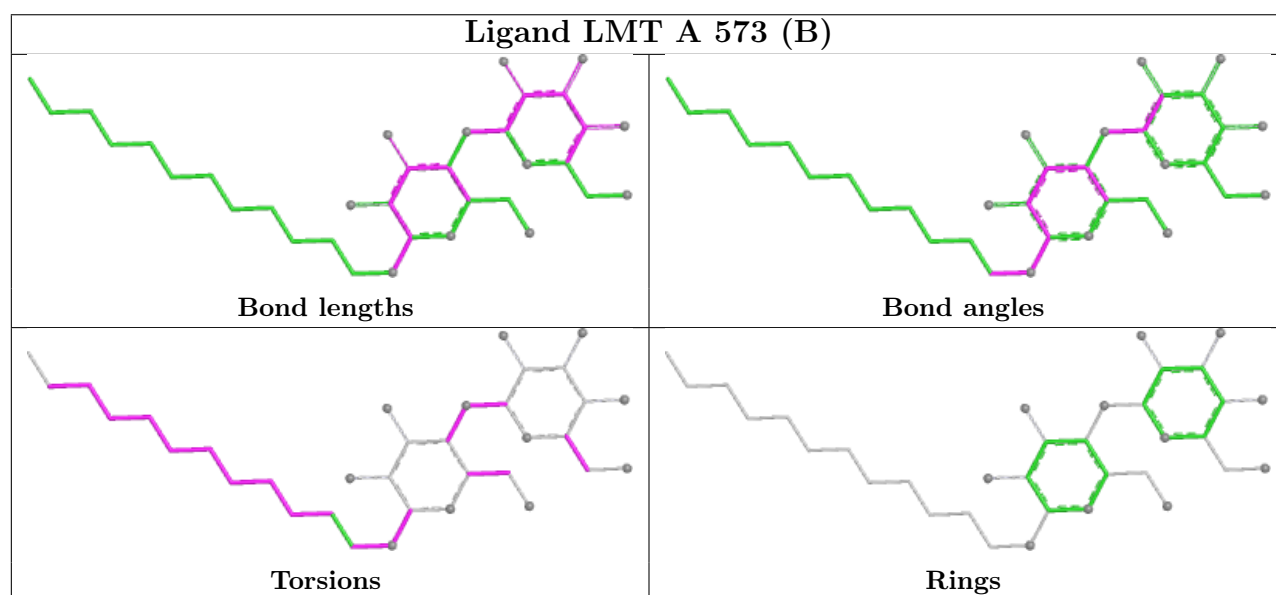
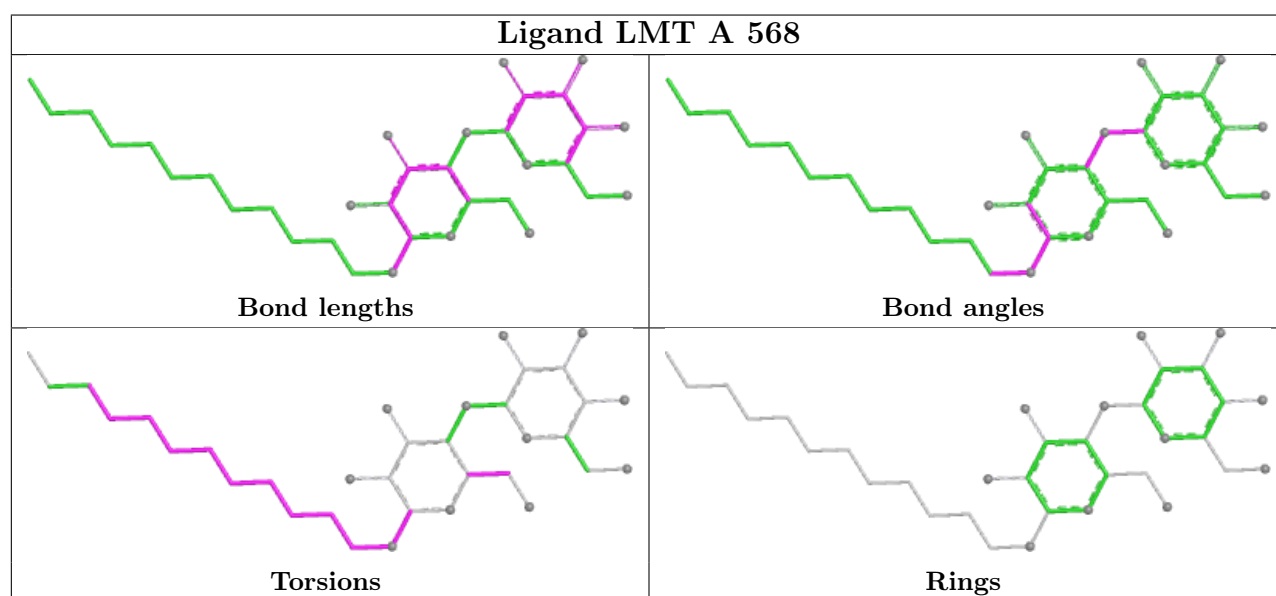
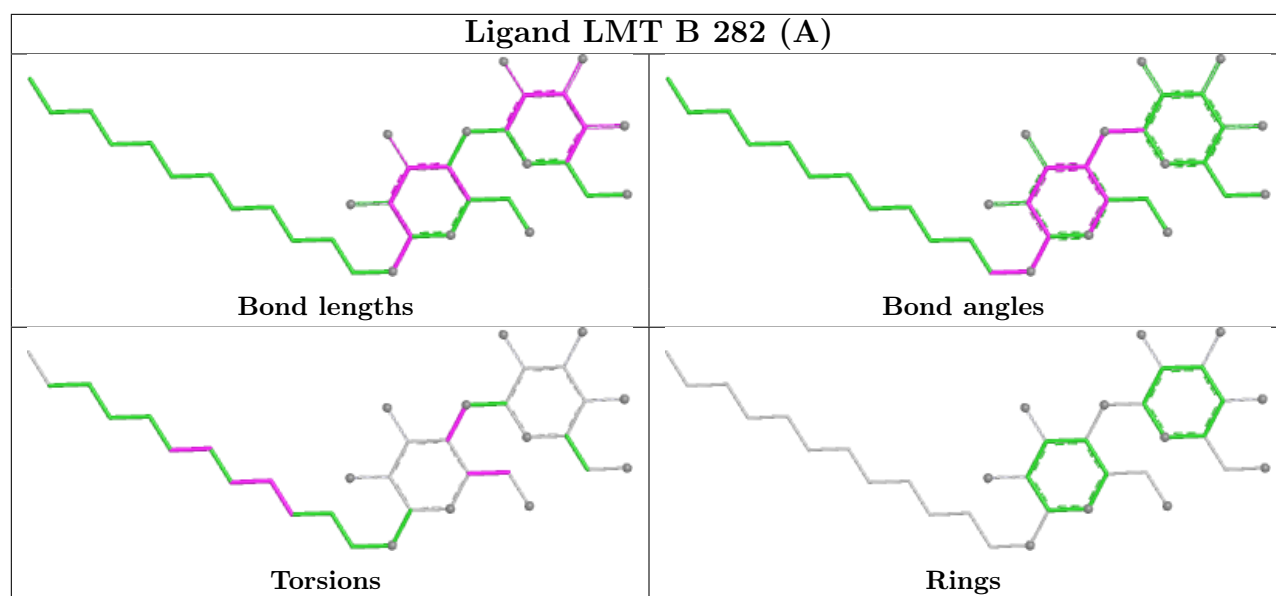


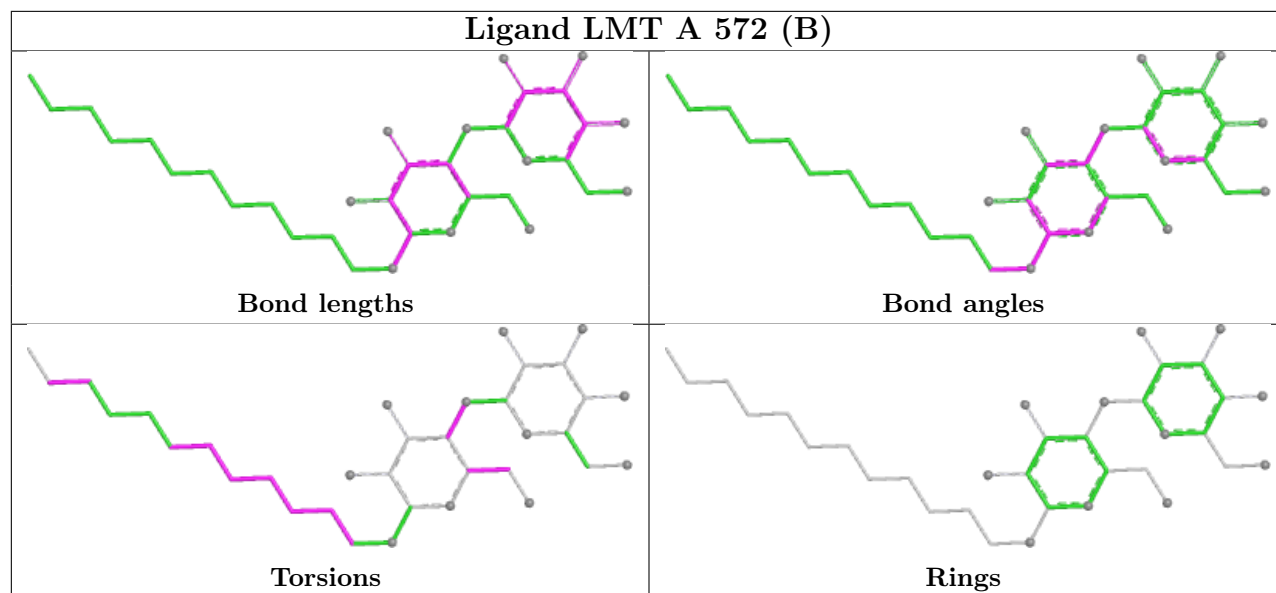












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	529/558 (94%)	-0.31	8 (1%) 71 73	18, 39, 62, 101	2 (0%)
2	B	252/298 (84%)	-0.59	0 100 100	15, 32, 50, 63	2 (0%)
3	C	118/127 (92%)	-0.19	2 (1%) 69 70	20, 45, 65, 74	2 (1%)
4	D	108/120 (90%)	-0.31	0 100 100	21, 41, 61, 69	0
All	All	1007/1103 (91%)	-0.37	10 (0%) 79 80	15, 38, 61, 101	6 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	118	SER	3.7
1	A	175	ALA	3.7
1	A	545	THR	3.5
1	A	173	THR	2.8
3	C	9	GLY	2.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

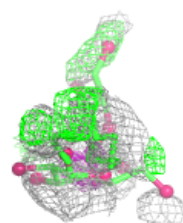
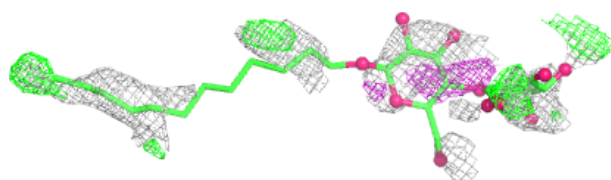
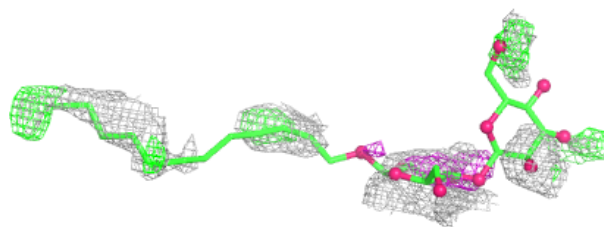
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	LDA	B	277	16/16	0.44	0.28	141,150,156,156	0
9	LDA	A	566	16/16	0.49	0.25	120,125,127,127	0
10	LMT	A	574[A]	35/35	0.53	0.29	140,155,159,159	12
10	LMT	A	574[B]	35/35	0.53	0.29	140,157,159,159	12
9	LDA	B	276	16/16	0.58	0.25	96,115,127,127	0
10	LMT	A	569	35/35	0.61	0.19	70,97,101,102	0
10	LMT	A	572[A]	35/35	0.64	0.24	100,105,108,108	23
10	LMT	A	572[B]	35/35	0.64	0.24	100,106,108,108	23
9	LDA	A	567	16/16	0.65	0.27	81,99,113,114	0
10	LMT	B	280	35/35	0.65	0.21	88,130,134,134	0
10	LMT	A	571[B]	35/35	0.66	0.25	79,104,112,112	12
10	LMT	A	571[A]	35/35	0.66	0.25	79,110,112,112	12
10	LMT	B	283[A]	35/35	0.67	0.19	71,86,88,88	23
10	LMT	B	283[B]	35/35	0.67	0.19	71,76,84,85	23
10	LMT	B	282[A]	35/35	0.68	0.18	57,120,122,122	12
10	LMT	B	282[B]	35/35	0.68	0.18	57,118,122,122	12
10	LMT	B	279	35/35	0.69	0.15	70,89,106,107	0
9	LDA	B	275	16/16	0.69	0.30	138,141,144,144	0
9	LDA	A	565	16/16	0.69	0.22	91,107,124,124	0
9	LDA	B	273	16/16	0.70	0.25	99,105,113,113	0
10	LMT	A	575[A]	35/35	0.70	0.23	91,121,127,127	12
10	LMT	A	575[B]	35/35	0.70	0.23	91,117,127,127	12
10	LMT	B	281	35/35	0.72	0.17	68,110,125,126	0
10	LMT	B	278	35/35	0.73	0.17	52,73,107,107	0
9	LDA	B	274	16/16	0.73	0.17	60,82,106,107	0
10	LMT	A	573[A]	35/35	0.74	0.20	50,102,107,108	12
10	LMT	A	573[B]	35/35	0.74	0.20	50,102,107,108	12
10	LMT	A	568	35/35	0.76	0.17	88,110,114,114	0
9	LDA	A	564	16/16	0.77	0.17	44,80,111,113	0
9	LDA	B	272	16/16	0.86	0.14	26,37,86,87	0
10	LMT	A	570	35/35	0.87	0.11	54,87,103,107	0
5	HEA	A	560	60/60	0.97	0.08	20,36,45,53	0
5	HEA	A	559	60/60	0.97	0.08	11,23,36,51	0
11	PEO	A	576	2/2	0.98	0.10	17,17,17,32	0
6	CU1	B	270	1/1	0.99	0.02	35,35,35,35	0
6	CU1	B	271	1/1	0.99	0.02	32,32,32,32	0
7	MN	A	562	1/1	0.99	0.02	34,34,34,34	0
8	CA	A	563	1/1	0.99	0.02	35,35,35,35	0
6	CU1	A	561	1/1	1.00	0.04	43,43,43,43	0

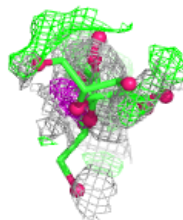
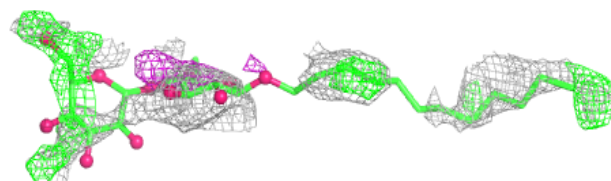
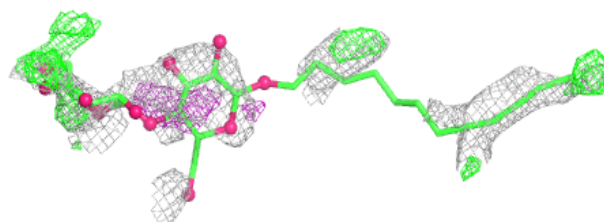
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 574 (A):

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

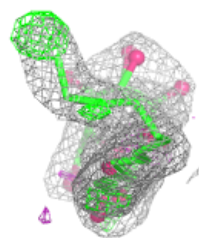
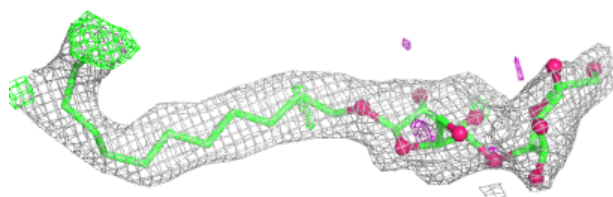
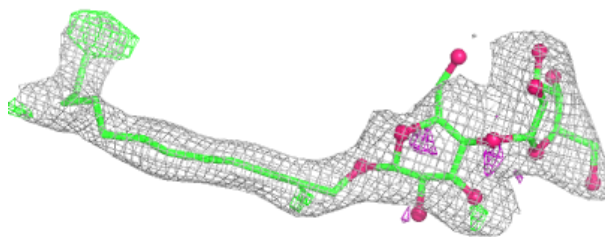
**Electron density around LMT A 574 (B):**

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

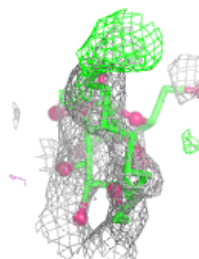
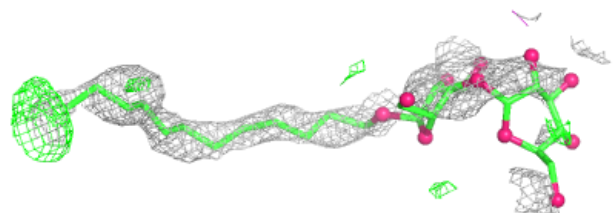
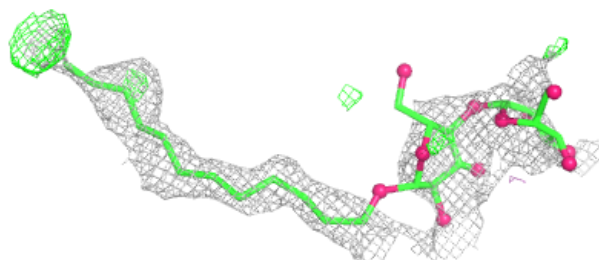


Electron density around LMT A 569:

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

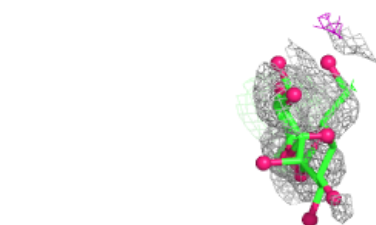
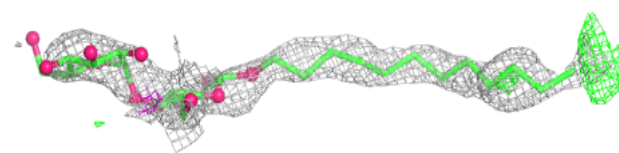
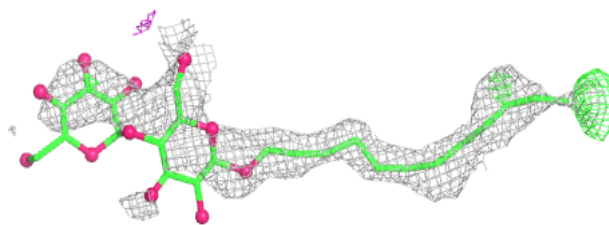
**Electron density around LMT A 572 (A):**

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

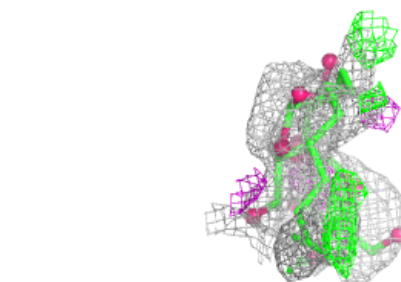
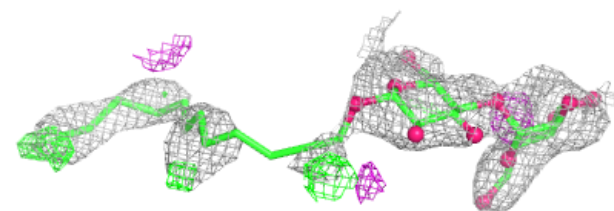
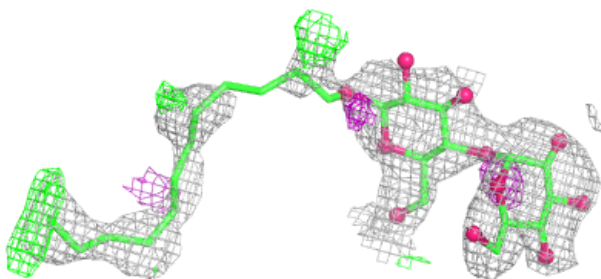


Electron density around LMT A 572 (B):

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

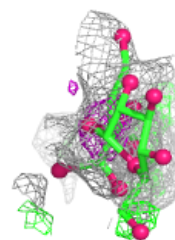
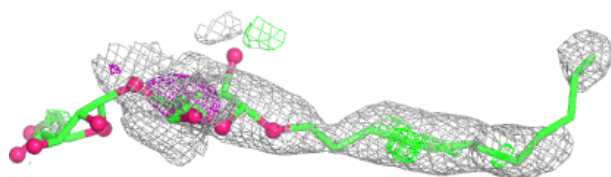
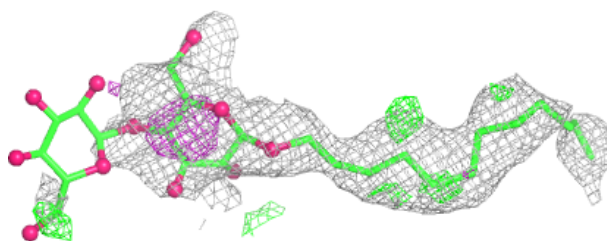
**Electron density around LMT B 280:**

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

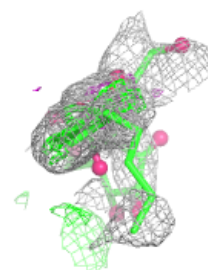
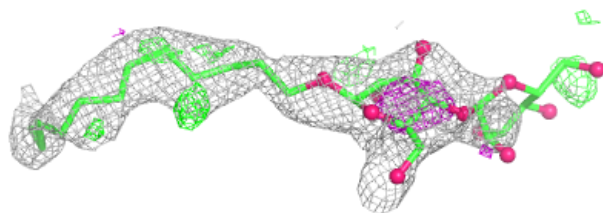
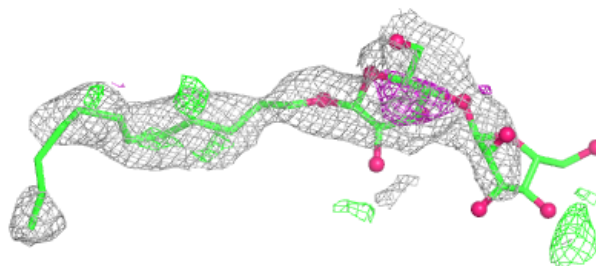


Electron density around LMT A 571 (B):

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

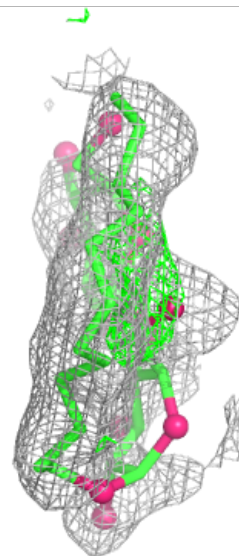
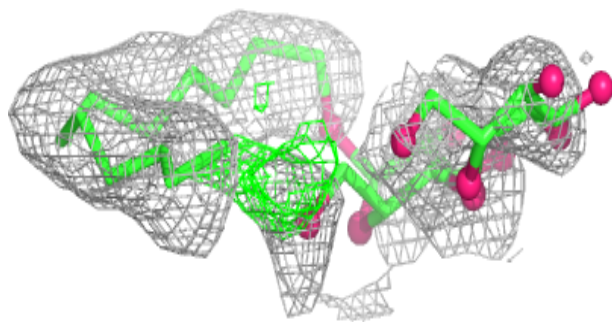
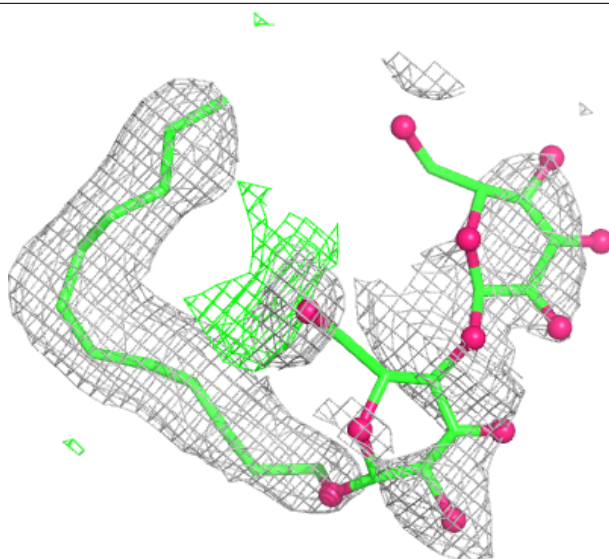
**Electron density around LMT A 571 (A):**

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



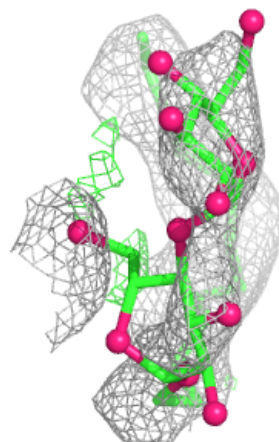
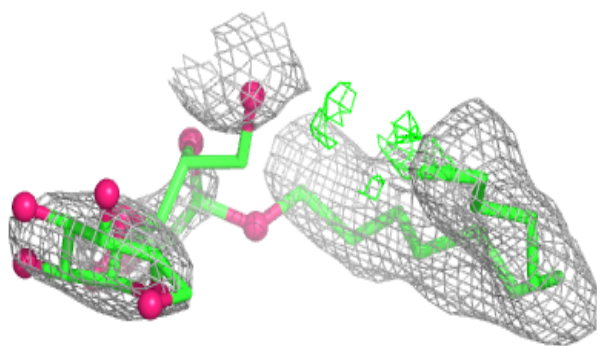
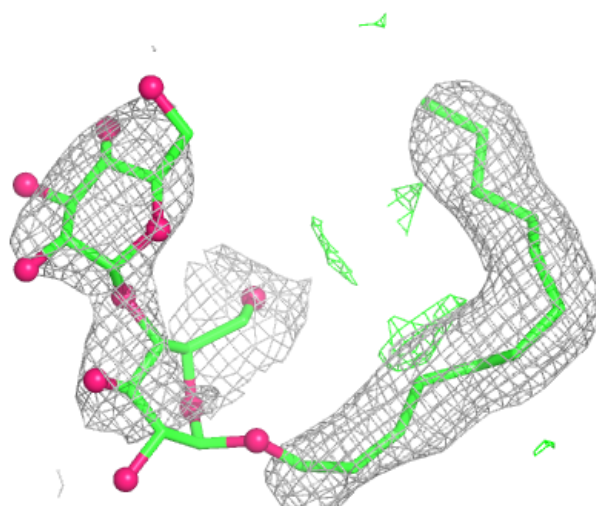
Electron density around LMT B 283 (A):

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



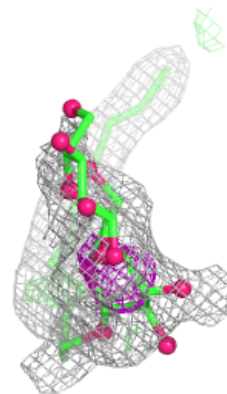
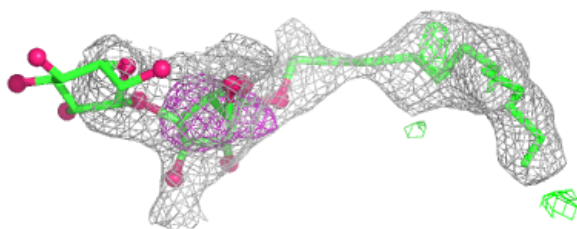
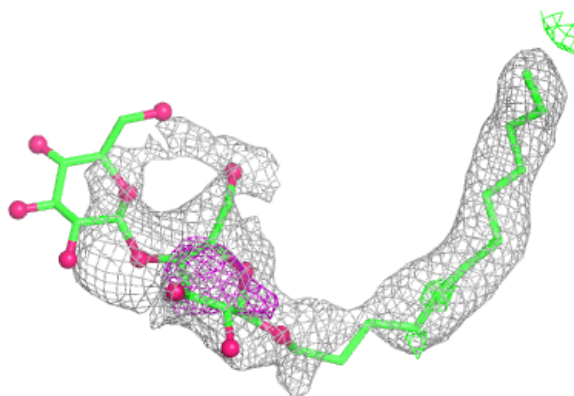
Electron density around LMT B 283 (B):

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

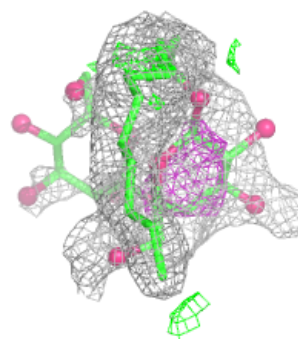
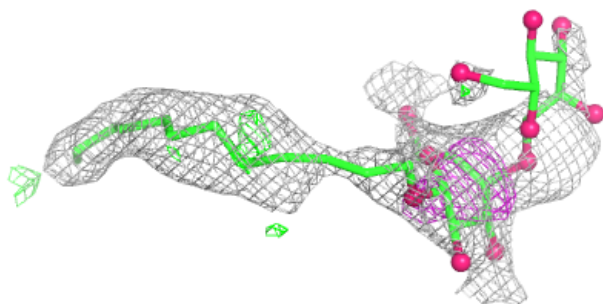
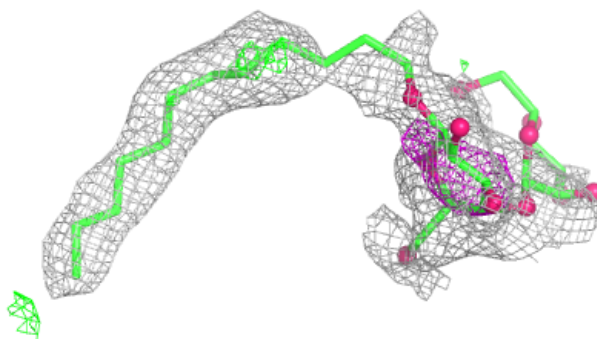


Electron density around LMT B 282 (A):

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

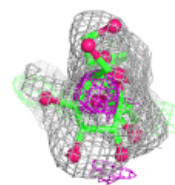
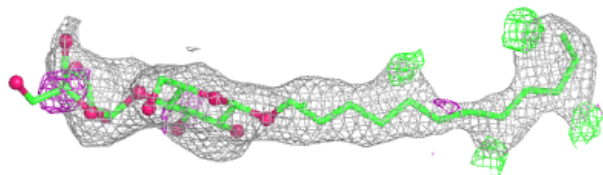
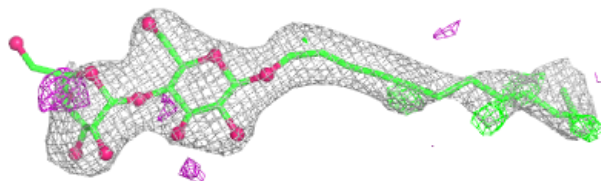
**Electron density around LMT B 282 (B):**

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

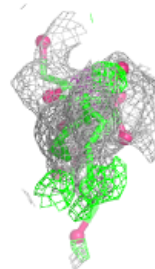
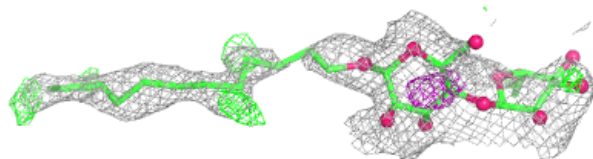
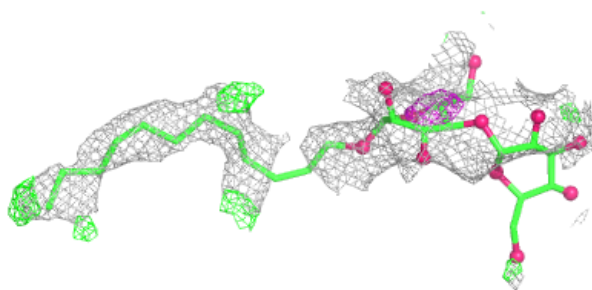


Electron density around LMT B 279:

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

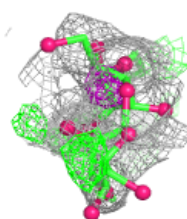
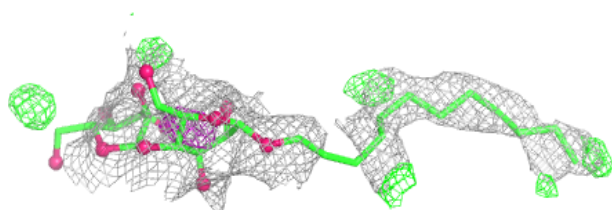
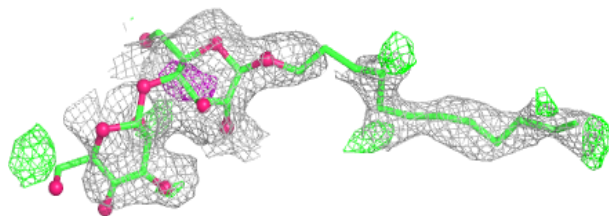
**Electron density around LMT A 575 (A):**

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

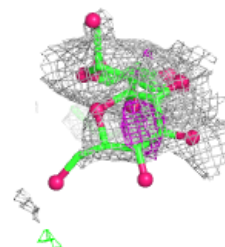
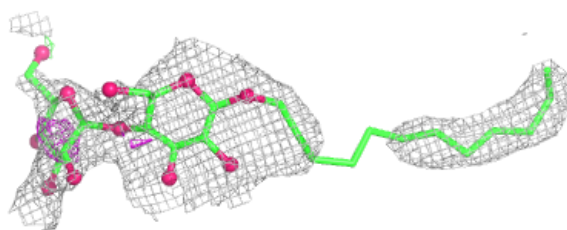
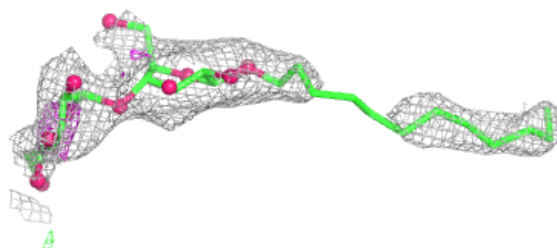


Electron density around LMT A 575 (B):

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

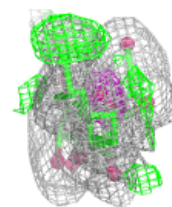
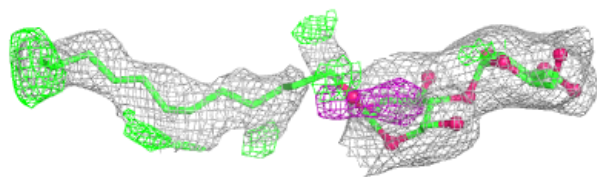
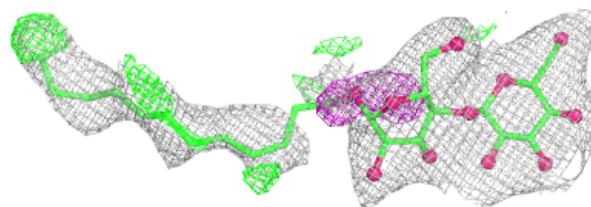
**Electron density around LMT B 281:**

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

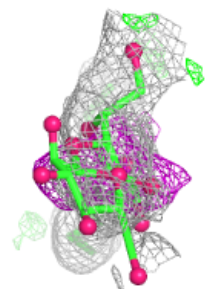
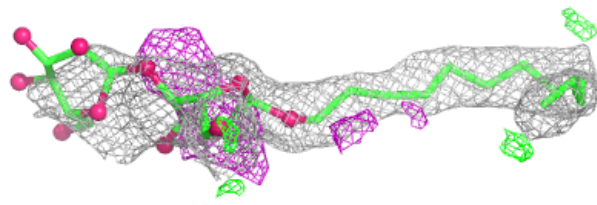
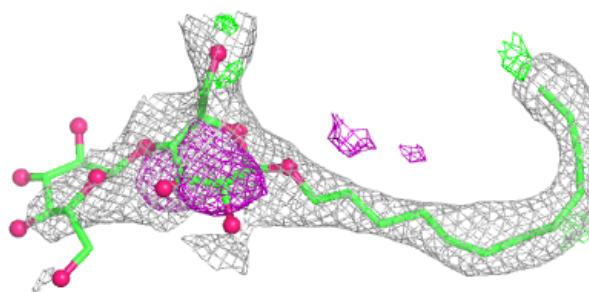


Electron density around LMT B 278:

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

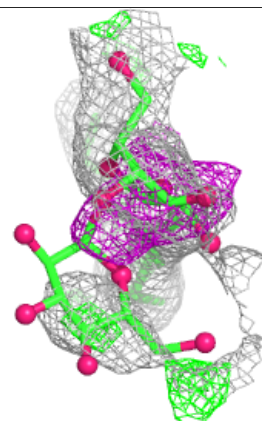
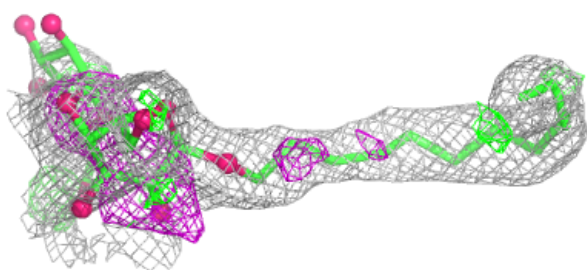
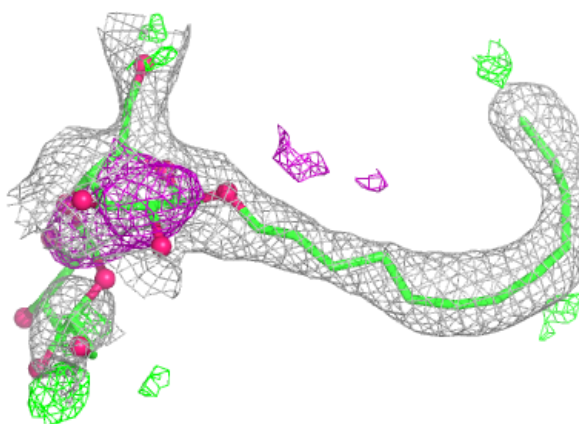
**Electron density around LMT A 573 (A):**

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

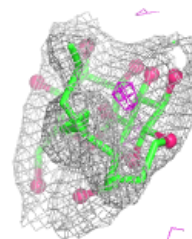
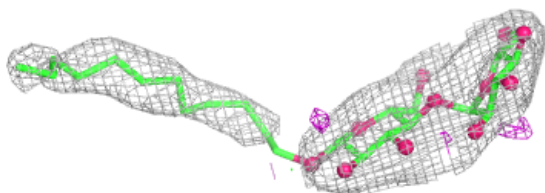
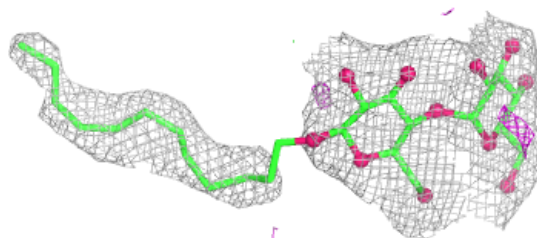


Electron density around LMT A 573 (B):

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

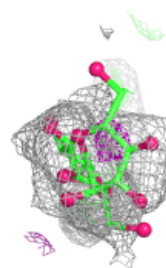
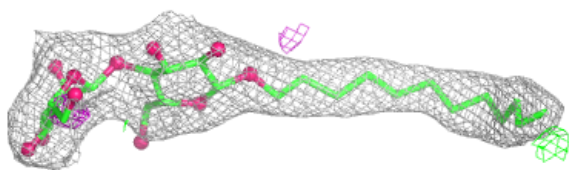
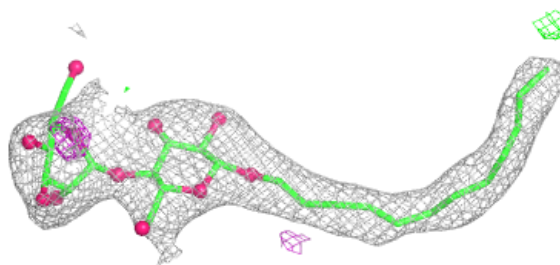
**Electron density around LMT A 568:**

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

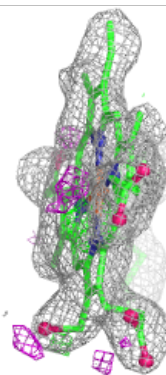
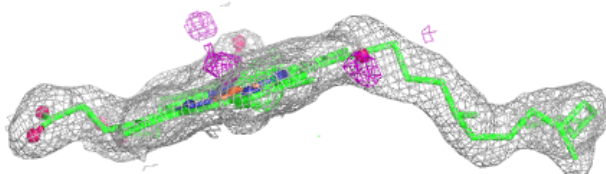
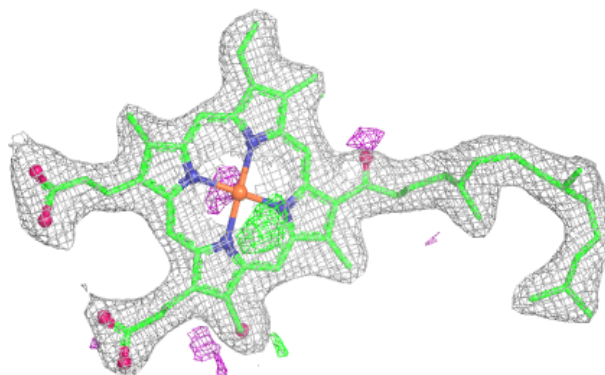


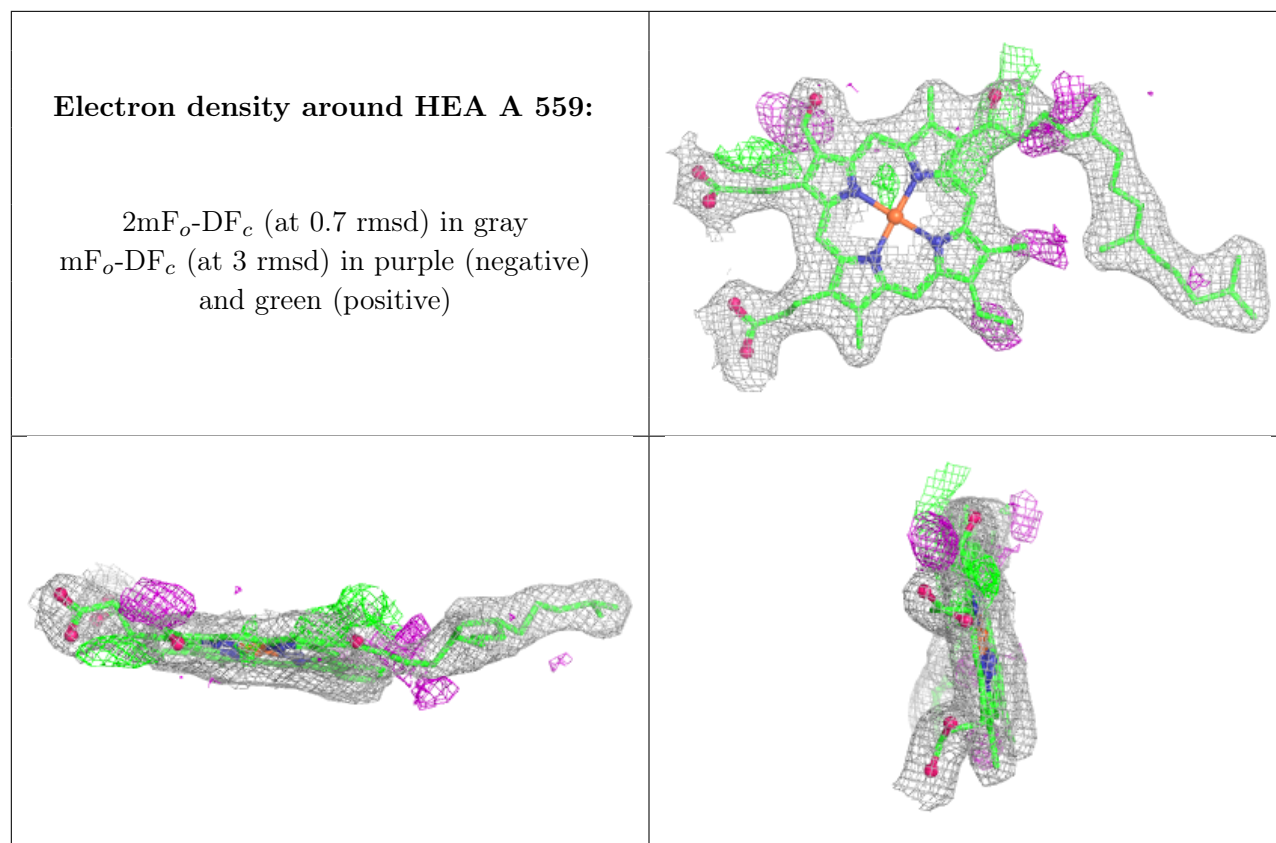
Electron density around LMT A 570:

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

**Electron density around HEA A 560:**

$2mF_o-DF_c$ (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.