



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:21 AM UTC

PDB ID : 9GCX / pdb_00009gcx
Title : Crystal structure of bovine Cytochrome bc1 in complex with inhibitor F8
Authors : Pinthong, N.; Hong, W.; O'Neill, P.W.; Antonyuk, S.V.
Deposited on : 2024-08-03
Resolution : 3.52 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

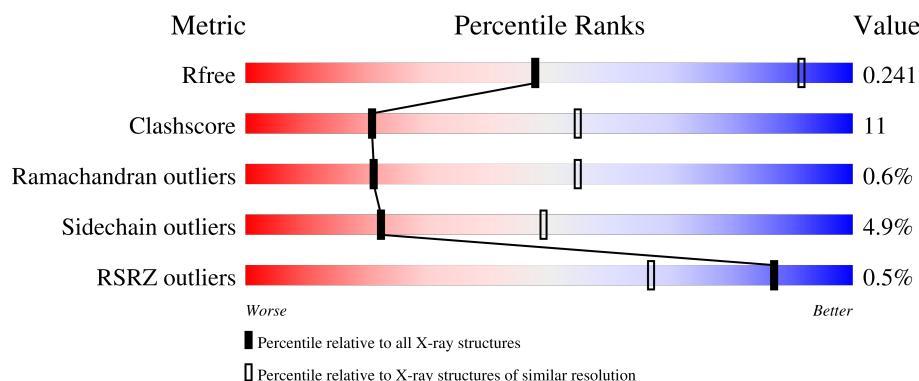
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	480	
2	B	453	
3	C	379	
4	D	325	
5	E	274	

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Mol	Chain	Length	Quality of chain
5	I	274	 5% . . 90%
6	F	111	 70% 15% . . 12%
7	G	82	 46% 30% 13% 10%
8	H	109	 39% 18% . 40%
9	J	64	 59% 23% 5% 12%
10	K	56	 5% 55% 12% . 30%

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
12	CDL	A	502	-	-	X	-
14	A1IKG	C	505	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 16707 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3402	2129	600	653	20			

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	1	0
			3112	1952	552	601	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	2	0
			3008	2019	470	500	19			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1901	1213	326	347	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1505	946	262	290	7			
5	I	27	Total	C	N	O	S	0	0	0
			191	117	38	35	1			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			860	547	155	156	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	405	116	98	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			529	321	96	107	5			

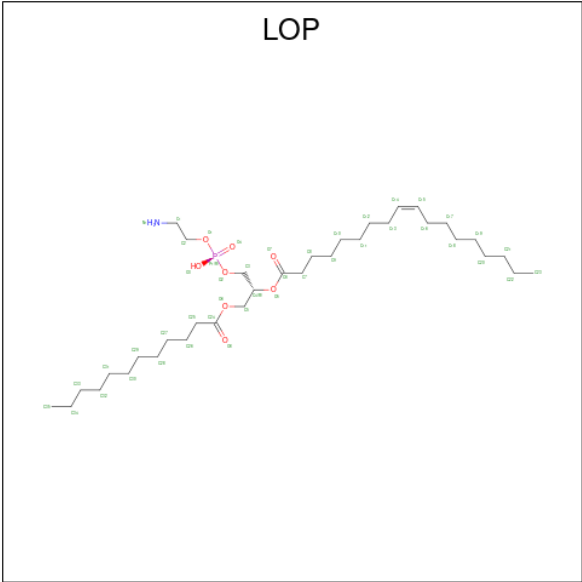
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	56	Total	C	N	O	S	0	0	0
			466	307	81	78				

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

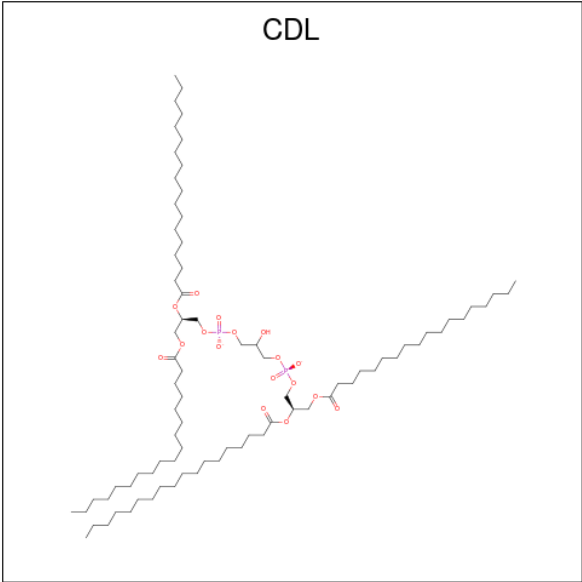
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	39	Total	C	N	O	S	0	0	0
			290	192	49	49				

- Molecule 11 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



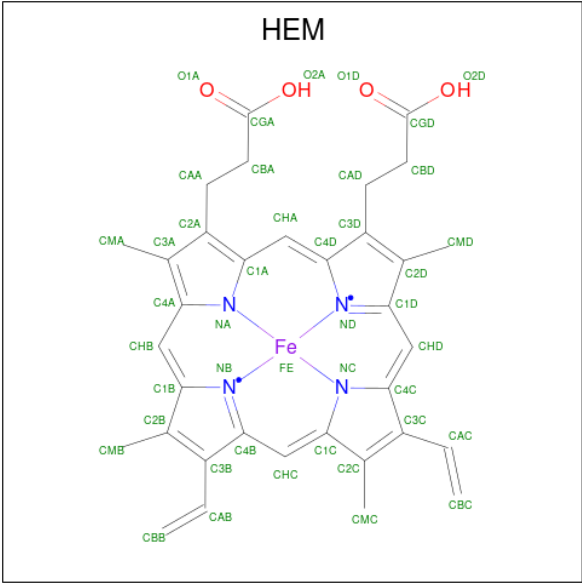
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	E	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



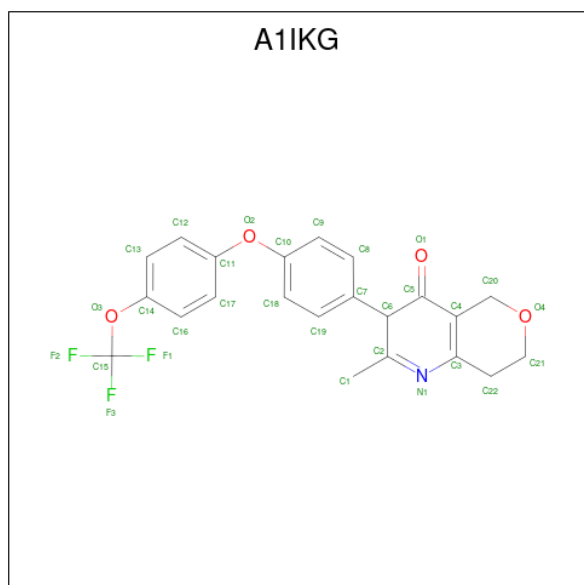
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			84	65	17	2		
12	C	1	Total	C	O	P	0	0
			100	81	17	2		
12	D	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



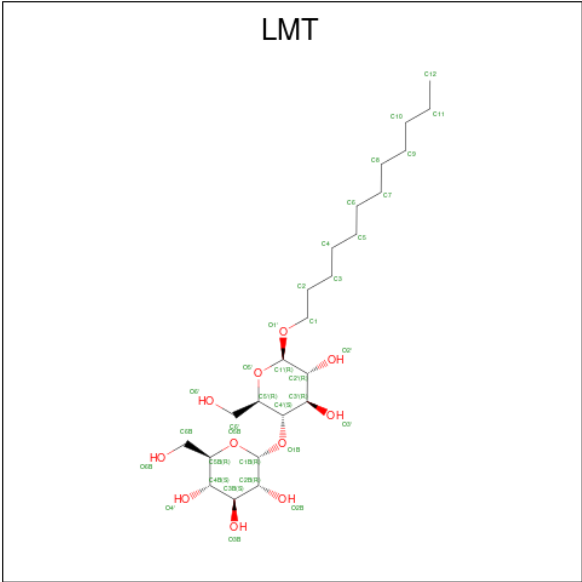
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is 2-methyl-3-(4-(4-(trifluoromethoxy)phenoxy)phenyl)-1,5,7,8-tetrahydro-4H-pyrano[4,3-b]pyridin-4-one (CCD ID: A1IKG) (formula: $C_{22}H_{18}F_3NO_4$).



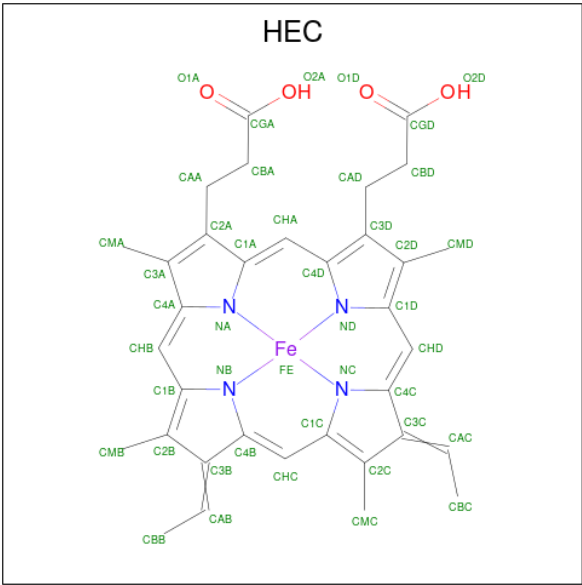
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	F	N	O	0	0
			30	22	3	1	4		

- Molecule 15 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



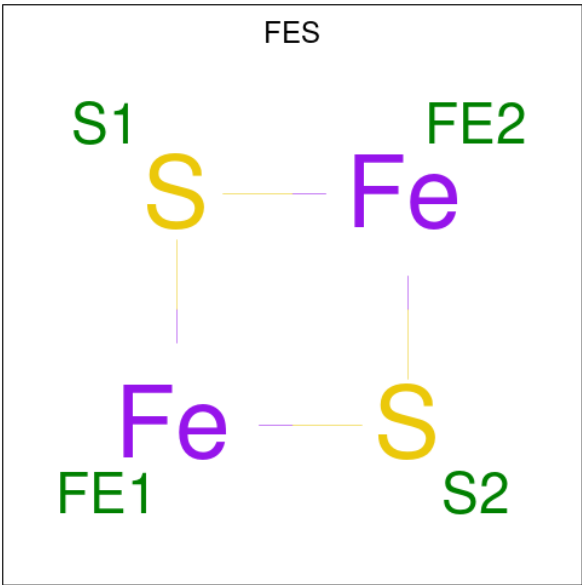
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



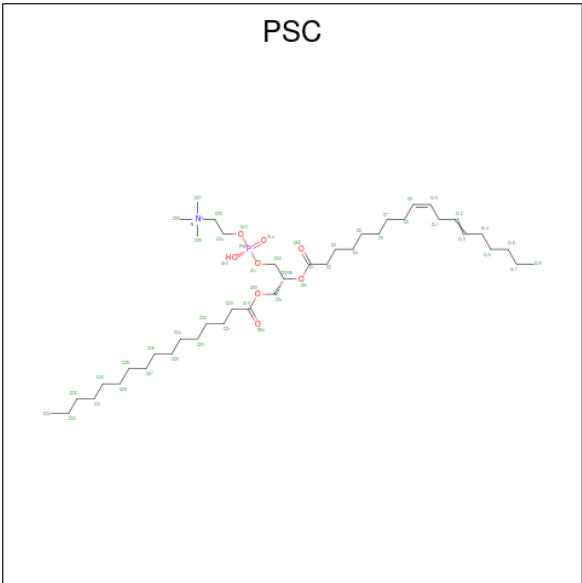
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



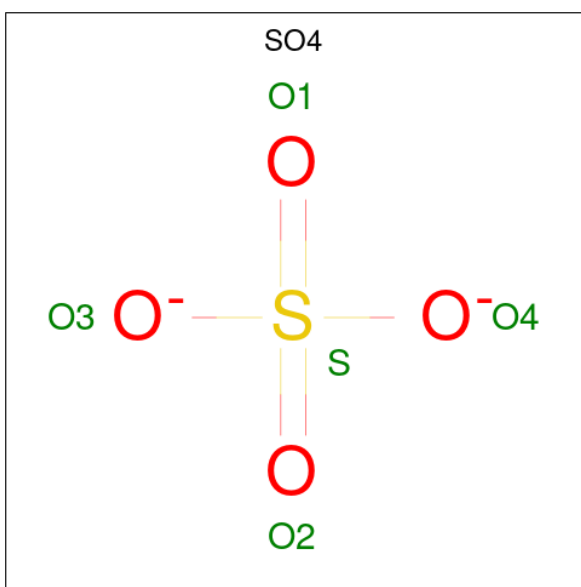
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 18 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		

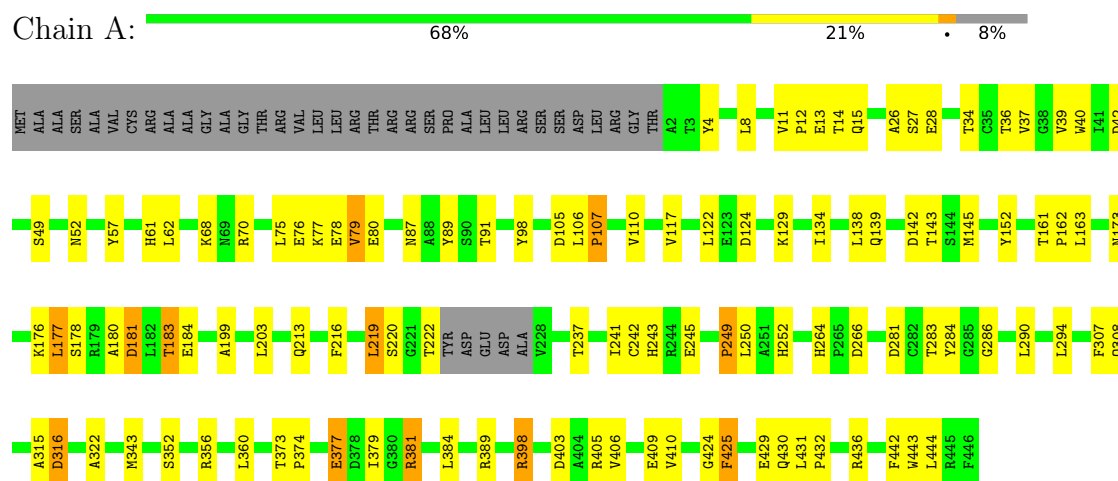
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	3	Total	O	0	0
			3	3		
20	B	1	Total	O	0	0
			1	1		
20	C	4	Total	O	0	0
			4	4		
20	E	1	Total	O	0	0
			1	1		
20	F	1	Total	O	0	0
			1	1		

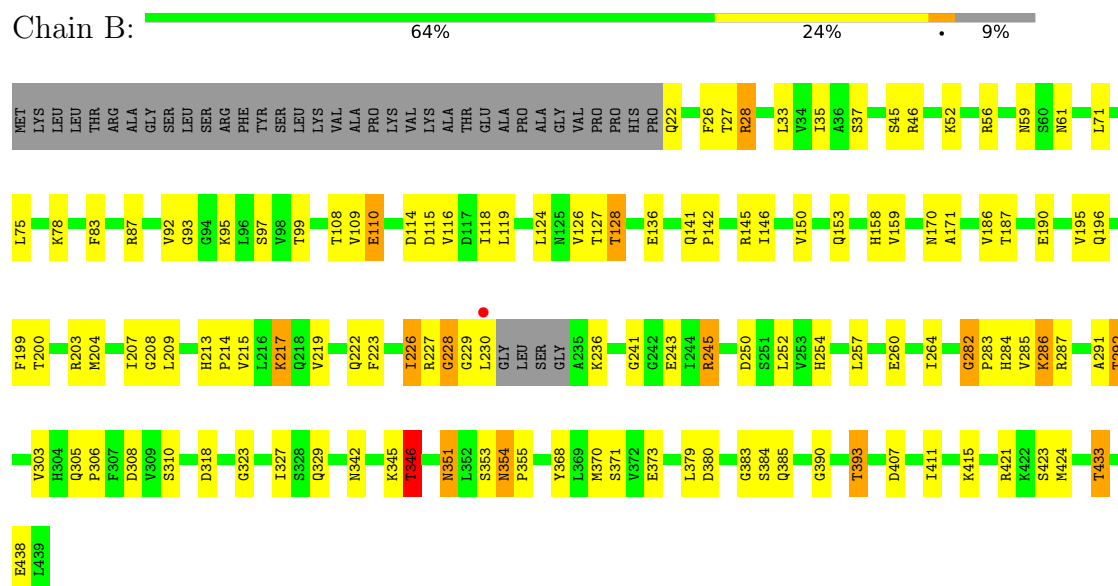
3 Residue-property plots

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 b-c1 complex subunit 1, mitochondrial

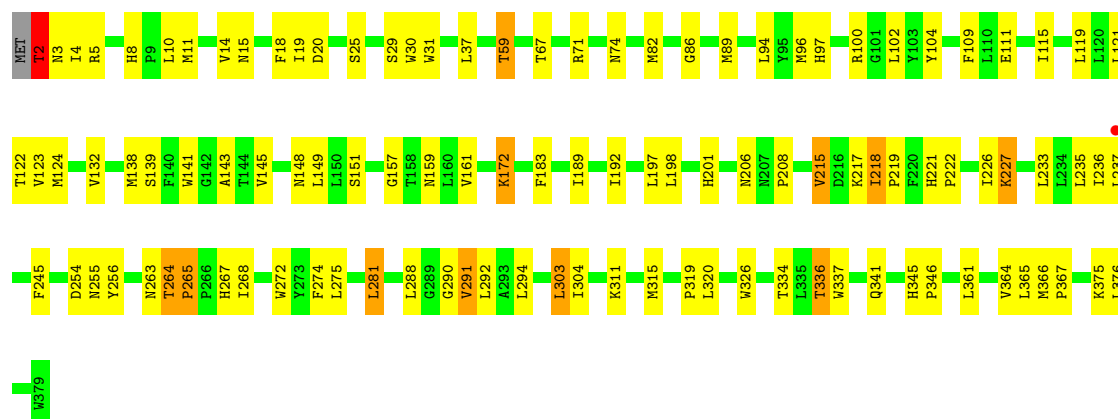


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



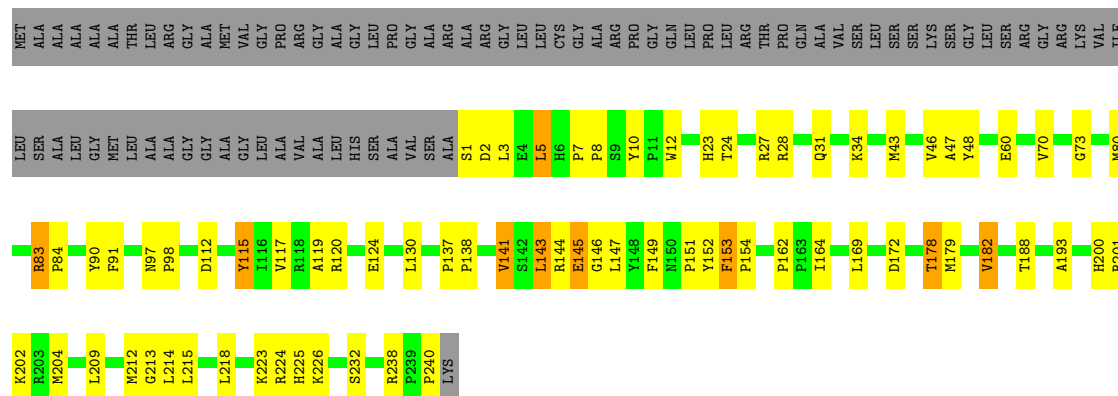
- Molecule 3: Cytochrome b

Chain C: 



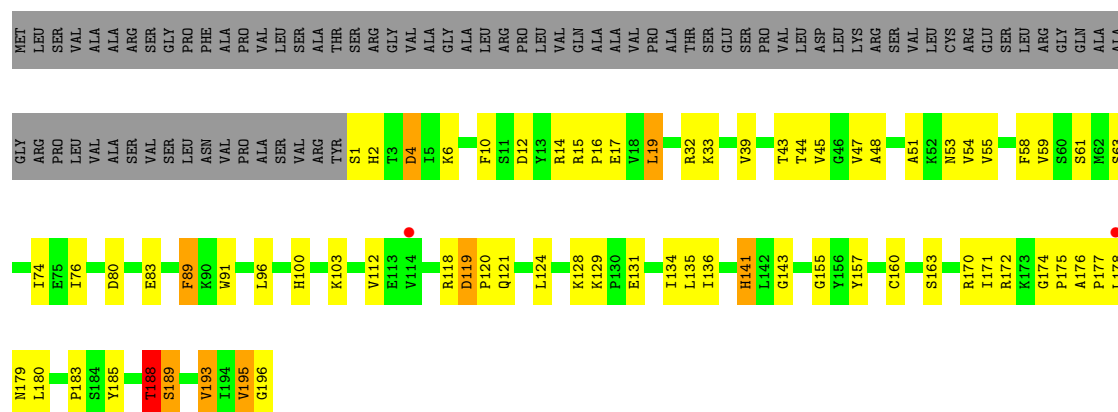
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 



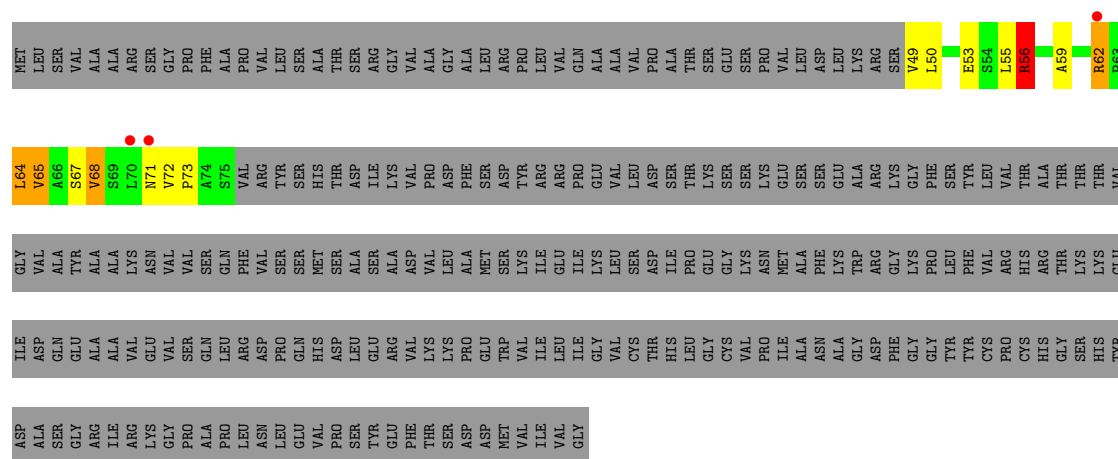
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

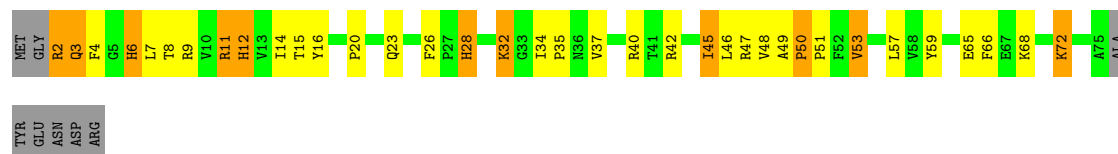
Chain I: 



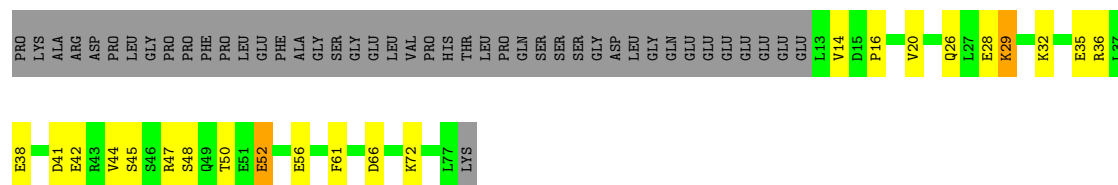
- Molecule 6: Cytochrome b-c1 complex subunit 7



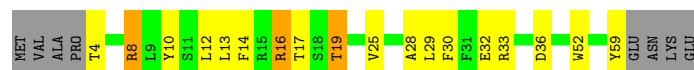
- Molecule 7: Cytochrome b-c1 complex subunit 8



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	210.08Å 210.08Å 344.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.52 30.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.52) 98.9 (30.00-3.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.188 , 0.241 0.188 , 0.241	Depositor DCC
R_{free} test set	2830 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: PSC, FES, A1IKG, CDL, HEC, SO4, LMT, LOP, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/3473	1.40	29/4713 (0.6%)
2	B	0.57	0/3167	1.40	28/4297 (0.7%)
3	C	0.54	0/3111	1.36	23/4259 (0.5%)
4	D	0.55	0/1960	1.35	13/2665 (0.5%)
5	E	0.57	0/1538	1.35	11/2082 (0.5%)
5	I	0.91	0/192	1.83	5/260 (1.9%)
6	F	0.52	0/879	1.51	13/1180 (1.1%)
7	G	0.61	0/641	1.64	13/869 (1.5%)
8	H	0.52	0/534	1.74	13/718 (1.8%)
9	J	0.57	0/478	1.42	5/644 (0.8%)
10	K	0.67	0/300	1.45	1/414 (0.2%)
All	All	0.57	0/16273	1.42	154/22101 (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
1	A	0	2
2	B	0	2
4	D	0	2
5	E	0	1
5	I	0	1
6	F	0	2
7	G	0	3
9	J	0	1
All	All	0	14

There are no bond length outliers.

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	THR	CA-CB-OG1	-11.05	93.03	109.60
6	F	77	LYS	CB-CG-CD	9.34	132.78	111.30
1	A	183	THR	CA-CB-OG1	-8.99	96.12	109.60
2	B	209	LEU	N-CA-CB	-8.94	96.53	110.57
7	G	2	ARG	CA-CB-CG	8.74	131.57	114.10
8	H	52	GLU	CB-CA-C	-8.70	93.53	109.54
3	C	265	PRO	N-CA-CB	8.58	107.68	103.22
1	A	143	THR	CA-CB-OG1	-8.55	96.78	109.60
5	E	157	TYR	N-CA-CB	8.21	123.46	110.65
3	C	74	ASN	CB-CA-C	8.17	122.51	110.26
8	H	29	LYS	N-CA-CB	-8.08	98.24	110.12
1	A	124	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	184	GLU	N-CA-CB	7.95	121.79	109.94
8	H	29	LYS	CB-CA-C	7.90	123.91	110.79
5	E	17	GLU	CB-CG-CD	7.87	125.98	112.60
6	F	63	LYS	N-CA-CB	7.62	121.50	110.06
1	A	13	GLU	N-CA-CB	-7.59	98.37	109.83
1	A	14	THR	CA-CB-OG1	-7.46	98.40	109.60
3	C	97	HIS	CA-CB-CG	7.45	121.25	113.80
6	F	44	LYS	CG-CD-CE	7.34	128.19	111.30
2	B	128	THR	CA-CB-OG1	-7.34	98.59	109.60
4	D	48	TYR	CB-CA-C	7.31	122.93	110.79
2	B	127	THR	CA-CB-OG1	-7.28	98.68	109.60
9	J	8	ARG	CB-CA-C	7.20	122.18	110.88
5	E	44	THR	CA-CB-OG1	-7.18	98.83	109.60
6	F	77	LYS	CG-CD-CE	7.17	127.79	111.30
3	C	201	HIS	CB-CA-C	7.14	125.24	110.31
9	J	8	ARG	CG-CD-NE	7.02	127.45	112.00
4	D	188	THR	CA-CB-OG1	-6.98	99.13	109.60
2	B	52	LYS	CG-CD-CE	6.97	127.32	111.30
8	H	42	GLU	CB-CA-C	-6.89	99.41	110.84
5	I	64	LEU	N-CA-CB	6.86	120.72	110.29
3	C	375	LYS	CB-CG-CD	6.69	126.69	111.30
1	A	184	GLU	CB-CA-C	-6.69	100.11	110.81
1	A	284	TYR	N-CA-CB	6.68	119.92	109.69
2	B	110	GLU	CB-CG-CD	6.68	123.95	112.60
8	H	28	GLU	CA-C-N	6.58	129.09	120.28
8	H	28	GLU	C-N-CA	6.58	129.09	120.28
3	C	336	THR	CA-CB-OG1	-6.52	99.83	109.60
7	G	16	TYR	N-CA-CB	6.51	121.17	110.69
1	A	377	GLU	CB-CG-CD	-6.51	101.53	112.60
7	G	3	GLN	CB-CA-C	-6.51	97.41	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	VAL	N-CA-CB	-6.48	103.51	111.67
1	A	425	PHE	N-CA-CB	-6.46	99.56	111.13
7	G	8	THR	CA-CB-OG1	-6.42	99.97	109.60
3	C	334	THR	CA-CB-OG1	-6.39	100.01	109.60
2	B	108	THR	CA-CB-OG1	-6.38	100.03	109.60
5	I	56	ARG	CB-CG-CD	6.36	125.93	111.30
8	H	29	LYS	CB-CG-CD	6.30	125.79	111.30
2	B	415	LYS	CB-CA-C	6.29	120.76	110.88
1	A	284	TYR	CB-CA-C	-6.26	100.13	109.90
7	G	15	THR	CA-CB-OG1	-6.26	100.21	109.60
3	C	2	THR	CA-CB-OG1	6.24	118.96	109.60
2	B	433	THR	CA-CB-OG1	-6.20	100.30	109.60
6	F	60	PHE	CA-CB-CG	-6.19	107.61	113.80
6	F	105	GLU	CB-CG-CD	6.16	123.07	112.60
3	C	255	ASN	CB-CA-C	6.15	121.32	110.37
2	B	438	GLU	CB-CG-CD	6.13	123.02	112.60
5	E	119	ASP	CB-CA-C	6.11	117.00	110.65
4	D	153	PHE	CB-CA-C	6.04	117.56	108.86
6	F	73	GLN	CB-CA-C	-6.04	98.34	110.30
2	B	227	ARG	N-CA-CB	6.00	118.99	109.51
2	B	26	PHE	CA-CB-CG	5.94	119.74	113.80
5	I	53	GLU	CB-CG-CD	5.93	122.68	112.60
3	C	18	PHE	CA-CB-CG	5.89	119.69	113.80
5	E	6	LYS	N-CA-CB	5.85	121.01	110.83
2	B	126	VAL	N-CA-CB	5.83	121.33	110.77
7	G	50	PRO	N-CA-C	5.83	117.82	110.70
2	B	292	THR	CA-CB-OG1	-5.79	100.91	109.60
5	I	64	LEU	CB-CG-CD1	5.79	128.07	110.70
7	G	68	LYS	CA-CB-CG	5.77	125.63	114.10
3	C	183	PHE	CA-CB-CG	5.72	119.53	113.80
4	D	238	ARG	CB-CA-C	5.72	119.30	111.41
3	C	59	THR	CA-CB-OG1	-5.72	101.02	109.60
2	B	393	THR	CA-CB-OG1	-5.69	101.06	109.60
5	E	89	PHE	CA-CB-CG	5.68	119.48	113.80
4	D	34	LYS	N-CA-CB	5.68	118.56	110.16
8	H	50	THR	OG1-CB-CG2	5.67	120.63	109.30
4	D	7	PRO	N-CA-C	5.63	117.58	110.70
1	A	219	LEU	N-CA-CB	-5.63	101.08	109.69
7	G	72	LYS	CB-CG-CD	5.61	124.21	111.30
8	H	61	PHE	N-CA-CB	5.61	118.15	110.01
4	D	202	LYS	CB-CA-C	5.59	121.41	110.67
1	A	398	ARG	CB-CA-C	-5.58	99.00	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	240	PRO	N-CA-C	5.57	126.03	112.10
9	J	30	PHE	N-CA-CB	5.57	118.91	110.28
9	J	30	PHE	CA-CB-CG	5.55	119.36	113.80
1	A	316	ASP	CA-CB-CG	5.54	118.14	112.60
5	E	4	ASP	CB-CA-C	5.53	119.92	111.02
7	G	2	ARG	CD-NE-CZ	5.52	132.12	124.40
1	A	249	PRO	N-CA-CB	-5.50	97.48	103.25
8	H	26	GLN	CB-CA-C	-5.49	100.47	110.63
1	A	181	ASP	CA-CB-CG	5.46	118.06	112.60
4	D	141	VAL	N-CA-CB	-5.46	104.77	111.00
3	C	267	HIS	CB-CA-C	5.43	118.84	110.14
4	D	145	GLU	N-CA-CB	5.43	118.54	110.29
1	A	183	THR	OG1-CB-CG2	5.43	120.15	109.30
2	B	26	PHE	N-CA-CB	-5.43	101.42	111.13
7	G	16	TYR	CB-CA-C	-5.42	99.62	109.38
2	B	99	THR	CA-CB-OG1	-5.42	101.47	109.60
2	B	260	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	79	VAL	N-CA-CB	5.41	118.31	110.52
1	A	176	LYS	CB-CA-C	5.41	118.15	109.07
3	C	159	ASN	CB-CA-C	-5.40	101.82	110.79
1	A	12	PRO	CA-C-N	5.39	128.36	120.71
1	A	12	PRO	C-N-CA	5.39	128.36	120.71
4	D	60	GLU	CB-CA-C	-5.39	101.85	110.79
7	G	6	HIS	CB-CA-C	5.38	120.30	111.74
8	H	72	LYS	CB-CA-C	5.38	118.44	109.56
6	F	38	HIS	CB-CA-C	5.38	118.85	109.65
5	E	17	GLU	CB-CA-C	5.37	121.66	110.32
3	C	8	HIS	CB-CA-C	5.37	117.71	109.50
6	F	18	LYS	CB-CG-CD	5.37	123.64	111.30
5	E	80	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	39	VAL	N-CA-CB	-5.33	104.75	111.46
1	A	105	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	176	LYS	CG-CD-CE	5.32	123.53	111.30
1	A	68	LYS	CB-CG-CD	5.26	123.39	111.30
6	F	86	ASP	CA-CB-CG	5.25	117.85	112.60
5	I	65	VAL	N-CA-CB	-5.25	105.39	112.10
8	H	52	GLU	N-CA-CB	5.22	117.69	110.17
2	B	217	LYS	CB-CG-CD	5.22	123.31	111.30
4	D	91	PHE	CB-CA-C	-5.21	99.91	110.17
2	B	260	GLU	CB-CA-C	5.19	118.91	109.62
2	B	245	ARG	CD-NE-CZ	-5.17	117.16	124.40
3	C	122	THR	CA-CB-OG1	-5.17	101.84	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	LYS	N-CA-CB	5.16	117.62	109.94
2	B	351	ASN	CB-CA-C	-5.15	103.05	111.50
7	G	32	LYS	CG-CD-CE	5.13	123.11	111.30
4	D	112	ASP	CA-CB-CG	5.13	117.73	112.60
5	E	10	PHE	CA-CB-CG	-5.12	108.68	113.80
7	G	66	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	129	LYS	N-CA-CB	5.12	117.43	110.01
3	C	2	THR	CB-CA-C	5.12	120.36	109.10
8	H	72	LYS	CB-CG-CD	5.11	123.05	111.30
1	A	283	THR	CA-CB-OG1	-5.10	101.95	109.60
6	F	44	LYS	CA-CB-CG	5.09	124.27	114.10
5	E	128	LYS	CB-CA-C	5.08	117.26	109.03
2	B	92	VAL	N-CA-CB	-5.08	105.57	112.22
1	A	213	GLN	CB-CA-C	5.07	119.21	110.79
2	B	286	LYS	CB-CG-CD	5.07	122.95	111.30
1	A	281	ASP	CA-CB-CG	5.06	117.66	112.60
3	C	219	PRO	N-CA-C	-5.06	103.25	111.19
10	K	43	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	370	MET	CG-SD-CE	5.05	112.02	100.90
3	C	311	LYS	CB-CA-C	5.03	119.96	109.95
3	C	109	PHE	CA-CB-CG	5.02	118.82	113.80
3	C	18	PHE	CB-CA-C	-5.02	102.64	110.37
9	J	19	THR	CA-CB-OG1	-5.02	102.07	109.60
2	B	196	GLN	CB-CA-C	5.01	119.89	110.63
3	C	264	THR	CA-C-N	5.00	123.26	119.66
3	C	264	THR	C-N-CA	5.00	123.26	119.66
6	F	38	HIS	CA-CB-CG	5.00	118.80	113.80
6	F	77	LYS	N-CA-CB	5.00	117.56	110.06

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Sidechain
1	A	398	ARG	Sidechain
2	B	282	GLY	Peptide
2	B	421	ARG	Sidechain
4	D	201	ARG	Sidechain
4	D	83	ARG	Sidechain
5	E	172	ARG	Sidechain
6	F	61	ARG	Sidechain
6	F	99	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	G	11	ARG	Sidechain
7	G	2	ARG	Sidechain
7	G	42	ARG	Sidechain
5	I	62	ARG	Sidechain
9	J	16	ARG	Sidechain

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	3402	0	3306	64	0
2	B	3112	0	3078	76	1
3	C	3008	0	3074	76	0
4	D	1901	0	1833	49	0
5	E	1505	0	1478	38	1
5	I	191	0	203	12	0
6	F	860	0	851	4	0
7	G	620	0	619	23	0
8	H	529	0	511	8	0
9	J	466	0	469	19	0
10	K	290	0	260	8	0
11	A	45	0	67	11	0
11	C	135	0	201	9	0
11	E	45	0	67	7	0
11	G	45	0	67	4	0
12	A	84	0	121	21	0
12	C	100	0	156	11	0
12	D	94	0	141	12	0
13	C	86	0	60	8	0
14	C	30	0	0	0	0
15	C	35	0	46	3	0
16	D	43	0	30	2	0
17	E	4	0	0	0	0
18	E	52	0	80	5	0
19	F	5	0	0	0	0
19	G	10	0	0	0	0
20	A	3	0	0	0	0
20	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	4	0	0	0	0
20	E	1	0	0	0	0
20	F	1	0	0	0	0
All	All	16707	0	16718	371	1

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 11.

All (371) 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)
12:A:502:CDL:HA22	12:A:502:CDL:H112	1.50	0.93
12:A:502:CDL:H422	12:A:502:CDL:H341	1.54	0.89
1:A:406:VAL:O	1:A:410:VAL:HG23	1.71	0.89
12:D:502:CDL:H342	12:D:502:CDL:H171	1.52	0.88
12:A:502:CDL:H162	3:C:11:MET:HE1	1.55	0.87
11:A:501:LOP:H352	18:E:203:PSC:H242	1.56	0.87
13:C:502:HEM:HBC2	13:C:502:HEM:HMC2	1.57	0.87
12:C:504:CDL:HA62	12:C:504:CDL:H351	1.57	0.86
1:A:444:LEU:HD11	11:A:501:LOP:H32	1.56	0.85
12:C:504:CDL:HB62	12:C:504:CDL:OB7	1.77	0.83
15:C:508:LMT:H61	15:C:508:LMT:H22	1.61	0.82
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.63	0.80
12:A:502:CDL:H872	12:A:502:CDL:H381	1.66	0.78
12:A:502:CDL:H422	12:A:502:CDL:C34	2.16	0.75
2:B:109:VAL:HB	2:B:119:LEU:HD23	1.69	0.75
3:C:141:TRP:CH2	3:C:264:THR:HG22	2.22	0.74
2:B:200:THR:HG21	2:B:229:GLY:H	1.53	0.73
11:E:202:LOP:H12	9:J:36:ASP:OD2	1.89	0.72
3:C:337:TRP:CH2	7:G:59:TYR:HA	2.24	0.72
2:B:385:GLN:HE22	2:B:393:THR:H	1.37	0.72
4:D:5:LEU:HD23	4:D:151:PRO:HB2	1.70	0.71
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.25	0.71
11:A:501:LOP:H332	12:A:502:CDL:H792	1.72	0.71
3:C:141:TRP:O	3:C:145:VAL:HG23	1.92	0.70
9:J:13:LEU:O	9:J:19:THR:HG22	1.92	0.69
3:C:345:HIS:HB2	15:C:508:LMT:O3'	1.93	0.68
1:A:178:SER:HB3	1:A:181:ASP:OD2	1.94	0.68
12:D:502:CDL:H251	12:D:502:CDL:H591	1.76	0.68
3:C:15:ASN:HA	3:C:19:ILE:HD12	1.76	0.67
3:C:138:MET:HE3	3:C:138:MET:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:GLY:HA2	4:D:80:MET:HE1	1.77	0.66
5:E:58:PHE:CZ	11:E:202:LOP:H352	2.30	0.66
1:A:444:LEU:HA	9:J:17:THR:HG21	1.78	0.66
1:A:360:LEU:HD23	2:B:93:GLY:HA2	1.77	0.66
12:A:502:CDL:H341	12:A:502:CDL:C42	2.26	0.66
5:E:16:PRO:HA	5:E:19:LEU:HD12	1.78	0.66
3:C:320[A]:LEU:CD2	11:G:101:LOP:H251	2.26	0.65
2:B:229:GLY:O	2:B:230:LEU:HG	1.97	0.65
3:C:148:ASN:O	3:C:151:SER:OG	2.08	0.64
4:D:12:TRP:CZ2	4:D:124:GLU:HB3	2.33	0.64
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.63	0.64
3:C:29:SER:OG	12:C:504:CDL:HA61	1.98	0.64
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.79	0.64
2:B:236:LYS:HE2	2:B:318:ASP:HB2	1.79	0.64
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.26	0.64
2:B:327:ILE:HG21	5:I:55:LEU:HD11	1.81	0.63
5:E:1:SER:O	5:E:4:ASP:OD1	2.16	0.63
3:C:294:LEU:HD11	11:C:506:LOP:H12	1.80	0.63
2:B:215:VAL:O	2:B:219:VAL:HG23	1.99	0.63
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.79	0.63
2:B:222:GLN:HB2	2:B:223:PHE:HD1	1.63	0.63
11:A:501:LOP:H52	18:E:203:PSC:H012	1.80	0.62
11:G:101:LOP:H121	11:G:101:LOP:H321	1.81	0.62
7:G:28:HIS:HB2	7:G:32:LYS:HE2	1.82	0.61
3:C:237:LEU:HA	4:D:212:MET:HE3	1.82	0.61
12:D:502:CDL:HA32	7:G:37:VAL:HG23	1.82	0.61
6:F:101:ARG:O	6:F:105:GLU:HG3	2.00	0.61
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.83	0.61
11:A:501:LOP:H302	11:A:501:LOP:O6	2.00	0.61
12:D:502:CDL:H511	12:D:502:CDL:H132	1.83	0.61
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.83	0.60
2:B:241:GLY:HA2	2:B:423:SER:OG	2.00	0.60
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.83	0.60
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.82	0.60
8:H:47:ARG:HD3	8:H:48:SER:H	1.66	0.60
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.84	0.59
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	1.83	0.59
3:C:30:TRP:CH2	12:C:504:CDL:H312	2.37	0.59
8:H:16:PRO:O	8:H:20:VAL:HG23	2.02	0.59
5:I:72:VAL:HG13	5:I:73:PRO:HD2	1.84	0.59
12:A:502:CDL:H812	12:A:502:CDL:H232	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:SER:HA	2:B:208:GLY:O	2.03	0.58
2:B:145:ARG:NH2	20:B:501:HOH:O	2.35	0.58
3:C:361:LEU:HD23	3:C:365:LEU:HD12	1.84	0.58
2:B:380:ASP:O	2:B:384:SER:HB2	2.03	0.58
9:J:29:LEU:CD1	10:K:34:TRP:HB2	2.34	0.58
3:C:5:ARG:NH1	3:C:20:ASP:OD2	2.35	0.58
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.68	0.58
9:J:33:ARG:NH2	10:K:51:LYS:O	2.37	0.57
12:A:502:CDL:H232	12:A:502:CDL:C80	2.35	0.57
5:E:76:ILE:HB	5:E:193:VAL:HG12	1.87	0.57
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.86	0.56
4:D:204:MET:SD	11:E:202:LOP:H51	2.45	0.56
3:C:303:LEU:HD13	11:C:506:LOP:H233	1.86	0.56
4:D:24:THR:HG22	4:D:28:ARG:NH1	2.21	0.56
16:D:501:HEC:CMB	16:D:501:HEC:HBB3	2.36	0.56
3:C:96:MET:HE2	3:C:96:MET:HA	1.88	0.56
16:D:501:HEC:HBB3	16:D:501:HEC:HMB1	1.88	0.56
1:A:138:LEU:HB3	5:E:1:SER:HB2	1.87	0.56
2:B:236:LYS:CE	2:B:318:ASP:HB2	2.37	0.55
3:C:102:LEU:HD21	3:C:304:ILE:HD13	1.88	0.55
12:A:502:CDL:OA7	12:A:502:CDL:C51	2.55	0.55
12:A:502:CDL:H182	3:C:14:VAL:HG11	1.89	0.55
3:C:123:VAL:HG22	3:C:189:ILE:HD13	1.88	0.55
1:A:249:PRO:O	1:A:250:LEU:HD23	2.08	0.54
3:C:96:MET:CE	11:C:503:LOP:H14	2.37	0.54
3:C:132:VAL:HA	3:C:139:SER:HB3	1.89	0.54
5:E:48:ALA:HB1	10:K:34:TRP:CH2	2.42	0.54
2:B:200:THR:O	2:B:204:MET:HG3	2.08	0.54
5:E:129:LYS:HB3	5:E:131:GLU:OE1	2.08	0.54
7:G:72:LYS:HD3	8:H:56:GLU:OE2	2.08	0.54
11:A:501:LOP:H262	4:D:226:LYS:NZ	2.22	0.54
3:C:89:MET:HE2	3:C:235:LEU:HD12	1.89	0.54
1:A:180:ALA:O	1:A:183:THR:HB	2.07	0.54
3:C:25:SER:HA	3:C:218:ILE:HD13	1.89	0.54
13:C:501:HEM:CMB	13:C:501:HEM:HBB2	2.38	0.54
12:C:504:CDL:H752	7:G:48:VAL:HG12	1.90	0.54
5:E:118:ARG:O	5:E:120:PRO:HD3	2.07	0.54
1:A:15:GLN:O	1:A:26:ALA:HA	2.08	0.54
12:A:502:CDL:H342	12:A:502:CDL:H432	1.88	0.53
4:D:164:ILE:HG22	4:D:179:MET:CG	2.39	0.53
5:E:141:HIS:CD2	5:E:175:PRO:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASP:OD1	1:A:406:VAL:HG23	2.08	0.53
2:B:213:HIS:N	2:B:214:PRO:CD	2.72	0.53
3:C:138:MET:HE1	3:C:268:ILE:HA	1.90	0.53
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.08	0.53
9:J:33:ARG:HB2	10:K:48:ILE:HD13	1.91	0.53
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.44	0.53
3:C:320[A]:LEU:HD22	11:G:101:LOP:H251	1.89	0.53
4:D:213:GLY:HA2	12:D:502:CDL:H622	1.91	0.53
11:A:501:LOP:H92	12:A:502:CDL:H212	1.90	0.53
2:B:170:ASN:OD1	2:B:170:ASN:N	2.42	0.52
3:C:71:ARG:NH2	4:D:193:ALA:O	2.35	0.52
13:C:502:HEM:HBC2	13:C:502:HEM:CMC	2.35	0.52
5:E:51:ALA:O	5:E:55:VAL:HG23	2.08	0.52
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.24	0.52
5:E:83:GLU:HG2	5:E:100:HIS:CE1	2.44	0.52
7:G:9:ARG:HG3	7:G:9:ARG:HH11	1.74	0.52
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.10	0.52
12:A:502:CDL:OA7	12:A:502:CDL:CB5	2.57	0.52
3:C:149:LEU:HB3	3:C:291:VAL:CG2	2.40	0.52
12:D:502:CDL:H391	7:G:26:PHE:CE2	2.45	0.52
1:A:28:GLU:OE2	1:A:389:ARG:NH1	2.42	0.51
1:A:430:GLN:O	1:A:430:GLN:HG2	2.09	0.51
2:B:407:ASP:O	2:B:411:ILE:HG13	2.10	0.51
12:C:504:CDL:OB9	12:C:504:CDL:H731	2.10	0.51
3:C:236:ILE:HD13	11:E:202:LOP:H301	1.92	0.51
3:C:272:TRP:HA	3:C:275:LEU:HG	1.91	0.51
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.93	0.51
10:K:51:LYS:O	10:K:52:PHE:C	2.53	0.51
1:A:8:LEU:O	1:A:11:VAL:HG23	2.10	0.51
1:A:436:ARG:NH1	3:C:221:HIS:O	2.42	0.51
2:B:286:LYS:HG2	2:B:287:ARG:HG3	1.93	0.51
3:C:96:MET:HE1	11:C:503:LOP:H132	1.93	0.51
3:C:121:LEU:HB3	11:C:506:LOP:H251	1.92	0.51
5:E:121:GLN:O	5:E:170:ARG:HD3	2.11	0.51
2:B:45:SER:HB2	2:B:116:VAL:CG1	2.41	0.51
2:B:59:ASN:OD1	2:B:61:ASN:HB2	2.11	0.51
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.42	0.50
2:B:200:THR:HB	2:B:228:GLY:HA2	1.93	0.50
1:A:220:SER:OG	1:A:222:THR:HG22	2.11	0.50
11:A:501:LOP:H91	12:A:502:CDL:H732	1.92	0.50
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.94	0.50
4:D:200:HIS:NE2	4:D:204:MET:HE3	2.26	0.50
9:J:29:LEU:HD12	10:K:34:TRP:CD1	2.47	0.50
5:E:43:THR:O	5:E:47:VAL:HG23	2.11	0.50
1:A:145:MET:HE3	1:A:425:PHE:CD2	2.46	0.50
2:B:354:ASN:N	2:B:355:PRO:HD2	2.27	0.50
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.27	0.50
2:B:346:THR:HG23	2:B:351:ASN:HB2	1.93	0.49
1:A:57:TYR:CE2	1:A:61:HIS:HE1	2.29	0.49
1:A:308:GLN:O	1:A:322:ALA:HA	2.12	0.49
3:C:149:LEU:HB3	3:C:291:VAL:HG22	1.93	0.49
11:C:503:LOP:H291	12:C:504:CDL:H162	1.93	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.46	0.49
3:C:111:GLU:O	3:C:115:ILE:HG12	2.12	0.49
1:A:405:ARG:O	1:A:409:GLU:HB2	2.13	0.49
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.95	0.49
13:C:501:HEM:HBC2	13:C:501:HEM:CMC	2.43	0.49
4:D:31:GLN:HE22	4:D:172:ASP:CG	2.21	0.49
18:E:203:PSC:H082	9:J:17:THR:OG1	2.12	0.49
9:J:13:LEU:O	9:J:19:THR:CG2	2.61	0.49
2:B:95:LYS:HE2	2:B:97:SER:HB3	1.95	0.49
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.78	0.49
5:E:118:ARG:HH11	5:E:171:ILE:HG13	1.78	0.49
2:B:308:ASP:OD2	5:I:59:ALA:CB	2.61	0.48
5:E:175:PRO:O	5:E:176:ALA:C	2.56	0.48
1:A:106:LEU:O	1:A:110:VAL:HG23	2.14	0.48
3:C:366:MET:N	3:C:367:PRO:CD	2.76	0.48
3:C:31:TRP:CZ3	3:C:208:PRO:HG3	2.48	0.48
3:C:96:MET:CE	11:C:503:LOP:H132	2.44	0.48
2:B:115:ASP:HB3	2:B:118:ILE:HD12	1.94	0.48
1:A:139:GLN:HB2	5:I:50:LEU:HD12	1.95	0.48
5:E:55:VAL:O	5:E:59:VAL:HG23	2.13	0.48
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.96	0.48
1:A:237:THR:HG21	5:E:14:ARG:NH2	2.28	0.48
3:C:226:ILE:HG12	4:D:223:LYS:HA	1.95	0.48
3:C:141:TRP:CZ3	3:C:264:THR:HG22	2.49	0.48
4:D:164:ILE:HD12	4:D:182:VAL:HG21	1.96	0.48
7:G:45:ILE:HG13	7:G:49:ALA:HB2	1.94	0.48
1:A:27:SER:HA	1:A:199:ALA:O	2.14	0.47
2:B:124:LEU:O	2:B:128:THR:HB	2.14	0.47
4:D:27:ARG:CZ	9:J:59:TYR:CE2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:504:CDL:H581	12:D:502:CDL:H131	1.97	0.47
1:A:436:ARG:NH2	3:C:20:ASP:OD1	2.45	0.47
11:A:501:LOP:O8	3:C:221:HIS:HE1	1.97	0.47
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.95	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.97	0.47
2:B:33:LEU:HD23	2:B:204:MET:HB2	1.95	0.47
1:A:243:HIS:O	1:A:425:PHE:HA	2.15	0.47
3:C:206:ASN:HB3	13:C:502:HEM:O2D	2.15	0.47
3:C:67:THR:HG21	4:D:115:TYR:HE2	1.80	0.46
3:C:157:GLY:O	3:C:161:VAL:HG12	2.14	0.46
3:C:256:TYR:HB2	4:D:119:ALA:HB2	1.96	0.46
4:D:144:ARG:HH21	4:D:147:LEU:HD11	1.80	0.46
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.97	0.46
3:C:275:LEU:HB2	3:C:336:THR:HG23	1.97	0.46
3:C:346:PRO:HG3	7:G:65:GLU:HB3	1.96	0.46
5:E:141:HIS:HA	5:E:177:PRO:HD2	1.97	0.46
1:A:152:TYR:HB3	1:A:241:ILE:HG21	1.96	0.46
2:B:200:THR:OG1	2:B:203:ARG:HG2	2.16	0.46
3:C:319:PRO:HB3	7:G:47:ARG:NH2	2.30	0.46
1:A:75:LEU:O	1:A:79:VAL:HG23	2.15	0.46
2:B:71:LEU:HD23	5:I:68:VAL:HG21	1.98	0.46
5:E:118:ARG:NH1	5:E:171:ILE:HG13	2.31	0.46
1:A:42:ASP:OD2	1:A:384:LEU:HD22	2.16	0.45
12:A:502:CDL:H232	12:A:502:CDL:C81	2.44	0.45
2:B:283:PRO:HG3	5:I:56:ARG:HD2	1.97	0.45
5:E:91:TRP:HZ2	5:E:196:GLY:HA2	1.81	0.45
12:A:502:CDL:H422	12:A:502:CDL:C35	2.45	0.45
1:A:249:PRO:HD2	1:A:250:LEU:H	1.81	0.45
1:A:252:HIS:O	1:A:424:GLY:HA2	2.17	0.45
2:B:150:VAL:O	2:B:153:GLN:HB2	2.17	0.45
5:E:54:VAL:HG22	11:E:202:LOP:H261	1.99	0.45
2:B:368:TYR:O	2:B:371:SER:OG	2.29	0.45
1:A:161:THR:HB	1:A:162:PRO:CD	2.47	0.45
2:B:282:GLY:HA2	5:I:56:ARG:CZ	2.47	0.45
12:D:502:CDL:HB62	12:D:502:CDL:H712	1.64	0.45
5:E:53:ASN:O	5:E:54:VAL:C	2.60	0.45
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.97	0.44
8:H:44:VAL:HG22	8:H:52:GLU:HB2	1.97	0.44
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.52	0.44
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.53	0.44
1:A:286:GLY:HA3	1:A:290:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ILE:H	2:B:226:ILE:HG12	1.52	0.44
3:C:2:THR:HG23	3:C:3:ASN:H	1.82	0.44
3:C:215:VAL:O	6:F:63:LYS:HE2	2.17	0.44
3:C:281:LEU:HD12	3:C:290:GLY:C	2.42	0.44
11:C:506:LOP:H252	11:C:506:LOP:H281	1.56	0.44
12:D:502:CDL:H311	12:D:502:CDL:HA61	1.76	0.44
1:A:173:ASN:O	1:A:177:LEU:HB2	2.18	0.44
12:A:502:CDL:H172	12:A:502:CDL:H201	1.71	0.44
4:D:145:GLU:HG2	4:D:146:GLY:H	1.83	0.44
5:E:96:LEU:HD21	5:E:195:VAL:HG21	2.00	0.44
4:D:145:GLU:HG2	4:D:146:GLY:N	2.32	0.44
1:A:62:LEU:HD13	1:A:122:LEU:HD23	2.00	0.44
1:A:242:CYS:O	7:G:14:ILE:HA	2.18	0.44
12:C:504:CDL:H462	12:C:504:CDL:H652	2.00	0.44
8:H:32:LYS:O	8:H:36:ARG:HG3	2.17	0.44
2:B:282:GLY:HA2	5:I:56:ARG:NH2	2.33	0.43
3:C:102:LEU:CD2	3:C:304:ILE:HD13	2.47	0.43
12:C:504:CDL:H522	7:G:40:ARG:NH2	2.33	0.43
2:B:207:ILE:HG13	2:B:383:GLY:HA2	2.00	0.43
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.86	0.43
5:E:163:SER:HA	5:E:174:GLY:HA3	2.00	0.43
2:B:342:ASN:HA	2:B:345:LYS:HD3	2.00	0.43
2:B:346:THR:CG2	2:B:351:ASN:HB2	2.49	0.43
3:C:245:PHE:CE2	4:D:209:LEU:HD11	2.54	0.43
4:D:204:MET:HE2	11:E:202:LOP:H31	2.00	0.43
12:D:502:CDL:HA32	7:G:37:VAL:CG2	2.46	0.43
5:E:33:LYS:HE3	9:J:10:TYR:CE2	2.53	0.43
9:J:4:THR:O	9:J:8:ARG:HD3	2.18	0.43
2:B:245:ARG:NH2	2:B:433:THR:O	2.45	0.43
2:B:308:ASP:OD1	5:I:56:ARG:HD3	2.18	0.43
3:C:82:MET:O	3:C:86:GLY:N	2.41	0.43
4:D:137:PRO:HB3	4:D:141:VAL:CG1	2.48	0.43
4:D:164:ILE:HD12	4:D:182:VAL:CG2	2.49	0.43
2:B:195:VAL:O	2:B:199:PHE:HB2	2.19	0.43
3:C:198:LEU:O	3:C:198:LEU:HD12	2.18	0.43
4:D:23:HIS:HD2	9:J:52:TRP:HB2	1.83	0.43
12:A:502:CDL:H391	12:A:502:CDL:H861	2.01	0.43
12:C:504:CDL:H462	12:C:504:CDL:H672	2.01	0.43
4:D:138:PRO:HG2	4:D:141:VAL:HG21	2.00	0.43
18:E:203:PSC:H081	9:J:14:PHE:O	2.18	0.43
1:A:429:GLU:O	1:A:429:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PRO:HG3	8:H:66:ASP:HB3	2.01	0.43
2:B:46:ARG:HG2	2:B:379:LEU:HD22	2.00	0.43
11:E:202:LOP:H12	9:J:36:ASP:CG	2.42	0.43
1:A:76:GLU:HB2	2:B:285:VAL:HG21	2.01	0.43
2:B:159:VAL:HG21	2:B:254:HIS:CB	2.49	0.43
1:A:87:ASN:HB3	1:A:98:TYR:CZ	2.54	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.19	0.43
1:A:442:PHE:CD1	1:A:442:PHE:C	2.97	0.42
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.42
5:I:71:ASN:OD1	5:I:71:ASN:N	2.52	0.42
1:A:34:THR:HB	2:B:373:GLU:OE1	2.19	0.42
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.54	0.42
10:K:51:LYS:HD2	10:K:51:LYS:HA	1.75	0.42
11:A:501:LOP:H352	18:E:203:PSC:C24	2.38	0.42
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.01	0.42
2:B:254:HIS:CD2	2:B:327:ILE:HG12	2.54	0.42
2:B:385:GLN:NE2	2:B:393:THR:H	2.12	0.42
3:C:59:THR:HG23	3:C:172:LYS:HA	2.02	0.42
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.02	0.42
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.54	0.42
2:B:141:GLN:NE2	2:B:186:VAL:O	2.52	0.42
2:B:286:LYS:O	2:B:287:ARG:HB2	2.20	0.42
1:A:106:LEU:HD22	1:A:203:LEU:HB3	2.02	0.42
1:A:237:THR:CG2	5:E:14:ARG:HH22	2.32	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.55	0.42
1:A:379:ILE:HG12	1:A:389:ARG:HD2	2.02	0.42
2:B:27:THR:HG23	2:B:213:HIS:NE2	2.35	0.42
2:B:250:ASP:C	2:B:252:LEU:H	2.27	0.42
3:C:132:VAL:HG22	3:C:143:ALA:HB2	2.01	0.42
4:D:1:SER:O	4:D:2:ASP:C	2.63	0.42
6:F:62:ILE:HG22	6:F:66:LEU:HD12	2.00	0.42
2:B:306:PRO:HG2	2:B:329:GLN:NE2	2.35	0.42
3:C:30:TRP:CE2	11:C:503:LOP:H82	2.54	0.42
4:D:215:LEU:HD23	4:D:215:LEU:HA	1.91	0.42
5:E:136:ILE:HD11	5:E:183:PRO:HB3	2.02	0.42
1:A:315:ALA:O	1:A:316:ASP:HB2	2.19	0.41
2:B:146:ILE:O	2:B:150:VAL:HG23	2.20	0.41
3:C:37:LEU:HD22	3:C:94:LEU:HD13	2.01	0.41
3:C:100:ARG:HD2	3:C:100:ARG:C	2.44	0.41
3:C:315:MET:HE1	3:C:366:MET:CE	2.50	0.41
4:D:8:PRO:HG2	4:D:10:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ARG:HB2	4:D:84:PRO:CD	2.50	0.41
4:D:164:ILE:HD13	4:D:164:ILE:HA	1.89	0.41
5:E:188:THR:OG1	5:E:189:SER:N	2.52	0.41
9:J:4:THR:N	9:J:8:ARG:NH1	2.68	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.02	0.41
1:A:36:THR:HG21	1:A:373:THR:HA	2.02	0.41
11:A:501:LOP:H353	12:A:502:CDL:H822	2.03	0.41
3:C:141:TRP:CD1	3:C:265:PRO:HD3	2.56	0.41
13:C:502:HEM:HBB2	13:C:502:HEM:CMB	2.50	0.41
5:E:15:ARG:HD2	5:E:32:ARG:HG2	2.02	0.41
1:A:216:PHE:O	1:A:219:LEU:HB2	2.20	0.41
12:A:502:CDL:H872	12:A:502:CDL:C38	2.44	0.41
2:B:28:ARG:HH22	2:B:390:GLY:HA3	1.85	0.41
3:C:288:LEU:O	3:C:292:LEU:HG	2.21	0.41
3:C:337:TRP:O	3:C:341:GLN:HG2	2.20	0.41
8:H:32:LYS:HA	8:H:32:LYS:HE2	2.03	0.41
1:A:37:VAL:HG23	1:A:199:ALA:HB2	2.03	0.41
2:B:385:GLN:HE22	2:B:393:THR:N	2.10	0.41
4:D:153:PHE:CD1	4:D:154:PRO:HD2	2.56	0.41
12:D:502:CDL:H362	12:D:502:CDL:H392	1.59	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.90	0.41
3:C:345:HIS:CE1	15:C:508:LMT:H31	2.55	0.41
5:E:103:LYS:HD2	5:E:103:LYS:HA	1.88	0.41
9:J:25:VAL:HG22	10:K:30:VAL:HG12	2.03	0.41
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.41
13:C:502:HEM:HBB2	13:C:502:HEM:HMB1	2.03	0.41
2:B:95:LYS:HD3	2:B:110:GLU:OE1	2.21	0.41
3:C:119:LEU:CD2	3:C:192:ILE:HG22	2.51	0.41
3:C:215:VAL:H	3:C:215:VAL:HG13	1.52	0.41
4:D:144:ARG:HE	4:D:147:LEU:HD11	1.86	0.41
4:D:178:THR:O	4:D:182:VAL:HG13	2.21	0.41
8:H:41:ASP:O	8:H:45:SER:CB	2.69	0.41
1:A:70:ARG:HD3	1:A:78:GLU:OE2	2.21	0.41
4:D:138:PRO:HD3	4:D:149:PHE:CZ	2.56	0.41
5:E:76:ILE:HG23	5:E:89:PHE:CZ	2.56	0.41
7:G:53:VAL:O	7:G:57:LEU:HG	2.21	0.41
2:B:310:SER:HB2	5:I:56:ARG:HH22	1.86	0.40
3:C:218:ILE:C	7:G:4:PHE:HZ	2.29	0.40
5:E:33:LYS:HE3	9:J:10:TYR:CZ	2.57	0.40
1:A:77:LYS:HG2	2:B:291:ALA:HB3	2.02	0.40
1:A:343:MET:HB3	1:A:443:TRP:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:SER:HB3	5:I:59:ALA:HB1	2.04	0.40
1:A:49:SER:N	1:A:52:ASN:OD1	2.55	0.40
1:A:373:THR:N	1:A:374:PRO:HD2	2.37	0.40
2:B:207:ILE:HG13	2:B:383:GLY:CA	2.51	0.40
3:C:227:LYS:HE2	12:D:502:CDL:OB9	2.22	0.40
5:E:119:ASP:HB3	5:E:179:ASN:OD1	2.21	0.40
5:E:134:ILE:O	5:E:135:LEU:HD23	2.22	0.40
1:A:264:HIS:HD2	1:A:266:ASP:H	1.68	0.40
1:A:356:ARG:HH11	1:A:356:ARG:HD3	1.70	0.40
3:C:320[A]:LEU:HD22	11:G:101:LOP:H271	2.03	0.40
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.40
2:B:353:SER:HB2	2:B:355:PRO:HD2	2.03	0.40
7:G:11:ARG:O	7:G:12:HIS:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLN:NE2	5:E:112:VAL:O[5_555]	1.67	0.53

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	436/480 (91%)	423 (97%)	13 (3%)	0	100	100
2	B	411/453 (91%)	383 (93%)	26 (6%)	2 (0%)	24	58
3	C	378/379 (100%)	362 (96%)	16 (4%)	0	100	100
4	D	238/325 (73%)	227 (95%)	9 (4%)	2 (1%)	16	50
5	E	194/274 (71%)	174 (90%)	15 (8%)	5 (3%)	4	27
5	I	25/274 (9%)	21 (84%)	4 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	96/111 (86%)	94 (98%)	2 (2%)	0	100	100
7	G	72/82 (88%)	66 (92%)	5 (7%)	1 (1%)	9	38
8	H	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
9	J	54/64 (84%)	54 (100%)	0	0	100	100
10	K	35/56 (62%)	28 (80%)	5 (14%)	2 (6%)	1	13
All	All	2002/2607 (77%)	1893 (95%)	97 (5%)	12 (1%)	21	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	228	GLY
5	E	141	HIS
5	E	143	GLY
5	E	155	GLY
10	K	12	GLN
10	K	14	ALA
2	B	158	HIS
5	E	160	CYS
4	D	5	LEU
4	D	162	PRO
5	E	188	THR
7	G	12	HIS

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	364/394 (92%)	356 (98%)	8 (2%)	45	66
2	B	324/355 (91%)	316 (98%)	8 (2%)	42	64
3	C	327/327 (100%)	311 (95%)	16 (5%)	22	49
4	D	203/257 (79%)	193 (95%)	10 (5%)	22	49
5	E	165/228 (72%)	152 (92%)	13 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	21/228 (9%)	14 (67%)	7 (33%)	0	2
6	F	90/99 (91%)	83 (92%)	7 (8%)	11	37
7	G	65/72 (90%)	59 (91%)	6 (9%)	8	32
8	H	62/99 (63%)	58 (94%)	4 (6%)	15	42
9	J	47/54 (87%)	44 (94%)	3 (6%)	16	43
10	K	25/46 (54%)	24 (96%)	1 (4%)	28	54
All	All	1693/2159 (78%)	1610 (95%)	83 (5%)	22	49

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

Mol	Chain	Res	Type
1	A	89	TYR
1	A	91	THR
1	A	107	PRO
1	A	117	VAL
1	A	177	LEU
1	A	245	GLU
1	A	352	SER
1	A	381	ARG
2	B	22	GLN
2	B	28	ARG
2	B	78	LYS
2	B	226	ILE
2	B	264	ILE
2	B	292	THR
2	B	346	THR
2	B	354	ASN
3	C	2	THR
3	C	4	ILE
3	C	10	LEU
3	C	172	LYS
3	C	215	VAL
3	C	218	ILE
3	C	222	PRO
3	C	227	LYS
3	C	233	LEU
3	C	254	ASP
3	C	263	ASN
3	C	281	LEU
3	C	291	VAL

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Mol	Chain	Res	Type
3	C	303	LEU
3	C	364	VAL
3	C	376	LEU
4	D	3	LEU
4	D	70	VAL
4	D	115	TYR
4	D	117	VAL
4	D	130	LEU
4	D	143	LEU
4	D	169	LEU
4	D	178	THR
4	D	182	VAL
4	D	214	LEU
5	E	12	ASP
5	E	19	LEU
5	E	61	SER
5	E	63	SER
5	E	74	ILE
5	E	124	LEU
5	E	178	LEU
5	E	180	LEU
5	E	185	TYR
5	E	188	THR
5	E	189	SER
5	E	193	VAL
5	E	195	VAL
6	F	13	LEU
6	F	38	HIS
6	F	59	VAL
6	F	63	LYS
6	F	84	GLU
6	F	95	LYS
6	F	106	GLU
7	G	3	GLN
7	G	6	HIS
7	G	28	HIS
7	G	45	ILE
7	G	46	LEU
7	G	53	VAL
8	H	14	VAL
8	H	29	LYS
8	H	35	GLU

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Mol	Chain	Res	Type
8	H	38	GLU
5	I	49	VAL
5	I	56	ARG
5	I	62	ARG
5	I	64	LEU
5	I	65	VAL
5	I	67	SER
5	I	68	VAL
9	J	12	LEU
9	J	16	ARG
9	J	32	GLU
10	K	48	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	61	HIS
1	A	126	GLN
1	A	136	GLN
1	A	159	GLN
1	A	215	HIS
1	A	264	HIS
1	A	301	ASN
1	A	308	GLN
2	B	104	ASN
2	B	158	HIS
2	B	270	ASN
2	B	277	HIS
2	B	329	GLN
2	B	351	ASN
2	B	385	GLN
3	C	54	HIS
3	C	68	HIS
3	C	85	ASN
3	C	201	HIS
3	C	267	HIS
3	C	341	GLN
4	D	23	HIS
4	D	31	GLN
4	D	181	GLN
4	D	198	HIS

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Mol	Chain	Res	Type
4	D	225	HIS
5	E	57	GLN
5	E	164	HIS
7	G	23	GLN
7	G	28	HIS
10	K	49	ASN

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 ⓘ

19 ligands are modelled in this entry.

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	$\# Z > 2$
15	LMT	C	508	-	36,36,36	0.52	0	47,47,47	0.85	2 (4%)
11	LOP	C	503	-	44,44,44	0.58	0	47,49,49	0.96	3 (6%)
18	PSC	E	203	-	51,51,51	0.58	0	57,59,59	1.29	4 (7%)
16	HEC	D	501	4	46,50,50	2.57	25 (54%)	58,82,82	2.87	27 (46%)
14	A1IKG	C	505	-	32,33,33	1.79	6 (18%)	40,48,48	1.32	7 (17%)
13	HEM	C	501	3	50,50,50	1.75	12 (24%)	67,82,82	1.85	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CDL	A	502	-	83,83,99	0.53	0	89,95,111	0.89	3 (3%)
11	LOP	G	101	-	44,44,44	0.45	0	47,49,49	1.26	3 (6%)
17	FES	E	201	5	0,4,4	-	-	-		
19	SO4	F	201	-	4,4,4	0.28	0	6,6,6	0.17	0
19	SO4	G	102	-	4,4,4	0.32	0	6,6,6	0.15	0
19	SO4	G	103	-	4,4,4	0.29	0	6,6,6	0.14	0
11	LOP	A	501	-	44,44,44	0.50	0	47,49,49	0.81	0
13	HEM	C	502	3	50,50,50	1.72	11 (22%)	67,82,82	1.43	13 (19%)
11	LOP	C	506	-	44,44,44	0.65	0	47,49,49	0.91	1 (2%)
11	LOP	E	202	-	44,44,44	0.46	0	47,49,49	0.93	2 (4%)
11	LOP	C	507	-	44,44,44	0.57	0	47,49,49	0.77	2 (4%)
12	CDL	C	504	-	99,99,99	0.44	0	105,111,111	0.80	2 (1%)
12	CDL	D	502	-	93,93,99	0.45	0	99,105,111	0.64	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
15	LMT	C	508	-	-	8/21/61/61	0/2/2/2
12	CDL	C	504	-	-	53/110/110/110	-
11	LOP	C	507	-	-	32/48/48/48	-
12	CDL	A	502	-	-	51/93/93/110	-
11	LOP	A	501	-	-	21/48/48/48	-
11	LOP	C	503	-	-	16/48/48/48	-
11	LOP	G	101	-	-	25/48/48/48	-
18	PSC	E	203	-	-	28/55/55/55	-
16	HEC	D	501	4	-	6/14/54/54	-
13	HEM	C	502	3	-	4/14/54/54	-
17	FES	E	201	5	-	-	0/1/1/1
11	LOP	C	506	-	-	18/48/48/48	-
14	A1IKG	C	505	-	1/1/6/6	0/13/40/40	0/4/4/4
12	CDL	D	502	-	-	48/104/104/110	-
13	HEM	C	501	3	-	4/14/54/54	-
11	LOP	E	202	-	-	22/48/48/48	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	505	A1IKG	C6-C2	-6.22	1.42	1.52
13	C	502	HEM	C1B-NB	-5.28	1.31	1.40
14	C	505	A1IKG	C6-C5	-5.17	1.42	1.52
16	D	501	HEC	C2A-C3A	5.01	1.47	1.36
16	D	501	HEC	CAB-C3B	5.00	1.51	1.35
16	D	501	HEC	CHA-C1A	4.55	1.47	1.38
13	C	501	HEM	FE-NB	4.54	2.08	1.94
16	D	501	HEC	CHD-C4C	4.41	1.47	1.38
16	D	501	HEC	CAC-C3C	4.40	1.49	1.35
16	D	501	HEC	CHB-C4A	4.19	1.46	1.38
13	C	502	HEM	FE-NB	3.85	2.06	1.94
14	C	505	A1IKG	C5-C4	-3.57	1.39	1.47
16	D	501	HEC	CHC-C1C	3.55	1.47	1.39
13	C	502	HEM	C4B-NB	-3.54	1.31	1.38
13	C	502	HEM	FE-NC	3.50	2.06	1.95
13	C	501	HEM	C1B-NB	-3.48	1.34	1.40
16	D	501	HEC	CHC-C4B	3.46	1.45	1.38
13	C	501	HEM	C1D-ND	-3.36	1.32	1.38
16	D	501	HEC	C4A-NA	-3.34	1.33	1.39
16	D	501	HEC	C4C-NC	-3.31	1.33	1.39
16	D	501	HEC	C3D-C2D	3.24	1.47	1.38
13	C	502	HEM	C4D-ND	-3.23	1.34	1.40
16	D	501	HEC	C1A-NA	-3.22	1.33	1.39
16	D	501	HEC	C1D-C2D	3.22	1.50	1.43
13	C	501	HEM	C4D-ND	-3.21	1.34	1.40
13	C	501	HEM	C4B-NB	-3.15	1.32	1.38
16	D	501	HEC	CHA-C4D	3.06	1.46	1.39
16	D	501	HEC	CHD-C1D	3.04	1.46	1.39
13	C	501	HEM	FE-NC	3.00	2.05	1.95
16	D	501	HEC	C1B-NB	-2.98	1.34	1.39
13	C	501	HEM	C4C-NC	-2.95	1.34	1.39
16	D	501	HEC	C1D-ND	-2.93	1.34	1.39
14	C	505	A1IKG	C7-C6	-2.92	1.49	1.53
16	D	501	HEC	C1C-C2C	2.70	1.49	1.43
16	D	501	HEC	CHB-C1B	2.68	1.45	1.39
16	D	501	HEC	C4B-NB	-2.67	1.34	1.39
13	C	501	HEM	FE-ND	-2.60	1.86	1.94
14	C	505	A1IKG	C4-C3	2.55	1.42	1.37
16	D	501	HEC	C4D-ND	-2.55	1.34	1.39
13	C	502	HEM	O1A-CGA	2.49	1.30	1.22
13	C	502	HEM	C1C-C2C	-2.46	1.40	1.45
13	C	502	HEM	C1D-ND	-2.42	1.34	1.38
13	C	501	HEM	C4D-C3D	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	C1C-NC	-2.35	1.35	1.39
16	D	501	HEC	C4D-C3D	2.30	1.49	1.44
13	C	501	HEM	C1C-NC	-2.24	1.35	1.39
16	D	501	HEC	C1A-C2A	2.21	1.49	1.45
13	C	501	HEM	C3C-C4C	-2.19	1.42	1.46
13	C	502	HEM	C4A-NA	-2.18	1.35	1.39
16	D	501	HEC	C1B-C2B	2.16	1.48	1.43
13	C	502	HEM	FE-ND	-2.11	1.88	1.94
14	C	505	A1IKG	O1-C5	2.11	1.26	1.22
16	D	501	HEC	C3C-C2C	2.05	1.48	1.41
13	C	501	HEM	C3B-C4B	2.01	1.48	1.44

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	CBC-CAC-C3C	-8.96	109.53	127.43
16	D	501	HEC	CBB-CAB-C3B	-8.50	110.45	127.43
18	E	203	PSC	O01-C1-C2	6.48	125.50	111.48
16	D	501	HEC	C3D-C4D-ND	6.34	117.18	110.15
11	G	101	LOP	O5-C6-C7	6.28	125.06	111.48
16	D	501	HEC	C2A-C1A-NA	5.16	115.30	110.32
16	D	501	HEC	C2B-C1B-NB	4.81	117.86	110.14
13	C	502	HEM	CHC-C4B-NB	4.74	129.52	124.42
13	C	501	HEM	CHC-C4B-NB	4.70	129.48	124.42
13	C	501	HEM	CAD-C3D-C4D	4.42	132.39	124.70
16	D	501	HEC	C1D-C2D-C3D	-4.23	101.98	106.82
16	D	501	HEC	C1A-C2A-C3A	-4.11	101.70	107.11
16	D	501	HEC	C2D-C1D-ND	4.02	116.59	110.14
14	C	505	A1IKG	C6-C5-C4	3.95	120.18	111.40
11	E	202	LOP	O5-C4-C5	-3.94	94.20	108.34
13	C	501	HEM	CHB-C1B-NB	3.79	129.05	124.37
12	A	502	CDL	CB4-OB6-CB5	3.73	124.43	117.85
16	D	501	HEC	CMD-C2D-C1D	3.71	131.07	125.42
12	C	504	CDL	OB6-CB5-C51	-3.66	103.57	111.48
11	E	202	LOP	O5-C4-C3	3.62	121.33	108.34
13	C	501	HEM	CMD-C2D-C1D	3.61	130.68	125.03
13	C	501	HEM	CBA-CAA-C2A	-3.59	102.60	112.53
13	C	502	HEM	C1B-NB-C4B	3.58	109.44	105.21
16	D	501	HEC	C2C-C1C-NC	3.51	115.78	110.14
11	C	506	LOP	O5-C6-C7	3.45	118.94	111.48
14	C	505	A1IKG	C7-C6-C5	3.44	117.98	111.46
13	C	501	HEM	CHD-C4C-NC	3.30	128.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	203	PSC	O01-C1-O02	-3.28	116.03	123.70
16	D	501	HEC	CMB-C2B-C1B	3.26	130.38	125.42
12	C	504	CDL	OB6-CB4-CB3	-3.24	96.74	108.34
16	D	501	HEC	C4D-C3D-C2D	-3.20	101.91	106.87
16	D	501	HEC	CAA-CBA-CGA	-3.15	105.31	113.67
13	C	501	HEM	C1B-NB-C4B	3.05	108.82	105.21
11	C	503	LOP	C5-C4-C3	2.97	118.72	111.78
13	C	501	HEM	C3B-C4B-NB	-2.95	107.35	109.47
16	D	501	HEC	CMC-C2C-C1C	2.94	129.90	125.42
16	D	501	HEC	C3A-C4A-NA	2.87	114.94	109.64
12	A	502	CDL	OB6-CB5-C51	2.85	116.17	111.09
14	C	505	A1IKG	O1-C5-C6	-2.83	121.14	126.56
13	C	501	HEM	CHB-C1B-C2B	-2.75	119.14	126.95
11	C	503	LOP	O5-C6-C7	2.72	117.36	111.48
18	E	203	PSC	O11-P-O14	2.71	119.66	108.94
15	C	508	LMT	O1'-C1'-C2'	2.68	112.34	108.27
11	C	507	LOP	O5-C6-C7	2.67	117.26	111.48
16	D	501	HEC	CHC-C1C-C2C	-2.61	119.84	127.43
16	D	501	HEC	C4A-C3A-C2A	-2.57	103.15	106.97
11	G	101	LOP	O5-C6-O7	-2.57	117.70	123.70
13	C	501	HEM	O2D-CGD-CBD	2.56	122.09	114.00
13	C	502	HEM	CHD-C1D-ND	2.49	127.10	124.42
16	D	501	HEC	CHB-C1B-C2B	-2.45	120.31	127.43
13	C	502	HEM	CHB-C1B-NB	2.45	127.40	124.37
11	C	507	LOP	O6-C5-C4	2.44	115.44	108.40
16	D	501	HEC	C4B-NB-C1B	-2.44	101.84	105.82
14	C	505	A1IKG	C1-C2-N1	-2.43	116.23	119.71
13	C	501	HEM	O2D-CGD-O1D	-2.42	117.12	123.33
13	C	501	HEM	CHA-C1A-NA	2.40	128.21	123.86
14	C	505	A1IKG	C4-C3-N1	-2.37	120.31	123.68
11	G	101	LOP	C4-O5-C6	2.37	123.47	117.80
16	D	501	HEC	O2A-CGA-CBA	2.37	121.48	114.00
15	C	508	LMT	C1-O1'-C1'	2.34	117.68	113.68
13	C	502	HEM	CHA-C4D-C3D	-2.32	120.95	125.23
16	D	501	HEC	CMC-C2C-C3C	2.28	131.92	126.55
13	C	501	HEM	C3C-C2C-C1C	-2.28	104.89	107.05
13	C	502	HEM	CHD-C1D-C2D	-2.26	121.46	125.03
13	C	502	HEM	CHA-C1A-NA	2.24	127.92	123.86
16	D	501	HEC	O2D-CGD-CBD	2.23	121.06	114.00
13	C	501	HEM	C4A-CHB-C1B	-2.22	121.02	126.25
14	C	505	A1IKG	O1-C5-C4	-2.22	118.59	122.42
13	C	502	HEM	CAD-C3D-C4D	2.21	128.56	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	CHA-C1A-C2A	-2.21	121.38	124.86
16	D	501	HEC	CHC-C4B-C3B	-2.21	121.49	125.21
16	D	501	HEC	CHB-C4A-C3A	-2.20	120.91	125.49
13	C	502	HEM	CBA-CAA-C2A	-2.20	106.45	112.53
13	C	501	HEM	O2A-CGA-CBA	2.19	120.92	114.00
13	C	501	HEM	C4D-C3D-C2D	-2.18	103.72	106.89
13	C	501	HEM	CHA-C4D-C3D	-2.16	121.24	125.23
13	C	502	HEM	CHD-C4C-NC	2.14	126.78	124.45
13	C	502	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
16	D	501	HEC	C4D-ND-C1D	-2.14	102.34	105.82
13	C	501	HEM	CAD-C3D-C2D	-2.13	123.87	127.87
12	A	502	CDL	OB7-CB5-C51	-2.11	117.30	124.77
14	C	505	A1IKG	C5-C4-C3	-2.08	118.98	120.68
11	C	503	LOP	O6-C5-C4	-2.08	102.41	108.40
13	C	502	HEM	C3B-C4B-NB	-2.05	108.00	109.47
16	D	501	HEC	CHD-C1D-ND	-2.04	120.15	123.86
13	C	502	HEM	C4C-CHD-C1D	-2.04	121.68	126.02
13	C	501	HEM	CMA-C3A-C4A	2.03	128.51	125.42
18	E	203	PSC	O13-P-O11	-2.02	98.41	107.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	A1IKG	C6

All (336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	LOP	N1-C1-C2-O1
11	A	501	LOP	C2-O1-P1-O2
11	A	501	LOP	C2-O1-P1-O4
11	C	507	LOP	N1-C1-C2-O1
11	C	507	LOP	C2-O1-P1-O2
11	C	507	LOP	C2-O1-P1-O3
11	C	507	LOP	C2-O1-P1-O4
11	C	507	LOP	C3-O2-P1-O1
11	C	507	LOP	C3-O2-P1-O3
11	C	507	LOP	C3-O2-P1-O4
11	E	202	LOP	O2-C3-C4-O5
11	G	101	LOP	C3-O2-P1-O1
11	G	101	LOP	C3-O2-P1-O4
11	G	101	LOP	O7-C6-O5-C4

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Mol	Chain	Res	Type	Atoms
11	G	101	LOP	C7-C6-O5-C4
12	A	502	CDL	OA6-CA4-CA6-OA8
12	C	504	CDL	CA2-OA2-PA1-OA3
12	C	504	CDL	CA2-OA2-PA1-OA5
12	D	502	CDL	CB2-OB2-PB2-OB4
12	D	502	CDL	CB2-OB2-PB2-OB5
16	D	501	HEC	C2B-C3B-CAB-CBB
16	D	501	HEC	C4B-C3B-CAB-CBB
16	D	501	HEC	C2C-C3C-CAC-CBC
16	D	501	HEC	C4C-C3C-CAC-CBC
18	E	203	PSC	C04-O12-P-O11
18	E	203	PSC	O02-C1-O01-C02
18	E	203	PSC	C2-C1-O01-C02
11	A	501	LOP	O8-C24-O6-C5
12	D	502	CDL	OA9-CA7-OA8-CA6
12	D	502	CDL	OB9-CB7-OB8-CB6
11	A	501	LOP	C25-C24-O6-C5
12	D	502	CDL	C31-CA7-OA8-CA6
12	D	502	CDL	C71-CB7-OB8-CB6
12	A	502	CDL	OA9-CA7-OA8-CA6
12	A	502	CDL	C31-CA7-OA8-CA6
11	A	501	LOP	C18-C19-C20-C21
12	C	504	CDL	CA7-C31-C32-C33
15	C	508	LMT	O5B-C5B-C6B-O6B
12	D	502	CDL	C36-C37-C38-C39
12	C	504	CDL	C63-C64-C65-C66
15	C	508	LMT	C2'-C1'-O1'-C1
18	E	203	PSC	C1-C2-C3-C4
11	C	506	LOP	C25-C26-C27-C28
11	A	501	LOP	O5-C4-C5-O6
11	A	501	LOP	C30-C31-C32-C33
11	C	507	LOP	C24-C25-C26-C27
12	C	504	CDL	CB5-C51-C52-C53
12	D	502	CDL	CB5-C51-C52-C53
15	C	508	LMT	O1'-C1-C2-C3
11	C	503	LOP	C24-C25-C26-C27
18	E	203	PSC	C19-C20-C21-C22
15	C	508	LMT	C4B-C5B-C6B-O6B
11	C	507	LOP	C6-C7-C8-C9
12	A	502	CDL	CA7-C31-C32-C33
12	C	504	CDL	CA5-C11-C12-C13
12	D	502	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
12	A	502	CDL	C17-C18-C19-C20
12	C	504	CDL	CB6-CB4-OB6-CB5
12	A	502	CDL	C11-CA5-OA6-CA4
12	A	502	CDL	C36-C37-C38-C39
11	A	501	LOP	C27-C28-C29-C30
11	C	507	LOP	C26-C27-C28-C29
12	D	502	CDL	C22-C23-C24-C25
12	A	502	CDL	C23-C24-C25-C26
12	D	502	CDL	C12-C13-C14-C15
11	C	503	LOP	C18-C19-C20-C21
12	C	504	CDL	C36-C37-C38-C39
12	D	502	CDL	C74-C75-C76-C77
15	C	508	LMT	C2-C1-O1'-C1'
12	C	504	CDL	C73-C74-C75-C76
11	C	507	LOP	C25-C26-C27-C28
12	C	504	CDL	C82-C83-C84-C85
12	D	502	CDL	C83-C84-C85-C86
11	C	506	LOP	C11-C10-C9-C8
11	C	507	LOP	C19-C20-C21-C22
12	C	504	CDL	C56-C57-C58-C59
11	A	501	LOP	C29-C30-C31-C32
12	C	504	CDL	C55-C56-C57-C58
12	A	502	CDL	C41-C42-C43-C44
12	A	502	CDL	C16-C17-C18-C19
12	D	502	CDL	C37-C38-C39-C40
18	E	203	PSC	C5-C6-C7-C8
11	C	507	LOP	C3-C4-C5-O6
11	C	503	LOP	C7-C8-C9-C10
11	C	506	LOP	C30-C31-C32-C33
12	C	504	CDL	C19-C20-C21-C22
12	C	504	CDL	C23-C24-C25-C26
15	C	508	LMT	C5-C6-C7-C8
11	G	101	LOP	C19-C20-C21-C22
12	A	502	CDL	C39-C40-C41-C42
12	C	504	CDL	C15-C16-C17-C18
18	E	203	PSC	C22-C23-C24-C25
18	E	203	PSC	C26-C27-C28-C29
12	A	502	CDL	C83-C84-C85-C86
12	C	504	CDL	C61-C62-C63-C64
12	C	504	CDL	C77-C78-C79-C80
12	D	502	CDL	C61-C62-C63-C64
11	C	503	LOP	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
12	C	504	CDL	C35-C36-C37-C38
12	A	502	CDL	C24-C25-C26-C27
11	A	501	LOP	C31-C32-C33-C34
11	C	506	LOP	C10-C11-C12-C13
11	G	101	LOP	C29-C30-C31-C32
11	G	101	LOP	C25-C26-C27-C28
11	G	101	LOP	C11-C10-C9-C8
12	A	502	CDL	C11-C12-C13-C14
12	C	504	CDL	C83-C84-C85-C86
12	C	504	CDL	C41-C42-C43-C44
12	A	502	CDL	C15-C16-C17-C18
12	C	504	CDL	C14-C15-C16-C17
12	C	504	CDL	C16-C17-C18-C19
11	E	202	LOP	C7-C6-O5-C4
12	D	502	CDL	C51-CB5-OB6-CB4
12	D	502	CDL	C55-C56-C57-C58
11	C	507	LOP	C17-C18-C19-C20
11	C	503	LOP	C28-C29-C30-C31
11	G	101	LOP	C25-C24-O6-C5
11	C	503	LOP	C16-C17-C18-C19
12	A	502	CDL	C34-C35-C36-C37
12	A	502	CDL	C74-C75-C76-C77
11	G	101	LOP	C7-C8-C9-C10
12	C	504	CDL	C80-C81-C82-C83
11	C	506	LOP	C26-C27-C28-C29
11	C	503	LOP	C15-C16-C17-C18
11	C	506	LOP	C15-C16-C17-C18
12	A	502	CDL	OB6-CB4-CB6-OB8
11	C	503	LOP	C29-C30-C31-C32
12	C	504	CDL	C39-C40-C41-C42
11	E	202	LOP	C28-C29-C30-C31
11	A	501	LOP	C26-C27-C28-C29
12	A	502	CDL	C38-C39-C40-C41
12	C	504	CDL	C43-C44-C45-C46
12	D	502	CDL	C54-C55-C56-C57
18	E	203	PSC	C3-C4-C5-C6
11	A	501	LOP	C16-C17-C18-C19
11	C	503	LOP	C30-C31-C32-C33
12	A	502	CDL	C12-C13-C14-C15
11	E	202	LOP	O2-C3-C4-C5
11	E	202	LOP	C26-C27-C28-C29
12	C	504	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
18	E	203	PSC	C2-C3-C4-C5
12	C	504	CDL	C22-C23-C24-C25
11	C	507	LOP	C25-C24-O6-C5
12	C	504	CDL	CB3-CB4-CB6-OB8
11	E	202	LOP	C11-C12-C13-C14
18	E	203	PSC	C6-C7-C8-C9
12	A	502	CDL	C14-C15-C16-C17
12	A	502	CDL	C33-C34-C35-C36
12	C	504	CDL	C31-CA7-OA8-CA6
11	E	202	LOP	C30-C31-C32-C33
12	C	504	CDL	C52-C53-C54-C55
11	A	501	LOP	C19-C20-C21-C22
11	C	507	LOP	C30-C31-C32-C33
11	E	202	LOP	C17-C18-C19-C20
11	C	507	LOP	C11-C10-C9-C8
12	A	502	CDL	CA5-C11-C12-C13
11	C	506	LOP	C19-C20-C21-C22
11	A	501	LOP	C15-C16-C17-C18
12	D	502	CDL	CA5-C11-C12-C13
12	D	502	CDL	C33-C34-C35-C36
12	C	504	CDL	OB5-CB3-CB4-OB6
12	C	504	CDL	C44-C45-C46-C47
12	D	502	CDL	C84-C85-C86-C87
12	A	502	CDL	C20-C21-C22-C23
12	D	502	CDL	C53-C54-C55-C56
11	C	503	LOP	C10-C11-C12-C13
18	E	203	PSC	C29-C30-C31-C32
12	D	502	CDL	C34-C35-C36-C37
18	E	203	PSC	C24-C25-C26-C27
12	D	502	CDL	C16-C17-C18-C19
15	C	508	LMT	C9-C10-C11-C12
18	E	203	PSC	C27-C28-C29-C30
12	A	502	CDL	C71-CB7-OB8-CB6
11	C	506	LOP	C27-C28-C29-C30
12	A	502	CDL	C43-C44-C45-C46
12	D	502	CDL	C17-C18-C19-C20
11	C	507	LOP	O2-C3-C4-C5
12	C	504	CDL	C54-C55-C56-C57
11	C	506	LOP	C29-C30-C31-C32
11	C	506	LOP	C31-C32-C33-C34
12	D	502	CDL	C80-C81-C82-C83
11	A	501	LOP	C3-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
12	A	502	CDL	CA3-CA4-CA6-OA8
12	A	502	CDL	CB3-CB4-CB6-OB8
18	E	203	PSC	O03-C01-C02-C03
12	A	502	CDL	C75-C76-C77-C78
11	C	507	LOP	C10-C11-C12-C13
12	C	504	CDL	C81-C82-C83-C84
12	A	502	CDL	OA7-CA5-OA6-CA4
11	C	507	LOP	O2-C3-C4-O5
11	G	101	LOP	C9-C10-C11-C12
11	E	202	LOP	C24-C25-C26-C27
11	G	101	LOP	O5-C4-C5-O6
12	D	502	CDL	C32-C33-C34-C35
18	E	203	PSC	C21-C22-C23-C24
11	E	202	LOP	C14-C15-C16-C17
18	E	203	PSC	C7-C8-C9-C10
11	C	507	LOP	C9-C10-C11-C12
12	D	502	CDL	C24-C25-C26-C27
11	C	507	LOP	C7-C6-O5-C4
12	C	504	CDL	C57-C58-C59-C60
11	G	101	LOP	C27-C28-C29-C30
12	C	504	CDL	C74-C75-C76-C77
11	C	507	LOP	C12-C13-C14-C15
12	C	504	CDL	C51-CB5-OB6-CB4
11	E	202	LOP	C18-C19-C20-C21
11	E	202	LOP	C19-C20-C21-C22
12	D	502	CDL	OB5-CB3-CB4-CB6
11	G	101	LOP	C31-C32-C33-C34
12	D	502	CDL	C63-C64-C65-C66
12	D	502	CDL	C81-C82-C83-C84
11	G	101	LOP	O8-C24-O6-C5
11	E	202	LOP	C6-C7-C8-C9
12	A	502	CDL	C44-C45-C46-C47
12	D	502	CDL	OB7-CB5-OB6-CB4
12	A	502	CDL	C77-C78-C79-C80
12	A	502	CDL	C21-C22-C23-C24
11	C	507	LOP	O5-C4-C5-O6
11	G	101	LOP	C15-C16-C17-C18
18	E	203	PSC	O03-C01-C02-O01
12	C	504	CDL	C51-C52-C53-C54
11	C	507	LOP	C7-C8-C9-C10
11	E	202	LOP	C16-C17-C18-C19
11	C	507	LOP	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	E	202	LOP	C9-C10-C11-C12
12	C	504	CDL	C71-C72-C73-C74
18	E	203	PSC	C15-C16-C17-C18
12	C	504	CDL	OB5-CB3-CB4-CB6
12	A	502	CDL	C79-C80-C81-C82
12	D	502	CDL	C72-C73-C74-C75
12	D	502	CDL	OB5-CB3-CB4-OB6
18	E	203	PSC	O01-C02-C03-O11
11	A	501	LOP	C32-C33-C34-C35
11	C	503	LOP	C26-C27-C28-C29
12	D	502	CDL	C23-C24-C25-C26
12	C	504	CDL	OB6-CB4-CB6-OB8
12	D	502	CDL	C76-C77-C78-C79
11	G	101	LOP	C3-C4-C5-O6
18	E	203	PSC	C25-C26-C27-C28
11	C	507	LOP	O8-C24-O6-C5
12	D	502	CDL	C79-C80-C81-C82
11	C	506	LOP	N1-C1-C2-O1
11	C	506	LOP	C3-O2-P1-O4
11	E	202	LOP	C2-O1-P1-O3
11	G	101	LOP	C2-O1-P1-O2
11	G	101	LOP	C3-O2-P1-O3
12	A	502	CDL	CA2-OA2-PA1-OA5
12	A	502	CDL	CB2-OB2-PB2-OB5
12	A	502	CDL	CB3-OB5-PB2-OB2
12	A	502	CDL	CB3-OB5-PB2-OB3
12	A	502	CDL	CB3-OB5-PB2-OB4
12	C	504	CDL	CA2-OA2-PA1-OA4
18	E	203	PSC	C04-O12-P-O14
12	A	502	CDL	C73-C74-C75-C76
11	C	507	LOP	C31-C32-C33-C34
11	E	202	LOP	C32-C33-C34-C35
12	D	502	CDL	CA2-C1-CB2-OB2
11	G	101	LOP	C24-C25-C26-C27
11	G	101	LOP	C28-C29-C30-C31
12	C	504	CDL	C21-C22-C23-C24
12	C	504	CDL	CA4-CA3-OA5-PA1
11	A	501	LOP	C11-C12-C13-C14
18	E	203	PSC	C4-C5-C6-C7
12	A	502	CDL	C13-C14-C15-C16
12	D	502	CDL	C18-C19-C20-C21
11	C	506	LOP	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
11	C	503	LOP	C25-C26-C27-C28
12	D	502	CDL	C52-C53-C54-C55
11	E	202	LOP	O7-C6-O5-C4
11	C	503	LOP	C12-C13-C14-C15
12	C	504	CDL	C31-C32-C33-C34
11	E	202	LOP	C10-C11-C12-C13
12	A	502	CDL	C35-C36-C37-C38
11	G	101	LOP	C4-C3-O2-P1
12	D	502	CDL	C35-C36-C37-C38
12	C	504	CDL	C42-C43-C44-C45
11	C	507	LOP	C27-C28-C29-C30
11	C	506	LOP	O2-C3-C4-C5
12	D	502	CDL	OA6-CA4-CA6-OA8
11	C	507	LOP	C18-C19-C20-C21
13	C	501	HEM	CAA-CBA-CGA-O2A
12	A	502	CDL	C78-C79-C80-C81
13	C	502	HEM	CAA-CBA-CGA-O1A
13	C	501	HEM	CAA-CBA-CGA-O1A
11	E	202	LOP	C11-C10-C9-C8
12	C	504	CDL	OA9-CA7-OA8-CA6
11	C	503	LOP	C3-C4-C5-O6
12	C	504	CDL	CA3-CA4-CA6-OA8
13	C	502	HEM	CAA-CBA-CGA-O2A
12	D	502	CDL	C58-C59-C60-C61
12	A	502	CDL	CB2-C1-CA2-OA2
12	A	502	CDL	CA2-C1-CB2-OB2
11	C	503	LOP	O2-C3-C4-C5
18	E	203	PSC	C01-C02-C03-O11
11	A	501	LOP	C12-C13-C14-C15
11	C	507	LOP	C14-C15-C16-C17
13	C	501	HEM	CAD-CBD-CGD-O2D
11	E	202	LOP	C27-C28-C29-C30
18	E	203	PSC	C23-C24-C25-C26
12	D	502	CDL	C77-C78-C79-C80
11	G	101	LOP	C14-C15-C16-C17
12	D	502	CDL	C52-C51-CB5-OB6
18	E	203	PSC	C04-C05-N-C06
12	D	502	CDL	C15-C16-C17-C18
11	C	503	LOP	C20-C21-C22-C23
12	A	502	CDL	C72-C71-CB7-OB8
18	E	203	PSC	C04-C05-N-C08
13	C	501	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	D	502	CDL	C13-C14-C15-C16
11	C	506	LOP	C16-C17-C18-C19
11	A	501	LOP	C25-C26-C27-C28
11	C	506	LOP	O6-C24-C25-C26
12	C	504	CDL	C20-C21-C22-C23
18	E	203	PSC	C04-C05-N-C07
11	G	101	LOP	O5-C6-C7-C8
11	E	202	LOP	O5-C4-C5-O6
12	C	504	CDL	C59-C60-C61-C62
12	A	502	CDL	C71-C72-C73-C74
11	C	506	LOP	O5-C6-C7-C8
12	C	504	CDL	C53-C54-C55-C56
11	A	501	LOP	C14-C15-C16-C17
12	A	502	CDL	C72-C71-CB7-OB9
13	C	502	HEM	CAD-CBD-CGD-O2D
12	D	502	CDL	C52-C51-CB5-OB7
12	A	502	CDL	OB9-CB7-OB8-CB6
16	D	501	HEC	CAD-CBD-CGD-O1D
16	D	501	HEC	CAD-CBD-CGD-O2D
12	C	504	CDL	C52-C51-CB5-OB7
15	C	508	LMT	C5'-C4'-O1B-C1B
13	C	502	HEM	CAD-CBD-CGD-O1D
11	G	101	LOP	O7-C6-C7-C8
12	A	502	CDL	O1-C1-CA2-OA2
11	C	507	LOP	C32-C33-C34-C35
12	C	504	CDL	C11-CA5-OA6-CA4
11	C	506	LOP	O8-C24-C25-C26
12	A	502	CDL	C12-C11-CA5-OA7

There are no ring outliers.

13 monomers are involved in 84 short contacts:

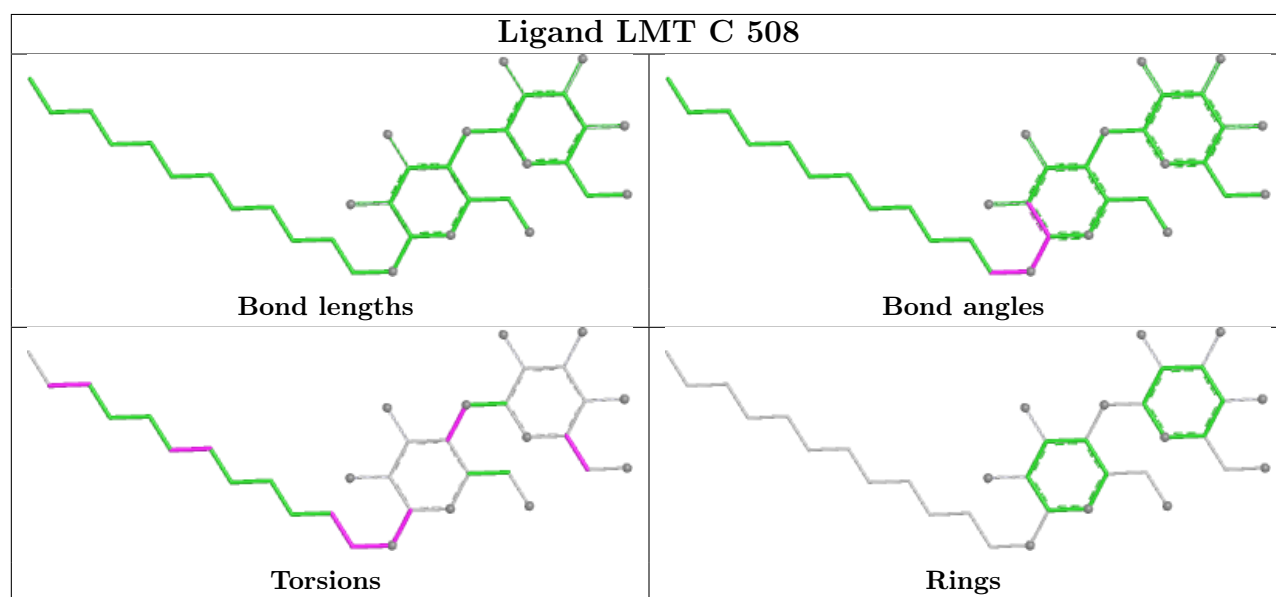
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	508	LMT	3	0
11	C	503	LOP	5	0
18	E	203	PSC	5	0
16	D	501	HEC	2	0
13	C	501	HEM	3	0
12	A	502	CDL	21	0
11	G	101	LOP	4	0
11	A	501	LOP	11	0
13	C	502	HEM	5	0

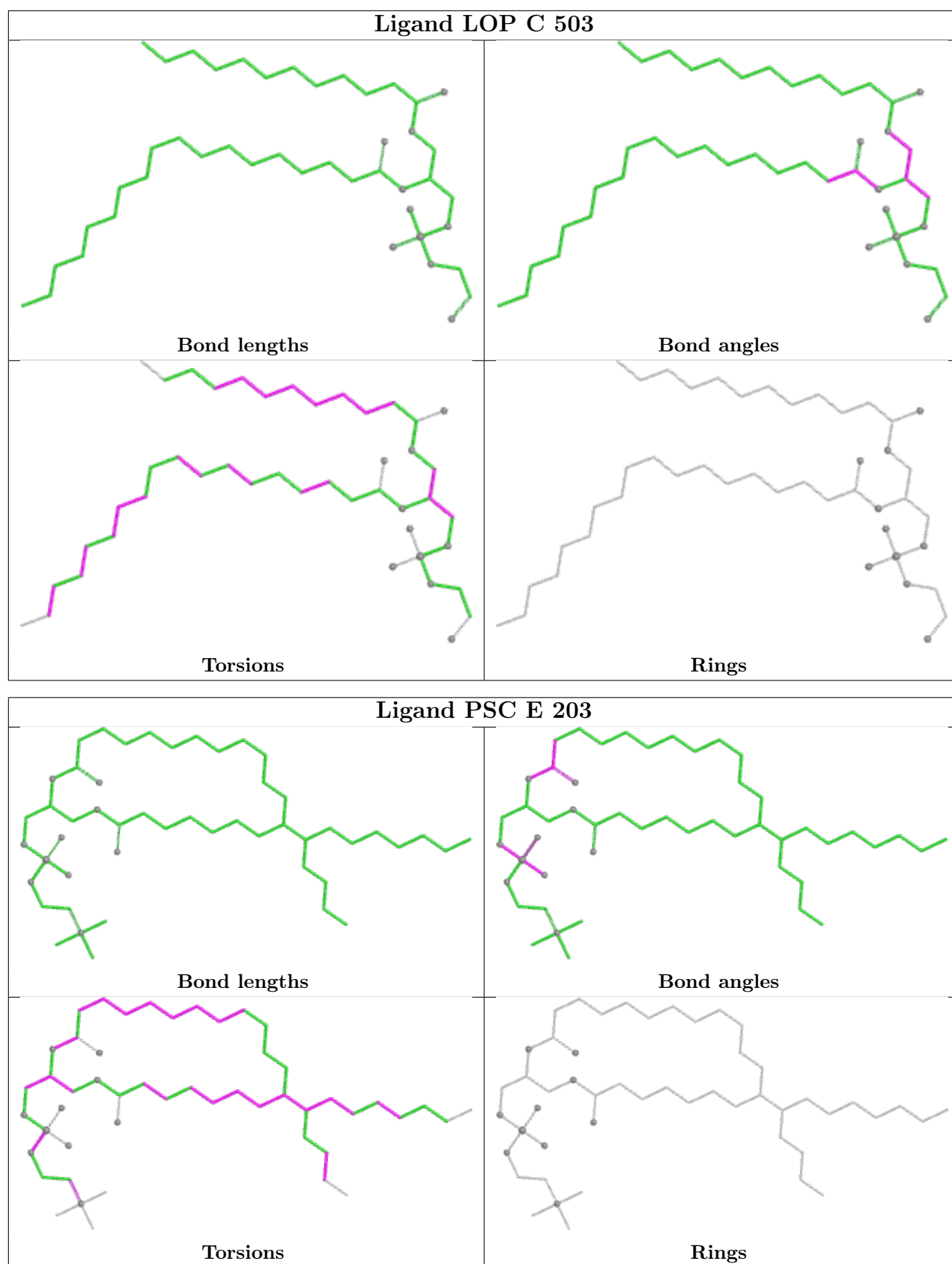
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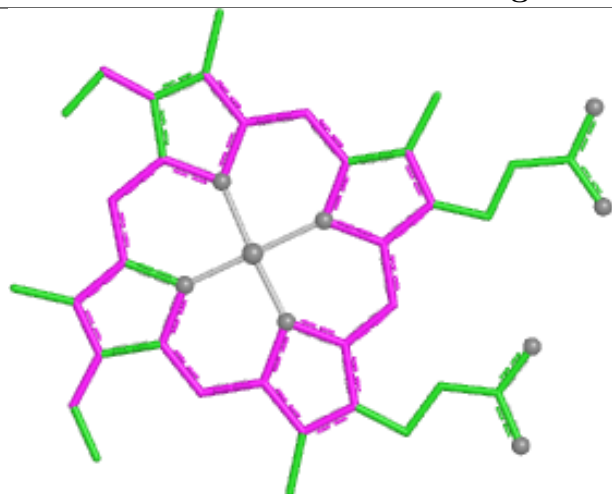
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	506	LOP	4	0
11	E	202	LOP	7	0
12	C	504	CDL	11	0
12	D	502	CDL	12	0

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.

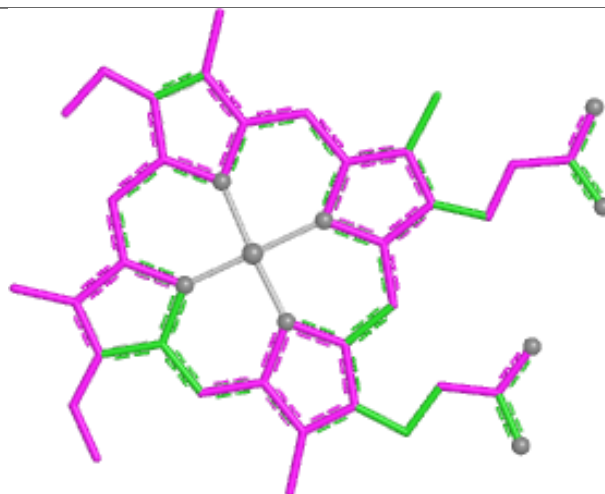




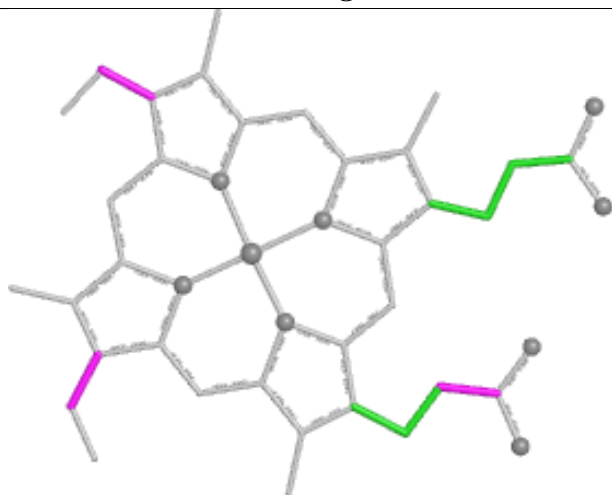
Ligand HEC D 501



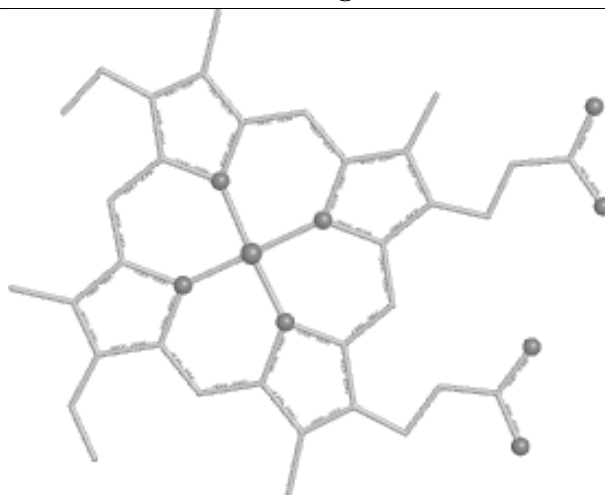
Bond lengths



Bond angles

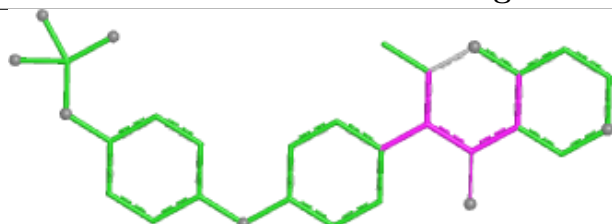


Torsions

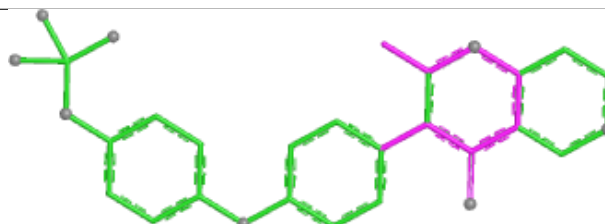


Rings

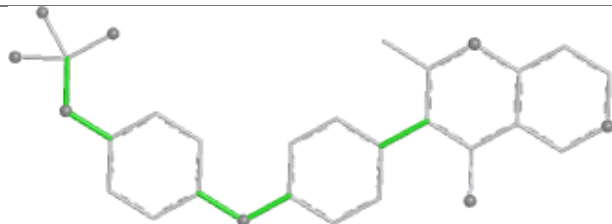
Ligand A1IKG C 505



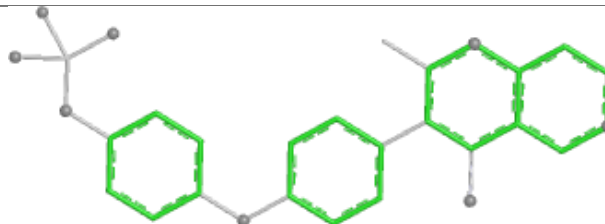
Bond lengths



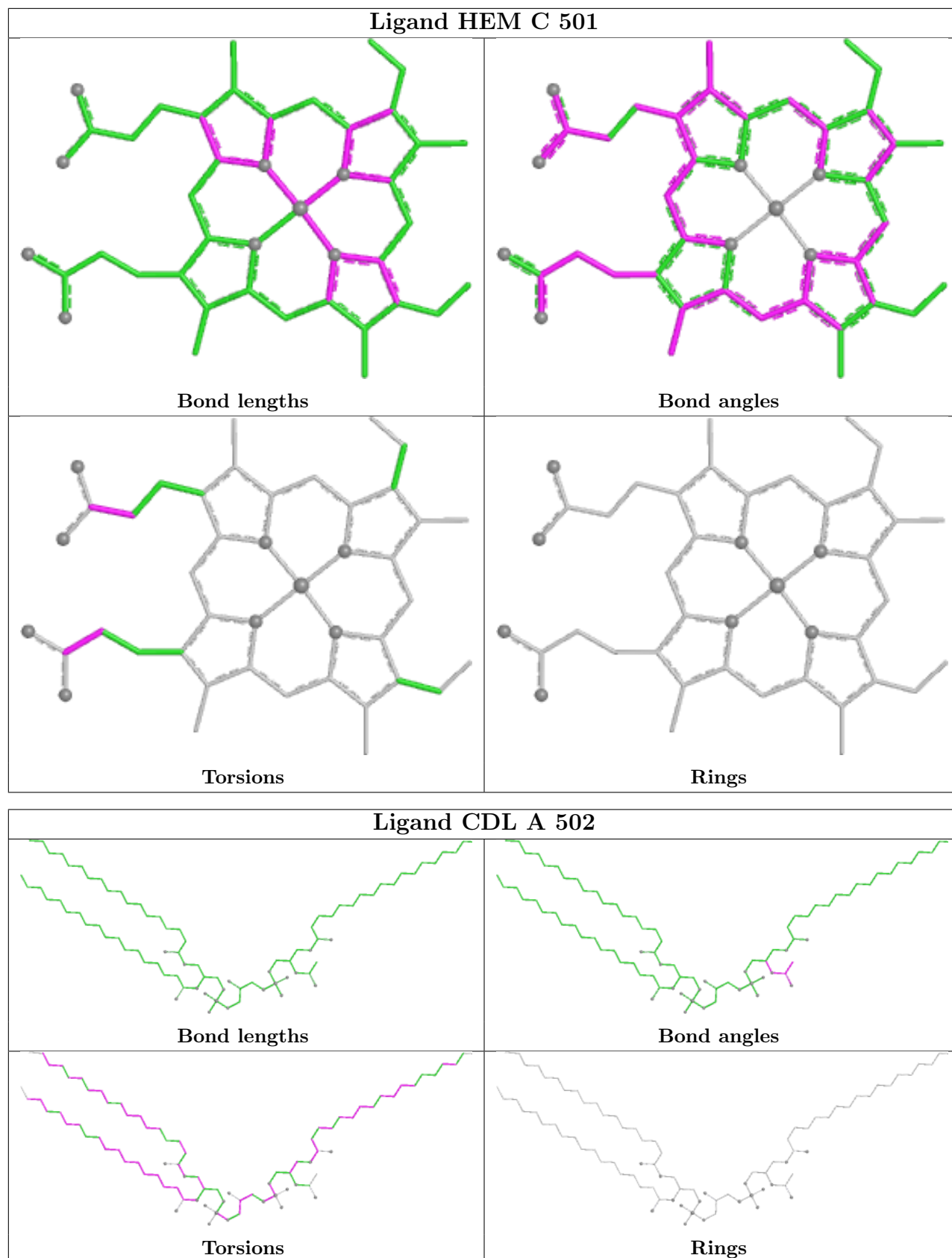
Bond angles

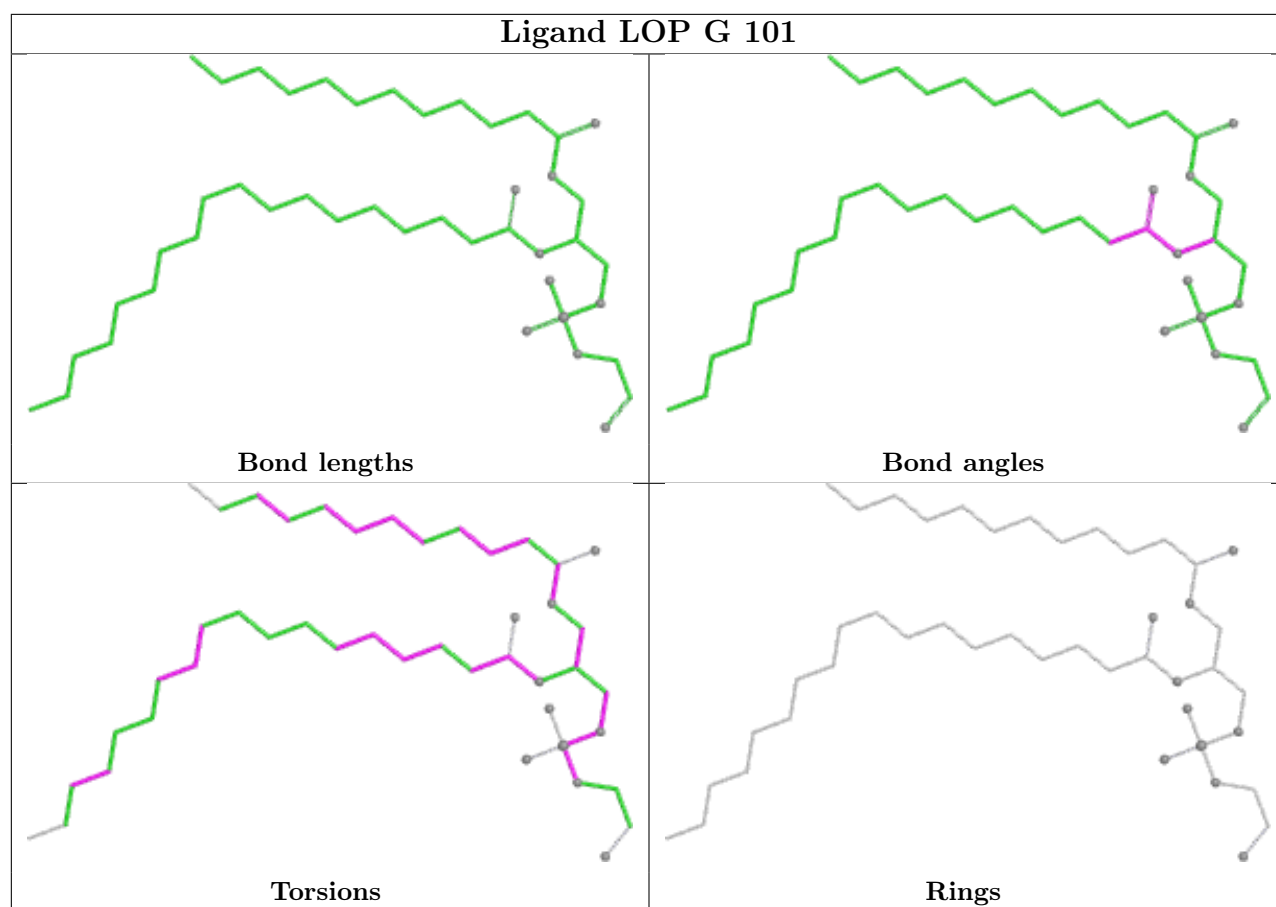


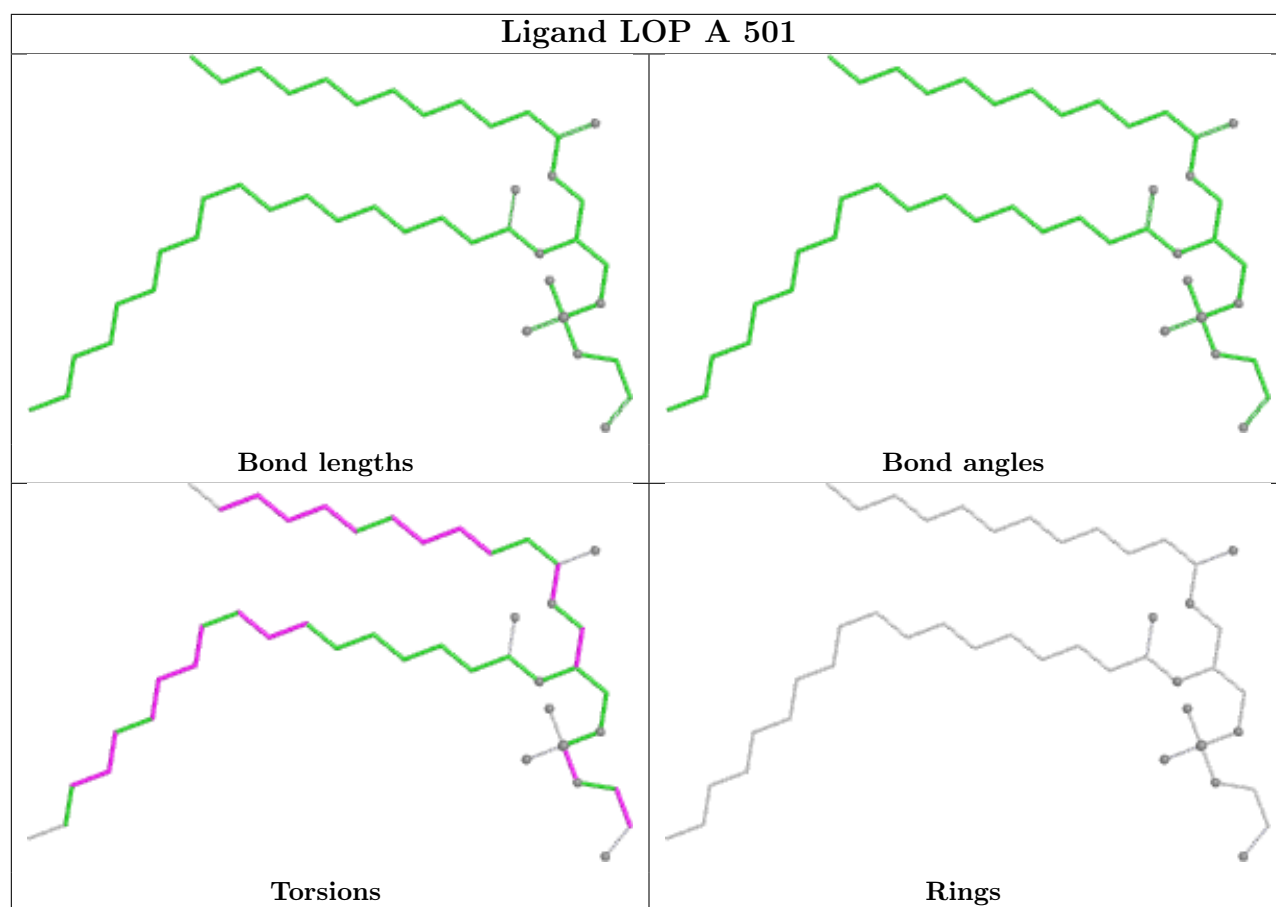
Torsions

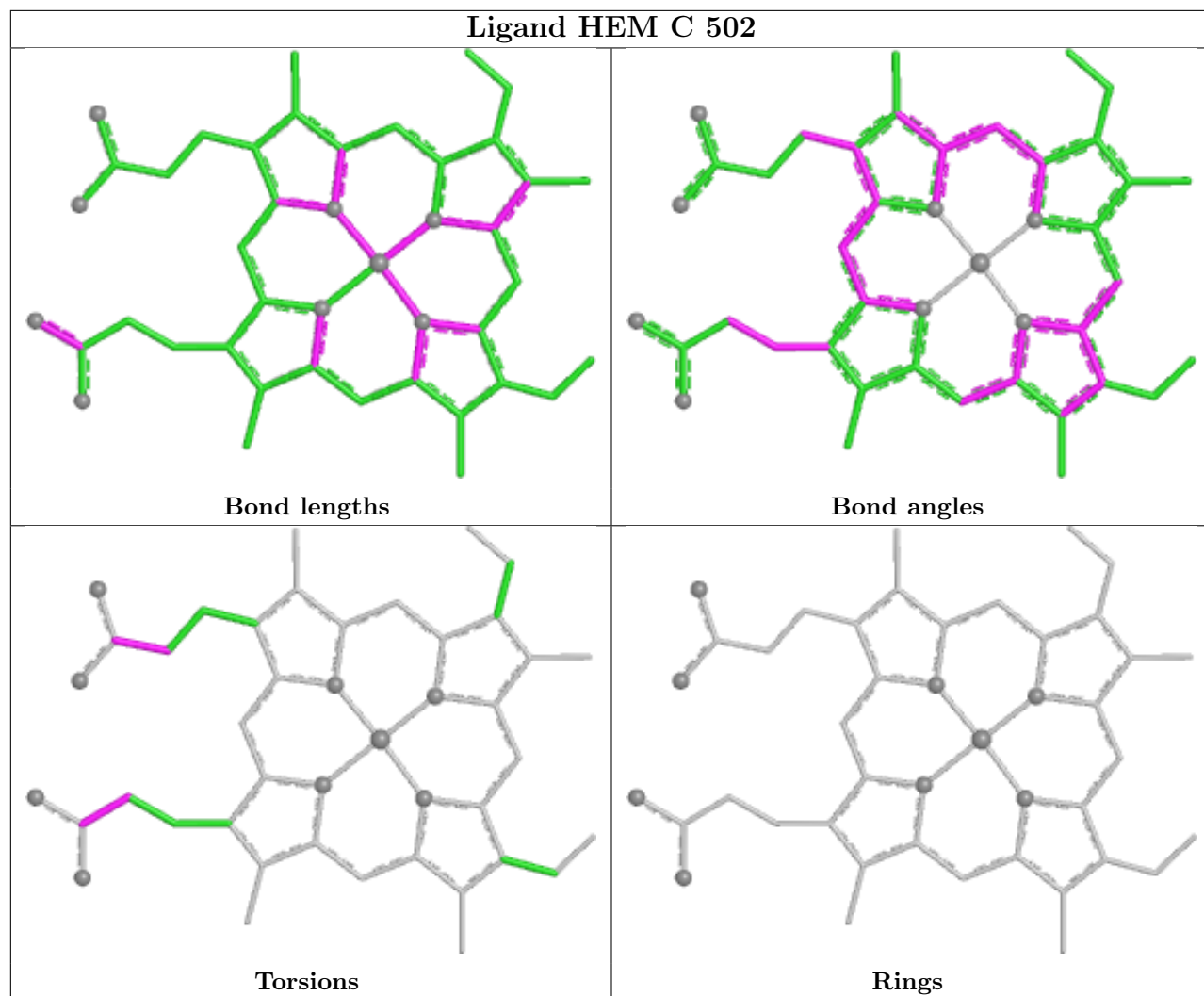


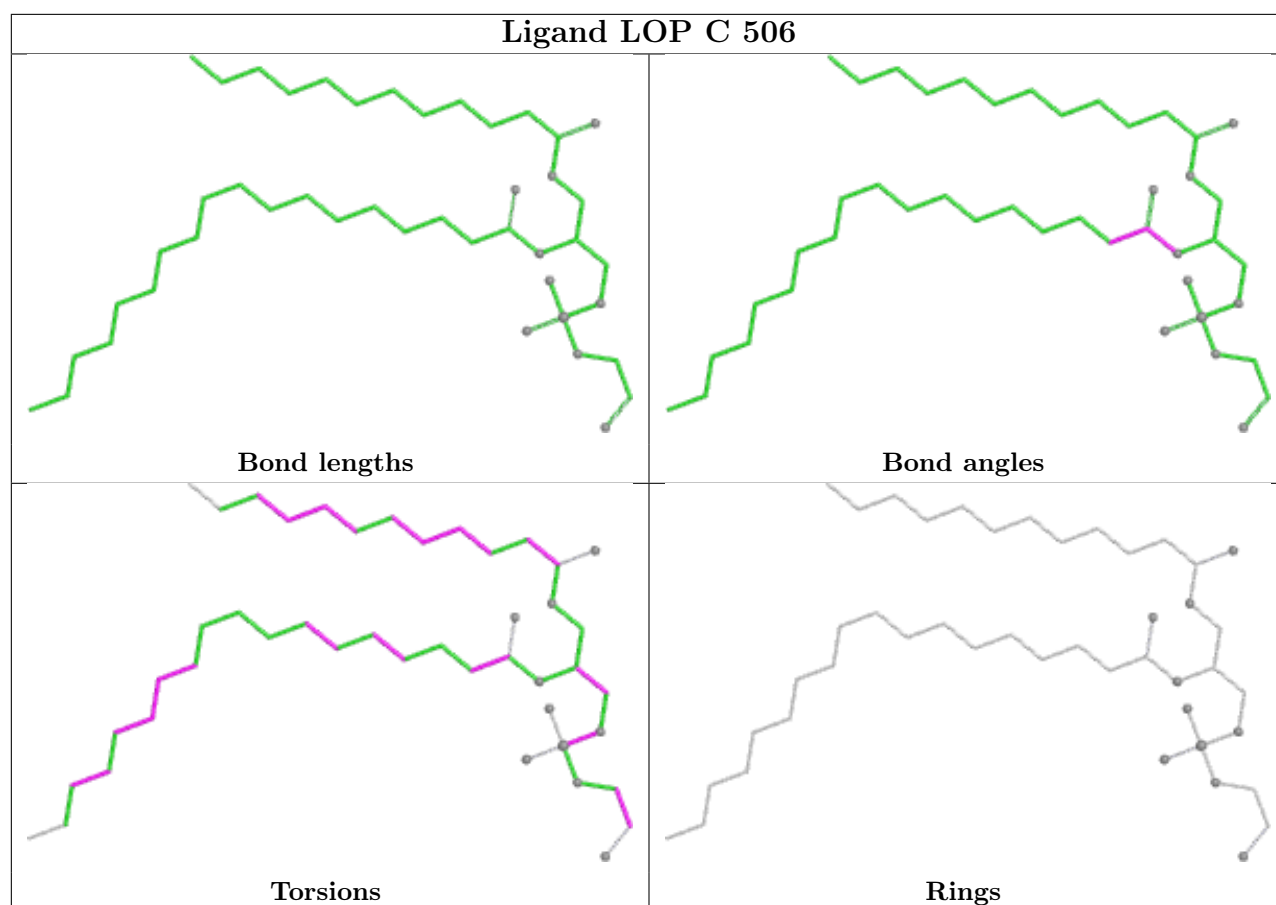
Rings

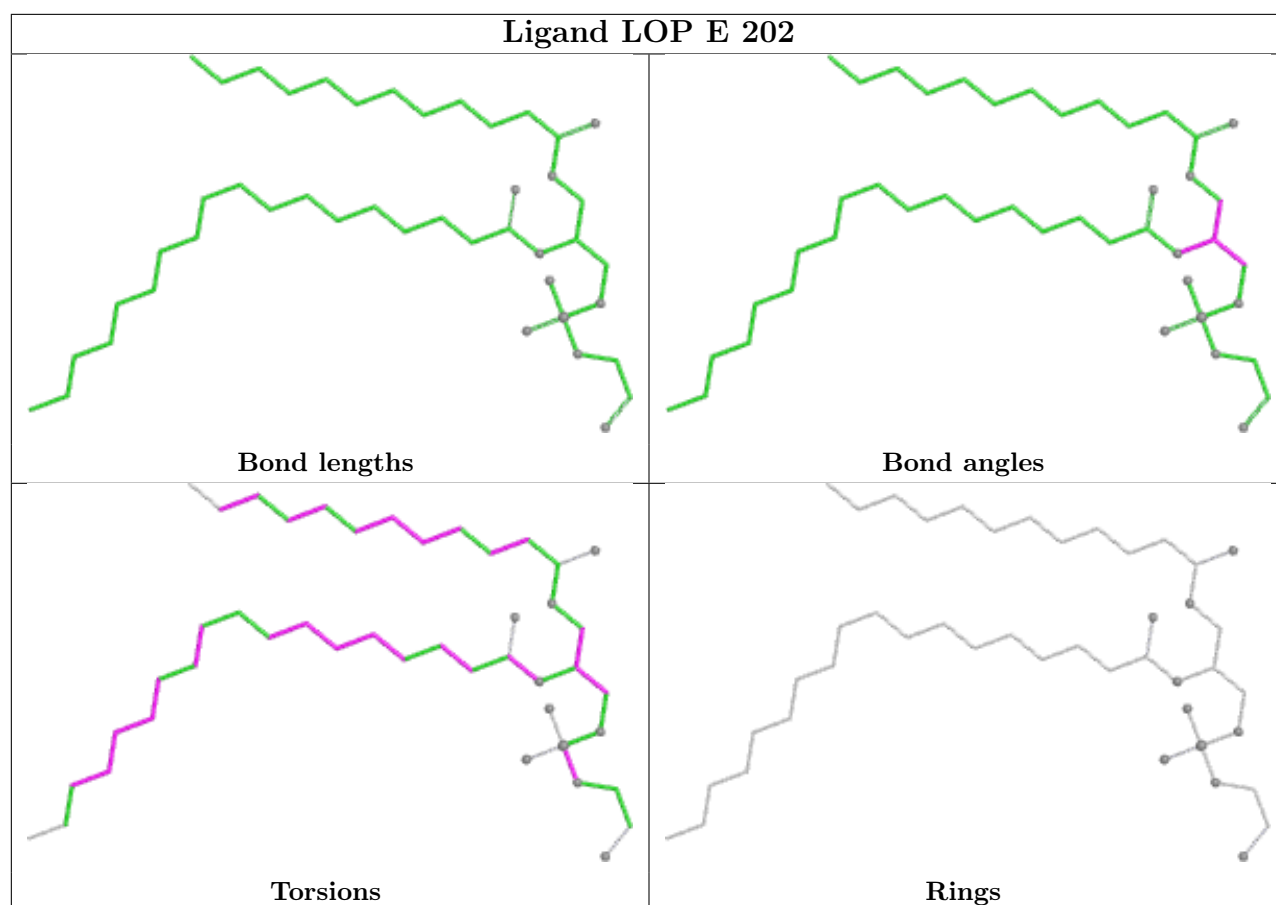


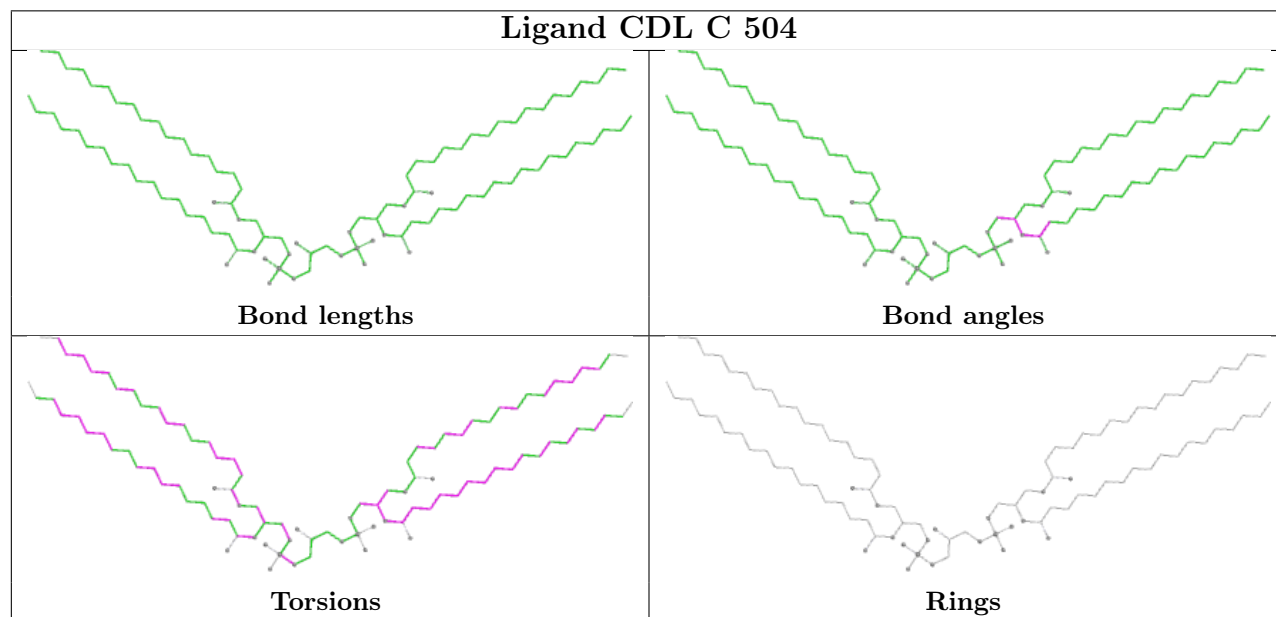
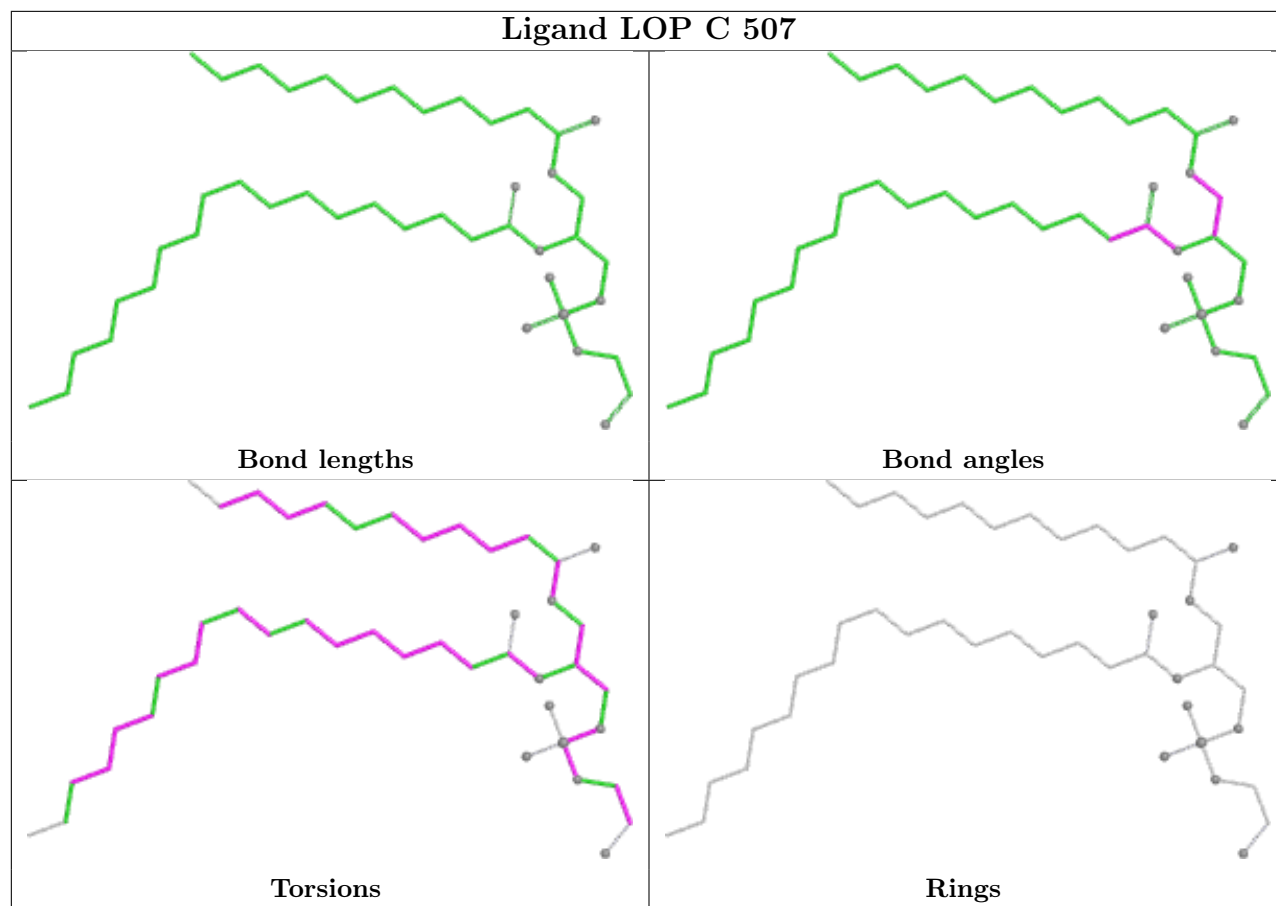


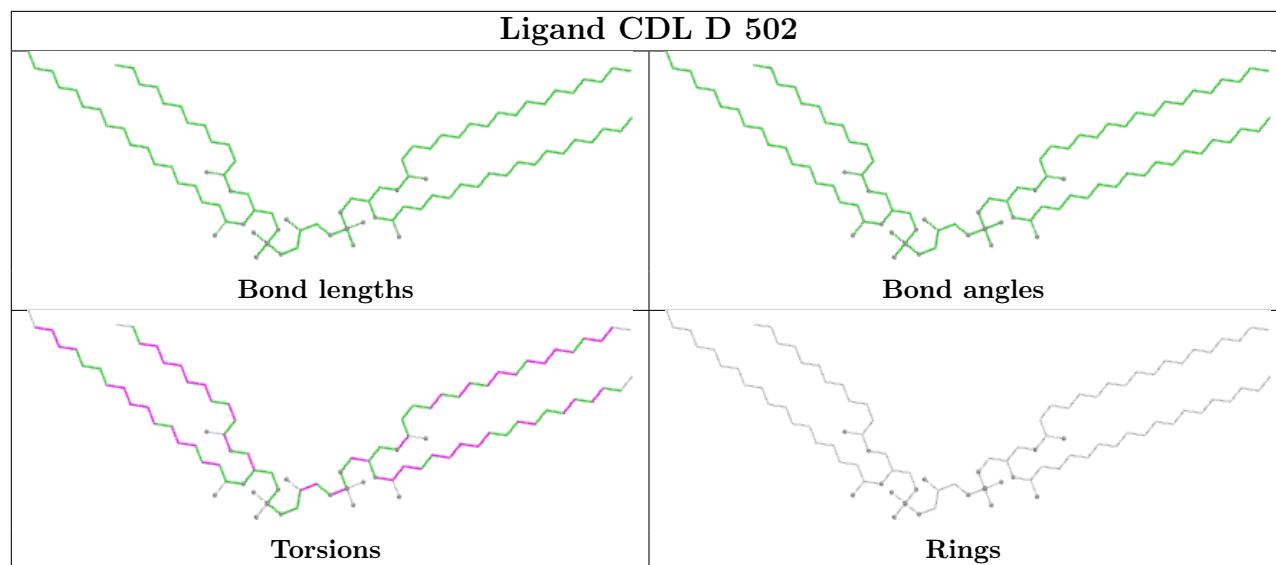












5.7 Other polymers [i](#)

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	440/480 (91%)	-0.77	0 100 100	70, 111, 146, 195	0
2	B	414/453 (91%)	-0.70	1 (0%) 91 81	47, 112, 148, 230	1 (0%)
3	C	378/379 (99%)	-0.63	1 (0%) 90 75	28, 104, 140, 195	3 (0%)
4	D	240/325 (73%)	-0.53	0 100 100	91, 140, 171, 199	0
5	E	196/274 (71%)	-0.31	2 (1%) 79 54	88, 156, 199, 240	0
5	I	27/274 (9%)	0.30	3 (11%) 10 7	101, 143, 177, 188	0
6	F	98/111 (88%)	-0.56	0 100 100	82, 107, 149, 167	0
7	G	74/82 (90%)	-0.61	0 100 100	80, 115, 155, 176	0
8	H	65/109 (59%)	-0.35	0 100 100	126, 164, 182, 200	0
9	J	56/64 (87%)	-0.59	0 100 100	101, 121, 149, 167	0
10	K	39/56 (69%)	0.61	3 (7%) 19 13	152, 185, 233, 265	0
All	All	2027/2607 (77%)	-0.58	10 (0%) 87 67	28, 116, 177, 265	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	LEU	4.0
5	E	114	VAL	3.1
3	C	237	LEU	2.6
5	E	178	LEU	2.5
10	K	13	LEU	2.5
5	I	70	LEU	2.4
5	I	71	ASN	2.4
10	K	34	TRP	2.3
10	K	48	ILE	2.2
5	I	62	ARG	2.1

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](#)

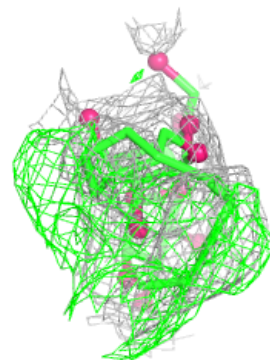
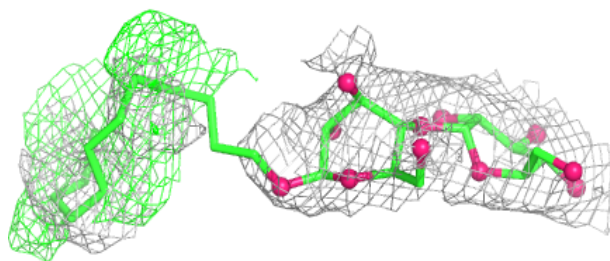
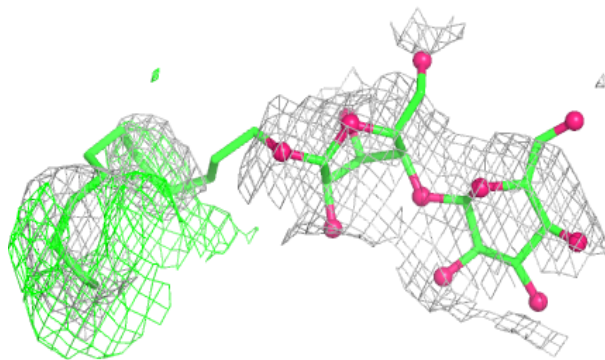
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	LMT	C	508	35/35	0.55	0.15	127,200,240,296	0
11	LOP	C	506	45/45	0.77	0.27	66,143,208,276	0
19	SO4	G	102	5/5	0.77	0.07	160,182,202,241	0
19	SO4	F	201	5/5	0.85	0.16	145,161,171,183	0
11	LOP	G	101	45/45	0.86	0.23	105,180,215,234	0
19	SO4	G	103	5/5	0.88	0.09	139,145,164,170	0
11	LOP	C	507	45/45	0.90	0.20	76,140,205,246	0
11	LOP	A	501	45/45	0.90	0.18	81,186,233,251	0
12	CDL	A	502	84/100	0.91	0.15	109,172,285,348	0
12	CDL	D	502	94/100	0.91	0.16	88,156,187,215	0
18	PSC	E	203	52/52	0.92	0.17	99,147,207,260	0
14	A1IKG	C	505	30/30	0.93	0.12	98,134,186,196	0
12	CDL	C	504	100/100	0.93	0.14	94,149,200,240	0
11	LOP	E	202	45/45	0.96	0.11	93,113,175,262	0
11	LOP	C	503	45/45	0.98	0.09	80,106,125,172	0
17	FES	E	201	4/4	0.98	0.06	220,233,252,274	0
16	HEC	D	501	43/43	0.99	0.07	116,138,150,162	0
13	HEM	C	501	43/43	0.99	0.05	86,94,105,128	0
13	HEM	C	502	43/43	0.99	0.06	62,96,111,124	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.

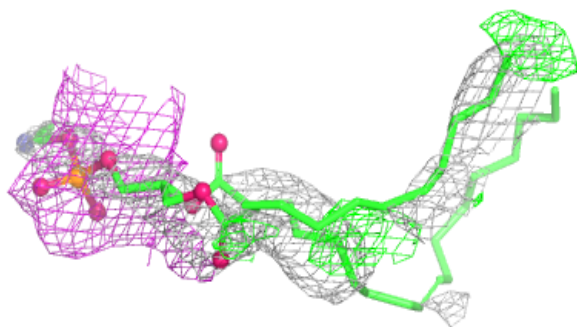
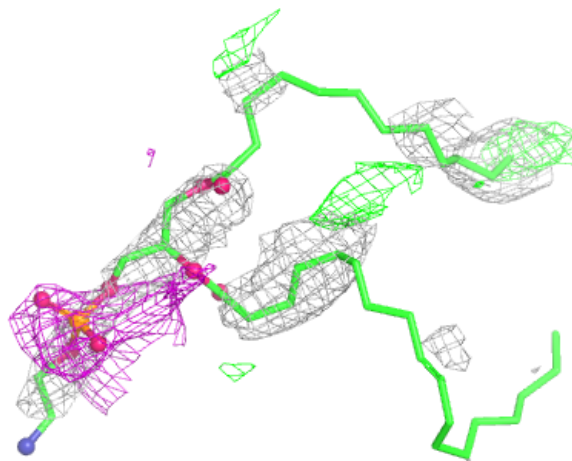
Electron density around LMT C 508:

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



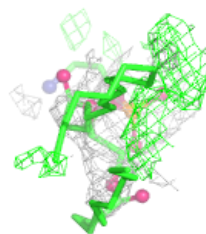
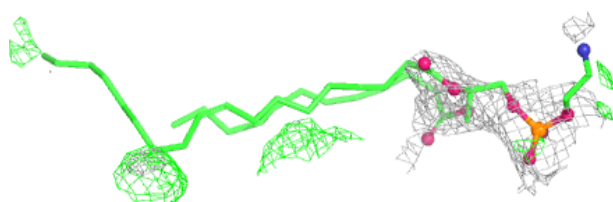
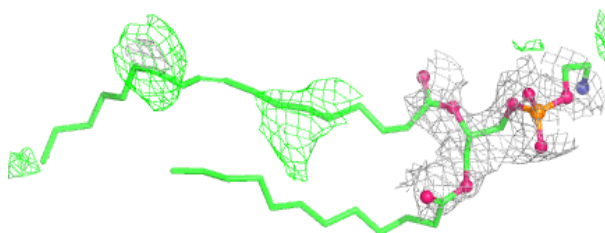
Electron density around LOP C 506:

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

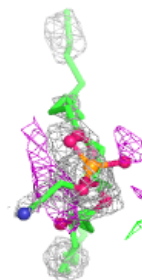
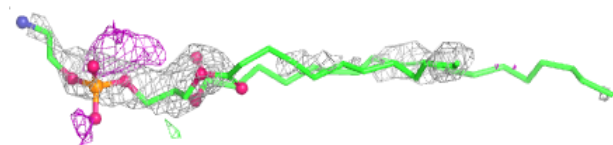
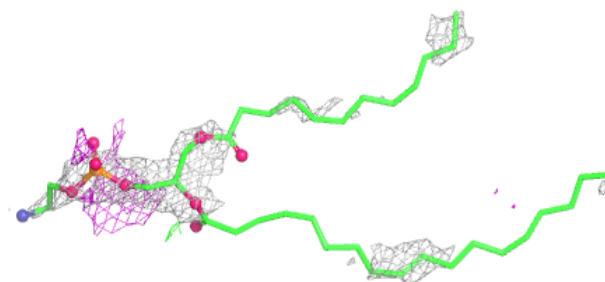


Electron density around LOP G 101:

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

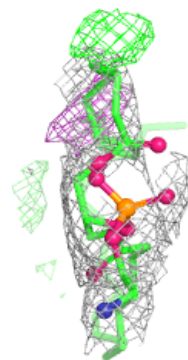
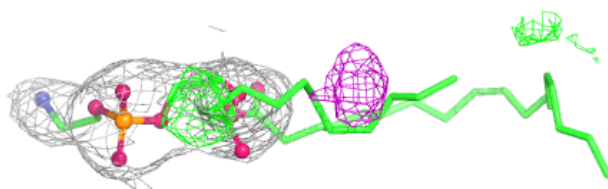
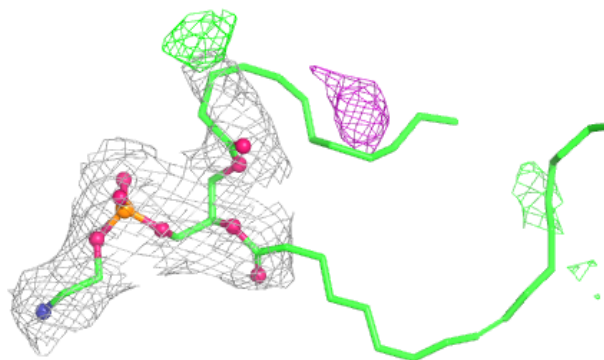
**Electron density around LOP C 507:**

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

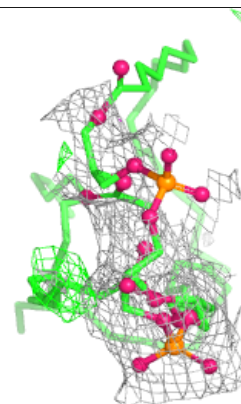
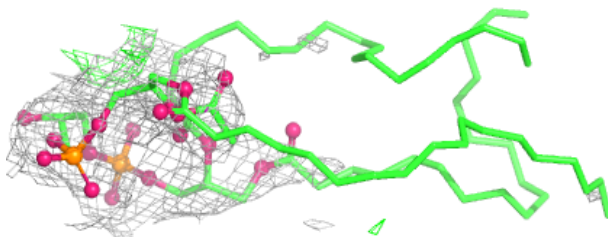
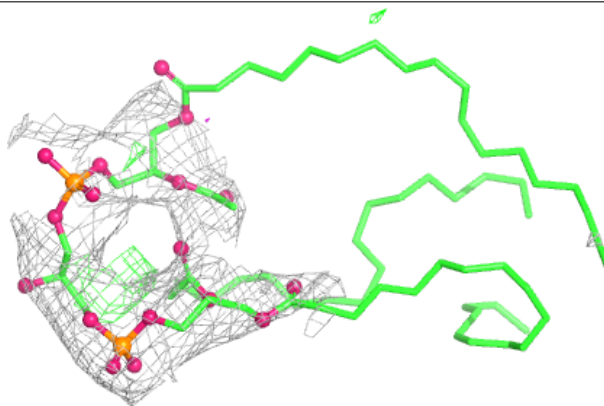


Electron density around LOP A 501:

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

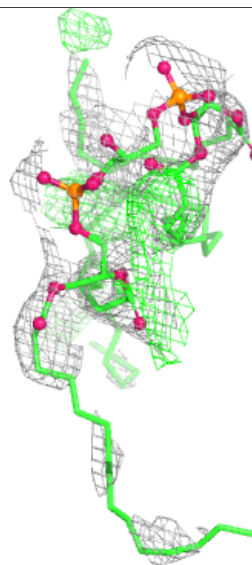
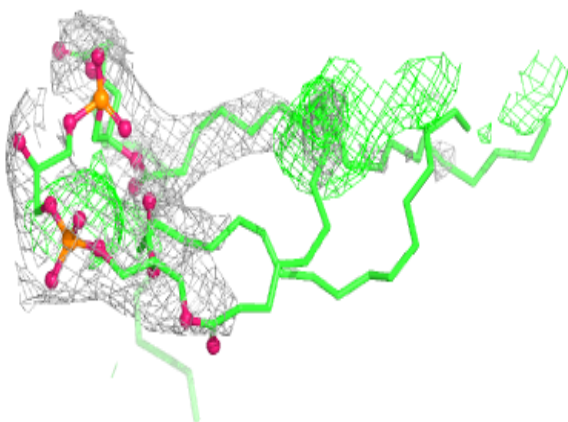
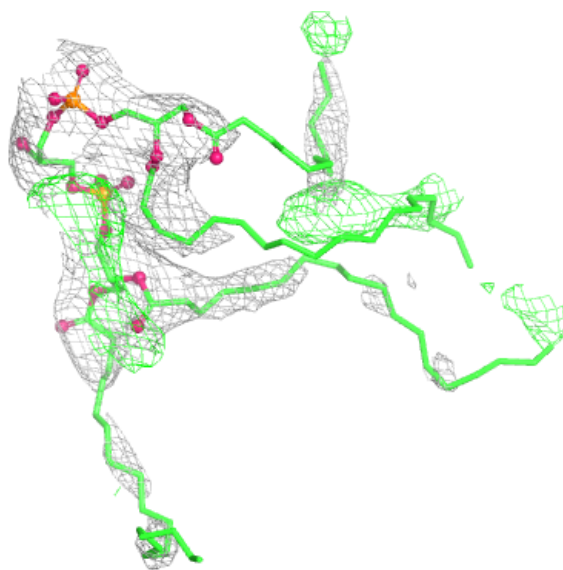
**Electron density around CDL A 502:**

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and green (positive)



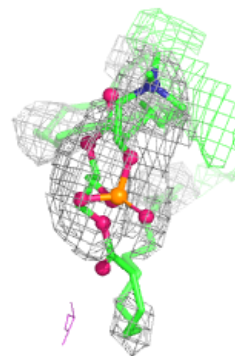
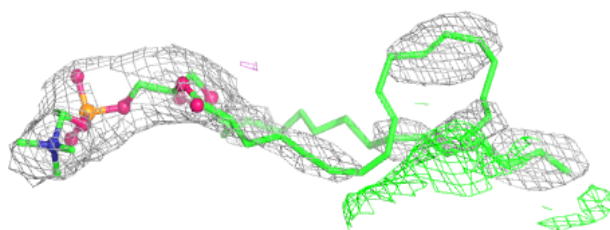
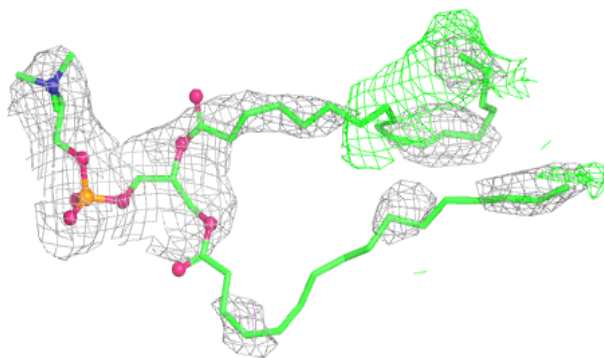
Electron density around CDL D 502:

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

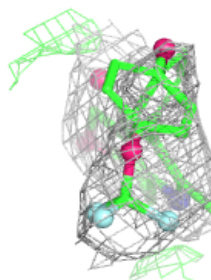
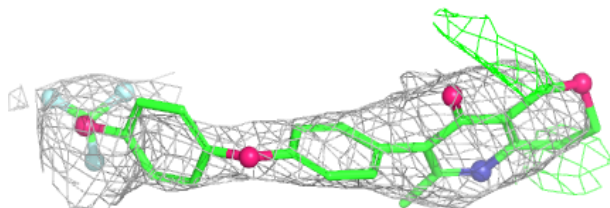
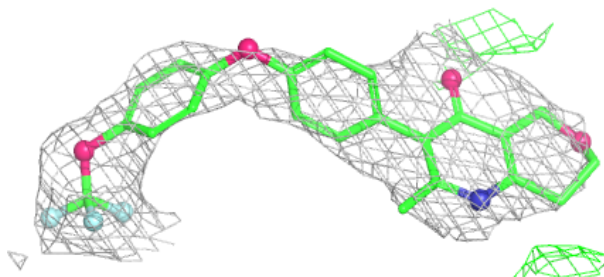


Electron density around PSC E 203:

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

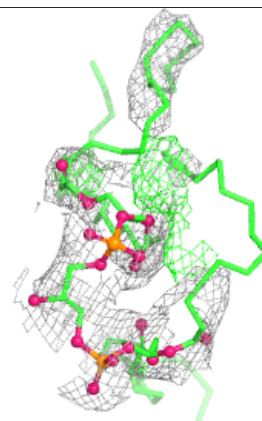
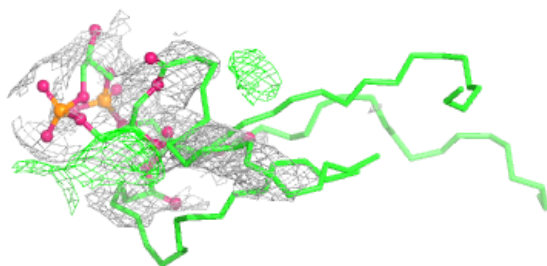
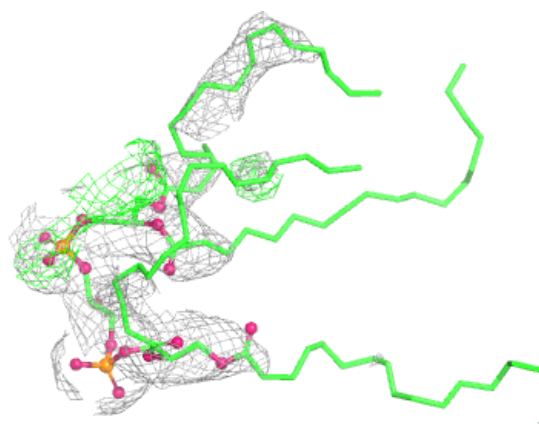
**Electron density around A1IKG C 505:**

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

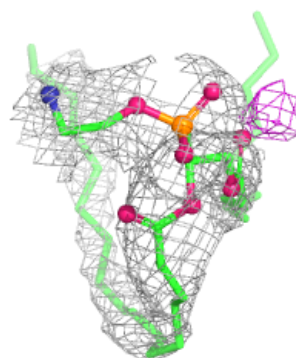
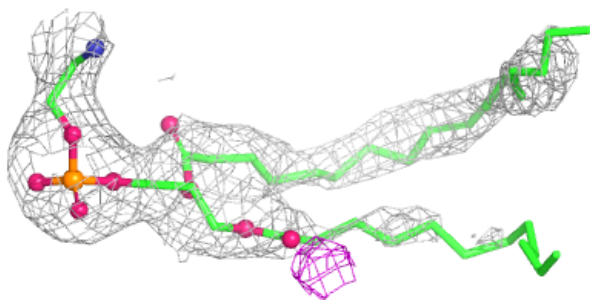
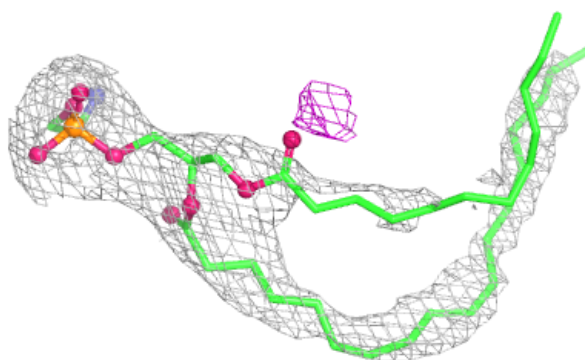


Electron density around CDL C 504:

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

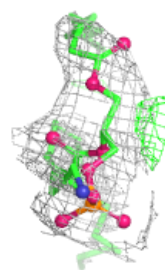
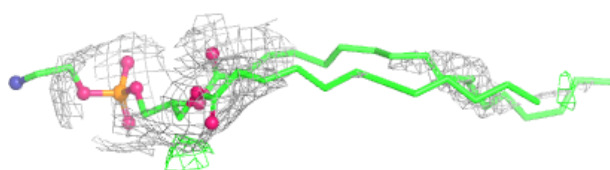
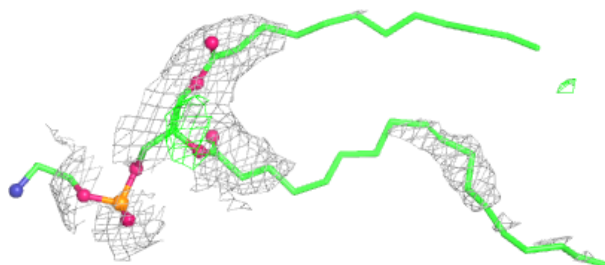
**Electron density around LOP E 202:**

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

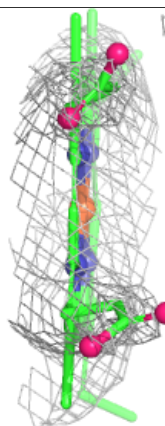
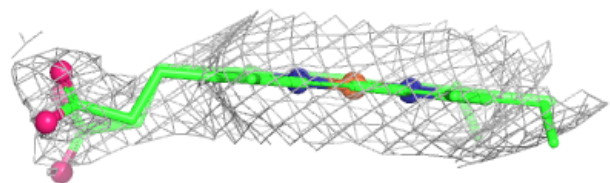
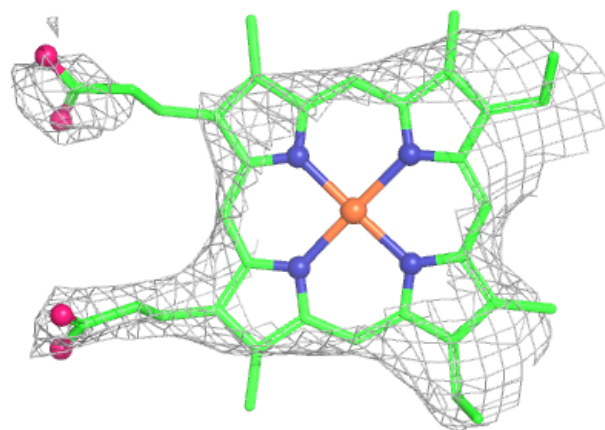


Electron density around LOP C 503:

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

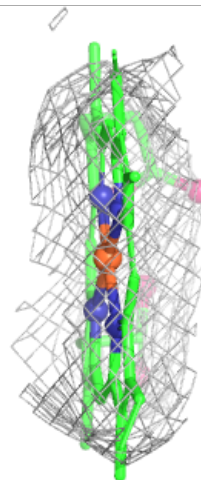
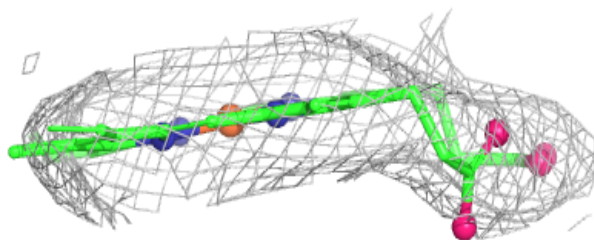
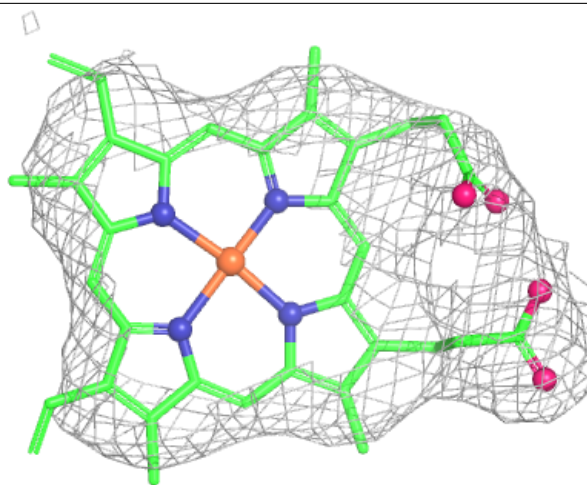
**Electron density around HEC D 501:**

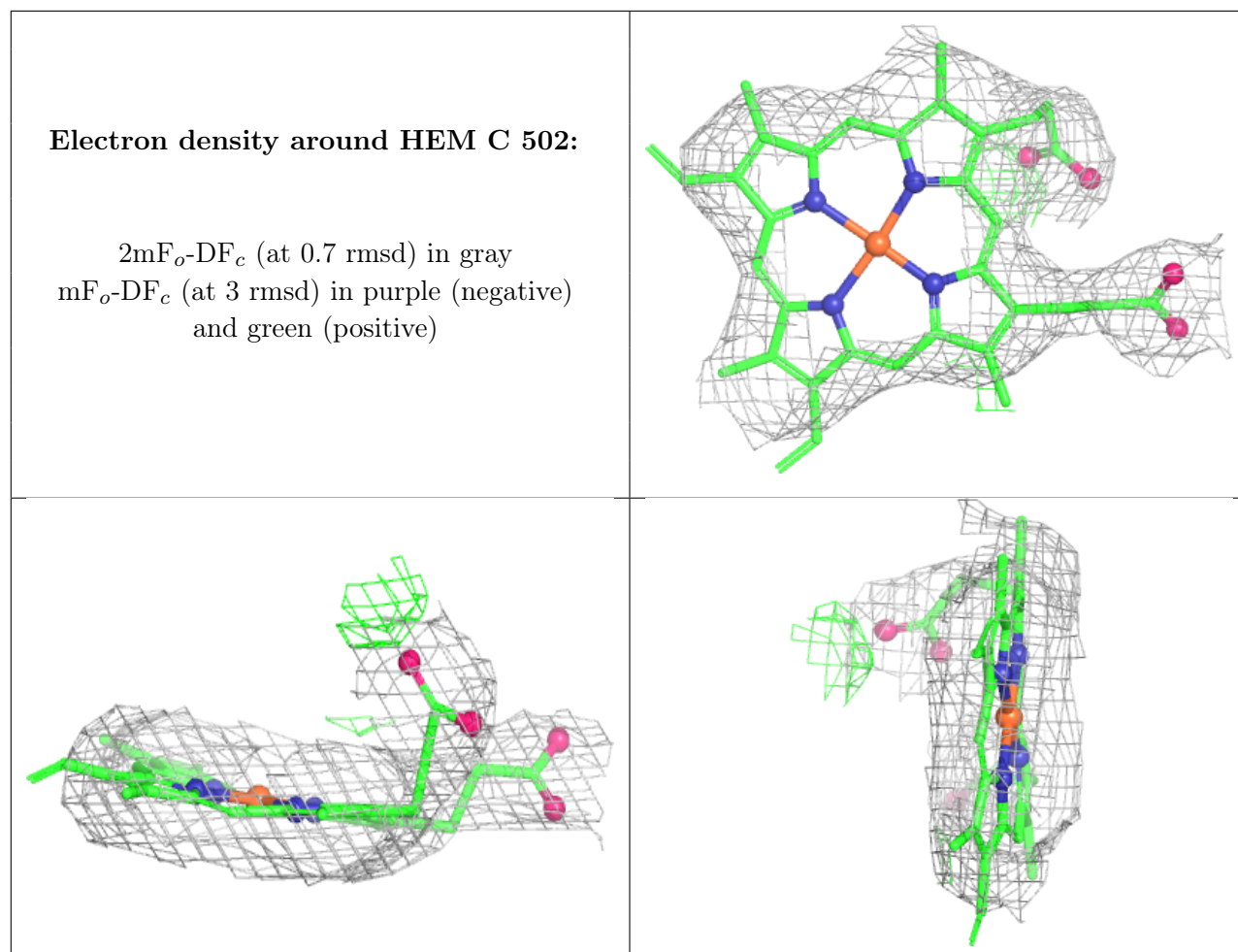
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

$2mF_o-DF_c$ (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.