



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:17 PM UTC

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

This is a 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

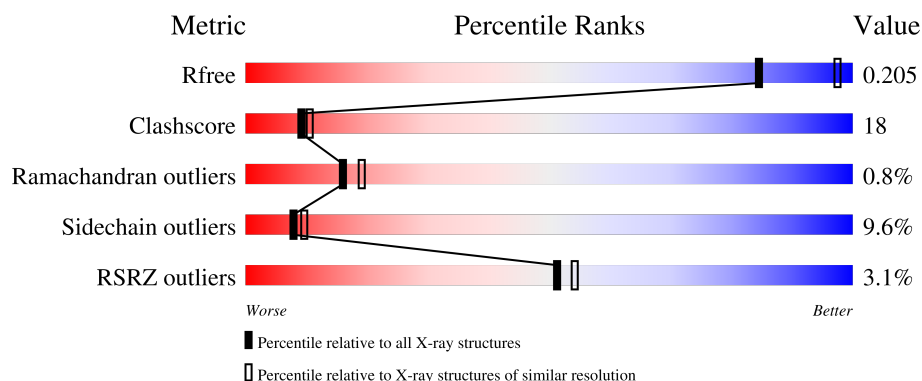
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 57% 29% 8% 5%
2	B	298	% 53% 25% 5% 15%
3	C	127	3% 57% 28% 9% 6%
4	D	120	2% 53% 28% 8% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PER	A	576	-	X	-	-
5	HEA	A	559	X	-	-	-
5	HEA	A	560	X	X	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9036 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	3	1
			4199	2818	656	692	33			

There is a discrepancy between the modelled and reference sequences:

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

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

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

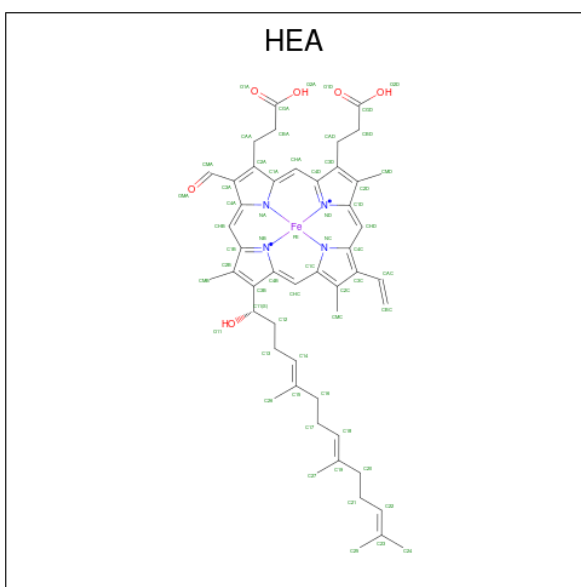
- Molecule 3 is a protein called FV fragment Chain H.

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

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

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

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



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

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

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

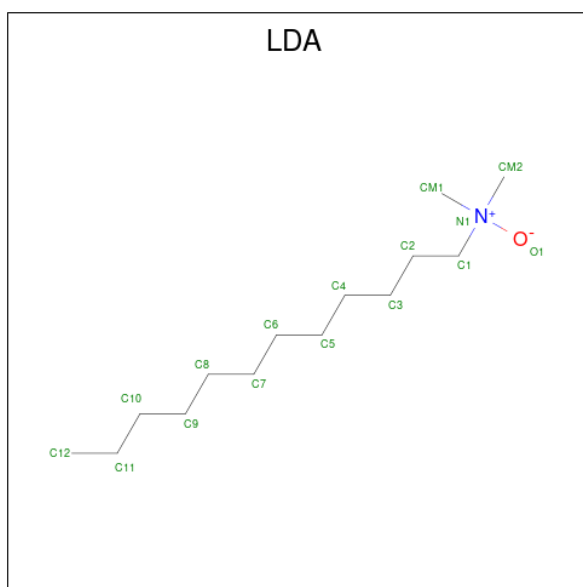
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

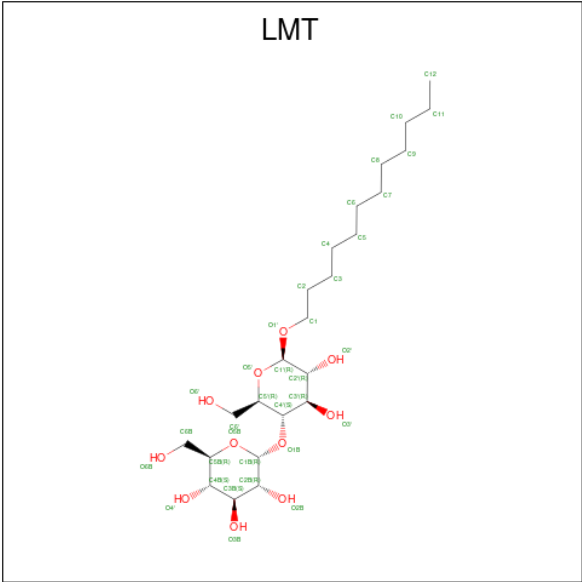
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

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



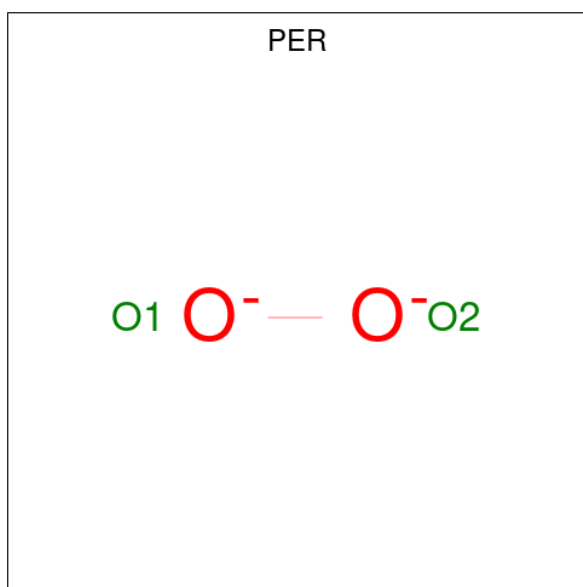
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
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	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	0
			35	24	11		
10	B	1	Total	C	O	0	1
			47	36	11		
10	B	1	Total	C	O	0	0
			35	24	11		
10	B	1	Total	C	O	0	0
			35	24	11		
10	D	1	Total	C	O	0	0
			35	24	11		

- Molecule 11 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

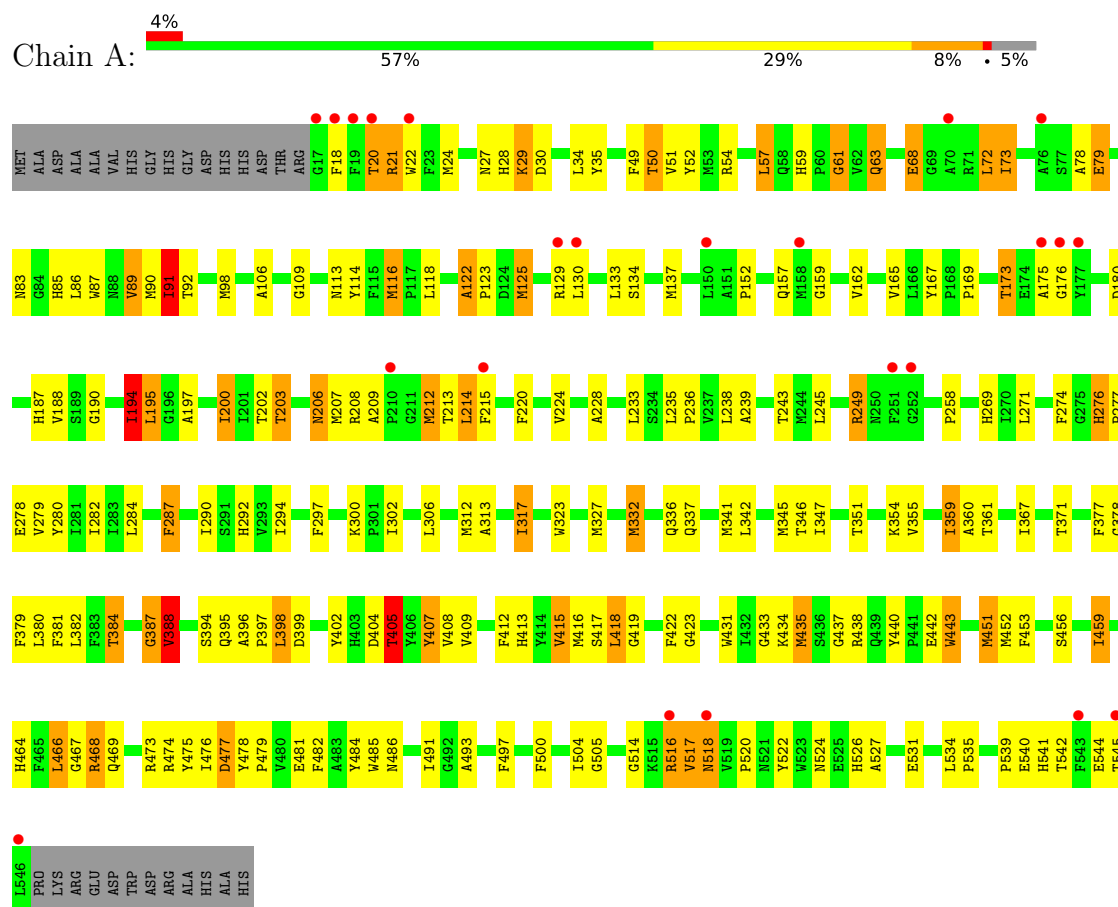
- Molecule 12 is water.

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

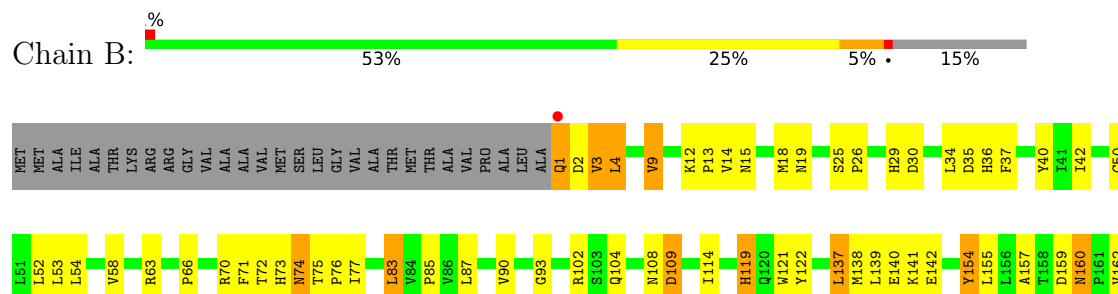
3 Residue-property plots

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



4 Data and refinement statistics

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

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

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: MG, HEA, CA, CU, LDA, PER, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.44	22/4367 (0.5%)	1.43	39/5959 (0.7%)
2	B	1.67	26/2043 (1.3%)	1.56	20/2801 (0.7%)
3	C	1.37	4/973 (0.4%)	1.30	7/1316 (0.5%)
4	D	1.55	10/853 (1.2%)	1.54	14/1158 (1.2%)
All	All	1.51	62/8236 (0.8%)	1.46	80/11234 (0.7%)

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

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

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	HIS	CA-C	8.91	1.62	1.52
2	B	222	ILE	CG1-CD1	8.53	1.85	1.51
2	B	178	ASP	CA-C	8.18	1.59	1.52
2	B	155	LEU	N-CA	8.06	1.56	1.46
4	D	98	THR	CA-CB	7.88	1.65	1.53
4	D	4	LEU	CA-C	-7.75	1.43	1.52
1	A	384	THR	CA-C	7.50	1.62	1.52
4	D	51	ALA	CA-CB	7.09	1.65	1.53
1	A	545	THR	C-N	-7.07	1.23	1.33
2	B	182	ALA	CA-CB	6.88	1.66	1.53
1	A	371	THR	CA-CB	-6.77	1.47	1.54
1	A	306	LEU	C-O	-6.51	1.18	1.24
4	D	3	GLU	CA-C	-6.41	1.45	1.52
1	A	476	ILE	CA-CB	6.33	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	236	GLN	CA-C	6.32	1.60	1.52
2	B	240	GLU	C-O	-6.20	1.16	1.24
1	A	399	ASP	CA-C	6.17	1.61	1.52
2	B	252	ALA	C-N	-6.11	1.24	1.33
2	B	244	ALA	CA-CB	6.10	1.62	1.53
2	B	3	VAL	CA-C	6.09	1.61	1.52
4	D	69	THR	CA-CB	6.07	1.63	1.53
3	C	118	SER	C-N	-6.07	1.24	1.33
1	A	89	VAL	CA-CB	5.93	1.61	1.54
2	B	119	HIS	CA-C	-5.82	1.45	1.52
4	D	31	SER	N-CA	5.77	1.53	1.46
2	B	157	ALA	N-CA	5.74	1.53	1.46
4	D	92	TYR	CA-C	5.74	1.59	1.52
4	D	95	PRO	CA-C	5.73	1.57	1.52
1	A	527	ALA	CA-CB	5.69	1.60	1.52
2	B	195	VAL	CA-C	5.68	1.57	1.53
1	A	287	PHE	CA-C	5.65	1.60	1.52
3	C	45	LEU	CA-C	-5.65	1.45	1.52
1	A	477	ASP	N-CA	5.63	1.53	1.45
4	D	108	LYS	C-N	-5.62	1.25	1.33
2	B	176	ALA	CA-CB	5.59	1.62	1.53
2	B	58	VAL	C-O	-5.57	1.17	1.23
1	A	282	ILE	CA-CB	5.55	1.61	1.54
3	C	37	VAL	CA-CB	5.44	1.62	1.54
2	B	12	LYS	C-O	-5.39	1.18	1.24
1	A	443	TRP	CA-C	5.38	1.59	1.52
2	B	2	ASP	C-O	-5.35	1.17	1.23
1	A	302	ILE	CA-CB	5.30	1.60	1.54
1	A	360	ALA	CA-C	5.27	1.59	1.52
1	A	423	GLY	N-CA	5.26	1.52	1.45
2	B	160	ASN	CA-C	5.24	1.59	1.52
1	A	451	MET	C-O	-5.23	1.18	1.24
1	A	106	ALA	CA-CB	5.22	1.61	1.53
1	A	409	VAL	CA-CB	5.20	1.61	1.54
2	B	66	PRO	CA-C	-5.20	1.45	1.52
2	B	200	ALA	C-O	-5.19	1.17	1.23
1	A	220	PHE	N-CA	5.18	1.52	1.46
1	A	387	GLY	C-O	-5.15	1.17	1.23
4	D	32	TYR	CA-C	-5.15	1.47	1.53
2	B	12	LYS	CA-C	5.13	1.57	1.52
3	C	70	ILE	CA-C	-5.11	1.46	1.52
2	B	218	GLU	C-O	5.10	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	222	ILE	CA-CB	5.09	1.63	1.54
2	B	211	VAL	CA-CB	5.08	1.61	1.54
1	A	188	VAL	CA-C	5.05	1.59	1.52
2	B	30	ASP	C-O	5.05	1.29	1.24
2	B	168	LYS	CA-C	-5.03	1.46	1.52
2	B	203	TRP	CA-C	-5.01	1.46	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	TYR	CA-C-N	-11.99	103.46	122.65
2	B	154	TYR	C-N-CA	-11.99	103.46	122.65
4	D	58	VAL	CA-C-N	-10.27	110.36	120.52
4	D	58	VAL	C-N-CA	-10.27	110.36	120.52
2	B	66	PRO	N-CA-C	-10.26	95.07	111.38
1	A	522	TYR	N-CA-C	-9.23	101.33	112.59
2	B	154	TYR	N-CA-C	8.72	121.74	111.71
1	A	459	ILE	N-CA-C	8.70	118.71	110.53
1	A	162	VAL	N-CA-C	8.11	119.92	112.29
1	A	54	ARG	NE-CZ-NH2	-7.96	112.03	119.20
1	A	175	ALA	N-CA-C	7.70	120.75	111.82
2	B	227	MET	CA-C-N	7.63	129.38	119.84
2	B	227	MET	C-N-CA	7.63	129.38	119.84
3	C	8	GLY	N-CA-C	7.57	125.90	115.00
2	B	109	ASP	CA-C-N	-7.54	112.56	120.03
2	B	109	ASP	C-N-CA	-7.54	112.56	120.03
2	B	166	VAL	CB-CA-C	-7.46	99.16	111.32
1	A	167	TYR	CA-C-N	7.36	127.96	120.38
1	A	167	TYR	C-N-CA	7.36	127.96	120.38
1	A	468	ARG	NE-CZ-NH2	-7.14	112.77	119.20
1	A	292	HIS	N-CA-C	7.14	118.71	111.07
4	D	94	THR	CA-C-N	-7.06	113.11	120.38
4	D	94	THR	C-N-CA	-7.06	113.11	120.38
1	A	61	GLY	N-CA-C	-6.95	96.72	113.18
1	A	435	MET	N-CA-C	-6.95	103.80	112.90
1	A	91	ILE	N-CA-C	6.88	117.02	110.42
1	A	200	ILE	N-CA-C	-6.86	103.62	110.62
3	C	10	ASP	N-CA-C	6.81	119.21	108.79
4	D	79	LEU	CA-C-N	6.73	127.00	119.32
4	D	79	LEU	C-N-CA	6.73	127.00	119.32
1	A	466	LEU	N-CA-C	-6.61	104.07	111.28
1	A	407	TYR	N-CA-C	-6.58	104.03	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215[A]	PHE	CB-CA-C	6.42	121.79	110.37
1	A	422	PHE	CA-C-N	6.39	127.03	119.94
1	A	422	PHE	C-N-CA	6.39	127.03	119.94
2	B	36	HIS	CA-C-N	6.39	128.74	120.44
2	B	36	HIS	C-N-CA	6.39	128.74	120.44
1	A	459	ILE	CB-CA-C	-6.33	103.73	112.02
1	A	159	GLY	CA-C-O	-6.17	117.07	121.88
1	A	405	THR	N-CA-CB	-6.11	101.31	111.20
1	A	468	ARG	CG-CD-NE	-6.07	98.65	112.00
4	D	84	GLY	N-CA-C	-6.00	102.47	110.58
2	B	154	TYR	O-C-N	-6.00	115.20	122.22
4	D	43	SER	CA-C-N	-5.93	113.67	119.78
4	D	43	SER	C-N-CA	-5.93	113.67	119.78
2	B	162	VAL	CA-C-N	-5.90	115.49	123.10
2	B	162	VAL	C-N-CA	-5.90	115.49	123.10
4	D	107	ILE	CB-CA-C	-5.71	103.39	111.21
1	A	194	ILE	N-CA-C	5.66	116.39	110.62
1	A	378	GLY	N-CA-C	-5.61	105.99	112.50
3	C	117	SER	N-CA-C	5.58	118.34	109.81
1	A	122	ALA	CA-C-N	-5.57	114.02	119.64
1	A	122	ALA	C-N-CA	-5.57	114.02	119.64
1	A	540	GLU	N-CA-C	5.51	116.96	111.07
2	B	179	VAL	N-CA-CB	-5.48	104.85	112.52
1	A	409	VAL	N-CA-C	-5.47	105.04	111.00
1	A	35	TYR	N-CA-C	5.43	116.88	111.07
3	C	48	VAL	CB-CA-C	5.38	115.92	110.65
1	A	195	LEU	N-CA-C	-5.37	105.43	111.28
2	B	174	VAL	CB-CA-C	5.33	118.57	110.62
3	C	4	LEU	N-CA-C	-5.30	99.31	108.69
1	A	497	PHE	N-CA-C	-5.27	105.45	111.14
2	B	205	SER	N-CA-C	-5.26	100.12	109.06
4	D	60	SER	CA-C-N	5.25	127.31	120.28
4	D	60	SER	C-N-CA	5.25	127.31	120.28
3	C	9	GLY	N-CA-C	-5.20	100.86	113.18
1	A	415	VAL	N-CA-C	5.20	115.92	110.62
2	B	139	LEU	N-CA-C	5.18	117.17	109.25
3	C	96	CYS	N-CA-C	-5.17	101.27	109.96
2	B	9	VAL	N-CA-C	5.16	115.70	108.89
4	D	5	THR	CA-C-N	-5.12	115.93	123.00
4	D	5	THR	C-N-CA	-5.12	115.93	123.00
1	A	522	TYR	CA-C-N	-5.12	111.76	121.54
1	A	522	TYR	C-N-CA	-5.12	111.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLN	CA-CB-CG	5.12	124.34	114.10
1	A	388	VAL	CG1-CB-CG2	5.05	121.92	110.80
2	B	195	VAL	N-CA-C	5.04	113.47	107.73
1	A	59	HIS	CA-C-N	-5.04	115.38	120.21
1	A	59	HIS	C-N-CA	-5.04	115.38	120.21
1	A	203	THR	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	8	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4199	0	4116	185	0
2	B	1982	0	1965	63	0
3	C	941	0	898	29	0
4	D	832	0	807	26	0
5	A	120	0	104	21	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	64	0	124	5	0
9	B	80	0	155	15	0
10	A	280	0	335	26	0
10	B	117	0	133	8	0
10	D	35	0	39	3	0
11	A	2	0	0	0	0
12	A	117	0	0	4	0
12	B	138	0	0	5	0
12	C	70	0	0	4	0
12	D	54	0	0	2	0
All	All	9036	0	8676	316	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:CD1	2:B:222:ILE:CG1	1.85	1.55
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.07	1.44
1:A:276:HIS:NE2	1:A:280:TYR:CE2	1.96	1.31
10:A:575:LMT:O6B	10:A:575:LMT:C6B	1.81	1.28
1:A:342:LEU:HA	1:A:345:MET:CE	1.78	1.13
1:A:342:LEU:HD23	1:A:345:MET:HE1	1.28	1.10
1:A:276:HIS:CE1	1:A:280:TYR:HE2	1.71	1.06
1:A:208:ARG:NH1	1:A:212:MET:O	1.93	1.01
2:B:1:GLN:HB2	2:B:4:LEU:HB2	1.42	1.00
2:B:29:HIS:HD2	12:B:386:HOH:O	1.51	0.93
1:A:169:PRO:O	1:A:173:THR:HB	1.67	0.93
10:A:570:LMT:H2B	10:A:570:LMT:H6E	1.47	0.93
10:A:575:LMT:H3B	10:A:575:LMT:H4'	1.51	0.93
1:A:342:LEU:HA	1:A:345:MET:HE3	1.53	0.89
1:A:342:LEU:HA	1:A:345:MET:HE2	1.55	0.88
1:A:342:LEU:HD23	1:A:345:MET:CE	2.04	0.87
1:A:342:LEU:CD2	1:A:345:MET:HE1	2.05	0.86
1:A:402:TYR:O	1:A:405:THR:HB	1.75	0.86
2:B:74:ASN:OD1	2:B:76:PRO:HD2	1.75	0.86
4:D:8:PRO:O	4:D:103:THR:HB	1.74	0.86
1:A:418:LEU:HD12	1:A:418:LEU:N	1.93	0.83
1:A:276:HIS:CE1	1:A:280:TYR:CE2	2.55	0.82
1:A:317:ILE:C	1:A:317:ILE:HD12	2.07	0.80
3:C:5:GLN:HG3	12:C:171:HOH:O	1.81	0.80
1:A:98:MET:HB3	5:A:559:HEA:CAC	2.13	0.79
10:A:571:LMT:H1B	10:A:571:LMT:O3'	1.80	0.78
1:A:29[A]:LYS:HG2	1:A:114:TYR:CZ	2.19	0.78
1:A:417:SER:C	1:A:418:LEU:HD12	2.10	0.76
1:A:468:ARG:NH2	2:B:35:ASP:OD2	2.19	0.76
1:A:469:GLN:HE22	2:B:14:VAL:H	1.33	0.76
3:C:35:SER:OG	3:C:99:HIS:HE1	1.69	0.75
1:A:83:ASN:HD21	1:A:157:GLN:HE22	1.32	0.75
1:A:83:ASN:HD21	1:A:157:GLN:NE2	1.85	0.74
4:D:50:ASN:H	4:D:91:HIS:HE1	1.35	0.74
1:A:116:MET:CE	1:A:200:ILE:HG23	2.19	0.73
4:D:50:ASN:H	4:D:91:HIS:CE1	2.06	0.73
1:A:405:THR:CG2	1:A:407:TYR:H	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:THR:HG22	3:C:116:VAL:H	1.54	0.72
1:A:91:ILE:HD12	1:A:92:THR:N	2.04	0.72
3:C:93:MET:HE3	3:C:93:MET:HA	1.71	0.71
1:A:98:MET:HG3	5:A:559:HEA:C3C	2.25	0.67
3:C:1:GLU:OE2	3:C:26:GLY:O	2.13	0.67
1:A:415:VAL:O	1:A:419:GLY:HA3	1.95	0.67
1:A:418:LEU:N	1:A:418:LEU:CD1	2.57	0.66
1:A:116:MET:HE3	1:A:200:ILE:HG23	1.79	0.65
1:A:452:MET:HE1	5:A:559:HEA:C14	2.26	0.65
2:B:154:TYR:CD1	2:B:154:TYR:O	2.49	0.65
1:A:206:ASN:N	1:A:206:ASN:ND2	2.45	0.65
1:A:206:ASN:N	1:A:206:ASN:HD22	1.95	0.65
4:D:6:GLN:NE2	4:D:103:THR:HG23	2.11	0.65
1:A:152:PRO:O	1:A:176:GLY:HA3	1.97	0.65
2:B:1:GLN:HB2	2:B:4:LEU:HD22	1.78	0.64
1:A:21:ARG:HD3	1:A:22:TRP:CD1	2.33	0.64
9:B:272:LDA:H11	9:B:275:LDA:HM22	1.78	0.64
1:A:130:LEU:HD22	1:A:195:LEU:HD22	1.80	0.64
1:A:190:GLY:O	1:A:194:ILE:HG13	1.97	0.64
4:D:6:GLN:HE21	4:D:103:THR:HG23	1.63	0.64
1:A:337:GLN:HE22	2:B:104:GLN:NE2	1.96	0.63
4:D:104:LYS:HE2	4:D:106:GLU:OE2	1.97	0.63
1:A:405:THR:HG22	1:A:407:TYR:H	1.63	0.63
1:A:202:THR:O	1:A:206:ASN:ND2	2.31	0.63
5:A:560:HEA:HHC	5:A:560:HEA:O11	1.98	0.63
1:A:245:LEU:O	1:A:249:ARG:HG3	1.98	0.63
9:A:565:LDA:HM23	10:A:571:LMT:H5'	1.81	0.63
2:B:37:PHE:HD1	9:B:273:LDA:H11	1.64	0.63
1:A:337:GLN:HE22	2:B:104:GLN:HE21	1.44	0.63
1:A:312:MET:HE3	1:A:354:LYS:HZ3	1.63	0.62
1:A:269:HIS:HD2	1:A:323:TRP:HE1	1.46	0.62
2:B:1:GLN:CB	2:B:4:LEU:HB2	2.23	0.62
1:A:342:LEU:HD22	10:A:574:LMT:H81	1.81	0.62
3:C:93:MET:CE	3:C:112:THR:C	2.73	0.62
1:A:336:GLN:HE22	9:A:566:LDA:H22	1.65	0.61
1:A:433:GLY:HA2	1:A:438:ARG:O	1.99	0.61
1:A:473:ARG:O	1:A:474:ARG:HB2	2.00	0.61
1:A:381:PHE:CD2	1:A:382:LEU:CD2	2.84	0.61
1:A:381:PHE:CD2	1:A:382:LEU:HD23	2.35	0.61
4:D:24:ARG:HD2	4:D:70:GLN:HE22	1.64	0.61
1:A:485:TRP:HH2	10:B:278:LMT:H11	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:MET:HE1	1:A:200:ILE:HG23	1.83	0.61
2:B:227:MET:N	2:B:228:PRO:CD	2.64	0.60
1:A:187:HIS:CE1	1:A:243:THR:HG22	2.36	0.60
1:A:269:HIS:CE1	1:A:327:MET:HE1	2.36	0.60
1:A:284:LEU:O	1:A:287:PHE:HB2	2.02	0.60
1:A:412:PHE:CD2	5:A:560:HEA:HAD1	2.36	0.60
1:A:239:ALA:O	1:A:243:THR:HG23	2.01	0.60
3:C:57:ARG:HG3	3:C:57:ARG:HH11	1.67	0.60
1:A:129:ARG:HG3	10:A:575:LMT:H31	1.84	0.59
1:A:297:PHE:O	1:A:367:ILE:HA	2.01	0.59
1:A:351:THR:HG21	5:A:560:HEA:H14	1.84	0.59
1:A:484:TYR:H	2:B:15:ASN:HD21	1.51	0.59
1:A:452:MET:HE1	5:A:559:HEA:H14	1.84	0.59
4:D:69:THR:HG22	4:D:70:GLN:HG2	1.84	0.59
3:C:93:MET:HE2	3:C:112:THR:N	2.17	0.59
1:A:78:ALA:O	1:A:79:GLU:C	2.46	0.58
1:A:287:PHE:HB3	1:A:312:MET:CE	2.34	0.58
1:A:125:MET:HE3	1:A:203:THR:HG21	1.84	0.58
1:A:464:HIS:O	1:A:468:ARG:HG3	2.02	0.58
1:A:83:ASN:ND2	1:A:157:GLN:HE22	2.01	0.58
1:A:451:MET:HG2	10:A:572:LMT:H92	1.86	0.58
3:C:47:TRP:HE1	3:C:50:SER:HB2	1.69	0.58
10:A:574:LMT:H91	2:B:90:VAL:HA	1.86	0.57
1:A:341:MET:HG3	1:A:394:SER:O	2.04	0.57
1:A:468:ARG:HD3	2:B:18:MET:O	2.04	0.57
1:A:85:HIS:O	1:A:89:VAL:HG23	2.03	0.57
2:B:75:THR:O	2:B:76:PRO:C	2.46	0.57
9:B:274:LDA:H12	10:B:279:LMT:H121	1.85	0.57
1:A:412:PHE:CB	5:A:560:HEA:C2D	2.83	0.57
1:A:443:TRP:HZ2	10:A:569:LMT:H11	1.69	0.56
1:A:68:GLU:H	1:A:68:GLU:CD	2.13	0.56
3:C:88:SER:O	3:C:91:THR:HG23	2.05	0.56
3:C:91:THR:HB	3:C:115:THR:HA	1.88	0.56
1:A:27:ASN:HB3	1:A:30:ASP:OD2	2.06	0.55
2:B:19:ASN:ND2	9:B:272:LDA:H32	2.20	0.55
3:C:47:TRP:CZ2	4:D:95:PRO:HB3	2.41	0.55
4:D:6:GLN:HG2	4:D:103:THR:HG22	1.88	0.55
1:A:129:ARG:CG	10:A:575:LMT:H31	2.36	0.55
2:B:3:VAL:HG13	2:B:4:LEU:HD13	1.89	0.55
2:B:19:ASN:HD21	9:B:272:LDA:H51	1.70	0.55
1:A:412:PHE:HB3	5:A:560:HEA:C2D	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:NH1	2:B:19:ASN:OD1	2.40	0.55
10:A:570:LMT:H6E	10:A:570:LMT:C2B	2.30	0.55
1:A:485:TRP:CH2	10:B:278:LMT:H11	2.42	0.55
3:C:87:LYS:HE2	12:C:135:HOH:O	2.07	0.55
1:A:109:GLY:O	1:A:113:ASN:HB2	2.07	0.54
1:A:276:HIS:O	1:A:279:VAL:HG22	2.07	0.54
4:D:40:GLN:HB2	12:D:132:HOH:O	2.07	0.54
2:B:109:ASP:HB3	12:B:372:HOH:O	2.07	0.54
1:A:405:THR:HG23	1:A:407:TYR:H	1.71	0.54
1:A:412:PHE:CE1	1:A:413:HIS:CE1	2.96	0.54
1:A:57:LEU:HD22	1:A:87:TRP:HH2	1.74	0.53
2:B:19:ASN:HD21	9:B:272:LDA:H32	1.73	0.53
3:C:86:LEU:HB3	3:C:116:VAL:HG21	1.90	0.53
1:A:18:PHE:HB3	1:A:21:ARG:HB2	1.91	0.53
4:D:79:LEU:HB3	4:D:80:PRO:HD2	1.90	0.53
1:A:379:PHE:CD1	1:A:379:PHE:C	2.86	0.53
1:A:274:PHE:CZ	1:A:278[A]:GLU:HG3	2.44	0.53
1:A:346:THR:HG22	10:A:574:LMT:H41	1.91	0.53
1:A:481:GLU:HG2	2:B:13:PRO:O	2.09	0.53
2:B:73:HIS:O	2:B:74:ASN:HB2	2.09	0.53
2:B:83:LEU:O	2:B:87:LEU:HD23	2.08	0.52
1:A:346:THR:HG22	10:A:574:LMT:H22	1.91	0.52
1:A:395:GLN:C	1:A:397:PRO:HD2	2.35	0.52
3:C:39:GLN:HB2	3:C:45:LEU:HD23	1.91	0.52
1:A:313:ALA:O	1:A:317:ILE:HG23	2.09	0.52
10:A:571:LMT:O3'	10:A:571:LMT:C1B	2.56	0.52
2:B:40:TYR:HE1	9:B:275:LDA:H31	1.74	0.52
10:D:121:LMT:H1B	10:D:121:LMT:O3'	2.09	0.52
1:A:524:ASN:OD1	1:A:526:HIS:HB2	2.09	0.52
1:A:412:PHE:HB2	5:A:560:HEA:HMD3	1.92	0.52
4:D:61:ARG:HG3	4:D:61:ARG:HH11	1.75	0.52
2:B:138:MET:HG3	2:B:228:PRO:HG3	1.92	0.52
1:A:300:LYS:HD3	1:A:361:THR:O	2.10	0.51
1:A:290:ILE:O	1:A:294:ILE:HG13	2.10	0.51
1:A:416:MET:HG2	5:A:560:HEA:HBC2	1.91	0.51
1:A:478:TYR:O	1:A:479:PRO:C	2.53	0.51
1:A:21:ARG:HD3	1:A:22:TRP:NE1	2.25	0.51
1:A:206:ASN:HD22	1:A:206:ASN:H	1.59	0.51
1:A:438:ARG:NH2	1:A:514:GLY:O	2.41	0.51
1:A:516:ARG:NH2	1:A:518:ASN:HB3	2.25	0.51
1:A:287:PHE:HB3	1:A:312:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:ILE:HG23	4:D:103:THR:HG21	1.92	0.51
1:A:187:HIS:HE1	1:A:243:THR:HG22	1.76	0.51
1:A:287:PHE:CB	1:A:312:MET:HE2	2.41	0.51
1:A:394:SER:HA	5:A:560:HEA:OMA	2.10	0.51
1:A:416:MET:HG2	5:A:560:HEA:CBC	2.41	0.50
2:B:52:LEU:HD13	10:B:279:LMT:H102	1.92	0.50
5:A:559:HEA:HHC	5:A:559:HEA:C12	2.42	0.50
3:C:17:SER:HB2	3:C:84:SER:HA	1.93	0.50
1:A:27:ASN:ND2	1:A:29[B]:LYS:HB2	2.27	0.50
2:B:73:HIS:C	2:B:73:HIS:CD2	2.90	0.50
1:A:504:ILE:CD1	10:A:570:LMT:H122	2.42	0.50
3:C:83:MET:HB3	3:C:86:LEU:HD21	1.94	0.50
1:A:440:TYR:OH	1:A:442:GLU:OE1	2.19	0.49
1:A:317:ILE:C	1:A:317:ILE:CD1	2.83	0.49
4:D:6:GLN:HG2	4:D:103:THR:CG2	2.42	0.49
2:B:1:GLN:HB2	2:B:4:LEU:CD2	2.42	0.49
1:A:342:LEU:CA	1:A:345:MET:HE2	2.34	0.49
1:A:122:ALA:HB2	1:A:207:MET:O	2.12	0.49
10:A:568:LMT:O2B	10:A:568:LMT:O3'	2.30	0.48
1:A:355:VAL:HG21	5:A:560:HEA:H18	1.94	0.48
1:A:27:ASN:HD21	1:A:29[C]:LYS:HE2	1.76	0.48
1:A:405:THR:HG23	1:A:467:GLY:HA2	1.94	0.48
1:A:456:SER:HA	1:A:459:ILE:HD12	1.96	0.48
2:B:216:CYS:HB2	2:B:227:MET:HG3	1.96	0.48
1:A:52:TYR:HD2	1:A:90:MET:HE2	1.78	0.48
1:A:396:ALA:HB3	1:A:397:PRO:HD3	1.95	0.48
2:B:121:TRP:CD2	2:B:223:ASN:HB2	2.49	0.48
2:B:174:VAL:HG23	2:B:194:ALA:HB2	1.95	0.48
2:B:40:TYR:CE1	9:B:275:LDA:H31	2.49	0.47
2:B:164:VAL:O	2:B:233:ALA:HA	2.13	0.47
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.49	0.47
3:C:94:TYR:O	3:C:111:GLY:HA2	2.14	0.47
1:A:453:PHE:C	1:A:453:PHE:CD2	2.92	0.47
10:A:574:LMT:H11	10:A:574:LMT:O2'	2.14	0.47
1:A:133:LEU:O	1:A:137:MET:HG2	2.14	0.47
1:A:484:TYR:N	2:B:15:ASN:HD21	2.11	0.47
9:A:566:LDA:H22	9:A:566:LDA:HM12	1.80	0.47
2:B:25:SER:HB2	2:B:26:PRO:HD2	1.95	0.47
1:A:125:MET:CE	1:A:203:THR:CB	2.93	0.47
4:D:28:ASN:OD1	4:D:68:GLY:HA2	2.15	0.47
1:A:98:MET:HE3	5:A:559:HEA:HMC2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HD11	1:A:493:ALA:HA	1.97	0.47
1:A:518:ASN:HD22	1:A:518:ASN:H	1.63	0.46
1:A:520:PRO:HA	1:A:534:LEU:O	2.16	0.46
9:A:564:LDA:HM23	9:A:564:LDA:H21	1.67	0.46
1:A:49:PHE:HA	1:A:90:MET:HE1	1.98	0.46
1:A:491:ILE:HD13	10:A:572:LMT:H6'1	1.98	0.46
12:A:606:HOH:O	2:B:198:ARG:HD2	2.15	0.46
9:B:276:LDA:HM21	9:B:276:LDA:H21	1.70	0.46
3:C:40:THR:HB	3:C:41:PRO:HD2	1.98	0.46
1:A:271:LEU:O	1:A:271:LEU:HG	2.04	0.46
3:C:5:GLN:OE1	3:C:110[B]:GLN:NE2	2.49	0.46
1:A:29[B]:LYS:HD2	1:A:114:TYR:OH	2.15	0.46
1:A:398:LEU:HD13	2:B:34:LEU:HD23	1.97	0.45
2:B:19:ASN:HB3	12:B:309:HOH:O	2.16	0.45
1:A:541:HIS:NE2	12:A:609:HOH:O	2.32	0.45
2:B:70:ARG:HG3	12:B:391:HOH:O	2.16	0.45
1:A:187:HIS:CE1	1:A:243:THR:CG2	2.99	0.45
5:A:559:HEA:HHC	5:A:559:HEA:H122	1.97	0.45
1:A:332:MET:HG3	1:A:337:GLN:HG3	1.98	0.45
1:A:516:ARG:O	1:A:517:VAL:HG23	2.16	0.45
1:A:125:MET:CE	1:A:203:THR:OG1	2.65	0.45
1:A:412:PHE:HB2	5:A:560:HEA:CMD	2.47	0.45
1:A:118:LEU:HD23	12:A:674:HOH:O	2.17	0.44
1:A:484:TYR:C	1:A:484:TYR:CD2	2.95	0.44
1:A:516:ARG:CZ	1:A:518:ASN:HB3	2.46	0.44
4:D:92:TYR:C	4:D:92:TYR:CD2	2.95	0.44
1:A:388:VAL:HG13	2:B:42:ILE:HD12	2.00	0.44
1:A:387:GLY:HA3	5:A:560:HEA:C15	2.47	0.44
1:A:209:ALA:O	1:A:212:MET:HB3	2.18	0.44
1:A:381:PHE:HD2	1:A:382:LEU:CD2	2.30	0.44
1:A:431:TRP:O	1:A:435:MET:HG3	2.18	0.44
2:B:109:ASP:OD1	2:B:109:ASP:N	2.49	0.44
1:A:395:GLN:C	1:A:397:PRO:CD	2.90	0.44
2:B:114:ILE:O	2:B:172:VAL:HA	2.17	0.44
4:D:61:ARG:NE	4:D:82:ASP:OD2	2.35	0.44
1:A:384:THR:O	1:A:388:VAL:HB	2.18	0.44
10:D:121:LMT:H12	10:D:121:LMT:O2'	2.17	0.44
1:A:276:HIS:CD2	1:A:280:TYR:CE2	2.95	0.44
1:A:341:MET:C	1:A:345:MET:HE2	2.43	0.43
1:A:355:VAL:O	1:A:359:ILE:HG13	2.17	0.43
1:A:336:GLN:HE22	9:A:566:LDA:HM12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:PHE:CZ	10:B:279:LMT:H32	2.54	0.43
2:B:74:ASN:HD22	10:B:279:LMT:H12	1.84	0.43
1:A:354:LYS:HB3	1:A:354:LYS:HE3	1.88	0.43
4:D:83:PHE:CZ	4:D:107:ILE:HG23	2.53	0.43
1:A:235:LEU:N	1:A:236:PRO:CD	2.81	0.43
4:D:2:ILE:HD12	4:D:2:ILE:C	2.43	0.43
4:D:24:ARG:HD2	4:D:70:GLN:NE2	2.33	0.43
1:A:165:VAL:HB	1:A:271:LEU:CD2	2.48	0.43
1:A:505:GLY:HA3	10:A:569:LMT:H62	2.01	0.43
1:A:404:ASP:CG	12:A:677:HOH:O	2.61	0.43
10:D:121:LMT:O3'	10:D:121:LMT:C1B	2.66	0.43
3:C:52:ASN:HB2	12:C:178:HOH:O	2.18	0.43
1:A:28:HIS:HD2	1:A:113:ASN:O	2.00	0.42
1:A:180:ASP:OD1	1:A:249:ARG:HD3	2.19	0.42
3:C:44:ARG:HE	3:C:44:ARG:HB2	1.54	0.42
2:B:227:MET:HA	2:B:228:PRO:HD2	1.80	0.42
9:B:274:LDA:H12	10:B:279:LMT:C12	2.50	0.42
3:C:39:GLN:HA	3:C:44:ARG:O	2.19	0.42
1:A:98:MET:HB3	5:A:559:HEA:CBC	2.50	0.42
1:A:381:PHE:CD2	1:A:382:LEU:HD21	2.54	0.42
1:A:500:PHE:HB2	5:A:559:HEA:H261	2.01	0.42
1:A:437:GLY:O	1:A:516:ARG:NH1	2.43	0.42
1:A:50:THR:HG22	1:A:51:VAL:N	2.34	0.42
1:A:91:ILE:HD12	1:A:91:ILE:C	2.44	0.42
1:A:258:PRO:HG3	2:B:196:PRO:HB2	2.02	0.42
2:B:37:PHE:CD1	9:B:273:LDA:H11	2.48	0.42
2:B:166:VAL:HG22	2:B:234:VAL:C	2.45	0.42
9:B:274:LDA:H41	9:B:274:LDA:H72	1.77	0.42
9:B:274:LDA:HM21	10:B:279:LMT:H121	2.00	0.42
9:B:275:LDA:H21	9:B:275:LDA:HM23	1.80	0.42
1:A:61:GLY:N	1:A:477:ASP:OD1	2.51	0.42
1:A:30:ASP:O	1:A:34:LEU:HG	2.19	0.42
1:A:197:ALA:HB1	1:A:228:ALA:HB1	2.02	0.41
10:A:574:LMT:H4'	10:A:574:LMT:H3B	2.01	0.41
10:A:575:LMT:H3B	10:A:575:LMT:C4'	2.37	0.41
3:C:3:LYS:HD3	12:C:171:HOH:O	2.19	0.41
4:D:8:PRO:O	4:D:103:THR:CB	2.58	0.41
4:D:24:ARG:CD	4:D:70:GLN:NE2	2.82	0.41
1:A:72:LEU:C	1:A:73:ILE:HD13	2.45	0.41
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.93	0.41
2:B:160:ASN:ND2	12:B:394:HOH:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CD1	1:A:440:TYR:C	2.98	0.41
2:B:102:ARG:HD3	12:D:159:HOH:O	2.20	0.41
4:D:35:TRP:O	4:D:47:LEU:HB2	2.21	0.41
1:A:213:THR:O	1:A:214:LEU:C	2.64	0.41
2:B:159:ASP:OD1	2:B:160:ASN:N	2.51	0.41
1:A:535:PRO:HD2	1:A:539:PRO:HD3	2.03	0.41
10:A:568:LMT:H31	10:A:568:LMT:H61	1.71	0.41
2:B:122:TYR:CB	2:B:137:LEU:HD22	2.50	0.41
2:B:236:GLN:O	2:B:240:GLU:HG3	2.20	0.41
9:B:273:LDA:HM23	9:B:273:LDA:H22	1.76	0.41
1:A:208:ARG:HB3	1:A:212:MET:HG2	2.03	0.41
1:A:405:THR:HG23	1:A:467:GLY:CA	2.50	0.41
1:A:381:PHE:CD1	2:B:50:CYS:SG	3.14	0.41
1:A:434:LYS:HE3	1:A:531:GLU:O	2.21	0.41
1:A:49:PHE:HA	1:A:90:MET:CE	2.51	0.41
3:C:57:ARG:HG3	3:C:57:ARG:NH1	2.34	0.41
3:C:73:ASP:OD2	3:C:76:LYS:HG3	2.21	0.41
1:A:123:PRO:HB3	1:A:542:THR:O	2.20	0.41
1:A:482:PHE:O	1:A:486:ASN:OD1	2.39	0.41
1:A:491:ILE:HG23	10:A:572:LMT:H2'	2.03	0.41
2:B:227:MET:N	2:B:228:PRO:HD3	2.35	0.41
4:D:24:ARG:CD	4:D:70:GLN:HE22	2.33	0.41
3:C:109:GLY:O	4:D:43:SER:OG	2.31	0.40
10:A:574:LMT:H92	2:B:93:GLY:HA3	2.03	0.40
2:B:72:THR:O	2:B:73:HIS:HB3	2.21	0.40
2:B:119:HIS:O	2:B:121:TRP:HA	2.20	0.40
1:A:20:THR:O	1:A:24:MET:HB2	2.22	0.40
1:A:238:LEU:HD22	1:A:274:PHE:CE1	2.56	0.40
1:A:280:TYR:O	1:A:284:LEU:HD23	2.22	0.40
1:A:475:TYR:CZ	2:B:225:ALA:HA	2.57	0.40
10:A:574:LMT:H4'	10:A:574:LMT:H5B	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	ASN
3	C	118	SER
1	A	79	GLU
4	D	77	SER
2	B	235	SER
1	A	544	GLU
1	A	517	VAL
4	D	68	GLY

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%)	397 (91%)	38 (9%)	9	12
2	B	212/243 (87%)	190 (90%)	22 (10%)	7	8
3	C	103/107 (96%)	92 (89%)	11 (11%)	6	7
4	D	92/104 (88%)	80 (87%)	12 (13%)	4	4
All	All	842/908 (93%)	759 (90%)	83 (10%)	8	9

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ARG
1	A	29[A]	LYS
1	A	29[B]	LYS
1	A	29[C]	LYS
1	A	50	THR
1	A	57	LEU
1	A	63	GLN
1	A	68	GLU
1	A	72	LEU
1	A	73	ILE
1	A	86	LEU
1	A	91	ILE
1	A	116	MET
1	A	125	MET
1	A	134	SER
1	A	173	THR
1	A	194	ILE
1	A	206	ASN
1	A	212	MET
1	A	214	LEU
1	A	224	VAL
1	A	233	LEU
1	A	249	ARG
1	A	277	PRO
1	A	317	ILE
1	A	332	MET
1	A	347	ILE
1	A	359	ILE
1	A	377	PHE
1	A	380	LEU
1	A	388	VAL
1	A	398	LEU
1	A	405	THR
1	A	408	VAL
1	A	418	LEU
1	A	516	ARG
1	A	518	ASN
2	B	1	GLN
2	B	4	LEU
2	B	9	VAL
2	B	53	LEU
2	B	54	LEU

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Mol	Chain	Res	Type
2	B	63	ARG
2	B	77	ILE
2	B	83	LEU
2	B	85	PRO
2	B	108	ASN
2	B	137	LEU
2	B	140[A]	GLU
2	B	140[B]	GLU
2	B	141	LYS
2	B	142	GLU
2	B	163	VAL
2	B	166	VAL
2	B	174	VAL
2	B	179	VAL
2	B	186	PRO
2	B	198	ARG
2	B	222	ILE
3	C	3	LYS
3	C	5	GLN
3	C	13	GLN
3	C	17	SER
3	C	33	THR
3	C	42	GLU
3	C	48	VAL
3	C	57	ARG
3	C	87	LYS
3	C	91	THR
3	C	93	MET
4	D	1	ASP
4	D	3	GLU
4	D	15	VAL
4	D	24	ARG
4	D	42	LYS
4	D	45	GLN
4	D	48	VAL
4	D	63	SER
4	D	69	THR
4	D	77	SER
4	D	103	THR
4	D	107	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	28	HIS
1	A	59	HIS
1	A	155	ASN
1	A	157	GLN
1	A	206	ASN
1	A	254	GLN
1	A	268	GLN
1	A	269	HIS
1	A	469	GLN
1	A	486	ASN
1	A	518	ASN
1	A	526	HIS
2	B	15	ASN
2	B	21	GLN
2	B	29	HIS
2	B	73	HIS
2	B	104	GLN
2	B	120	GLN
2	B	192	GLN
2	B	208	GLN
3	C	99	HIS
4	D	6	GLN
4	D	37	GLN
4	D	90	HIS
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 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 for Mogul analysis.

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

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

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (283) bond length outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	OMA-CMA	8.93	1.41	1.22
10	A	571	LMT	C4B-C5B	-8.68	1.34	1.53
10	A	569	LMT	O2B-C2B	-8.47	1.22	1.43
10	B	277[A]	LMT	O4'-C4B	-8.45	1.22	1.43
10	B	277[B]	LMT	O4'-C4B	-8.45	1.22	1.43
10	A	569	LMT	C4B-C5B	-8.39	1.35	1.53
5	A	560	HEA	C18-C19	8.37	1.52	1.33
10	A	569	LMT	O3B-C3B	-8.36	1.22	1.43
10	B	278	LMT	O4'-C4B	-8.33	1.22	1.43
10	A	574	LMT	C4B-C5B	-8.26	1.35	1.53
5	A	559	HEA	C22-C23	8.18	1.56	1.32
10	A	568	LMT	O3'-C3'	-8.15	1.22	1.43
10	B	279	LMT	O3'-C3'	-8.15	1.22	1.43
10	A	570	LMT	C4B-C5B	-8.10	1.35	1.53
5	A	559	HEA	C18-C19	8.07	1.51	1.33
10	A	570	LMT	O3B-C3B	-8.06	1.23	1.43
10	B	277[A]	LMT	O2B-C2B	-8.04	1.23	1.43
10	B	277[B]	LMT	O2B-C2B	-8.04	1.23	1.43
10	A	572	LMT	O3'-C3'	-8.02	1.23	1.43
10	A	568	LMT	O3B-C3B	-8.00	1.23	1.43
10	A	574	LMT	O3'-C3'	-8.00	1.23	1.43
10	B	278	LMT	C4B-C5B	-8.00	1.36	1.53
10	A	568	LMT	O2B-C2B	-7.99	1.23	1.43
10	B	279	LMT	C4B-C5B	-7.98	1.36	1.53
10	A	571	LMT	O4'-C4B	-7.98	1.23	1.43
10	A	574	LMT	O2B-C2B	-7.96	1.23	1.43
10	A	568	LMT	C4B-C5B	-7.95	1.36	1.53
10	A	574	LMT	O3B-C3B	-7.95	1.23	1.43
10	B	279	LMT	O3B-C3B	-7.94	1.23	1.43
10	A	570	LMT	O2B-C2B	-7.94	1.23	1.43
10	A	573	LMT	C4B-C5B	-7.92	1.36	1.53
10	B	278	LMT	O2B-C2B	-7.91	1.23	1.43
10	B	277[A]	LMT	C4B-C5B	-7.90	1.36	1.53
10	B	277[B]	LMT	C4B-C5B	-7.90	1.36	1.53
10	A	575	LMT	O2B-C2B	-7.89	1.23	1.43
10	B	278	LMT	O3'-C3'	-7.88	1.23	1.43
10	A	575	LMT	O3'-C3'	-7.88	1.23	1.43
10	B	278	LMT	O3B-C3B	-7.87	1.23	1.43
10	A	571	LMT	O3B-C3B	-7.86	1.23	1.43
10	A	575	LMT	O4'-C4B	-7.84	1.23	1.43
10	A	570	LMT	O4'-C4B	-7.83	1.23	1.43
10	A	573	LMT	O2B-C2B	-7.83	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	279	LMT	O4'-C4B	-7.82	1.23	1.43
10	B	279	LMT	O2B-C2B	-7.80	1.23	1.43
10	B	277[A]	LMT	O3'-C3'	-7.80	1.23	1.43
10	B	277[B]	LMT	O3'-C3'	-7.80	1.23	1.43
10	A	574	LMT	O4'-C4B	-7.78	1.23	1.43
10	A	575	LMT	C4B-C5B	-7.77	1.36	1.53
10	A	571	LMT	O3'-C3'	-7.74	1.23	1.43
10	A	573	LMT	O3B-C3B	-7.73	1.23	1.43
10	A	570	LMT	O3'-C3'	-7.72	1.23	1.43
10	D	121	LMT	O2B-C2B	-7.71	1.23	1.43
10	A	569	LMT	O3'-C3'	-7.71	1.23	1.43
10	A	572	LMT	O3B-C3B	-7.71	1.23	1.43
10	D	121	LMT	O3B-C3B	-7.67	1.24	1.43
10	A	568	LMT	O4'-C4B	-7.63	1.24	1.43
10	A	571	LMT	O2B-C2B	-7.61	1.24	1.43
10	D	121	LMT	O3'-C3'	-7.59	1.24	1.43
10	A	572	LMT	C4B-C5B	-7.54	1.37	1.53
5	A	559	HEA	C14-C15	7.54	1.50	1.33
10	A	568	LMT	C3'-C2'	-7.54	1.32	1.52
10	A	569	LMT	O4'-C4B	-7.52	1.24	1.43
10	A	573	LMT	O3'-C3'	-7.51	1.24	1.43
10	B	277[A]	LMT	O3B-C3B	-7.49	1.24	1.43
10	B	277[B]	LMT	O3B-C3B	-7.49	1.24	1.43
10	A	575	LMT	O3B-C3B	-7.48	1.24	1.43
10	A	572	LMT	O4'-C4B	-7.48	1.24	1.43
10	A	569	LMT	C3'-C2'	-7.44	1.33	1.52
10	A	572	LMT	O2B-C2B	-7.42	1.24	1.43
10	A	573	LMT	O4'-C4B	-7.35	1.24	1.43
5	A	560	HEA	FE-NA	7.32	2.19	1.95
5	A	560	HEA	C22-C23	7.27	1.54	1.32
10	A	569	LMT	C3B-C2B	-7.19	1.33	1.52
10	D	121	LMT	O4'-C4B	-7.12	1.25	1.43
10	B	278	LMT	C3'-C2'	-7.00	1.34	1.52
10	A	574	LMT	C3'-C2'	-6.90	1.34	1.52
10	A	568	LMT	C3B-C2B	-6.87	1.34	1.52
10	A	568	LMT	C4B-C3B	-6.74	1.34	1.52
10	A	569	LMT	C4B-C3B	-6.73	1.34	1.52
10	A	571	LMT	C1'-C2'	-6.72	1.32	1.52
10	B	279	LMT	C4'-C5'	-6.72	1.34	1.52
10	A	568	LMT	C3'-C4'	-6.69	1.34	1.52
10	A	570	LMT	C4'-C5'	-6.69	1.34	1.52
10	A	571	LMT	C4B-C3B	-6.69	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	573	LMT	C3B-C2B	-6.67	1.35	1.52
10	B	279	LMT	C3'-C2'	-6.67	1.35	1.52
10	D	121	LMT	C4'-C5'	-6.61	1.35	1.52
10	B	279	LMT	C4B-C3B	-6.61	1.35	1.52
10	A	575	LMT	C3'-C2'	-6.59	1.35	1.52
10	B	277[A]	LMT	C1B-C2B	-6.58	1.33	1.52
10	B	277[B]	LMT	C1B-C2B	-6.58	1.33	1.52
9	A	564	LDA	O1-N1	-6.57	1.26	1.42
9	B	276	LDA	O1-N1	-6.56	1.26	1.42
10	B	277[A]	LMT	C3'-C4'	-6.55	1.34	1.52
10	B	277[B]	LMT	C3'-C4'	-6.55	1.34	1.52
10	D	121	LMT	C3'-C2'	-6.54	1.35	1.52
10	A	570	LMT	C3B-C2B	-6.50	1.35	1.52
10	D	121	LMT	C4B-C5B	-6.48	1.39	1.53
9	B	273	LDA	O1-N1	-6.48	1.26	1.42
10	A	571	LMT	C3'-C2'	-6.48	1.35	1.52
10	B	278	LMT	C3B-C2B	-6.46	1.35	1.52
10	A	570	LMT	C3'-C2'	-6.45	1.35	1.52
10	A	574	LMT	C3B-C2B	-6.44	1.35	1.52
10	B	279	LMT	C3B-C2B	-6.43	1.35	1.52
10	B	277[A]	LMT	C4B-C3B	-6.43	1.35	1.52
10	B	277[B]	LMT	C4B-C3B	-6.43	1.35	1.52
10	A	570	LMT	C4B-C3B	-6.41	1.35	1.52
10	A	571	LMT	C3B-C2B	-6.41	1.35	1.52
10	A	570	LMT	C3'-C4'	-6.40	1.34	1.52
10	B	279	LMT	C3'-C4'	-6.38	1.34	1.52
9	A	567	LDA	O1-N1	-6.36	1.26	1.42
10	A	575	LMT	C4B-C3B	-6.34	1.35	1.52
9	B	274	LDA	O1-N1	-6.33	1.26	1.42
9	B	272	LDA	O1-N1	-6.33	1.26	1.42
10	B	278	LMT	C1B-C2B	-6.32	1.34	1.52
10	A	568	LMT	C1'-C2'	-6.30	1.34	1.52
10	B	279	LMT	C1B-C2B	-6.27	1.34	1.52
10	D	121	LMT	C3'-C4'	-6.27	1.35	1.52
10	A	574	LMT	C4B-C3B	-6.26	1.36	1.52
10	A	575	LMT	C3B-C2B	-6.26	1.36	1.52
10	A	568	LMT	C4'-C5'	-6.24	1.36	1.52
10	A	572	LMT	C4B-C3B	-6.23	1.36	1.52
10	A	572	LMT	C3'-C2'	-6.23	1.36	1.52
10	B	278	LMT	C4B-C3B	-6.23	1.36	1.52
10	A	575	LMT	C4'-C5'	-6.20	1.36	1.52
10	D	121	LMT	C3B-C2B	-6.18	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	275	LDA	O1-N1	-6.18	1.27	1.42
10	A	571	LMT	C4'-C5'	-6.17	1.36	1.52
10	B	277[A]	LMT	C3B-C2B	-6.17	1.36	1.52
10	B	277[B]	LMT	C3B-C2B	-6.17	1.36	1.52
10	D	121	LMT	C1'-C2'	-6.16	1.34	1.52
9	A	566	LDA	O1-N1	-6.13	1.27	1.42
9	A	565	LDA	O1-N1	-6.13	1.27	1.42
10	A	573	LMT	C4B-C3B	-6.09	1.36	1.52
10	A	569	LMT	C3'-C4'	-6.07	1.35	1.52
10	D	121	LMT	C4B-C3B	-6.03	1.36	1.52
10	A	574	LMT	C3'-C4'	-5.99	1.36	1.52
10	B	277[A]	LMT	C4'-C5'	-5.97	1.36	1.52
10	B	277[B]	LMT	C4'-C5'	-5.97	1.36	1.52
10	A	574	LMT	C1B-C2B	-5.97	1.35	1.52
10	B	278	LMT	C1'-C2'	-5.96	1.35	1.52
10	A	574	LMT	C4'-C5'	-5.96	1.36	1.52
10	A	574	LMT	C1'-C2'	-5.93	1.35	1.52
5	A	559	HEA	C3B-C2B	5.93	1.48	1.34
10	B	278	LMT	C4'-C5'	-5.93	1.36	1.52
10	A	575	LMT	C1'-C2'	-5.92	1.35	1.52
10	A	570	LMT	C1'-C2'	-5.90	1.35	1.52
10	A	569	LMT	C1'-C2'	-5.90	1.35	1.52
10	B	277[A]	LMT	O1'-C1'	5.90	1.50	1.40
10	B	277[B]	LMT	O1'-C1'	5.90	1.50	1.40
10	A	575	LMT	C3'-C4'	-5.83	1.36	1.52
10	A	573	LMT	C1B-C2B	-5.83	1.35	1.52
10	A	569	LMT	C1B-C2B	-5.80	1.35	1.52
10	A	572	LMT	C3B-C2B	-5.79	1.37	1.52
10	B	277[A]	LMT	C3'-C2'	-5.78	1.37	1.52
10	B	277[B]	LMT	C3'-C2'	-5.78	1.37	1.52
10	A	571	LMT	C3'-C4'	-5.77	1.36	1.52
10	A	570	LMT	C1B-C2B	-5.75	1.35	1.52
10	A	572	LMT	C4'-C5'	-5.68	1.37	1.52
10	A	575	LMT	C1B-C2B	-5.67	1.35	1.52
10	A	569	LMT	C4'-C5'	-5.64	1.37	1.52
10	A	573	LMT	C4'-C5'	-5.60	1.37	1.52
5	A	560	HEA	C3B-C2B	5.60	1.47	1.34
10	B	278	LMT	C3'-C4'	-5.57	1.37	1.52
10	A	568	LMT	C1B-C2B	-5.56	1.36	1.52
10	A	572	LMT	C3'-C4'	-5.54	1.37	1.52
10	A	573	LMT	C3'-C2'	-5.52	1.38	1.52
10	B	279	LMT	C1'-C2'	-5.51	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	572	LMT	C1'-C2'	-5.50	1.36	1.52
10	A	571	LMT	C1B-C2B	-5.50	1.36	1.52
5	A	559	HEA	FE-NC	5.33	2.12	1.95
10	D	121	LMT	C1B-C2B	-5.28	1.37	1.52
5	A	560	HEA	FE-NC	5.28	2.12	1.95
10	A	573	LMT	C1'-C2'	-5.27	1.37	1.52
5	A	559	HEA	C4C-NC	-5.20	1.29	1.39
10	A	573	LMT	C3'-C4'	-5.19	1.38	1.52
10	D	121	LMT	O1'-C1'	5.00	1.48	1.40
5	A	559	HEA	C3D-C2D	4.97	1.47	1.36
10	A	574	LMT	O1'-C1'	4.90	1.48	1.40
5	A	560	HEA	FE-NB	4.90	2.10	1.94
5	A	559	HEA	FE-NA	4.82	2.11	1.95
5	A	560	HEA	C4A-NA	-4.78	1.30	1.39
5	A	560	HEA	CHD-C1D	4.72	1.47	1.38
10	B	277[A]	LMT	C1'-C2'	-4.71	1.38	1.52
10	B	277[B]	LMT	C1'-C2'	-4.71	1.38	1.52
10	A	575	LMT	O1'-C1'	4.71	1.48	1.40
9	A	564	LDA	C1-N1	-4.70	1.46	1.51
10	A	568	LMT	O1'-C1'	4.69	1.48	1.40
10	A	572	LMT	C1B-C2B	-4.68	1.38	1.52
5	A	560	HEA	C3D-C2D	4.63	1.46	1.36
5	A	560	HEA	CHA-C1A	4.60	1.47	1.38
10	A	571	LMT	O1'-C1'	4.58	1.47	1.40
5	A	560	HEA	FE-ND	4.55	2.08	1.94
9	B	275	LDA	C1-N1	-4.52	1.46	1.51
5	A	559	HEA	C12-C11	-4.44	1.45	1.53
5	A	560	HEA	C3A-C2A	4.44	1.47	1.37
10	A	572	LMT	O1'-C1'	4.32	1.47	1.40
10	A	573	LMT	O1'-C1'	4.30	1.47	1.40
5	A	559	HEA	C1D-ND	-4.04	1.33	1.40
5	A	559	HEA	C1A-NA	-4.01	1.32	1.39
5	A	560	HEA	C4B-NB	-3.91	1.33	1.40
10	B	278	LMT	O1'-C1'	3.91	1.46	1.40
5	A	560	HEA	C1C-C2C	3.90	1.52	1.43
10	A	569	LMT	O1'-C1'	3.90	1.46	1.40
9	A	567	LDA	C1-N1	-3.87	1.47	1.51
10	A	570	LMT	O1'-C1'	3.85	1.46	1.40
5	A	560	HEA	CHC-C4B	3.84	1.46	1.38
9	B	272	LDA	C1-N1	-3.80	1.47	1.51
5	A	560	HEA	C4C-NC	-3.75	1.32	1.39
5	A	560	HEA	C1B-C2B	3.74	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	HEA	C3A-C2A	3.74	1.45	1.37
10	B	279	LMT	O1'-C1'	3.73	1.46	1.40
5	A	559	HEA	CHD-C1D	3.71	1.45	1.38
5	A	560	HEA	C1D-ND	-3.70	1.33	1.40
5	A	559	HEA	FE-ND	3.70	2.06	1.94
9	B	276	LDA	C1-N1	-3.64	1.47	1.51
5	A	560	HEA	C4B-C3B	3.64	1.51	1.44
5	A	559	HEA	C4A-NA	-3.64	1.32	1.39
5	A	559	HEA	CHB-C4A	3.57	1.45	1.38
5	A	560	HEA	C1A-NA	-3.56	1.32	1.39
9	A	565	LDA	C1-N1	-3.28	1.48	1.51
5	A	560	HEA	CHD-C4C	3.26	1.46	1.39
5	A	559	HEA	C1C-NC	-3.25	1.33	1.39
5	A	559	HEA	C4B-NB	-3.20	1.34	1.40
5	A	560	HEA	CHA-C4D	3.18	1.46	1.39
5	A	560	HEA	CHB-C4A	3.17	1.44	1.38
5	A	560	HEA	C4D-ND	-3.15	1.32	1.38
5	A	560	HEA	C3C-C2C	3.03	1.51	1.41
5	A	559	HEA	C1D-C2D	3.03	1.50	1.44
5	A	560	HEA	CHC-C1C	3.01	1.46	1.39
5	A	559	HEA	CHA-C4D	2.96	1.45	1.39
5	A	559	HEA	CHB-C1B	2.92	1.45	1.39
9	B	274	LDA	C1-N1	-2.91	1.48	1.51
5	A	560	HEA	C3A-C4A	2.87	1.51	1.46
10	B	277[A]	LMT	O5B-C1B	2.84	1.49	1.41
10	B	277[B]	LMT	O5B-C1B	2.84	1.49	1.41
10	A	569	LMT	O5B-C1B	2.81	1.49	1.41
9	A	566	LDA	C1-N1	-2.80	1.48	1.51
10	A	571	LMT	O5B-C1B	2.74	1.48	1.41
5	A	560	HEA	CHB-C1B	2.72	1.45	1.39
5	A	559	HEA	CHA-C1A	2.70	1.43	1.38
5	A	559	HEA	C1B-C2B	2.69	1.50	1.44
5	A	560	HEA	C1C-NC	-2.64	1.34	1.39
10	A	569	LMT	O5'-C1'	2.58	1.48	1.41
5	A	560	HEA	C13-C14	2.51	1.58	1.50
10	D	121	LMT	O1B-C1B	2.51	1.48	1.41
10	A	573	LMT	O1B-C1B	2.50	1.48	1.41
10	A	572	LMT	O5'-C1'	2.47	1.48	1.41
10	A	572	LMT	O5B-C1B	2.45	1.48	1.41
10	A	575	LMT	O1B-C1B	2.44	1.48	1.41
5	A	560	HEA	C3C-C4C	2.44	1.49	1.42
9	B	273	LDA	C1-N1	-2.43	1.49	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	C24-C23	2.39	1.56	1.50
10	A	571	LMT	O1B-C1B	2.39	1.48	1.41
10	A	572	LMT	O1B-C1B	2.38	1.48	1.41
11	A	576	PER	O2-O1	-2.38	1.09	1.42
10	A	570	LMT	O1B-C4'	2.27	1.49	1.43
5	A	560	HEA	CMA-C3A	2.26	1.50	1.45
10	A	573	LMT	O1B-C4'	2.25	1.49	1.43
5	A	559	HEA	CHC-C1C	2.25	1.44	1.39
10	A	575	LMT	O5'-C1'	2.24	1.47	1.41
5	A	560	HEA	C12-C11	-2.24	1.49	1.53
5	A	560	HEA	C1D-C2D	2.23	1.49	1.44
10	A	574	LMT	O5B-C1B	2.22	1.47	1.41
10	A	568	LMT	O5'-C1'	2.22	1.47	1.41
10	A	569	LMT	O1B-C1B	2.19	1.47	1.41
5	A	560	HEA	C4D-C3D	2.18	1.48	1.45
10	A	574	LMT	O1B-C1B	2.14	1.47	1.41
10	B	277[A]	LMT	O5'-C1'	2.13	1.47	1.41
10	B	277[B]	LMT	O5'-C1'	2.13	1.47	1.41
10	A	570	LMT	O5B-C1B	2.09	1.47	1.41
10	A	573	LMT	O5B-C1B	2.06	1.47	1.41
10	D	121	LMT	O2'-C2'	2.05	1.48	1.43
10	A	572	LMT	O2'-C2'	2.05	1.48	1.43
5	A	560	HEA	C11-C3B	-2.05	1.48	1.51
10	A	571	LMT	O5'-C1'	2.04	1.47	1.41
10	A	571	LMT	C12-C11	2.00	1.64	1.50
10	A	570	LMT	O1B-C1B	2.00	1.47	1.41

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	560	HEA	C13-C12-C11	-15.25	90.03	114.39
5	A	560	HEA	C12-C11-C3B	13.24	132.82	112.12
5	A	559	HEA	C12-C11-C3B	11.28	129.75	112.12
5	A	559	HEA	C17-C18-C19	-10.26	104.14	127.62
5	A	559	HEA	CHB-C1B-NB	10.07	135.26	124.42
5	A	559	HEA	CHB-C4A-NA	8.91	134.16	124.45
5	A	559	HEA	C12-C13-C14	-8.78	89.08	112.16
5	A	559	HEA	O11-C11-C3B	8.56	126.96	111.26
5	A	560	HEA	C13-C14-C15	-8.26	108.71	127.62
5	A	559	HEA	C16-C15-C14	-8.25	102.64	121.17
5	A	559	HEA	CHA-C1A-NA	8.13	133.31	124.45
5	A	560	HEA	CHB-C1B-NB	8.12	133.16	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	HEA	CHC-C4B-NB	7.94	134.19	124.37
10	D	121	LMT	C1-O1'-C1'	7.81	127.02	113.68
5	A	560	HEA	C27-C19-C18	-7.54	104.27	123.63
5	A	559	HEA	CHB-C1B-C2B	-7.50	113.18	125.03
5	A	559	HEA	C4A-CHB-C1B	-7.31	110.48	126.02
5	A	559	HEA	C13-C14-C15	-6.82	112.01	127.62
5	A	560	HEA	CHB-C4A-NA	6.78	131.84	124.45
5	A	560	HEA	CHB-C1B-C2B	-6.72	114.42	125.03
5	A	560	HEA	CHD-C1D-ND	6.59	132.52	124.37
10	A	569	LMT	O1'-C1'-C2'	6.56	118.23	108.27
5	A	559	HEA	CHA-C4D-ND	6.42	131.34	124.42
5	A	559	HEA	CHD-C1D-ND	6.39	132.28	124.37
5	A	560	HEA	CHA-C4D-ND	6.35	131.26	124.42
10	A	573	LMT	C1-O1'-C1'	6.33	124.50	113.68
5	A	560	HEA	CHA-C1A-NA	6.25	131.26	124.45
10	B	277[A]	LMT	O1'-C1'-C2'	6.21	117.70	108.27
10	B	277[B]	LMT	O1'-C1'-C2'	6.21	117.70	108.27
5	A	560	HEA	CHC-C4B-NB	6.15	131.98	124.37
5	A	560	HEA	C4A-CHB-C1B	-6.13	112.98	126.02
10	A	570	LMT	C1-O1'-C1'	6.11	124.11	113.68
5	A	560	HEA	C12-C13-C14	5.99	127.91	112.16
10	A	571	LMT	C1-O1'-C1'	5.75	123.51	113.68
10	A	575	LMT	C1-O1'-C1'	5.71	123.44	113.68
5	A	560	HEA	C1D-ND-C4D	5.70	111.96	105.21
5	A	560	HEA	C1B-C2B-C3B	-5.69	100.20	106.80
10	A	574	LMT	C1-O1'-C1'	5.60	123.25	113.68
10	B	278	LMT	O1'-C1'-C2'	5.58	116.75	108.27
10	D	121	LMT	C4B-C3B-C2B	5.56	120.60	110.83
5	A	559	HEA	C4C-CHD-C1D	-5.33	113.72	126.25
5	A	559	HEA	C4B-NB-C1B	5.32	111.51	105.21
5	A	559	HEA	C1B-C2B-C3B	-5.26	100.71	106.80
10	A	572	LMT	C1-O1'-C1'	5.13	122.45	113.68
5	A	559	HEA	CHC-C1C-NC	5.12	133.14	123.86
5	A	560	HEA	CHA-C1A-C2A	-5.10	116.81	124.86
5	A	560	HEA	C26-C15-C14	-5.08	110.58	123.63
5	A	559	HEA	CHB-C4A-C3A	-5.06	116.68	125.21
10	B	277[A]	LMT	C1-O1'-C1'	5.04	122.29	113.68
5	A	559	HEA	C13-C12-C11	-4.99	106.42	114.39
10	A	569	LMT	O2'-C2'-C1'	4.95	121.87	110.08
5	A	559	HEA	CAA-CBA-CGA	-4.89	100.70	113.67
5	A	559	HEA	CHA-C4D-C3D	-4.85	117.70	124.77
5	A	559	HEA	C27-C19-C18	-4.78	111.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	560	HEA	OMA-CMA-C3A	-4.77	114.86	125.62
10	A	574	LMT	O1'-C1'-C2'	4.73	115.45	108.27
5	A	559	HEA	C4A-NA-C1A	4.68	113.45	105.82
5	A	559	HEA	CHD-C4C-NC	4.62	132.25	123.86
10	B	277[A]	LMT	C3B-C4B-C5B	4.61	118.60	110.23
10	B	277[B]	LMT	C3B-C4B-C5B	4.61	118.60	110.23
5	A	560	HEA	CMB-C2B-C1B	4.60	132.22	125.03
5	A	560	HEA	CHB-C4A-C3A	-4.57	117.50	125.21
5	A	560	HEA	C4C-CHD-C1D	-4.57	115.50	126.25
10	A	568	LMT	C1-O1'-C1'	4.57	121.48	113.68
5	A	560	HEA	CAD-CBD-CGD	-4.55	101.61	113.67
5	A	560	HEA	C4B-NB-C1B	4.50	110.54	105.21
5	A	560	HEA	C3C-C2C-C1C	-4.50	101.86	107.17
5	A	559	HEA	C3C-C2C-C1C	-4.50	101.86	107.17
5	A	559	HEA	C20-C19-C18	-4.49	111.09	121.17
10	D	121	LMT	C1B-C2B-C3B	4.46	119.40	110.01
10	D	121	LMT	C3B-C4B-C5B	4.45	118.30	110.23
10	A	572	LMT	O1'-C1'-C2'	4.42	114.98	108.27
5	A	559	HEA	CMC-C2C-C3C	4.41	136.93	126.55
10	A	573	LMT	C2'-C3'-C4'	4.39	119.65	109.68
5	A	560	HEA	C3A-C2A-C1A	-4.34	102.94	107.05
5	A	559	HEA	C1D-C2D-C3D	-4.34	102.42	106.98
5	A	559	HEA	C27-C19-C20	-4.30	107.77	115.23
5	A	560	HEA	CAA-CBA-CGA	-4.27	102.33	113.67
10	D	121	LMT	C1B-O5B-C5B	-4.26	105.40	113.72
5	A	559	HEA	CBA-CAA-C2A	4.24	124.27	112.53
10	A	575	LMT	O5B-C5B-C4B	4.15	117.17	109.70
10	B	279	LMT	C1-O1'-C1'	4.09	120.66	113.68
5	A	559	HEA	CHC-C1C-C2C	-4.06	115.63	127.43
10	A	574	LMT	O5'-C5'-C4'	4.04	118.07	109.72
5	A	560	HEA	C4C-NC-C1C	4.02	112.37	105.82
10	B	277[A]	LMT	C1'-O5'-C5'	-3.99	105.92	113.72
10	B	277[B]	LMT	C1'-O5'-C5'	-3.99	105.92	113.72
5	A	559	HEA	C1C-CHC-C4B	-3.99	116.86	126.25
5	A	560	HEA	C26-C15-C16	-3.97	108.34	115.23
5	A	560	HEA	CHD-C4C-NC	3.91	130.95	123.86
10	A	570	LMT	O1B-C4'-C5'	3.88	119.66	109.48
5	A	560	HEA	C17-C18-C19	-3.87	118.78	127.62
10	B	277[A]	LMT	O5B-C5B-C4B	3.86	116.65	109.70
10	B	277[B]	LMT	O5B-C5B-C4B	3.86	116.65	109.70
5	A	559	HEA	C24-C23-C22	-3.85	111.10	122.66
10	A	569	LMT	C1'-C2'-C3'	-3.80	102.03	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	HEA	C26-C15-C16	-3.79	108.64	115.23
5	A	559	HEA	CHD-C1D-C2D	-3.78	116.19	126.95
5	A	559	HEA	C4C-NC-C1C	3.74	111.92	105.82
5	A	559	HEA	C26-C15-C14	-3.74	114.03	123.63
10	A	572	LMT	O1B-C1B-C2B	3.73	117.26	108.09
5	A	559	HEA	C1D-ND-C4D	3.71	109.60	105.21
5	A	560	HEA	C17-C16-C15	-3.66	101.05	113.19
5	A	560	HEA	CHA-C4D-C3D	-3.62	119.49	124.77
5	A	559	HEA	C4A-C3A-C2A	-3.55	103.74	106.81
5	A	559	HEA	C2A-C1A-NA	-3.54	106.91	110.32
5	A	560	HEA	C4A-C3A-C2A	-3.52	103.76	106.81
10	A	570	LMT	C1B-O5B-C5B	-3.47	106.94	113.72
5	A	560	HEA	CHC-C1C-NC	3.46	130.13	123.86
10	A	574	LMT	C2'-C3'-C4'	3.44	117.49	109.68
10	B	279	LMT	C1'-O5'-C5'	-3.43	107.01	113.72
10	A	569	LMT	O3'-C3'-C4'	3.33	118.48	109.94
5	A	559	HEA	C1A-CHA-C4D	-3.32	118.95	126.02
5	A	560	HEA	CHD-C1D-C2D	-3.32	117.51	126.95
5	A	560	HEA	O11-C11-C3B	3.32	117.34	111.26
10	A	571	LMT	C2'-C3'-C4'	3.32	117.20	109.68
5	A	560	HEA	C1D-C2D-C3D	-3.29	103.52	106.98
5	A	560	HEA	CAD-C3D-C4D	3.26	130.37	124.70
5	A	560	HEA	C21-C22-C23	-3.24	116.84	127.64
5	A	559	HEA	CHA-C1A-C2A	-3.22	119.78	124.86
5	A	559	HEA	CHC-C4B-C3B	-3.20	117.72	125.80
10	A	573	LMT	O1'-C1'-C2'	3.18	113.10	108.27
10	A	573	LMT	C1'-C2'-C3'	3.15	116.64	110.01
10	A	574	LMT	C3'-C4'-C5'	3.11	117.82	110.93
10	A	575	LMT	C3B-C4B-C5B	3.10	115.85	110.23
10	A	568	LMT	O1B-C1B-C2B	3.06	115.61	108.09
10	A	569	LMT	O1'-C1-C2	3.05	119.71	109.37
10	B	278	LMT	C1B-O5B-C5B	-3.03	107.79	113.72
10	A	575	LMT	O6B-C6B-C5B	-2.98	101.20	111.33
10	A	575	LMT	O1B-C1B-C2B	2.97	115.40	108.09
10	A	572	LMT	O5'-C5'-C4'	2.96	115.85	109.72
5	A	560	HEA	C4A-NA-C1A	2.96	110.65	105.82
5	A	560	HEA	C25-C23-C22	-2.96	113.78	122.66
5	A	560	HEA	C24-C23-C22	-2.95	113.81	122.66
10	B	278	LMT	O5B-C1B-C2B	-2.92	104.37	110.37
10	A	569	LMT	C2'-C3'-C4'	-2.91	103.08	109.68
5	A	560	HEA	CMC-C2C-C3C	2.85	133.26	126.55
5	A	560	HEA	CAA-C2A-C1A	2.84	130.63	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	278	LMT	C1'-C2'-C3'	-2.82	104.08	110.01
5	A	560	HEA	CHC-C1C-C2C	-2.80	119.30	127.43
5	A	560	HEA	CMD-C2D-C1D	2.80	129.40	125.03
5	A	559	HEA	CMC-C2C-C1C	-2.79	121.17	125.42
10	A	571	LMT	C3'-C4'-C5'	2.76	117.05	110.93
10	B	277[A]	LMT	O5B-C5B-C6B	2.69	113.11	106.44
10	B	277[B]	LMT	O5B-C5B-C6B	2.69	113.11	106.44
5	A	559	HEA	O2D-CGD-O1D	-2.68	116.45	123.33
5	A	559	HEA	C21-C22-C23	-2.67	118.75	127.64
10	D	121	LMT	C2'-C3'-C4'	2.67	115.73	109.68
10	A	569	LMT	O5'-C5'-C4'	2.66	115.23	109.72
10	A	572	LMT	O2B-C2B-C1B	2.66	116.42	110.08
5	A	559	HEA	C21-C20-C19	-2.65	104.41	113.19
10	A	575	LMT	O1B-C4'-C3'	2.64	113.94	107.23
10	B	277[A]	LMT	C6B-C5B-C4B	-2.60	106.62	113.02
10	B	277[B]	LMT	C6B-C5B-C4B	-2.60	106.62	113.02
5	A	559	HEA	CMB-C2B-C1B	2.60	129.10	125.03
10	A	573	LMT	C1'-O5'-C5'	-2.60	108.64	113.72
5	A	560	HEA	C16-C15-C14	2.59	126.98	121.17
10	A	573	LMT	O1B-C1B-C2B	2.59	114.46	108.09
10	B	279	LMT	C1B-O5B-C5B	-2.52	108.80	113.72
10	B	277[A]	LMT	C1'-C2'-C3'	2.52	115.30	110.01
10	B	277[B]	LMT	C1'-C2'-C3'	2.52	115.30	110.01
5	A	560	HEA	CHC-C4B-C3B	-2.50	119.49	125.80
10	A	569	LMT	O1B-C1B-C2B	2.49	114.21	108.09
10	B	279	LMT	O1'-C1'-C2'	2.49	112.05	108.27
10	D	121	LMT	O5'-C5'-C4'	2.48	114.84	109.72
10	B	278	LMT	C2'-C3'-C4'	2.47	115.29	109.68
10	A	569	LMT	C3-C2-C1	-2.46	102.76	113.47
5	A	559	HEA	CBD-CAD-C3D	-2.46	105.72	112.53
10	B	277[A]	LMT	O1B-C1B-O5B	2.40	117.01	110.69
10	B	277[B]	LMT	O1B-C1B-O5B	2.40	117.01	110.69
10	A	570	LMT	O1B-C1B-C2B	2.40	113.99	108.09
10	B	278	LMT	O2'-C2'-C1'	2.39	115.76	110.08
10	A	569	LMT	O4'-C4B-C5B	2.37	115.16	109.32
5	A	559	HEA	CMD-C2D-C1D	2.36	128.73	125.03
10	A	569	LMT	C4-C3-C2	2.34	126.19	114.37
10	B	279	LMT	O5'-C5'-C6'	2.33	112.20	106.44
10	A	571	LMT	O5B-C1B-C2B	2.32	115.13	110.37
5	A	559	HEA	OMA-CMA-C3A	-2.32	120.39	125.62
10	A	574	LMT	O1B-C1B-C2B	2.31	113.77	108.09
10	A	569	LMT	O5B-C1B-C2B	2.29	115.07	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	278	LMT	O1B-C1B-O5B	-2.26	104.73	110.69
10	A	568	LMT	O5'-C5'-C4'	2.25	114.37	109.72
5	A	559	HEA	O11-C11-C12	-2.23	103.22	109.14
10	B	278	LMT	O5B-C5B-C6B	2.21	111.93	106.44
5	A	560	HEA	C2B-C1B-NB	2.18	112.42	109.90
10	D	121	LMT	O1B-C1B-C2B	2.18	113.45	108.09
10	D	121	LMT	O5B-C5B-C4B	2.17	113.62	109.70
10	A	571	LMT	C4-C3-C2	2.17	125.33	114.37
10	B	277[B]	LMT	C1-O1'-C1'	2.16	117.37	113.68
10	A	569	LMT	C1B-C2B-C3B	2.16	114.55	110.01
10	A	570	LMT	O5'-C5'-C6'	-2.15	101.11	106.44
10	A	571	LMT	C1B-O1B-C4'	-2.12	112.94	117.98
10	A	575	LMT	O1'-C1'-C2'	2.11	111.48	108.27
10	D	121	LMT	C3'-C4'-C5'	2.07	115.51	110.93
10	D	121	LMT	C1'-O5'-C5'	2.06	117.75	113.72
5	A	560	HEA	C20-C19-C18	-2.05	116.57	121.17
10	D	121	LMT	O4'-C4B-C5B	2.04	114.36	109.32
10	A	568	LMT	O1'-C1'-C2'	2.04	111.37	108.27
10	B	278	LMT	O2B-C2B-C3B	2.04	115.17	110.38
10	A	571	LMT	C3B-C4B-C5B	-2.03	106.54	110.23
10	A	573	LMT	O5'-C5'-C4'	2.02	113.90	109.72
10	A	573	LMT	O5B-C5B-C4B	2.02	113.34	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 (259) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	559	HEA	C2A-C3A-CMA-OMA
5	A	559	HEA	C4A-C3A-CMA-OMA
5	A	559	HEA	O11-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C2B
5	A	559	HEA	C12-C11-C3B-C4B
5	A	559	HEA	O11-C11-C12-C13
5	A	559	HEA	C17-C18-C19-C27
5	A	560	HEA	O11-C11-C3B-C2B
5	A	560	HEA	C12-C11-C3B-C2B
5	A	560	HEA	O11-C11-C3B-C4B

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Mol	Chain	Res	Type	Atoms
5	A	560	HEA	C3B-C11-C12-C13
5	A	560	HEA	C11-C12-C13-C14
5	A	560	HEA	C17-C18-C19-C20
9	A	564	LDA	C2-C1-N1-CM2
9	A	565	LDA	C2-C1-N1-CM2
9	A	566	LDA	C2-C1-N1-CM1
9	A	567	LDA	C2-C1-N1-CM1
9	A	567	LDA	C2-C1-N1-CM2
9	B	272	LDA	C2-C1-N1-CM1
9	B	272	LDA	N1-C1-C2-C3
9	B	273	LDA	C2-C1-N1-O1
9	B	273	LDA	C2-C1-N1-CM1
9	B	273	LDA	C2-C1-N1-CM2
9	B	274	LDA	C2-C1-N1-CM1
9	B	274	LDA	C2-C1-N1-CM2
9	B	276	LDA	C2-C1-N1-O1
9	B	276	LDA	C2-C1-N1-CM1
9	B	276	LDA	C2-C1-N1-CM2
9	B	276	LDA	N1-C1-C2-C3
10	A	572	LMT	C2'-C1'-O1'-C1
10	A	572	LMT	O5'-C1'-O1'-C1
10	A	574	LMT	O5'-C1'-O1'-C1
10	A	574	LMT	C2-C1-O1'-C1'
10	B	277[B]	LMT	C2'-C1'-O1'-C1
10	D	121	LMT	C2'-C1'-O1'-C1
10	A	570	LMT	C5'-C4'-O1B-C1B
10	A	575	LMT	C2B-C1B-O1B-C4'
5	A	560	HEA	C21-C22-C23-C25
10	A	569	LMT	C2B-C1B-O1B-C4'
10	A	574	LMT	O5B-C1B-O1B-C4'
5	A	559	HEA	C21-C22-C23-C25
5	A	559	HEA	C13-C14-C15-C26
5	A	560	HEA	C13-C14-C15-C26
5	A	560	HEA	C17-C18-C19-C27
10	A	569	LMT	O5B-C5B-C6B-O6B
10	A	572	LMT	C4'-C5'-C6'-O6'
10	A	575	LMT	C4B-C5B-C6B-O6B
10	A	574	LMT	O5B-C5B-C6B-O6B
10	A	575	LMT	O5B-C5B-C6B-O6B
10	B	278	LMT	O5B-C5B-C6B-O6B
10	A	571	LMT	C4B-C5B-C6B-O6B
10	B	278	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
10	A	569	LMT	C4'-C5'-C6'-O6'
10	A	568	LMT	O5'-C5'-C6'-O6'
10	A	572	LMT	O5'-C5'-C6'-O6'
10	A	571	LMT	O5'-C1'-O1'-C1
10	B	277[B]	LMT	O5'-C1'-O1'-C1
10	D	121	LMT	O5'-C1'-O1'-C1
10	A	575	LMT	O5'-C5'-C6'-O6'
10	B	279	LMT	O5'-C5'-C6'-O6'
10	A	571	LMT	O5B-C5B-C6B-O6B
10	A	574	LMT	O5'-C5'-C6'-O6'
10	B	279	LMT	O5B-C5B-C6B-O6B
10	D	121	LMT	O5B-C5B-C6B-O6B
10	B	279	LMT	C1-C2-C3-C4
10	A	574	LMT	C4'-C5'-C6'-O6'
10	B	279	LMT	C4B-C5B-C6B-O6B
10	B	279	LMT	C4'-C5'-C6'-O6'
10	A	568	LMT	C4'-C5'-C6'-O6'
10	A	569	LMT	C4B-C5B-C6B-O6B
10	A	571	LMT	C2'-C1'-O1'-C1
10	B	277[A]	LMT	C2'-C1'-O1'-C1
10	A	574	LMT	C4B-C5B-C6B-O6B
10	A	568	LMT	O1'-C1-C2-C3
10	A	574	LMT	O1'-C1-C2-C3
10	D	121	LMT	C4B-C5B-C6B-O6B
10	D	121	LMT	C4'-C5'-C6'-O6'
10	A	569	LMT	O5'-C5'-C6'-O6'
10	A	570	LMT	C4B-C5B-C6B-O6B
10	B	278	LMT	C4B-C5B-C6B-O6B
10	A	574	LMT	C2B-C1B-O1B-C4'
9	B	274	LDA	C4-C5-C6-C7
10	A	575	LMT	O1'-C1-C2-C3
5	A	560	HEA	C18-C19-C20-C21
10	B	279	LMT	C2'-C1'-O1'-C1
5	A	560	HEA	C19-C20-C21-C22
10	A	571	LMT	C3'-C4'-O1B-C1B
10	A	573	LMT	C3'-C4'-O1B-C1B
10	B	277[B]	LMT	O1'-C1-C2-C3
10	A	570	LMT	O5B-C5B-C6B-O6B
10	B	278	LMT	O5'-C5'-C6'-O6'
10	B	279	LMT	O5'-C1'-O1'-C1
10	B	278	LMT	C2B-C1B-O1B-C4'
10	B	278	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
10	A	573	LMT	C6-C7-C8-C9
10	A	574	LMT	C2-C3-C4-C5
10	A	568	LMT	C3-C4-C5-C6
10	A	571	LMT	C2-C1-O1'-C1'
10	A	573	LMT	C2-C1-O1'-C1'
10	B	279	LMT	C5-C6-C7-C8
10	A	574	LMT	C1-C2-C3-C4
10	B	277[A]	LMT	C6-C7-C8-C9
10	B	277[A]	LMT	C1-C2-C3-C4
10	A	571	LMT	C1-C2-C3-C4
10	D	121	LMT	O5B-C1B-O1B-C4'
10	A	575	LMT	C4'-C5'-C6'-O6'
9	B	273	LDA	C5-C6-C7-C8
10	B	278	LMT	C5-C6-C7-C8
10	B	278	LMT	C6-C7-C8-C9
10	A	572	LMT	C1-C2-C3-C4
9	B	274	LDA	C7-C8-C9-C10
10	A	568	LMT	C2-C3-C4-C5
10	A	570	LMT	C2-C3-C4-C5
10	A	573	LMT	C5'-C4'-O1B-C1B
10	A	571	LMT	C2-C3-C4-C5
9	A	567	LDA	C2-C3-C4-C5
9	A	564	LDA	C11-C10-C9-C8
9	A	565	LDA	C2-C3-C4-C5
10	A	570	LMT	C5-C6-C7-C8
10	A	574	LMT	C6-C7-C8-C9
10	B	278	LMT	C11-C10-C9-C8
10	A	572	LMT	C3-C4-C5-C6
9	A	566	LDA	C3-C4-C5-C6
10	A	569	LMT	C11-C10-C9-C8
10	A	572	LMT	C6-C7-C8-C9
9	B	273	LDA	C4-C5-C6-C7
9	B	274	LDA	C5-C6-C7-C8
9	A	566	LDA	C1-C2-C3-C4
10	A	571	LMT	C6-C7-C8-C9
10	A	572	LMT	C11-C10-C9-C8
10	A	571	LMT	C5-C6-C7-C8
10	A	570	LMT	C11-C10-C9-C8
10	A	575	LMT	C5-C6-C7-C8
9	B	273	LDA	C7-C8-C9-C10
10	B	277[A]	LMT	C11-C10-C9-C8
10	A	572	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
10	B	277[A]	LMT	C7-C8-C9-C10
10	A	571	LMT	C5'-C4'-O1B-C1B
10	A	568	LMT	C7-C8-C9-C10
10	A	573	LMT	C2-C3-C4-C5
10	B	278	LMT	C2-C3-C4-C5
10	B	279	LMT	C4-C5-C6-C7
10	B	279	LMT	C7-C8-C9-C10
9	A	565	LDA	C6-C7-C8-C9
10	A	572	LMT	C4-C5-C6-C7
10	A	573	LMT	C3-C4-C5-C6
10	A	571	LMT	O5'-C5'-C6'-O6'
9	B	276	LDA	C3-C4-C5-C6
9	B	276	LDA	C7-C8-C9-C10
9	B	276	LDA	C2-C3-C4-C5
9	A	564	LDA	C6-C7-C8-C9
10	B	277[A]	LMT	C2-C3-C4-C5
9	B	275	LDA	C6-C7-C8-C9
10	A	568	LMT	C6-C7-C8-C9
9	A	565	LDA	C11-C10-C9-C8
10	A	572	LMT	O5B-C5B-C6B-O6B
10	A	571	LMT	C11-C10-C9-C8
10	A	572	LMT	O1'-C1-C2-C3
9	A	567	LDA	C7-C8-C9-C10
10	D	121	LMT	C3'-C4'-O1B-C1B
10	A	568	LMT	C5-C6-C7-C8
9	A	564	LDA	C9-C10-C11-C12
9	A	566	LDA	N1-C1-C2-C3
9	B	273	LDA	N1-C1-C2-C3
9	B	275	LDA	N1-C1-C2-C3
10	A	570	LMT	C9-C10-C11-C12
10	B	277[A]	LMT	C4-C5-C6-C7
10	B	278	LMT	C9-C10-C11-C12
10	A	573	LMT	C11-C10-C9-C8
10	A	574	LMT	C2'-C1'-O1'-C1
9	B	275	LDA	C9-C10-C11-C12
10	A	573	LMT	C9-C10-C11-C12
9	A	564	LDA	C5-C6-C7-C8
9	B	273	LDA	C1-C2-C3-C4
10	A	572	LMT	C2-C3-C4-C5
10	A	570	LMT	C2B-C1B-O1B-C4'
9	A	567	LDA	C11-C10-C9-C8
9	A	567	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	D	121	LMT	O5'-C5'-C6'-O6'
9	A	567	LDA	C9-C10-C11-C12
10	A	569	LMT	C9-C10-C11-C12
9	B	272	LDA	C9-C10-C11-C12
10	D	121	LMT	C5'-C4'-O1B-C1B
10	A	570	LMT	O5B-C1B-O1B-C4'
10	B	279	LMT	C6-C7-C8-C9
9	A	566	LDA	C9-C10-C11-C12
10	A	574	LMT	C11-C10-C9-C8
10	A	575	LMT	C9-C10-C11-C12
9	A	567	LDA	C3-C4-C5-C6
9	A	565	LDA	C7-C8-C9-C10
9	A	565	LDA	C2-C1-N1-CM1
9	B	272	LDA	C2-C1-N1-CM2
10	B	278	LMT	C1-C2-C3-C4
10	A	568	LMT	C2-C1-O1'-C1'
10	A	575	LMT	C2-C1-O1'-C1'
10	B	277[A]	LMT	C2-C1-O1'-C1'
5	A	560	HEA	C15-C16-C17-C18
10	A	574	LMT	C9-C10-C11-C12
9	B	275	LDA	C4-C5-C6-C7
10	A	568	LMT	C1-C2-C3-C4
10	A	574	LMT	C7-C8-C9-C10
10	D	121	LMT	C5-C6-C7-C8
10	A	575	LMT	C4-C5-C6-C7
10	D	121	LMT	C9-C10-C11-C12
9	B	272	LDA	C1-C2-C3-C4
9	A	564	LDA	C4-C5-C6-C7
5	A	560	HEA	C4A-C3A-CMA-OMA
9	A	565	LDA	C2-C1-N1-O1
9	A	567	LDA	C2-C1-N1-O1
9	B	274	LDA	C2-C1-N1-O1
10	A	569	LMT	O5B-C1B-O1B-C4'
5	A	560	HEA	C12-C11-C3B-C4B
9	A	566	LDA	C6-C7-C8-C9
9	A	565	LDA	C9-C10-C11-C12
9	B	274	LDA	C11-C10-C9-C8
10	A	573	LMT	C4-C5-C6-C7
10	B	279	LMT	C11-C10-C9-C8
10	D	121	LMT	C2B-C1B-O1B-C4'
10	A	569	LMT	C1-C2-C3-C4
10	B	279	LMT	C2-C1-O1'-C1'

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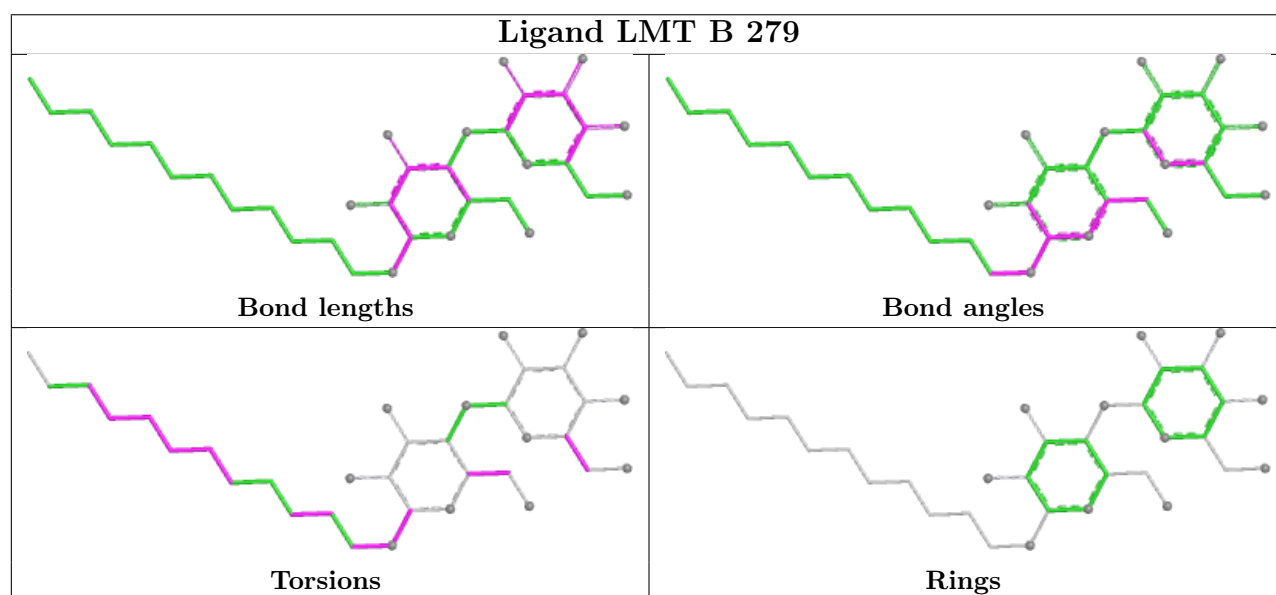
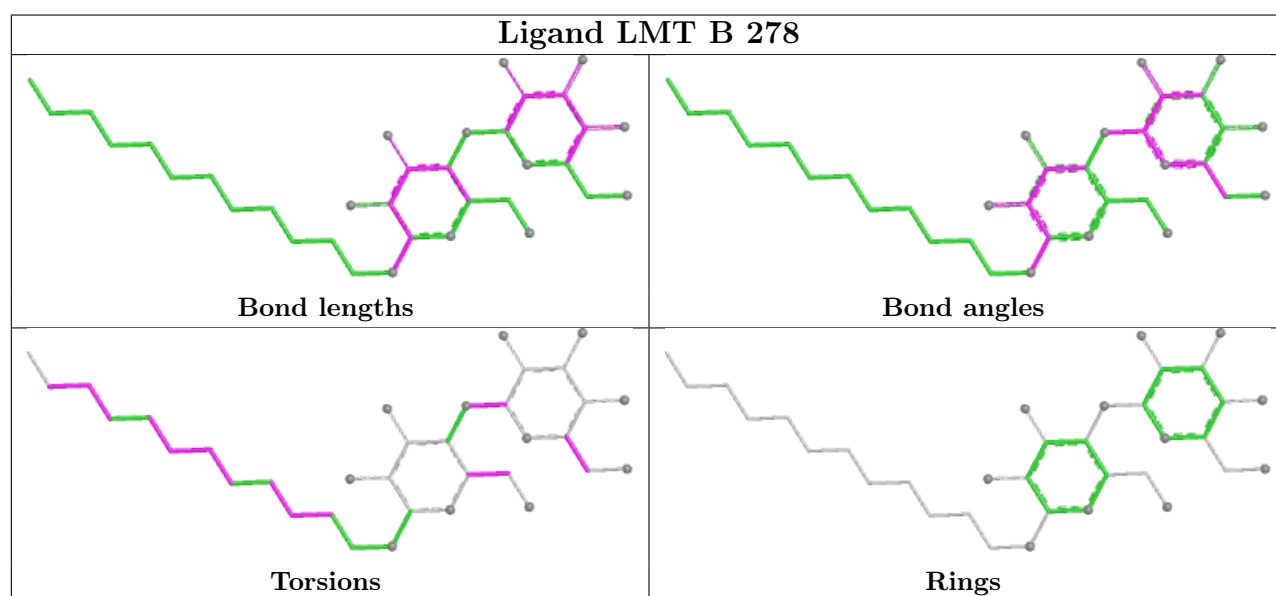
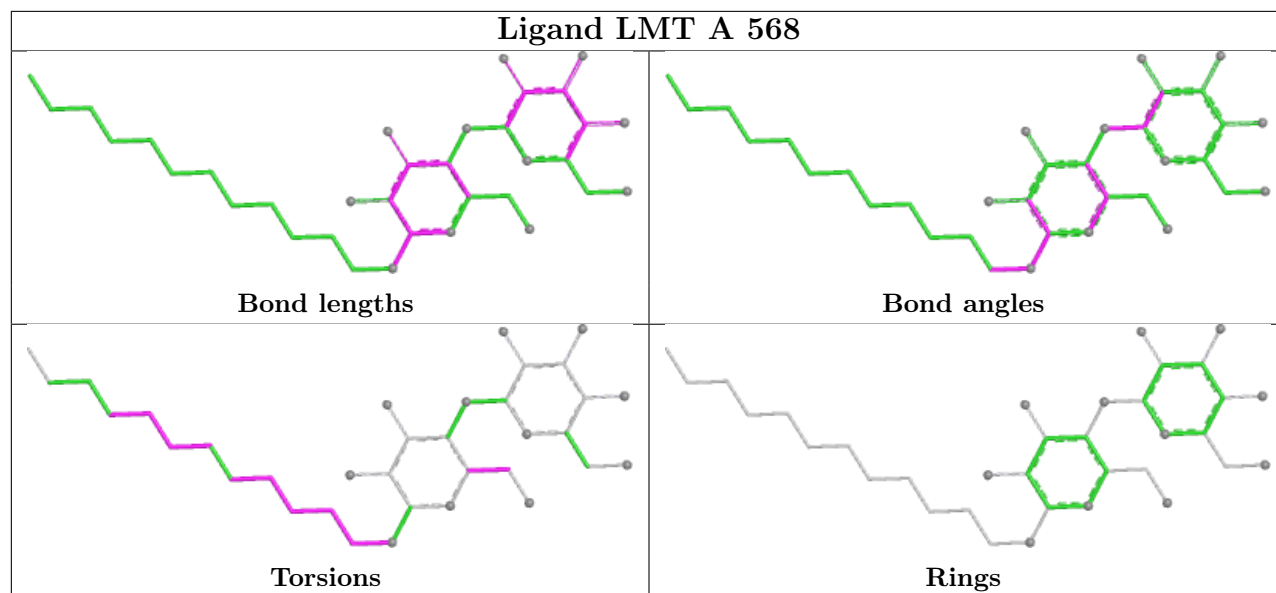
Mol	Chain	Res	Type	Atoms
10	D	121	LMT	C1-C2-C3-C4
10	A	575	LMT	C3-C4-C5-C6
9	B	276	LDA	C5-C6-C7-C8
10	A	570	LMT	O1'-C1-C2-C3
5	A	559	HEA	C27-C19-C20-C21
10	A	575	LMT	C6-C7-C8-C9
5	A	560	HEA	CAD-CBD-CGD-O1D
10	D	121	LMT	C3-C4-C5-C6
9	B	274	LDA	C2-C3-C4-C5
9	A	564	LDA	C2-C3-C4-C5
9	B	272	LDA	C3-C4-C5-C6
10	B	278	LMT	C4-C5-C6-C7
10	A	573	LMT	C5-C6-C7-C8
10	A	571	LMT	C9-C10-C11-C12
5	A	559	HEA	CAD-CBD-CGD-O2D
5	A	560	HEA	CAD-CBD-CGD-O2D
5	A	559	HEA	CAD-CBD-CGD-O1D
10	A	571	LMT	C3-C4-C5-C6
10	A	575	LMT	C1-C2-C3-C4
10	A	575	LMT	O5B-C1B-O1B-C4'
10	A	575	LMT	C11-C10-C9-C8
5	A	560	HEA	CAA-CBA-CGA-O2A
10	B	277[A]	LMT	O5B-C5B-C6B-O6B
10	B	277[B]	LMT	O5B-C5B-C6B-O6B
10	A	570	LMT	C4'-C5'-C6'-O6'
9	B	274	LDA	C1-C2-C3-C4
5	A	559	HEA	CAA-CBA-CGA-O2A
5	A	560	HEA	CAA-CBA-CGA-O1A
5	A	559	HEA	CAA-CBA-CGA-O1A
5	A	559	HEA	C26-C15-C16-C17
9	A	566	LDA	C7-C8-C9-C10
10	B	277[A]	LMT	C5-C6-C7-C8
5	A	559	HEA	C14-C15-C16-C17
10	B	277[B]	LMT	C2-C3-C4-C5
9	B	273	LDA	C6-C7-C8-C9
10	A	570	LMT	O5'-C5'-C6'-O6'
5	A	559	HEA	O11-C11-C3B-C4B
10	A	573	LMT	C4'-C5'-C6'-O6'
9	B	274	LDA	C9-C10-C11-C12

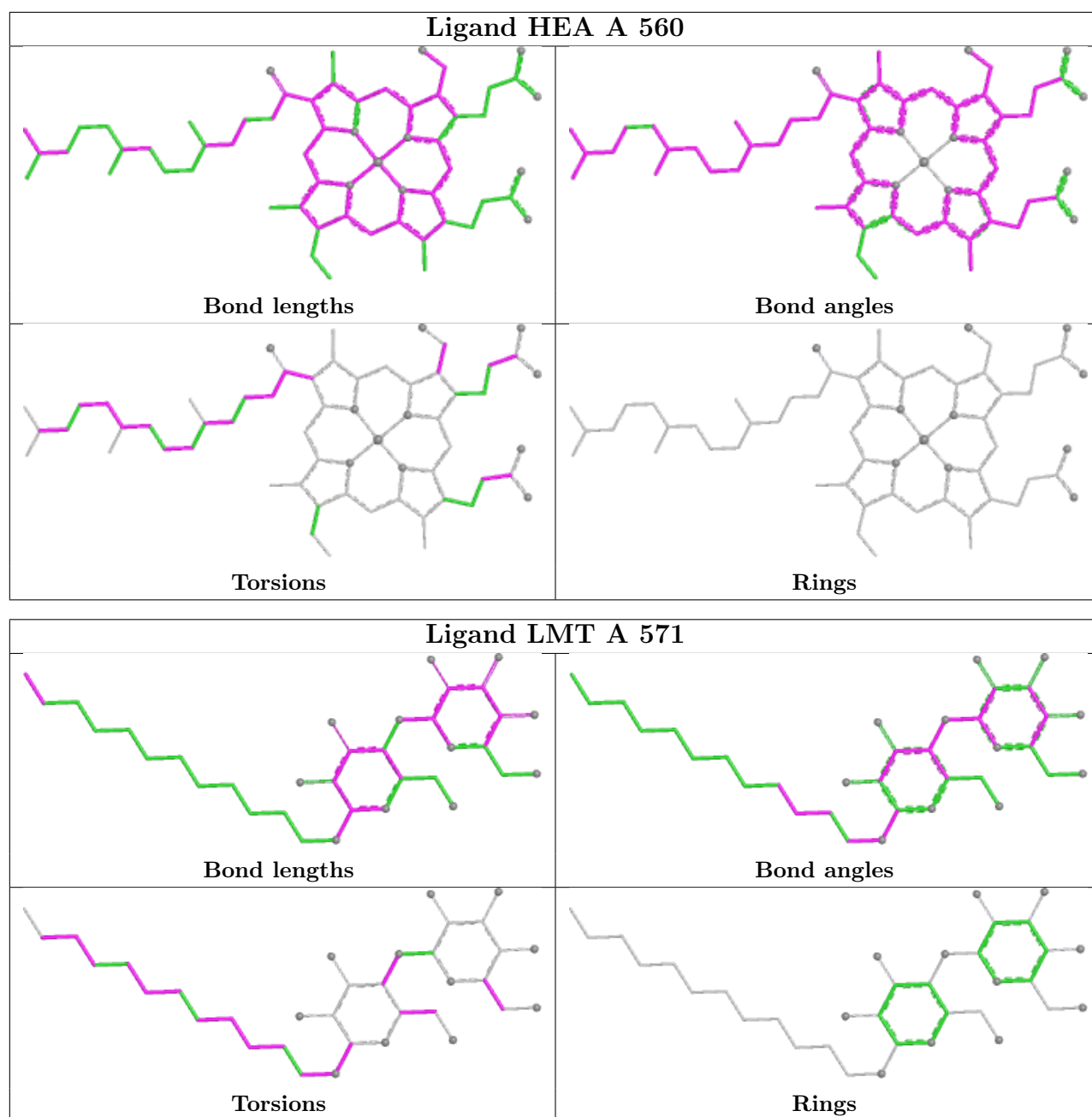
There are no ring outliers.

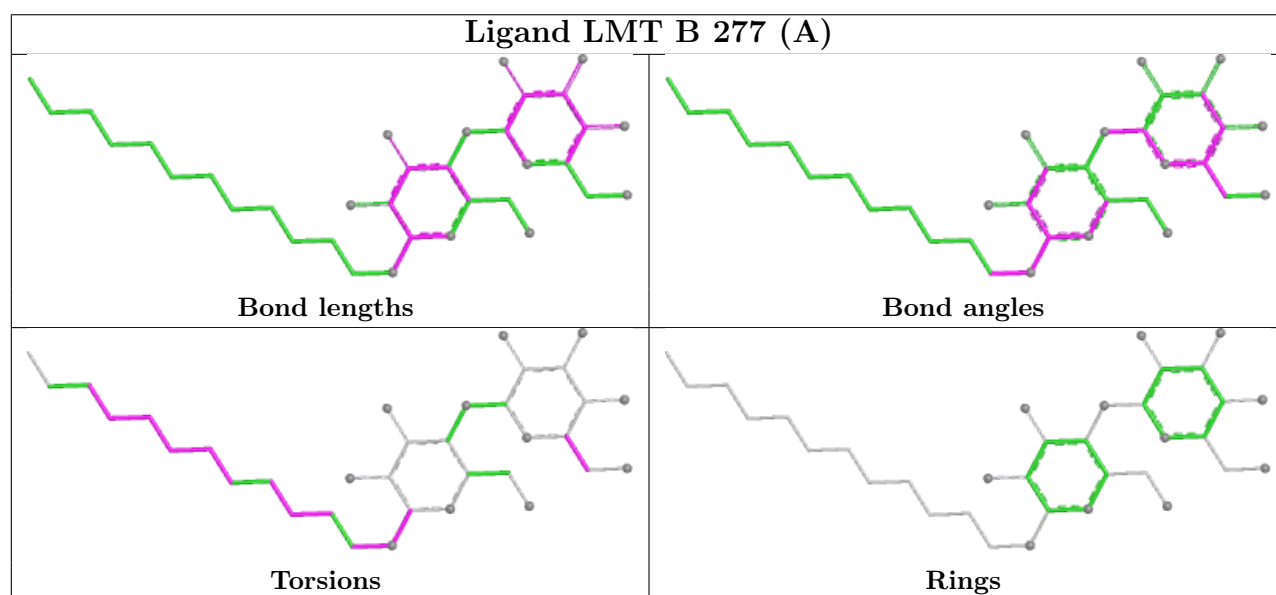
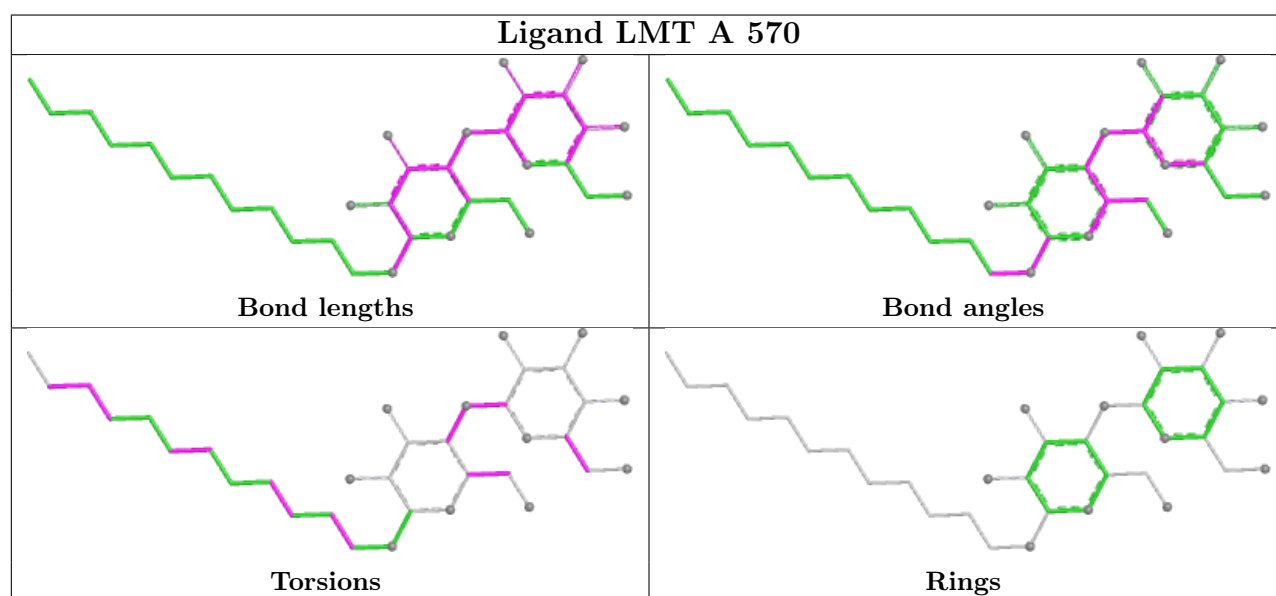
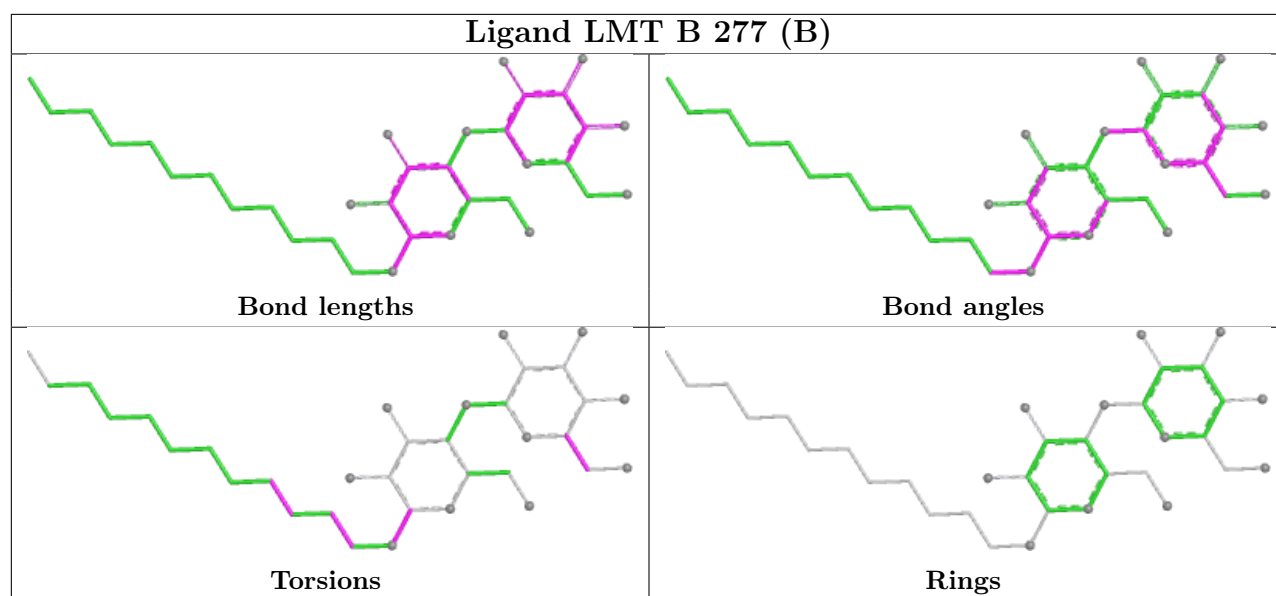
20 monomers are involved in 74 short contacts:

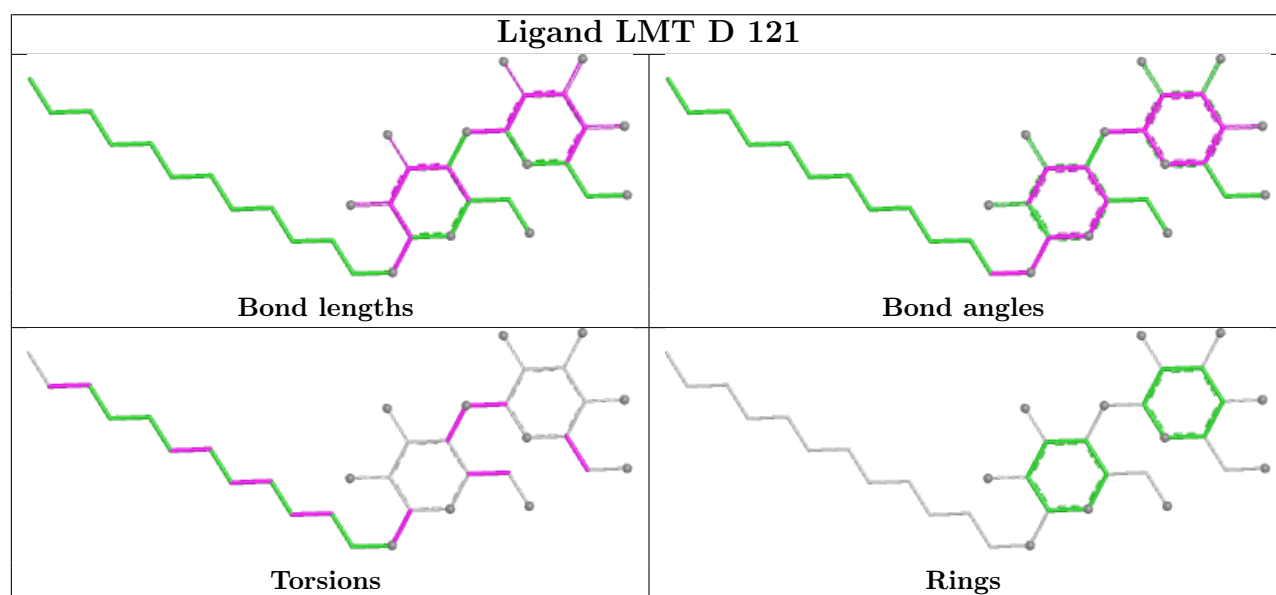
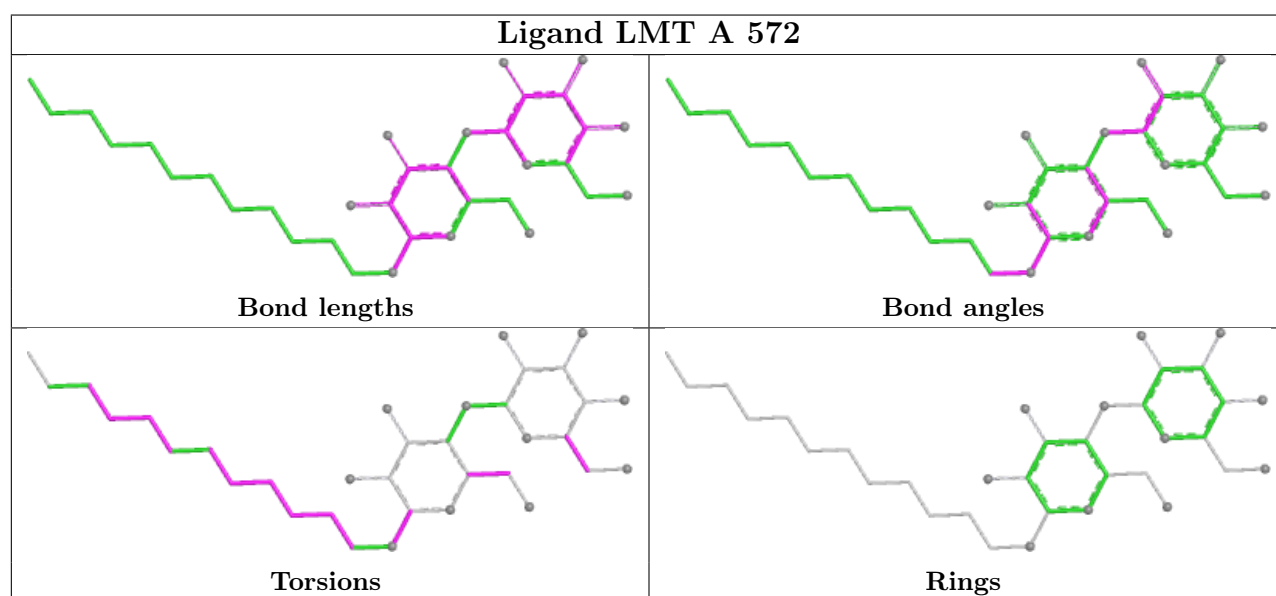
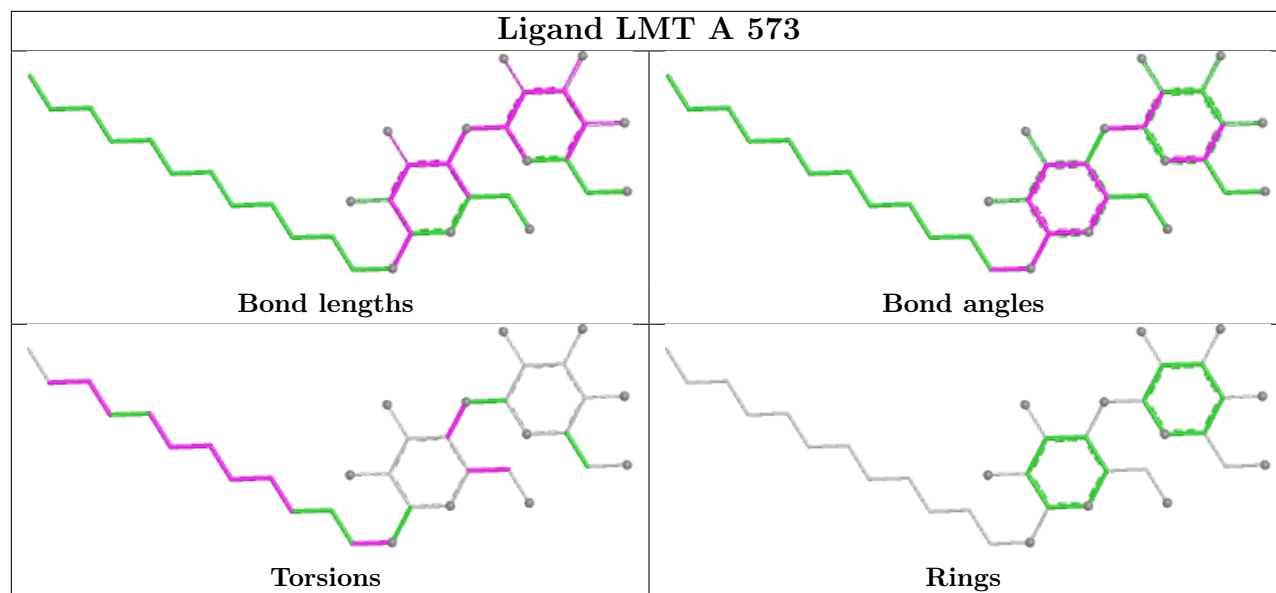
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	568	LMT	2	0
10	B	278	LMT	2	0
9	B	272	LDA	4	0
10	B	279	LMT	6	0
5	A	560	HEA	12	0
10	A	571	LMT	3	0
10	A	570	LMT	3	0
9	A	565	LDA	1	0
9	B	276	LDA	1	0
10	A	572	LMT	3	0
10	D	121	LMT	3	0
9	B	274	LDA	4	0
10	A	569	LMT	2	0
10	A	574	LMT	8	0
9	B	275	LDA	4	0
9	A	564	LDA	1	0
9	A	566	LDA	3	0
10	A	575	LMT	5	0
5	A	559	HEA	9	0
9	B	273	LDA	3	0

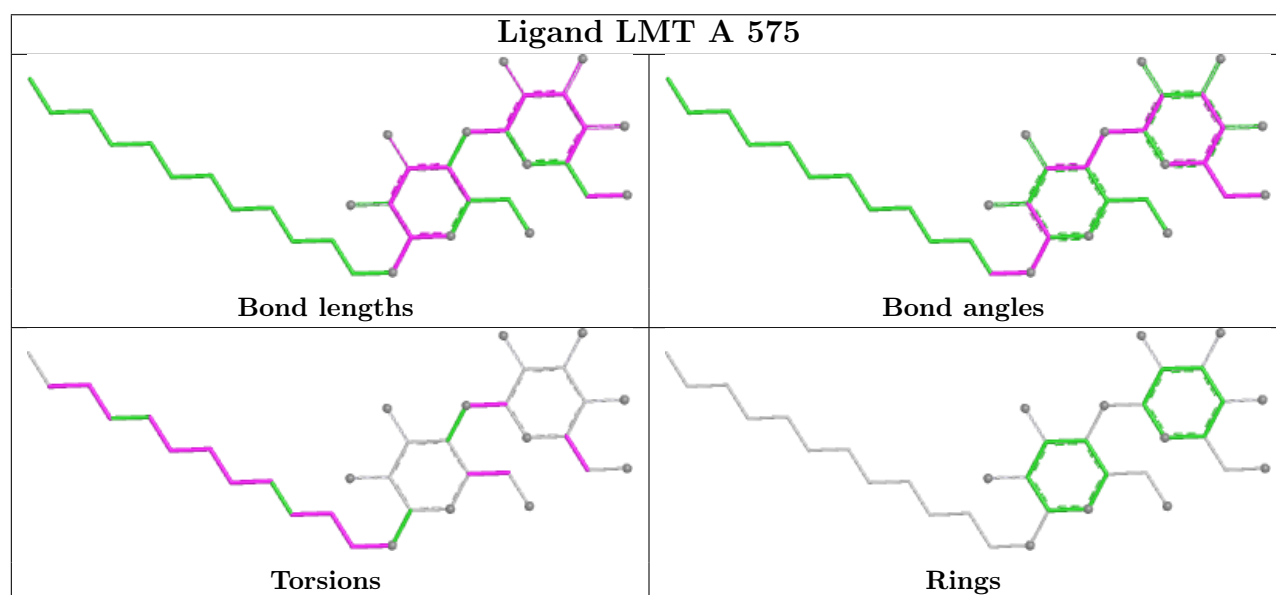
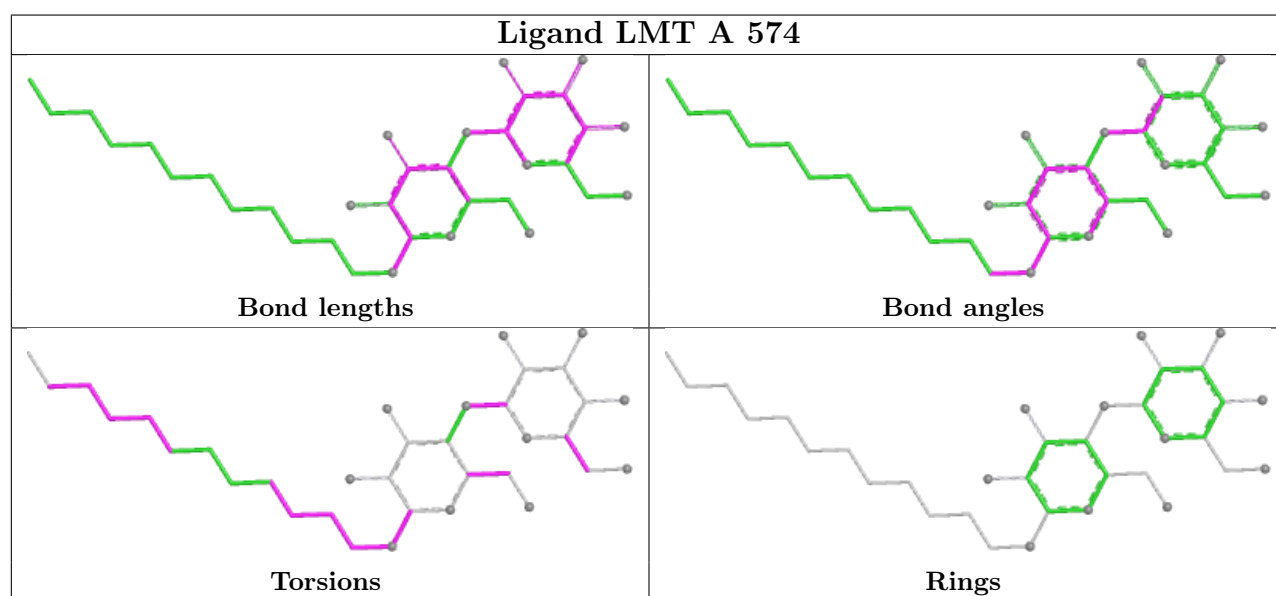
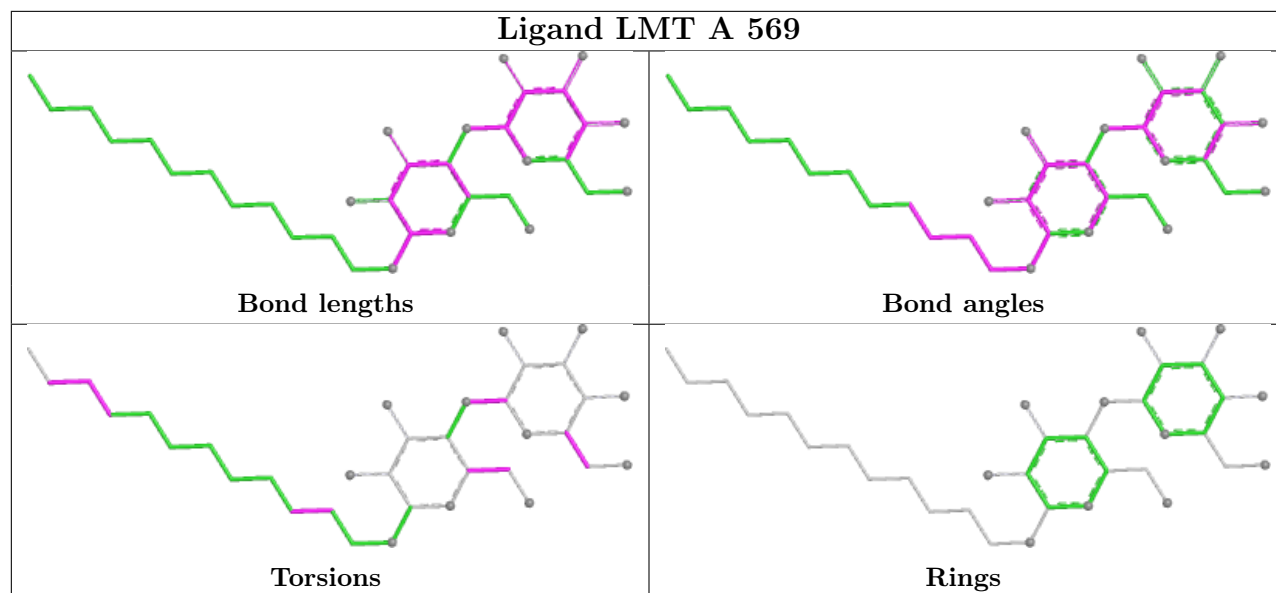
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

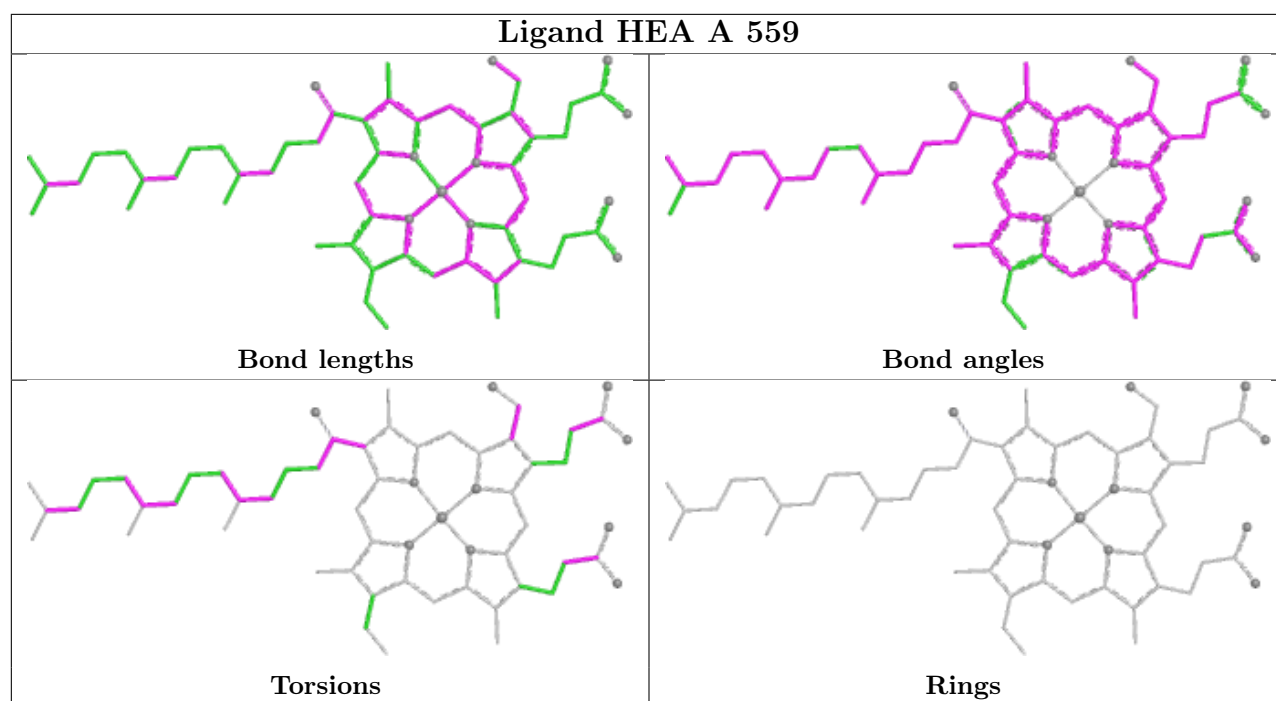












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	118	SER	4.9
1	A	20	THR	4.8
2	B	1	GLN	4.4
1	A	175	ALA	4.1
3	C	119	ALA	3.9
1	A	18	PHE	3.8
1	A	177	TYR	3.8
4	D	109	ARG	3.4
1	A	176	GLY	3.2
1	A	545	THR	3.0
1	A	543	PHE	2.9
3	C	117	SER	2.9
1	A	215[A]	PHE	2.8
1	A	252	GLY	2.8
1	A	158	MET	2.8
1	A	70	ALA	2.7
1	A	19	PHE	2.7
1	A	518	ASN	2.6
1	A	76	ALA	2.5
4	D	1	ASP	2.5
1	A	22	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	129	ARG	2.4
1	A	516	ARG	2.4
1	A	130	LEU	2.4
1	A	17	GLY	2.3
1	A	210	PRO	2.3
1	A	150	LEU	2.1
1	A	546	LEU	2.1
3	C	11	LEU	2.1
2	B	222	ILE	2.1
1	A	251	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LMT	A	575	35/35	0.39	0.28	97,142,149,150	0
10	LMT	A	572	35/35	0.46	0.25	84,112,123,123	0
10	LMT	D	121	35/35	0.53	0.27	93,103,108,110	0
10	LMT	A	571	35/35	0.54	0.27	81,116,145,146	0
10	LMT	A	573	35/35	0.63	0.21	65,102,131,132	0
10	LMT	A	574	35/35	0.63	0.20	64,134,147,148	0
10	LMT	A	569	35/35	0.64	0.23	84,98,111,111	0
9	LDA	B	276	16/16	0.65	0.27	121,128,130,130	0
10	LMT	B	277[A]	35/35	0.71	0.25	67,81,87,88	12
10	LMT	B	277[B]	35/35	0.71	0.25	65,78,87,88	12
10	LMT	A	568	35/35	0.71	0.17	83,103,108,109	0
9	LDA	A	567	16/16	0.72	0.28	96,103,104,105	0
9	LDA	B	274	16/16	0.73	0.24	83,98,111,111	0

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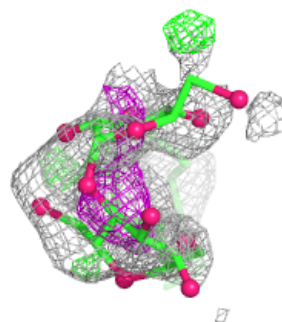
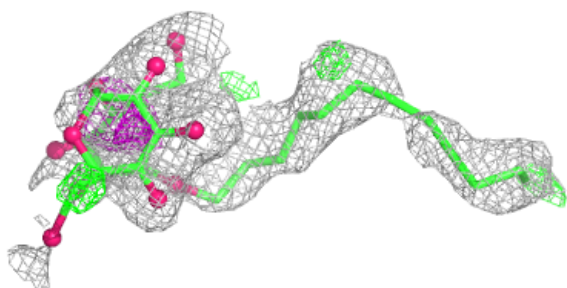
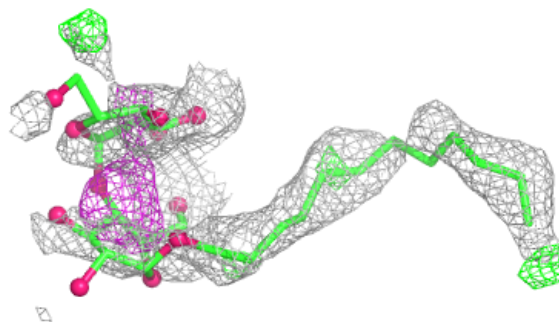
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	LMT	B	279	35/35	0.73	0.18	68,120,136,137	0
9	LDA	A	566	16/16	0.73	0.27	92,97,113,113	0
9	LDA	A	564	16/16	0.74	0.26	68,75,106,109	0
9	LDA	B	275	16/16	0.75	0.19	55,81,113,115	0
10	LMT	B	278	35/35	0.75	0.15	68,86,99,100	0
9	LDA	A	565	16/16	0.76	0.19	72,85,94,95	0
9	LDA	B	273	16/16	0.79	0.24	81,85,98,100	0
9	LDA	B	272	16/16	0.79	0.19	46,67,114,117	0
10	LMT	A	570	35/35	0.81	0.15	69,104,122,125	0
5	HEA	A	559	60/60	0.95	0.13	37,47,51,56	0
5	HEA	A	560	60/60	0.96	0.11	34,52,54,62	0
7	MG	A	562	1/1	0.98	0.11	28,28,28,28	0
8	CA	A	563	1/1	0.98	0.04	53,53,53,53	0
6	CU	B	270	1/1	0.98	0.03	48,48,48,48	0
11	PER	A	576	2/2	0.98	0.10	49,49,49,56	0
6	CU	B	271	1/1	0.99	0.03	50,50,50,50	0
6	CU	A	561	1/1	1.00	0.05	54,54,54,54	0

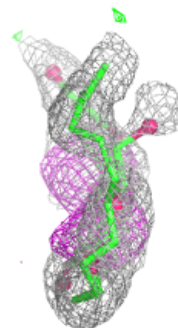
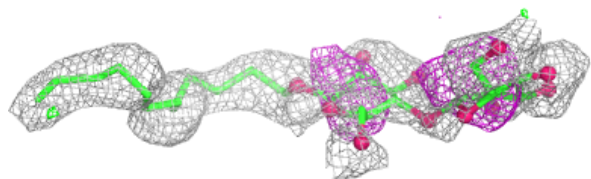
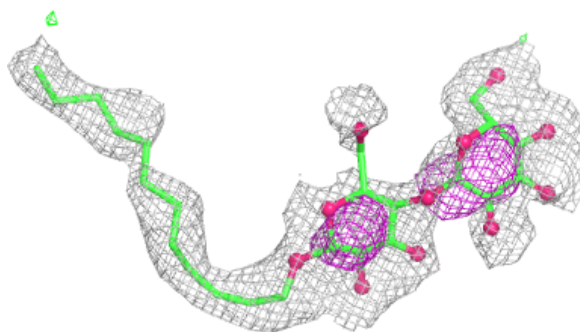
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 575:

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

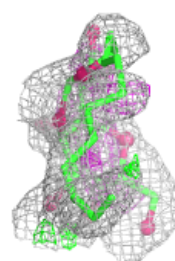
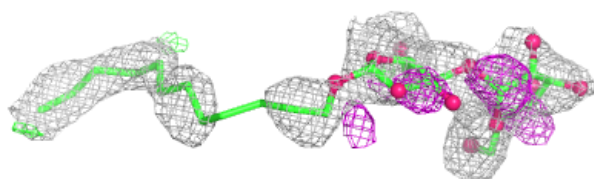
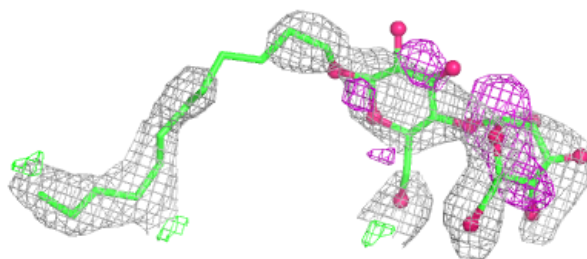
**Electron density around LMT A 572:**

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

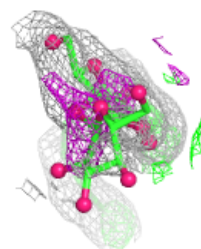
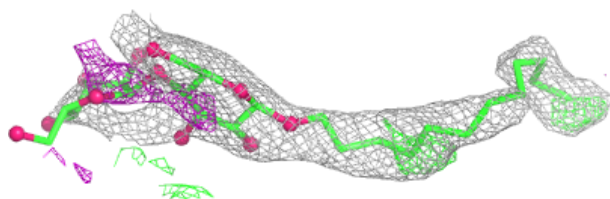
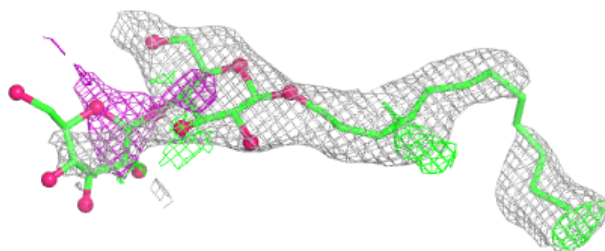


Electron density around LMT D 121:

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

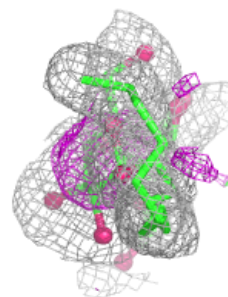
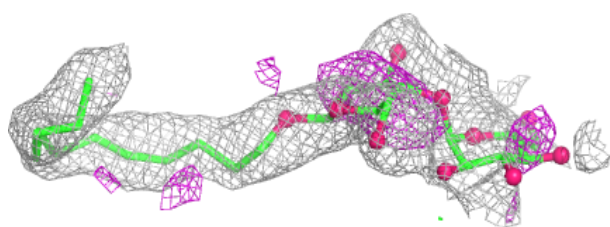
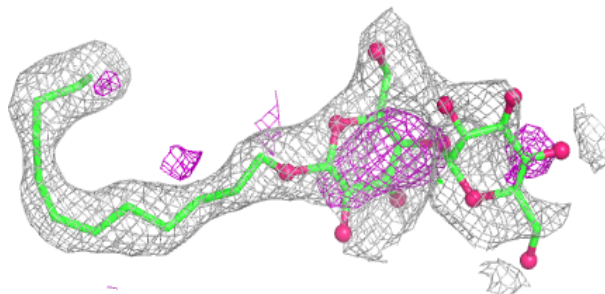
**Electron density around LMT A 571:**

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

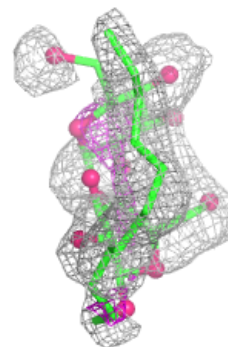
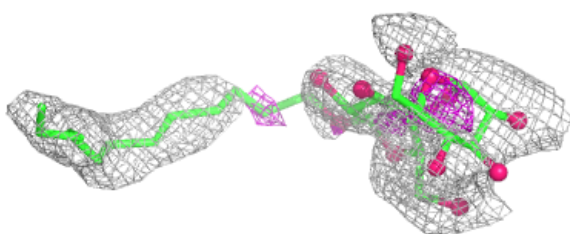
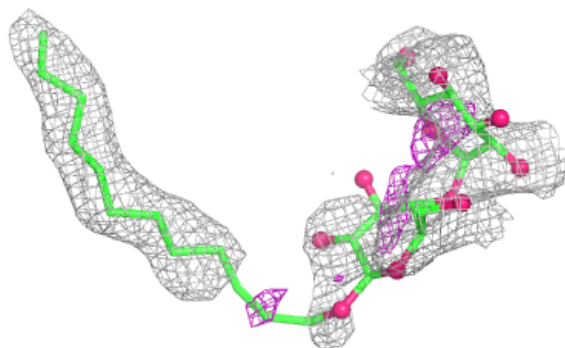


Electron density around LMT A 573:

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

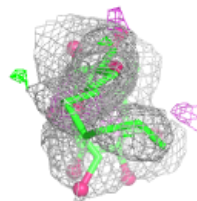
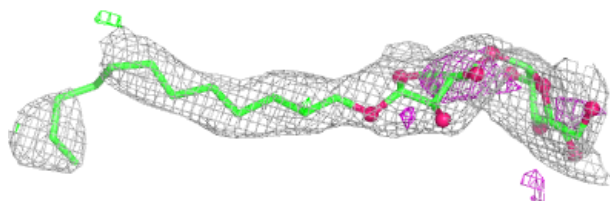
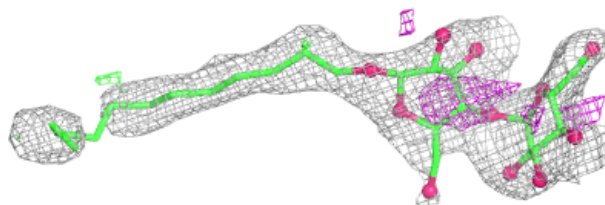
**Electron density around LMT A 574:**

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

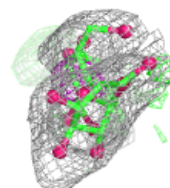
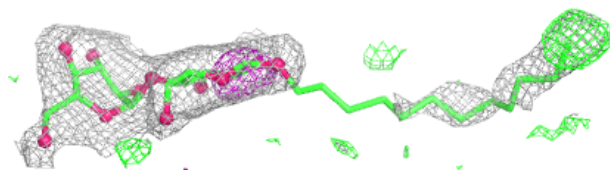
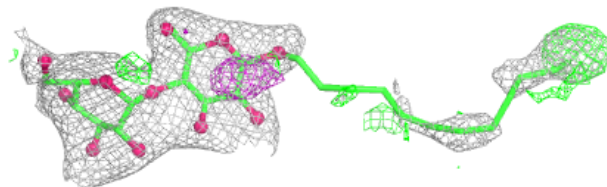


Electron density around LMT A 569:

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

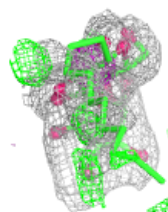
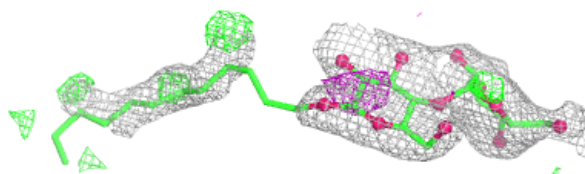
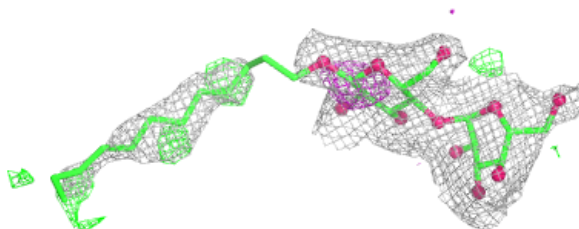
**Electron density around LMT B 277 (A):**

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

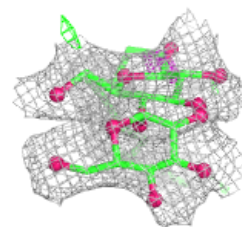
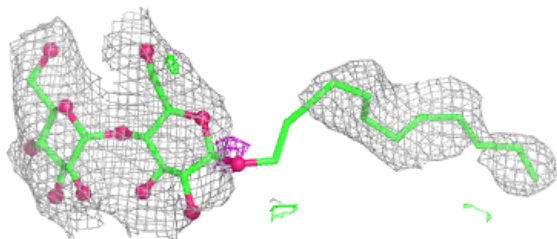
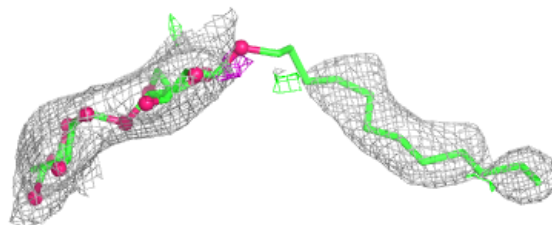


Electron density around LMT B 277 (B):

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

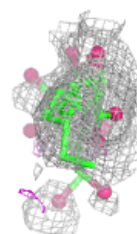
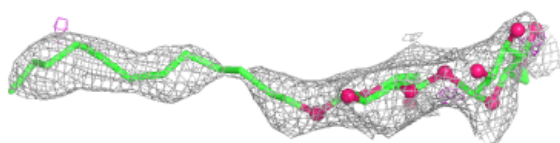
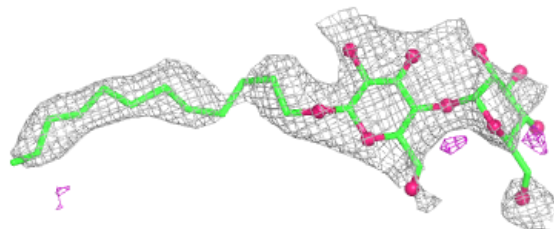
**Electron density around LMT A 568:**

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

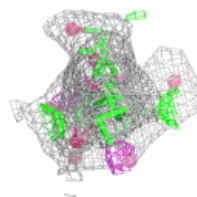
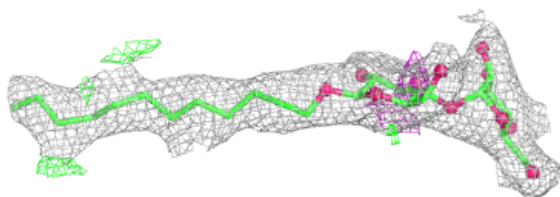
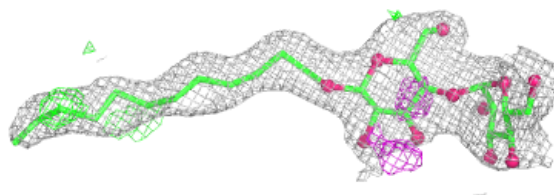


Electron density around LMT B 279:

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

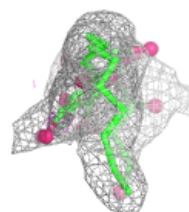
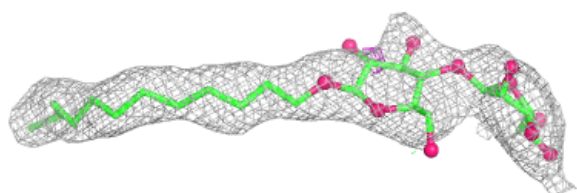
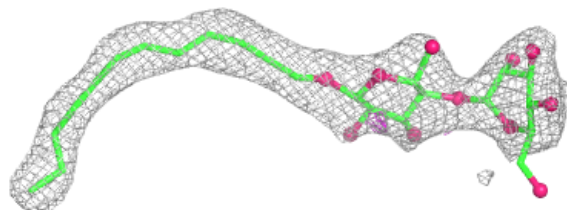
**Electron density around LMT B 278:**

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

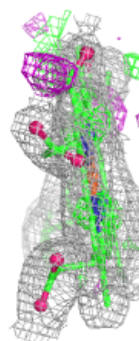
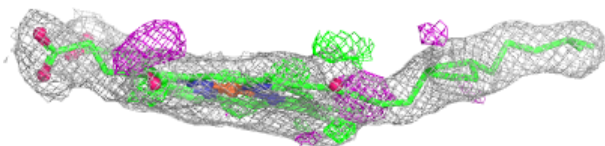
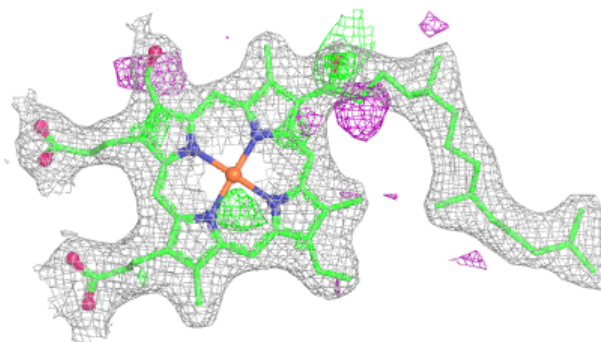


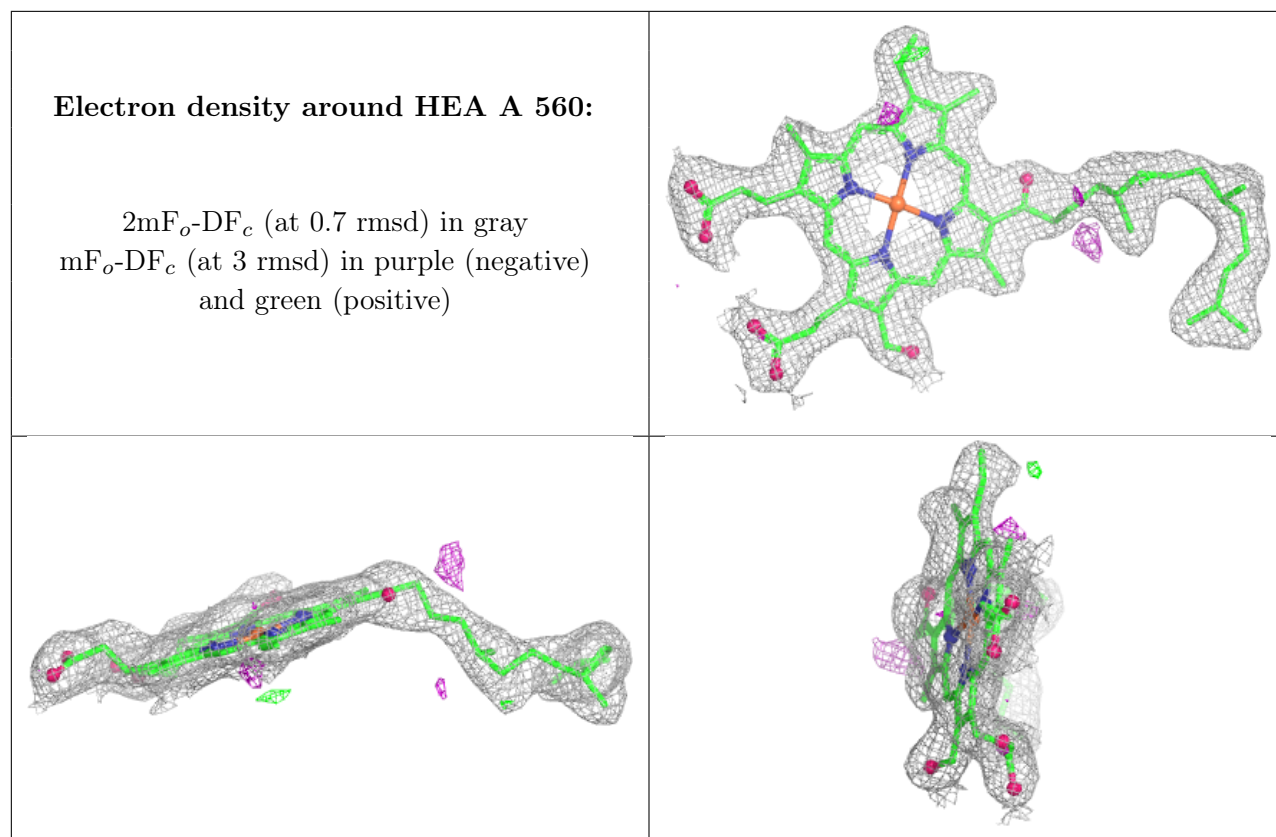
Electron density around LMT A 570:

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

**Electron density around HEA A 559:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.