wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 06:09 PM EDT

PDB ID	:	3EHB / pdb_00003ehb
Title	:	A D-Pathway Mutation Decouples the Paracoccus Denitrificans Cytochrome c Oxidase by Altering the side chain orientation of a distant, conserved Glutamate
Authors	:	Koepke, J.; Mueller, H.; Peng, G.
Deposited on	:	2008-09-12
Resolution	:	2.32 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

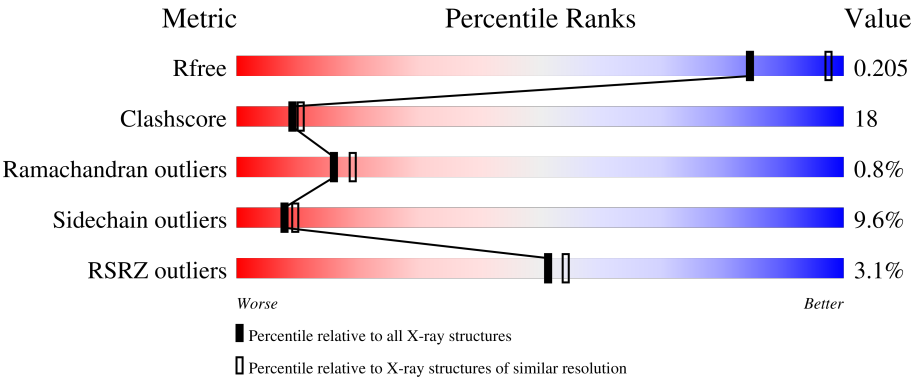
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	4% 57% 29% 8% • 5%
2	B	298	% 53% 25% 5% • 15%
3	C	127	3% 57% 28% 9% 6%
4	D	120	2% 53% 28% 8% • 9%

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
11	PER	A	576	-	X	-	-
5	HEA	A	559	X	-	-	-
5	HEA	A	560	X	X	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 9036 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	530	Total	C	N	O	S	0	3	1
			4199	2818	656	692	33			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	ASP	ASN	engineered mutation	UNP P98002

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	1	1
			1982	1298	320	356	8			

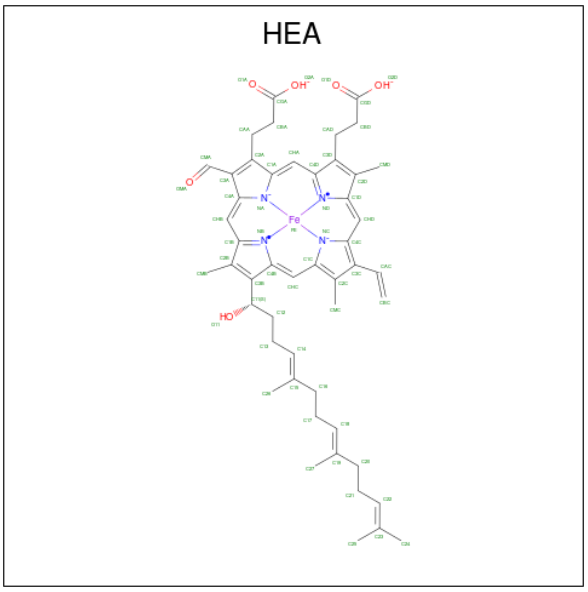
- Molecule 3 is a protein called FV fragment Chain H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	119	Total	C	N	O	S	0	2	1
			941	591	159	185	6			

- Molecule 4 is a protein called FV fragment Chain L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	109	Total	C	N	O	S	0	0	1
			832	530	136	164	2			

- Molecule 5 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (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		

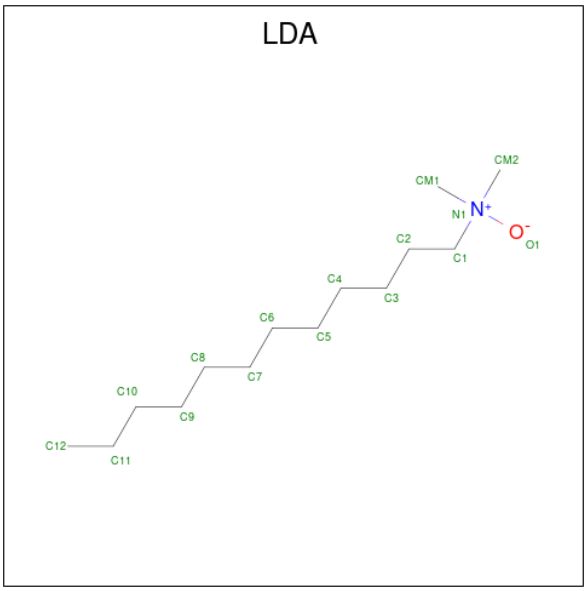
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

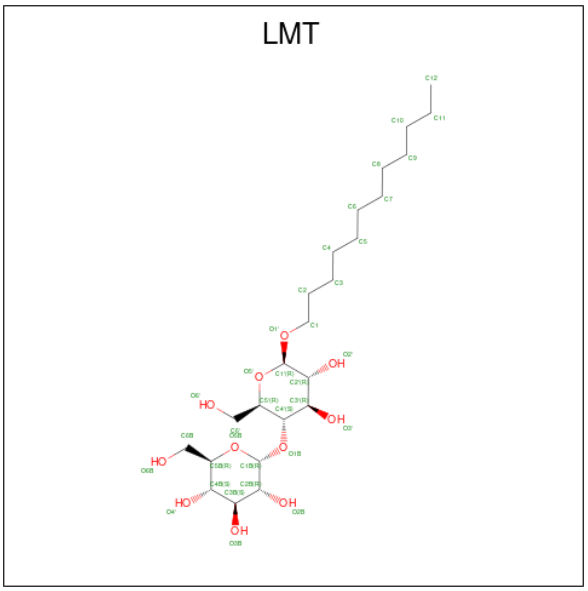
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



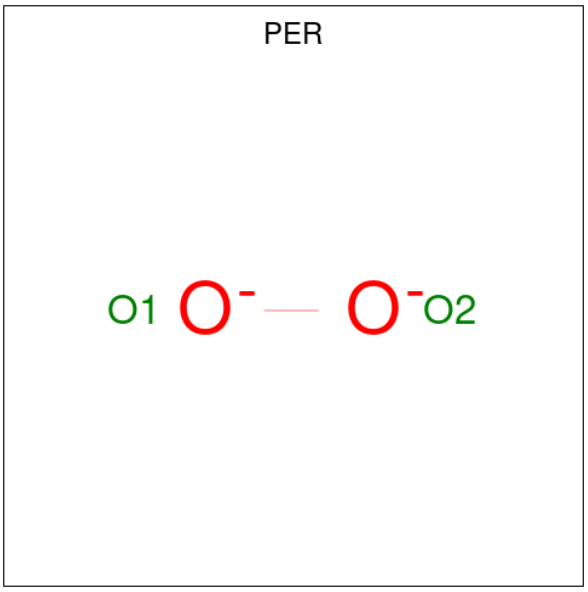
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	B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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	B	1	Total C O 47 36 11	0	1
10	B	1	Total C O 35 24 11	0	0
10	B	1	Total C O 35 24 11	0	0
10	D	1	Total C O 35 24 11	0	0

- Molecule 11 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	117	Total O 117 117	0	0
12	B	138	Total O 138 138	0	0
12	C	70	Total O 70 70	0	0
12	D	54	Total O 54 54	0	0

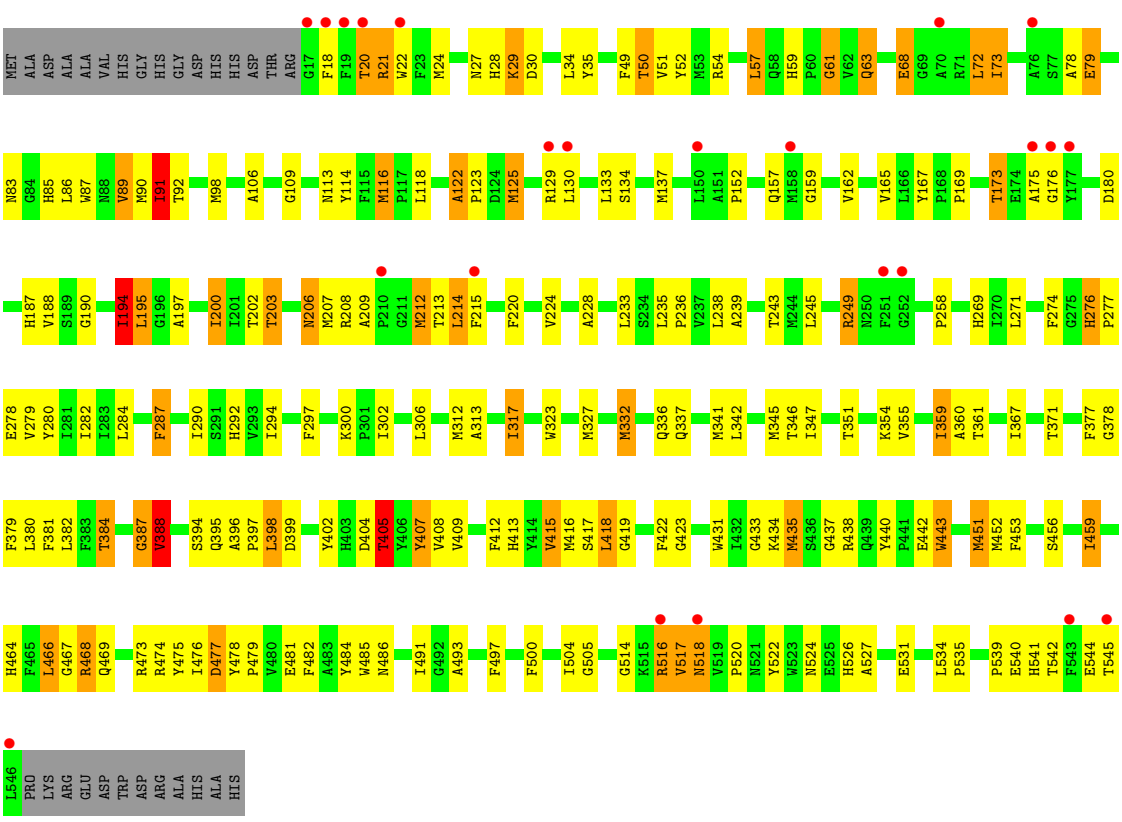
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1-beta

Chain A:

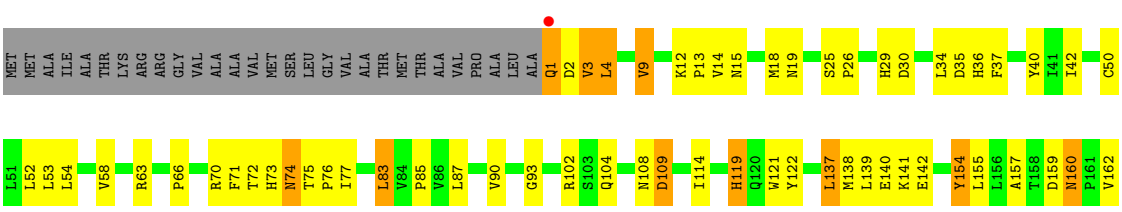




• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

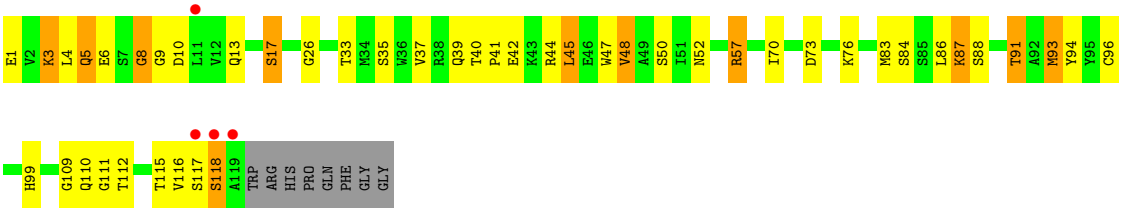






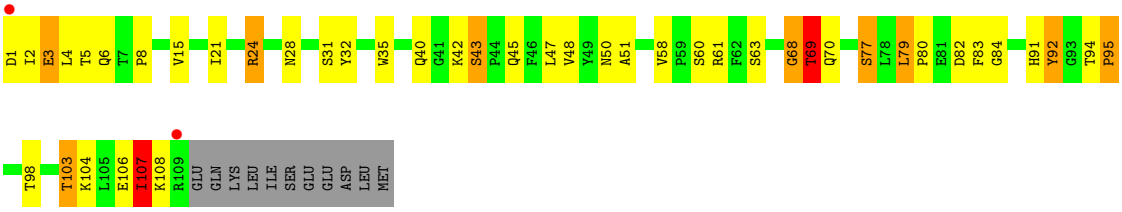
• Molecule 3: FV fragment Chain H





• Molecule 4: FV fragment Chain L





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.46Å 151.33Å 157.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 2.32 19.69 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.69-2.32) 98.8 (19.69-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.242 0.204 , 0.205	Depositor DCC
R_{free} test set	2629 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9036	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, PER, LMT, LDA, CU, MG, CA

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	1.44	22/4367 (0.5%)	1.43	39/5959 (0.7%)
2	B	1.67	26/2043 (1.3%)	1.56	20/2801 (0.7%)
3	C	1.37	4/973 (0.4%)	1.30	7/1316 (0.5%)
4	D	1.55	10/853 (1.2%)	1.54	14/1158 (1.2%)
All	All	1.51	62/8236 (0.8%)	1.46	80/11234 (0.7%)

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
3	C	0	1

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	HIS	CA-C	8.91	1.62	1.52
2	B	222	ILE	CG1-CD1	8.53	1.85	1.51
2	B	178	ASP	CA-C	8.18	1.59	1.52
2	B	155	LEU	N-CA	8.06	1.56	1.46
4	D	98	THR	CA-CB	7.88	1.65	1.53

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	154	TYR	CA-C-N	-11.99	103.46	122.65
2	B	154	TYR	C-N-CA	-11.99	103.46	122.65
4	D	58	VAL	CA-C-N	-10.27	110.36	120.52
4	D	58	VAL	C-N-CA	-10.27	110.36	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	PRO	N-CA-C	-10.26	95.07	111.38

There are no chirality outliers.

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	4199	0	4116	185	0
2	B	1982	0	1965	63	0
3	C	941	0	898	29	0
4	D	832	0	807	26	0
5	A	120	0	104	21	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	80	0	155	15	0
10	A	280	0	335	26	0
10	B	117	0	133	8	0
10	D	35	0	39	3	0
11	A	2	0	0	0	0
12	A	117	0	0	4	0
12	B	138	0	0	5	0
12	C	70	0	0	4	0
12	D	54	0	0	2	0
All	All	9036	0	8676	316	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 18.

The worst 5 of 316 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	1.85	1.55
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.07	1.44
1:A:276:HIS:NE2	1:A:280:TYR:CE2	1.96	1.31
10:A:575:LMT:O6B	10:A:575:LMT:C6B	1.81	1.28
1:A:342:LEU:HA	1:A:345:MET:CE	1.78	1.13

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	531/558 (95%)	494 (93%)	34 (6%)	3 (1%)	21	25
2	B	252/298 (85%)	240 (95%)	10 (4%)	2 (1%)	16	19
3	C	119/127 (94%)	110 (92%)	8 (7%)	1 (1%)	16	19
4	D	107/120 (89%)	101 (94%)	4 (4%)	2 (2%)	6	5
All	All	1009/1103 (92%)	945 (94%)	56 (6%)	8 (1%)	16	19

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	ASN
3	C	118	SER
1	A	79	GLU
4	D	77	SER
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%)	397 (91%)	38 (9%)	9 12
2	B	212/243 (87%)	190 (90%)	22 (10%)	7 8
3	C	103/107 (96%)	92 (89%)	11 (11%)	6 7
4	D	92/104 (88%)	80 (87%)	12 (13%)	4 4
All	All	842/908 (93%)	759 (90%)	83 (10%)	8 9

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	186	PRO
4	D	1	ASP
2	B	222	ILE
3	C	42	GLU
4	D	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	GLN
2	B	104	GLN
4	D	90	HIS
2	B	73	HIS
2	B	120	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 30 ligands modelled in this entry, 5 are 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	$\#\|Z\| > 2$
9	LDA	B	272	-	13,15,15	2.08	2 (15%)	14,17,17	0.68	0
10	LMT	B	277[A]	-	36,36,36	4.20	15 (41%)	47,47,47	1.91	9 (19%)
10	LMT	A	570	-	36,36,36	4.19	16 (44%)	47,47,47	1.46	5 (10%)
9	LDA	A	564	-	13,15,15	2.27	2 (15%)	14,17,17	0.64	0
10	LMT	B	278	-	36,36,36	4.16	13 (36%)	47,47,47	1.63	9 (19%)
10	LMT	A	571	-	36,36,36	4.25	17 (47%)	47,47,47	1.52	7 (14%)
10	LMT	A	573	-	36,36,36	3.98	16 (44%)	47,47,47	1.64	8 (17%)
9	LDA	B	273	-	13,15,15	1.98	2 (15%)	14,17,17	0.60	0
9	LDA	B	274	-	13,15,15	2.00	2 (15%)	14,17,17	0.49	0
10	LMT	A	575	-	36,36,36	4.40	16 (44%)	47,47,47	1.56	7 (14%)
9	LDA	A	566	-	13,15,15	1.91	2 (15%)	14,17,17	0.55	0
5	HEA	A	560	11,1	67,67,67	3.88	40 (59%)	81,103,103	4.33	50 (61%)
10	LMT	B	279	-	36,36,36	4.19	13 (36%)	47,47,47	1.24	5 (10%)
5	HEA	A	559	1	67,67,67	3.31	26 (38%)	81,103,103	4.52	53 (65%)
9	LDA	A	567	-	13,15,15	2.14	2 (15%)	14,17,17	0.40	0
10	LMT	A	572	-	36,36,36	3.98	17 (47%)	47,47,47	1.53	5 (10%)
10	LMT	D	121	-	36,36,36	4.04	15 (41%)	47,47,47	2.16	12 (25%)
9	LDA	B	276	-	13,15,15	2.13	2 (15%)	14,17,17	0.44	0
9	LDA	A	565	-	13,15,15	1.98	2 (15%)	14,17,17	0.49	0
9	LDA	B	275	-	13,15,15	2.16	2 (15%)	14,17,17	0.60	0
11	PER	A	576	5,6	1,1,1	2.38	1 (100%)	-		
10	LMT	A	574	-	36,36,36	4.21	15 (41%)	47,47,47	1.64	6 (12%)
10	LMT	A	569	-	36,36,36	4.29	16 (44%)	47,47,47	1.97	13 (27%)
10	LMT	A	568	-	36,36,36	4.28	14 (38%)	47,47,47	1.23	4 (8%)
10	LMT	B	277[B]	-	36,36,36	4.20	15 (41%)	47,47,47	1.82	9 (19%)

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
9	LDA	B	272	-	-	6/13/13/13	-
10	LMT	B	277[A]	-	-	10/21/61/61	0/2/2/2
10	LMT	A	570	-	-	12/21/61/61	0/2/2/2
9	LDA	A	564	-	-	7/13/13/13	-
10	LMT	B	278	-	-	13/21/61/61	0/2/2/2
10	LMT	A	571	-	-	15/21/61/61	0/2/2/2
10	LMT	A	573	-	-	11/21/61/61	0/2/2/2
9	LDA	B	273	-	-	9/13/13/13	-
9	LDA	B	274	-	-	10/13/13/13	-
10	LMT	A	575	-	-	15/21/61/61	0/2/2/2
9	LDA	A	566	-	-	7/13/13/13	-
5	HEA	A	560	11,1	1/1/7/16	18/36/76/76	-
10	LMT	B	279	-	-	13/21/61/61	0/2/2/2
5	HEA	A	559	1	1/1/7/16	17/36/76/76	-
9	LDA	A	567	-	-	9/13/13/13	-
10	LMT	A	572	-	-	13/21/61/61	0/2/2/2
10	LMT	D	121	-	-	14/21/61/61	0/2/2/2
9	LDA	B	276	-	-	8/13/13/13	-
9	LDA	A	565	-	-	8/13/13/13	-
9	LDA	B	275	-	-	4/13/13/13	-
10	LMT	A	574	-	-	16/21/61/61	0/2/2/2
10	LMT	A	569	-	-	9/21/61/61	0/2/2/2
10	LMT	A	568	-	-	10/21/61/61	0/2/2/2
10	LMT	B	277[B]	-	-	5/21/61/61	0/2/2/2

The worst 5 of 283 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	O11-C11	-12.12	1.16	1.42
5	A	560	HEA	C14-C15	11.09	1.58	1.33
5	A	559	HEA	O11-C11	-9.26	1.22	1.42
10	A	575	LMT	O6B-C6B	9.22	1.81	1.42
5	A	559	HEA	OMA-CMA	9.09	1.42	1.22

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	560	HEA	C13-C12-C11	-15.25	90.03	114.39
5	A	560	HEA	C12-C11-C3B	13.24	132.82	112.12
5	A	559	HEA	C12-C11-C3B	11.28	129.75	112.12
5	A	559	HEA	C17-C18-C19	-10.26	104.14	127.62
5	A	559	HEA	CHB-C1B-NB	10.07	135.26	124.42

All (2) chirality outliers are listed below:

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

5 of 259 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	559	HEA	C2A-C3A-CMA-OMA
5	A	559	HEA	C4A-C3A-CMA-OMA
5	A	559	HEA	O11-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C4B

There are no ring outliers.

20 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	272	LDA	4	0
10	A	570	LMT	3	0
9	A	564	LDA	1	0
10	B	278	LMT	2	0
10	A	571	LMT	3	0
9	B	273	LDA	3	0
9	B	274	LDA	4	0
10	A	575	LMT	5	0
9	A	566	LDA	3	0
5	A	560	HEA	12	0
10	B	279	LMT	6	0
5	A	559	HEA	9	0
10	A	572	LMT	3	0
10	D	121	LMT	3	0
9	B	276	LDA	1	0
9	A	565	LDA	1	0

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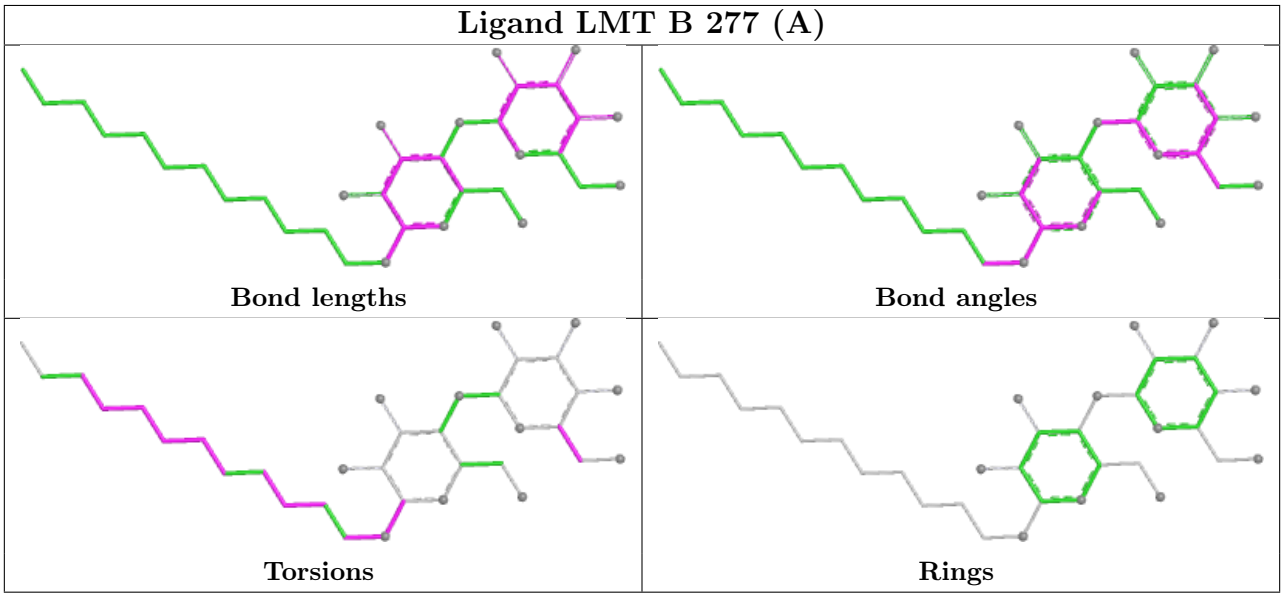
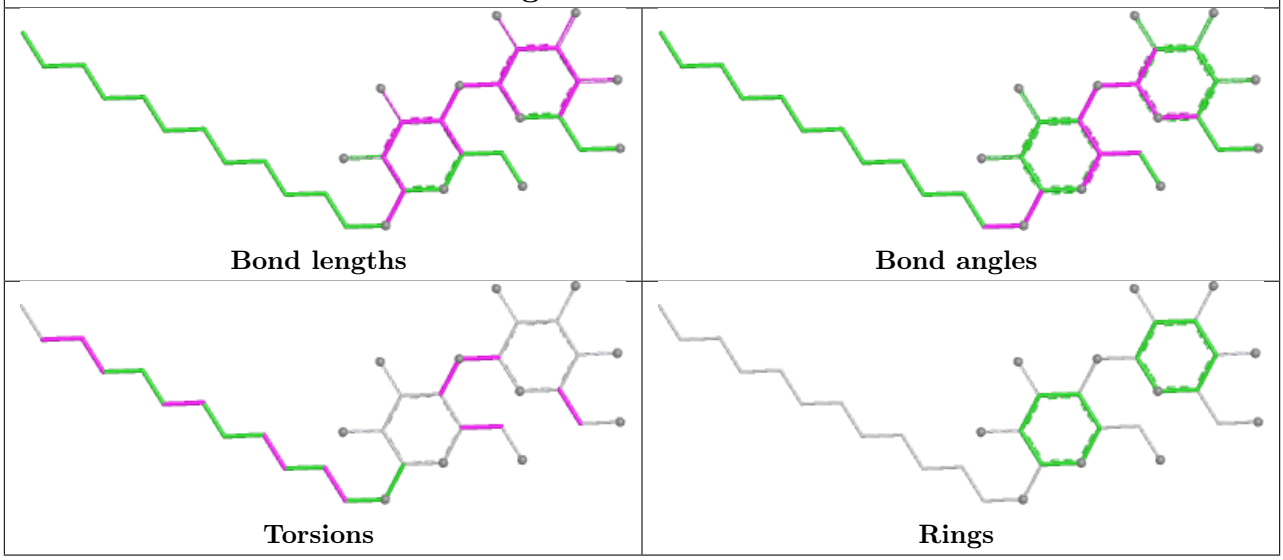
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	275	LDA	4	0
10	A	574	LMT	8	0
10	A	569	LMT	2	0
10	A	568	LMT	2	0

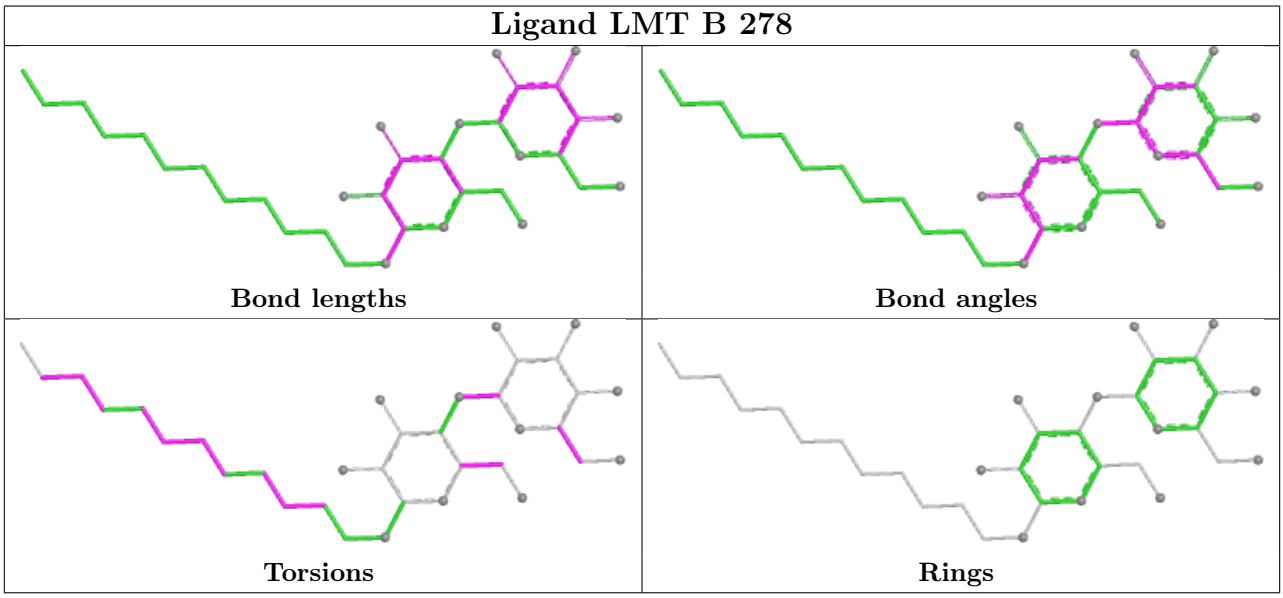
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



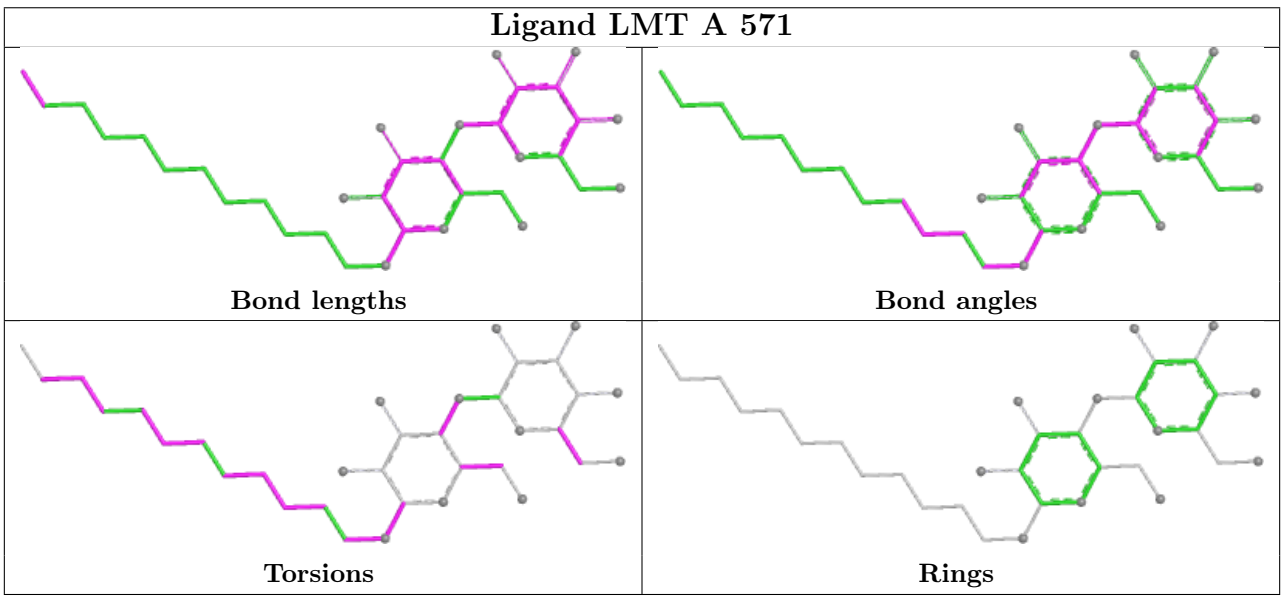
Ligand LMT A 570



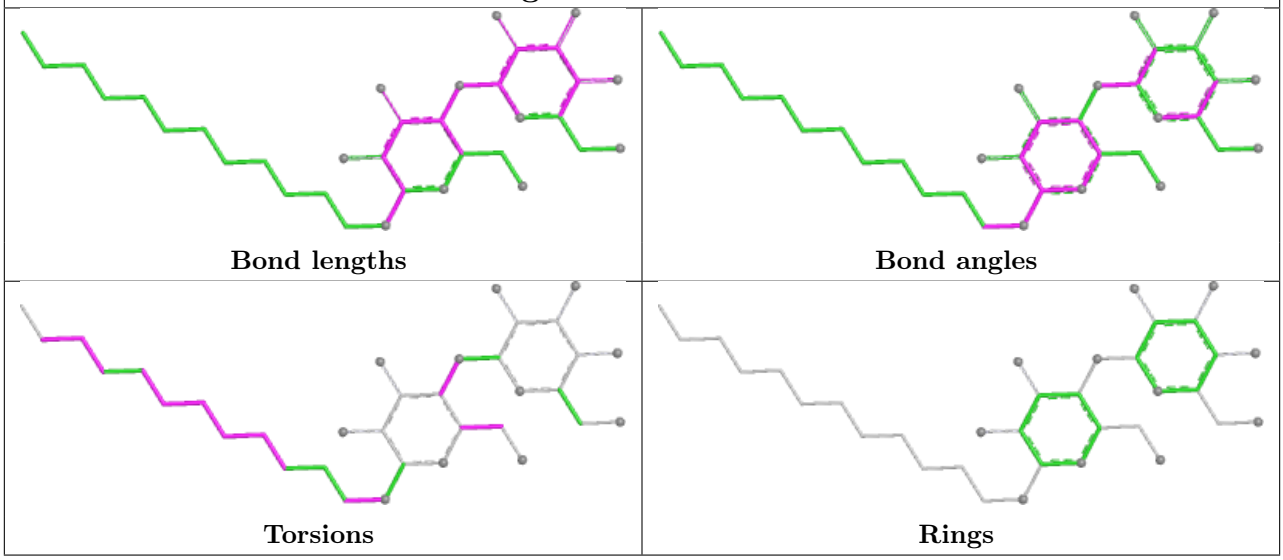
Ligand LMT B 278



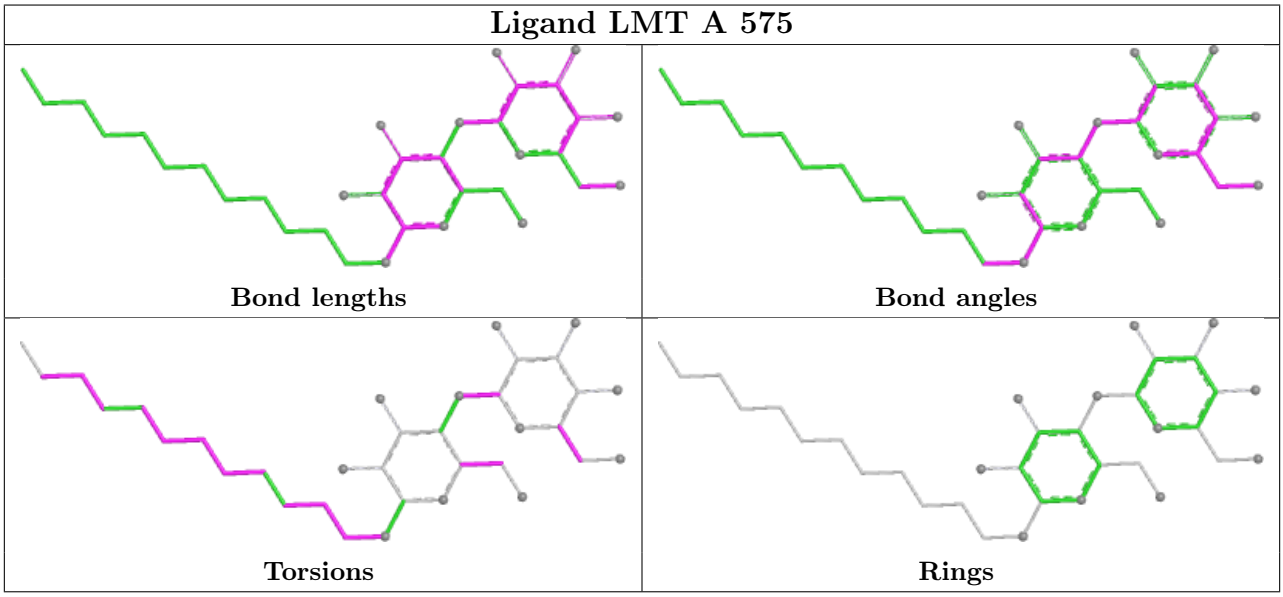
Ligand LMT A 571



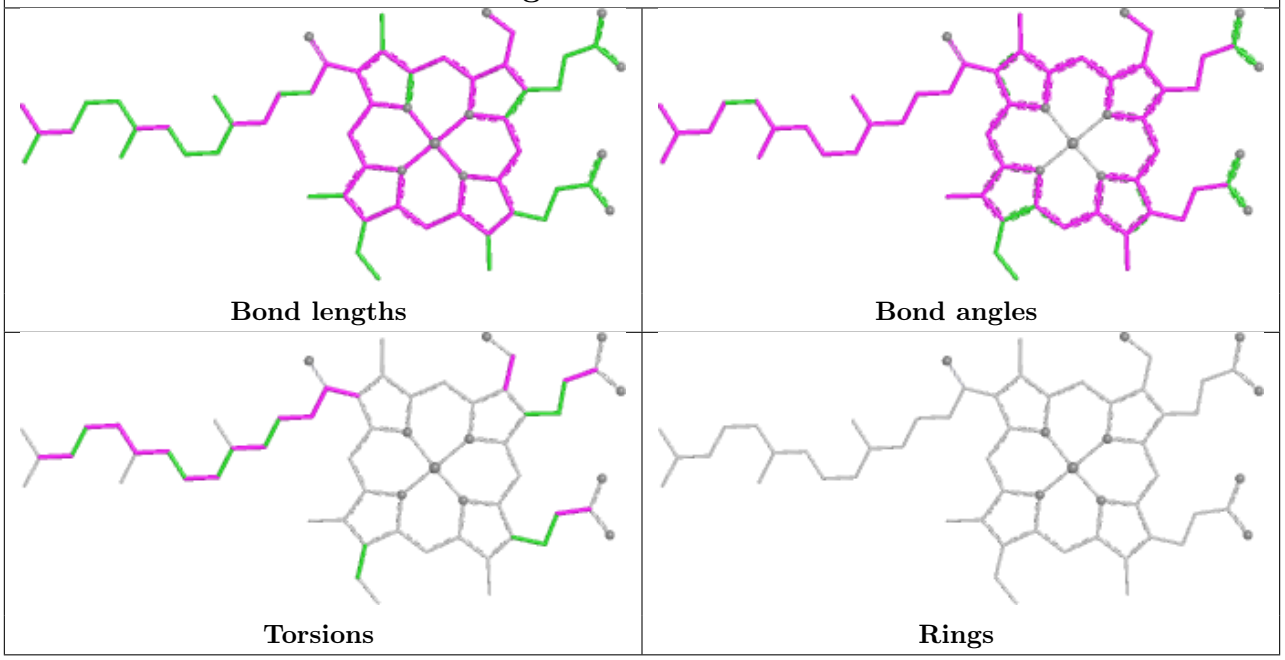
Ligand LMT A 573



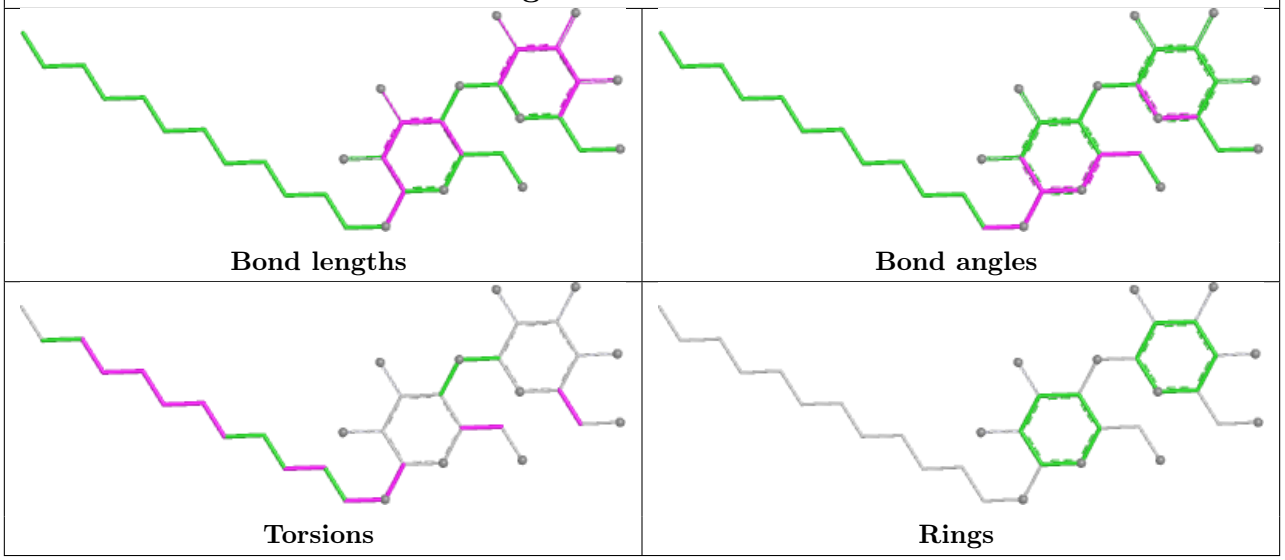
Ligand LMT A 575



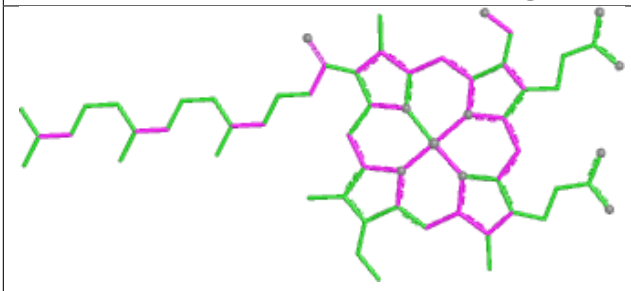
Ligand HEA A 560



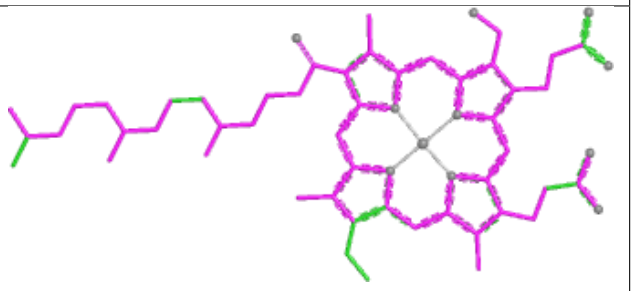
Ligand LMT B 279



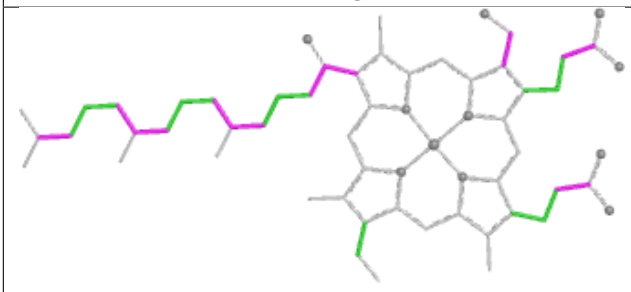
Ligand HEA A 559



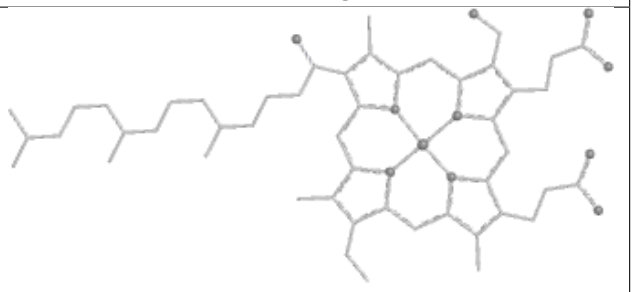
Bond lengths



Bond angles

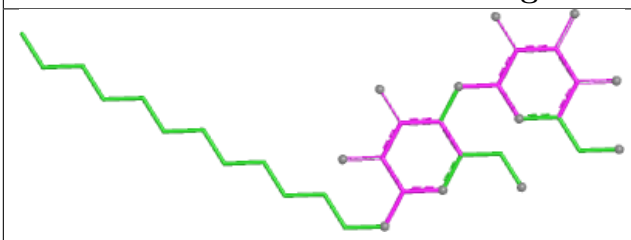


Torsions

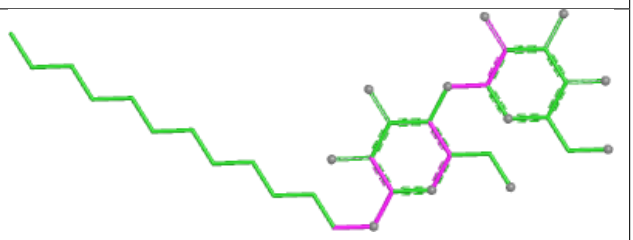


Rings

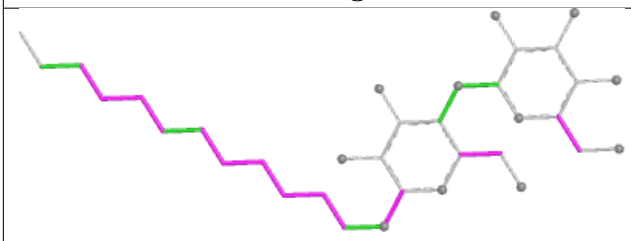
Ligand LMT A 572



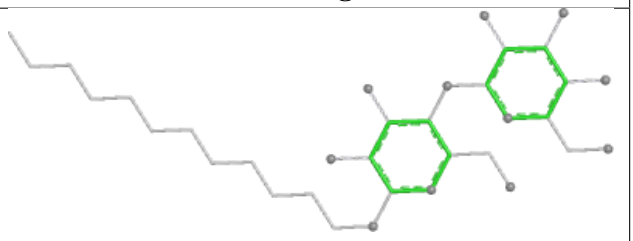
Bond lengths



Bond angles

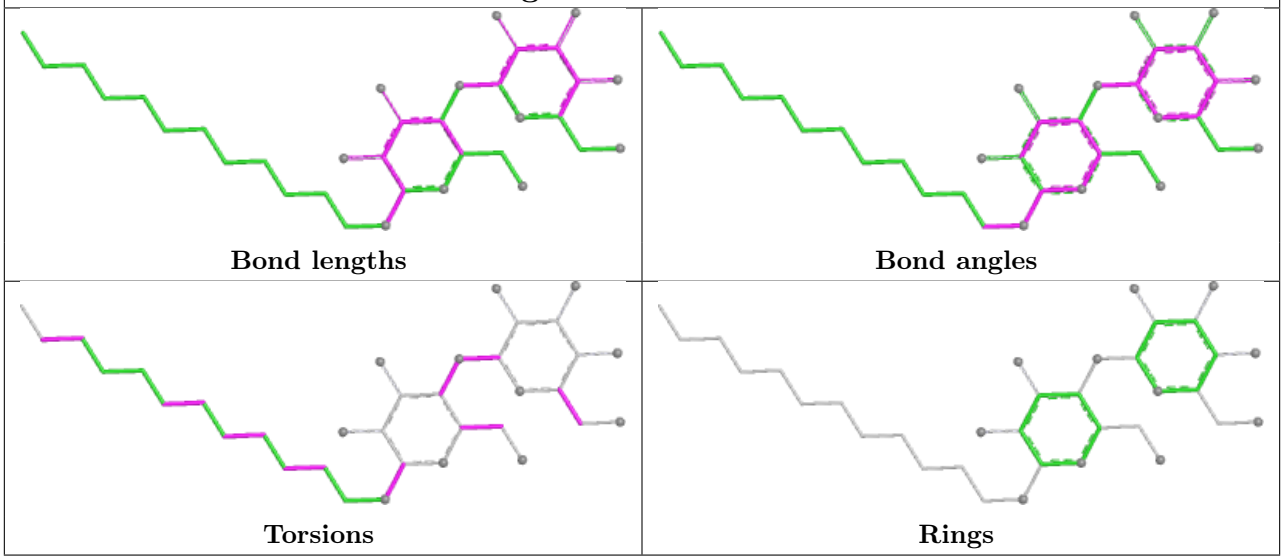


Torsions

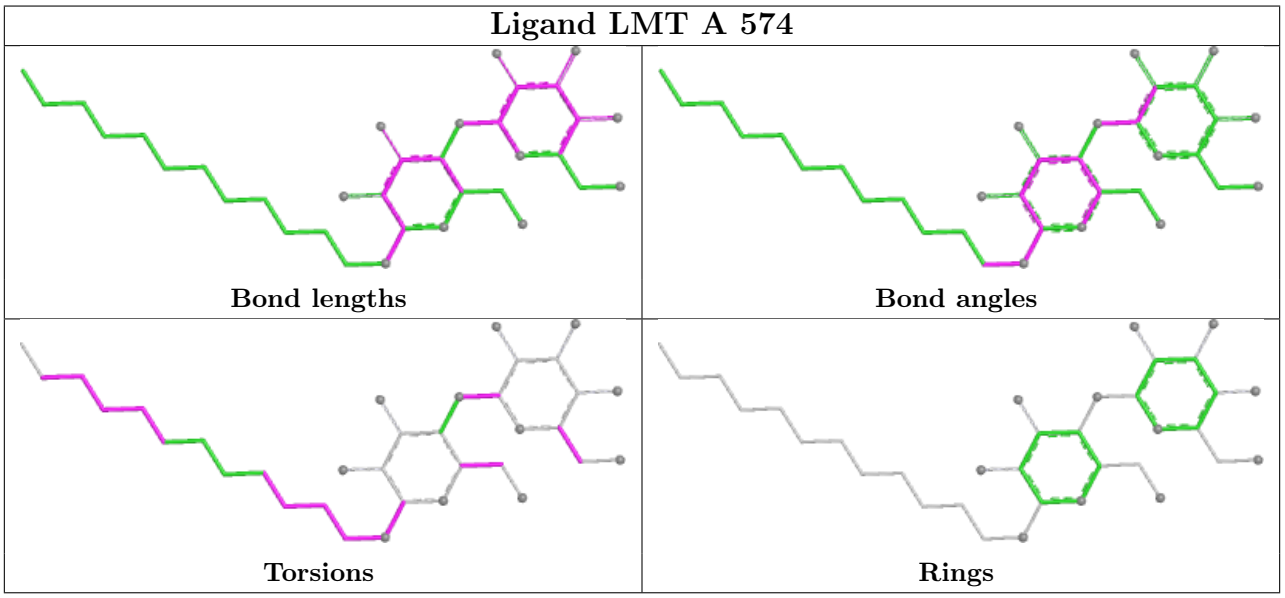


Rings

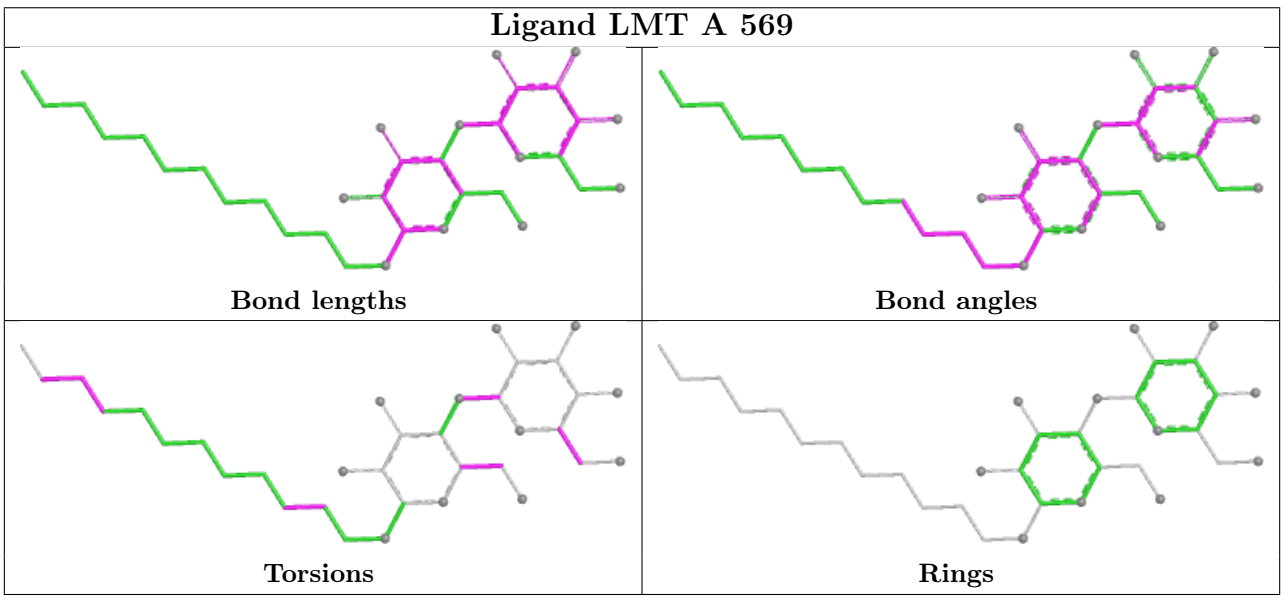
Ligand LMT D 121

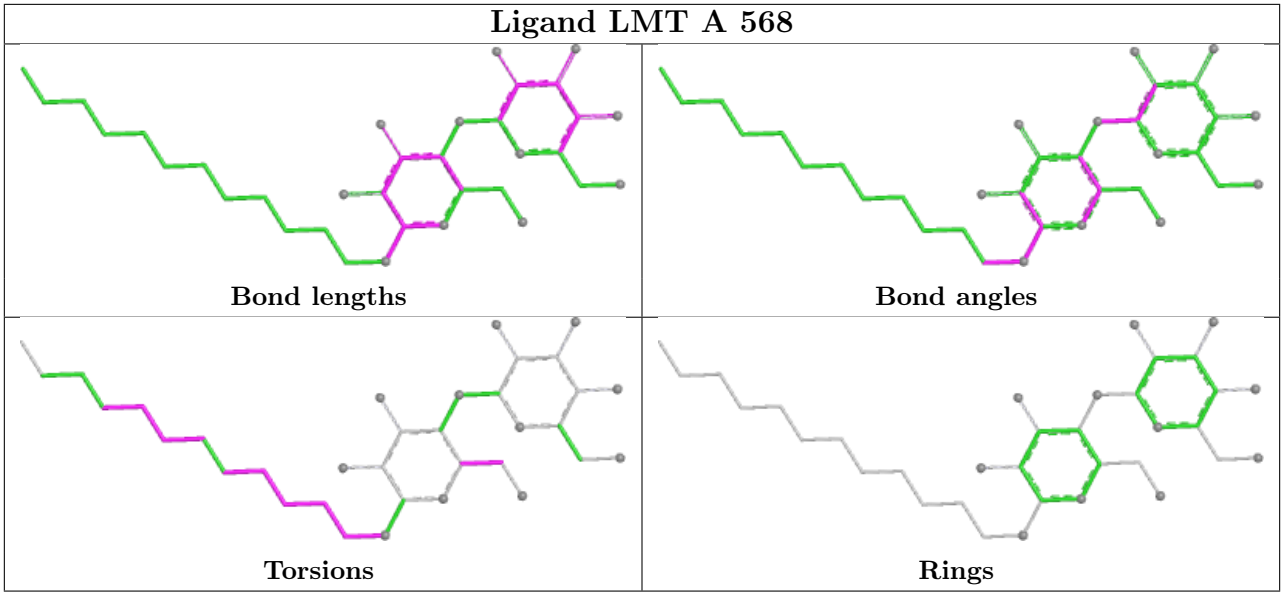


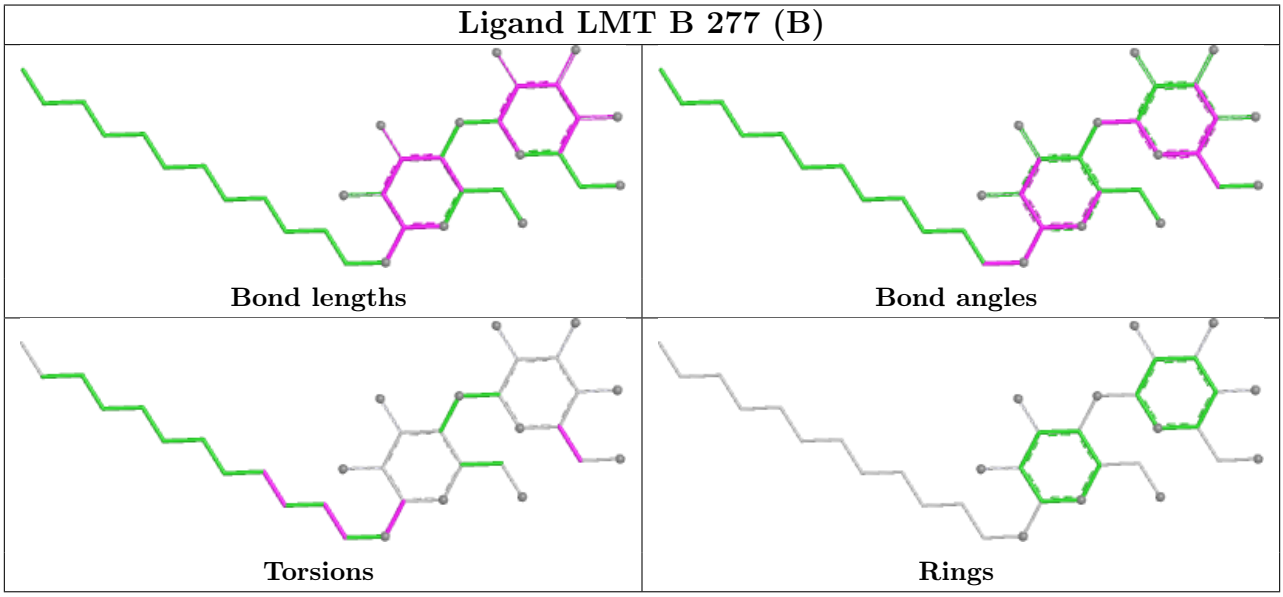
Ligand LMT A 574



Ligand LMT A 569







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	530/558 (94%)	0.48	23 (4%) 40 42	25, 55, 79, 125	2 (0%)
2	B	253/298 (84%)	0.06	2 (0%) 82 84	31, 50, 70, 86	1 (0%)
3	C	119/127 (93%)	0.52	4 (3%) 48 51	36, 60, 82, 112	2 (1%)
4	D	109/120 (90%)	0.36	2 (1%) 67 70	42, 57, 71, 82	0
All	All	1011/1103 (91%)	0.37	31 (3%) 51 54	25, 55, 77, 125	5 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	118	SER	4.9
1	A	20	THR	4.8
2	B	1	GLN	4.4
1	A	175	ALA	4.1
3	C	119	ALA	3.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

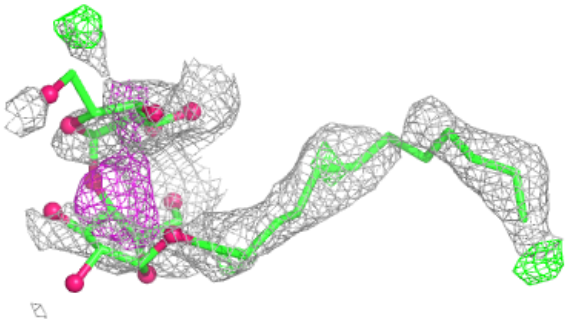
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

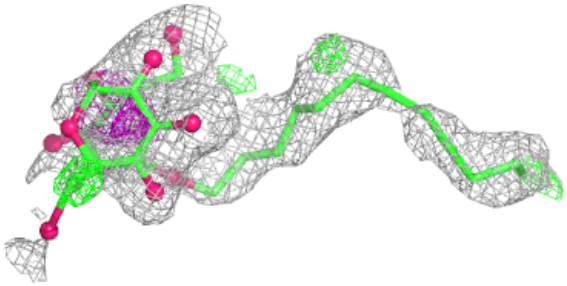
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	LMT	A	575	35/35	0.39	0.28	97,142,149,150	0
10	LMT	A	572	35/35	0.46	0.25	84,112,123,123	0
10	LMT	D	121	35/35	0.53	0.27	93,103,108,110	0
10	LMT	A	571	35/35	0.54	0.27	81,116,145,146	0
10	LMT	A	573	35/35	0.63	0.21	65,102,131,132	0
10	LMT	A	574	35/35	0.63	0.20	64,134,147,148	0
10	LMT	A	569	35/35	0.64	0.23	84,98,111,111	0
9	LDA	B	276	16/16	0.65	0.27	121,128,130,130	0
10	LMT	B	277[A]	35/35	0.71	0.25	67,81,87,88	12
10	LMT	B	277[B]	35/35	0.71	0.25	65,78,87,88	12
10	LMT	A	568	35/35	0.71	0.17	83,103,108,109	0
9	LDA	A	567	16/16	0.72	0.28	96,103,104,105	0
9	LDA	B	274	16/16	0.73	0.24	83,98,111,111	0
10	LMT	B	279	35/35	0.73	0.18	68,120,136,137	0
9	LDA	A	566	16/16	0.73	0.27	92,97,113,113	0
9	LDA	A	564	16/16	0.74	0.26	68,75,106,109	0
9	LDA	B	275	16/16	0.75	0.19	55,81,113,115	0
10	LMT	B	278	35/35	0.75	0.15	68,86,99,100	0
9	LDA	A	565	16/16	0.76	0.19	72,85,94,95	0
9	LDA	B	273	16/16	0.79	0.24	81,85,98,100	0
9	LDA	B	272	16/16	0.79	0.19	46,67,114,117	0
10	LMT	A	570	35/35	0.81	0.15	69,104,122,125	0
5	HEA	A	559	60/60	0.95	0.13	37,47,51,56	0
5	HEA	A	560	60/60	0.96	0.11	34,52,54,62	0
7	MG	A	562	1/1	0.98	0.11	28,28,28,28	0
8	CA	A	563	1/1	0.98	0.04	53,53,53,53	0
6	CU	B	270	1/1	0.98	0.03	48,48,48,48	0
11	PER	A	576	2/2	0.98	0.10	49,49,49,56	0
6	CU	B	271	1/1	0.99	0.03	50,50,50,50	0
6	CU	A	561	1/1	1.00	0.05	54,54,54,54	0

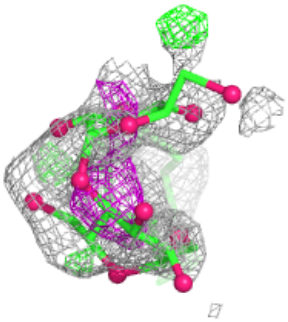
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 575:

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

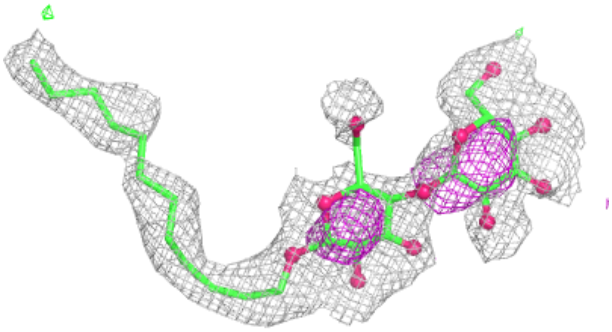


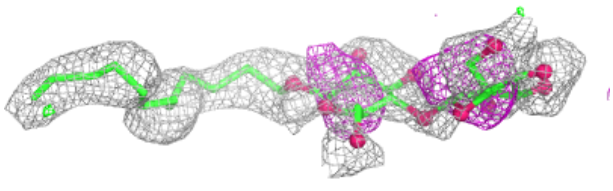


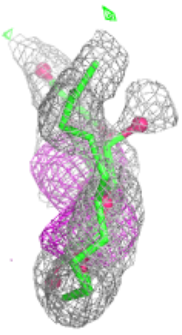


Electron density around LMT A 572:

$2mF_o$-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 D 121:

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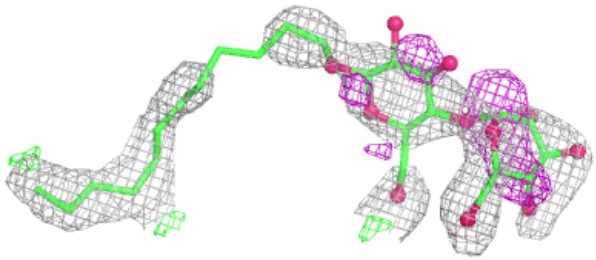
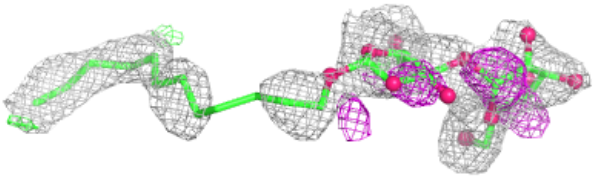
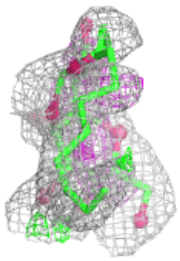
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

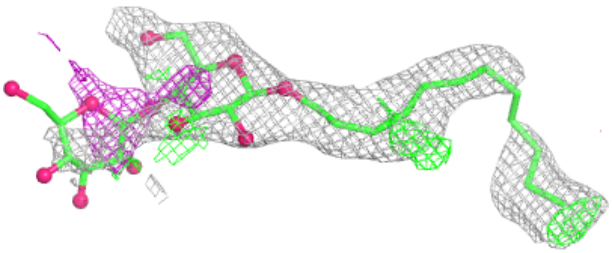


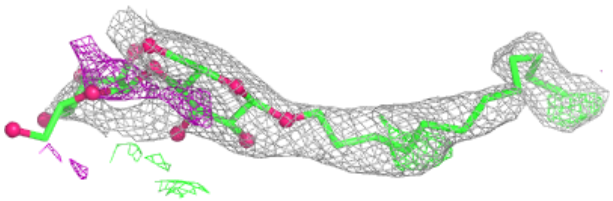


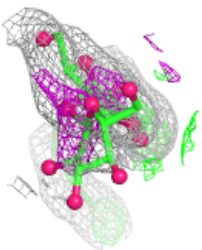


Electron density around LMT A 571:

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

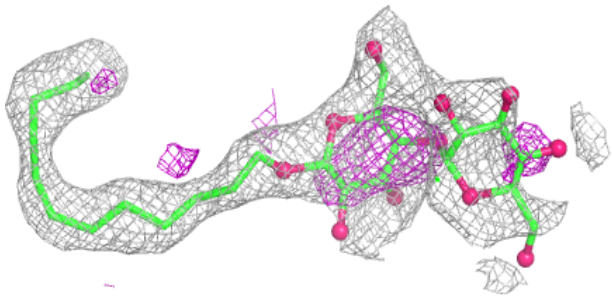


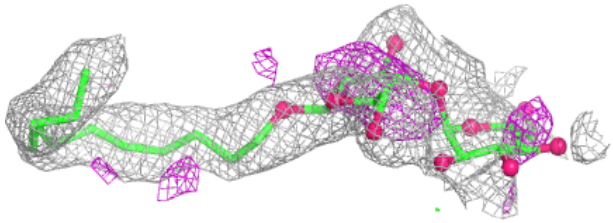


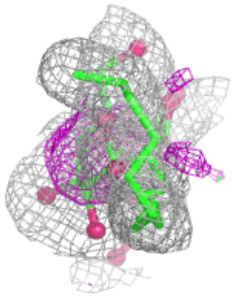


Electron density around LMT A 573:

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

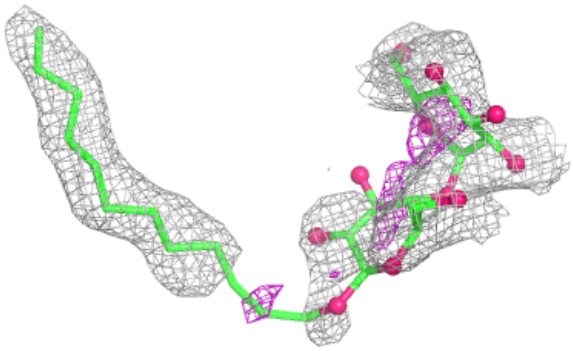


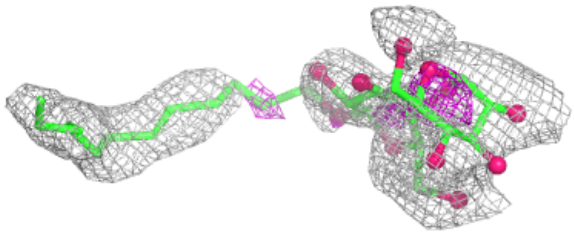


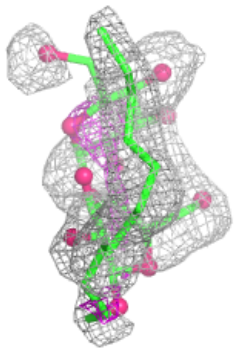


Electron density around LMT A 574:

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



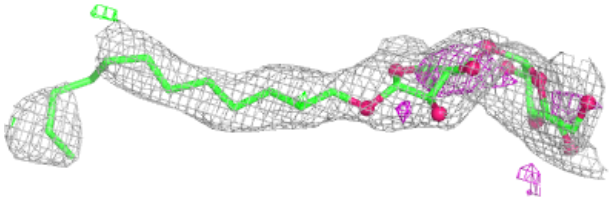


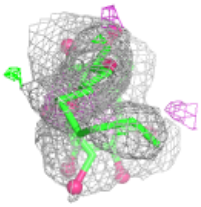


Electron density around LMT A 569:

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

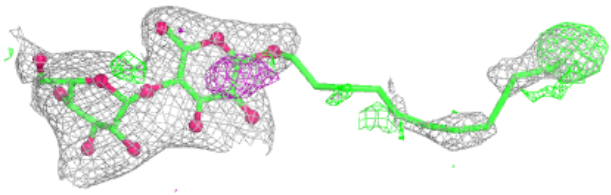


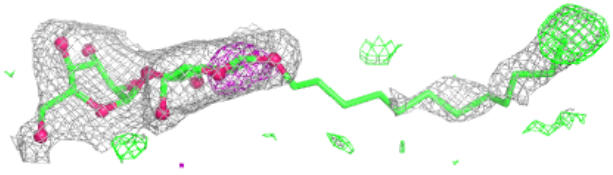


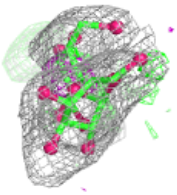


Electron density around LMT B 277 (A):

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

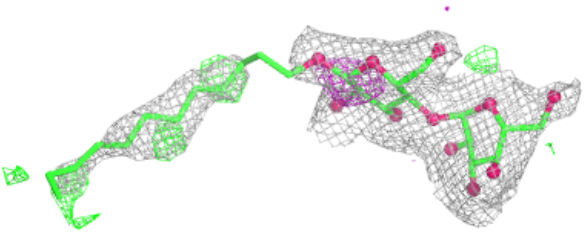


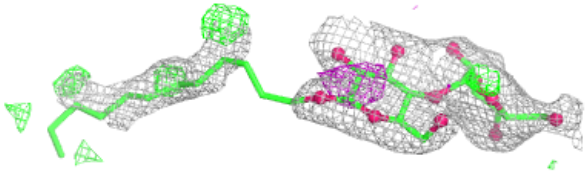




Electron density around LMT B 277 (B):

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

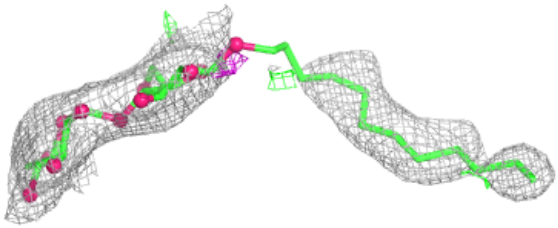


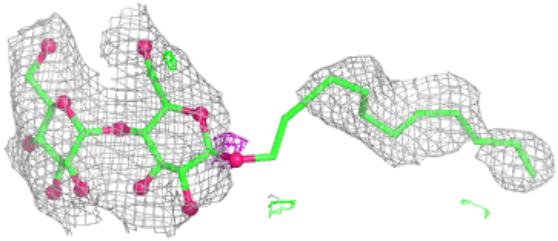


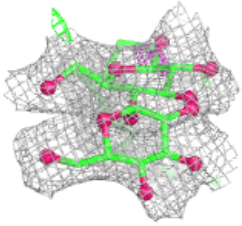


Electron density around LMT A 568:

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

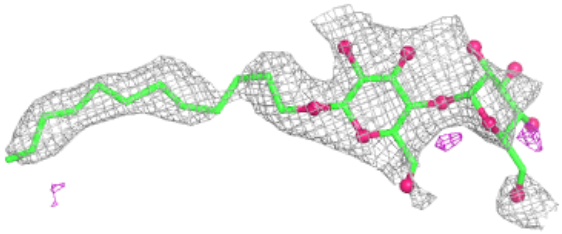


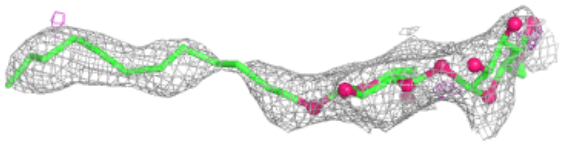


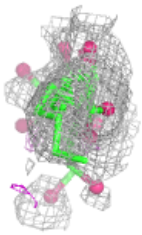


Electron density around LMT B 279:

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

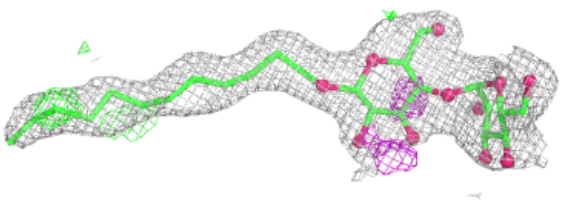


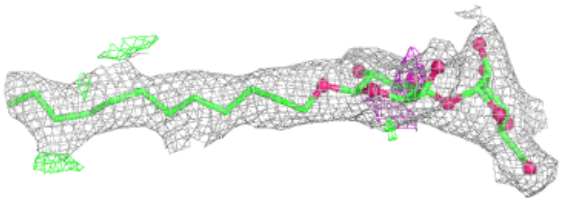


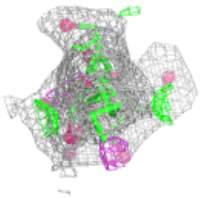


Electron density around LMT B 278:

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

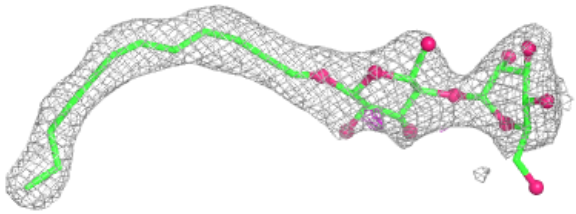


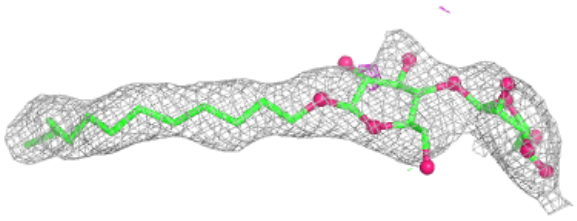


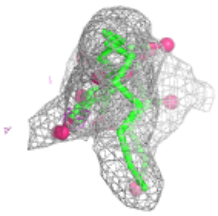


Electron density around LMT A 570:

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

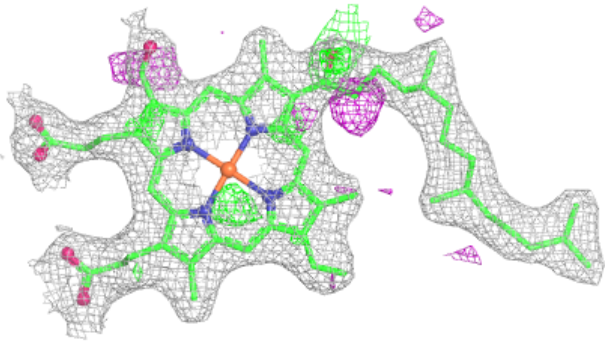


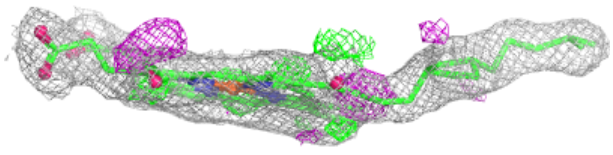


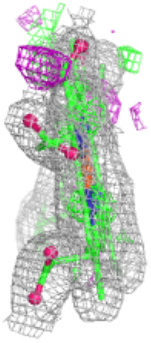


Electron density around HEA A 559:

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

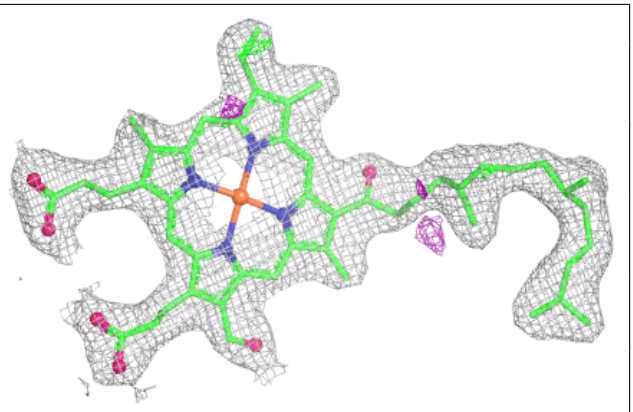


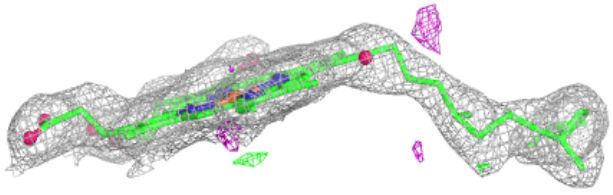


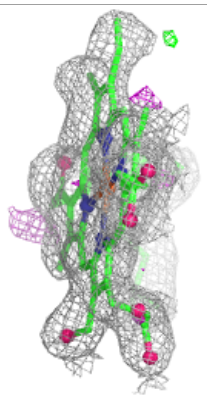


Electron density around HEA A 560:

$2mF_o$-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.