



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:55 AM EDT

PDB ID : 3HB3 / pdb_00003hb3
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (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

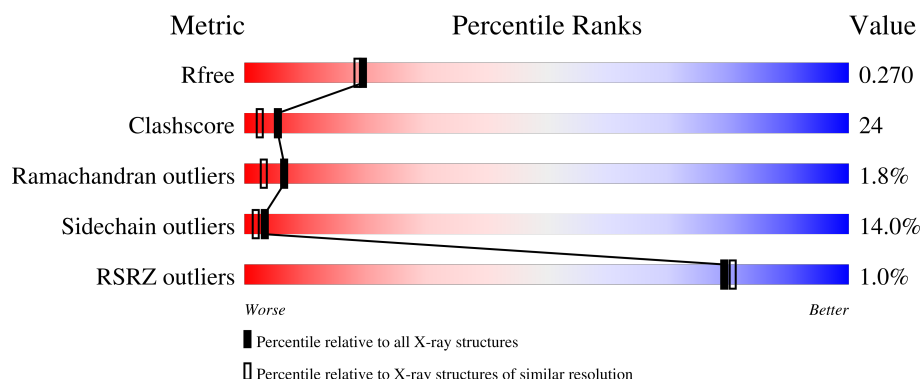
1 Overall quality at a glance

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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	46% 35% 12% 5%
2	B	298	37% 33% 14% 15%
3	C	127	2% 40% 39% 12% 7%
4	D	120	50% 27% 13% 10%

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	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			

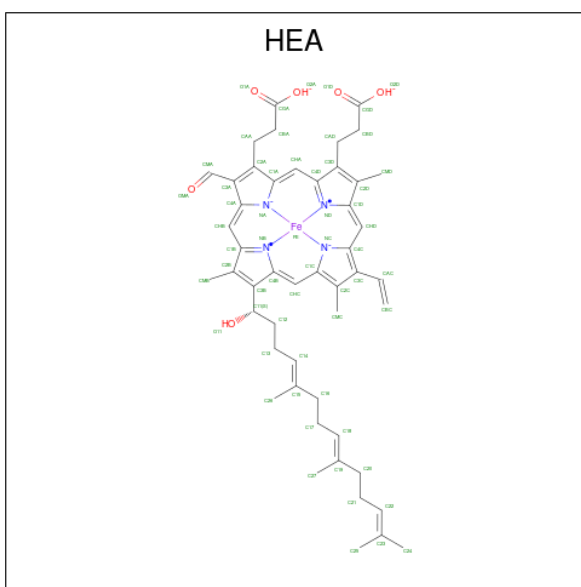
- Molecule 3 is a protein called ANTIBODY FV FRAGMENT.

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 (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	
			60	49	1	4	6	0
5	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

- Molecule 6 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

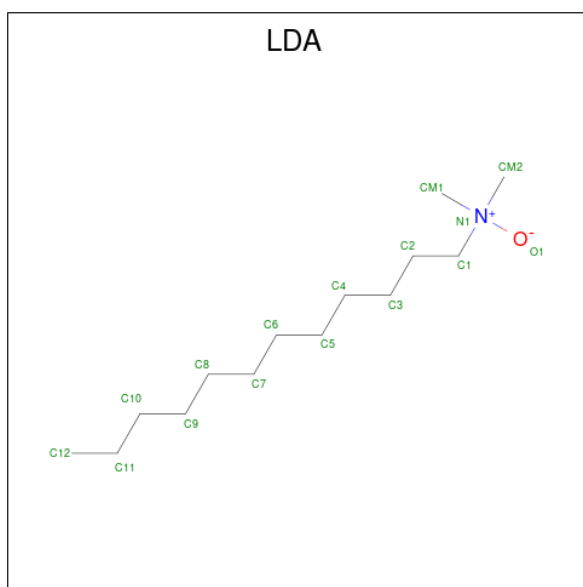
- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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

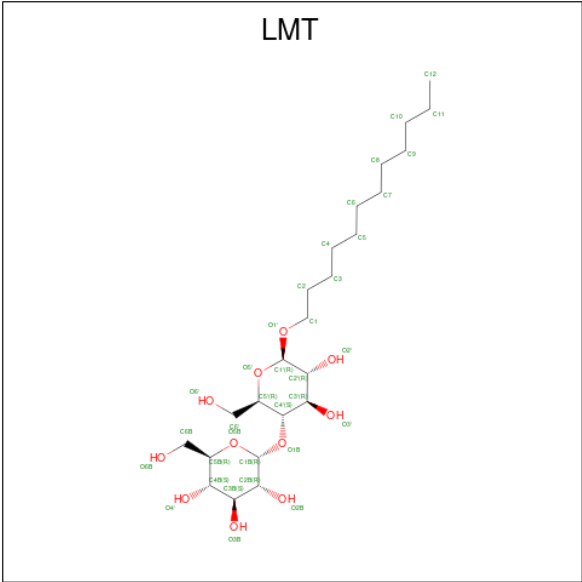
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca		
			1	1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



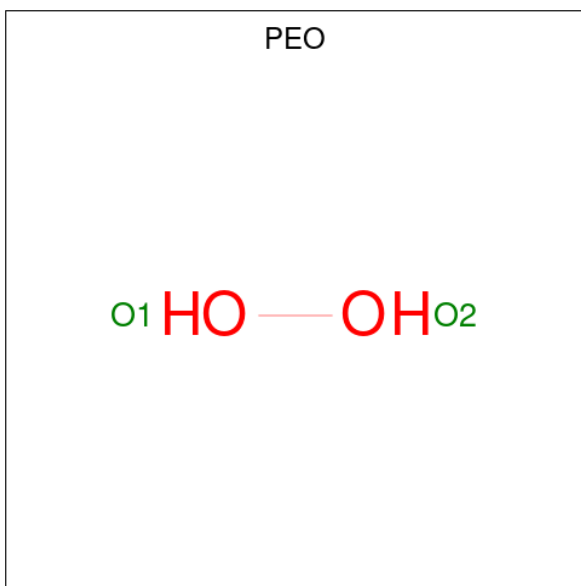
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 11 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



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

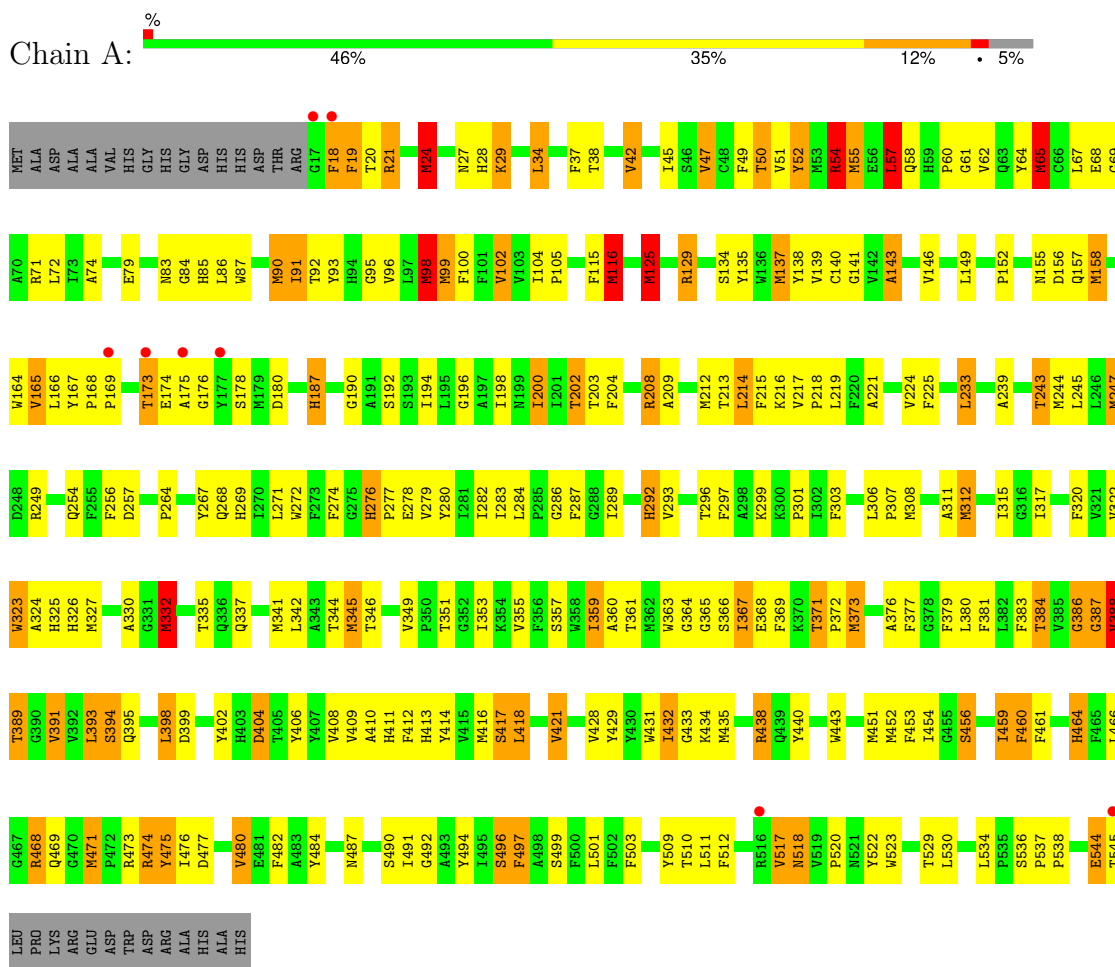
- Molecule 12 is water.

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		

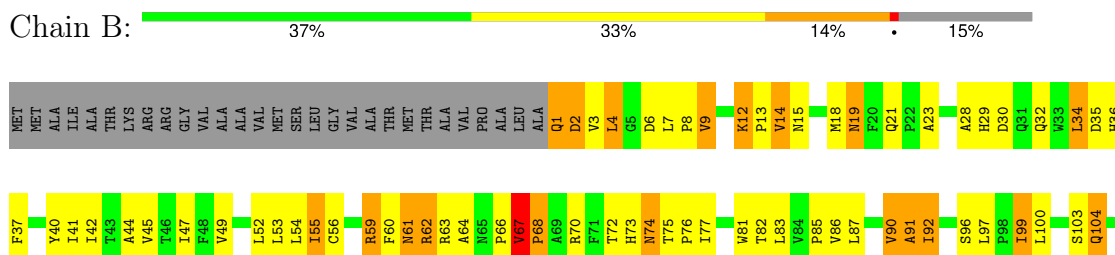
3 Residue-property plots

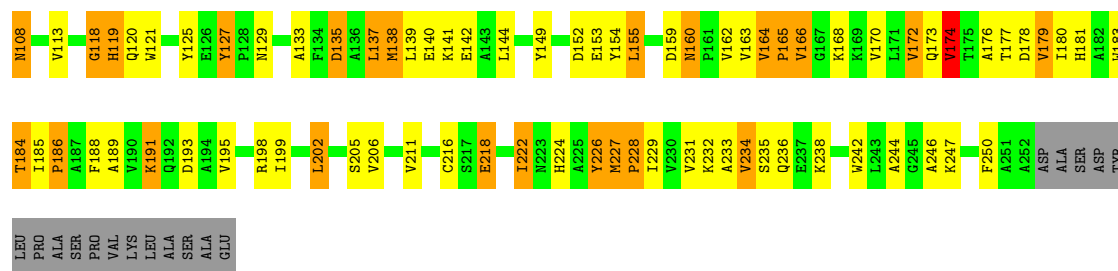
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

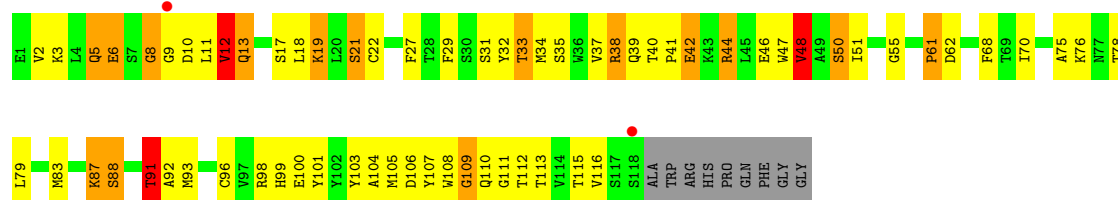


• Molecule 2: Cytochrome c oxidase subunit 2

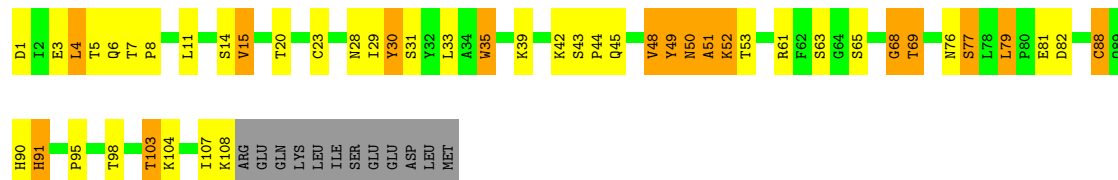




• Molecule 3: ANTIBODY FV FRAGMENT



• 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 (2.99%)	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: LMT, LDA, PEO, HEA, CU1, CA, MN

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	1.75	73/4368 (1.7%)	1.57	66/5959 (1.1%)
2	B	2.03	46/2050 (2.2%)	1.85	50/2810 (1.8%)
3	C	1.53	9/972 (0.9%)	1.48	8/1314 (0.6%)
4	D	1.68	12/852 (1.4%)	1.52	7/1156 (0.6%)
All	All	1.79	140/8242 (1.7%)	1.63	131/11239 (1.2%)

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

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GLU	C-O	16.05	1.42	1.24
2	B	178	ASP	CA-C	11.82	1.62	1.52
1	A	65	MET	SD-CE	9.83	2.04	1.79
1	A	373	MET	SD-CE	9.43	2.03	1.79
1	A	388	VAL	CA-C	8.95	1.64	1.52
2	B	155	LEU	N-CA	8.94	1.56	1.46
1	A	312	MET	SD-CE	8.94	2.01	1.79
1	A	349	VAL	CA-CB	8.86	1.65	1.54
2	B	206	VAL	CA-CB	8.58	1.65	1.54
2	B	195	VAL	CA-CB	8.54	1.65	1.54
1	A	24	MET	SD-CE	8.29	2.00	1.79
1	A	47	VAL	CA-CB	8.20	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	52	LYS	CA-C	8.18	1.63	1.52
2	B	236	GLN	CA-C	8.05	1.63	1.52
1	A	353	ILE	C-O	7.86	1.33	1.24
1	A	64	TYR	CA-C	-7.71	1.42	1.52
2	B	119	HIS	CA-C	-7.71	1.43	1.52
2	B	191	LYS	CA-C	-7.63	1.43	1.52
1	A	158	MET	SD-CE	7.55	1.98	1.79
3	C	91	THR	CA-CB	7.47	1.63	1.53
2	B	222	ILE	CG1-CD1	7.45	1.80	1.51
1	A	116	MET	C-O	-7.41	1.17	1.24
1	A	42	VAL	CA-CB	-7.40	1.44	1.54
2	B	199	ILE	CA-CB	7.40	1.63	1.54
2	B	191	LYS	N-CA	-7.36	1.37	1.46
1	A	332	MET	SD-CE	7.32	1.97	1.79
1	A	361	THR	CA-CB	-7.32	1.42	1.53
1	A	125	MET	SD-CE	-7.30	1.61	1.79
2	B	113	VAL	CA-CB	-7.24	1.45	1.54
2	B	184	THR	CA-CB	7.20	1.65	1.53
4	D	3	GLU	CA-C	-7.16	1.43	1.52
1	A	501	LEU	CA-C	7.13	1.61	1.52
1	A	244	MET	SD-CE	7.11	1.97	1.79
1	A	480	VAL	CA-CB	7.07	1.63	1.54
2	B	226	TYR	C-O	7.04	1.31	1.23
1	A	399	ASP	CA-C	7.04	1.62	1.52
1	A	474	ARG	C-O	-7.03	1.15	1.24
2	B	34	LEU	N-CA	-6.98	1.38	1.46
2	B	211	VAL	CA-C	6.92	1.61	1.52
1	A	386	GLY	C-O	6.77	1.31	1.23
1	A	432	ILE	CA-CB	6.70	1.62	1.54
1	A	361	THR	C-O	-6.67	1.16	1.24
1	A	57	LEU	CA-C	-6.64	1.43	1.52
4	D	4	LEU	CA-C	-6.63	1.44	1.52
2	B	118	GLY	CA-C	-6.62	1.47	1.52
2	B	172	VAL	CA-CB	-6.57	1.46	1.54
4	D	69	THR	CA-CB	6.50	1.65	1.53
2	B	91	ALA	CA-CB	-6.48	1.43	1.53
2	B	242	TRP	CA-CB	6.47	1.63	1.53
1	A	491	ILE	CA-CB	-6.46	1.47	1.54
1	A	402	TYR	CA-CB	6.41	1.63	1.53
1	A	459	ILE	CA-CB	-6.32	1.47	1.54
1	A	175	ALA	CA-CB	6.32	1.61	1.53
3	C	107	TYR	C-O	6.30	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	VAL	CA-C	6.27	1.60	1.52
1	A	384	THR	CA-CB	6.27	1.63	1.53
1	A	464	HIS	CA-CB	6.27	1.63	1.53
1	A	52	TYR	C-O	6.25	1.31	1.24
2	B	127	TYR	CA-CB	-6.24	1.46	1.53
2	B	99	ILE	CA-C	6.11	1.60	1.52
4	D	5	THR	CA-C	-6.10	1.45	1.52
2	B	164	VAL	CA-CB	6.08	1.64	1.54
1	A	344	THR	CA-CB	6.08	1.63	1.53
2	B	170	VAL	C-O	-6.04	1.17	1.24
1	A	218	PRO	CA-C	6.01	1.60	1.52
2	B	9	VAL	CA-C	5.99	1.59	1.52
1	A	61	GLY	C-O	-5.99	1.17	1.24
2	B	49	VAL	CA-CB	-5.97	1.46	1.54
1	A	391	VAL	CA-C	5.95	1.60	1.52
2	B	165	PRO	CA-C	5.95	1.59	1.52
1	A	90	MET	N-CA	-5.94	1.39	1.46
1	A	367	ILE	CB-CG2	5.94	1.72	1.52
1	A	476	ILE	CA-CB	5.94	1.63	1.54
1	A	454	ILE	CA-CB	-5.89	1.47	1.54
3	C	105	MET	SD-CE	-5.89	1.64	1.79
1	A	409	VAL	CA-CB	5.88	1.61	1.54
2	B	3	VAL	CA-C	5.88	1.60	1.52
1	A	349	VAL	CA-C	5.85	1.59	1.52
2	B	185	ILE	CA-CB	5.83	1.61	1.54
1	A	326	HIS	CA-C	5.81	1.63	1.52
1	A	477	ASP	N-CA	5.81	1.53	1.45
2	B	183	TRP	CA-CB	5.80	1.61	1.53
1	A	98	MET	SD-CE	-5.79	1.65	1.79
2	B	189	ALA	CA-CB	5.78	1.62	1.53
1	A	146	VAL	CA-CB	5.77	1.61	1.54
1	A	376	ALA	CA-CB	-5.77	1.44	1.53
1	A	296	THR	CA-C	-5.74	1.45	1.52
2	B	234	VAL	CA-CB	5.71	1.63	1.55
4	D	90	HIS	CA-CB	5.71	1.60	1.53
1	A	219	LEU	CA-C	5.70	1.61	1.52
2	B	246	ALA	CA-CB	5.69	1.63	1.53
2	B	211	VAL	CA-CB	5.69	1.62	1.54
1	A	60	PRO	CA-C	5.68	1.60	1.52
2	B	118	GLY	C-O	5.68	1.31	1.23
4	D	15	VAL	CA-CB	5.60	1.60	1.54
1	A	404	ASP	CA-C	-5.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	135	ASP	N-CA	-5.58	1.39	1.45
1	A	289	ILE	CA-CB	5.57	1.61	1.54
1	A	428	VAL	CA-CB	5.56	1.60	1.54
3	C	5	GLN	CA-C	-5.54	1.46	1.52
1	A	367	ILE	CA-C	-5.54	1.45	1.52
2	B	12	LYS	CA-C	5.50	1.58	1.52
2	B	67	VAL	CA-CB	5.49	1.61	1.54
1	A	387	GLY	C-O	-5.48	1.17	1.23
2	B	100	LEU	C-O	5.46	1.30	1.24
1	A	276	HIS	CA-C	5.46	1.58	1.52
2	B	168	LYS	CA-C	-5.43	1.45	1.52
1	A	381	PHE	CA-C	5.41	1.59	1.52
2	B	97	LEU	CA-C	5.41	1.59	1.52
3	C	61	PRO	CA-C	5.41	1.59	1.52
1	A	50	THR	CA-CB	5.40	1.61	1.53
4	D	35	TRP	CA-C	5.39	1.59	1.52
3	C	103	TYR	CA-C	-5.38	1.46	1.52
1	A	468	ARG	NE-CZ	-5.37	1.27	1.33
2	B	244	ALA	CA-CB	5.36	1.61	1.53
1	A	292	HIS	CA-CB	-5.33	1.45	1.53
4	D	20	THR	C-O	-5.33	1.17	1.23
3	C	37	VAL	N-CA	-5.31	1.40	1.46
1	A	345	MET	SD-CE	-5.28	1.66	1.79
3	C	100	GLU	CA-C	5.27	1.59	1.52
2	B	206	VAL	C-O	-5.26	1.18	1.24
1	A	247	MET	SD-CE	5.24	1.92	1.79
2	B	188	PHE	CA-CB	5.22	1.61	1.54
1	A	523	TRP	CA-C	5.21	1.59	1.52
4	D	98	THR	CA-CB	5.20	1.62	1.53
1	A	409	VAL	CA-C	5.19	1.59	1.52
4	D	31	SER	N-CA	5.18	1.53	1.46
4	D	49	TYR	CA-C	5.17	1.59	1.52
1	A	497	PHE	C-O	-5.16	1.18	1.24
1	A	283	ILE	CA-C	5.14	1.59	1.52
1	A	57	LEU	CA-CB	-5.13	1.44	1.53
2	B	99	ILE	C-O	5.11	1.30	1.24
2	B	52	LEU	N-CA	-5.09	1.40	1.46
1	A	471	MET	C-O	-5.08	1.18	1.24
1	A	421	VAL	CA-CB	5.07	1.61	1.54
1	A	395	GLN	CA-C	5.05	1.59	1.52
1	A	62	VAL	CA-CB	-5.05	1.48	1.54
1	A	365	GLY	C-O	5.03	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	VAL	N-CA	-5.03	1.40	1.46
3	C	38	ARG	CA-C	-5.02	1.46	1.52

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	TYR	CA-C-N	-14.78	98.93	122.73
2	B	154	TYR	C-N-CA	-14.78	98.93	122.73
2	B	166	VAL	CB-CA-C	-11.99	94.74	111.28
2	B	2	ASP	N-CA-C	-11.17	99.16	113.12
1	A	394	SER	N-CA-C	-10.53	100.18	113.23
2	B	44	ALA	N-CA-C	-10.08	99.29	111.69
2	B	66	PRO	N-CA-C	-9.68	95.99	111.38
1	A	165	VAL	N-CA-C	9.24	120.13	111.91
3	C	33	THR	N-CA-C	-9.18	94.70	109.76
1	A	453	PHE	N-CA-C	-8.98	99.97	112.45
3	C	10	ASP	N-CA-C	8.83	122.30	109.14
2	B	154	TYR	O-C-N	-8.75	112.05	122.11
1	A	468	ARG	N-CA-C	-8.56	102.03	111.36
2	B	62	ARG	N-CA-C	8.53	121.43	111.02
2	B	13	PRO	CA-C-O	-7.88	112.09	121.95
3	C	75	ALA	N-CA-C	-7.88	102.58	112.90
1	A	37	PHE	N-CA-C	-7.87	101.50	112.45
2	B	174	VAL	CB-CA-C	7.86	122.26	110.63
1	A	494	TYR	N-CA-C	-7.80	101.88	111.40
1	A	196	GLY	N-CA-C	-7.53	103.76	112.50
1	A	45	ILE	N-CA-C	-7.42	103.56	110.53
2	B	155	LEU	N-CA-C	7.41	121.17	112.72
2	B	137	LEU	N-CA-C	-7.40	97.76	109.23
1	A	55	MET	N-CA-C	-7.36	103.26	111.28
1	A	398	LEU	N-CA-C	-7.36	103.93	113.12
1	A	365	GLY	N-CA-C	-7.25	102.23	112.60
1	A	501	LEU	N-CA-C	-7.24	103.32	111.14
2	B	231	VAL	N-CA-C	-7.20	97.24	107.75
2	B	184	THR	OG1-CB-CG2	-7.17	94.96	109.30
1	A	468	ARG	CG-CD-NE	-7.15	96.28	112.00
2	B	149	TYR	N-CA-C	6.96	120.77	110.48
4	D	90	HIS	N-CA-C	-6.94	97.41	108.73
3	C	12	VAL	N-CA-C	6.91	123.71	109.34
1	A	54	ARG	NE-CZ-NH2	-6.86	113.02	119.20
2	B	100	LEU	N-CA-C	-6.86	103.73	111.14
1	A	215[A]	PHE	CB-CA-C	6.80	122.48	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	SER	N-CA-C	-6.80	103.89	111.71
2	B	179	VAL	N-CA-CB	-6.78	104.53	112.32
1	A	477	ASP	CA-C-N	-6.73	111.50	122.26
1	A	477	ASP	C-N-CA	-6.73	111.50	122.26
2	B	144	LEU	N-CA-C	6.62	118.29	111.14
1	A	399	ASP	N-CA-C	6.62	119.34	111.33
2	B	191	LYS	N-CA-C	-6.62	97.47	108.32
2	B	28	ALA	N-CA-C	-6.58	104.74	112.89
1	A	29[A]	LYS	N-CA-C	-6.53	104.01	112.23
1	A	29[B]	LYS	N-CA-C	-6.53	104.01	112.23
1	A	29[C]	LYS	N-CA-C	-6.53	104.01	112.23
1	A	143	ALA	N-CA-C	-6.42	103.57	111.40
1	A	52	TYR	N-CA-C	-6.41	103.92	111.03
1	A	464	HIS	N-CA-C	-6.33	102.92	112.04
2	B	205	SER	N-CA-C	-6.28	99.13	108.99
2	B	55	ILE	N-CA-C	-6.21	104.58	110.42
4	D	88	CYS	N-CA-C	-6.17	101.33	110.46
1	A	475	TYR	N-CA-C	6.13	118.51	108.52
1	A	497	PHE	N-CA-C	-6.12	104.53	111.14
1	A	389	THR	CA-CB-CG2	6.12	120.90	110.50
1	A	50	THR	N-CA-CB	-6.11	101.14	110.12
1	A	202	THR	N-CA-C	-6.07	103.41	111.24
1	A	360	ALA	N-CA-C	-6.06	104.75	111.36
2	B	23	ALA	N-CA-C	-6.04	100.66	110.20
2	B	179	VAL	N-CA-C	-6.03	101.17	108.53
1	A	280	TYR	CB-CA-C	6.03	121.74	110.70
2	B	218	GLU	CA-C-O	5.95	126.92	120.32
1	A	276	HIS	N-CA-CB	5.90	118.61	110.11
2	B	59	ARG	N-CA-C	-5.85	107.13	114.56
1	A	99	MET	CG-SD-CE	-5.82	88.10	100.90
1	A	388	VAL	N-CA-CB	-5.76	101.93	110.58
1	A	428	VAL	N-CA-C	-5.76	105.01	110.42
4	D	51	ALA	CA-C-N	-5.71	113.09	121.99
4	D	51	ALA	C-N-CA	-5.71	113.09	121.99
1	A	503	PHE	N-CA-C	5.68	118.21	111.33
2	B	129	ASN	N-CA-C	-5.67	106.02	113.17
2	B	195	VAL	N-CA-C	5.65	114.05	107.89
1	A	99	MET	N-CA-C	5.64	120.22	113.23
2	B	165	PRO	CA-C-O	-5.62	114.73	121.48
2	B	6	ASP	N-CA-C	5.61	120.08	113.23
2	B	90	VAL	N-CA-C	-5.61	105.05	110.72
1	A	409	VAL	N-CA-C	-5.59	105.08	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	VAL	N-CA-C	5.58	116.26	108.89
1	A	286	GLY	N-CA-C	-5.56	105.66	112.77
2	B	160	ASN	N-CA-C	5.54	117.65	109.62
1	A	386	GLY	N-CA-C	5.53	119.85	112.77
2	B	19	ASN	N-CA-C	5.53	118.62	109.94
2	B	82	THR	OG1-CB-CG2	-5.50	98.29	109.30
3	C	106	ASP	N-CA-C	5.46	118.16	111.82
1	A	141	GLY	N-CA-C	-5.46	106.17	112.83
3	C	2	VAL	N-CA-CB	5.44	117.00	110.31
1	A	451	MET	N-CA-C	-5.40	105.31	111.14
1	A	55	MET	CG-SD-CE	-5.36	89.10	100.90
1	A	93	TYR	N-CA-C	-5.36	105.88	112.90
1	A	496	SER	N-CA-C	5.34	118.02	111.82
2	B	162	VAL	CA-C-N	-5.32	116.24	123.10
2	B	162	VAL	C-N-CA	-5.32	116.24	123.10
1	A	388	VAL	CA-CB-CG1	5.31	119.42	110.40
2	B	202	LEU	N-CA-C	-5.27	101.06	109.07
1	A	353	ILE	CB-CA-C	5.26	118.61	111.88
1	A	530	LEU	N-CA-C	5.25	117.69	111.33
1	A	61	GLY	CA-C-O	-5.23	115.34	121.31
1	A	388	VAL	N-CA-C	5.23	116.00	110.72
2	B	68	PRO	CB-CA-C	-5.22	104.14	110.98
2	B	67	VAL	N-CA-C	5.21	120.14	108.88
1	A	388	VAL	CB-CA-C	5.21	119.41	112.22
2	B	154	TYR	N-CA-C	5.21	119.97	111.37
2	B	191	LYS	CA-C-O	-5.21	113.79	120.14
1	A	65	MET	CA-C-N	5.20	128.94	121.50
1	A	65	MET	C-N-CA	5.20	128.94	121.50
3	C	48	VAL	CB-CA-C	5.20	119.82	111.29
1	A	34	LEU	N-CA-C	-5.19	105.52	111.07
2	B	179	VAL	CA-CB-CG1	5.18	119.21	110.40
1	A	225	PHE	N-CA-C	-5.18	105.71	112.23
1	A	272	TRP	N-CA-C	-5.17	106.47	112.89
1	A	323	TRP	N-CA-C	5.17	117.66	111.71
2	B	228	PRO	N-CD-CG	5.17	110.96	103.20
1	A	522	TYR	N-CA-C	-5.14	106.24	112.88
1	A	460	PHE	CA-C-N	-5.14	113.38	120.26
1	A	460	PHE	C-N-CA	-5.14	113.38	120.26
4	D	91	HIS	N-CA-C	5.14	118.86	112.59
1	A	61	GLY	N-CA-C	-5.13	99.55	111.04
1	A	292	HIS	N-CA-C	5.13	117.26	111.11
2	B	227	MET	CG-SD-CE	-5.12	89.62	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	231	VAL	N-CA-CB	5.11	118.29	111.64
2	B	47	ILE	N-CA-C	-5.07	105.45	112.50
2	B	41	ILE	N-CA-CB	-5.07	105.10	110.62
4	D	4	LEU	CA-C-N	-5.06	115.86	122.99
4	D	4	LEU	C-N-CA	-5.06	115.86	122.99
3	C	78	THR	OG1-CB-CG2	-5.06	99.19	109.30
2	B	231	VAL	CA-C-N	-5.05	115.61	122.93
2	B	231	VAL	C-N-CA	-5.05	115.61	122.93
1	A	383	PHE	N-CA-C	-5.04	107.08	113.18
1	A	280	TYR	CA-C-N	5.01	127.59	120.53
1	A	280	TYR	C-N-CA	5.01	127.59	120.53

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	241	0
2	B	1985	0	1967	105	0
3	C	940	0	898	51	0
4	D	831	0	807	27	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	0
12	C	87	0	0	10	0
12	D	81	0	0	2	0
All	All	9393	0	8665	420	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 24.

All (420) 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
3:C:93:MET:HE3	3:C:93:MET:HA	1.28	1.13
1:A:254:GLN:HB3	1:A:257:ASP:HB3	1.27	1.12
1:A:545:THR:HB	12:A:637:HOH:O	1.49	1.09
1:A:518:ASN:N	1:A:518:ASN:HD22	1.53	1.06
1:A:389:THR:HG21	12:A:852:HOH:O	1.55	1.04
4:D:45:GLN:HG3	12:D:1196:HOH:O	1.62	0.99
4:D:28:ASN:OD1	4:D:68:GLY:HA2	1.62	0.97
1:A:83:ASN:HD21	1:A:157:GLN:HE22	1.02	0.95
2:B:1:GLN:N	12:B:1235:HOH:O	1.95	0.95
1:A:72:LEU:HD23	9:A:567:LDA:H52	1.50	0.92
2:B:227:MET:N	2:B:228:PRO:HD3	1.84	0.91
1:A:518:ASN:H	1:A:518:ASN:ND2	1.68	0.90
1:A:98:MET:HG3	5:A:559:HEA:C3C	2.03	0.89
1:A:239:ALA:O	1:A:243:THR:HG23	1.74	0.88
1:A:369:PHE:H	10:A:573[B]:LMT:H4B	1.39	0.88
1:A:342:LEU:HD23	1:A:345:MET:HE1	1.57	0.86
1:A:518:ASN:HD22	1:A:518:ASN:H	0.88	0.86
1:A:83:ASN:HD21	1:A:157:GLN:NE2	1.74	0.85
1:A:102:VAL:O	1:A:105:PRO:HD2	1.76	0.85
2:B:227:MET:O	2:B:227:MET:HG2	1.77	0.83
3:C:31:SER:OG	12:C:1225:HOH:O	1.97	0.82
1:A:342:LEU:HA	1:A:345:MET:HE3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:TYR:HE1	9:B:274:LDA:H31	1.43	0.80
3:C:93:MET:HE1	3:C:112:THR:C	2.07	0.80
2:B:227:MET:N	2:B:228:PRO:CD	2.44	0.79
1:A:487:ASN:ND2	10:A:572[B]:LMT:O6'	2.12	0.79
1:A:52:TYR:HD2	1:A:90:MET:HE2	1.48	0.79
1:A:243:THR:O	1:A:247:MET:HG3	1.83	0.78
1:A:187:HIS:CE1	1:A:243:THR:HG22	2.19	0.78
1:A:308:MET:HE2	1:A:357:SER:HB3	1.63	0.78
1:A:83:ASN:ND2	1:A:157:GLN:HE22	1.81	0.77
3:C:93:MET:HE3	3:C:93:MET:CA	2.13	0.76
1:A:54:ARG:HD3	1:A:490:SER:OG	1.86	0.74
1:A:468:ARG:NH2	2:B:35:ASP:OD2	2.20	0.74
4:D:6:GLN:HG2	4:D:103:THR:HG22	1.69	0.73
5:A:560:HEA:HHC	5:A:560:HEA:O11	1.88	0.73
1:A:57:LEU:CD2	1:A:87:TRP:HH2	2.01	0.73
4:D:50:ASN:O	4:D:52:LYS:N	2.20	0.73
2:B:227:MET:H	2:B:228:PRO:HD3	1.54	0.73
1:A:337:GLN:HE22	2:B:104:GLN:HE21	1.37	0.73
1:A:342:LEU:HA	1:A:345:MET:CE	2.19	0.73
1:A:27:ASN:HD21	1:A:29[B]:LYS:HB2	1.55	0.71
1:A:190:GLY:O	1:A:194:ILE:HG13	1.90	0.71
1:A:518:ASN:N	1:A:518:ASN:ND2	2.30	0.71
3:C:62:ASP:HB2	12:C:1238:HOH:O	1.90	0.71
1:A:245:LEU:O	1:A:249:ARG:HG3	1.92	0.69
2:B:135:ASP:OD2	12:B:1284:HOH:O	2.10	0.69
4:D:6:GLN:HE21	4:D:103:THR:HG23	1.57	0.69
1:A:57:LEU:HD21	1:A:87:TRP:CH2	2.28	0.69
1:A:57:LEU:CD2	1:A:87:TRP:CH2	2.77	0.68
1:A:98:MET:HB3	5:A:559:HEA:CAC	2.23	0.68
1:A:452:MET:O	1:A:456:SER:HB2	1.94	0.68
1:A:254:GLN:CB	1:A:257:ASP:HB3	2.17	0.67
1:A:91:ILE:HD12	1:A:92:THR:N	2.09	0.67
1:A:308:MET:HE2	1:A:357:SER:CB	2.25	0.66
2:B:138:MET:HE1	2:B:226:TYR:HB3	1.77	0.66
2:B:32:GLN:OE1	12:B:610:HOH:O	2.13	0.66
1:A:269:HIS:HD2	1:A:323:TRP:HE1	1.41	0.66
1:A:57:LEU:HD22	1:A:87:TRP:HH2	1.60	0.66
1:A:152:PRO:O	1:A:176:GLY:HA3	1.96	0.66
3:C:113:THR:HG23	12:C:925:HOH:O	1.94	0.66
3:C:91:THR:CG2	3:C:116:VAL:H	2.08	0.65
1:A:20:THR:HA	1:A:24:MET:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:HE22	2:B:14:VAL:H	1.44	0.65
2:B:74:ASN:HB2	10:B:281:LMT:H12	1.78	0.65
1:A:379:PHE:CD1	1:A:379:PHE:C	2.74	0.65
1:A:418:LEU:HD12	1:A:418:LEU:N	2.12	0.65
3:C:9:GLY:HA3	12:C:935:HOH:O	1.96	0.65
4:D:8:PRO:O	4:D:103:THR:HB	1.96	0.65
3:C:91:THR:HB	3:C:115:THR:HA	1.79	0.64
1:A:187:HIS:HE1	1:A:243:THR:HG22	1.62	0.63
4:D:29:ILE:O	4:D:30:TYR:HB2	1.98	0.63
3:C:70:ILE:O	12:C:918:HOH:O	2.16	0.63
1:A:413:HIS:CG	1:A:460:PHE:CE1	2.86	0.63
3:C:109:GLY:O	4:D:43:SER:OG	2.14	0.62
1:A:342:LEU:HD23	1:A:345:MET:CE	2.27	0.62
1:A:52:TYR:CD2	1:A:90:MET:HE2	2.33	0.62
1:A:284:LEU:O	1:A:287:PHE:HB2	1.99	0.62
1:A:307:PRO:HB2	12:A:1014:HOH:O	1.99	0.62
1:A:366:SER:OG	2:B:62:ARG:HG3	2.00	0.62
3:C:32:TYR:CD2	3:C:98:ARG:HD2	2.34	0.62
3:C:40:THR:HB	3:C:41:PRO:CD	2.30	0.61
4:D:33:LEU:HD21	4:D:88:CYS:HB2	1.82	0.61
2:B:180:ILE:HG22	2:B:218:GLU:HG2	1.82	0.61
3:C:93:MET:HA	3:C:93:MET:CE	2.16	0.61
1:A:484:TYR:H	2:B:15[A]:ASN:HD21	1.49	0.61
1:A:155:ASN:HD21	2:B:222:ILE:HB	1.65	0.61
1:A:393:LEU:C	5:A:560:HEA:HMA	2.26	0.61
3:C:93:MET:CE	3:C:112:THR:C	2.73	0.61
1:A:452:MET:HE1	5:A:559:HEA:C14	2.30	0.61
12:B:307:HOH:O	4:D:30:TYR:HA	1.99	0.61
4:D:50:ASN:H	4:D:91:HIS:CE1	2.20	0.60
1:A:54:ARG:HD2	1:A:490:SER:HA	1.84	0.60
1:A:301:PRO:HG2	2:B:72:THR:HG22	1.84	0.60
2:B:164:VAL:O	2:B:233:ALA:HA	2.02	0.60
2:B:70:ARG:HB3	12:B:659:HOH:O	2.01	0.60
3:C:35:SER:OG	3:C:50:SER:OG	2.17	0.59
4:D:4:LEU:HD22	4:D:23:CYS:SG	2.43	0.59
1:A:27:ASN:HD21	1:A:29[C]:LYS:HB2	1.67	0.59
3:C:47:TRP:CZ2	4:D:95:PRO:HB3	2.38	0.59
9:A:564:LDA:H12	10:A:572[A]:LMT:H5'	1.83	0.59
1:A:406:TYR:CE1	1:A:471:MET:HE2	2.37	0.59
1:A:440:TYR:HA	1:A:510:THR:OG1	2.02	0.59
1:A:155:ASN:HD22	2:B:222:ILE:HD12	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:TRP:HB2	4:D:48:VAL:HG13	1.85	0.58
2:B:181:HIS:HB3	2:B:216:CYS:SG	2.43	0.58
4:D:6:GLN:HG2	4:D:103:THR:CG2	2.32	0.58
1:A:413:HIS:CD2	1:A:460:PHE:CZ	2.91	0.58
3:C:91:THR:HG22	3:C:116:VAL:H	1.67	0.58
1:A:412:PHE:CD2	5:A:560:HEA:HAD1	2.38	0.58
1:A:21:ARG:NH1	10:A:570:LMT:H4B	2.19	0.58
1:A:91:ILE:HD12	1:A:91:ILE:C	2.28	0.58
1:A:129:ARG:HB3	10:A:574[A]:LMT:H6'1	1.86	0.58
1:A:268:GLN:NE2	12:A:1110:HOH:O	2.36	0.57
4:D:50:ASN:H	4:D:91:HIS:HE1	1.50	0.57
1:A:269:HIS:CD2	1:A:323:TRP:HE1	2.23	0.57
5:A:559:HEA:HHC	5:A:559:HEA:H122	1.85	0.57
2:B:36:HIS:CD2	9:B:273:LDA:HM23	2.39	0.57
1:A:27:ASN:ND2	1:A:29[B]:LYS:HB2	2.20	0.57
1:A:371:THR:HG21	1:A:429:TYR:CD1	2.40	0.57
2:B:238:LYS:NZ	12:B:756:HOH:O	2.34	0.57
2:B:36:HIS:HD2	9:B:273:LDA:HM23	1.68	0.57
1:A:158:MET:HG2	12:A:1038:HOH:O	2.05	0.57
3:C:93:MET:HE2	3:C:112:THR:N	2.20	0.57
1:A:18:PHE:O	1:A:20:THR:N	2.38	0.56
1:A:511:LEU:HD21	10:A:570:LMT:H22	1.88	0.56
2:B:61:ASN:C	2:B:61:ASN:HD22	2.13	0.56
3:C:99:HIS:HD2	3:C:104:ALA:O	1.88	0.56
1:A:355:VAL:O	1:A:359:ILE:HG13	2.06	0.56
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.88	0.55
1:A:308:MET:CE	1:A:357:SER:HB2	2.36	0.55
2:B:141:LYS:HE2	12:B:1156:HOH:O	2.05	0.55
1:A:85:HIS:CD2	1:A:157:GLN:HB3	2.42	0.55
9:B:273:LDA:HM21	9:B:276:LDA:HM21	1.88	0.55
1:A:105:PRO:HD3	12:A:969:HOH:O	2.06	0.55
1:A:297:PHE:O	1:A:367:ILE:HA	2.05	0.55
1:A:337:GLN:HE22	2:B:104:GLN:NE2	2.03	0.55
1:A:398:LEU:CD1	2:B:34:LEU:HD23	2.36	0.55
5:A:560:HEA:H22	2:B:45:VAL:HG11	1.89	0.55
2:B:138:MET:HB2	2:B:228:PRO:HD2	1.89	0.55
3:C:44:ARG:HG2	12:C:1236:HOH:O	2.07	0.55
1:A:473:ARG:O	1:A:474:ARG:HB2	2.07	0.55
3:C:76:LYS:HD3	12:C:813:HOH:O	2.07	0.54
3:C:93:MET:HE2	3:C:111:GLY:C	2.32	0.54
1:A:74:ALA:HB3	10:A:571[A]:LMT:H4B	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD22	1:A:87:TRP:CH2	2.41	0.54
12:A:1324:HOH:O	2:B:198:ARG:HD3	2.08	0.54
2:B:227:MET:O	2:B:227:MET:CG	2.50	0.54
3:C:19[A]:LYS:HE2	12:C:907:HOH:O	2.08	0.54
1:A:475:TYR:HE1	2:B:224:HIS:NE2	2.06	0.54
2:B:73:HIS:HB2	12:B:1057:HOH:O	2.08	0.54
2:B:81:TRP:CE3	10:B:281:LMT:C12	2.90	0.54
1:A:413:HIS:CD2	1:A:460:PHE:CE1	2.96	0.54
3:C:27:PHE:CE2	3:C:29:PHE:HA	2.43	0.54
1:A:202:THR:O	1:A:203:THR:C	2.51	0.54
2:B:29:HIS:HD2	12:B:863:HOH:O	1.90	0.54
1:A:137:MET:O	1:A:138:TYR:C	2.48	0.53
2:B:138:MET:CE	2:B:226:TYR:HB3	2.39	0.53
1:A:135:TYR:O	1:A:139:VAL:HG23	2.09	0.53
1:A:308:MET:CE	1:A:357:SER:CB	2.86	0.53
2:B:81:TRP:CE3	10:B:281:LMT:H121	2.43	0.53
1:A:102:VAL:C	1:A:105:PRO:HD2	2.33	0.52
1:A:393:LEU:CB	5:A:560:HEA:HMA	2.39	0.52
1:A:410:ALA:O	1:A:411:HIS:C	2.53	0.52
1:A:387:GLY:HA3	5:A:560:HEA:C15	2.40	0.52
1:A:239:ALA:O	1:A:243:THR:CG2	2.50	0.52
3:C:35:SER:OG	3:C:99:HIS:HE1	1.92	0.52
1:A:116:MET:CE	1:A:200:ILE:HG23	2.39	0.52
2:B:118:GLY:H	2:B:176:ALA:HA	1.74	0.52
2:B:108:ASN:ND2	2:B:108:ASN:H	2.07	0.52
1:A:464:HIS:O	1:A:468:ARG:HG3	2.10	0.52
1:A:475:TYR:CE1	2:B:224:HIS:CD2	2.98	0.51
5:A:559:HEA:HHC	5:A:559:HEA:C12	2.41	0.51
2:B:172:VAL:HG12	2:B:174:VAL:HG12	1.93	0.51
1:A:208:ARG:HG2	1:A:212:MET:HG2	1.90	0.51
2:B:81:TRP:HE3	10:B:281:LMT:C12	2.23	0.51
1:A:67:LEU:C	1:A:69:GLY:H	2.17	0.51
1:A:278:GLU:O	1:A:282:ILE:HG13	2.10	0.51
1:A:276:HIS:O	1:A:279:VAL:HG22	2.11	0.51
2:B:21:GLN:NE2	12:B:295:HOH:O	2.41	0.51
1:A:369:PHE:HB2	10:A:573[B]:LMT:H6'2	1.93	0.51
2:B:159:ASP:OD1	2:B:160:ASN:N	2.43	0.51
3:C:22:CYS:HB3	3:C:79:LEU:HB3	1.92	0.51
1:A:364:GLY:HA2	2:B:60:PHE:CE1	2.47	0.51
2:B:1:GLN:HA	2:B:1:GLN:OE1	2.11	0.51
1:A:165:VAL:HB	1:A:271:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ALA:HA	2:B:193:ASP:OD2	2.11	0.50
1:A:509:TYR:CD1	1:A:509:TYR:C	2.89	0.50
1:A:47:VAL:O	1:A:51:VAL:HG23	2.12	0.50
1:A:473:ARG:HG3	1:A:474:ARG:HD2	1.92	0.50
2:B:19:ASN:HD21	9:B:272:LDA:H21	1.76	0.50
3:C:88:SER:O	3:C:91:THR:HG23	2.12	0.50
1:A:277:PRO:O	1:A:278:GLU:C	2.55	0.50
2:B:61:ASN:C	2:B:61:ASN:ND2	2.70	0.50
3:C:93:MET:CE	3:C:112:THR:N	2.74	0.50
1:A:38:THR:CG2	1:A:138:TYR:CE2	2.94	0.50
1:A:65:MET:CE	1:A:65:MET:CG	2.88	0.50
3:C:42:GLU:CD	3:C:42:GLU:H	2.19	0.50
3:C:101:TYR:HB3	4:D:49:TYR:CD2	2.46	0.49
2:B:138:MET:SD	2:B:155:LEU:HD23	2.52	0.49
2:B:155:LEU:HD21	2:B:226:TYR:CE1	2.47	0.49
1:A:418:LEU:N	1:A:418:LEU:CD1	2.74	0.49
1:A:459:ILE:HD13	5:A:559:HEA:HMB2	1.94	0.49
4:D:61:ARG:CZ	4:D:79:LEU:HD23	2.42	0.49
1:A:18:PHE:O	1:A:21:ARG:N	2.33	0.49
1:A:27:ASN:HD21	1:A:29[A]:LYS:CG	2.25	0.49
1:A:209:ALA:O	1:A:212:MET:HB3	2.11	0.49
2:B:119:HIS:HE1	2:B:177:THR:HG21	1.77	0.49
2:B:19:ASN:HB3	12:B:314:HOH:O	2.12	0.49
10:A:575[B]:LMT:O2B	10:A:575[B]:LMT:H5B	2.13	0.49
1:A:168:PRO:HD2	1:A:267:TYR:CD2	2.48	0.48
1:A:391:VAL:O	1:A:394:SER:OG	2.28	0.48
3:C:108:TRP:CE3	4:D:44:PRO:HD2	2.48	0.48
1:A:92:THR:O	1:A:96:VAL:HG23	2.14	0.48
3:C:38:ARG:HD3	3:C:48:VAL:HG21	1.94	0.48
1:A:27:ASN:HD21	1:A:29[A]:LYS:HG3	1.78	0.48
1:A:125:MET:HA	1:A:125:MET:HE3	1.95	0.48
1:A:412:PHE:CB	5:A:560:HEA:C2D	2.91	0.48
1:A:452:MET:O	1:A:452:MET:HG3	2.12	0.48
2:B:61:ASN:ND2	2:B:64:ALA:H	2.11	0.48
3:C:8:GLY:O	3:C:18:LEU:HD11	2.13	0.48
3:C:39:GLN:O	3:C:92:ALA:HB1	2.13	0.48
4:D:81:GLU:OE1	4:D:81:GLU:N	2.44	0.48
1:A:363:TRP:CD1	10:B:281:LMT:H61	2.48	0.48
1:A:460:PHE:O	1:A:461:PHE:C	2.52	0.48
10:A:570:LMT:H2B	10:A:570:LMT:H6E	1.95	0.48
1:A:384:THR:O	1:A:388:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ALA:O	2:B:250:PHE:HB3	2.13	0.48
1:A:38:THR:HG21	1:A:138:TYR:CE2	2.49	0.48
1:A:373:MET:O	1:A:377:PHE:HB2	2.14	0.48
1:A:520:PRO:HA	1:A:534:LEU:O	2.14	0.48
2:B:81:TRP:CZ3	10:B:281:LMT:H121	2.49	0.48
3:C:51:ILE:HD11	3:C:55:GLY:HA2	1.96	0.48
1:A:386:GLY:HA2	1:A:389:THR:HG22	1.96	0.48
2:B:19:ASN:HD21	9:B:272:LDA:H41	1.78	0.48
1:A:115:PHE:CZ	1:A:431:TRP:CG	3.02	0.47
1:A:379:PHE:CD1	1:A:379:PHE:O	2.67	0.47
2:B:1:GLN:N	2:B:4:LEU:HB2	2.28	0.47
3:C:93:MET:HE1	3:C:112:THR:CA	2.44	0.47
1:A:98:MET:HG3	5:A:559:HEA:CAC	2.45	0.47
1:A:452:MET:HE1	5:A:559:HEA:H161	1.95	0.47
1:A:99:MET:HE3	1:A:278:GLU:OE2	2.15	0.47
1:A:169:PRO:O	1:A:173:THR:HB	2.13	0.47
2:B:140[B]:GLU:OE2	12:B:1161:HOH:O	2.20	0.47
1:A:292:HIS:H	1:A:292:HIS:CD2	2.32	0.47
2:B:120:GLN:HB3	2:B:121:TRP:CE2	2.50	0.47
1:A:115:PHE:O	1:A:116:MET:C	2.53	0.47
1:A:417:SER:C	1:A:418:LEU:HD12	2.39	0.47
1:A:393:LEU:HB3	5:A:560:HEA:HMA	1.97	0.47
5:A:559:HEA:HMC1	5:A:559:HEA:HBC1	1.96	0.47
2:B:127:TYR:N	2:B:127:TYR:CD1	2.81	0.47
10:B:280:LMT:O3'	10:B:280:LMT:H1B	2.14	0.47
1:A:217:VAL:CG1	1:A:221:ALA:HB3	2.45	0.46
3:C:44:ARG:CG	12:C:1236:HOH:O	2.63	0.46
1:A:68:GLU:H	1:A:68:GLU:CD	2.22	0.46
1:A:398:LEU:HD13	2:B:34:LEU:HD23	1.98	0.46
1:A:416:MET:HG2	5:A:560:HEA:CBC	2.46	0.46
2:B:72:THR:O	2:B:73:HIS:HB3	2.16	0.46
4:D:61:ARG:NE	4:D:82:ASP:OD2	2.42	0.46
1:A:388:VAL:HG13	2:B:42:ILE:HD12	1.96	0.46
1:A:68:GLU:OE1	1:A:68:GLU:N	2.37	0.46
1:A:292:HIS:CD2	1:A:292:HIS:N	2.84	0.46
1:A:389:THR:CG2	1:A:411:HIS:HA	2.45	0.46
1:A:18:PHE:HD2	1:A:18:PHE:H	1.62	0.46
1:A:303:PHE:CD1	1:A:303:PHE:C	2.93	0.46
1:A:364:GLY:HA2	2:B:60:PHE:CD1	2.51	0.46
1:A:116:MET:HE3	1:A:200:ILE:HG23	1.97	0.46
1:A:233:LEU:HB3	1:A:320:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:HE3	1:A:203:THR:OG1	2.16	0.45
2:B:40:TYR:CE1	9:B:274:LDA:H31	2.36	0.45
1:A:167:TYR:HB2	12:A:1274:HOH:O	2.16	0.45
1:A:311:ALA:O	1:A:315:ILE:HD12	2.16	0.45
1:A:54:ARG:CD	1:A:490:SER:HA	2.46	0.45
1:A:322:VAL:O	1:A:325:HIS:ND1	2.49	0.45
2:B:202:LEU:HD12	2:B:202:LEU:C	2.41	0.45
1:A:484:TYR:OH	10:B:279:LMT:H5'	2.16	0.45
1:A:137:MET:HB2	1:A:192:SER:HB2	1.98	0.45
1:A:432:ILE:HD13	1:A:510:THR:HG21	1.97	0.45
1:A:545:THR:CB	12:A:637:HOH:O	2.32	0.45
2:B:67:VAL:HA	2:B:68:PRO:HD2	1.82	0.45
4:D:50:ASN:C	4:D:52:LYS:H	2.18	0.45
1:A:452:MET:HE1	5:A:559:HEA:H14	1.99	0.45
3:C:87:LYS:H	3:C:87:LYS:HG2	1.62	0.45
1:A:71:ARG:NH2	1:A:79:GLU:O	2.50	0.45
1:A:140:CYS:O	1:A:143:ALA:N	2.45	0.45
1:A:200:ILE:HD12	1:A:200:ILE:HA	1.87	0.45
1:A:306:LEU:N	1:A:307:PRO:HD2	2.32	0.45
1:A:267:TYR:OH	1:A:271:LEU:HD13	2.16	0.45
2:B:165:PRO:HA	2:B:234:VAL:O	2.16	0.45
2:B:228:PRO:C	2:B:229:ILE:HG13	2.42	0.45
1:A:98:MET:HG3	5:A:559:HEA:C2C	2.47	0.44
1:A:116:MET:CE	1:A:204:PHE:HB2	2.48	0.44
1:A:308:MET:HE1	1:A:357:SER:HB2	1.98	0.44
1:A:475:TYR:HE1	2:B:224:HIS:CD2	2.36	0.44
3:C:68:PHE:CD1	3:C:68:PHE:N	2.85	0.44
1:A:324:ALA:HB1	1:A:332:MET:HE1	2.00	0.44
1:A:475:TYR:CE1	2:B:224:HIS:NE2	2.84	0.44
1:A:34:LEU:HB3	1:A:135:TYR:CE1	2.53	0.44
4:D:6:GLN:NE2	4:D:103:THR:HG23	2.28	0.44
1:A:325:HIS:HB2	5:A:560:HEA:OMA	2.17	0.44
1:A:29[C]:LYS:HE3	1:A:538:PRO:HB2	2.00	0.44
1:A:312:MET:CE	1:A:312:MET:CG	2.93	0.44
5:A:559:HEA:O11	5:A:559:HEA:HMB1	2.16	0.44
2:B:125:TYR:O	2:B:133:ALA:HA	2.18	0.44
1:A:468:ARG:HD3	2:B:18:MET:O	2.18	0.44
9:A:564:LDA:H21	10:A:572[A]:LMT:H6'2	2.00	0.44
1:A:104:ILE:HB	12:A:969:HOH:O	2.17	0.43
2:B:81:TRP:CE3	10:B:281:LMT:H123	2.53	0.43
10:A:572[B]:LMT:H5'	10:A:572[B]:LMT:O2B	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:HIS:HE1	12:A:857:HOH:O	2.01	0.43
1:A:155:ASN:ND2	2:B:222:ILE:HD12	2.33	0.43
1:A:306:LEU:N	1:A:307:PRO:CD	2.81	0.43
5:A:560:HEA:O11	5:A:560:HEA:CHC	2.61	0.43
1:A:83:ASN:O	1:A:84:GLY:C	2.60	0.43
1:A:443:TRP:HZ2	10:A:569:LMT:H1'	1.84	0.43
1:A:213:THR:O	1:A:214:LEU:C	2.61	0.43
9:A:565:LDA:HM23	9:A:565:LDA:H21	1.59	0.43
2:B:34:LEU:O	2:B:37:PHE:HB3	2.19	0.43
2:B:155:LEU:HD21	2:B:226:TYR:HE1	1.84	0.43
4:D:7:THR:HA	4:D:8:PRO:C	2.44	0.43
4:D:76:ASN:O	4:D:77:SER:C	2.61	0.43
2:B:138:MET:HE1	2:B:226:TYR:CB	2.47	0.43
9:B:273:LDA:HM12	9:B:273:LDA:H21	1.51	0.43
3:C:93:MET:HE2	3:C:111:GLY:CA	2.49	0.43
1:A:52:TYR:HD2	1:A:90:MET:CE	2.24	0.43
1:A:431:TRP:O	1:A:435:MET:HG3	2.19	0.43
3:C:93:MET:CE	3:C:111:GLY:C	2.91	0.43
1:A:165:VAL:HB	1:A:271:LEU:CD2	2.49	0.43
2:B:180:ILE:CG2	2:B:218:GLU:HG2	2.48	0.42
3:C:6:GLU:HA	3:C:21:SER:O	2.19	0.42
4:D:6:GLN:N	12:D:643:HOH:O	2.50	0.42
1:A:433:GLY:HA2	1:A:438:ARG:O	2.18	0.42
2:B:127:TYR:N	2:B:127:TYR:HD1	2.17	0.42
3:C:6:GLU:OE2	3:C:109:GLY:HA3	2.19	0.42
1:A:149:LEU:O	1:A:149:LEU:HG	2.18	0.42
1:A:276:HIS:HB3	1:A:277:PRO:HD3	2.01	0.42
1:A:327:MET:HE2	1:A:327:MET:HB3	1.81	0.42
2:B:12:LYS:HE3	2:B:153:GLU:CG	2.49	0.42
2:B:30:ASP:HB3	2:B:99:ILE:HG23	2.01	0.42
1:A:416:MET:HG2	5:A:560:HEA:HBC2	2.02	0.42
5:A:559:HEA:H211	5:A:559:HEA:H253	1.67	0.42
5:A:560:HEA:H252	2:B:45:VAL:HG21	2.01	0.42
2:B:138:MET:HE1	2:B:226:TYR:CD1	2.54	0.42
3:C:34:MET:HE3	3:C:34:MET:HB3	1.64	0.42
1:A:116:MET:HE1	1:A:200:ILE:HG23	2.02	0.42
1:A:116:MET:HE1	1:A:200:ILE:O	2.20	0.42
1:A:416:MET:CG	5:A:560:HEA:HAC	2.50	0.42
2:B:1:GLN:H1	2:B:4:LEU:HB2	1.83	0.42
2:B:7:LEU:HA	2:B:8:PRO:HD2	1.89	0.42
2:B:91:ALA:O	2:B:92:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:VAL:O	3:C:61:PRO:HD2	2.20	0.42
1:A:351:THR:HG21	5:A:560:HEA:H14	2.01	0.42
2:B:103:SER:OG	2:B:104:GLN:N	2.52	0.42
1:A:155:ASN:HD22	2:B:222:ILE:CD1	2.33	0.41
3:C:6:GLU:OE1	3:C:96:CYS:N	2.49	0.41
5:A:559:HEA:HHA	5:A:559:HEA:HAA2	1.90	0.41
1:A:155:ASN:ND2	2:B:222:ILE:CD1	2.84	0.41
1:A:341:MET:HG3	1:A:394:SER:O	2.20	0.41
1:A:389:THR:HG23	1:A:411:HIS:HA	2.02	0.41
1:A:459:ILE:HD13	1:A:459:ILE:HG21	1.92	0.41
2:B:119:HIS:CE1	2:B:177:THR:CG2	3.03	0.41
1:A:21:ARG:HH12	10:A:570:LMT:H4B	1.84	0.41
1:A:72:LEU:HB2	9:A:567:LDA:H32	2.02	0.41
1:A:116:MET:HE1	1:A:204:PHE:HB2	2.01	0.41
1:A:249:ARG:HH11	1:A:249:ARG:HD3	1.74	0.41
1:A:293:VAL:O	1:A:297:PHE:HD1	2.03	0.41
1:A:371:THR:N	1:A:372:PRO:CD	2.83	0.41
3:C:12:VAL:HB	3:C:13:GLN:H	1.67	0.41
1:A:95:GLY:O	1:A:99:MET:HG2	2.21	0.41
1:A:256:PHE:HB3	1:A:264:PRO:HA	2.02	0.41
2:B:141:LYS:CE	12:B:1156:HOH:O	2.66	0.41
1:A:18:PHE:O	1:A:19:PHE:C	2.64	0.41
1:A:18:PHE:C	1:A:20:THR:N	2.78	0.41
1:A:125:MET:HE2	1:A:125:MET:HB3	1.79	0.41
1:A:414:TYR:CE1	1:A:418:LEU:HD22	2.56	0.41
2:B:138:MET:HE2	2:B:226:TYR:C	2.46	0.41
1:A:65:MET:O	1:A:83:ASN:HB3	2.20	0.41
1:A:137:MET:H	1:A:137:MET:HG2	1.54	0.41
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.90	0.41
1:A:480:VAL:HG11	12:B:1312:HOH:O	2.20	0.41
4:D:49:TYR:CE1	4:D:53:THR:CG2	3.04	0.41
1:A:57:LEU:O	1:A:58:GLN:C	2.64	0.41
2:B:152:ASP:OD1	2:B:152:ASP:C	2.64	0.41
1:A:42:VAL:H	1:A:42:VAL:HG23	1.66	0.41
1:A:180:ASP:OD2	1:A:249:ARG:NH1	2.53	0.41
1:A:536:SER:HA	1:A:537:PRO:HA	1.80	0.41
2:B:119:HIS:HE1	2:B:177:THR:CG2	2.34	0.41
2:B:55:ILE:O	2:B:56:CYS:C	2.64	0.41
2:B:222:ILE:CD1	2:B:222:ILE:CB	2.87	0.41
1:A:164:TRP:CE2	1:A:165:VAL:HG13	2.56	0.40
1:A:341:MET:HG2	1:A:345:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG21	5:A:559:HEA:HMB2	2.03	0.40
1:A:416:MET:HG2	5:A:560:HEA:CAC	2.52	0.40
2:B:75:THR:N	2:B:76:PRO:HD2	2.36	0.40
1:A:49:PHE:N	1:A:49:PHE:CD1	2.87	0.40
5:A:559:HEA:H263	5:A:559:HEA:H132	1.62	0.40
2:B:139:LEU:HD23	2:B:139:LEU:HA	1.89	0.40
3:C:62:ASP:N	12:C:1238:HOH:O	2.53	0.40
1:A:27:ASN:ND2	1:A:29[A]:LYS:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/558 (95%)	462 (87%)	61 (12%)	7 (1%)	9	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	3
4	D	106/120 (88%)	99 (93%)	3 (3%)	4 (4%)	2	1
All	All	1006/1103 (91%)	882 (88%)	106 (10%)	18 (2%)	6	3

All (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
3	C	109	GLY
4	D	68	GLY

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Mol	Chain	Res	Type
4	D	77	SER
1	A	299	LYS
1	A	482	PHE
1	A	492	GLY
4	D	30	TYR
4	D	51	ALA
1	A	393	LEU
2	B	92	ILE
2	B	67	VAL
1	A	517	VAL
2	B	186	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/454 (96%)	383 (88%)	52 (12%)	5	3
2	B	213/243 (88%)	182 (85%)	31 (15%)	3	1
3	C	103/107 (96%)	84 (82%)	19 (18%)	1	0
4	D	92/104 (88%)	76 (83%)	16 (17%)	2	0
All	All	843/908 (93%)	725 (86%)	118 (14%)	3	2

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	21	ARG
1	A	24	MET
1	A	50	THR
1	A	54	ARG
1	A	55	MET
1	A	57	LEU
1	A	65	MET
1	A	86	LEU
1	A	91	ILE

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Mol	Chain	Res	Type
1	A	98	MET
1	A	100	PHE
1	A	116	MET
1	A	125	MET
1	A	129	ARG
1	A	134	SER
1	A	137	MET
1	A	156	ASP
1	A	166	LEU
1	A	173	THR
1	A	174	GLU
1	A	178	SER
1	A	187	HIS
1	A	198	ILE
1	A	200	ILE
1	A	208	ARG
1	A	214	LEU
1	A	216	LYS
1	A	224	VAL
1	A	233	LEU
1	A	243	THR
1	A	274	PHE
1	A	317	ILE
1	A	332	MET
1	A	335	THR
1	A	359	ILE
1	A	368	GLU
1	A	371	THR
1	A	380	LEU
1	A	388	VAL
1	A	404	ASP
1	A	408	VAL
1	A	417	SER
1	A	418	LEU
1	A	421	VAL
1	A	434	LYS
1	A	438	ARG
1	A	456	SER
1	A	496	SER
1	A	518	ASN
1	A	529	THR
1	A	544	GLU

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Mol	Chain	Res	Type
2	B	1	GLN
2	B	2	ASP
2	B	4	LEU
2	B	9	VAL
2	B	14	VAL
2	B	53	LEU
2	B	54	LEU
2	B	59	ARG
2	B	61	ASN
2	B	63	ARG
2	B	77	ILE
2	B	83	LEU
2	B	85	PRO
2	B	87	LEU
2	B	90	VAL
2	B	96	SER
2	B	104	GLN
2	B	108	ASN
2	B	137	LEU
2	B	138	MET
2	B	142	GLU
2	B	163	VAL
2	B	166	VAL
2	B	173	GLN
2	B	174	VAL
2	B	179	VAL
2	B	184	THR
2	B	186	PRO
2	B	191	LYS
2	B	232	LYS
2	B	247	LYS
3	C	3	LYS
3	C	5	GLN
3	C	6	GLU
3	C	11	LEU
3	C	13	GLN
3	C	17	SER
3	C	19[A]	LYS
3	C	19[B]	LYS
3	C	21	SER
3	C	33	THR
3	C	42	GLU

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Mol	Chain	Res	Type
3	C	44	ARG
3	C	46	GLU
3	C	48	VAL
3	C	50	SER
3	C	83	MET
3	C	87	LYS
3	C	88	SER
3	C	91	THR
4	D	1	ASP
4	D	11	LEU
4	D	14	SER
4	D	15	VAL
4	D	39	LYS
4	D	42	LYS
4	D	48	VAL
4	D	50	ASN
4	D	63	SER
4	D	65	SER
4	D	69	THR
4	D	79	LEU
4	D	103	THR
4	D	104	LYS
4	D	107	ILE
4	D	108	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	85	HIS
1	A	132	ASN
1	A	155	ASN
1	A	157	GLN
1	A	187	HIS
1	A	269	HIS
1	A	469	GLN
1	A	486	ASN
1	A	487	ASN
1	A	518	ASN
2	B	21	GLN
2	B	29	HIS
2	B	61	ASN

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Mol	Chain	Res	Type
2	B	73	HIS
2	B	104	GLN
2	B	108	ASN
2	B	192	GLN
2	B	208	GLN
3	C	13	GLN
3	C	99	HIS
4	D	45	GLN
4	D	70	GLN
4	D	91	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	574[B]	-	36,36,36	4.42	13 (36%)	47,47,47	1.07	2 (4%)
10	LMT	B	281	-	36,36,36	4.35	13 (36%)	47,47,47	1.19	5 (10%)
9	LDA	B	273	-	13,15,15	2.37	2 (15%)	14,17,17	0.42	0

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
10	LMT	B	283[A]	-	36,36,36	4.46	13 (36%)	47,47,47	1.21	2 (4%)
10	LMT	A	575[B]	-	36,36,36	4.36	13 (36%)	47,47,47	1.49	8 (17%)
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
5	HEA	A	560	11,1	67,67,67	3.86	39 (58%)	81,103,103	4.14	52 (64%)
5	HEA	A	559	1	67,67,67	3.23	28 (41%)	81,103,103	4.59	56 (69%)
9	LDA	B	272	-	13,15,15	2.25	2 (15%)	14,17,17	0.62	0
10	LMT	B	279	-	36,36,36	4.36	13 (36%)	47,47,47	1.47	5 (10%)
10	LMT	B	282[B]	-	36,36,36	4.38	13 (36%)	47,47,47	1.27	6 (12%)
10	LMT	A	571[A]	-	36,36,36	4.33	13 (36%)	47,47,47	1.64	6 (12%)
9	LDA	B	277	-	13,15,15	2.39	2 (15%)	14,17,17	0.44	0
11	PEO	A	576	5,6	1,1,1	0.45	0	-		
10	LMT	A	570	-	36,36,36	4.38	13 (36%)	47,47,47	1.24	4 (8%)
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%)
10	LMT	A	572[A]	-	36,36,36	4.44	13 (36%)	47,47,47	1.23	2 (4%)
10	LMT	A	573[B]	-	36,36,36	4.38	14 (38%)	47,47,47	1.35	5 (10%)
9	LDA	A	564	-	13,15,15	2.29	2 (15%)	14,17,17	0.47	0
10	LMT	A	574[A]	-	36,36,36	4.40	13 (36%)	47,47,47	1.34	5 (10%)
10	LMT	A	571[B]	-	36,36,36	4.33	13 (36%)	47,47,47	1.65	7 (14%)
9	LDA	A	567	-	13,15,15	2.31	2 (15%)	14,17,17	0.50	0
10	LMT	B	280	-	36,36,36	4.40	13 (36%)	47,47,47	1.16	3 (6%)
9	LDA	B	276	-	13,15,15	2.34	2 (15%)	14,17,17	0.42	0
10	LMT	A	575[A]	-	36,36,36	4.37	13 (36%)	47,47,47	1.43	8 (17%)
9	LDA	B	274	-	13,15,15	2.32	2 (15%)	14,17,17	0.41	0
10	LMT	B	282[A]	-	36,36,36	4.38	13 (36%)	47,47,47	1.30	7 (14%)
10	LMT	A	568	-	36,36,36	4.36	13 (36%)	47,47,47	1.00	3 (6%)
9	LDA	B	275	-	13,15,15	2.40	2 (15%)	14,17,17	0.45	0
10	LMT	A	569	-	36,36,36	4.39	13 (36%)	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	574[B]	-	-	12/21/61/61	0/2/2/2
10	LMT	B	281	-	-	17/21/61/61	0/2/2/2
9	LDA	B	273	-	-	12/13/13/13	-
9	LDA	A	566	-	-	6/13/13/13	-
10	LMT	B	283[A]	-	-	11/21/61/61	0/2/2/2
10	LMT	A	575[B]	-	-	14/21/61/61	0/2/2/2
10	LMT	A	573[A]	-	-	17/21/61/61	0/2/2/2
9	LDA	A	565	-	-	8/13/13/13	-
5	HEA	A	560	11,1	1/1/7/16	20/36/76/76	-
5	HEA	A	559	1	1/1/7/16	14/36/76/76	-
9	LDA	B	272	-	-	8/13/13/13	-
10	LMT	B	279	-	-	7/21/61/61	0/2/2/2
10	LMT	B	282[B]	-	-	6/21/61/61	0/2/2/2
10	LMT	A	571[A]	-	-	14/21/61/61	0/2/2/2
9	LDA	B	277	-	-	12/13/13/13	-
10	LMT	A	570	-	-	11/21/61/61	0/2/2/2
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
10	LMT	A	572[A]	-	-	15/21/61/61	0/2/2/2
10	LMT	A	573[B]	-	-	18/21/61/61	0/2/2/2
9	LDA	A	564	-	-	9/13/13/13	-
10	LMT	A	574[A]	-	-	12/21/61/61	0/2/2/2
10	LMT	A	571[B]	-	-	15/21/61/61	0/2/2/2
9	LDA	A	567	-	-	9/13/13/13	-
10	LMT	B	280	-	-	14/21/61/61	0/2/2/2
9	LDA	B	276	-	-	7/13/13/13	-
10	LMT	A	575[A]	-	-	14/21/61/61	0/2/2/2
9	LDA	B	274	-	-	8/13/13/13	-
10	LMT	B	282[A]	-	-	6/21/61/61	0/2/2/2
10	LMT	A	568	-	-	14/21/61/61	0/2/2/2
9	LDA	B	275	-	-	6/13/13/13	-
10	LMT	A	569	-	-	10/21/61/61	0/2/2/2
10	LMT	A	572[B]	-	-	10/21/61/61	0/2/2/2

All (361) 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
10	A	572[B]	LMT	C4B-C5B	-9.09	1.33	1.53
10	A	575[B]	LMT	C4B-C5B	-9.09	1.33	1.53
10	A	573[A]	LMT	C4B-C5B	-9.08	1.33	1.53
10	B	282[A]	LMT	C4B-C5B	-9.08	1.33	1.53
10	A	572[A]	LMT	C4B-C5B	-9.07	1.33	1.53
10	A	574[B]	LMT	C4B-C5B	-9.04	1.33	1.53
10	A	574[A]	LMT	C4B-C5B	-9.03	1.33	1.53
10	A	571[B]	LMT	C4B-C5B	-9.02	1.33	1.53
10	B	282[B]	LMT	C4B-C5B	-9.01	1.33	1.53
10	B	283[B]	LMT	C4B-C5B	-9.01	1.33	1.53
10	A	575[A]	LMT	C4B-C5B	-8.96	1.33	1.53
10	A	568	LMT	C4B-C5B	-8.86	1.34	1.53
10	B	280	LMT	C4B-C5B	-8.84	1.34	1.53
10	B	278	LMT	C4B-C5B	-8.84	1.34	1.53
10	B	281	LMT	C4B-C5B	-8.77	1.34	1.53
10	A	570	LMT	C4B-C5B	-8.70	1.34	1.53
10	A	569	LMT	C4B-C5B	-8.68	1.34	1.53
5	A	559	HEA	O11-C11	-8.63	1.24	1.42
5	A	560	HEA	C18-C19	8.61	1.52	1.33
5	A	560	HEA	OMA-CMA	8.58	1.40	1.22
5	A	559	HEA	C22-C23	8.51	1.57	1.32
10	B	279	LMT	C4B-C5B	-8.43	1.35	1.53
10	B	283[B]	LMT	O3'-C3'	-8.37	1.22	1.43
10	B	279	LMT	O2B-C2B	-8.33	1.22	1.43
10	B	280	LMT	O3B-C3B	-8.29	1.22	1.43
10	B	283[A]	LMT	O3'-C3'	-8.29	1.22	1.43
10	B	282[B]	LMT	O3B-C3B	-8.28	1.22	1.43
10	A	572[A]	LMT	O2B-C2B	-8.28	1.22	1.43
10	B	283[B]	LMT	O4'-C4B	-8.28	1.22	1.43
10	B	282[B]	LMT	O4'-C4B	-8.27	1.22	1.43
10	B	283[A]	LMT	O2B-C2B	-8.27	1.22	1.43
10	B	283[B]	LMT	O3B-C3B	-8.27	1.22	1.43
10	A	575[B]	LMT	O4'-C4B	-8.26	1.22	1.43
10	B	283[A]	LMT	O3B-C3B	-8.26	1.22	1.43
10	A	573[B]	LMT	O2B-C2B	-8.26	1.22	1.43
10	A	573[B]	LMT	O3B-C3B	-8.26	1.22	1.43
10	A	572[B]	LMT	O4'-C4B	-8.26	1.22	1.43
10	A	574[B]	LMT	O3B-C3B	-8.26	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	283[B]	LMT	O2B-C2B	-8.26	1.22	1.43
10	A	575[A]	LMT	O2B-C2B	-8.25	1.22	1.43
10	B	282[A]	LMT	O2B-C2B	-8.24	1.22	1.43
10	A	575[B]	LMT	O3B-C3B	-8.24	1.22	1.43
10	A	572[A]	LMT	O3'-C3'	-8.24	1.22	1.43
10	A	575[A]	LMT	O3B-C3B	-8.24	1.22	1.43
10	A	573[B]	LMT	O4'-C4B	-8.24	1.22	1.43
10	A	574[A]	LMT	O2B-C2B	-8.24	1.22	1.43
10	A	571[B]	LMT	O4'-C4B	-8.24	1.22	1.43
10	A	572[B]	LMT	O2B-C2B	-8.24	1.22	1.43
10	A	574[A]	LMT	O3B-C3B	-8.24	1.22	1.43
10	A	574[B]	LMT	O2B-C2B	-8.24	1.22	1.43
10	B	282[B]	LMT	O2B-C2B	-8.23	1.22	1.43
10	A	574[A]	LMT	O4'-C4B	-8.23	1.22	1.43
10	A	571[A]	LMT	O3B-C3B	-8.23	1.22	1.43
10	A	573[A]	LMT	O4'-C4B	-8.23	1.22	1.43
10	A	571[A]	LMT	O2B-C2B	-8.23	1.22	1.43
10	A	571[B]	LMT	O3B-C3B	-8.23	1.22	1.43
10	A	573[A]	LMT	O2B-C2B	-8.23	1.22	1.43
10	A	574[B]	LMT	O4'-C4B	-8.23	1.22	1.43
10	A	575[A]	LMT	O4'-C4B	-8.23	1.22	1.43
10	B	283[A]	LMT	O4'-C4B	-8.23	1.22	1.43
10	B	282[A]	LMT	O4'-C4B	-8.22	1.22	1.43
10	A	572[B]	LMT	O3B-C3B	-8.22	1.22	1.43
10	B	280	LMT	O3'-C3'	-8.21	1.22	1.43
10	A	572[A]	LMT	O4'-C4B	-8.21	1.22	1.43
10	A	572[A]	LMT	O3B-C3B	-8.20	1.22	1.43
10	A	570	LMT	O3B-C3B	-8.20	1.22	1.43
10	B	279	LMT	O3'-C3'	-8.20	1.22	1.43
10	A	572[B]	LMT	O3'-C3'	-8.19	1.22	1.43
10	B	280	LMT	O2B-C2B	-8.19	1.22	1.43
10	A	570	LMT	O2B-C2B	-8.19	1.22	1.43
10	B	282[A]	LMT	O3B-C3B	-8.18	1.22	1.43
10	A	574[A]	LMT	O3'-C3'	-8.18	1.22	1.43
10	A	574[B]	LMT	O3'-C3'	-8.18	1.22	1.43
10	A	571[B]	LMT	O2B-C2B	-8.18	1.22	1.43
10	A	569	LMT	O4'-C4B	-8.17	1.22	1.43
10	A	575[B]	LMT	O2B-C2B	-8.17	1.22	1.43
10	A	571[A]	LMT	O4'-C4B	-8.17	1.22	1.43
10	A	569	LMT	O2B-C2B	-8.16	1.22	1.43
10	A	573[A]	LMT	O3B-C3B	-8.16	1.22	1.43
10	A	568	LMT	O4'-C4B	-8.16	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	278	LMT	O3'-C3'	-8.16	1.22	1.43
10	B	280	LMT	O4'-C4B	-8.15	1.22	1.43
10	A	570	LMT	O4'-C4B	-8.14	1.22	1.43
10	A	568	LMT	O3'-C3'	-8.12	1.22	1.43
10	B	281	LMT	O2B-C2B	-8.12	1.22	1.43
10	A	570	LMT	O3'-C3'	-8.11	1.22	1.43
10	B	281	LMT	O4'-C4B	-8.10	1.22	1.43
10	A	569	LMT	O3B-C3B	-8.10	1.22	1.43
10	A	569	LMT	O3'-C3'	-8.10	1.22	1.43
10	B	279	LMT	O3B-C3B	-8.09	1.22	1.43
10	A	568	LMT	O3B-C3B	-8.08	1.22	1.43
10	A	575[A]	LMT	O3'-C3'	-8.07	1.23	1.43
10	A	575[B]	LMT	O3'-C3'	-8.07	1.23	1.43
10	A	568	LMT	O2B-C2B	-8.07	1.23	1.43
10	B	281	LMT	O3B-C3B	-8.07	1.23	1.43
10	B	281	LMT	O3'-C3'	-8.06	1.23	1.43
10	B	279	LMT	O4'-C4B	-8.04	1.23	1.43
10	B	282[A]	LMT	O3'-C3'	-8.02	1.23	1.43
10	B	282[B]	LMT	O3'-C3'	-8.02	1.23	1.43
10	A	571[A]	LMT	O3'-C3'	-8.00	1.23	1.43
10	A	571[B]	LMT	O3'-C3'	-8.00	1.23	1.43
10	A	573[A]	LMT	O3'-C3'	-8.00	1.23	1.43
10	A	573[B]	LMT	O3'-C3'	-8.00	1.23	1.43
10	B	278	LMT	O2B-C2B	-8.00	1.23	1.43
10	B	278	LMT	O3B-C3B	-7.99	1.23	1.43
5	A	559	HEA	C14-C15	7.98	1.51	1.33
10	B	278	LMT	O4'-C4B	-7.93	1.23	1.43
5	A	559	HEA	C18-C19	7.67	1.50	1.33
5	A	559	HEA	OMA-CMA	7.58	1.38	1.22
10	B	283[B]	LMT	C3B-C2B	-7.35	1.33	1.52
10	A	569	LMT	C3'-C2'	-7.30	1.33	1.52
10	B	283[A]	LMT	C3'-C2'	-7.27	1.33	1.52
10	B	279	LMT	C3B-C2B	-7.26	1.33	1.52
10	A	574[B]	LMT	C4B-C3B	-7.25	1.33	1.52
10	A	569	LMT	C3B-C2B	-7.23	1.33	1.52
10	B	283[B]	LMT	C3'-C2'	-7.23	1.33	1.52
10	A	573[B]	LMT	C4B-C3B	-7.23	1.33	1.52
5	A	560	HEA	C22-C23	7.22	1.54	1.32
10	B	283[B]	LMT	C4B-C3B	-7.22	1.33	1.52
10	B	283[A]	LMT	C4B-C3B	-7.18	1.33	1.52
10	B	281	LMT	C3'-C2'	-7.17	1.33	1.52
10	A	574[B]	LMT	C3B-C2B	-7.16	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	575[A]	LMT	C3B-C2B	-7.16	1.33	1.52
10	B	283[A]	LMT	C3B-C2B	-7.15	1.33	1.52
10	A	572[B]	LMT	C4B-C3B	-7.14	1.33	1.52
10	B	282[A]	LMT	C4B-C3B	-7.14	1.33	1.52
10	A	570	LMT	C3'-C2'	-7.14	1.33	1.52
10	A	572[A]	LMT	C3'-C2'	-7.13	1.33	1.52
10	A	575[A]	LMT	C4B-C3B	-7.13	1.33	1.52
10	B	282[B]	LMT	C4B-C3B	-7.13	1.33	1.52
10	B	282[A]	LMT	C3B-C2B	-7.13	1.33	1.52
10	A	574[A]	LMT	C3'-C2'	-7.12	1.33	1.52
10	A	574[B]	LMT	C3'-C2'	-7.12	1.33	1.52
10	A	575[B]	LMT	C4B-C3B	-7.10	1.33	1.52
10	B	280	LMT	C3'-C2'	-7.10	1.33	1.52
10	B	280	LMT	C3B-C2B	-7.09	1.33	1.52
10	A	572[A]	LMT	C4B-C3B	-7.09	1.33	1.52
10	A	568	LMT	C3'-C2'	-7.09	1.34	1.52
10	A	572[A]	LMT	C3B-C2B	-7.08	1.34	1.52
10	A	571[B]	LMT	C4B-C3B	-7.08	1.34	1.52
10	A	572[B]	LMT	C3B-C2B	-7.07	1.34	1.52
10	A	572[A]	LMT	C4'-C5'	-7.07	1.33	1.52
10	A	571[B]	LMT	C3B-C2B	-7.06	1.34	1.52
10	A	573[A]	LMT	C3B-C2B	-7.06	1.34	1.52
10	B	282[B]	LMT	C3B-C2B	-7.06	1.34	1.52
10	A	574[A]	LMT	C4B-C3B	-7.05	1.34	1.52
10	B	278	LMT	C3'-C2'	-7.05	1.34	1.52
10	A	573[A]	LMT	C4B-C3B	-7.05	1.34	1.52
10	A	571[A]	LMT	C4B-C3B	-7.04	1.34	1.52
10	A	570	LMT	C4B-C3B	-7.04	1.34	1.52
10	A	568	LMT	C3B-C2B	-7.03	1.34	1.52
10	B	279	LMT	C3'-C2'	-7.02	1.34	1.52
10	B	283[B]	LMT	C4'-C5'	-7.01	1.33	1.52
10	A	568	LMT	C4B-C3B	-7.01	1.34	1.52
10	B	281	LMT	C3B-C2B	-7.01	1.34	1.52
10	B	280	LMT	C4B-C3B	-7.01	1.34	1.52
10	A	573[B]	LMT	C3B-C2B	-7.00	1.34	1.52
10	A	569	LMT	C4B-C3B	-7.00	1.34	1.52
10	A	572[B]	LMT	C3'-C2'	-7.00	1.34	1.52
10	A	572[B]	LMT	C4'-C5'	-6.99	1.33	1.52
10	A	570	LMT	C3B-C2B	-6.99	1.34	1.52
10	A	574[A]	LMT	C3B-C2B	-6.99	1.34	1.52
10	B	282[A]	LMT	C3'-C2'	-6.98	1.34	1.52
10	B	282[B]	LMT	C3'-C2'	-6.98	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	575[B]	LMT	C3B-C2B	-6.98	1.34	1.52
10	A	571[A]	LMT	C3B-C2B	-6.97	1.34	1.52
10	B	278	LMT	C3B-C2B	-6.96	1.34	1.52
10	A	570	LMT	C4'-C5'	-6.95	1.34	1.52
10	B	281	LMT	C4B-C3B	-6.95	1.34	1.52
10	B	283[B]	LMT	C3'-C4'	-6.95	1.33	1.52
10	B	283[A]	LMT	C4'-C5'	-6.93	1.34	1.52
10	B	278	LMT	C4B-C3B	-6.91	1.34	1.52
10	B	279	LMT	C4B-C3B	-6.90	1.34	1.52
10	A	575[A]	LMT	C4'-C5'	-6.87	1.34	1.52
10	A	575[B]	LMT	C4'-C5'	-6.87	1.34	1.52
10	B	279	LMT	C4'-C5'	-6.86	1.34	1.52
10	B	283[A]	LMT	C3'-C4'	-6.86	1.33	1.52
10	A	572[A]	LMT	C3'-C4'	-6.84	1.33	1.52
10	A	568	LMT	C4'-C5'	-6.84	1.34	1.52
9	A	566	LDA	O1-N1	-6.81	1.25	1.42
10	A	571[A]	LMT	C4'-C5'	-6.78	1.34	1.52
10	A	571[B]	LMT	C4'-C5'	-6.78	1.34	1.52
9	B	277	LDA	O1-N1	-6.77	1.25	1.42
9	B	275	LDA	O1-N1	-6.75	1.25	1.42
9	A	565	LDA	O1-N1	-6.75	1.25	1.42
10	B	280	LMT	C4'-C5'	-6.74	1.34	1.52
9	B	273	LDA	O1-N1	-6.73	1.25	1.42
10	A	569	LMT	C4'-C5'	-6.73	1.34	1.52
10	A	573[A]	LMT	C3'-C2'	-6.71	1.34	1.52
10	A	573[B]	LMT	C3'-C2'	-6.71	1.34	1.52
10	A	570	LMT	C3'-C4'	-6.71	1.34	1.52
9	B	276	LDA	O1-N1	-6.68	1.25	1.42
10	A	574[A]	LMT	C4'-C5'	-6.67	1.34	1.52
10	A	574[B]	LMT	C4'-C5'	-6.67	1.34	1.52
10	B	281	LMT	C4'-C5'	-6.66	1.34	1.52
10	A	575[A]	LMT	C3'-C2'	-6.64	1.35	1.52
10	A	575[B]	LMT	C3'-C2'	-6.64	1.35	1.52
10	A	568	LMT	C3'-C4'	-6.64	1.34	1.52
9	A	564	LDA	O1-N1	-6.63	1.25	1.42
9	B	274	LDA	O1-N1	-6.63	1.25	1.42
10	B	281	LMT	C3'-C4'	-6.63	1.34	1.52
9	A	567	LDA	O1-N1	-6.63	1.25	1.42
10	B	278	LMT	C3'-C4'	-6.59	1.34	1.52
10	B	280	LMT	C3'-C4'	-6.59	1.34	1.52
10	A	569	LMT	C3'-C4'	-6.58	1.34	1.52
10	A	572[B]	LMT	C3'-C4'	-6.54	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	573[A]	LMT	C4'-C5'	-6.54	1.35	1.52
10	A	573[B]	LMT	C4'-C5'	-6.54	1.35	1.52
10	B	283[B]	LMT	C1B-C2B	-6.52	1.33	1.52
10	A	572[B]	LMT	C1'-C2'	-6.51	1.33	1.52
10	B	282[A]	LMT	C4'-C5'	-6.51	1.35	1.52
10	B	282[B]	LMT	C4'-C5'	-6.51	1.35	1.52
9	B	272	LDA	O1-N1	-6.50	1.26	1.42
10	A	574[A]	LMT	C3'-C4'	-6.49	1.34	1.52
10	A	574[B]	LMT	C3'-C4'	-6.49	1.34	1.52
10	A	570	LMT	C1'-C2'	-6.49	1.33	1.52
10	B	280	LMT	C1'-C2'	-6.48	1.33	1.52
10	B	278	LMT	C4'-C5'	-6.47	1.35	1.52
10	B	279	LMT	C1B-C2B	-6.47	1.33	1.52
10	B	283[A]	LMT	C1'-C2'	-6.42	1.33	1.52
10	A	571[A]	LMT	C3'-C2'	-6.42	1.35	1.52
10	A	571[B]	LMT	C3'-C2'	-6.42	1.35	1.52
10	A	569	LMT	C1'-C2'	-6.42	1.33	1.52
10	A	575[A]	LMT	C3'-C4'	-6.41	1.34	1.52
10	A	575[B]	LMT	C3'-C4'	-6.41	1.34	1.52
10	A	574[A]	LMT	C1'-C2'	-6.41	1.33	1.52
10	A	574[B]	LMT	C1'-C2'	-6.41	1.33	1.52
10	B	279	LMT	C3'-C4'	-6.40	1.34	1.52
10	B	282[A]	LMT	C1'-C2'	-6.40	1.33	1.52
10	B	282[B]	LMT	C1'-C2'	-6.40	1.33	1.52
10	B	281	LMT	C1'-C2'	-6.37	1.33	1.52
10	A	572[A]	LMT	C1B-C2B	-6.35	1.33	1.52
5	A	560	HEA	FE-NC	6.33	2.16	1.95
10	B	282[A]	LMT	C3'-C4'	-6.33	1.35	1.52
10	B	282[B]	LMT	C3'-C4'	-6.33	1.35	1.52
10	A	574[A]	LMT	C1B-C2B	-6.32	1.34	1.52
10	B	282[A]	LMT	C1B-C2B	-6.32	1.34	1.52
10	A	572[A]	LMT	C1'-C2'	-6.31	1.34	1.52
10	A	573[A]	LMT	C3'-C4'	-6.31	1.35	1.52
10	A	573[B]	LMT	C3'-C4'	-6.31	1.35	1.52
10	A	573[A]	LMT	C1B-C2B	-6.30	1.34	1.52
10	B	283[B]	LMT	C1'-C2'	-6.30	1.34	1.52
10	B	282[B]	LMT	C1B-C2B	-6.29	1.34	1.52
10	B	281	LMT	C1B-C2B	-6.28	1.34	1.52
10	A	568	LMT	C1'-C2'	-6.28	1.34	1.52
10	A	575[A]	LMT	C1B-C2B	-6.28	1.34	1.52
10	A	569	LMT	C1B-C2B	-6.28	1.34	1.52
10	B	279	LMT	C1'-C2'	-6.26	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	571[A]	LMT	C3'-C4'	-6.25	1.35	1.52
10	A	571[B]	LMT	C3'-C4'	-6.25	1.35	1.52
5	A	560	HEA	C3B-C2B	6.24	1.48	1.34
10	A	570	LMT	C1B-C2B	-6.24	1.34	1.52
10	B	280	LMT	C1B-C2B	-6.23	1.34	1.52
10	A	568	LMT	C1B-C2B	-6.23	1.34	1.52
10	B	283[A]	LMT	C1B-C2B	-6.23	1.34	1.52
10	A	572[B]	LMT	C1B-C2B	-6.23	1.34	1.52
10	A	575[B]	LMT	C1B-C2B	-6.22	1.34	1.52
10	B	278	LMT	C1'-C2'	-6.21	1.34	1.52
10	A	574[B]	LMT	C1B-C2B	-6.20	1.34	1.52
10	A	571[A]	LMT	C1B-C2B	-6.20	1.34	1.52
10	A	573[B]	LMT	C1B-C2B	-6.13	1.34	1.52
10	A	571[B]	LMT	C1B-C2B	-6.13	1.34	1.52
10	A	573[A]	LMT	C1'-C2'	-6.11	1.34	1.52
10	A	573[B]	LMT	C1'-C2'	-6.11	1.34	1.52
10	A	571[A]	LMT	C1'-C2'	-6.07	1.34	1.52
10	A	571[B]	LMT	C1'-C2'	-6.07	1.34	1.52
10	B	278	LMT	C1B-C2B	-6.05	1.34	1.52
10	A	575[A]	LMT	C1'-C2'	-5.98	1.35	1.52
10	A	575[B]	LMT	C1'-C2'	-5.98	1.35	1.52
5	A	560	HEA	FE-NA	5.82	2.14	1.95
5	A	560	HEA	FE-ND	5.78	2.12	1.94
5	A	560	HEA	C3D-C2D	5.61	1.48	1.36
5	A	559	HEA	C3D-C2D	5.58	1.48	1.36
9	B	275	LDA	C1-N1	-5.31	1.46	1.51
9	B	277	LDA	C1-N1	-5.26	1.46	1.51
9	A	566	LDA	C1-N1	-5.18	1.46	1.51
9	B	273	LDA	C1-N1	-5.16	1.46	1.51
5	A	560	HEA	C4A-NA	-5.15	1.29	1.39
5	A	560	HEA	CHA-C1A	5.09	1.48	1.38
9	A	565	LDA	C1-N1	-5.07	1.46	1.51
5	A	559	HEA	C3B-C2B	5.06	1.46	1.34
9	B	276	LDA	C1-N1	-5.01	1.46	1.51
9	A	567	LDA	C1-N1	-4.96	1.46	1.51
9	B	274	LDA	C1-N1	-4.96	1.46	1.51
5	A	559	HEA	FE-NC	4.89	2.11	1.95
9	A	564	LDA	C1-N1	-4.82	1.46	1.51
9	B	272	LDA	C1-N1	-4.81	1.46	1.51
5	A	559	HEA	C1D-C2D	4.79	1.54	1.44
5	A	559	HEA	C4A-NA	-4.69	1.30	1.39
5	A	560	HEA	CHD-C1D	4.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	HEA	C1D-ND	-4.59	1.32	1.40
5	A	560	HEA	C3A-C2A	4.53	1.47	1.37
5	A	560	HEA	FE-NB	4.50	2.08	1.94
5	A	559	HEA	C1A-NA	-4.47	1.31	1.39
5	A	559	HEA	C4C-NC	-4.27	1.31	1.39
10	B	278	LMT	O1'-C1'	4.08	1.47	1.40
5	A	560	HEA	CHB-C4A	4.02	1.46	1.38
5	A	559	HEA	CHB-C1B	3.98	1.48	1.39
10	A	573[A]	LMT	O1'-C1'	3.96	1.46	1.40
10	A	573[B]	LMT	O1'-C1'	3.96	1.46	1.40
5	A	560	HEA	CHD-C4C	3.92	1.48	1.39
5	A	560	HEA	CHC-C4B	3.89	1.46	1.38
10	A	569	LMT	O1'-C1'	3.86	1.46	1.40
10	A	575[A]	LMT	O1'-C1'	3.86	1.46	1.40
10	A	575[B]	LMT	O1'-C1'	3.86	1.46	1.40
10	B	280	LMT	O1'-C1'	3.85	1.46	1.40
10	B	283[A]	LMT	O1'-C1'	3.82	1.46	1.40
10	A	574[A]	LMT	O1'-C1'	3.80	1.46	1.40
10	A	574[B]	LMT	O1'-C1'	3.80	1.46	1.40
5	A	559	HEA	FE-NA	3.80	2.07	1.95
5	A	560	HEA	C4B-NB	-3.79	1.33	1.40
10	A	572[A]	LMT	O1'-C1'	3.76	1.46	1.40
5	A	560	HEA	C1A-NA	-3.75	1.32	1.39
10	B	283[B]	LMT	O1'-C1'	3.71	1.46	1.40
10	B	282[A]	LMT	O1'-C1'	3.71	1.46	1.40
10	B	282[B]	LMT	O1'-C1'	3.71	1.46	1.40
10	B	279	LMT	O1'-C1'	3.69	1.46	1.40
5	A	559	HEA	CHB-C4A	3.69	1.45	1.38
10	A	568	LMT	O1'-C1'	3.69	1.46	1.40
10	A	571[A]	LMT	O1'-C1'	3.61	1.46	1.40
10	A	571[B]	LMT	O1'-C1'	3.61	1.46	1.40
5	A	559	HEA	C1C-NC	-3.58	1.32	1.39
5	A	559	HEA	C1B-C2B	3.50	1.51	1.44
10	B	281	LMT	O1'-C1'	3.43	1.45	1.40
5	A	560	HEA	CHA-C4D	3.41	1.47	1.39
10	A	572[B]	LMT	O1'-C1'	3.41	1.45	1.40
5	A	559	HEA	CHC-C4B	3.39	1.45	1.38
5	A	559	HEA	C12-C11	-3.37	1.47	1.53
5	A	560	HEA	C1C-NC	-3.34	1.33	1.39
10	A	570	LMT	O1'-C1'	3.32	1.45	1.40
5	A	560	HEA	C1B-C2B	3.31	1.51	1.44
5	A	560	HEA	C4B-C3B	3.28	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	HEA	C1A-C2A	-3.08	1.39	1.45
5	A	560	HEA	C4D-ND	-3.05	1.32	1.38
5	A	560	HEA	C1C-C2C	3.02	1.50	1.43
5	A	560	HEA	C3C-C4C	2.87	1.51	1.42
5	A	560	HEA	C1D-ND	-2.75	1.35	1.40
5	A	559	HEA	C3A-C4A	-2.74	1.41	1.46
5	A	560	HEA	C3C-C2C	2.70	1.50	1.41
5	A	560	HEA	C4D-C3D	2.67	1.49	1.45
5	A	560	HEA	C1A-C2A	2.61	1.49	1.45
5	A	559	HEA	CHC-C1C	2.60	1.45	1.39
5	A	559	HEA	CBD-CAD	2.55	1.60	1.51
5	A	560	HEA	C4C-NC	-2.47	1.35	1.39
5	A	560	HEA	CMA-C3A	2.42	1.50	1.45
5	A	560	HEA	C12-C11	-2.32	1.49	1.53
5	A	560	HEA	C1B-NB	-2.32	1.34	1.38
5	A	560	HEA	C1D-C2D	2.30	1.49	1.44
5	A	560	HEA	C17-C18	2.29	1.57	1.50
5	A	559	HEA	CHD-C4C	2.28	1.44	1.39
5	A	559	HEA	CHA-C1A	2.26	1.42	1.38
5	A	560	HEA	CHB-C1B	2.23	1.44	1.39
5	A	559	HEA	CBD-CGD	2.14	1.55	1.50
5	A	560	HEA	C24-C23	2.13	1.56	1.50
5	A	559	HEA	O1D-CGD	2.02	1.28	1.22
10	A	573[B]	LMT	O1B-C1B	2.01	1.47	1.41

All (212) 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	CHB-C1B-NB	10.41	135.63	124.42
5	A	559	HEA	CHB-C4A-NA	10.31	135.68	124.45
5	A	560	HEA	OMA-CMA-C3A	-10.03	102.99	125.62
5	A	559	HEA	CHA-C1A-NA	9.29	134.57	124.45
5	A	559	HEA	C4A-CHB-C1B	-9.07	106.74	126.02
5	A	559	HEA	C17-C18-C19	-8.76	107.57	127.62
5	A	559	HEA	CHA-C4D-ND	8.39	133.45	124.42
5	A	559	HEA	C13-C14-C15	-8.38	108.45	127.62
5	A	559	HEA	O11-C11-C3B	8.31	126.50	111.26
5	A	559	HEA	C16-C15-C14	-8.18	102.81	121.17
5	A	559	HEA	CHA-C4D-C3D	-8.14	112.90	124.77
5	A	559	HEA	C12-C13-C14	-8.00	91.13	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	HEA	CHC-C4B-NB	7.81	134.03	124.37
5	A	560	HEA	C17-C18-C19	-7.75	109.89	127.62
5	A	560	HEA	CHB-C4A-NA	7.71	132.85	124.45
5	A	559	HEA	C21-C22-C23	-7.09	103.99	127.64
5	A	560	HEA	CHC-C4B-NB	7.04	133.07	124.37
5	A	560	HEA	C13-C14-C15	-6.80	112.07	127.62
5	A	559	HEA	C12-C11-C3B	6.76	122.68	112.12
5	A	559	HEA	CHB-C1B-C2B	-6.71	114.44	125.03
5	A	559	HEA	C4C-CHD-C1D	-6.68	110.54	126.25
5	A	559	HEA	CHD-C4C-NC	6.25	135.20	123.86
10	B	283[A]	LMT	C1-O1'-C1'	6.09	124.08	113.68
5	A	559	HEA	C20-C19-C18	-6.03	107.63	121.17
5	A	560	HEA	CAA-CBA-CGA	-6.03	97.67	113.67
5	A	560	HEA	C21-C22-C23	-5.99	107.68	127.64
5	A	559	HEA	CHD-C1D-ND	5.86	131.62	124.37
5	A	560	HEA	CHB-C1B-NB	5.83	130.70	124.42
5	A	560	HEA	C4A-CHB-C1B	-5.64	114.04	126.02
5	A	560	HEA	CHA-C1A-NA	5.58	130.53	124.45
10	A	572[A]	LMT	C1-O1'-C1'	5.56	123.17	113.68
5	A	560	HEA	C1D-C2D-C3D	-5.53	101.16	106.98
5	A	560	HEA	CHB-C1B-C2B	-5.42	116.47	125.03
10	A	571[A]	LMT	C1'-C2'-C3'	5.40	121.37	110.01
10	A	571[B]	LMT	C1'-C2'-C3'	5.40	121.37	110.01
10	A	574[A]	LMT	C1-O1'-C1'	5.17	122.50	113.68
10	A	574[B]	LMT	C1-O1'-C1'	5.17	122.50	113.68
10	A	571[A]	LMT	C2'-C3'-C4'	5.16	121.39	109.68
10	A	571[B]	LMT	C2'-C3'-C4'	5.16	121.39	109.68
10	B	283[B]	LMT	C1-O1'-C1'	5.10	122.39	113.68
10	B	280	LMT	C1-O1'-C1'	5.09	122.38	113.68
10	B	279	LMT	C1-O1'-C1'	5.03	122.27	113.68
5	A	560	HEA	CHB-C4A-C3A	-4.96	116.84	125.21
10	A	571[A]	LMT	C1-O1'-C1'	4.96	122.16	113.68
10	A	571[B]	LMT	C1-O1'-C1'	4.96	122.16	113.68
10	B	278	LMT	C1-O1'-C1'	4.91	122.08	113.68
5	A	559	HEA	C4B-NB-C1B	4.84	110.94	105.21
5	A	560	HEA	C1B-C2B-C3B	-4.84	101.19	106.80
5	A	560	HEA	CHD-C1D-ND	4.82	130.33	124.37
5	A	559	HEA	CHA-C1A-C2A	-4.81	117.27	124.86
5	A	559	HEA	C26-C15-C14	-4.73	111.48	123.63
10	B	279	LMT	O5B-C5B-C4B	4.69	118.15	109.70
5	A	559	HEA	CMB-C2B-C1B	4.62	132.26	125.03
10	A	575[A]	LMT	C1'-C2'-C3'	4.61	119.72	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	575[B]	LMT	C1'-C2'-C3'	4.61	119.72	110.01
5	A	559	HEA	C4A-NA-C1A	4.59	113.31	105.82
5	A	559	HEA	CHB-C4A-C3A	-4.59	117.47	125.21
5	A	560	HEA	C1D-ND-C4D	4.51	110.55	105.21
5	A	559	HEA	OMA-CMA-C3A	-4.47	115.53	125.62
10	A	573[A]	LMT	C1-O1'-C1'	4.46	121.29	113.68
10	A	573[B]	LMT	C1-O1'-C1'	4.46	121.29	113.68
5	A	559	HEA	CAA-CBA-CGA	-4.45	101.86	113.67
5	A	559	HEA	C13-C12-C11	-4.40	107.36	114.39
5	A	560	HEA	CAD-CBD-CGD	-4.28	102.31	113.67
5	A	560	HEA	C3A-C2A-C1A	-4.28	103.00	107.05
5	A	560	HEA	C25-C23-C22	-4.19	110.07	122.66
5	A	560	HEA	C4B-NB-C1B	4.18	110.16	105.21
5	A	560	HEA	CHA-C4D-ND	4.15	128.89	124.42
5	A	559	HEA	C1C-CHC-C4B	-4.10	116.61	126.25
5	A	559	HEA	C1A-CHA-C4D	-4.05	117.41	126.02
10	A	574[A]	LMT	O1B-C4'-C3'	4.05	117.53	107.23
5	A	560	HEA	O11-C11-C3B	4.01	118.61	111.26
5	A	560	HEA	C4A-NA-C1A	4.00	112.34	105.82
5	A	560	HEA	C3C-C2C-C1C	-3.95	102.51	107.17
5	A	559	HEA	C24-C23-C22	-3.90	110.94	122.66
10	B	279	LMT	C3B-C4B-C5B	3.87	117.24	110.23
5	A	560	HEA	C20-C19-C18	-3.86	112.50	121.17
5	A	559	HEA	CHC-C1C-NC	3.82	130.78	123.86
10	A	570	LMT	C1-O1'-C1'	3.80	120.16	113.68
5	A	559	HEA	CHC-C4B-C3B	-3.76	116.31	125.80
10	A	569	LMT	C1-O1'-C1'	3.75	120.08	113.68
10	A	573[A]	LMT	C2'-C3'-C4'	3.74	118.18	109.68
10	A	573[B]	LMT	C2'-C3'-C4'	3.74	118.18	109.68
10	A	568	LMT	C1-O1'-C1'	3.71	120.02	113.68
10	B	282[A]	LMT	O5'-C5'-C4'	3.71	117.39	109.72
10	B	282[B]	LMT	O5'-C5'-C4'	3.71	117.39	109.72
5	A	559	HEA	CHD-C1D-C2D	-3.67	116.52	126.95
10	A	569	LMT	O5'-C5'-C4'	3.67	117.31	109.72
10	A	575[A]	LMT	C1-O1'-C1'	3.65	119.91	113.68
10	A	575[B]	LMT	C1-O1'-C1'	3.65	119.91	113.68
10	A	573[A]	LMT	O1B-C4'-C3'	3.64	116.48	107.23
10	A	575[A]	LMT	C2'-C3'-C4'	3.62	117.89	109.68
10	A	575[B]	LMT	C2'-C3'-C4'	3.62	117.89	109.68
10	B	281	LMT	C1-O1'-C1'	3.62	119.86	113.68
5	A	560	HEA	CMB-C2B-C1B	3.61	130.67	125.03
5	A	560	HEA	C4C-CHD-C1D	-3.60	117.78	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	571[A]	LMT	C1'-O5'-C5'	-3.59	106.71	113.72
10	A	571[B]	LMT	C1'-O5'-C5'	-3.59	106.71	113.72
5	A	559	HEA	C27-C19-C20	-3.59	109.00	115.23
10	A	572[B]	LMT	C1-O1'-C1'	3.58	119.80	113.68
5	A	559	HEA	C4C-NC-C1C	3.57	111.64	105.82
10	B	282[A]	LMT	C3'-C4'-C5'	3.57	118.83	110.93
10	B	282[B]	LMT	C3'-C4'-C5'	3.57	118.83	110.93
10	B	281	LMT	O5'-C5'-C4'	3.55	117.07	109.72
5	A	560	HEA	CHC-C4B-C3B	-3.52	116.91	125.80
5	A	559	HEA	CMD-C2D-C1D	3.51	130.52	125.03
10	A	572[B]	LMT	C1'-O5'-C5'	-3.50	106.89	113.72
5	A	560	HEA	C26-C15-C16	-3.50	109.15	115.23
5	A	560	HEA	C26-C15-C14	-3.49	114.67	123.63
5	A	560	HEA	CHA-C1A-C2A	-3.48	119.37	124.86
5	A	559	HEA	C3D-C4D-ND	3.40	113.64	110.35
5	A	560	HEA	CHD-C1D-C2D	-3.40	117.29	126.95
10	A	569	LMT	O5B-C5B-C4B	3.33	115.69	109.70
10	A	570	LMT	C1B-O5B-C5B	-3.30	107.28	113.72
5	A	559	HEA	C1D-C2D-C3D	-3.29	103.52	106.98
5	A	559	HEA	CMB-C2B-C3B	-3.27	123.95	130.28
5	A	560	HEA	CHD-C4C-NC	3.27	129.79	123.86
10	A	570	LMT	O1B-C4'-C5'	3.25	118.01	109.48
10	B	282[A]	LMT	C1-O1'-C1'	3.21	119.16	113.68
10	B	282[B]	LMT	C1-O1'-C1'	3.21	119.16	113.68
5	A	559	HEA	C26-C15-C16	3.17	120.73	115.23
10	A	575[A]	LMT	C1'-O5'-C5'	-3.14	107.59	113.72
10	A	575[B]	LMT	C1'-O5'-C5'	-3.14	107.59	113.72
10	A	572[B]	LMT	O1'-C1'-C2'	3.08	112.95	108.27
10	A	570	LMT	O1B-C4'-C3'	3.03	114.94	107.23
5	A	560	HEA	O2A-CGA-O1A	-3.02	115.56	123.33
5	A	560	HEA	CHC-C1C-C2C	-3.00	118.73	127.43
5	A	560	HEA	C4A-C3A-C2A	-2.97	104.24	106.81
5	A	559	HEA	CHD-C4C-C3C	-2.90	114.79	127.37
10	A	575[B]	LMT	C1B-O5B-C5B	-2.87	108.11	113.72
5	A	559	HEA	CBA-CAA-C2A	2.86	120.45	112.53
5	A	559	HEA	C27-C19-C18	-2.86	116.29	123.63
10	B	282[A]	LMT	C2'-C3'-C4'	2.83	116.11	109.68
10	B	282[B]	LMT	C2'-C3'-C4'	2.83	116.11	109.68
5	A	560	HEA	CMD-C2D-C1D	2.83	129.46	125.03
10	A	571[A]	LMT	C4B-C3B-C2B	2.82	115.78	110.83
5	A	560	HEA	C17-C16-C15	2.81	122.50	113.19
10	A	573[A]	LMT	C1'-C2'-C3'	2.79	115.88	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	573[B]	LMT	C1'-C2'-C3'	2.79	115.88	110.01
10	A	573[A]	LMT	C1B-O5B-C5B	-2.78	108.30	113.72
10	B	278	LMT	C1B-O5B-C5B	-2.76	108.32	113.72
10	A	572[A]	LMT	O1B-C4'-C3'	2.73	114.16	107.23
10	A	571[B]	LMT	O1B-C1B-C2B	2.72	114.78	108.09
5	A	559	HEA	CHC-C1C-C2C	-2.72	119.54	127.43
5	A	559	HEA	C25-C23-C22	-2.71	114.51	122.66
5	A	559	HEA	CAD-C3D-C4D	2.71	129.42	124.70
10	B	281	LMT	O1'-C1'-C2'	2.70	112.37	108.27
5	A	560	HEA	C4C-NC-C1C	2.69	110.21	105.82
5	A	559	HEA	C1B-C2B-C3B	-2.66	103.71	106.80
10	B	282[A]	LMT	O1'-C1'-C2'	2.65	112.29	108.27
10	B	282[B]	LMT	O1'-C1'-C2'	2.65	112.29	108.27
10	A	574[A]	LMT	C1B-O5B-C5B	-2.65	108.55	113.72
10	A	573[A]	LMT	C3'-C4'-C5'	2.63	116.75	110.93
10	A	573[B]	LMT	C3'-C4'-C5'	2.63	116.75	110.93
10	A	569	LMT	O1B-C1B-C2B	2.62	114.55	108.09
10	A	568	LMT	O1'-C1'-C2'	2.61	112.24	108.27
5	A	560	HEA	CHC-C1C-NC	2.57	128.52	123.86
5	A	559	HEA	C2A-C1A-NA	-2.52	107.89	110.32
5	A	559	HEA	C4D-C3D-C2D	-2.50	103.25	106.89
5	A	560	HEA	O2A-CGA-CBA	2.47	121.81	114.00
10	A	572[B]	LMT	O5'-C1'-C2'	-2.46	105.31	110.37
5	A	560	HEA	C4C-C3C-C2C	-2.46	104.24	107.30
10	B	278	LMT	C1'-C2'-C3'	2.46	115.19	110.01
10	A	574[A]	LMT	O1B-C4'-C5'	2.45	115.91	109.48
10	B	282[B]	LMT	C1B-O5B-C5B	-2.42	108.98	113.72
10	A	571[A]	LMT	C1B-C2B-C3B	2.42	115.11	110.01
10	B	281	LMT	C3'-C4'-C5'	2.41	116.28	110.93
5	A	559	HEA	CBD-CAD-C3D	-2.41	105.87	112.53
10	A	575[A]	LMT	O1'-C1'-C2'	2.40	111.92	108.27
10	A	575[B]	LMT	O1'-C1'-C2'	2.40	111.92	108.27
10	A	573[B]	LMT	O1B-C1B-C2B	2.39	113.98	108.09
5	A	560	HEA	C2B-C1B-NB	2.38	112.66	109.90
10	B	282[A]	LMT	C1B-O1B-C4'	-2.38	112.34	117.98
10	A	574[A]	LMT	C1B-O1B-C4'	-2.37	112.35	117.98
10	A	572[B]	LMT	C1B-O5B-C5B	-2.37	109.08	113.72
5	A	559	HEA	C3C-C2C-C1C	-2.37	104.38	107.17
5	A	559	HEA	O2A-CGA-CBA	2.36	121.46	114.00
5	A	560	HEA	C12-C13-C14	2.36	118.36	112.16
10	A	571[B]	LMT	C1B-O5B-C5B	-2.36	109.12	113.72
5	A	560	HEA	C16-C17-C18	2.35	123.62	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	560	HEA	C27-C19-C18	-2.33	117.65	123.63
10	B	280	LMT	O1'-C1'-C2'	2.32	111.80	108.27
10	B	278	LMT	O5B-C5B-C6B	2.31	112.17	106.44
10	B	283[A]	LMT	O1'-C1'-C2'	2.30	111.77	108.27
10	B	279	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
10	A	569	LMT	O1'-C1'-C2'	2.28	111.74	108.27
10	A	572[B]	LMT	O1B-C4'-C3'	2.28	113.02	107.23
10	A	568	LMT	C1B-O1B-C4'	-2.27	112.60	117.98
10	B	279	LMT	O1'-C1'-C2'	2.26	111.70	108.27
10	B	283[B]	LMT	O1'-C1'-C2'	2.24	111.68	108.27
5	A	560	HEA	C2D-C1D-ND	2.21	112.38	109.84
10	B	278	LMT	C2'-C3'-C4'	2.19	114.66	109.68
10	A	571[B]	LMT	O1B-C4'-C3'	2.18	112.76	107.23
10	B	282[A]	LMT	O1B-C4'-C3'	2.15	112.70	107.23
10	B	278	LMT	O1B-C1B-C2B	2.15	113.37	108.09
10	A	575[A]	LMT	O1B-C4'-C3'	2.14	112.68	107.23
5	A	559	HEA	C1D-ND-C4D	2.12	107.72	105.21
10	B	283[B]	LMT	O5B-C5B-C4B	2.12	113.51	109.70
5	A	559	HEA	C21-C20-C19	-2.11	106.21	113.19
10	A	575[A]	LMT	C1B-O1B-C4'	-2.09	113.03	117.98
10	B	280	LMT	O1B-C1B-C2B	2.09	113.22	108.09
10	A	575[A]	LMT	O5'-C1'-C2'	2.08	114.65	110.37
10	A	575[B]	LMT	O5'-C1'-C2'	2.08	114.65	110.37
5	A	559	HEA	C4C-C3C-C2C	-2.06	104.74	107.30
5	A	560	HEA	CHA-C4D-C3D	-2.06	121.77	124.77
5	A	560	HEA	C24-C23-C22	-2.03	116.57	122.66
10	A	574[B]	LMT	O1B-C4'-C5'	-2.02	104.17	109.48
5	A	560	HEA	CBD-CAD-C3D	-2.01	106.98	112.53
10	A	575[B]	LMT	O5B-C5B-C6B	2.01	111.41	106.44
10	B	281	LMT	O5B-C5B-C4B	2.00	113.30	109.70

All (2) chirality outliers are listed below:

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

All (380) 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

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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
5	A	560	HEA	C2A-C3A-CMA-OMA
5	A	560	HEA	C4A-C3A-CMA-OMA
5	A	560	HEA	O11-C11-C3B-C2B
5	A	560	HEA	C12-C11-C3B-C2B
5	A	560	HEA	O11-C11-C3B-C4B
5	A	560	HEA	C3B-C11-C12-C13
5	A	560	HEA	C13-C14-C15-C16
5	A	560	HEA	C13-C14-C15-C26
5	A	560	HEA	C17-C18-C19-C27
5	A	560	HEA	C21-C22-C23-C25
9	A	564	LDA	C2-C1-N1-CM2
9	A	565	LDA	C2-C1-N1-O1
9	A	565	LDA	C2-C1-N1-CM1
9	A	565	LDA	C2-C1-N1-CM2
9	A	567	LDA	C2-C1-N1-CM1
9	A	567	LDA	C2-C1-N1-CM2
9	A	567	LDA	N1-C1-C2-C3
9	B	272	LDA	N1-C1-C2-C3
9	B	273	LDA	C2-C1-N1-CM1
9	B	273	LDA	C2-C1-N1-CM2
9	B	273	LDA	N1-C1-C2-C3
9	B	274	LDA	C2-C1-N1-O1
9	B	274	LDA	C2-C1-N1-CM1
9	B	274	LDA	C2-C1-N1-CM2
9	B	276	LDA	C2-C1-N1-CM2
9	B	277	LDA	C2-C1-N1-CM1
9	B	277	LDA	C2-C1-N1-CM2
10	A	573[A]	LMT	C2'-C1'-O1'-C1
10	A	573[A]	LMT	O5'-C1'-O1'-C1
10	A	573[B]	LMT	C2'-C1'-O1'-C1
10	A	573[B]	LMT	O5'-C1'-O1'-C1
10	A	575[A]	LMT	C2'-C1'-O1'-C1
10	A	575[A]	LMT	O5'-C1'-O1'-C1
10	A	575[B]	LMT	C2'-C1'-O1'-C1
10	A	575[B]	LMT	O5'-C1'-O1'-C1
10	B	278	LMT	O5'-C1'-O1'-C1
10	B	281	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
10	B	281	LMT	O5'-C1'-O1'-C1
10	B	282[B]	LMT	C5'-C4'-O1B-C1B
10	A	571[A]	LMT	C3'-C4'-O1B-C1B
10	A	575[B]	LMT	O5B-C1B-O1B-C4'
10	A	575[B]	LMT	C3'-C4'-O1B-C1B
10	A	573[A]	LMT	O5B-C1B-O1B-C4'
10	A	575[B]	LMT	C2B-C1B-O1B-C4'
10	A	569	LMT	O5B-C1B-O1B-C4'
10	A	572[A]	LMT	O5B-C1B-O1B-C4'
10	A	571[B]	LMT	O5B-C1B-O1B-C4'
10	B	283[B]	LMT	C4B-C5B-C6B-O6B
10	A	575[A]	LMT	O5B-C1B-O1B-C4'
10	A	568	LMT	O5'-C5'-C6'-O6'
10	A	570	LMT	C5'-C4'-O1B-C1B
10	A	574[B]	LMT	C3'-C4'-O1B-C1B
10	A	572[A]	LMT	O5B-C5B-C6B-O6B
10	B	283[B]	LMT	O5B-C5B-C6B-O6B
10	A	573[B]	LMT	C3'-C4'-O1B-C1B
10	A	573[A]	LMT	C3'-C4'-O1B-C1B
10	A	575[A]	LMT	O5'-C5'-C6'-O6'
10	A	575[B]	LMT	O5'-C5'-C6'-O6'
10	B	281	LMT	C4B-C5B-C6B-O6B
10	B	281	LMT	O5B-C5B-C6B-O6B
10	A	574[A]	LMT	C4'-C5'-C6'-O6'
10	A	574[B]	LMT	C4'-C5'-C6'-O6'
10	A	572[B]	LMT	C3'-C4'-O1B-C1B
10	A	571[A]	LMT	O5B-C5B-C6B-O6B
10	A	572[A]	LMT	O5'-C5'-C6'-O6'
10	B	280	LMT	O5B-C5B-C6B-O6B
10	A	575[A]	LMT	C4'-C5'-C6'-O6'
10	A	575[B]	LMT	C4'-C5'-C6'-O6'
5	A	560	HEA	C21-C22-C23-C24
10	A	574[A]	LMT	O5B-C5B-C6B-O6B
10	B	281	LMT	O5'-C5'-C6'-O6'
10	A	568	LMT	C4'-C5'-C6'-O6'
10	A	571[A]	LMT	C4B-C5B-C6B-O6B
10	A	574[B]	LMT	C4B-C5B-C6B-O6B
10	A	574[A]	LMT	O5'-C5'-C6'-O6'
10	A	574[B]	LMT	O5B-C5B-C6B-O6B
10	A	574[B]	LMT	O5'-C5'-C6'-O6'
10	A	572[A]	LMT	C4B-C5B-C6B-O6B
5	A	559	HEA	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
10	A	569	LMT	O5'-C1'-O1'-C1
10	A	572[A]	LMT	O5'-C1'-O1'-C1
10	A	569	LMT	O5'-C5'-C6'-O6'
10	A	575[A]	LMT	O5B-C5B-C6B-O6B
5	A	559	HEA	C17-C18-C19-C27
10	B	279	LMT	O5B-C5B-C6B-O6B
10	B	282[A]	LMT	C4'-C5'-C6'-O6'
10	B	282[B]	LMT	C4'-C5'-C6'-O6'
10	B	279	LMT	C4B-C5B-C6B-O6B
10	A	569	LMT	C4'-C5'-C6'-O6'
10	A	575[A]	LMT	C4B-C5B-C6B-O6B
10	A	571[A]	LMT	C4-C5-C6-C7
10	A	571[B]	LMT	C4-C5-C6-C7
10	A	569	LMT	C2'-C1'-O1'-C1
10	A	572[A]	LMT	C2'-C1'-O1'-C1
10	B	280	LMT	C2'-C1'-O1'-C1
10	B	283[A]	LMT	C2'-C1'-O1'-C1
10	A	571[B]	LMT	O5B-C5B-C6B-O6B
10	A	574[A]	LMT	C4B-C5B-C6B-O6B
10	B	280	LMT	C4B-C5B-C6B-O6B
10	B	278	LMT	O5'-C5'-C6'-O6'
10	B	279	LMT	O1'-C1-C2-C3
10	B	280	LMT	O1'-C1-C2-C3
10	B	283[A]	LMT	C4B-C5B-C6B-O6B
10	B	283[B]	LMT	O1'-C1-C2-C3
10	B	278	LMT	O1'-C1-C2-C3
10	A	569	LMT	O1'-C1-C2-C3
10	A	574[A]	LMT	O1'-C1-C2-C3
10	A	574[B]	LMT	O1'-C1-C2-C3
10	B	283[B]	LMT	C4'-C5'-C6'-O6'
10	A	572[A]	LMT	C3'-C4'-O1B-C1B
10	A	571[A]	LMT	C2'-C1'-O1'-C1
10	A	571[B]	LMT	C2'-C1'-O1'-C1
5	A	560	HEA	C15-C16-C17-C18
10	B	281	LMT	O1'-C1-C2-C3
10	A	574[A]	LMT	C1-C2-C3-C4
10	A	574[B]	LMT	C1-C2-C3-C4
9	A	565	LDA	C3-C4-C5-C6
10	A	571[A]	LMT	C6-C7-C8-C9
10	A	571[B]	LMT	C6-C7-C8-C9
10	B	280	LMT	C1-C2-C3-C4
10	A	568	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
10	B	283[A]	LMT	C6-C7-C8-C9
10	B	283[B]	LMT	C6-C7-C8-C9
10	B	278	LMT	C2-C1-O1'-C1'
9	A	567	LDA	C5-C6-C7-C8
9	B	273	LDA	C7-C8-C9-C10
9	B	277	LDA	C4-C5-C6-C7
10	A	573[A]	LMT	C4-C5-C6-C7
10	A	573[B]	LMT	C4-C5-C6-C7
9	B	275	LDA	C7-C8-C9-C10
9	A	564	LDA	C11-C10-C9-C8
10	B	283[A]	LMT	C1-C2-C3-C4
10	B	283[B]	LMT	C1-C2-C3-C4
9	A	564	LDA	C4-C5-C6-C7
10	B	280	LMT	C3-C4-C5-C6
10	A	573[A]	LMT	C5'-C4'-O1B-C1B
10	A	571[A]	LMT	C7-C8-C9-C10
10	A	571[B]	LMT	C7-C8-C9-C10
10	A	571[A]	LMT	O1'-C1-C2-C3
10	A	571[B]	LMT	O1'-C1-C2-C3
10	B	281	LMT	C1-C2-C3-C4
10	A	569	LMT	C11-C10-C9-C8
10	A	570	LMT	C4'-C5'-C6'-O6'
9	A	566	LDA	C6-C7-C8-C9
5	A	560	HEA	C19-C20-C21-C22
10	A	572[B]	LMT	O1'-C1-C2-C3
10	B	282[A]	LMT	C3-C4-C5-C6
10	B	282[A]	LMT	C5-C6-C7-C8
10	B	282[B]	LMT	C3-C4-C5-C6
10	B	282[B]	LMT	C5-C6-C7-C8
10	B	281	LMT	C6-C7-C8-C9
10	A	568	LMT	C1-C2-C3-C4
9	A	565	LDA	C5-C6-C7-C8
10	A	568	LMT	C5-C6-C7-C8
10	A	573[A]	LMT	C7-C8-C9-C10
10	A	573[B]	LMT	C7-C8-C9-C10
10	A	574[A]	LMT	C6-C7-C8-C9
10	A	574[B]	LMT	C6-C7-C8-C9
10	A	568	LMT	O1'-C1-C2-C3
10	A	572[A]	LMT	C4-C5-C6-C7
10	A	572[B]	LMT	C4-C5-C6-C7
9	B	273	LDA	C4-C5-C6-C7
9	A	566	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	B	281	LMT	C7-C8-C9-C10
9	A	565	LDA	C4-C5-C6-C7
9	B	277	LDA	C11-C10-C9-C8
10	B	279	LMT	C9-C10-C11-C12
10	A	570	LMT	C4-C5-C6-C7
10	B	283[A]	LMT	O5B-C5B-C6B-O6B
9	A	567	LDA	C6-C7-C8-C9
9	B	275	LDA	C2-C3-C4-C5
10	A	571[A]	LMT	O5'-C1'-O1'-C1
10	A	571[B]	LMT	O5'-C1'-O1'-C1
10	A	571[A]	LMT	C1-C2-C3-C4
10	A	571[B]	LMT	C1-C2-C3-C4
10	A	572[A]	LMT	C4'-C5'-C6'-O6'
9	B	273	LDA	C3-C4-C5-C6
9	A	565	LDA	C1-C2-C3-C4
10	B	282[A]	LMT	O5'-C5'-C6'-O6'
10	B	282[B]	LMT	O5'-C5'-C6'-O6'
10	A	572[A]	LMT	C3-C4-C5-C6
10	A	572[B]	LMT	C3-C4-C5-C6
10	A	571[A]	LMT	C2-C3-C4-C5
10	A	571[B]	LMT	C2-C3-C4-C5
10	B	279	LMT	C4-C5-C6-C7
10	A	573[B]	LMT	C4B-C5B-C6B-O6B
10	A	572[A]	LMT	C5'-C4'-O1B-C1B
10	A	575[A]	LMT	C2-C3-C4-C5
10	A	575[B]	LMT	C2-C3-C4-C5
10	B	281	LMT	C4-C5-C6-C7
9	B	277	LDA	C5-C6-C7-C8
9	A	564	LDA	C1-C2-C3-C4
10	A	573[A]	LMT	C1-C2-C3-C4
10	A	573[B]	LMT	C1-C2-C3-C4
10	A	574[A]	LMT	O5B-C1B-O1B-C4'
9	B	275	LDA	C5-C6-C7-C8
9	A	567	LDA	C7-C8-C9-C10
9	A	566	LDA	C5-C6-C7-C8
9	B	276	LDA	C3-C4-C5-C6
10	A	573[A]	LMT	C11-C10-C9-C8
10	A	573[B]	LMT	C11-C10-C9-C8
9	B	275	LDA	C3-C4-C5-C6
10	A	573[A]	LMT	C2-C3-C4-C5
10	A	573[B]	LMT	C2-C3-C4-C5
10	A	572[A]	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	A	572[B]	LMT	C2-C3-C4-C5
9	B	277	LDA	C1-C2-C3-C4
10	A	570	LMT	O5'-C5'-C6'-O6'
10	A	573[B]	LMT	O5B-C5B-C6B-O6B
9	B	274	LDA	C1-C2-C3-C4
9	B	276	LDA	C1-C2-C3-C4
10	B	283[A]	LMT	C4'-C5'-C6'-O6'
10	A	568	LMT	C11-C10-C9-C8
10	B	283[A]	LMT	C7-C8-C9-C10
10	B	283[B]	LMT	C7-C8-C9-C10
9	B	272	LDA	C11-C10-C9-C8
10	A	573[A]	LMT	O5B-C5B-C6B-O6B
10	A	573[B]	LMT	O5B-C1B-O1B-C4'
9	B	272	LDA	C1-C2-C3-C4
10	A	573[A]	LMT	C3-C4-C5-C6
10	A	573[B]	LMT	C3-C4-C5-C6
10	A	568	LMT	C2-C3-C4-C5
10	B	283[A]	LMT	C3-C4-C5-C6
10	B	283[B]	LMT	C3-C4-C5-C6
9	B	277	LDA	C6-C7-C8-C9
10	A	571[A]	LMT	C11-C10-C9-C8
10	A	571[B]	LMT	C11-C10-C9-C8
10	A	575[A]	LMT	C11-C10-C9-C8
10	A	575[B]	LMT	C11-C10-C9-C8
10	A	571[B]	LMT	C4B-C5B-C6B-O6B
9	A	567	LDA	C1-C2-C3-C4
9	A	564	LDA	C5-C6-C7-C8
10	A	573[A]	LMT	C4'-C5'-C6'-O6'
10	A	573[B]	LMT	C4'-C5'-C6'-O6'
9	A	565	LDA	C9-C10-C11-C12
10	B	283[A]	LMT	C11-C10-C9-C8
10	B	283[B]	LMT	C11-C10-C9-C8
9	B	275	LDA	C4-C5-C6-C7
9	B	276	LDA	C5-C6-C7-C8
9	B	272	LDA	C3-C4-C5-C6
9	A	566	LDA	C7-C8-C9-C10
9	B	277	LDA	C9-C10-C11-C12
9	B	273	LDA	C5-C6-C7-C8
10	A	574[B]	LMT	C5'-C4'-O1B-C1B
9	A	564	LDA	C3-C4-C5-C6
9	B	273	LDA	C2-C3-C4-C5
10	A	573[A]	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
10	A	573[B]	LMT	C2-C1-O1'-C1'
10	A	570	LMT	C7-C8-C9-C10
10	B	279	LMT	C6-C7-C8-C9
10	B	280	LMT	O5B-C1B-O1B-C4'
10	B	278	LMT	C2'-C1'-O1'-C1
9	B	275	LDA	C9-C10-C11-C12
10	A	568	LMT	C6-C7-C8-C9
10	B	278	LMT	C11-C10-C9-C8
9	A	566	LDA	C4-C5-C6-C7
10	B	281	LMT	C5'-C4'-O1B-C1B
10	B	281	LMT	C4'-C5'-C6'-O6'
9	B	274	LDA	C6-C7-C8-C9
10	B	280	LMT	C9-C10-C11-C12
9	B	274	LDA	C4-C5-C6-C7
10	A	573[A]	LMT	C5-C6-C7-C8
10	A	573[B]	LMT	C5-C6-C7-C8
9	B	274	LDA	C9-C10-C11-C12
9	A	566	LDA	C11-C10-C9-C8
10	B	280	LMT	C11-C10-C9-C8
5	A	559	HEA	C26-C15-C16-C17
10	B	281	LMT	C9-C10-C11-C12
10	A	572[B]	LMT	C4'-C5'-C6'-O6'
10	A	570	LMT	C1-C2-C3-C4
10	A	572[B]	LMT	C5'-C4'-O1B-C1B
9	B	276	LDA	C11-C10-C9-C8
9	B	273	LDA	C6-C7-C8-C9
10	B	278	LMT	C9-C10-C11-C12
10	B	283[B]	LMT	O5'-C5'-C6'-O6'
9	B	273	LDA	C11-C10-C9-C8
9	B	277	LDA	C2-C3-C4-C5
10	A	574[A]	LMT	C5-C6-C7-C8
10	A	574[B]	LMT	C5-C6-C7-C8
10	A	572[A]	LMT	C5-C6-C7-C8
10	A	572[B]	LMT	C5-C6-C7-C8
10	A	575[A]	LMT	C6-C7-C8-C9
10	A	575[B]	LMT	C6-C7-C8-C9
10	A	572[A]	LMT	C9-C10-C11-C12
10	A	572[B]	LMT	C9-C10-C11-C12
9	A	564	LDA	C2-C1-N1-CM1
9	B	272	LDA	C2-C1-N1-CM1
9	B	272	LDA	C2-C1-N1-CM2
9	B	276	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
10	B	283[A]	LMT	C4-C5-C6-C7
10	B	283[B]	LMT	C4-C5-C6-C7
10	A	575[A]	LMT	O1'-C1-C2-C3
10	A	575[B]	LMT	O1'-C1-C2-C3
10	B	281	LMT	C2-C1-O1'-C1'
10	A	573[B]	LMT	C5'-C4'-O1B-C1B
9	B	272	LDA	C2-C3-C4-C5
9	B	277	LDA	C7-C8-C9-C10
10	A	575[A]	LMT	C7-C8-C9-C10
10	A	575[B]	LMT	C7-C8-C9-C10
10	B	280	LMT	C7-C8-C9-C10
9	B	274	LDA	C3-C4-C5-C6
9	A	564	LDA	C2-C1-N1-O1
9	B	276	LDA	C2-C1-N1-O1
9	B	277	LDA	C2-C1-N1-O1
10	A	573[A]	LMT	C9-C10-C11-C12
10	A	573[B]	LMT	C9-C10-C11-C12
9	B	273	LDA	C9-C10-C11-C12
10	A	574[A]	LMT	C3-C4-C5-C6
10	A	574[B]	LMT	C3-C4-C5-C6
5	A	560	HEA	C11-C12-C13-C14
10	A	569	LMT	C7-C8-C9-C10
10	B	278	LMT	C5-C6-C7-C8
10	B	280	LMT	C2B-C1B-O1B-C4'
5	A	560	HEA	C12-C11-C3B-C4B
10	B	278	LMT	C4-C5-C6-C7
10	A	574[A]	LMT	C2B-C1B-O1B-C4'
10	A	572[A]	LMT	C1-C2-C3-C4
10	A	572[B]	LMT	C1-C2-C3-C4
10	A	569	LMT	C2B-C1B-O1B-C4'
10	A	571[A]	LMT	C5-C6-C7-C8
10	A	571[B]	LMT	C5-C6-C7-C8
9	A	567	LDA	C9-C10-C11-C12
10	B	282[A]	LMT	C5'-C4'-O1B-C1B
10	A	575[A]	LMT	C1-C2-C3-C4
10	A	575[B]	LMT	C1-C2-C3-C4
10	A	573[A]	LMT	C6-C7-C8-C9
10	A	573[B]	LMT	C6-C7-C8-C9
10	A	568	LMT	C2-C1-O1'-C1'
10	A	570	LMT	O5B-C5B-C6B-O6B
10	A	570	LMT	C3'-C4'-O1B-C1B
5	A	559	HEA	CAD-CBD-CGD-O1D

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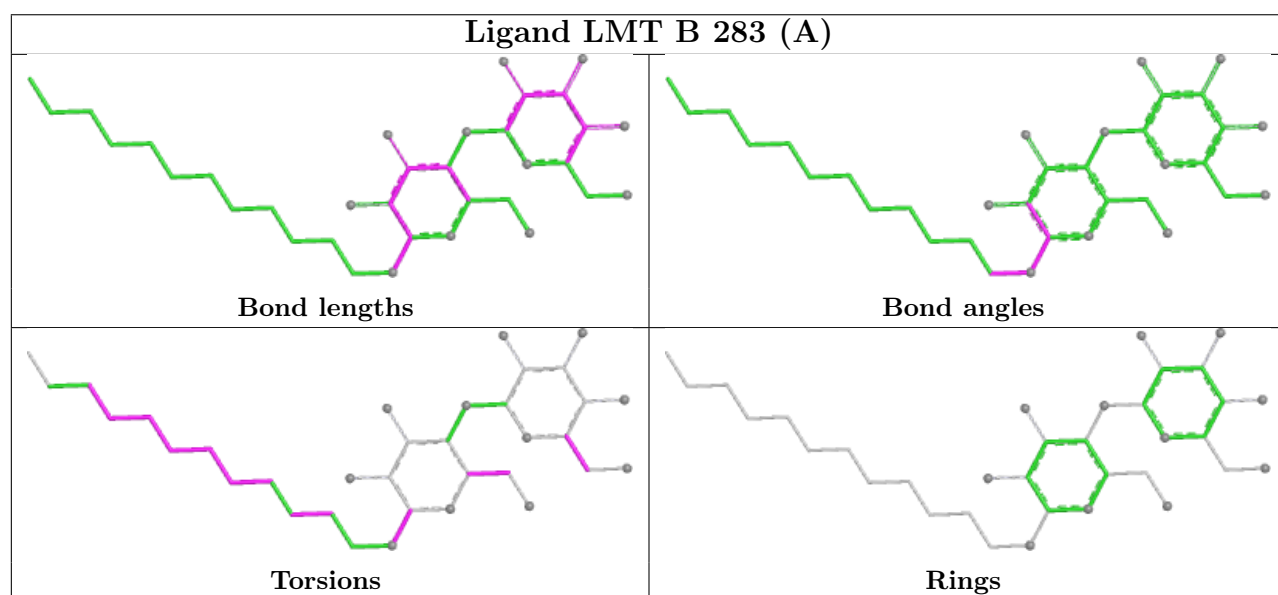
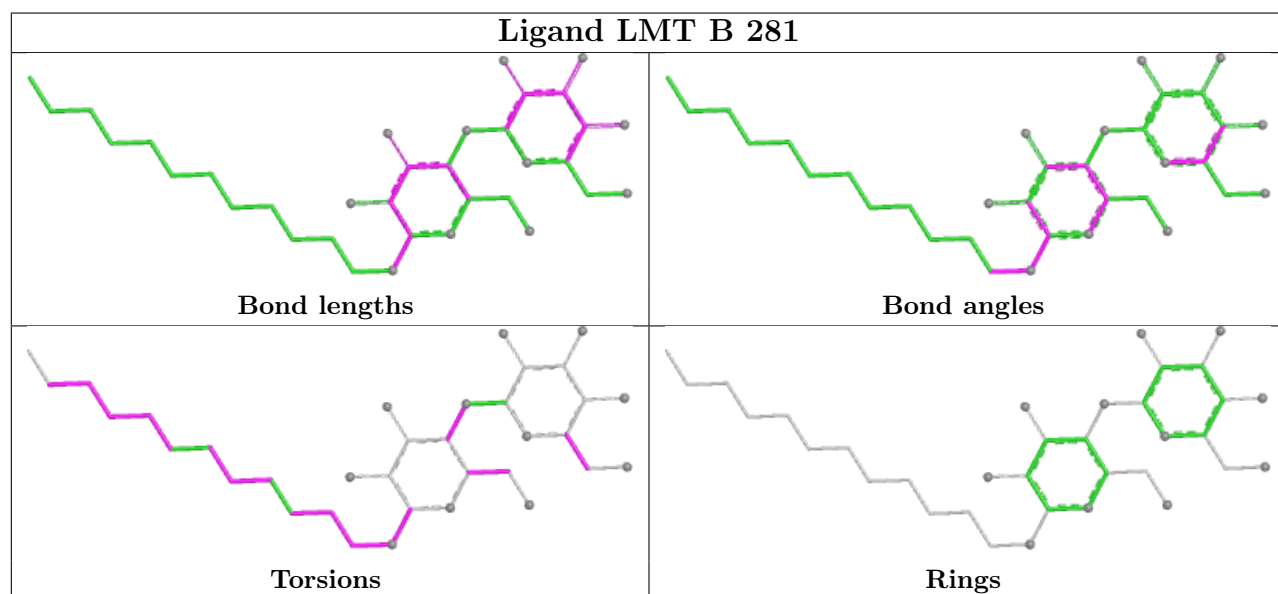
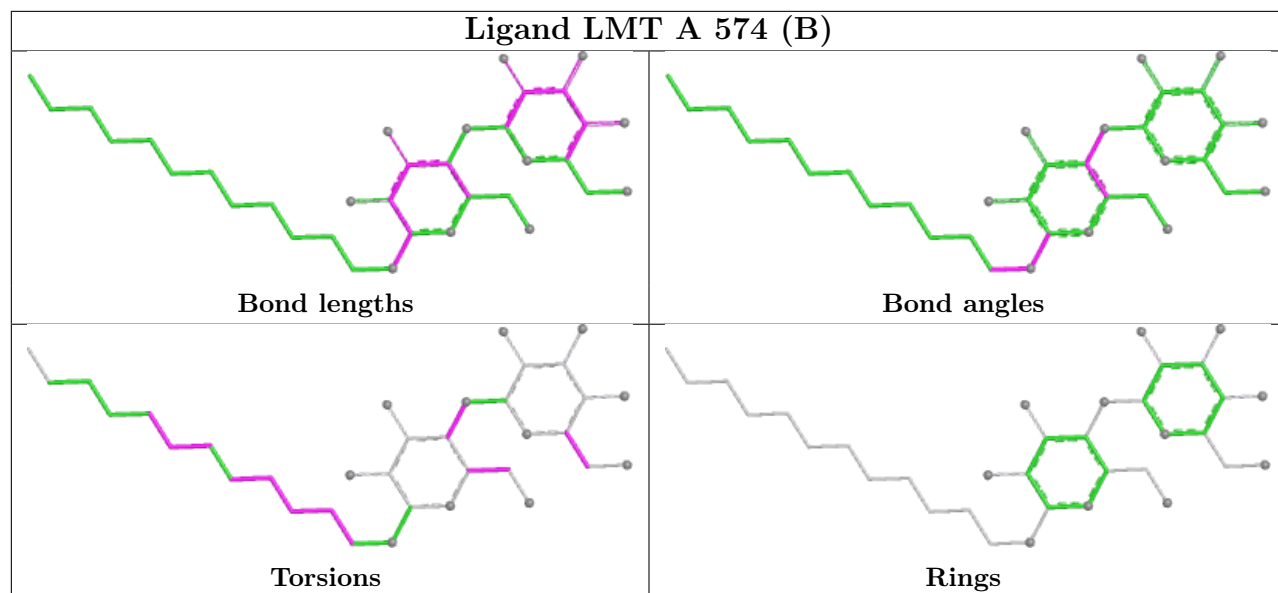
Mol	Chain	Res	Type	Atoms
10	B	282[A]	LMT	C2-C3-C4-C5
10	B	282[B]	LMT	C2-C3-C4-C5
5	A	560	HEA	CAD-CBD-CGD-O2D
5	A	560	HEA	CAA-CBA-CGA-O2A
10	B	278	LMT	C4'-C5'-C6'-O6'
10	A	571[B]	LMT	C2B-C1B-O1B-C4'
10	A	571[A]	LMT	C3-C4-C5-C6
10	A	571[B]	LMT	C3-C4-C5-C6
5	A	559	HEA	CAD-CBD-CGD-O2D
10	B	281	LMT	C3-C4-C5-C6
5	A	559	HEA	C27-C19-C20-C21
10	A	575[A]	LMT	C9-C10-C11-C12
10	A	575[B]	LMT	C9-C10-C11-C12
5	A	560	HEA	C2D-C3D-CAD-CBD
10	B	283[A]	LMT	C5-C6-C7-C8
10	B	283[B]	LMT	C5-C6-C7-C8
10	B	281	LMT	C3'-C4'-O1B-C1B
5	A	560	HEA	CAD-CBD-CGD-O1D
9	B	277	LDA	C3-C4-C5-C6
5	A	560	HEA	CAA-CBA-CGA-O1A
10	B	281	LMT	C11-C10-C9-C8
10	B	280	LMT	C3'-C4'-O1B-C1B
10	A	570	LMT	C3-C4-C5-C6
10	A	568	LMT	C4-C5-C6-C7
10	A	570	LMT	C2-C3-C4-C5
10	B	279	LMT	C5-C6-C7-C8
10	B	278	LMT	C4B-C5B-C6B-O6B
10	B	280	LMT	C4-C5-C6-C7
10	B	280	LMT	C5'-C4'-O1B-C1B
10	A	570	LMT	C11-C10-C9-C8
10	A	568	LMT	O5'-C1'-O1'-C1
10	A	568	LMT	C2'-C1'-O1'-C1
9	A	564	LDA	C6-C7-C8-C9
10	A	574[A]	LMT	C2-C3-C4-C5
10	A	574[B]	LMT	C2-C3-C4-C5
10	B	283[B]	LMT	C5'-C4'-O1B-C1B
10	A	568	LMT	C3-C4-C5-C6
9	A	567	LDA	C2-C1-N1-O1
9	B	272	LDA	C2-C1-N1-O1
9	B	273	LDA	C2-C1-N1-O1
10	A	569	LMT	C6-C7-C8-C9
5	A	559	HEA	O11-C11-C3B-C4B

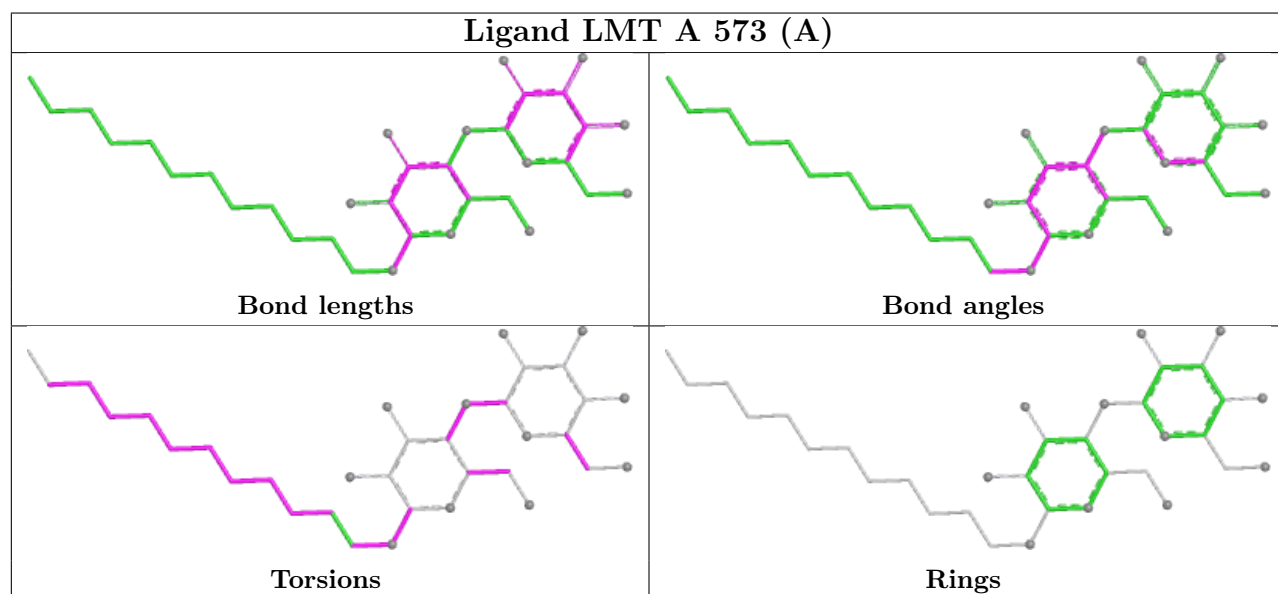
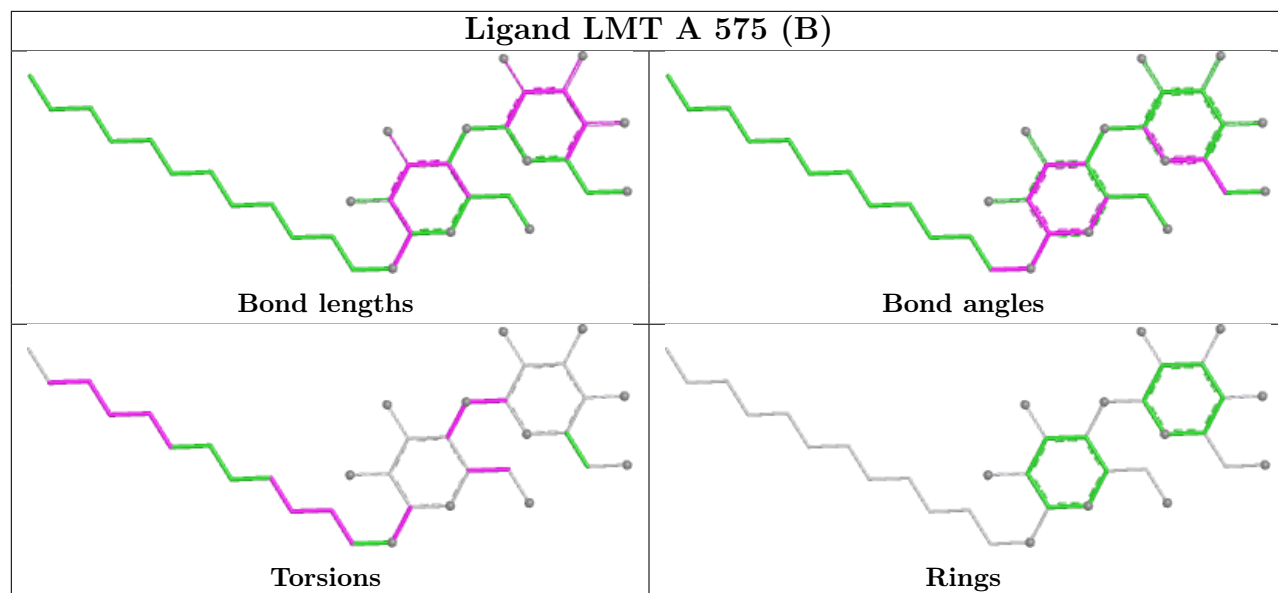
There are no ring outliers.

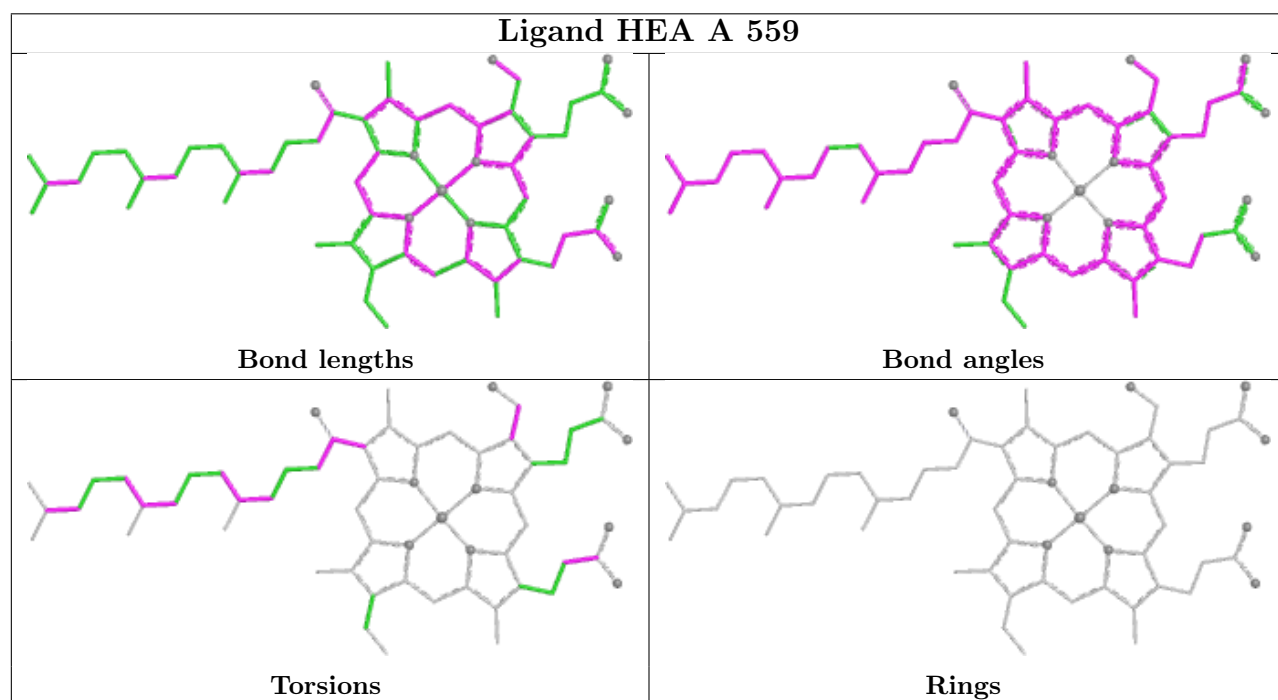
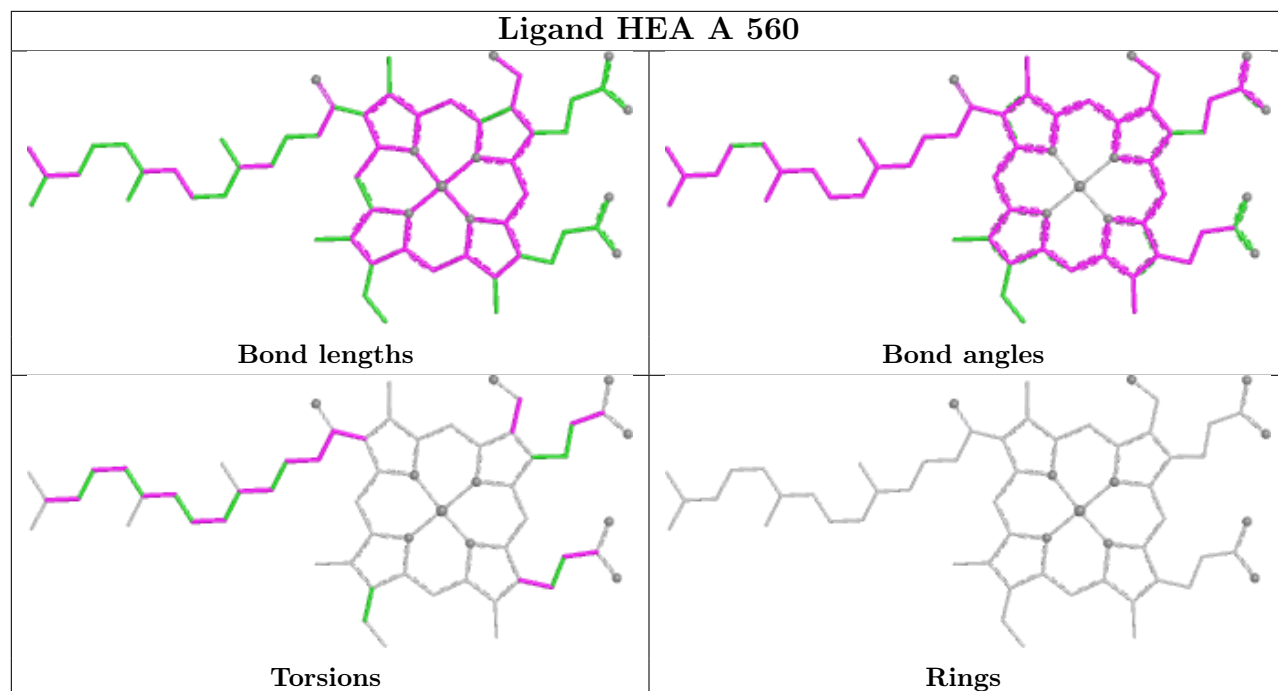
22 monomers are involved in 71 short contacts:

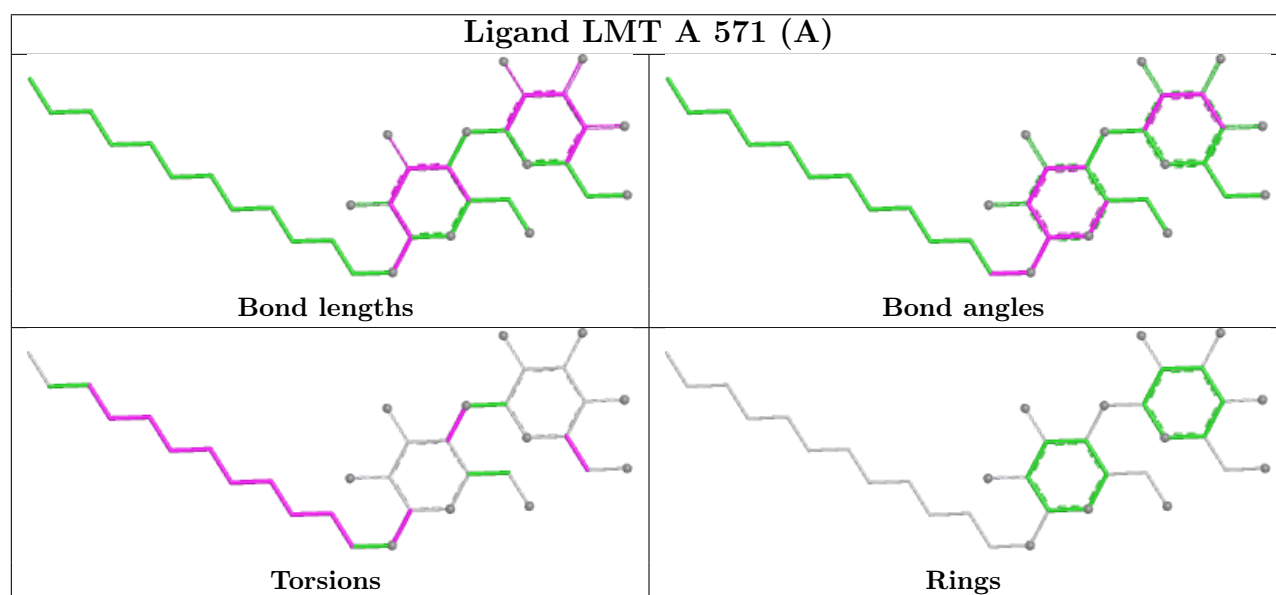
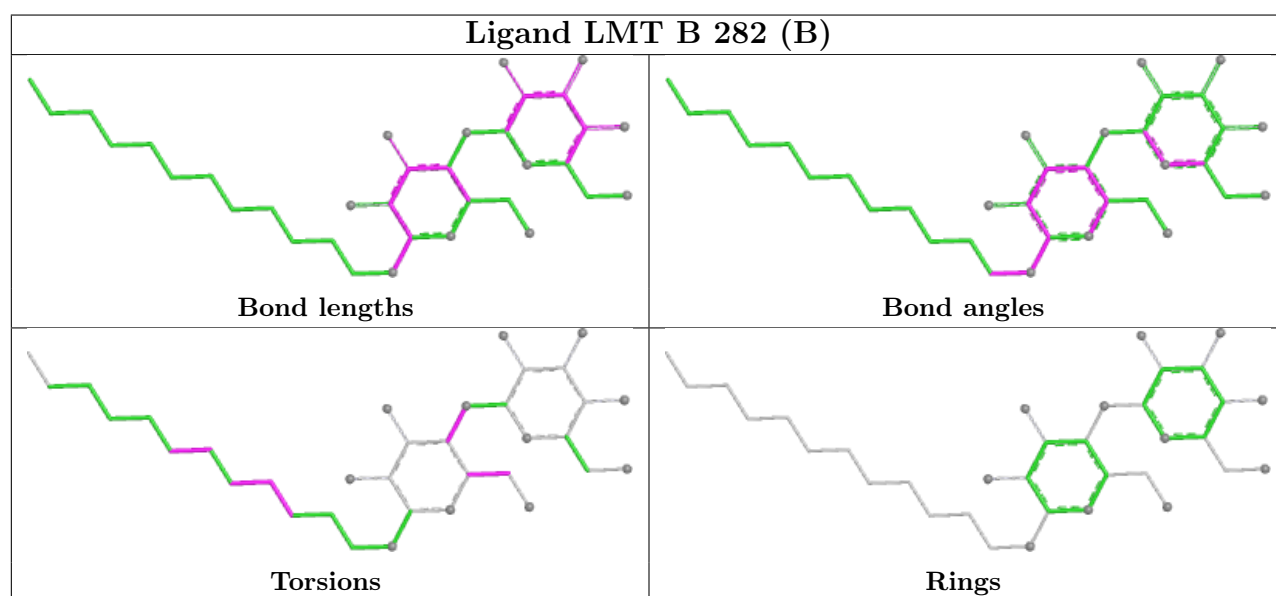
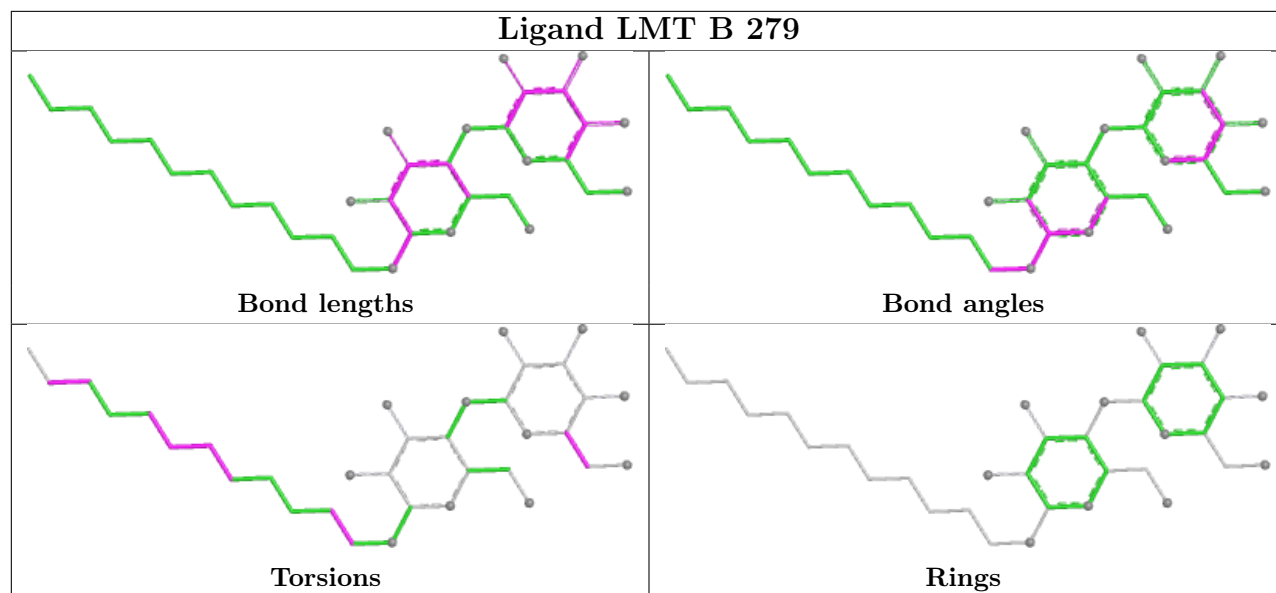
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	574[B]	LMT	2	0
10	B	281	LMT	7	0
9	B	273	LDA	4	0
10	A	575[B]	LMT	2	0
9	A	565	LDA	1	0
5	A	560	HEA	16	0
5	A	559	HEA	16	0
9	B	272	LDA	2	0
10	B	279	LMT	1	0
10	A	571[A]	LMT	1	0
10	A	570	LMT	4	0
10	A	572[A]	LMT	2	0
10	A	573[B]	LMT	3	0
9	A	564	LDA	2	0
10	A	574[A]	LMT	1	0
10	A	571[B]	LMT	1	0
9	A	567	LDA	2	0
10	B	280	LMT	1	0
9	B	276	LDA	1	0
9	B	274	LDA	2	0
10	A	569	LMT	1	0
10	A	572[B]	LMT	2	0

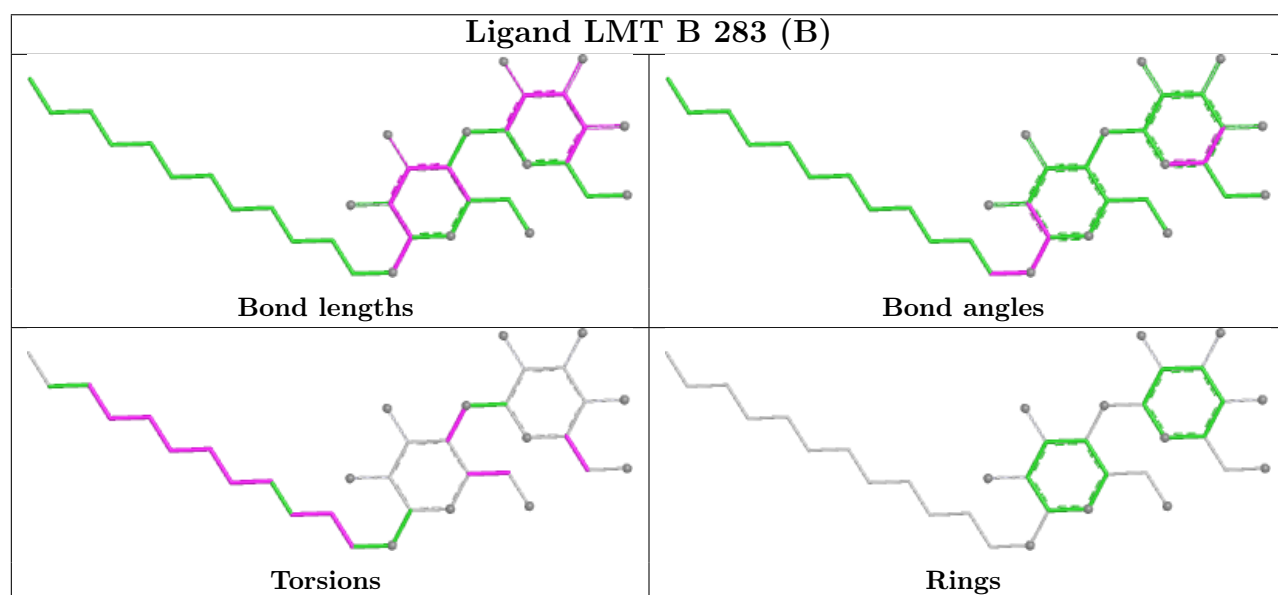
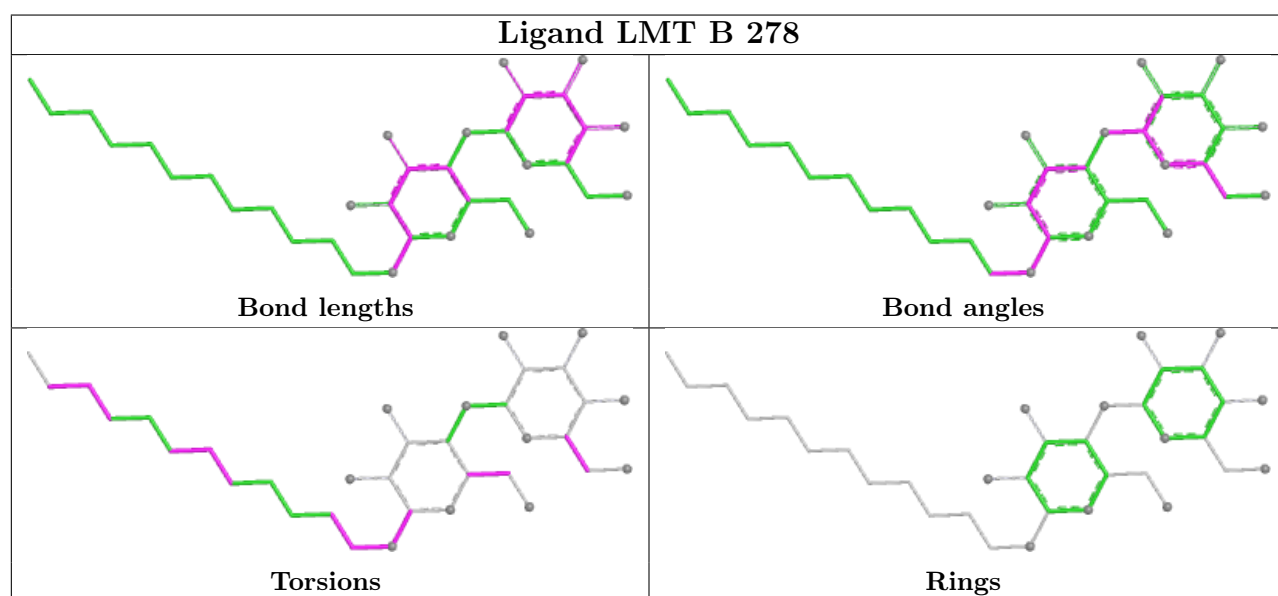
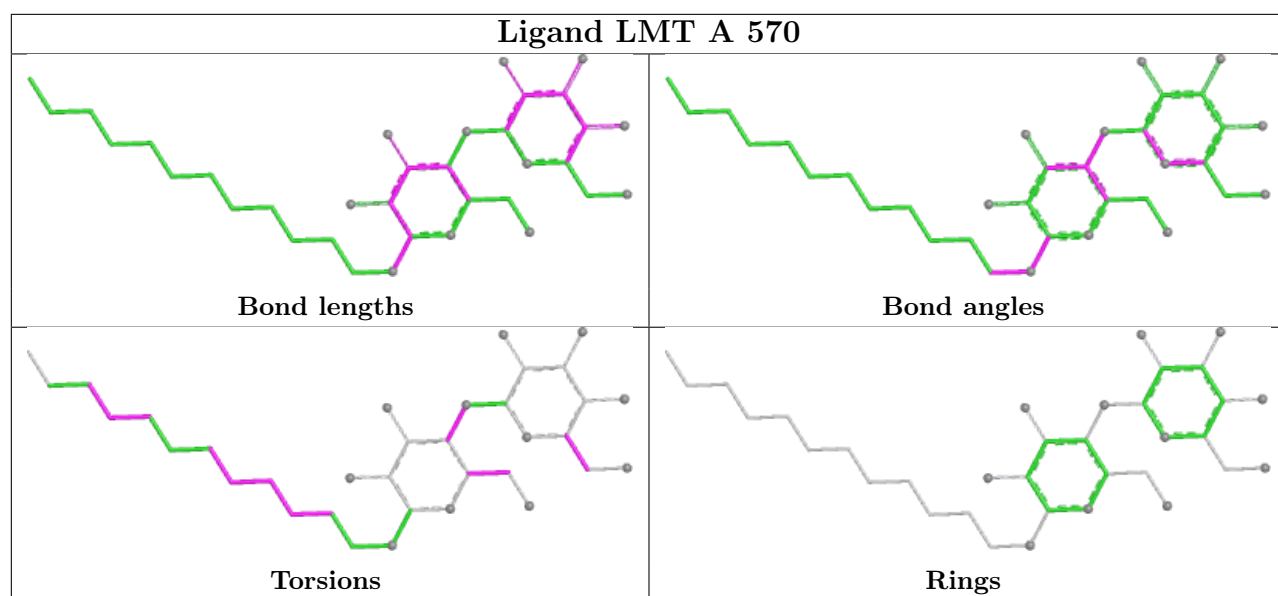
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

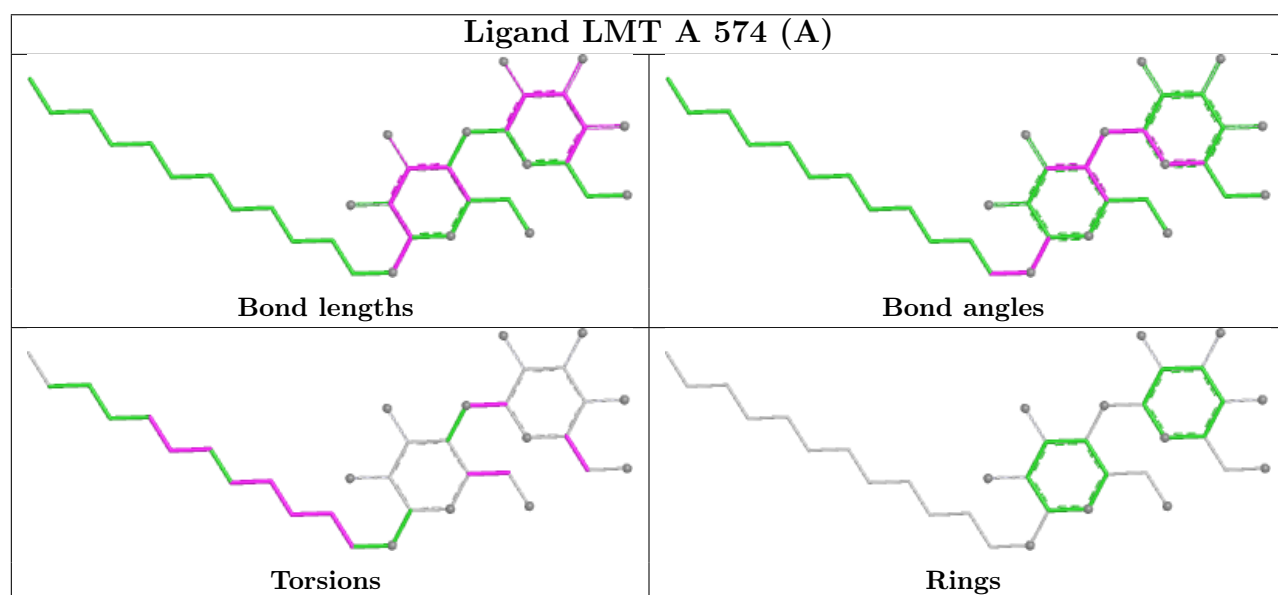
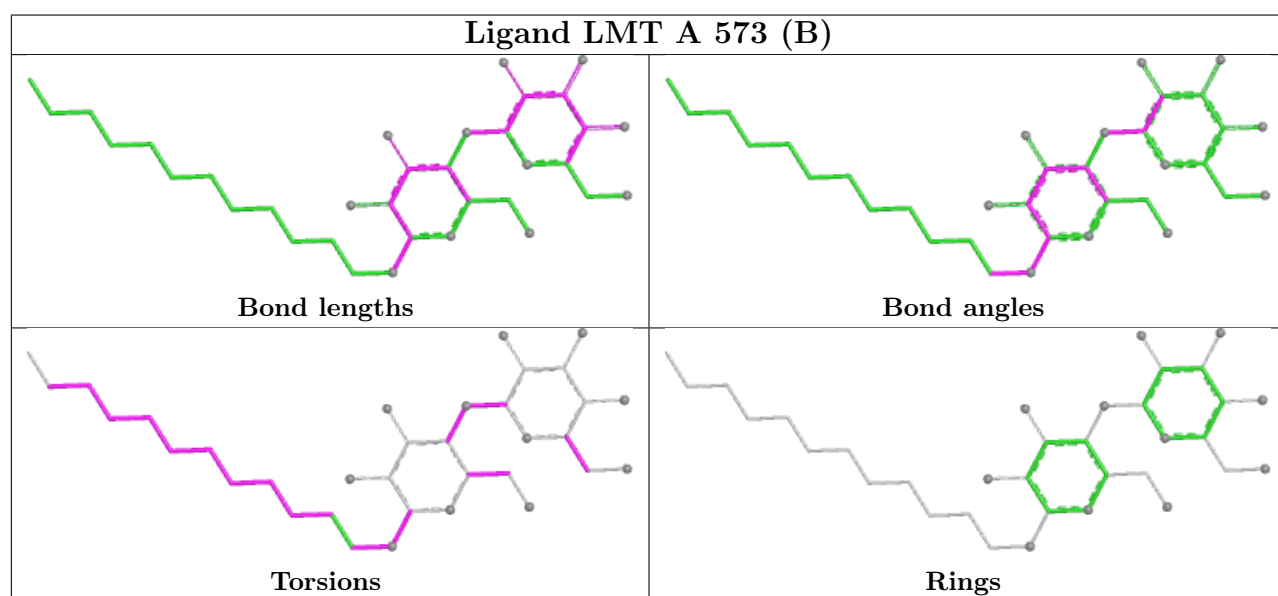
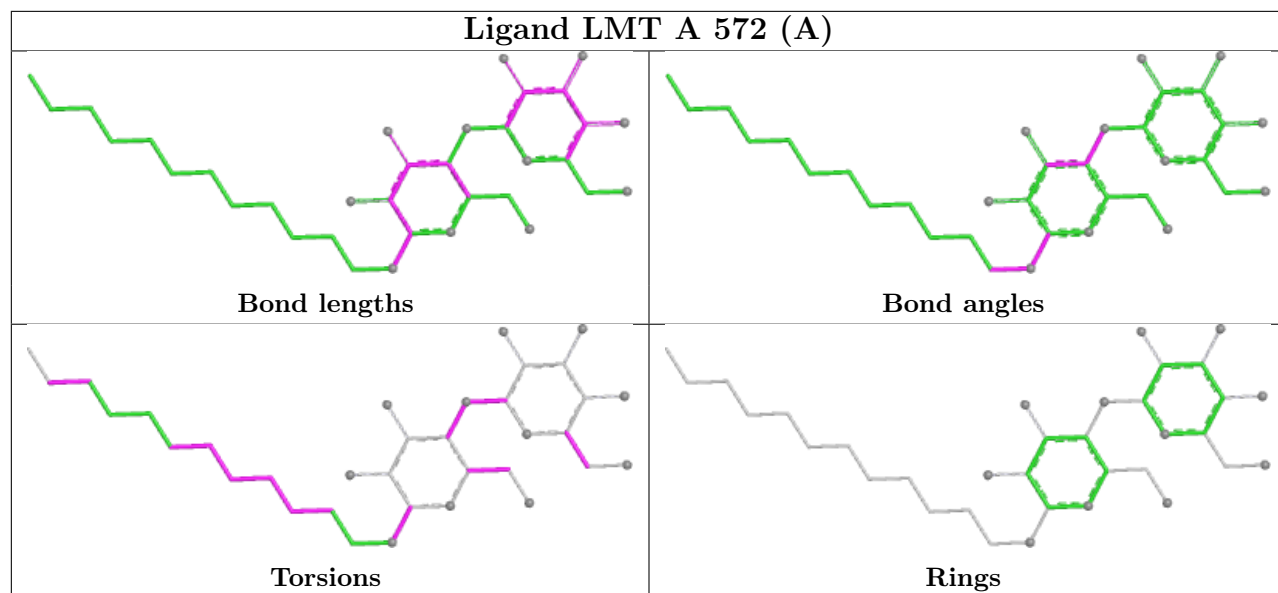


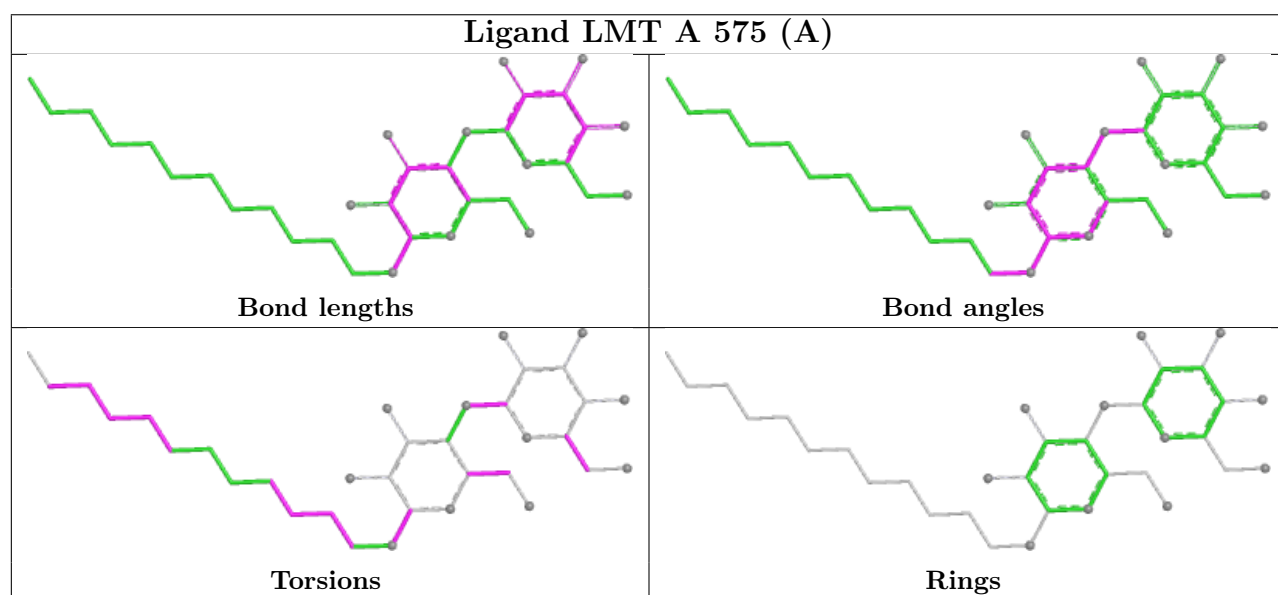
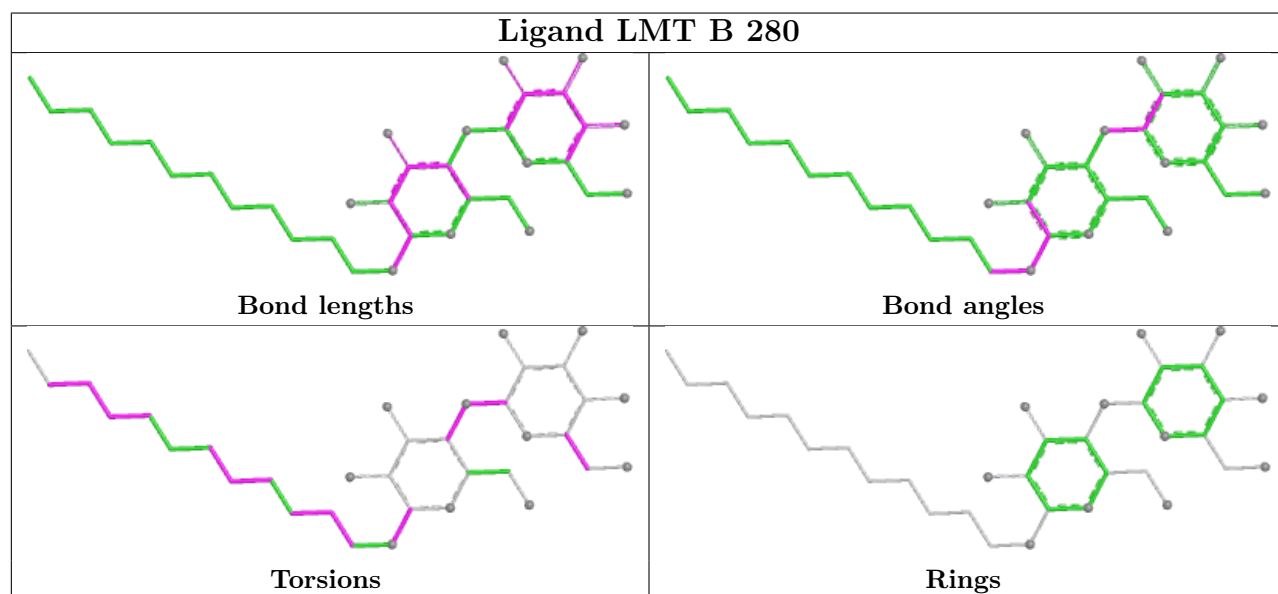
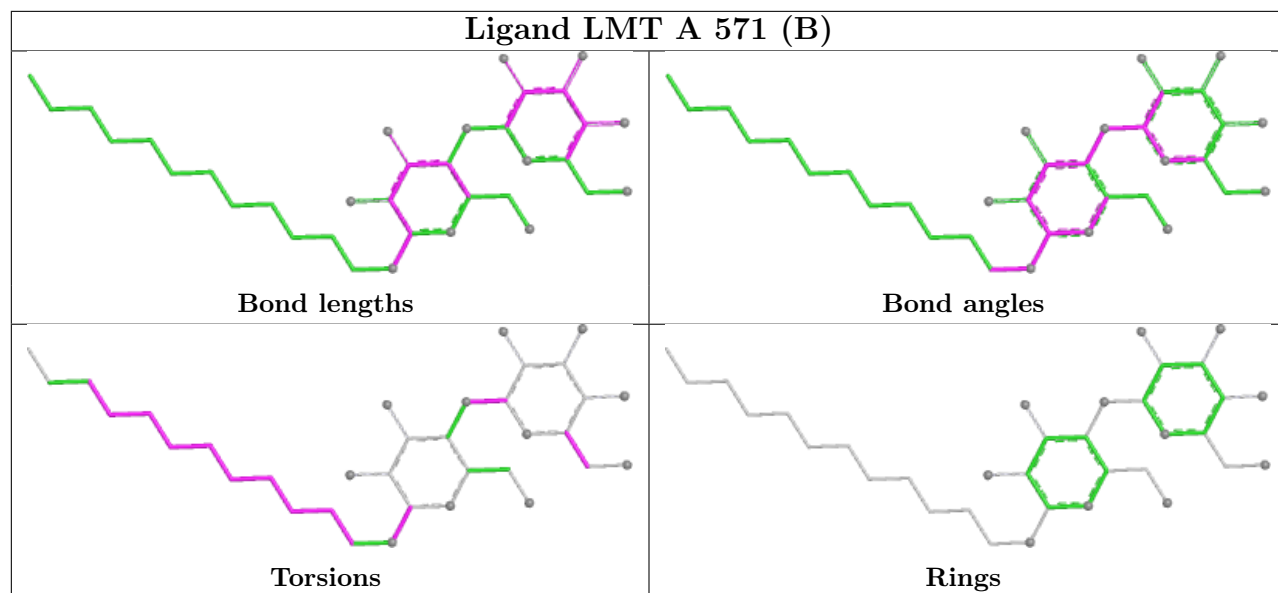


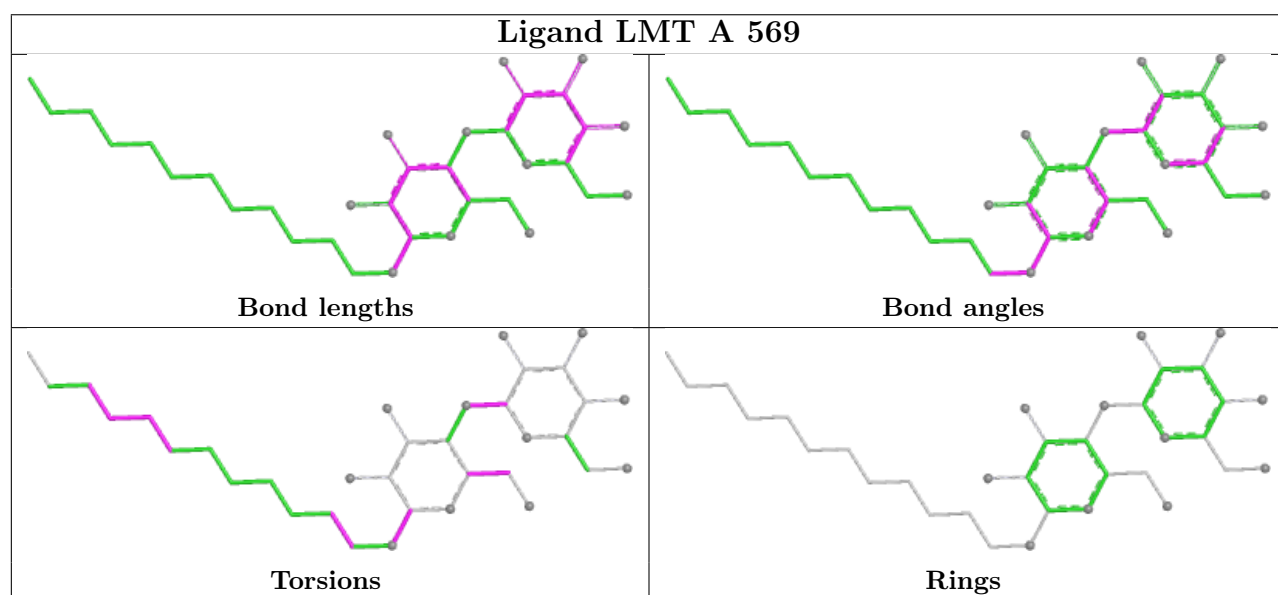
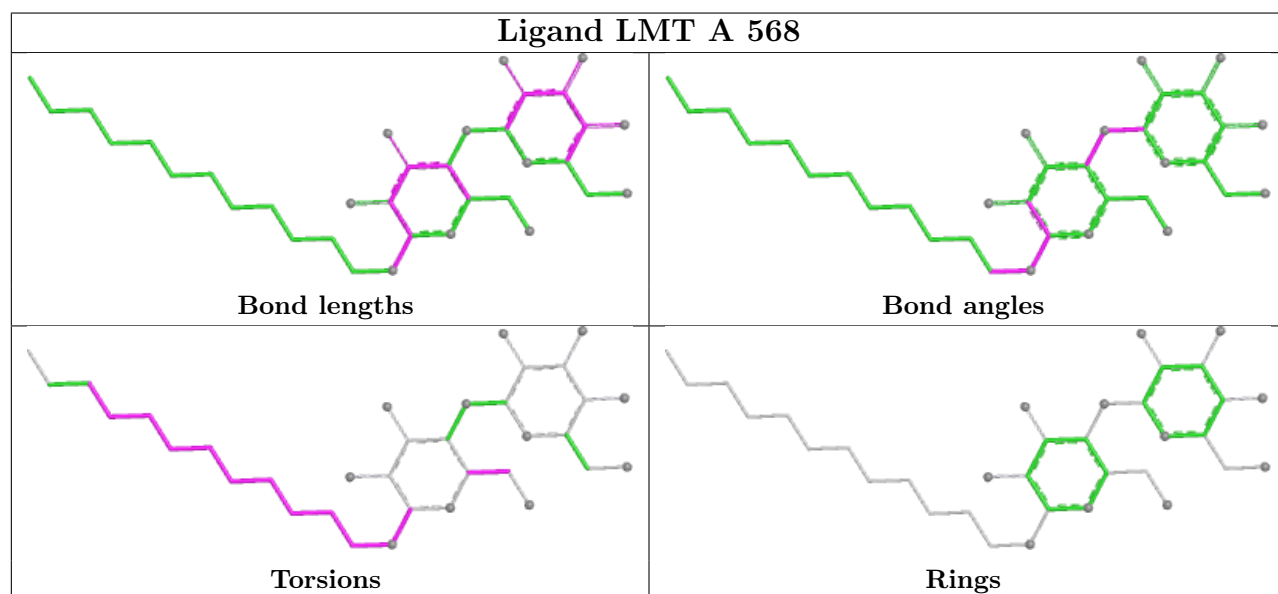
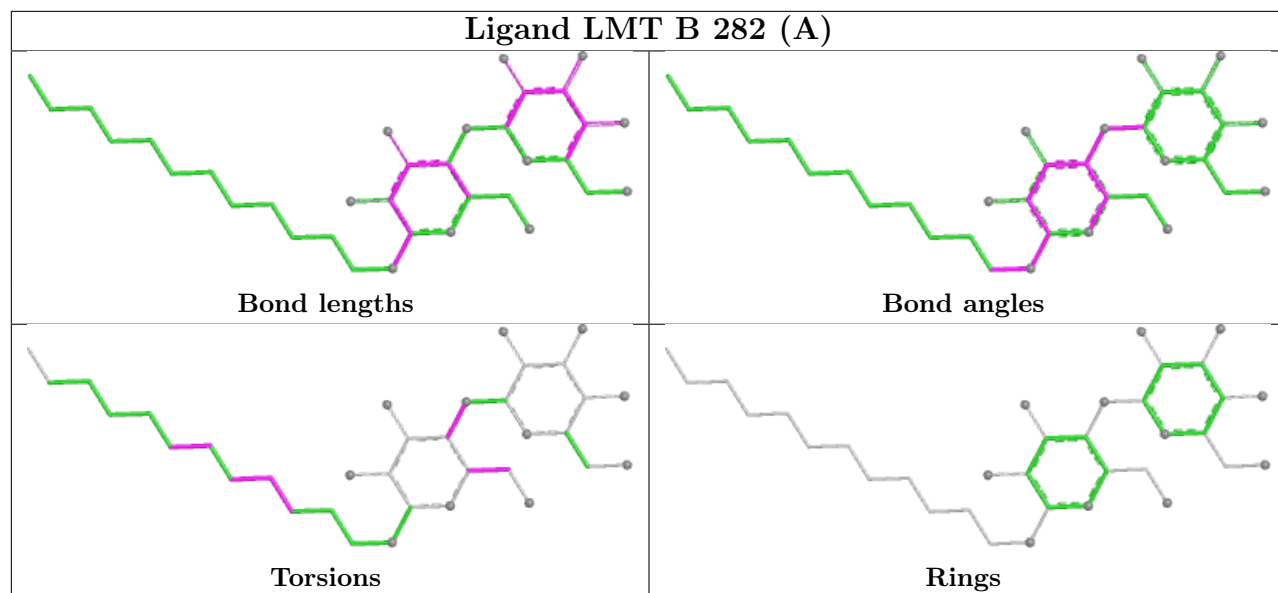


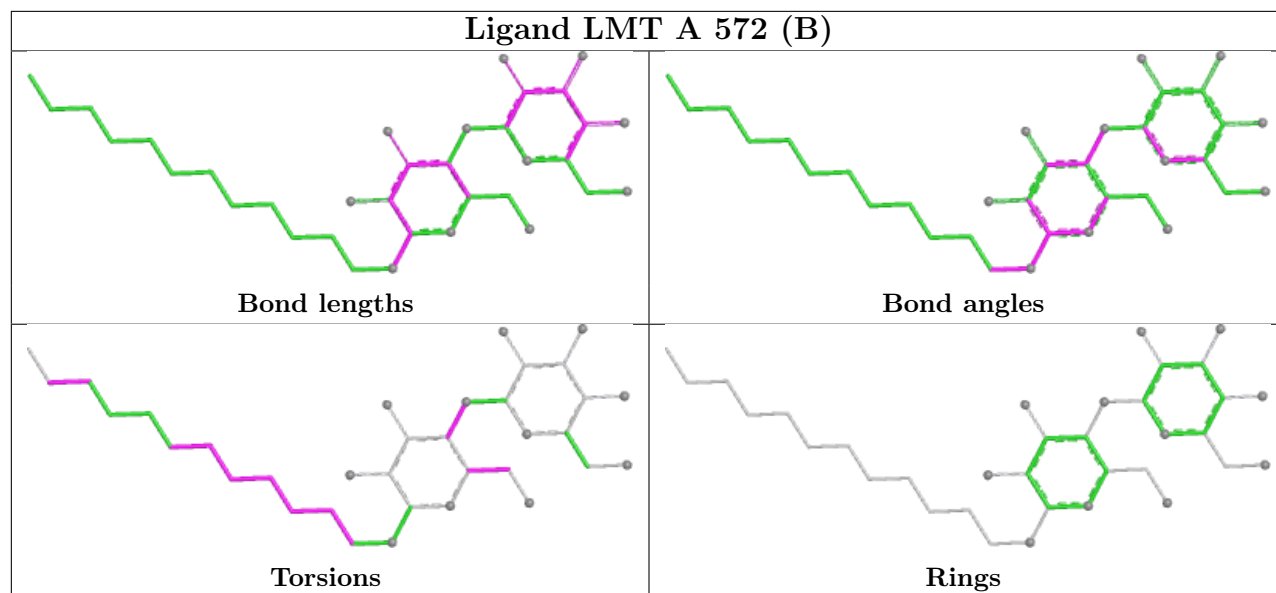












5.7 Other polymers [i](#)

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%)	-0.21	8 (1%) 72 73	18, 39, 62, 101	2 (0%)
2	B	252/298 (84%)	-0.48	0 100 100	15, 32, 50, 63	2 (0%)
3	C	118/127 (92%)	-0.09	2 (1%) 69 70	20, 45, 65, 74	2 (1%)
4	D	108/120 (90%)	-0.21	0 100 100	21, 41, 61, 69	0
All	All	1007/1103 (91%)	-0.26	10 (0%) 79 81	15, 38, 61, 101	6 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	3.8
3	C	118	SER	3.7
1	A	545	THR	3.6
1	A	173	THR	2.9
3	C	9	GLY	2.8
1	A	17	GLY	2.7
1	A	516[A]	ARG	2.6
1	A	18	PHE	2.4
1	A	177	TYR	2.3
1	A	169	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

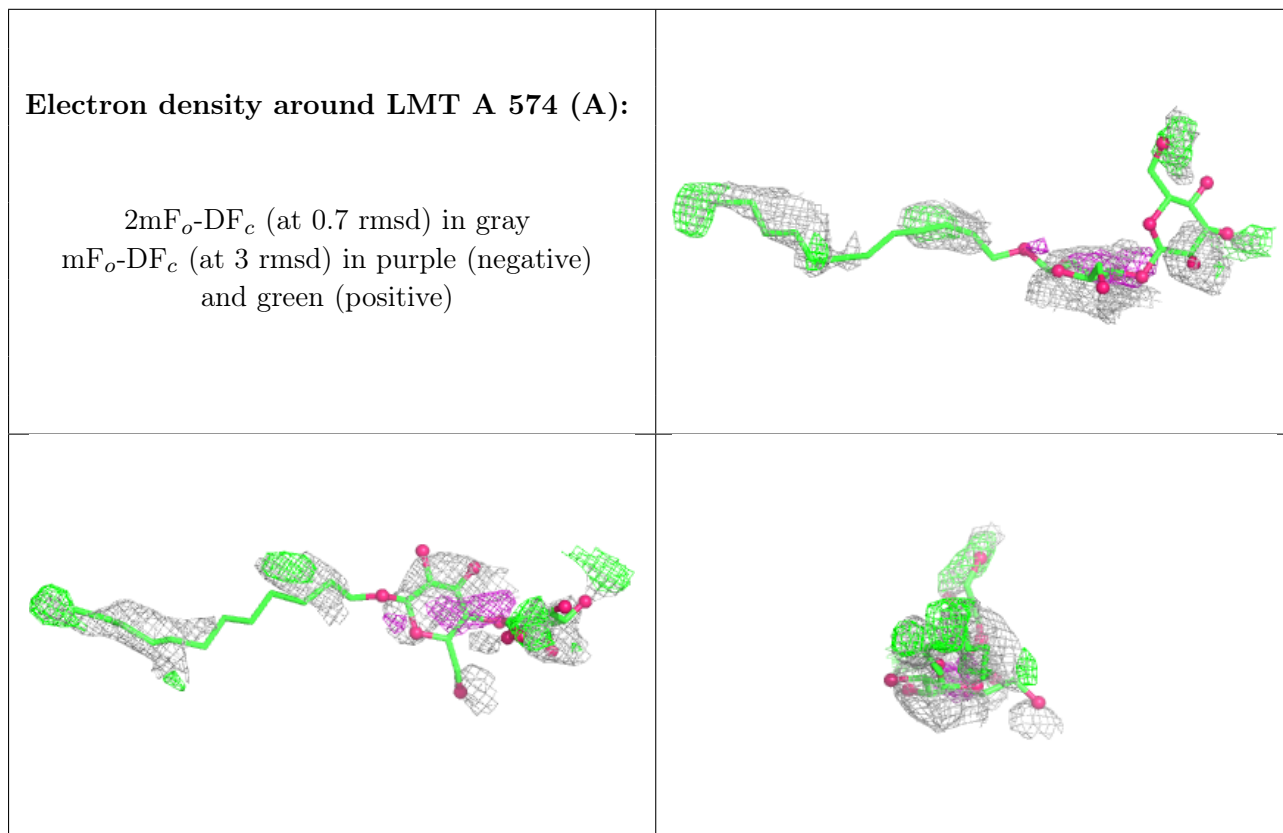
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LDA	B	277	16/16	0.44	0.28	141,150,156,156	0
9	LDA	A	566	16/16	0.49	0.25	120,125,127,127	0
10	LMT	A	574[A]	35/35	0.53	0.29	140,155,159,159	12
10	LMT	A	574[B]	35/35	0.53	0.29	140,157,159,159	12
9	LDA	B	276	16/16	0.58	0.25	96,115,127,127	0
10	LMT	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

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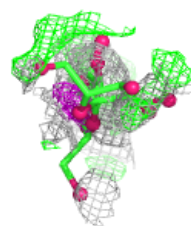
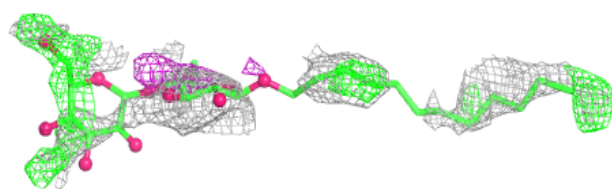
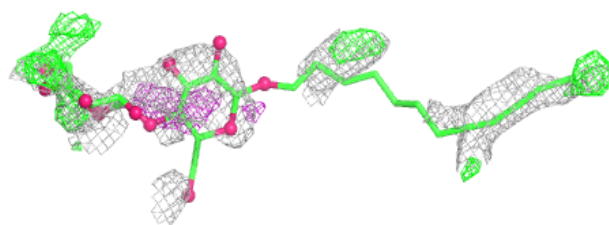
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	A	563	1/1	0.99	0.02	35,35,35,35	0
6	CU1	A	561	1/1	1.00	0.04	43,43,43,43	0

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.

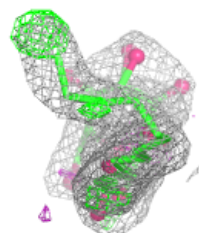
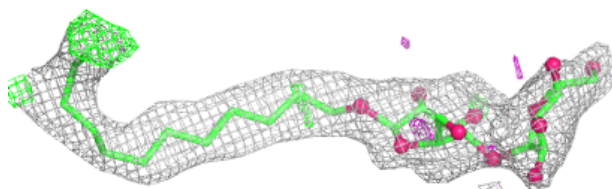
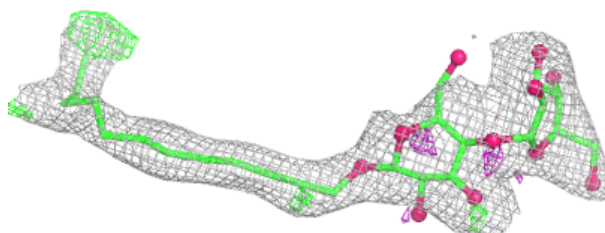


Electron density around LMT A 574 (B):

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

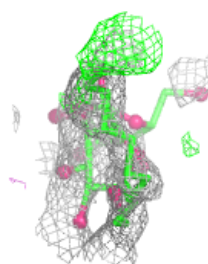
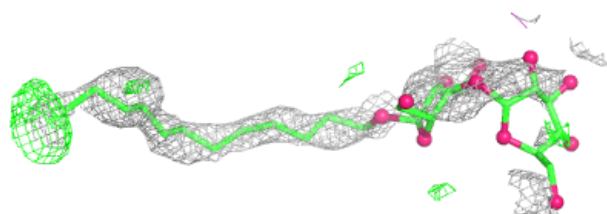
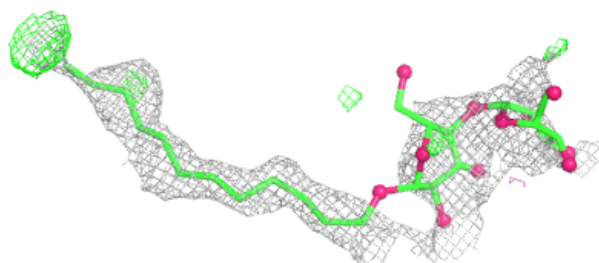
**Electron density around LMT A 569:**

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

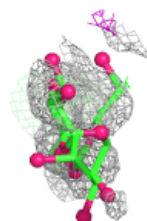
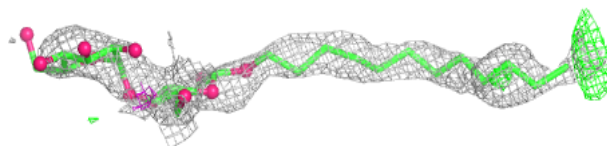
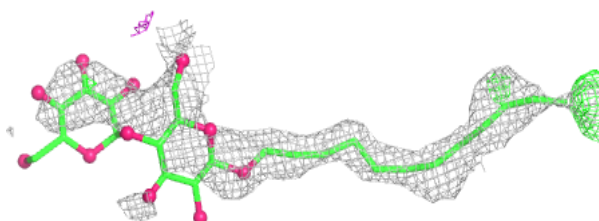


Electron density around LMT A 572 (A):

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

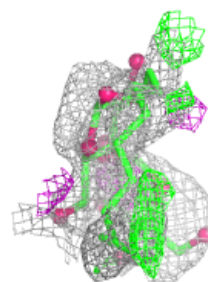
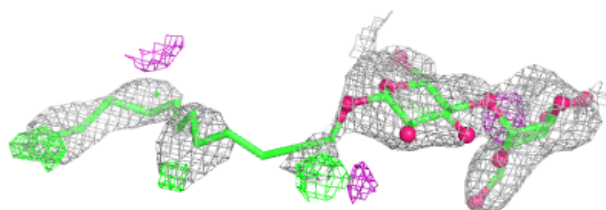
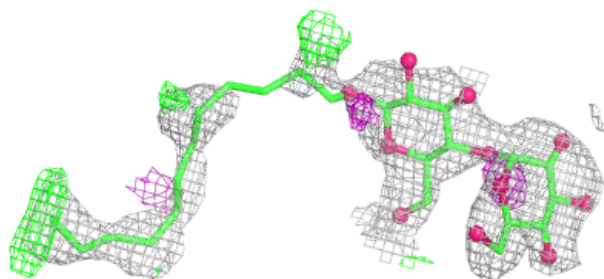
**Electron density around LMT A 572 (B):**

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

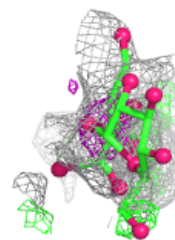
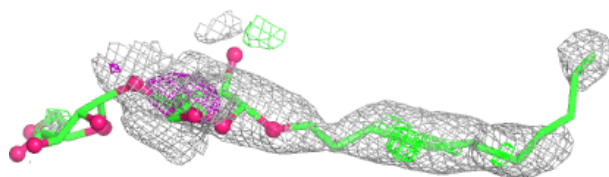
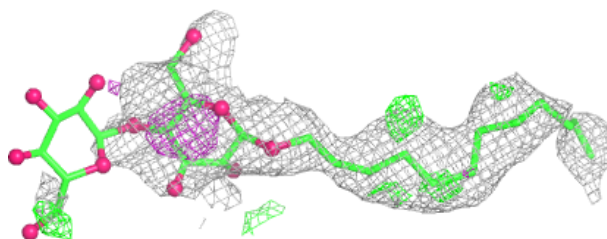


Electron density around LMT B 280:

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

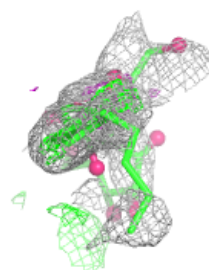
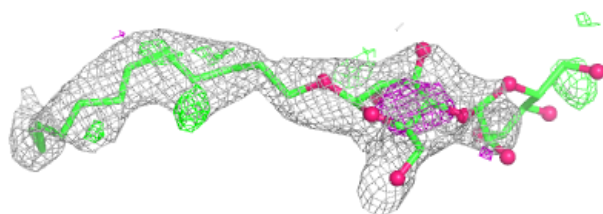
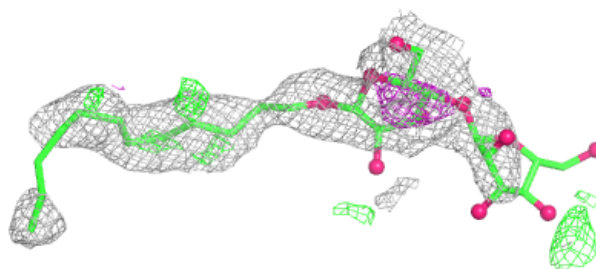
**Electron density around LMT A 571 (B):**

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



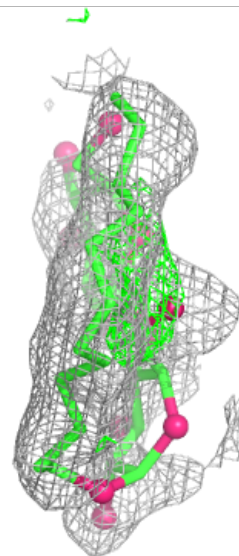
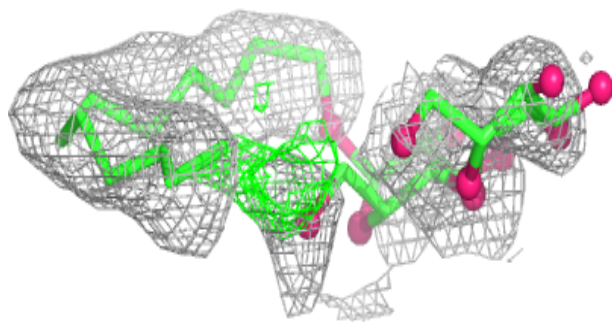
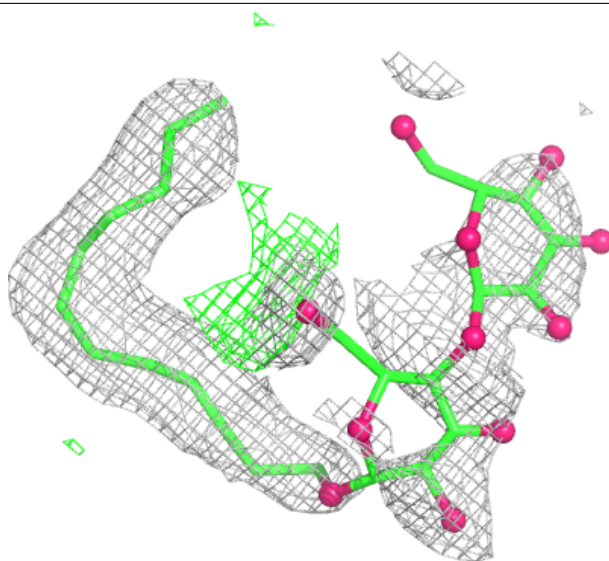
Electron density around LMT A 571 (A):

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



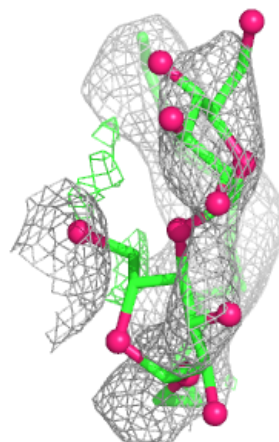
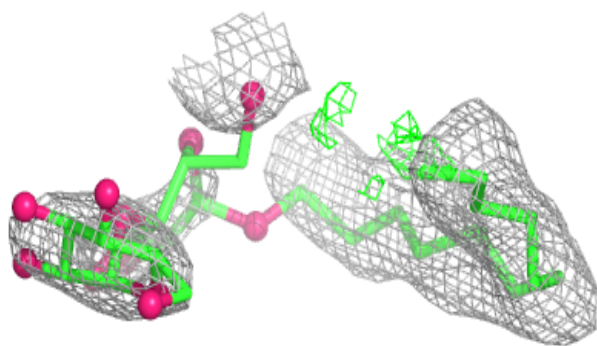
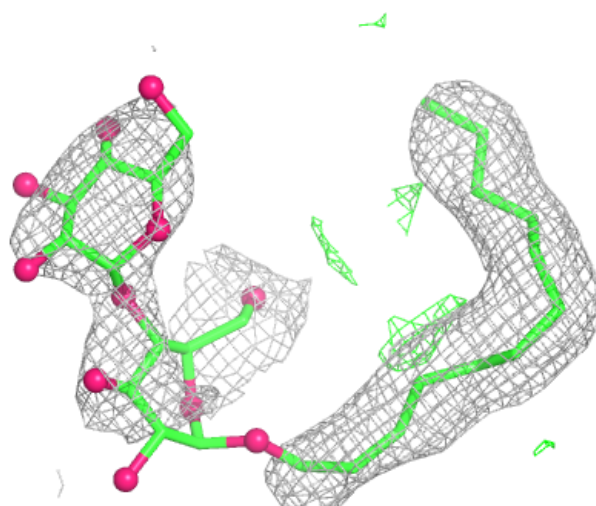
Electron density around LMT B 283 (A):

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



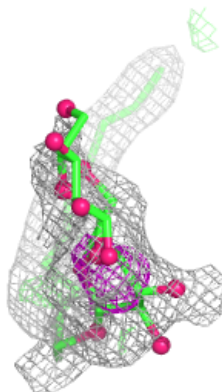
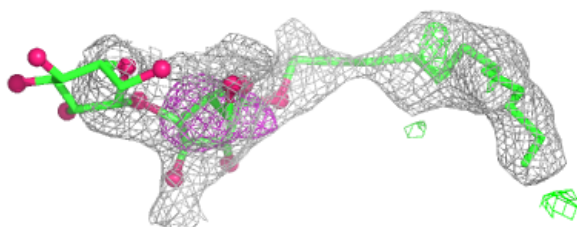
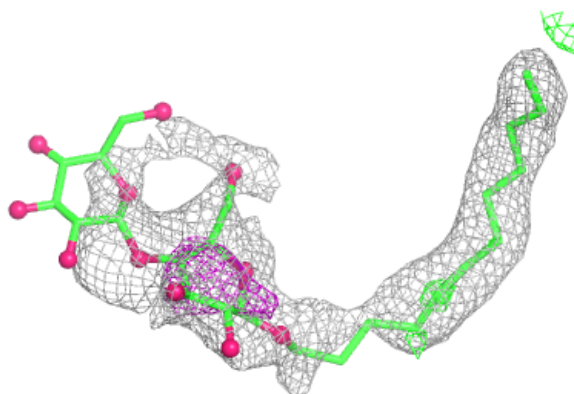
Electron density around LMT B 283 (B):

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

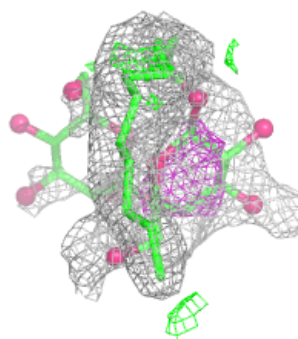
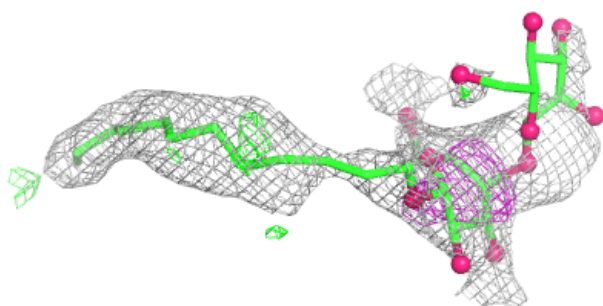
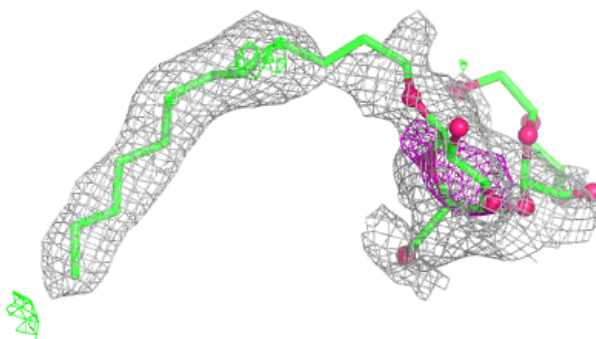


Electron density around LMT B 282 (A):

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

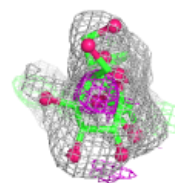
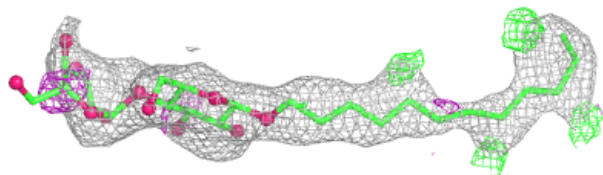
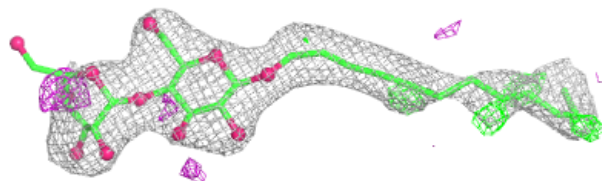
**Electron density around LMT B 282 (B):**

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

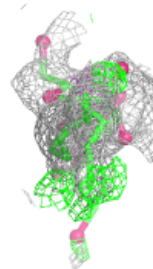
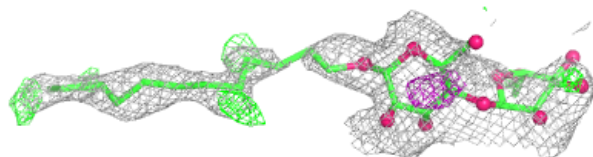
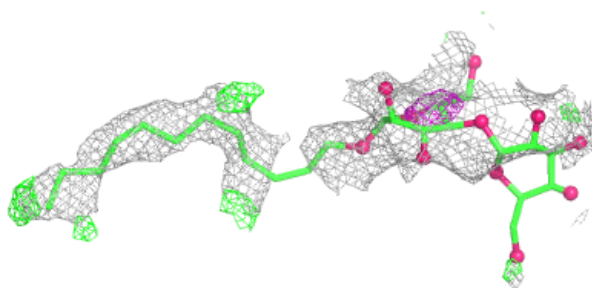


Electron density around LMT B 279:

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

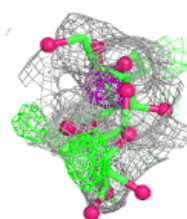
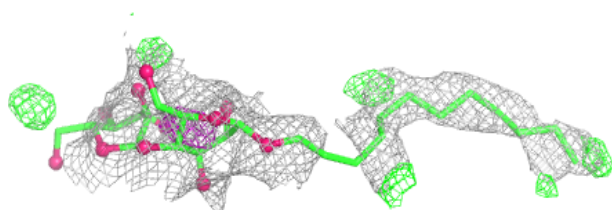
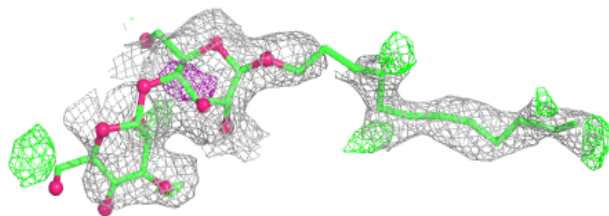
**Electron density around LMT A 575 (A):**

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

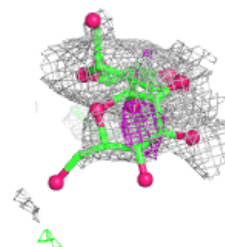
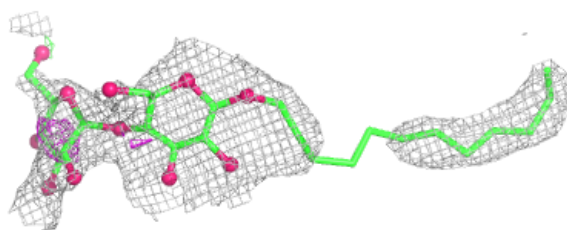
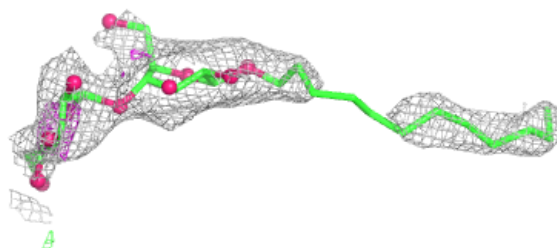


Electron density around LMT A 575 (B):

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

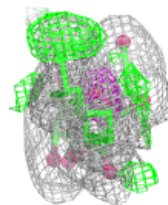
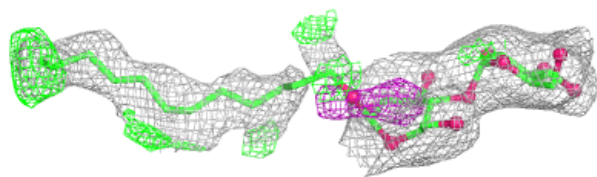
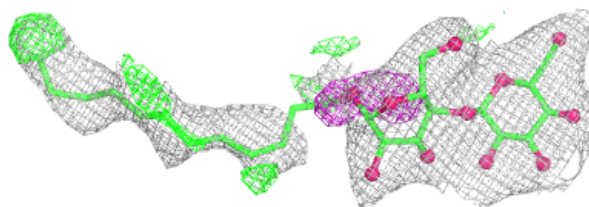
**Electron density around LMT B 281:**

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

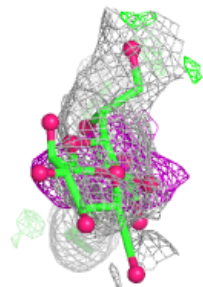
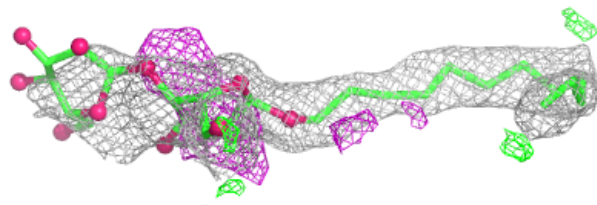
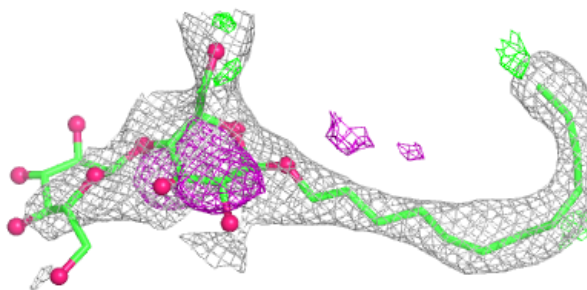


Electron density around LMT B 278:

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

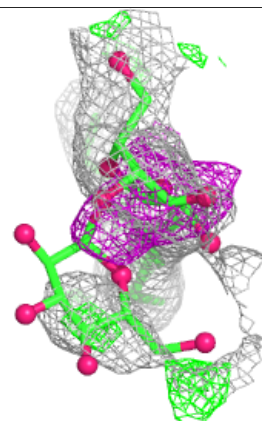
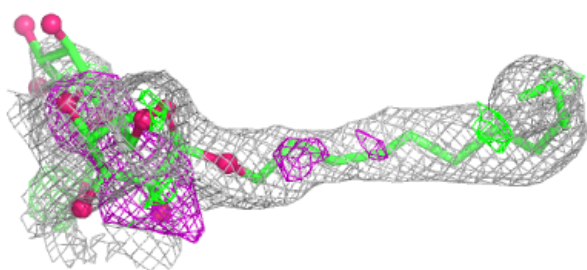
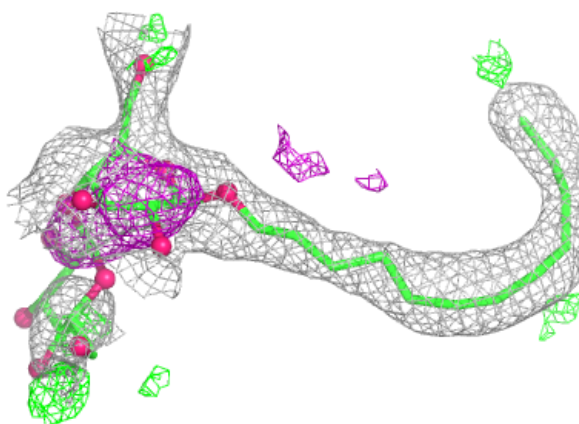
**Electron density around LMT A 573 (A):**

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

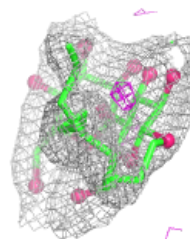
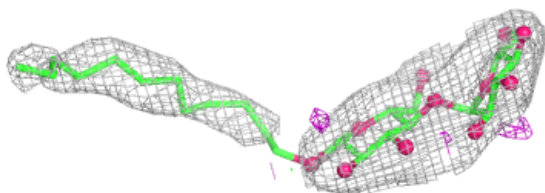
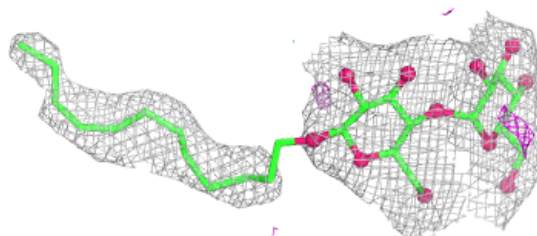


Electron density around LMT A 573 (B):

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

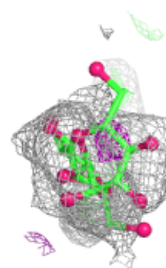
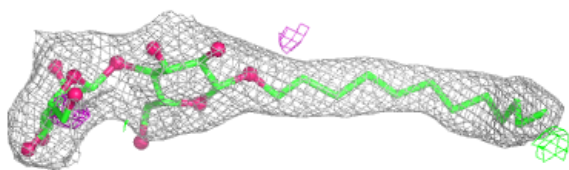
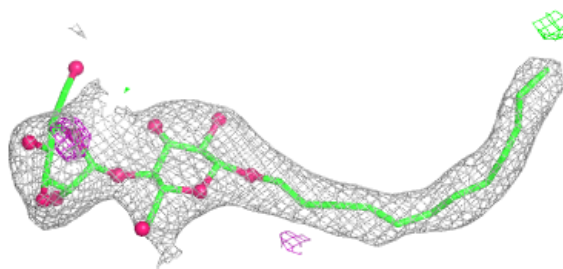
**Electron density around LMT A 568:**

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

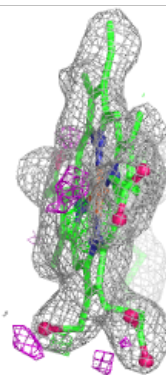
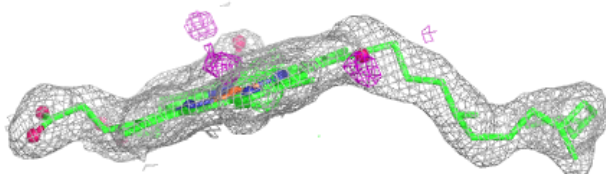
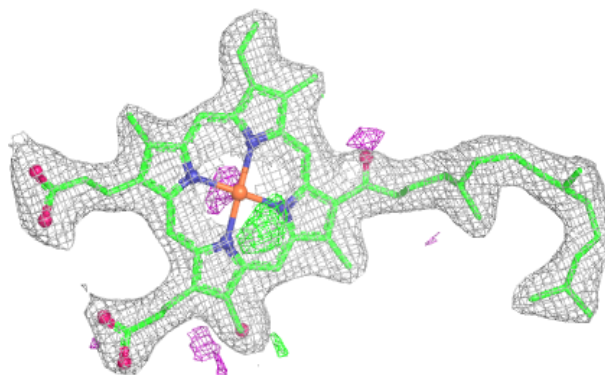


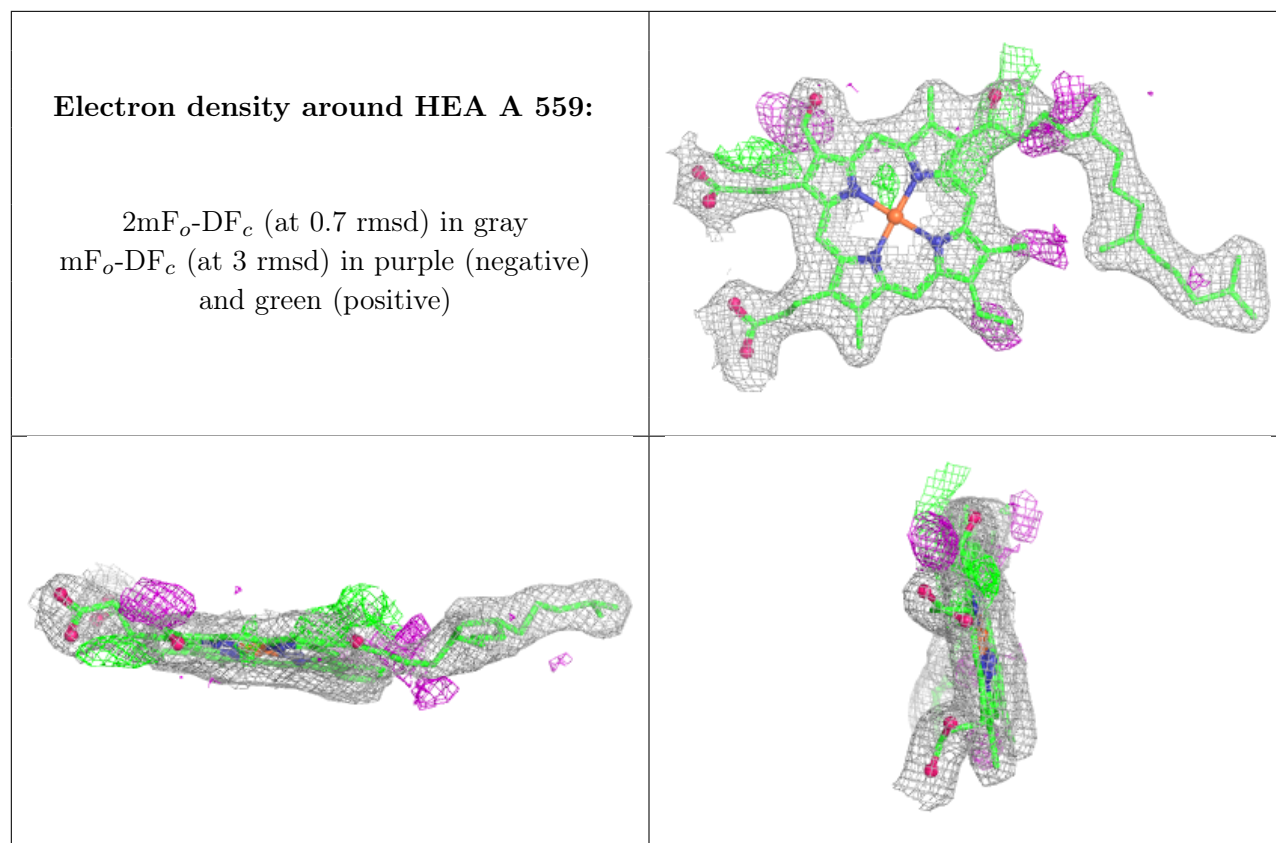
Electron density around LMT A 570:

$2mF_o-DF_c$ (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.