



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 02:54 AM EDT

PDB ID : 4U3F / pdb_00004u3f
Title : Cytochrome bc1 complex from chicken with designed inhibitor bound
Authors : Huang, L.-S.; Zhu, X.-L.; Yang, G.F.; Berry, E.A.
Deposited on : 2014-07-21
Resolution : 3.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

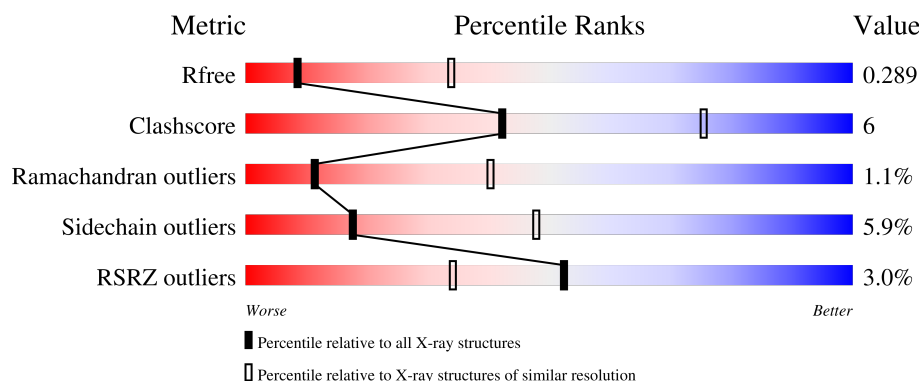
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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.



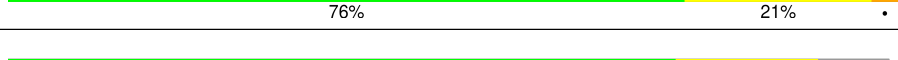
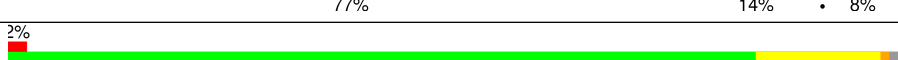
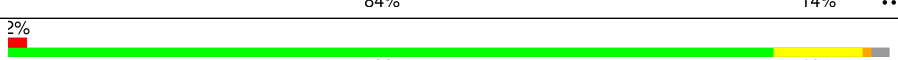
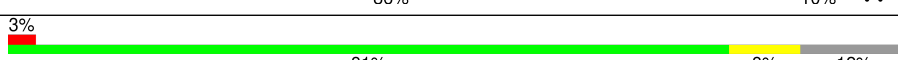
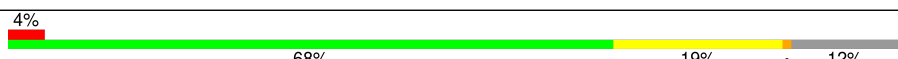
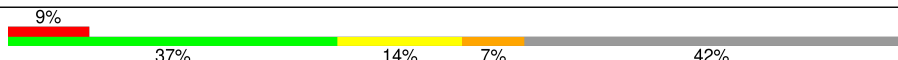
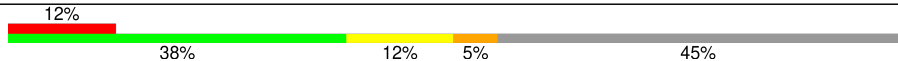
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	446	% 80% 18% ..
1	N	446	80% 18% ..
2	B	441	2% 71% 22% 5%
2	O	441	72% 21% . .
3	C	380	% 83% 16% .

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Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	76	
9	V	76	
10	J	61	
10	W	61	

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
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32790 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3137	1971	544	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3143	1974	545	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	1	0
			3022	2025	480	505	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	expression tag	UNP P18946
P	1	FME	-	expression tag	UNP P18946

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- 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
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	68	Total	C	N	O	S	0	0	0
			562	343	104	110	5			
8	U	68	Total	C	N	O	S	0	0	0
			558	341	104	108	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	44	Total	C	N	O	S	0	0	1
			266	157	54	53	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	42	Total	C	N	O	S	0	0	1
			265	157	55	51	2			

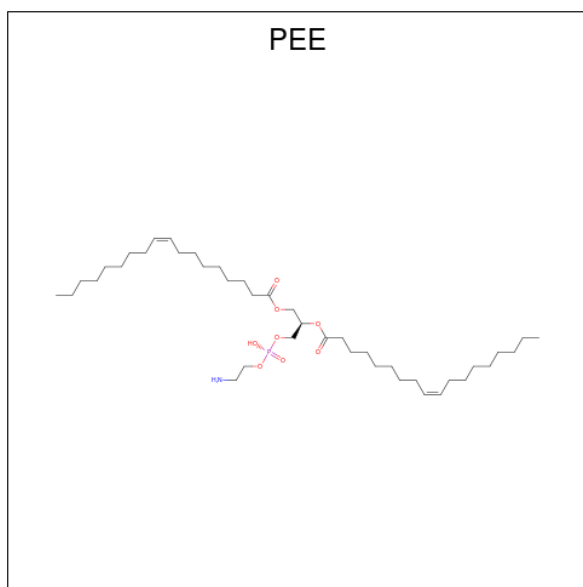
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	AME	-	expression tag	UNP Q5ZLR5
I	29	UNK	LEU	see remark 999	UNP Q5ZLR5
I	30	UNK	ALA	see remark 999	UNP Q5ZLR5
I	31	UNK	PRO	see remark 999	UNP Q5ZLR5
I	32	UNK	ALA	see remark 999	UNP Q5ZLR5
I	33	UNK	ALA	see remark 999	UNP Q5ZLR5
I	37	UNK	LEU	see remark 999	UNP Q5ZLR5
I	38	UNK	ARG	see remark 999	UNP Q5ZLR5
I	39	UNK	ALA	see remark 999	UNP Q5ZLR5
I	40	UNK	GLU	see remark 999	UNP Q5ZLR5
I	41	UNK	LYS	see remark 999	UNP Q5ZLR5
I	42	UNK	VAL	see remark 999	UNP Q5ZLR5
I	43	UNK	VAL	see remark 999	UNP Q5ZLR5
I	44	UNK	LEU	see remark 999	UNP Q5ZLR5
I	45	UNK	ASP	see remark 999	UNP Q5ZLR5
V	-1	AME	-	expression tag	UNP Q5ZLR5
V	27	UNK	LEU	see remark 999	UNP Q5ZLR5
V	28	UNK	ALA	see remark 999	UNP Q5ZLR5
V	29	UNK	PRO	see remark 999	UNP Q5ZLR5
V	30	UNK	ALA	see remark 999	UNP Q5ZLR5
V	31	UNK	ALA	see remark 999	UNP Q5ZLR5
V	32	UNK	LEU	see remark 999	UNP Q5ZLR5
V	33	UNK	ARG	see remark 999	UNP Q5ZLR5
V	37	UNK	ALA	see remark 999	UNP Q5ZLR5
V	38	UNK	GLU	see remark 999	UNP Q5ZLR5
V	39	UNK	LYS	see remark 999	UNP Q5ZLR5
V	40	UNK	VAL	see remark 999	UNP Q5ZLR5
V	41	UNK	VAL	see remark 999	UNP Q5ZLR5
V	42	UNK	LEU	see remark 999	UNP Q5ZLR5
V	43	UNK	ASP	see remark 999	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



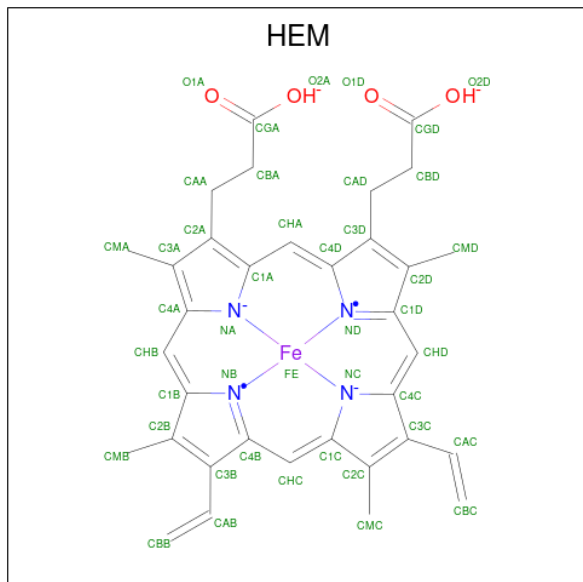
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
11	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
11	C	1	Total	C	O			0	0
			15	13	2				
11	E	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
11	E	1	Total	C				0	0
			15	15					
11	N	1	Total	C	N	O	P	0	0
			8	2	1	4	1		
11	P	1	Total	C	O			0	0
			15	13	2				

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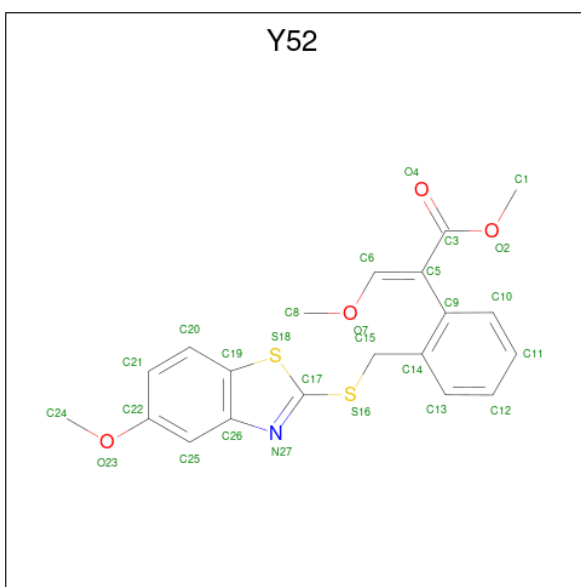
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			41	31	1	8	1		
11	P	1	Total	C	O			0	0
			12	10	2				
11	P	1	Total	C	N	O	P	0	0
			25	15	1	8	1		
11	R	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



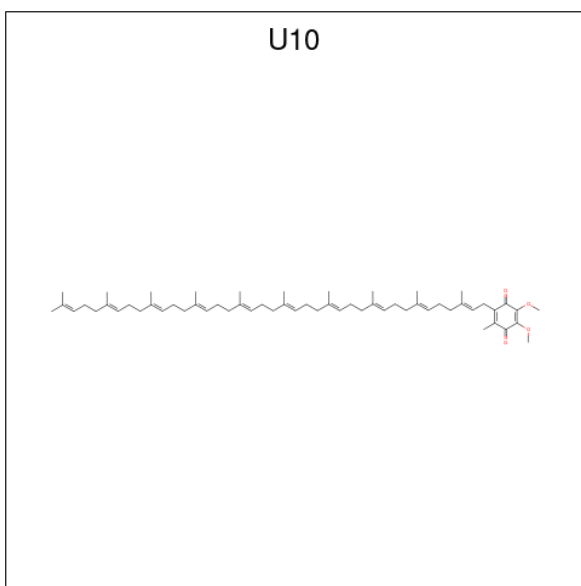
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is methyl (2E)-3-methoxy-2-(2-[(5-methoxy-1,3-benzothiazol-2-yl)sulfanyl]methyl}phenyl)prop-2-enoate (CCD ID: Y52) (formula: $C_{20}H_{19}NO_4S_2$).



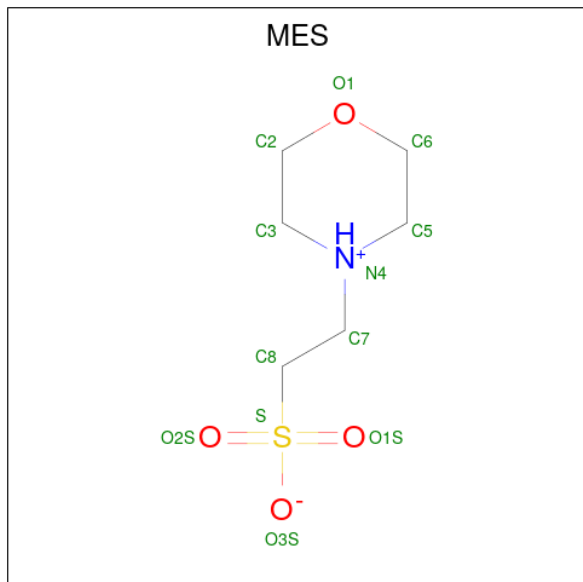
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 27	C 20	N 1	O 4	S 2	0	0
13	P	1	Total 27	C 20	N 1	O 4	S 2	0	0

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



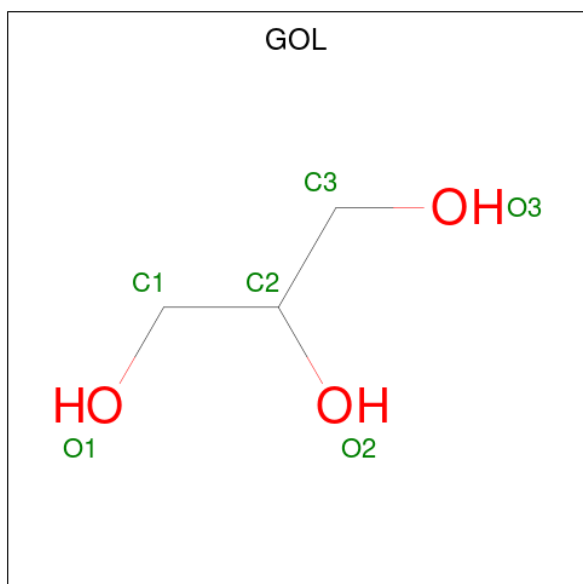
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



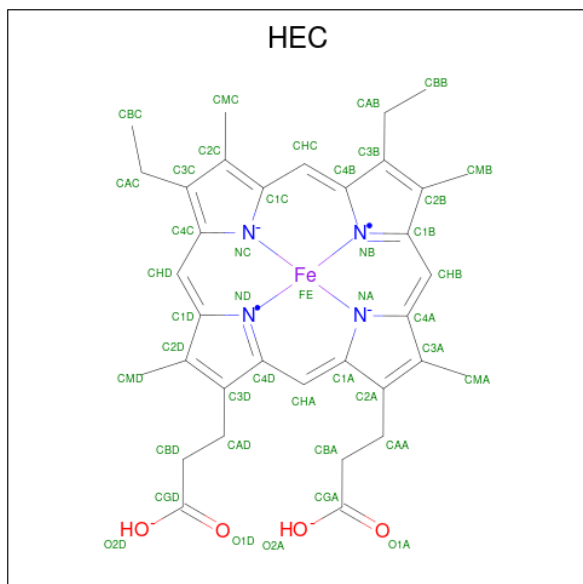
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		

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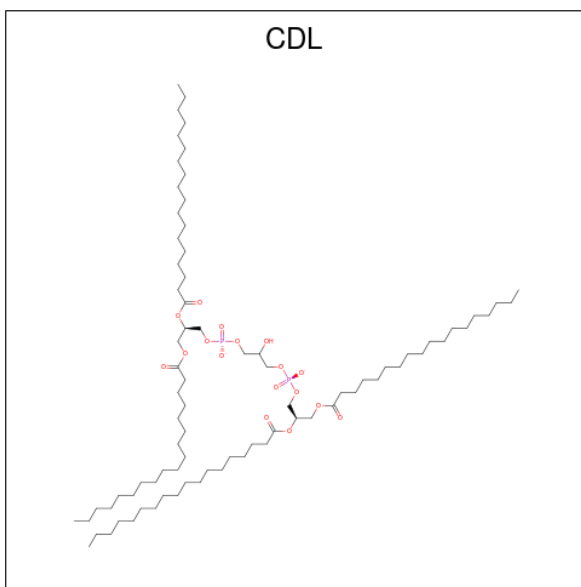
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



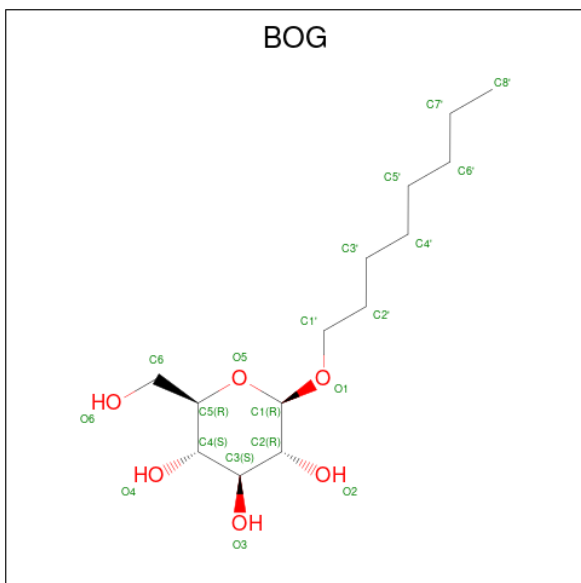
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



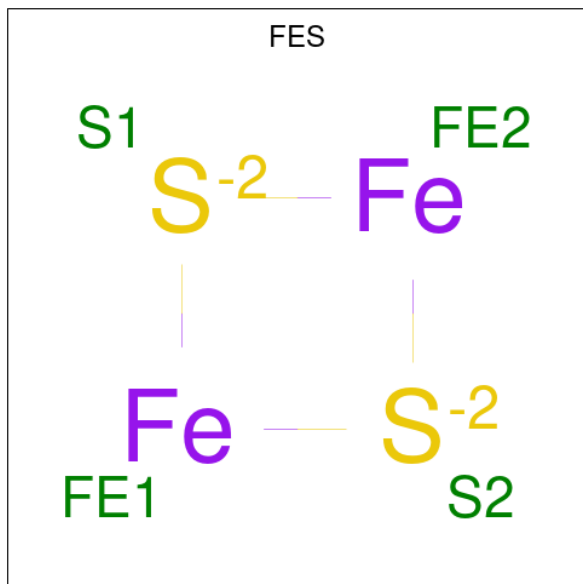
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			42	23	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		
18	Q	1	Total	C	O	P	0	0
			42	23	17	2		
18	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 19 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	C	O	0	0
			20	14	6		
19	P	1	Total	C	O	0	0
			20	14	6		
19	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	O	0	0
			2	2		
21	B	1	Total	O	0	0
			1	1		
21	C	2	Total	O	0	0
			2	2		
21	F	1	Total	O	0	0
			1	1		
21	N	1	Total	O	0	0
			1	1		

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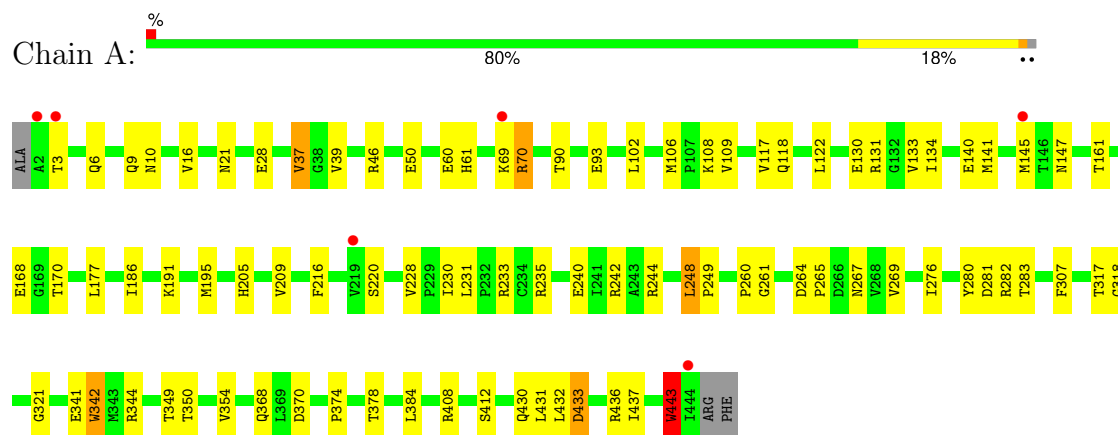
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	O	2	Total	O	0	0
			2	2		
21	P	2	Total	O	0	0
			2	2		

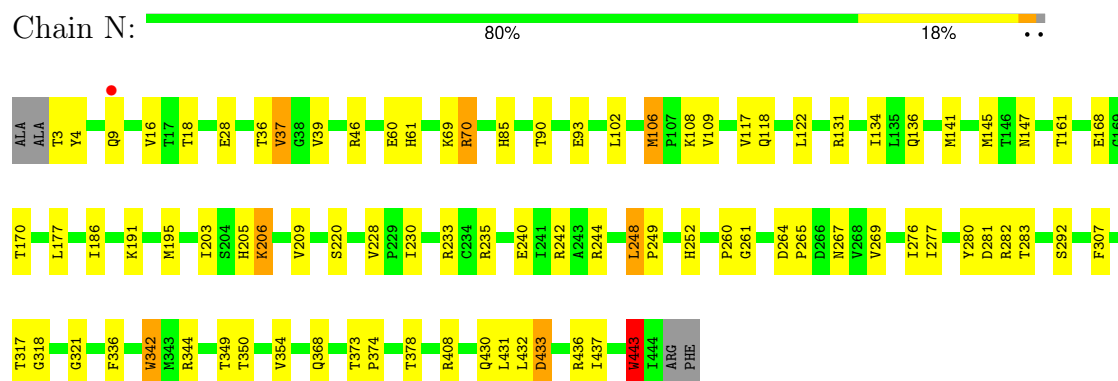
3 Residue-property plots

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.

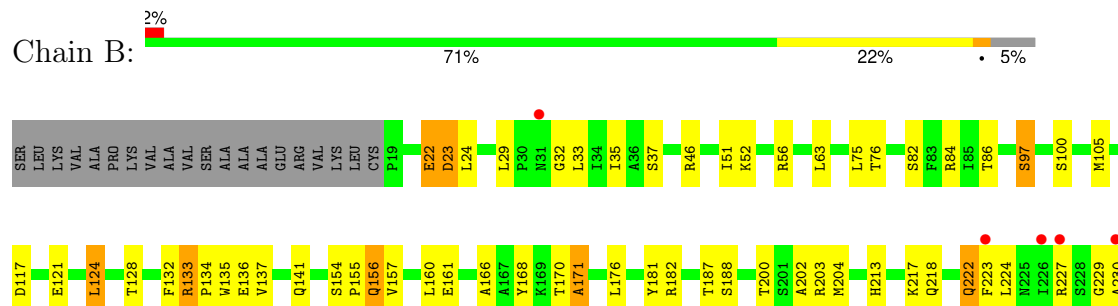
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

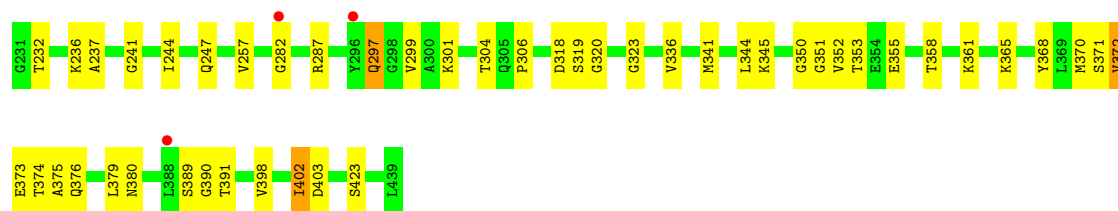


- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex protein 2





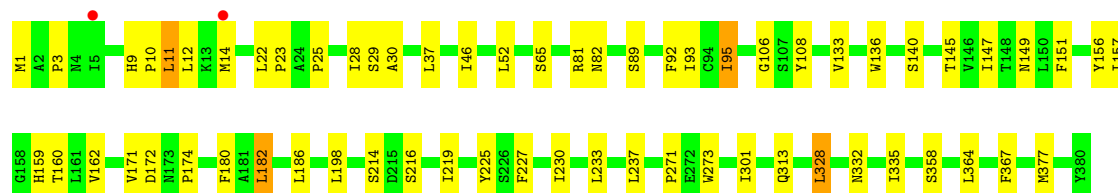
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain O: 72% 21%



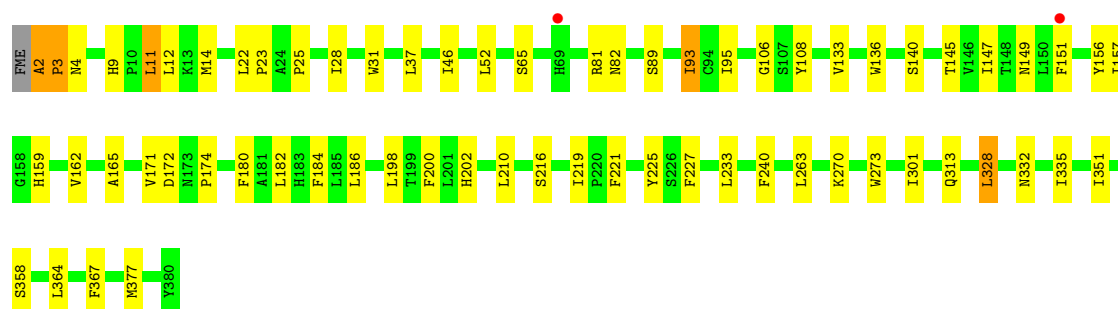
• Molecule 3: Cytochrome b

Chain C: 83% 16%

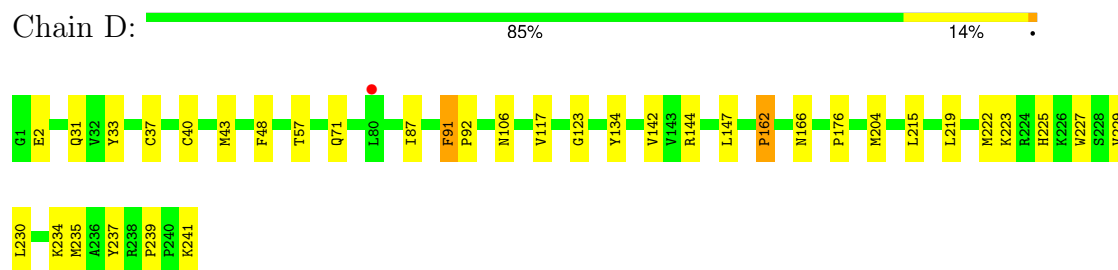


• Molecule 3: Cytochrome b

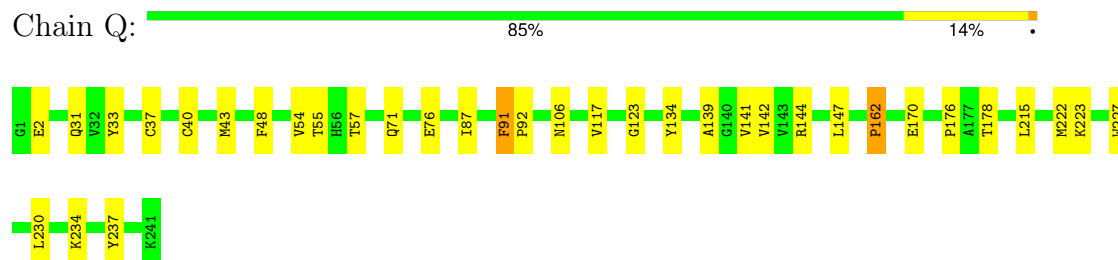
Chain P: 82% 16%



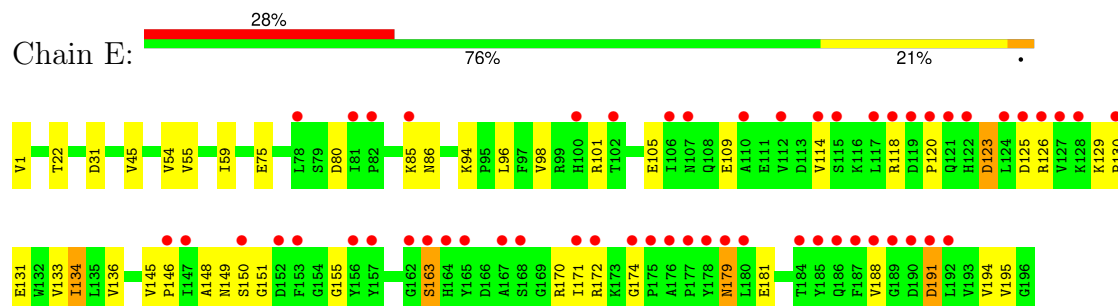
• Molecule 4: Mitochondrial cytochrome c1, heme protein



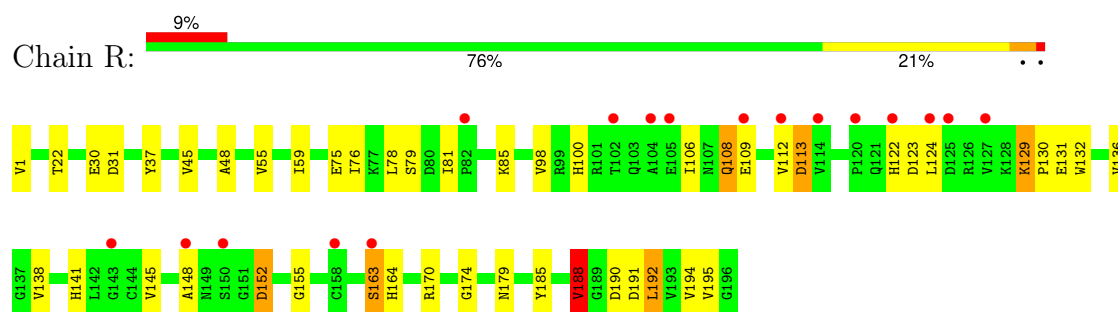
- Molecule 4: Mitochondrial cytochrome c1, heme protein



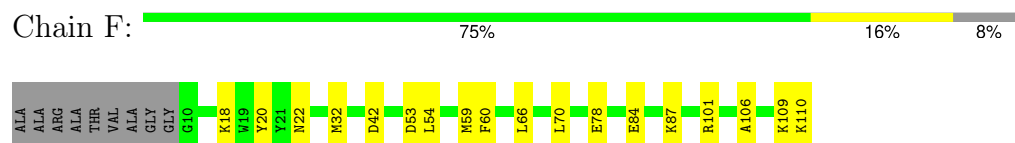
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



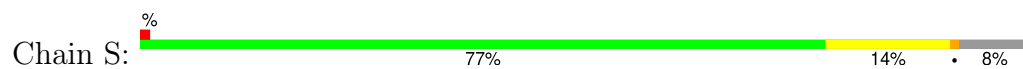
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



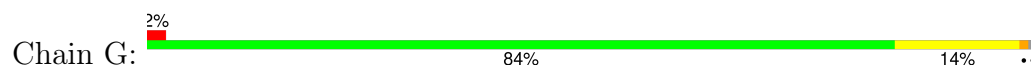
- Molecule 6: Cytochrome b-c1 complex subunit 7



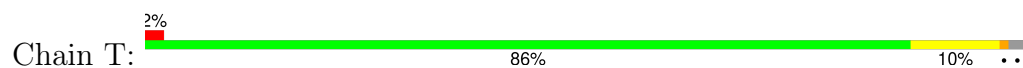
- Molecule 6: Cytochrome b-c1 complex subunit 7



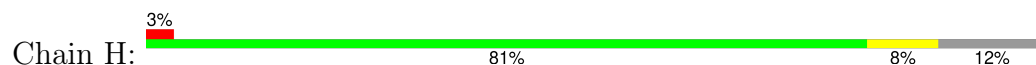
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



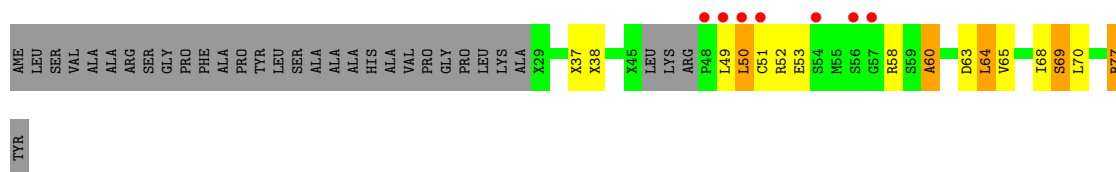
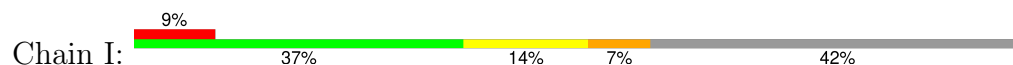
- Molecule 8: Cytochrome b-c1 complex subunit 6



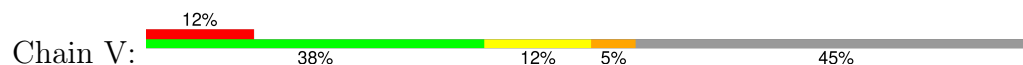
- Molecule 8: Cytochrome b-c1 complex subunit 6

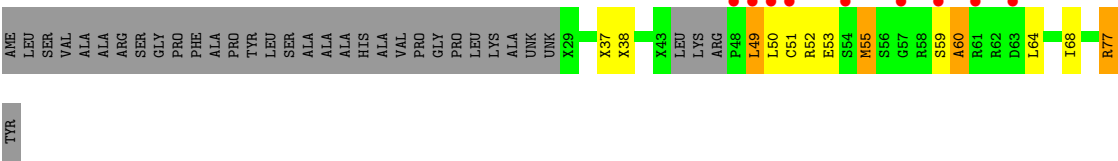


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

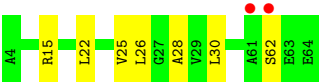
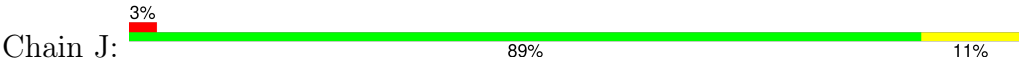


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

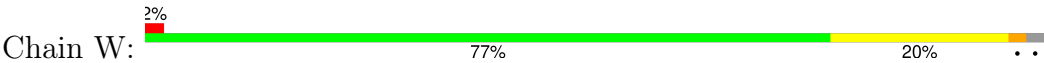




● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	167.25Å 181.48Å 239.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.23 15.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-3.23) 81.5 (15.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, R_{free}	0.236 , 0.284 0.246 , 0.289	Depositor DCC
R_{free} test set	2286 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	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	0.88	EDS
Total number of atoms	32790	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: Y52, MES, GOL, PEE, U10, FME, FES, HEC, CDL, HEM, BOG

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	0.27	0/3513	0.73	0/4760
1	N	0.27	0/3508	0.71	0/4753
2	B	0.28	0/3192	0.74	5/4330 (0.1%)
2	O	0.28	0/3198	0.77	6/4339 (0.1%)
3	C	0.30	0/3114	0.74	0/4263
3	P	0.29	0/3102	0.75	2/4245 (0.0%)
4	D	0.27	0/1956	0.75	2/2658 (0.1%)
4	Q	0.28	0/1956	0.76	2/2658 (0.1%)
5	E	0.27	0/1547	0.73	0/2103
5	R	0.26	0/1543	0.75	2/2098 (0.1%)
6	F	0.25	0/911	0.63	0/1219
6	S	0.25	0/911	0.65	0/1219
7	G	0.31	0/694	0.73	0/941
7	T	0.31	0/684	0.75	0/929
8	H	0.27	0/570	0.67	0/763
8	U	0.27	0/566	0.72	0/758
9	I	0.27	0/208	0.92	0/279
9	V	0.26	0/215	0.88	0/288
10	J	0.25	0/508	0.61	0/682
10	W	0.25	0/490	0.66	0/660
All	All	0.28	0/32386	0.73	19/43945 (0.0%)

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	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	18	CYS	CA-C-N	10.52	132.99	119.84
2	O	18	CYS	C-N-CA	10.52	132.99	119.84
3	P	2	ALA	CA-C-N	5.72	126.99	119.84
3	P	2	ALA	C-N-CA	5.72	126.99	119.84
4	D	91	PHE	CA-C-N	5.57	125.50	119.76
4	D	91	PHE	C-N-CA	5.57	125.50	119.76
2	B	133	ARG	CA-C-N	5.54	125.64	119.32
2	B	133	ARG	C-N-CA	5.54	125.64	119.32
2	O	133	ARG	CA-C-N	5.45	125.53	119.32
2	O	133	ARG	C-N-CA	5.45	125.53	119.32
4	Q	91	PHE	CA-C-N	5.39	125.31	119.76
4	Q	91	PHE	C-N-CA	5.39	125.31	119.76
5	R	129	LYS	CA-C-N	5.38	125.09	119.82
5	R	129	LYS	C-N-CA	5.38	125.09	119.82
2	B	32	GLY	N-CA-C	-5.20	107.51	115.00
2	B	282	GLY	CA-C-N	5.15	125.15	119.90
2	B	282	GLY	C-N-CA	5.15	125.15	119.90
2	O	282	GLY	CA-C-N	5.03	125.03	119.90
2	O	282	GLY	C-N-CA	5.03	125.03	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3354	45	0
1	N	3437	0	3349	42	0
2	B	3137	0	3131	58	0
2	O	3143	0	3135	59	0
3	C	3021	0	3068	40	0
3	P	3022	0	3064	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1898	0	1846	19	0
4	Q	1898	0	1846	18	0
5	E	1513	0	1480	21	0
5	R	1509	0	1476	22	0
6	F	891	0	893	10	0
6	S	891	0	893	11	0
7	G	672	0	653	10	0
7	T	662	0	645	10	0
8	H	562	0	545	2	0
8	U	558	0	541	8	0
9	I	266	0	223	15	0
9	V	265	0	239	11	0
10	J	497	0	490	3	0
10	W	479	0	478	6	0
11	A	26	0	26	1	0
11	C	122	0	174	2	0
11	E	63	0	99	6	0
11	N	8	0	7	0	0
11	P	142	0	193	7	0
11	R	49	0	75	5	0
12	C	86	0	60	7	0
12	P	86	0	60	8	0
13	C	27	0	19	2	0
13	P	27	0	19	1	0
14	C	19	0	17	0	0
14	P	19	0	17	1	0
15	C	12	0	13	0	0
16	C	6	0	8	1	0
16	P	6	0	8	1	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	42	0	28	1	0
18	G	40	0	24	1	0
18	Q	42	0	28	0	0
18	T	40	0	24	3	0
19	D	20	0	28	0	0
19	P	20	0	28	3	0
19	Q	20	0	28	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	2	0	0	0	0
21	F	1	0	0	0	0
21	N	1	0	0	0	0
21	O	2	0	0	1	0
21	P	2	0	0	1	0
All	All	32790	0	32392	408	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 6.

All (408) 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)
9:V:37:UNK:HG3	9:V:38:UNK:H	1.37	0.90
9:V:49:LEU:HB2	9:V:55:MET:HB3	1.57	0.85
9:I:37:UNK:HG3	9:I:38:UNK:N	1.94	0.81
9:I:37:UNK:HG3	9:I:38:UNK:H	1.47	0.78
2:B:361:LYS:HD2	2:B:403:ASP:HA	1.67	0.76
2:O:361:LYS:HD2	2:O:403:ASP:HA	1.66	0.76
9:V:37:UNK:CG	9:V:38:UNK:H	2.00	0.75
2:O:389:SER:O	2:O:391:THR:N	2.22	0.72
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.71	0.72
2:O:226:ILE:HG22	2:O:227:ARG:H	1.55	0.72
2:B:389:SER:O	2:B:391:THR:N	2.22	0.71
2:B:306:PRO:HB3	9:I:52:ARG:HB2	1.73	0.70
4:D:166:ASN:HD21	8:H:15:ASP:HB2	1.56	0.70
8:U:40:CYS:SG	8:U:43:ARG:NH2	2.64	0.70
1:N:248:LEU:HD13	1:N:249:PRO:HD2	1.73	0.70
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.73	0.69
1:A:248:LEU:HD13	1:A:249:PRO:HD2	1.73	0.69
2:B:52:LYS:O	2:B:203:ARG:NH2	2.26	0.69
2:B:236:LYS:HE3	2:B:318:ASP:HB2	1.75	0.69
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.76	0.68
9:V:37:UNK:HG3	9:V:38:UNK:N	2.01	0.68
5:R:188:VAL:HG23	5:R:192:LEU:HB3	1.76	0.68
9:I:37:UNK:CG	9:I:38:UNK:H	2.07	0.67
2:O:46:ARG:NH2	2:O:376:GLN:OE1	2.28	0.67
2:O:52:LYS:O	2:O:203:ARG:NH2	2.26	0.67
3:C:81:ARG:HH12	16:C:508:GOL:H2	1.60	0.66
1:A:261:GLY:O	1:A:267:ASN:ND2	2.28	0.66
1:A:244:ARG:HE	7:G:10:VAL:HB	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.78	0.66
11:E:502:PEE:H62	10:J:25:VAL:HG22	1.78	0.66
1:N:261:GLY:O	1:N:267:ASN:ND2	2.29	0.66
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.78	0.64
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.79	0.64
2:B:86:THR:HA	9:I:70:LEU:HD11	1.81	0.63
4:D:239:PRO:HG2	4:D:241:LYS:HB2	1.79	0.63
1:A:131:ARG:NH2	1:A:177:LEU:O	2.31	0.63
1:N:131:ARG:NH2	1:N:177:LEU:O	2.32	0.63
9:I:60:ALA:HA	9:I:77:ARG:HH22	1.64	0.62
3:C:216:SER:HB3	6:F:59:MET:HE2	1.82	0.62
3:P:89:SER:HG	3:P:273:TRP:HE1	1.47	0.61
2:B:46:ARG:NH2	2:B:376:GLN:OE1	2.33	0.61
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.61
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.84	0.60
5:E:101:ARG:NH2	5:E:130:PRO:O	2.34	0.60
6:F:106:ALA:HA	6:F:109:LYS:HE2	1.82	0.60
12:C:501:HEM:HBB2	12:C:501:HEM:HMB2	1.84	0.60
12:C:501:HEM:HMC1	12:C:501:HEM:HBC2	1.84	0.60
1:N:141:MET:HE3	1:N:147:ASN:HD21	1.67	0.60
7:T:40:ARG:NH1	18:T:101:CDL:OA4	2.35	0.60
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.34	0.59
1:A:412:SER:O	10:J:15:ARG:NH2	2.35	0.59
12:P:403:HEM:HMC2	12:P:403:HEM:HBC2	1.84	0.59
3:P:216:SER:HB3	6:S:59:MET:HE2	1.83	0.59
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.84	0.59
19:P:406:BOG:H4	11:R:502:PEE:H24	1.84	0.59
4:Q:178:THR:HG21	8:U:16:PRO:HD3	1.84	0.59
11:E:502:PEE:H42	11:E:503:PEE:H32	1.84	0.58
2:O:225:ASN:HD22	2:O:226:ILE:H	1.50	0.58
12:P:402:HEM:HMC1	12:P:402:HEM:HBC2	1.84	0.58
1:A:141:MET:HE3	1:A:147:ASN:HD21	1.68	0.58
11:A:501:PEE:H57	11:E:502:PEE:H57	1.86	0.58
4:D:144:ARG:HB3	4:D:147:LEU:HD12	1.85	0.58
3:C:89:SER:HG	3:C:273:TRP:HE1	1.48	0.58
12:P:402:HEM:HMB2	12:P:402:HEM:HBB2	1.84	0.58
4:Q:144:ARG:HB3	4:Q:147:LEU:HD12	1.85	0.58
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.86	0.58
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.37	0.58
1:N:60:GLU:OE1	2:O:287:ARG:NH2	2.37	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.70	0.57
5:E:118:ARG:NH1	5:E:172:ARG:O	2.37	0.57
3:P:202:HIS:NE2	14:P:405:U10:O2	2.38	0.57
2:B:56:ARG:HG2	2:B:171:ALA:HB1	1.87	0.57
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.87	0.57
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.86	0.57
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.87	0.57
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.69	0.56
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.86	0.56
4:D:204:MET:HE3	11:E:503:PEE:H16	1.87	0.56
5:R:113:ASP:OD2	5:R:113:ASP:N	2.34	0.56
2:O:287:ARG:HA	9:V:53:GLU:HB3	1.86	0.56
12:P:403:HEM:HMB1	12:P:403:HEM:HBB2	1.87	0.56
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.88	0.56
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.87	0.56
2:B:156:GLN:NE2	21:B:501:HOH:O	2.38	0.55
1:N:244:ARG:HE	7:T:10:VAL:HB	1.70	0.55
2:O:56:ARG:HG2	2:O:171:ALA:HB1	1.87	0.55
2:O:117:ASP:OD1	2:O:117:ASP:N	2.39	0.55
8:U:18:THR:HA	8:U:21:ARG:HB2	1.88	0.55
5:E:163:SER:HA	5:E:174:GLY:HA3	1.88	0.55
2:O:128:THR:HG21	2:O:224:LEU:HG	1.89	0.55
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.87	0.55
5:R:76:ILE:HD13	5:R:98:VAL:HG21	1.89	0.55
3:C:198:LEU:HD21	12:C:502:HEM:HMA3	1.88	0.55
1:A:349:THR:O	1:A:408:ARG:NH1	2.40	0.54
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.89	0.54
12:C:502:HEM:HMB1	12:C:502:HEM:HBB2	1.88	0.54
1:A:161:THR:HG21	1:A:235:ARG:H	1.71	0.54
3:P:198:LEU:HD21	12:P:403:HEM:HMA3	1.88	0.54
3:P:93:ILE:HD12	3:P:240:PHE:HZ	1.72	0.54
5:E:136:VAL:HB	5:E:181:GLU:HB3	1.89	0.54
2:O:350:GLY:O	2:O:352:VAL:N	2.39	0.54
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.89	0.54
1:N:349:THR:O	1:N:408:ARG:NH1	2.40	0.54
3:C:180:PHE:HE1	3:P:180:PHE:HE1	1.56	0.53
1:A:6:GLN:HA	1:A:9:GLN:HE21	1.73	0.53
8:U:13:LEU:HB2	8:U:14:VAL:HA	1.90	0.53
2:B:353:THR:HG22	2:B:355:GLU:H	1.73	0.53
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.91	0.53
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:PHE:O	2:B:188:SER:OG	2.27	0.52
3:C:147:ILE:HG13	13:C:503:Y52:H12	1.91	0.52
2:O:132:PHE:O	2:O:188:SER:OG	2.27	0.52
1:N:4:TYR:HB2	2:O:113:ARG:HB2	1.92	0.52
2:O:353:THR:HG22	2:O:355:GLU:H	1.73	0.52
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.92	0.52
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.91	0.52
6:F:32:MET:HE3	6:F:87:LYS:HE2	1.92	0.51
2:O:306:PRO:HB3	9:V:52:ARG:N	2.25	0.51
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.91	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.93	0.51
3:P:81:ARG:HH12	16:P:408:GOL:H2	1.74	0.51
5:R:79:SER:OG	5:R:191:ASP:OD2	2.29	0.51
2:O:189:GLU:N	2:O:189:GLU:OE2	2.43	0.51
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.93	0.51
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.92	0.51
3:C:182:LEU:HD21	11:C:509:PEE:H3	1.92	0.51
3:P:147:ILE:HG13	13:P:404:Y52:H12	1.91	0.51
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.92	0.51
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.92	0.51
2:O:37:SER:HB3	2:O:213:HIS:ND1	2.26	0.51
1:N:145:MET:HB3	1:N:252:HIS:CE1	2.46	0.51
1:A:244:ARG:NE	7:G:10:VAL:HB	2.26	0.51
2:O:157:VAL:HG23	9:V:64:LEU:HD11	1.93	0.51
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.93	0.51
2:B:117:ASP:OD1	2:B:117:ASP:N	2.39	0.50
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.76	0.50
2:B:154:SER:O	2:B:157:VAL:HG12	2.11	0.50
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.92	0.50
2:B:350:GLY:O	2:B:352:VAL:N	2.39	0.50
2:O:84:ARG:NH2	2:O:121:GLU:OE2	2.45	0.50
1:A:3:THR:OG1	1:A:6:GLN:OE1	2.23	0.50
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.93	0.50
2:O:154:SER:O	2:O:157:VAL:HG12	2.11	0.50
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.47	0.50
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.49
2:B:84:ARG:NH2	2:B:121:GLU:OE2	2.45	0.49
3:C:29:SER:HB2	18:G:101:CDL:HB21	1.94	0.49
2:O:31:ASN:OD1	2:O:31:ASN:N	2.43	0.49
5:R:122:HIS:CG	5:R:123:ASP:H	2.31	0.49
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:THR:HG21	1:N:235:ARG:H	1.77	0.49
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.48	0.49
2:O:161:GLU:OE1	2:O:176:LEU:N	2.45	0.49
1:A:141:MET:HE1	1:A:168:GLU:CD	2.38	0.49
2:O:365:LYS:HG3	2:O:402:ILE:HD12	1.95	0.49
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.48	0.49
2:B:128:THR:HG21	2:B:224:LEU:HD22	1.95	0.49
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.48	0.49
1:A:140:GLU:HG3	9:I:51:CYS:SG	2.52	0.49
2:B:137:VAL:O	2:B:141:GLN:HG2	2.13	0.48
9:I:49:LEU:HD21	9:I:58:ARG:NE	2.28	0.48
19:P:406:BOG:H3'2	11:R:502:PEE:H46	1.95	0.48
3:C:332:ASN:ND2	3:C:358:SER:OG	2.45	0.48
1:N:141:MET:HE1	1:N:168:GLU:CD	2.38	0.48
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.48	0.48
2:B:247:GLN:NE2	2:O:60:THR:OG1	2.46	0.48
2:B:365:LYS:HG3	2:B:402:ILE:HD12	1.95	0.48
5:E:125:ASP:HB3	5:E:126:ARG:HD2	1.95	0.48
2:B:161:GLU:OE1	2:B:176:LEU:N	2.46	0.48
2:B:157:VAL:HG23	9:I:64:LEU:HD11	1.96	0.48
3:C:52:LEU:HD11	3:C:81:ARG:HA	1.93	0.48
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.94	0.48
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.48
1:A:191:LYS:O	1:A:195:MET:HG3	2.14	0.48
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.95	0.48
4:D:235:MET:HB3	7:G:15:THR:HG22	1.96	0.48
1:N:102:LEU:HD12	1:N:102:LEU:H	1.79	0.48
2:B:203:ARG:HD2	2:B:230:ALA:O	2.14	0.48
5:E:129:LYS:HD2	5:E:130:PRO:HD2	1.96	0.48
1:N:191:LYS:O	1:N:195:MET:HG3	2.14	0.48
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.29	0.47
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.49	0.47
3:P:9:HIS:HB3	3:P:12:LEU:HB2	1.96	0.47
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.95	0.47
2:O:137:VAL:O	2:O:141:GLN:HG2	2.14	0.47
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.49	0.47
5:E:55:VAL:O	5:E:59:ILE:HG12	2.14	0.47
1:N:368:GLN:O	1:N:374:PRO:HB2	2.14	0.47
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.96	0.47
3:C:52:LEU:HD13	12:C:501:HEM:HBD1	1.96	0.47
5:R:55:VAL:O	5:R:59:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:SER:OG	3:C:273:TRP:NE1	2.31	0.47
6:F:53:ASP:OD1	6:F:54:LEU:N	2.48	0.47
3:C:145:THR:O	3:C:149:ASN:HB2	2.15	0.47
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.96	0.47
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.44	0.47
1:N:205:HIS:HB3	1:N:206:LYS:HE3	1.97	0.47
2:O:217:LYS:O	2:O:221:GLU:HG2	2.14	0.47
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.97	0.46
2:O:203:ARG:HD2	2:O:230:ALA:O	2.15	0.46
2:B:22:GLU:H	2:B:22:GLU:HG3	1.54	0.46
2:B:56:ARG:NH1	2:B:318:ASP:OD2	2.47	0.46
3:C:9:HIS:HB3	3:C:12:LEU:HB2	1.97	0.46
5:E:191:ASP:OD2	5:E:191:ASP:N	2.47	0.46
3:P:52:LEU:HD13	12:P:402:HEM:HBD1	1.96	0.46
3:P:351:ILE:HD11	7:T:61:TRP:HZ3	1.79	0.46
1:A:140:GLU:CD	9:I:50:LEU:H	2.20	0.46
3:P:332:ASN:ND2	3:P:358:SER:OG	2.45	0.46
5:R:30:GLU:OE1	10:W:7:ARG:NH2	2.49	0.46
3:C:10:PRO:HG2	3:P:200:PHE:CE1	2.50	0.46
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.97	0.46
5:R:152:ASP:HB2	5:R:164:HIS:CG	2.50	0.46
1:A:368:GLN:O	1:A:374:PRO:HB2	2.14	0.46
6:F:59:MET:HE3	6:F:59:MET:HA	1.98	0.46
1:A:102:LEU:HD12	1:A:102:LEU:H	1.79	0.46
3:P:145:THR:O	3:P:149:ASN:HB2	2.15	0.46
2:B:341:MET:HE3	2:B:345:LYS:HE3	1.98	0.46
5:E:94:LYS:HG2	3:P:263:LEU:HD21	1.98	0.46
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.79	0.46
2:O:56:ARG:NH1	2:O:318:ASP:OD2	2.49	0.46
1:N:37:VAL:HG13	1:N:109:VAL:HG11	1.98	0.46
3:P:25:PRO:O	3:P:225:TYR:OH	2.33	0.45
5:R:136:VAL:HG12	5:R:138:VAL:HG23	1.98	0.45
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.45
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.52	0.45
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.44	0.45
1:A:341:GLU:OE1	1:A:344:ARG:NH1	2.45	0.45
2:B:23:ASP:OD1	2:B:23:ASP:N	2.34	0.45
5:R:108:GLN:HE21	5:R:108:GLN:HB3	1.55	0.45
1:A:37:VAL:HG13	1:A:109:VAL:HG11	1.98	0.45
3:C:186:LEU:HD21	11:C:509:PEE:H2	1.99	0.45
5:E:150:SER:OG	5:E:151:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:37:TYR:CE2	11:R:502:PEE:H10	2.52	0.45
3:C:46:ILE:HA	12:C:501:HEM:HMC2	1.98	0.45
6:S:59:MET:HE3	6:S:59:MET:HA	1.98	0.45
1:A:317:THR:OG1	1:A:318:GLY:N	2.51	0.45
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.81	0.45
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.81	0.44
2:O:341:MET:HE3	2:O:345:LYS:HE3	1.97	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.52	0.44
1:A:191:LYS:HA	1:A:191:LYS:HE2	2.00	0.44
1:A:281:ASP:O	1:A:283:THR:N	2.50	0.44
3:C:133:VAL:HA	3:C:140:SER:HB3	1.99	0.44
2:O:206:LEU:HD23	2:O:220:ALA:HB2	2.00	0.44
3:P:89:SER:OG	3:P:273:TRP:NE1	2.30	0.44
3:P:133:VAL:HA	3:P:140:SER:HB3	2.00	0.44
4:Q:48:PHE:HB2	4:Q:87:ILE:HA	1.99	0.44
6:S:13:MET:O	6:S:17:ARG:HG2	2.18	0.44
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.24	0.44
3:P:165:ALA:HB1	11:P:409:PEE:H60	1.99	0.44
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.53	0.44
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.53	0.44
5:R:48:ALA:HB1	11:R:502:PEE:H66	1.99	0.44
2:B:168:TYR:CD2	2:B:237:ALA:HB1	2.53	0.44
4:D:48:PHE:HB2	4:D:87:ILE:HA	2.00	0.44
3:C:89:SER:HG	3:C:273:TRP:NE1	2.15	0.44
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.44
1:N:191:LYS:HE2	1:N:191:LYS:HA	2.00	0.44
6:S:18:LYS:O	6:S:22:ASN:ND2	2.50	0.44
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.52	0.44
2:B:287:ARG:HG2	9:I:53:GLU:HB3	2.00	0.44
2:B:370:MET:HA	2:B:373:GLU:HG3	2.00	0.44
1:N:281:ASP:O	1:N:283:THR:N	2.50	0.44
1:N:433:ASP:OD1	1:N:436:ARG:HG2	2.18	0.44
2:O:207:VAL:HG21	2:O:383:GLY:HA2	2.00	0.44
2:O:370:MET:HA	2:O:373:GLU:HG3	2.00	0.44
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	2.00	0.44
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.18	0.43
2:O:197:ASN:HB3	2:O:232:THR:HB	2.00	0.43
3:P:270:LYS:NZ	21:P:501:HOH:O	2.51	0.43
5:E:98:VAL:HG22	5:E:134:ILE:HG22	1.99	0.43
5:E:123:ASP:OD1	5:E:170:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.99	0.43
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.00	0.43
5:E:118:ARG:HD3	5:E:171:ILE:HG23	2.00	0.43
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.53	0.43
1:N:136:GLN:HE21	9:V:50:LEU:HB2	1.83	0.43
11:P:409:PEE:H10	11:P:409:PEE:H64	2.00	0.43
1:A:240:GLU:CD	1:A:242:ARG:HE	2.27	0.43
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.90	0.43
4:D:225:HIS:O	7:G:20:PRO:HB3	2.18	0.43
5:R:185:TYR:HB3	5:R:195:VAL:HG13	2.01	0.43
7:T:40:ARG:HD2	18:T:101:CDL:OA4	2.17	0.43
1:A:46:ARG:HD3	1:A:231:LEU:HD13	2.01	0.43
3:P:31:TRP:NE1	11:P:407:PEE:O4	2.51	0.43
3:P:46:ILE:HA	12:P:402:HEM:HMC2	1.99	0.43
3:P:210:LEU:HD12	6:S:66:LEU:HD23	2.01	0.43
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.53	0.43
6:F:18:LYS:O	6:F:22:ASN:ND2	2.50	0.43
1:N:36:THR:HG21	1:N:373:THR:HA	2.01	0.43
8:U:31:VAL:HA	8:U:34:ARG:HB3	1.99	0.43
9:I:63:ASP:CG	9:I:64:LEU:H	2.26	0.43
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.90	0.43
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.53	0.43
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.84	0.43
1:N:317:THR:OG1	1:N:318:GLY:N	2.50	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB1	1.84	0.42
2:O:29:LEU:HD12	2:O:33:LEU:HD23	2.01	0.42
4:D:223:LYS:HE2	4:D:227:TRP:CD1	2.54	0.42
1:N:122:LEU:HD11	1:N:186:ILE:HD12	2.02	0.42
1:N:244:ARG:NE	7:T:10:VAL:HB	2.34	0.42
2:B:368:TYR:O	2:B:372:VAL:HG23	2.20	0.42
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.53	0.42
2:O:166:ALA:HB2	2:O:244:ILE:HG13	2.01	0.42
2:O:241:GLY:HA2	2:O:423:SER:HB3	2.01	0.42
2:O:306:PRO:HB3	9:V:52:ARG:H	1.85	0.42
1:A:145:MET:HE3	1:A:248:LEU:HD11	2.01	0.42
3:C:25:PRO:O	3:C:225:TYR:OH	2.33	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.74	0.42
9:V:60:ALA:HA	9:V:77:ARG:HH22	1.85	0.42
2:B:368:TYR:O	2:B:371:SER:OG	2.34	0.42
1:N:240:GLU:CD	1:N:242:ARG:HE	2.27	0.42
3:P:9:HIS:CE1	3:P:11:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:SER:OG	2:B:320:GLY:N	2.53	0.42
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.85	0.42
3:C:230:ILE:HG22	4:D:219:LEU:HD13	2.01	0.42
5:E:96:LEU:HD21	5:E:195:VAL:HG21	2.01	0.42
19:P:406:BOG:H1'1	11:R:502:PEE:H33	2.02	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.49	0.42
4:D:33:TYR:CZ	4:D:43:MET:HG3	2.55	0.42
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.20	0.42
2:O:368:TYR:O	2:O:371:SER:OG	2.34	0.42
3:P:221:PHE:HE2	11:P:401:PEE:H26	1.84	0.42
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.60	0.42
4:Q:223:LYS:HE2	4:Q:227:TRP:CD1	2.54	0.42
3:C:37:LEU:HD21	3:C:233:LEU:HA	2.02	0.42
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.52	0.42
1:A:21:ASN:OD1	1:A:21:ASN:N	2.50	0.41
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.20	0.41
1:A:205:HIS:O	1:A:209:VAL:HG13	2.20	0.41
3:C:9:HIS:CE1	3:C:11:LEU:HB2	2.55	0.41
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.02	0.41
3:P:186:LEU:HD21	11:P:409:PEE:H1	2.02	0.41
5:R:163:SER:HA	5:R:174:GLY:HA3	2.01	0.41
3:C:271:PRO:HB3	13:C:503:Y52:C14	2.51	0.41
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.55	0.41
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.54	0.41
3:C:30:ALA:HB2	18:D:502:CDL:HA31	2.03	0.41
3:C:92:PHE:HA	3:C:95:ILE:HG22	2.02	0.41
1:N:145:MET:HE3	1:N:248:LEU:HD11	2.02	0.41
2:O:156:GLN:NE2	21:O:502:HOH:O	2.46	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.74	0.41
7:T:40:ARG:HB3	18:T:101:CDL:HA31	2.02	0.41
2:B:257:VAL:O	2:B:323:GLY:HA3	2.21	0.41
1:N:277:ILE:O	1:N:292:SER:OG	2.28	0.41
2:O:368:TYR:O	2:O:372:VAL:HG23	2.20	0.41
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.02	0.41
2:B:124:LEU:HD21	2:B:223:PHE:HB3	2.02	0.41
1:N:205:HIS:O	1:N:209:VAL:HG13	2.20	0.41
1:N:276:ILE:HD11	1:N:354:VAL:HG12	2.02	0.41
11:P:411:PEE:H50	11:P:411:PEE:H13	2.03	0.41
4:D:117:VAL:O	4:D:123:GLY:HA2	2.20	0.41
2:O:120:MET:HE1	2:O:206:LEU:HD11	2.03	0.41
2:O:223:PHE:HD2	2:O:223:PHE:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:297:GLN:O	2:O:301:LYS:HG3	2.20	0.41
3:P:37:LEU:HD21	3:P:233:LEU:HA	2.03	0.41
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.85	0.41
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	2.03	0.41
4:Q:141:VAL:HG21	8:U:55:THR:HG23	2.03	0.41
2:B:76:THR:HG22	2:B:82:SER:H	1.86	0.41
2:B:202:ALA:HB3	2:B:229:GLY:O	2.21	0.41
3:C:237:LEU:HD21	11:E:503:PEE:H29	2.02	0.41
1:N:106:MET:HG3	1:N:203:ILE:HD13	2.03	0.41
2:O:51:ILE:HG12	2:O:204:MET:HG2	2.03	0.41
11:P:407:PEE:H32	11:P:407:PEE:H25	1.92	0.41
4:Q:43:MET:HE3	4:Q:43:MET:HB3	1.94	0.41
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.20	0.41
5:R:45:VAL:HG13	10:W:28:ALA:HA	2.03	0.41
1:A:276:ILE:HD11	1:A:354:VAL:HG12	2.03	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.87	0.41
2:B:218:GLN:O	2:B:222:GLN:HB2	2.20	0.41
3:C:214:SER:HA	6:F:66:LEU:HD11	2.03	0.41
4:D:229:VAL:HG23	7:G:20:PRO:HG3	2.02	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.56	0.41
5:E:54:VAL:HG11	11:E:502:PEE:H43	2.03	0.41
7:G:24:ARG:NH2	7:G:28:ASN:H	2.18	0.41
8:H:17:LEU:HD21	8:H:21:ARG:HH21	1.86	0.41
9:I:51:CYS:HB3	9:I:52:ARG:H	1.70	0.41
2:O:200:THR:O	2:O:204:MET:HG3	2.20	0.41
3:P:2:ALA:HA	3:P:3:PRO:HD2	1.72	0.41
4:Q:33:TYR:CZ	4:Q:43:MET:HG3	2.55	0.41
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.85	0.41
1:A:370:ASP:CG	2:B:375:ALA:H	2.28	0.41
2:B:100:SER:HB2	2:B:105:MET:HG2	2.02	0.41
2:B:154:SER:HA	2:B:155:PRO:HD3	1.94	0.41
4:D:239:PRO:C	4:D:241:LYS:H	2.27	0.41
2:O:100:SER:HB2	2:O:105:MET:HG2	2.03	0.41
3:P:184:PHE:CZ	12:P:402:HEM:HBC1	2.56	0.41
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.57	0.40
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.55	0.40
2:O:19:PRO:HB3	2:O:41:PHE:CD1	2.56	0.40
10:W:38:GLY:O	10:W:42:ILE:HG13	2.21	0.40
2:B:51:ILE:HG12	2:B:204:MET:HG2	2.03	0.40
2:B:200:THR:O	2:B:204:MET:HG3	2.21	0.40
2:O:170:THR:O	2:O:172:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:359:LYS:HE3	2:O:359:LYS:HB2	1.91	0.40
10:W:52:TRP:O	10:W:56:LYS:HB2	2.22	0.40
1:A:384:LEU:HD12	1:A:384:LEU:HA	1.95	0.40
2:B:97:SER:HA	9:I:69:SER:HA	2.03	0.40
2:B:297:GLN:O	2:B:301:LYS:HG3	2.20	0.40
2:O:56:ARG:NH2	2:O:236:LYS:HA	2.37	0.40
8:U:37:LEU:O	8:U:41:ASP:N	2.49	0.40
5:E:105:GLU:O	5:E:109:GLU:HB2	2.21	0.40
1:A:130:GLU:HA	1:A:133:VAL:HB	2.04	0.40
1:A:281:ASP:C	1:A:283:THR:H	2.30	0.40
6:S:37:LEU:HD23	6:S:37:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	421 (96%)	16 (4%)	4 (1%)	14	44
1	N	440/446 (99%)	419 (95%)	17 (4%)	4 (1%)	14	44
2	B	419/441 (95%)	397 (95%)	18 (4%)	4 (1%)	12	42
2	O	420/441 (95%)	397 (94%)	17 (4%)	6 (1%)	9	35
3	C	378/380 (100%)	365 (97%)	11 (3%)	2 (0%)	24	56
3	P	378/380 (100%)	364 (96%)	12 (3%)	2 (0%)	24	56
4	D	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	16	47
4	Q	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16	47
5	E	194/196 (99%)	168 (87%)	20 (10%)	6 (3%)	3	19
5	R	194/196 (99%)	175 (90%)	14 (7%)	5 (3%)	4	23
6	F	99/110 (90%)	97 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	98 (99%)	1 (1%)	0	100	100
7	G	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
7	T	77/81 (95%)	72 (94%)	5 (6%)	0	100	100
8	H	66/77 (86%)	64 (97%)	2 (3%)	0	100	100
8	U	66/77 (86%)	56 (85%)	9 (14%)	1 (2%)	8	34
9	I	28/76 (37%)	17 (61%)	9 (32%)	2 (7%)	1	5
9	V	28/76 (37%)	19 (68%)	7 (25%)	2 (7%)	1	5
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	7	32
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	32
All	All	4000/4218 (95%)	3763 (94%)	193 (5%)	44 (1%)	11	40

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	390	GLY
2	O	19	PRO
2	O	226	ILE
2	O	390	GLY
9	V	59	SER
2	B	171	ALA
2	B	351	GLY
5	E	149	ASN
2	O	171	ALA
2	O	351	GLY
5	R	148	ALA
5	R	188	VAL
1	A	282	ARG
1	A	433	ASP
3	C	3	PRO
3	C	156	TYR
4	D	176	PRO
10	J	62	SER
1	N	282	ARG
1	N	433	ASP
2	O	223	PHE
3	P	3	PRO
4	Q	176	PRO
1	A	443	TRP
5	E	114	VAL

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Mol	Chain	Res	Type
5	E	179	ASN
9	I	60	ALA
1	N	443	TRP
8	U	12	GLU
2	B	227	ARG
5	E	120	PRO
5	E	155	GLY
5	E	163	SER
9	I	64	LEU
3	P	156	TYR
5	R	155	GLY
5	R	163	SER
9	V	60	ALA
10	W	15	ARG
5	R	141	HIS
4	D	162	PRO
4	Q	162	PRO
1	A	260	PRO
1	N	260	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	341 (93%)	24 (7%)	15	44
1	N	365/368 (99%)	338 (93%)	27 (7%)	13	40
2	B	331/347 (95%)	311 (94%)	20 (6%)	17	47
2	O	332/347 (96%)	312 (94%)	20 (6%)	17	47
3	C	328/328 (100%)	314 (96%)	14 (4%)	26	56
3	P	327/328 (100%)	314 (96%)	13 (4%)	28	58
4	D	200/200 (100%)	191 (96%)	9 (4%)	24	55
4	Q	200/200 (100%)	190 (95%)	10 (5%)	22	52
5	E	166/166 (100%)	155 (93%)	11 (7%)	15	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	165/166 (99%)	150 (91%)	15 (9%)	9	31
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	56
6	S	93/96 (97%)	89 (96%)	4 (4%)	26	56
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	56
7	T	70/71 (99%)	68 (97%)	2 (3%)	37	63
8	H	64/71 (90%)	61 (95%)	3 (5%)	23	54
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	53
9	I	22/45 (49%)	17 (77%)	5 (23%)	1	4
9	V	23/45 (51%)	18 (78%)	5 (22%)	1	5
10	J	49/49 (100%)	46 (94%)	3 (6%)	17	47
10	W	47/49 (96%)	42 (89%)	5 (11%)	6	26
All	All	3374/3482 (97%)	3174 (94%)	200 (6%)	18	48

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	16	VAL
1	A	28	GLU
1	A	37	VAL
1	A	39	VAL
1	A	50	GLU
1	A	70	ARG
1	A	106	MET
1	A	108	LYS
1	A	170	THR
1	A	220	SER
1	A	228	VAL
1	A	230	ILE
1	A	233	ARG
1	A	248	LEU
1	A	269	VAL
1	A	342	TRP
1	A	350	THR
1	A	378	THR
1	A	430	GLN
1	A	431	LEU
1	A	432	LEU

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Mol	Chain	Res	Type
1	A	437	ILE
1	A	443	TRP
2	B	22	GLU
2	B	23	ASP
2	B	24	LEU
2	B	97	SER
2	B	124	LEU
2	B	156	GLN
2	B	160	LEU
2	B	170	THR
2	B	187	THR
2	B	222	GLN
2	B	232	THR
2	B	297	GLN
2	B	304	THR
2	B	344	LEU
2	B	358	THR
2	B	372	VAL
2	B	374	THR
2	B	380	ASN
2	B	398	VAL
2	B	402	ILE
3	C	11	LEU
3	C	14	MET
3	C	22	LEU
3	C	65	SER
3	C	82	ASN
3	C	93	ILE
3	C	95	ILE
3	C	157	ILE
3	C	159	HIS
3	C	160	THR
3	C	182	LEU
3	C	313	GLN
3	C	328	LEU
3	C	367	PHE
4	D	2	GLU
4	D	31	GLN
4	D	40	CYS
4	D	57	THR
4	D	71	GLN
4	D	106	ASN

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Mol	Chain	Res	Type
4	D	142	VAL
4	D	215	LEU
4	D	234	LYS
5	E	1	VAL
5	E	22	THR
5	E	31	ASP
5	E	80	ASP
5	E	85	LYS
5	E	123	ASP
5	E	131	GLU
5	E	133	VAL
5	E	134	ILE
5	E	188	VAL
5	E	191	ASP
6	F	70	LEU
6	F	78	GLU
6	F	84	GLU
6	F	110	LYS
7	G	2	ILE
7	G	3	HIS
7	G	6	ASN
8	H	13	LEU
8	H	18	THR
8	H	49	HIS
9	I	50	LEU
9	I	65	VAL
9	I	68	ILE
9	I	69	SER
9	I	77	ARG
10	J	22	LEU
10	J	26	LEU
10	J	30	LEU
1	N	3	THR
1	N	9	GLN
1	N	16	VAL
1	N	18	THR
1	N	28	GLU
1	N	37	VAL
1	N	39	VAL
1	N	70	ARG
1	N	106	MET
1	N	108	LYS

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Mol	Chain	Res	Type
1	N	170	THR
1	N	206	LYS
1	N	220	SER
1	N	228	VAL
1	N	230	ILE
1	N	233	ARG
1	N	248	LEU
1	N	269	VAL
1	N	342	TRP
1	N	344	ARG
1	N	350	THR
1	N	378	THR
1	N	430	GLN
1	N	431	LEU
1	N	432	LEU
1	N	437	ILE
1	N	443	TRP
2	O	24	LEU
2	O	31	ASN
2	O	97	SER
2	O	124	LEU
2	O	156	GLN
2	O	160	LEU
2	O	170	THR
2	O	187	THR
2	O	223	PHE
2	O	225	ASN
2	O	232	THR
2	O	297	GLN
2	O	304	THR
2	O	344	LEU
2	O	358	THR
2	O	372	VAL
2	O	374	THR
2	O	380	ASN
2	O	398	VAL
2	O	402	ILE
3	P	11	LEU
3	P	14	MET
3	P	22	LEU
3	P	65	SER
3	P	82	ASN

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Mol	Chain	Res	Type
3	P	93	ILE
3	P	95	ILE
3	P	157	ILE
3	P	159	HIS
3	P	182	LEU
3	P	313	GLN
3	P	328	LEU
3	P	367	PHE
4	Q	2	GLU
4	Q	31	GLN
4	Q	40	CYS
4	Q	57	THR
4	Q	71	GLN
4	Q	106	ASN
4	Q	142	VAL
4	Q	170	GLU
4	Q	215	LEU
4	Q	234	LYS
5	R	1	VAL
5	R	22	THR
5	R	31	ASP
5	R	85	LYS
5	R	106	ILE
5	R	108	GLN
5	R	109	GLU
5	R	112	VAL
5	R	113	ASP
5	R	124	LEU
5	R	145	VAL
5	R	152	ASP
5	R	188	VAL
5	R	190	ASP
5	R	192	LEU
6	S	13	MET
6	S	70	LEU
6	S	78	GLU
6	S	84	GLU
7	T	3	HIS
7	T	6	ASN
8	U	36	ARG
8	U	47	ARG
8	U	55	THR

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Mol	Chain	Res	Type
9	V	49	LEU
9	V	51	CYS
9	V	55	MET
9	V	68	ILE
9	V	77	ARG
10	W	15	ARG
10	W	16	ARG
10	W	22	LEU
10	W	40	ASP
10	W	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	53	ASN
1	A	94	GLN
1	A	118	GLN
1	A	143	ASN
1	A	147	ASN
1	A	215	HIS
1	A	252	HIS
1	A	271	HIS
1	A	308	GLN
2	B	153	GLN
2	B	225	ASN
2	B	332	HIS
2	B	392	HIS
3	C	313	GLN
3	C	342	GLN
4	D	97	ASN
4	D	166	ASN
5	E	122	HIS
6	F	79	GLN
7	G	23	GLN
1	N	53	ASN
1	N	94	GLN
1	N	118	GLN
1	N	136	GLN
1	N	143	ASN
1	N	147	ASN
1	N	215	HIS

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Mol	Chain	Res	Type
1	N	252	HIS
1	N	271	HIS
1	N	308	GLN
1	N	339	GLN
2	O	156	GLN
2	O	225	ASN
2	O	270	ASN
2	O	332	HIS
3	P	4	ASN
3	P	149	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	6	HIS
4	Q	97	ASN
5	R	86	ASN
5	R	108	GLN
6	S	79	GLN
7	T	23	GLN
8	U	67	HIS
8	U	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	FME	C	1	3	7,8,10	2.08	1 (14%)	5,8,11	1.43	1 (20%)

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
3	FME	C	1	3	-	0/5/8/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CN-N	-5.39	1.33	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CN-N-CA	2.73	121.87	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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
12	HEM	P	402	3	50,50,50	1.45	9 (18%)	67,82,82	1.17	5 (7%)
20	FES	E	501	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	HEM	P	403	3	50,50,50	1.42	9 (18%)	67,82,82	1.15	6 (8%)
11	PEE	A	501	-	25,25,50	1.36	2 (8%)	28,30,55	1.58	5 (17%)
11	PEE	C	505	-	48,48,50	1.21	4 (8%)	51,53,55	1.24	5 (9%)
11	PEE	R	502	-	48,48,50	1.25	4 (8%)	51,53,55	1.19	6 (11%)
14	U10	P	405	-	19,19,63	2.25	2 (10%)	24,26,79	1.61	4 (16%)
11	PEE	P	407	-	48,48,50	1.24	4 (8%)	51,53,55	1.11	3 (5%)
12	HEM	C	501	3	50,50,50	1.44	9 (18%)	67,82,82	1.15	5 (7%)
13	Y52	C	503	-	29,29,29	0.50	0	39,39,39	0.88	2 (5%)
15	MES	C	506	-	12,12,12	2.31	1 (8%)	15,16,16	1.08	0
16	GOL	C	508	-	5,5,5	0.37	0	5,5,5	0.38	0
19	BOG	Q	503	-	20,20,20	0.55	1 (5%)	25,25,25	0.60	0
11	PEE	E	503	-	14,14,50	1.02	1 (7%)	13,13,55	0.91	1 (7%)
11	PEE	P	401	-	14,14,50	2.30	3 (21%)	14,14,55	1.29	2 (14%)
11	PEE	C	509	-	46,46,50	1.29	4 (8%)	49,51,55	1.21	4 (8%)
11	PEE	N	501	-	7,7,50	1.46	1 (14%)	9,9,55	1.27	1 (11%)
18	CDL	D	502	-	41,41,99	1.31	4 (9%)	47,53,111	1.29	6 (12%)
18	CDL	Q	502	-	41,41,99	1.31	4 (9%)	47,53,111	1.28	6 (12%)
11	PEE	P	409	-	40,40,50	1.19	3 (7%)	43,45,55	1.21	3 (6%)
11	PEE	E	502	-	47,47,50	1.25	4 (8%)	50,52,55	1.17	4 (8%)
17	HEC	D	501	4	50,50,50	1.34	5 (10%)	68,82,82	1.20	7 (10%)
20	FES	R	501	5	0,4,4	-	-	-	-	-
13	Y52	P	404	-	29,29,29	0.48	0	39,39,39	0.86	1 (2%)
11	PEE	C	507	-	10,10,50	0.52	0	11,12,55	0.56	0
18	CDL	T	101	-	39,39,99	1.36	4 (10%)	45,51,111	1.34	5 (11%)
11	PEE	P	411	-	24,24,50	1.30	2 (8%)	27,29,55	1.42	4 (14%)
11	PEE	C	510	-	14,14,50	2.31	3 (21%)	14,14,55	1.21	1 (7%)
16	GOL	P	408	-	5,5,5	0.38	0	5,5,5	0.33	0
19	BOG	D	503	-	20,20,20	0.56	1 (5%)	25,25,25	0.63	0
11	PEE	P	410	-	11,11,50	1.80	2 (18%)	11,11,55	1.30	2 (18%)
18	CDL	G	101	-	39,39,99	1.35	4 (10%)	45,51,111	1.33	6 (13%)
19	BOG	P	406	-	20,20,20	0.52	0	25,25,25	0.61	0
12	HEM	C	502	3	50,50,50	1.43	9 (18%)	67,82,82	1.15	6 (8%)
14	U10	C	504	-	19,19,63	2.19	2 (10%)	24,26,79	1.46	3 (12%)
17	HEC	Q	501	4	50,50,50	1.34	5 (10%)	68,82,82	1.20	7 (10%)

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
12	HEM	P	402	3	-	6/14/54/54	-
20	FES	E	501	5	-	-	0/1/1/1
12	HEM	P	403	3	-	4/14/54/54	-
11	PEE	A	501	-	-	11/29/29/54	-
11	PEE	C	505	-	-	21/52/52/54	-
11	PEE	R	502	-	-	20/52/52/54	-
14	U10	P	405	-	-	4/11/35/87	0/1/1/1
11	PEE	P	407	-	-	15/52/52/54	-
12	HEM	C	501	3	-	6/14/54/54	-
13	Y52	C	503	-	-	0/20/20/20	0/3/3/3
15	MES	C	506	-	-	3/6/14/14	0/1/1/1
16	GOL	C	508	-	-	4/4/4/4	-
19	BOG	Q	503	-	-	2/11/31/31	0/1/1/1
11	PEE	E	503	-	-	1/12/12/54	-
11	PEE	P	401	-	-	7/12/12/54	-
11	PEE	C	509	-	-	17/50/50/54	-
11	PEE	N	501	-	-	0/5/5/54	-
18	CDL	D	502	-	-	14/51/51/110	-
18	CDL	Q	502	-	-	14/51/51/110	-
11	PEE	P	409	-	-	17/44/44/54	-
11	PEE	E	502	-	-	20/51/51/54	-
17	HEC	D	501	4	1/1/3/7	2/14/54/54	-
20	FES	R	501	5	-	-	0/1/1/1
13	Y52	P	404	-	-	0/20/20/20	0/3/3/3
11	PEE	C	507	-	-	4/10/10/54	-
18	CDL	T	101	-	-	17/49/49/110	-
11	PEE	P	411	-	-	8/28/28/54	-
11	PEE	C	510	-	-	6/12/12/54	-
16	GOL	P	408	-	-	4/4/4/4	-
19	BOG	D	503	-	-	0/11/31/31	0/1/1/1
11	PEE	P	410	-	-	5/9/9/54	-
18	CDL	G	101	-	-	13/49/49/110	-
19	BOG	P	406	-	-	3/11/31/31	0/1/1/1
12	HEM	C	502	3	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	U10	C	504	-	-	4/11/35/87	0/1/1/1
17	HEC	Q	501	4	1/1/3/7	2/14/54/54	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	405	U10	C6-C1	8.81	1.51	1.35
14	C	504	U10	C6-C1	8.52	1.50	1.35
15	C	506	MES	C8-S	-7.74	1.66	1.77
11	C	510	PEE	O4-C10	7.31	1.46	1.22
11	P	401	PEE	O4-C10	7.26	1.45	1.22
11	A	501	PEE	O3-C30	4.67	1.46	1.33
11	C	509	PEE	O2-C10	4.64	1.47	1.34
11	P	410	PEE	O2-C10	4.59	1.46	1.30
11	R	502	PEE	O2-C10	4.54	1.47	1.34
11	C	509	PEE	O3-C30	4.45	1.46	1.33
11	E	502	PEE	O2-C10	4.39	1.46	1.34
18	T	101	CDL	OB8-CB7	4.35	1.46	1.33
11	R	502	PEE	O3-C30	4.32	1.45	1.33
18	G	101	CDL	OB8-CB7	4.29	1.45	1.33
11	P	409	PEE	O3-C30	4.29	1.45	1.33
18	D	502	CDL	OB8-CB7	4.28	1.45	1.33
11	P	407	PEE	O2-C10	4.28	1.46	1.34
11	E	502	PEE	O3-C30	4.25	1.45	1.33
11	P	409	PEE	O2-C10	4.23	1.46	1.34
11	P	411	PEE	O3-C30	4.22	1.45	1.33
11	P	407	PEE	O3-C30	4.21	1.45	1.33
18	Q	502	CDL	OB8-CB7	4.21	1.45	1.33
11	C	505	PEE	O3-C30	4.16	1.45	1.33
11	P	411	PEE	O2-C10	4.15	1.46	1.34
11	C	505	PEE	O2-C10	4.15	1.46	1.34
18	D	502	CDL	OA6-CA5	4.14	1.46	1.34
18	T	101	CDL	OA6-CA5	4.14	1.46	1.34
11	A	501	PEE	O2-C10	4.13	1.46	1.34
18	D	502	CDL	OB6-CB5	4.08	1.45	1.34
18	Q	502	CDL	OA6-CA5	4.08	1.45	1.34
18	G	101	CDL	OB6-CB5	4.08	1.45	1.34
18	Q	502	CDL	OB6-CB5	4.07	1.45	1.34
18	T	101	CDL	OB6-CB5	4.06	1.45	1.34
18	G	101	CDL	OA6-CA5	4.02	1.45	1.34
11	P	407	PEE	C39-C38	3.77	1.53	1.31
11	E	502	PEE	C39-C38	3.76	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	510	PEE	C18-C19	3.75	1.53	1.31
11	R	502	PEE	C39-C38	3.74	1.52	1.31
11	C	509	PEE	C39-C38	3.74	1.52	1.31
11	P	401	PEE	C18-C19	3.73	1.52	1.31
11	R	502	PEE	C18-C19	3.72	1.52	1.31
11	P	409	PEE	C39-C38	3.72	1.52	1.31
11	C	509	PEE	C18-C19	3.71	1.52	1.31
11	C	505	PEE	C39-C38	3.71	1.52	1.31
11	E	503	PEE	C18-C19	3.70	1.52	1.31
11	P	410	PEE	C19-C18	3.70	1.53	1.29
11	C	505	PEE	C18-C19	3.70	1.52	1.31
11	P	407	PEE	C18-C19	3.69	1.52	1.31
11	E	502	PEE	C18-C19	3.67	1.52	1.31
17	D	501	HEC	FE-NC	3.56	2.06	1.95
17	Q	501	HEC	FE-NB	3.55	2.05	1.94
12	C	501	HEM	FE-ND	3.55	2.05	1.94
14	C	504	U10	C4-C3	3.53	1.49	1.36
17	D	501	HEC	FE-NB	3.52	2.05	1.94
11	N	501	PEE	P-O1P	3.51	1.61	1.50
12	C	502	HEM	FE-NA	3.47	2.06	1.95
17	Q	501	HEC	FE-NC	3.47	2.06	1.95
14	P	405	U10	C4-C3	3.44	1.48	1.36
12	P	402	HEM	FE-ND	3.44	2.05	1.94
12	P	402	HEM	FE-NB	3.44	2.05	1.94
12	P	403	HEM	FE-NA	3.43	2.06	1.95
17	D	501	HEC	FE-ND	3.36	2.05	1.94
17	Q	501	HEC	FE-ND	3.32	2.05	1.94
12	C	501	HEM	FE-NB	3.27	2.05	1.94
12	P	403	HEM	FE-NB	3.19	2.04	1.94
12	C	502	HEM	FE-ND	3.19	2.04	1.94
12	C	502	HEM	CAC-C3C	3.18	1.55	1.47
12	P	403	HEM	CAC-C3C	3.18	1.55	1.47
12	C	502	HEM	FE-NB	3.17	2.04	1.94
12	P	403	HEM	CAB-C3B	3.17	1.55	1.47
12	C	501	HEM	CAB-C3B	3.17	1.55	1.47
12	C	502	HEM	CAB-C3B	3.16	1.55	1.47
12	P	403	HEM	FE-ND	3.15	2.04	1.94
12	P	402	HEM	CAB-C3B	3.14	1.55	1.47
12	C	501	HEM	FE-NA	3.14	2.05	1.95
12	P	402	HEM	FE-NA	3.14	2.05	1.95
12	C	501	HEM	CAC-C3C	3.11	1.55	1.47
12	P	402	HEM	FE-NC	3.11	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	402	HEM	CAC-C3C	3.10	1.55	1.47
17	Q	501	HEC	FE-NA	3.01	2.05	1.95
12	C	501	HEM	FE-NC	3.01	2.05	1.95
12	C	502	HEM	FE-NC	2.98	2.05	1.95
12	P	403	HEM	FE-NC	2.97	2.05	1.95
17	D	501	HEC	FE-NA	2.92	2.04	1.95
18	Q	502	CDL	OA8-CA7	2.58	1.45	1.33
18	G	101	CDL	OA8-CA7	2.56	1.45	1.33
18	T	101	CDL	OA8-CA7	2.56	1.45	1.33
11	P	401	PEE	O2-C10	-2.54	1.22	1.30
11	C	510	PEE	O2-C10	-2.53	1.22	1.30
18	D	502	CDL	OA8-CA7	2.49	1.45	1.33
17	D	501	HEC	CMB-C2B	2.28	1.55	1.50
17	Q	501	HEC	CMB-C2B	2.20	1.55	1.50
12	C	502	HEM	CMB-C2B	2.17	1.55	1.50
12	C	501	HEM	CMB-C2B	2.13	1.55	1.50
12	P	402	HEM	CMB-C2B	2.13	1.55	1.50
12	P	403	HEM	CMC-C2C	2.09	1.55	1.50
12	P	402	HEM	CMC-C2C	2.09	1.55	1.50
12	P	403	HEM	CMB-C2B	2.07	1.55	1.50
19	Q	503	BOG	O1-C1	2.06	1.43	1.40
12	C	501	HEM	CMC-C2C	2.05	1.55	1.50
19	D	503	BOG	O1-C1	2.05	1.43	1.40
12	C	502	HEM	CMC-C2C	2.04	1.55	1.50
12	C	502	HEM	CMA-C3A	2.03	1.54	1.50
12	P	403	HEM	CMA-C3A	2.02	1.54	1.50
12	P	402	HEM	CMA-C3A	2.01	1.54	1.50
12	C	501	HEM	CMA-C3A	2.00	1.54	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	101	CDL	OB6-CB5-C51	4.48	121.18	111.48
11	C	505	PEE	O2-C10-C11	4.48	121.17	111.48
18	Q	502	CDL	OB6-CB5-C51	4.39	120.98	111.48
11	P	411	PEE	O2-C10-C11	4.39	120.97	111.48
18	G	101	CDL	OB6-CB5-C51	4.35	120.90	111.48
14	C	504	U10	C7-C8-C9	-4.32	119.38	126.83
11	A	501	PEE	O2-C10-C11	4.25	120.68	111.48
18	D	502	CDL	OB6-CB5-C51	4.16	120.49	111.48
11	E	502	PEE	O2-C10-C11	4.03	120.21	111.48
14	P	405	U10	C7-C8-C9	-3.85	120.19	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	502	PEE	O2-C10-C11	3.84	119.78	111.48
11	P	409	PEE	O3-C30-C31	3.83	123.50	111.83
11	C	509	PEE	O2-C10-C11	3.68	119.43	111.48
11	A	501	PEE	O3-C30-C31	3.64	122.93	111.83
11	P	409	PEE	O2-C10-C11	3.59	119.25	111.48
18	T	101	CDL	CB4-OB6-CB5	-3.48	109.48	117.80
14	C	504	U10	C10-C9-C11	3.46	120.21	116.13
11	P	407	PEE	O2-C10-C11	3.40	118.84	111.48
11	C	505	PEE	O3-C30-C31	3.29	121.86	111.83
11	N	501	PEE	O2P-P-O3P	3.29	120.12	107.80
11	A	501	PEE	O3-C3-C2	3.27	117.83	108.40
18	G	101	CDL	CB4-OB6-CB5	-3.24	110.05	117.80
14	P	405	U10	C10-C9-C11	3.18	119.87	116.13
11	E	502	PEE	O3-C30-C31	3.13	121.38	111.83
18	T	101	CDL	OB8-CB7-C71	3.13	120.64	111.15
17	Q	501	HEC	C2A-C1A-NA	-3.01	107.41	110.32
17	D	501	HEC	C2A-C1A-NA	-2.96	107.47	110.32
11	A	501	PEE	O2-C10-O4	-2.93	116.85	123.70
14	P	405	U10	C7-C6-C5	-2.92	115.12	118.52
17	Q	501	HEC	C3D-C4D-ND	-2.85	107.60	110.35
17	D	501	HEC	C3D-C4D-ND	-2.85	107.60	110.35
11	C	509	PEE	O3-C30-C31	2.85	120.52	111.83
18	D	502	CDL	OB8-CB7-C71	2.85	120.51	111.83
18	G	101	CDL	OB8-CB7-C71	2.79	119.61	111.15
18	D	502	CDL	CB4-OB6-CB5	-2.74	111.24	117.80
14	P	405	U10	C8-C7-C6	2.72	118.78	112.08
11	P	407	PEE	O3-C30-C31	2.71	120.11	111.83
17	D	501	HEC	C1D-ND-C4D	2.71	108.42	105.21
12	P	403	HEM	C1B-NB-C4B	2.69	108.39	105.21
12	C	502	HEM	C4D-ND-C1D	2.66	108.36	105.21
18	Q	502	CDL	CB4-OB6-CB5	-2.66	111.44	117.80
11	C	505	PEE	O2-C10-O4	-2.65	117.50	123.70
17	Q	501	HEC	C1D-ND-C4D	2.65	108.35	105.21
11	C	509	PEE	O2-C2-C1	2.64	117.83	108.34
18	D	502	CDL	OA6-CA5-C11	2.64	120.63	110.93
12	C	502	HEM	C1B-NB-C4B	2.62	108.31	105.21
12	P	403	HEM	C4D-ND-C1D	2.59	108.28	105.21
11	P	411	PEE	O3-C30-C31	2.59	119.73	111.83
11	R	502	PEE	O2-C2-C1	2.59	117.63	108.34
11	C	509	PEE	C2-O2-C10	2.55	123.89	117.80
11	P	411	PEE	O2-C10-O4	-2.52	117.82	123.70
11	R	502	PEE	O3-C30-C31	2.48	119.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	C4D-ND-C1D	2.48	108.14	105.21
12	P	402	HEM	C1B-NB-C4B	2.47	108.14	105.21
11	P	401	PEE	C12-C11-C10	-2.45	108.11	114.51
12	P	402	HEM	C4D-ND-C1D	2.45	108.11	105.21
18	Q	502	CDL	OB8-CB7-C71	2.43	119.23	111.83
11	R	502	PEE	C2-O2-C10	2.43	123.60	117.80
18	Q	502	CDL	OA6-CA5-C11	2.42	119.81	110.93
12	P	402	HEM	C2A-C1A-NA	-2.40	107.48	110.15
12	P	402	HEM	C3B-C2B-C1B	2.40	108.21	106.41
12	C	501	HEM	C1B-NB-C4B	2.39	108.04	105.21
12	P	403	HEM	C3D-C4D-ND	-2.36	107.58	110.17
12	C	502	HEM	C3D-C4D-ND	-2.35	107.59	110.17
12	P	403	HEM	C2A-C1A-NA	-2.33	107.57	110.15
12	C	502	HEM	C3B-C2B-C1B	2.32	108.15	106.41
17	D	501	HEC	C4B-NB-C1B	2.31	107.94	105.21
11	C	505	PEE	O3-C30-O5	-2.31	117.86	123.63
12	C	501	HEM	C3B-C2B-C1B	2.30	108.14	106.41
12	C	501	HEM	C2A-C1A-NA	-2.29	107.61	110.15
17	Q	501	HEC	C4B-NB-C1B	2.29	107.92	105.21
12	P	403	HEM	C3B-C2B-C1B	2.29	108.13	106.41
17	Q	501	HEC	C3C-C4C-NC	-2.28	107.63	110.15
11	A	501	PEE	O3-C30-O5	-2.27	117.95	123.63
12	C	502	HEM	C2A-C1A-NA	-2.26	107.65	110.15
11	E	502	PEE	O3-C30-O5	-2.25	118.00	123.63
18	Q	502	CDL	OB6-CB5-OB7	-2.25	118.45	123.70
17	D	501	HEC	C3C-C4C-NC	-2.24	107.67	110.15
13	C	503	Y52	C25-C26-N27	-2.22	124.51	129.31
11	P	401	PEE	O2-C10-C11	2.20	120.96	114.00
18	T	101	CDL	OA6-CA5-C11	2.20	119.01	110.93
12	C	501	HEM	C3D-C4D-ND	-2.20	107.76	110.17
18	Q	502	CDL	CA4-OA6-CA5	-2.18	112.58	117.80
12	P	402	HEM	C3D-C4D-ND	-2.17	107.79	110.17
18	T	101	CDL	OB6-CB5-OB7	-2.15	118.69	123.70
13	P	404	Y52	C25-C26-N27	-2.14	124.69	129.31
17	Q	501	HEC	C3B-C4B-NB	-2.12	107.85	110.17
17	D	501	HEC	C2D-C1D-ND	-2.11	107.42	109.84
11	C	510	PEE	O2-C10-C11	2.10	120.64	114.00
17	Q	501	HEC	C2D-C1D-ND	-2.09	107.44	109.84
11	P	410	PEE	C17-C18-C19	-2.08	111.45	126.65
11	E	502	PEE	C3-C2-C1	-2.08	106.93	111.78
18	G	101	CDL	OA6-CA5-C11	2.08	118.56	110.93
11	R	502	PEE	O3-C3-C2	2.08	114.38	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	411	PEE	O3-C30-O5	-2.07	118.44	123.63
11	R	502	PEE	O3-C30-O5	-2.07	118.44	123.63
17	D	501	HEC	C3B-C4B-NB	-2.07	107.90	110.17
11	P	409	PEE	O3-C30-O5	-2.06	118.47	123.63
18	D	502	CDL	CA4-OA6-CA5	-2.06	112.87	117.80
18	D	502	CDL	OB6-CB5-OB7	-2.05	118.90	123.70
12	C	502	HEM	CBD-CAD-C3D	-2.05	106.86	112.53
18	G	101	CDL	OB6-CB5-OB7	-2.05	118.92	123.70
12	P	403	HEM	CBD-CAD-C3D	-2.04	106.89	112.53
11	P	410	PEE	O2-C10-C11	2.04	120.44	114.00
11	E	503	PEE	C20-C19-C18	-2.04	109.57	124.83
18	G	101	CDL	CA4-OA6-CA5	-2.04	112.92	117.80
14	C	504	U10	C8-C7-C6	2.03	117.09	112.08
13	C	503	Y52	C15-S16-C17	-2.03	98.97	102.46
11	P	407	PEE	C2-O2-C10	-2.03	112.94	117.80
11	C	505	PEE	C17-C18-C19	-2.03	109.65	124.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	D	501	HEC	NA
17	Q	501	HEC	NA

All (258) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	PEE	C1-O3P-P-O1P
11	A	501	PEE	C1-O3P-P-O4P
11	A	501	PEE	C4-O4P-P-O1P
11	C	505	PEE	C11-C10-O2-C2
11	C	505	PEE	C1-C2-O2-C10
11	C	505	PEE	C1-O3P-P-O4P
11	C	505	PEE	C4-O4P-P-O1P
11	C	507	PEE	C1-O3P-P-O4P
11	C	507	PEE	C4-O4P-P-O1P
11	C	509	PEE	C1-O3P-P-O2P
11	C	509	PEE	C1-O3P-P-O1P
11	C	509	PEE	C1-O3P-P-O4P
11	C	509	PEE	C4-O4P-P-O3P
11	E	502	PEE	C1-O3P-P-O2P
11	E	502	PEE	C1-O3P-P-O1P
11	E	502	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
11	E	502	PEE	C4-O4P-P-O1P
11	P	407	PEE	C1-O3P-P-O1P
11	P	409	PEE	C11-C10-O2-C2
11	P	409	PEE	C4-O4P-P-O3P
11	P	409	PEE	C4-O4P-P-O2P
11	P	411	PEE	C11-C10-O2-C2
11	P	411	PEE	C1-O3P-P-O2P
11	P	411	PEE	C1-O3P-P-O4P
11	R	502	PEE	C1-O3P-P-O4P
14	C	504	U10	C12-C11-C9-C10
14	P	405	U10	C1-C6-C7-C8
14	P	405	U10	C5-C6-C7-C8
14	P	405	U10	C12-C11-C9-C8
14	P	405	U10	C12-C11-C9-C10
16	C	508	GOL	O1-C1-C2-O2
16	C	508	GOL	C1-C2-C3-O3
16	P	408	GOL	O1-C1-C2-O2
16	P	408	GOL	C1-C2-C3-O3
18	D	502	CDL	CA3-OA5-PA1-OA2
18	G	101	CDL	CB2-C1-CA2-OA2
18	G	101	CDL	CA2-OA2-PA1-OA5
18	G	101	CDL	CB2-OB2-PB2-OB4
18	G	101	CDL	CB2-OB2-PB2-OB5
18	G	101	CDL	CB3-OB5-PB2-OB2
18	G	101	CDL	CB3-OB5-PB2-OB4
18	Q	502	CDL	CA2-OA2-PA1-OA3
18	Q	502	CDL	CA2-OA2-PA1-OA5
18	Q	502	CDL	CA3-OA5-PA1-OA2
18	Q	502	CDL	CB2-OB2-PB2-OB4
18	Q	502	CDL	CB2-OB2-PB2-OB5
18	Q	502	CDL	CB3-OB5-PB2-OB2
18	Q	502	CDL	CB3-OB5-PB2-OB4
18	T	101	CDL	CA2-OA2-PA1-OA5
18	T	101	CDL	CA3-OA5-PA1-OA2
18	T	101	CDL	CA3-OA5-PA1-OA4
18	T	101	CDL	CB2-OB2-PB2-OB3
18	T	101	CDL	CB2-OB2-PB2-OB4
18	T	101	CDL	CB2-OB2-PB2-OB5
18	T	101	CDL	CB3-OB5-PB2-OB2
18	T	101	CDL	CB3-OB5-PB2-OB4
18	T	101	CDL	C51-CB5-OB6-CB4
11	A	501	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
11	C	505	PEE	O4-C10-O2-C2
11	P	411	PEE	O4-C10-O2-C2
18	T	101	CDL	OB7-CB5-OB6-CB4
11	C	505	PEE	C17-C18-C19-C20
11	C	505	PEE	C37-C38-C39-C40
11	R	502	PEE	C37-C38-C39-C40
11	P	409	PEE	O4-C10-O2-C2
18	D	502	CDL	O1-C1-CA2-OA2
18	D	502	CDL	O1-C1-CB2-OB2
18	Q	502	CDL	O1-C1-CA2-OA2
11	A	501	PEE	C11-C10-O2-C2
18	G	101	CDL	C51-CB5-OB6-CB4
18	Q	502	CDL	C51-CB5-OB6-CB4
19	P	406	BOG	O5-C5-C6-O6
11	R	502	PEE	C17-C18-C19-C20
18	T	101	CDL	C71-CB7-OB8-CB6
11	C	510	PEE	C10-C11-C12-C13
11	C	505	PEE	O2-C2-C3-O3
11	P	407	PEE	O2-C2-C3-O3
11	P	407	PEE	C17-C18-C19-C20
16	P	408	GOL	O2-C2-C3-O3
18	T	101	CDL	OB9-CB7-OB8-CB6
11	E	502	PEE	C30-C31-C32-C33
18	G	101	CDL	O1-C1-CA2-OA2
18	G	101	CDL	OB7-CB5-OB6-CB4
18	Q	502	CDL	OB7-CB5-OB6-CB4
11	P	401	PEE	C10-C11-C12-C13
11	C	509	PEE	C31-C30-O3-C3
18	Q	502	CDL	C11-CA5-OA6-CA4
18	Q	502	CDL	OA7-CA5-OA6-CA4
11	C	510	PEE	C17-C18-C19-C20
12	C	501	HEM	C3D-CAD-CBD-CGD
12	P	402	HEM	C3D-CAD-CBD-CGD
19	Q	503	BOG	O1-C1'-C2'-C3'
16	C	508	GOL	O1-C1-C2-C3
16	P	408	GOL	O1-C1-C2-C3
11	C	509	PEE	C1-C2-O2-C10
11	P	411	PEE	C1-C2-O2-C10
11	R	502	PEE	C31-C32-C33-C34
11	C	509	PEE	O5-C30-O3-C3
19	Q	503	BOG	C1'-C2'-C3'-C4'
11	R	502	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
16	C	508	GOL	O2-C2-C3-O3
11	C	510	PEE	C11-C12-C13-C14
11	R	502	PEE	C11-C10-O2-C2
11	C	505	PEE	C32-C33-C34-C35
11	E	502	PEE	C13-C14-C15-C16
12	C	501	HEM	C1A-C2A-CAA-CBA
12	P	402	HEM	C1A-C2A-CAA-CBA
18	D	502	CDL	C11-CA5-OA6-CA4
11	C	509	PEE	C32-C33-C34-C35
11	E	502	PEE	C31-C32-C33-C34
11	C	509	PEE	C11-C10-O2-C2
11	C	510	PEE	C15-C16-C17-C18
11	C	509	PEE	O4-C10-O2-C2
11	E	502	PEE	C39-C40-C41-C42
18	D	502	CDL	OB6-CB4-CB6-OB8
11	E	502	PEE	C12-C13-C14-C15
11	R	502	PEE	C23-C24-C25-C26
18	Q	502	CDL	CB2-C1-CA2-OA2
11	P	409	PEE	C32-C33-C34-C35
11	P	409	PEE	C33-C34-C35-C36
11	R	502	PEE	C10-C11-C12-C13
11	R	502	PEE	C11-C12-C13-C14
11	P	410	PEE	C15-C16-C17-C18
19	P	406	BOG	C4-C5-C6-O6
18	D	502	CDL	OA7-CA5-OA6-CA4
11	C	505	PEE	C1-C2-C3-O3
11	R	502	PEE	C31-C30-O3-C3
11	P	407	PEE	C11-C12-C13-C14
11	A	501	PEE	C3-C2-O2-C10
11	R	502	PEE	C1-C2-O2-C10
18	G	101	CDL	OA5-CA3-CA4-OA6
11	P	411	PEE	O2-C2-C3-O3
11	P	401	PEE	C13-C14-C15-C16
11	C	505	PEE	O3P-C1-C2-C3
11	P	407	PEE	C1-C2-C3-O3
11	P	411	PEE	C1-C2-C3-O3
18	D	502	CDL	CB3-CB4-CB6-OB8
11	R	502	PEE	O5-C30-O3-C3
11	A	501	PEE	O3P-C1-C2-O2
18	D	502	CDL	OA6-CA4-CA6-OA8
11	P	410	PEE	C10-C11-C12-C13
11	E	502	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	C	506	MES	C7-C8-S-O3S
15	C	506	MES	C7-C8-S-O1S
15	C	506	MES	C7-C8-S-O2S
18	D	502	CDL	CB2-C1-CA2-OA2
18	D	502	CDL	CA2-C1-CB2-OB2
11	C	509	PEE	C11-C12-C13-C14
14	C	504	U10	C1-C6-C7-C8
11	C	505	PEE	O3P-C1-C2-O2
11	P	409	PEE	O3P-C1-C2-O2
11	P	407	PEE	C12-C13-C14-C15
11	R	502	PEE	C22-C23-C24-C25
14	C	504	U10	C5-C6-C7-C8
11	C	505	PEE	C12-C13-C14-C15
11	P	401	PEE	C11-C12-C13-C14
11	P	409	PEE	C13-C14-C15-C16
11	R	502	PEE	C12-C13-C14-C15
11	A	501	PEE	O3P-C1-C2-C3
11	P	409	PEE	O3P-C1-C2-C3
18	G	101	CDL	OA5-CA3-CA4-CA6
11	P	401	PEE	C18-C19-C20-C21
11	P	409	PEE	O5-C30-O3-C3
18	T	101	CDL	OB6-CB4-CB6-OB8
18	D	502	CDL	CA3-CA4-CA6-OA8
11	E	502	PEE	C34-C35-C36-C37
11	C	505	PEE	C1-O3P-P-O1P
11	C	507	PEE	C1-O3P-P-O1P
11	C	509	PEE	C4-O4P-P-O1P
11	P	407	PEE	C1-O3P-P-O4P
11	P	407	PEE	C4-O4P-P-O3P
11	P	407	PEE	C4-O4P-P-O2P
11	P	411	PEE	C4-O4P-P-O1P
11	R	502	PEE	C1-O3P-P-O1P
18	D	502	CDL	CA2-OA2-PA1-OA3
18	D	502	CDL	CA3-OA5-PA1-OA3
18	G	101	CDL	CA2-OA2-PA1-OA3
18	G	101	CDL	CB2-OB2-PB2-OB3
18	Q	502	CDL	CA3-OA5-PA1-OA3
18	T	101	CDL	CA2-OA2-PA1-OA3
17	Q	501	HEC	C2B-C3B-CAB-CBB
11	E	502	PEE	C10-C11-C12-C13
11	C	509	PEE	C18-C19-C20-C21
11	C	510	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	P	409	PEE	C41-C42-C43-C44
11	P	409	PEE	C31-C30-O3-C3
19	P	406	BOG	C3'-C4'-C5'-C6'
17	D	501	HEC	C2B-C3B-CAB-CBB
11	E	502	PEE	C15-C16-C17-C18
11	E	502	PEE	C14-C15-C16-C17
11	P	407	PEE	C23-C24-C25-C26
11	R	502	PEE	C38-C39-C40-C41
11	A	501	PEE	O5-C30-O3-C3
11	A	501	PEE	C31-C30-O3-C3
11	P	409	PEE	C44-C45-C46-C47
11	C	507	PEE	O3P-C1-C2-C3
12	P	403	HEM	CAA-CBA-CGA-O1A
11	P	407	PEE	O3P-C1-C2-C3
18	T	101	CDL	OA5-CA3-CA4-CA6
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	403	HEM	CAD-CBD-CGD-O1D
12	C	501	HEM	C3A-C2A-CAA-CBA
12	C	502	HEM	CAD-CBD-CGD-O1D
11	R	502	PEE	C24-C25-C26-C27
11	R	502	PEE	C33-C34-C35-C36
12	P	402	HEM	C3A-C2A-CAA-CBA
12	C	502	HEM	CAD-CBD-CGD-O2D
12	P	403	HEM	CAD-CBD-CGD-O2D
11	P	401	PEE	O2-C10-C11-C12
11	P	407	PEE	O3P-C1-C2-O2
18	T	101	CDL	OA5-CA3-CA4-OA6
11	P	409	PEE	C38-C39-C40-C41
12	P	403	HEM	CAA-CBA-CGA-O2A
11	P	410	PEE	O2-C10-C11-C12
11	P	410	PEE	C11-C12-C13-C14
11	E	502	PEE	O2-C2-C3-O3
11	C	505	PEE	C38-C39-C40-C41
12	C	502	HEM	CAA-CBA-CGA-O2A
11	P	410	PEE	O4-C10-C11-C12
11	E	502	PEE	C36-C37-C38-C39
11	P	401	PEE	O4-C10-C11-C12
11	P	409	PEE	C1-C2-O2-C10
11	E	502	PEE	C38-C39-C40-C41
11	P	401	PEE	C16-C17-C18-C19
11	P	407	PEE	C38-C39-C40-C41
11	P	407	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	C	509	PEE	C36-C37-C38-C39
11	E	502	PEE	O3P-C1-C2-O2
11	R	502	PEE	C1-C2-C3-O3
18	T	101	CDL	CB3-CB4-CB6-OB8
11	C	509	PEE	C16-C17-C18-C19
11	C	505	PEE	C18-C19-C20-C21
11	C	509	PEE	C38-C39-C40-C41
11	P	407	PEE	C18-C19-C20-C21
11	E	503	PEE	C16-C17-C18-C19
11	C	505	PEE	C11-C12-C13-C14
12	C	501	HEM	CAA-CBA-CGA-O1A
12	P	402	HEM	CAA-CBA-CGA-O1A
12	C	501	HEM	CAA-CBA-CGA-O2A
12	P	402	HEM	CAA-CBA-CGA-O2A
14	C	504	U10	C2-C3-O3-C3M
11	C	505	PEE	O2-C10-C11-C12
11	E	502	PEE	O3-C30-C31-C32
11	C	505	PEE	C31-C32-C33-C34
11	P	409	PEE	C3-C2-O2-C10
11	A	501	PEE	C10-C11-C12-C13
17	D	501	HEC	CAA-CBA-CGA-O2A
17	Q	501	HEC	CAA-CBA-CGA-O2A
11	R	502	PEE	C36-C37-C38-C39
11	P	409	PEE	O3-C30-C31-C32
11	C	509	PEE	O2-C2-C3-O3
11	C	505	PEE	O3-C30-C31-C32
11	C	510	PEE	O2-C10-C11-C12
12	C	501	HEM	C2C-C3C-CAC-CBC
12	P	402	HEM	C2C-C3C-CAC-CBC
11	E	502	PEE	O5-C30-C31-C32
18	D	502	CDL	C51-CB5-OB6-CB4
11	C	505	PEE	O5-C30-C31-C32

There are no ring outliers.

22 monomers are involved in 46 short contacts:

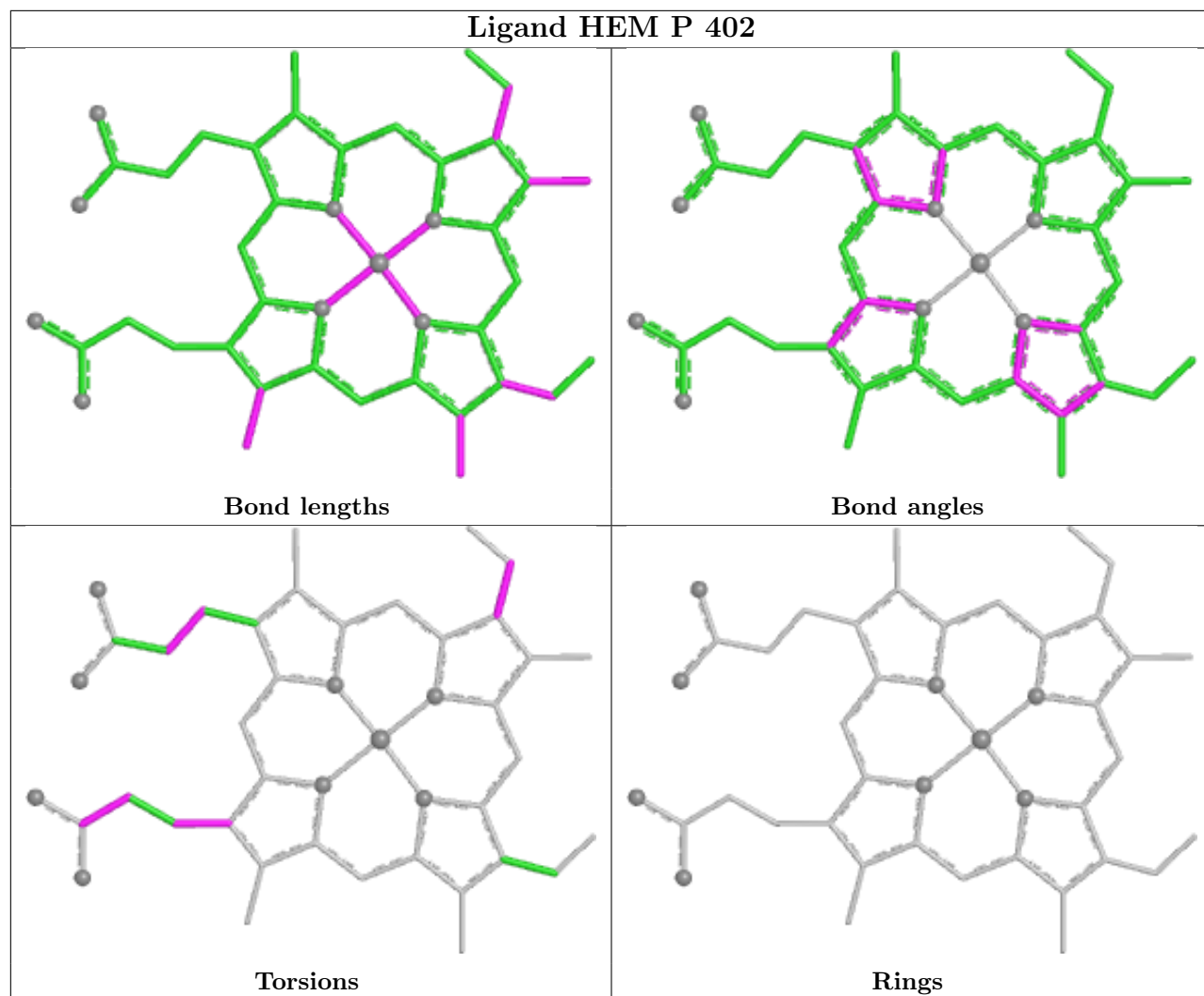
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	402	HEM	5	0
12	P	403	HEM	3	0
11	A	501	PEE	1	0
11	R	502	PEE	5	0
14	P	405	U10	1	0

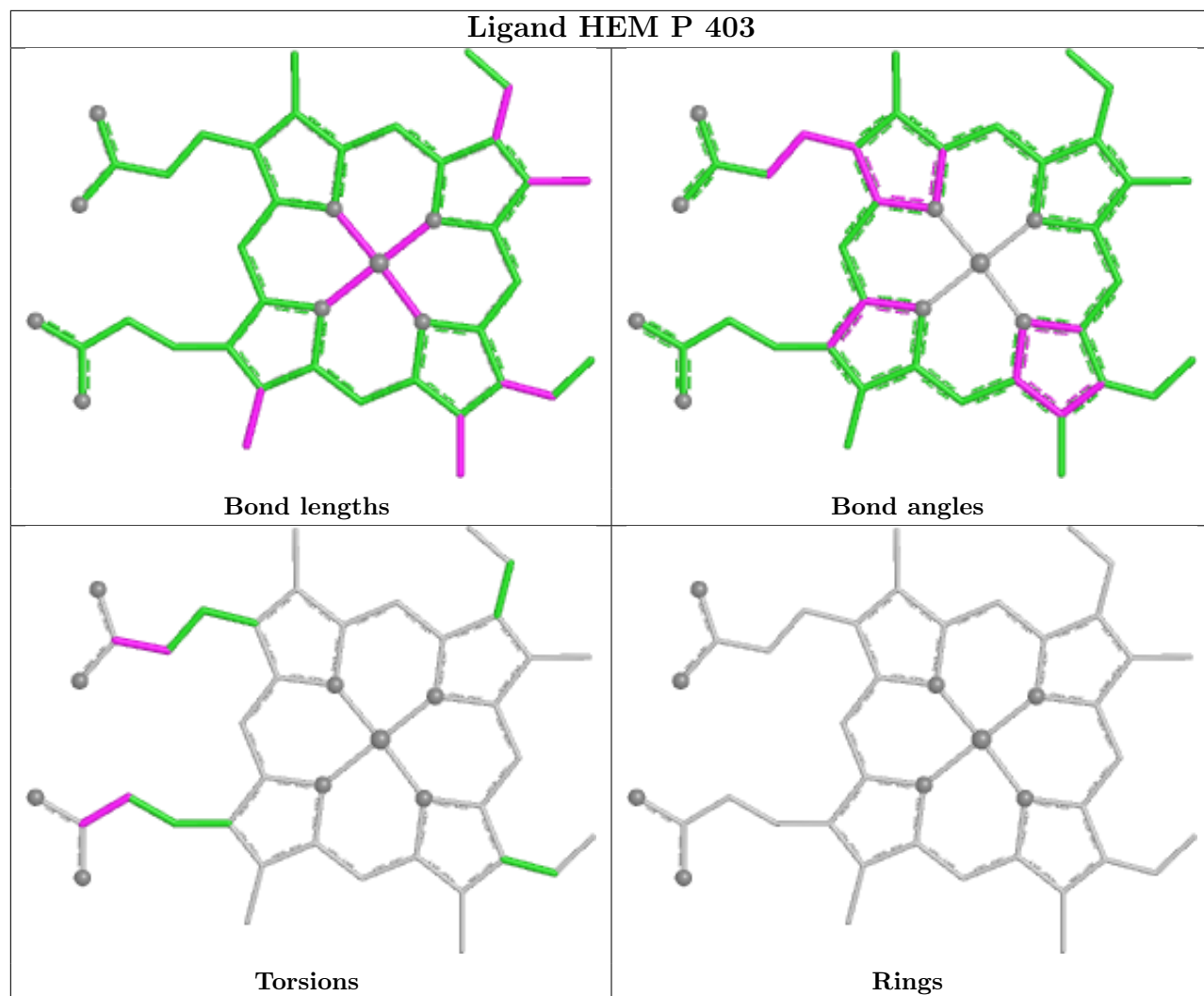
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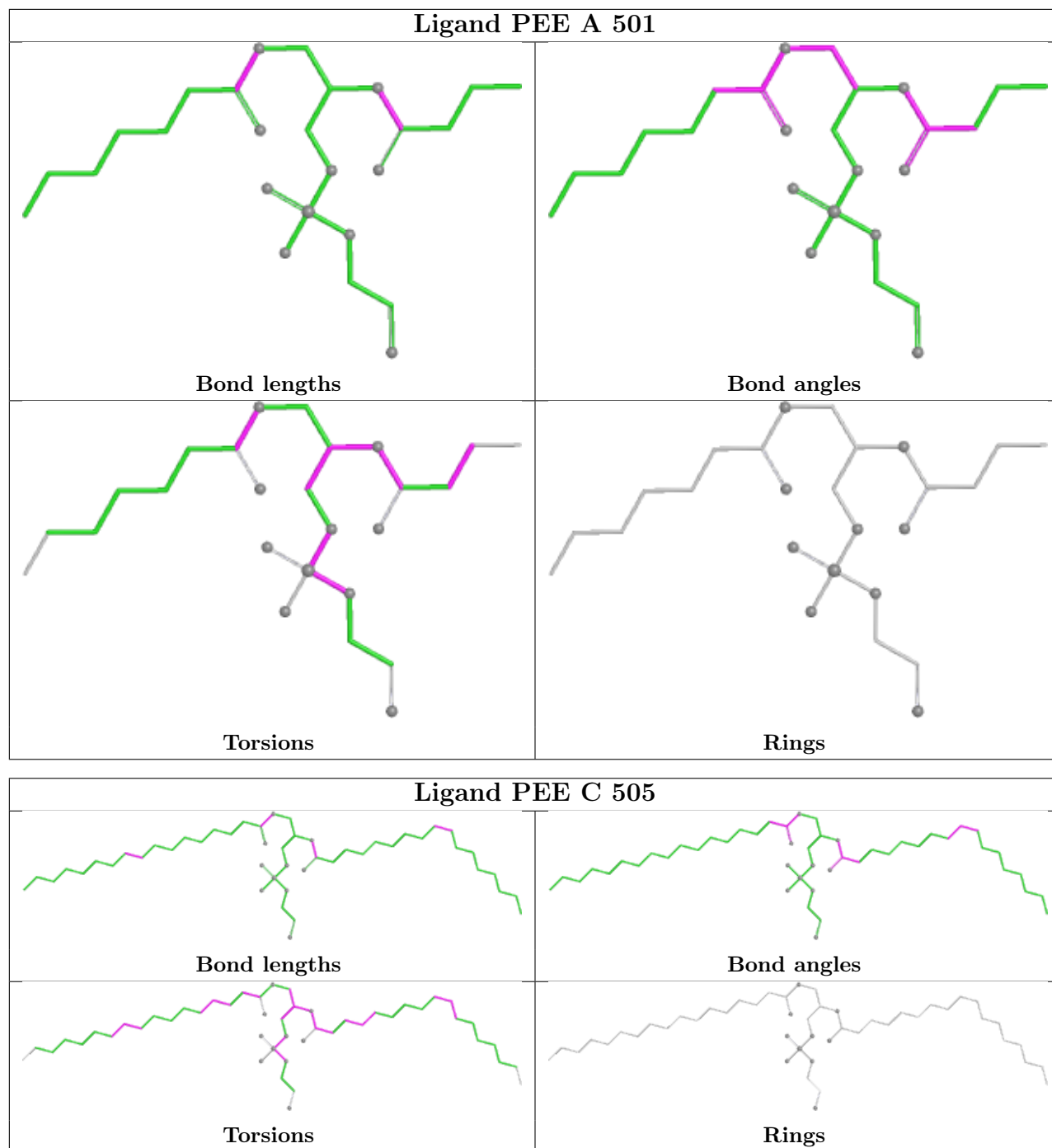
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	407	PEE	2	0
12	C	501	HEM	4	0
13	C	503	Y52	2	0
16	C	508	GOL	1	0
11	E	503	PEE	3	0
11	P	401	PEE	1	0
11	C	509	PEE	2	0
18	D	502	CDL	1	0
11	P	409	PEE	3	0
11	E	502	PEE	4	0
13	P	404	Y52	1	0
18	T	101	CDL	3	0
11	P	411	PEE	1	0
16	P	408	GOL	1	0
18	G	101	CDL	1	0
19	P	406	BOG	3	0
12	C	502	HEM	3	0

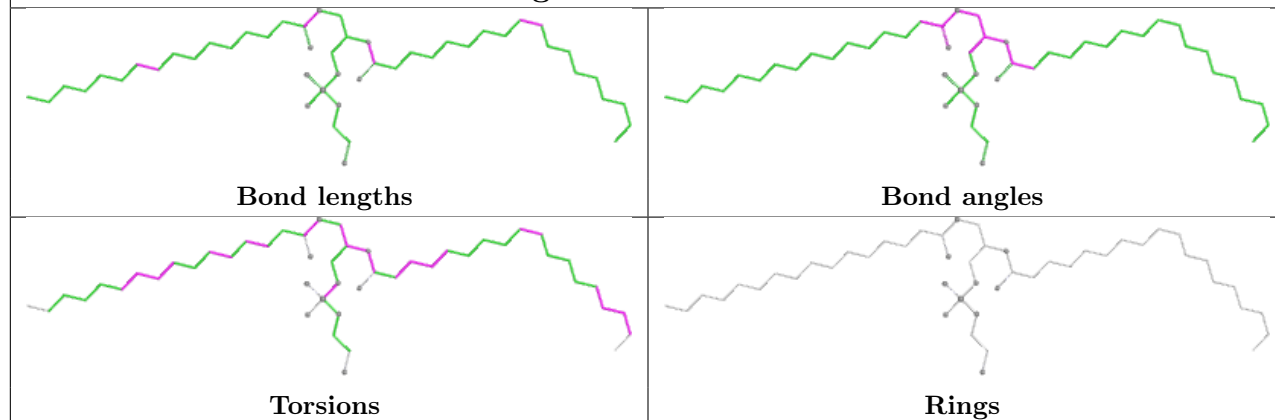
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



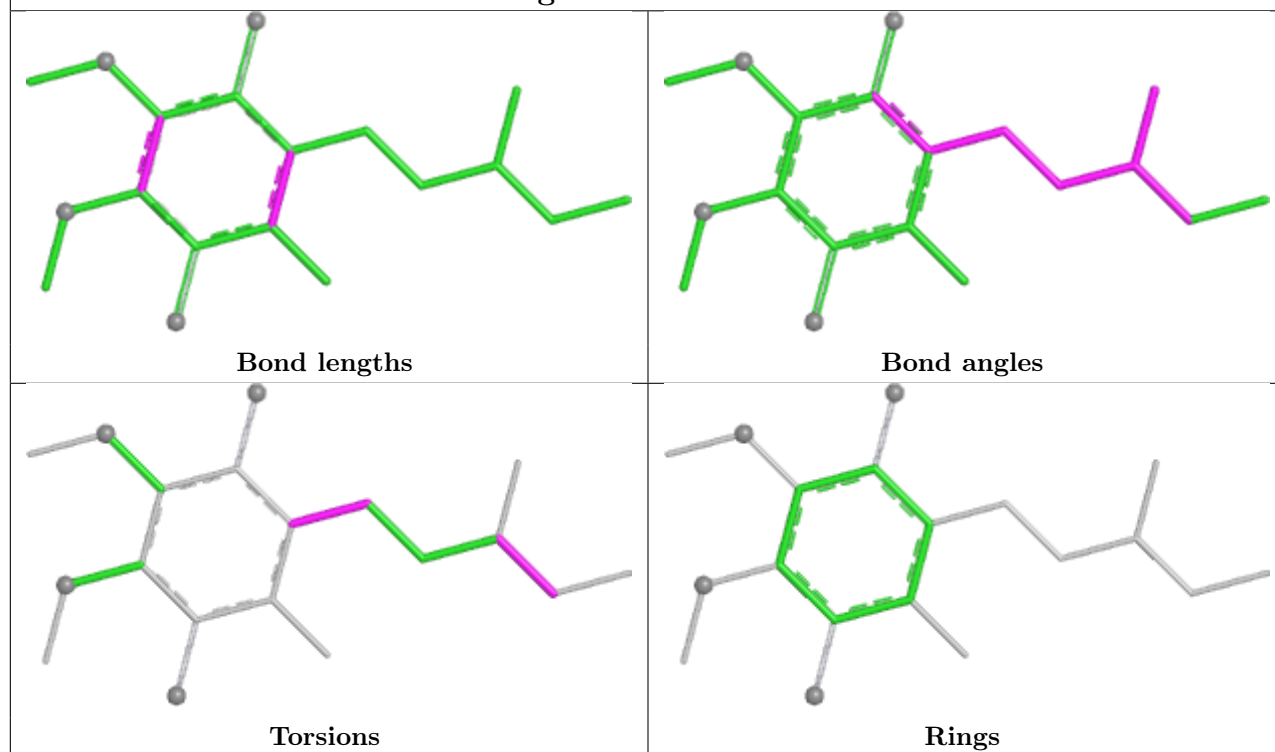




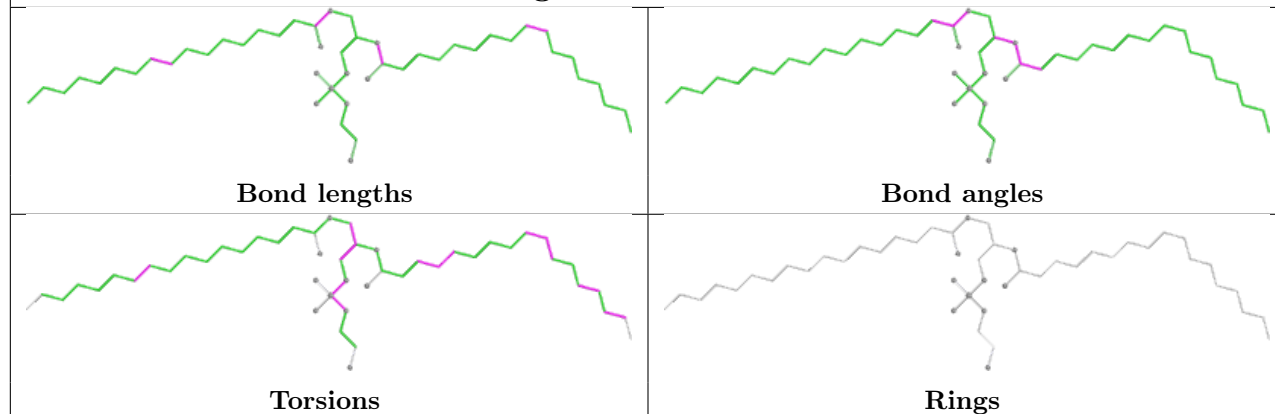
Ligand PEE R 502

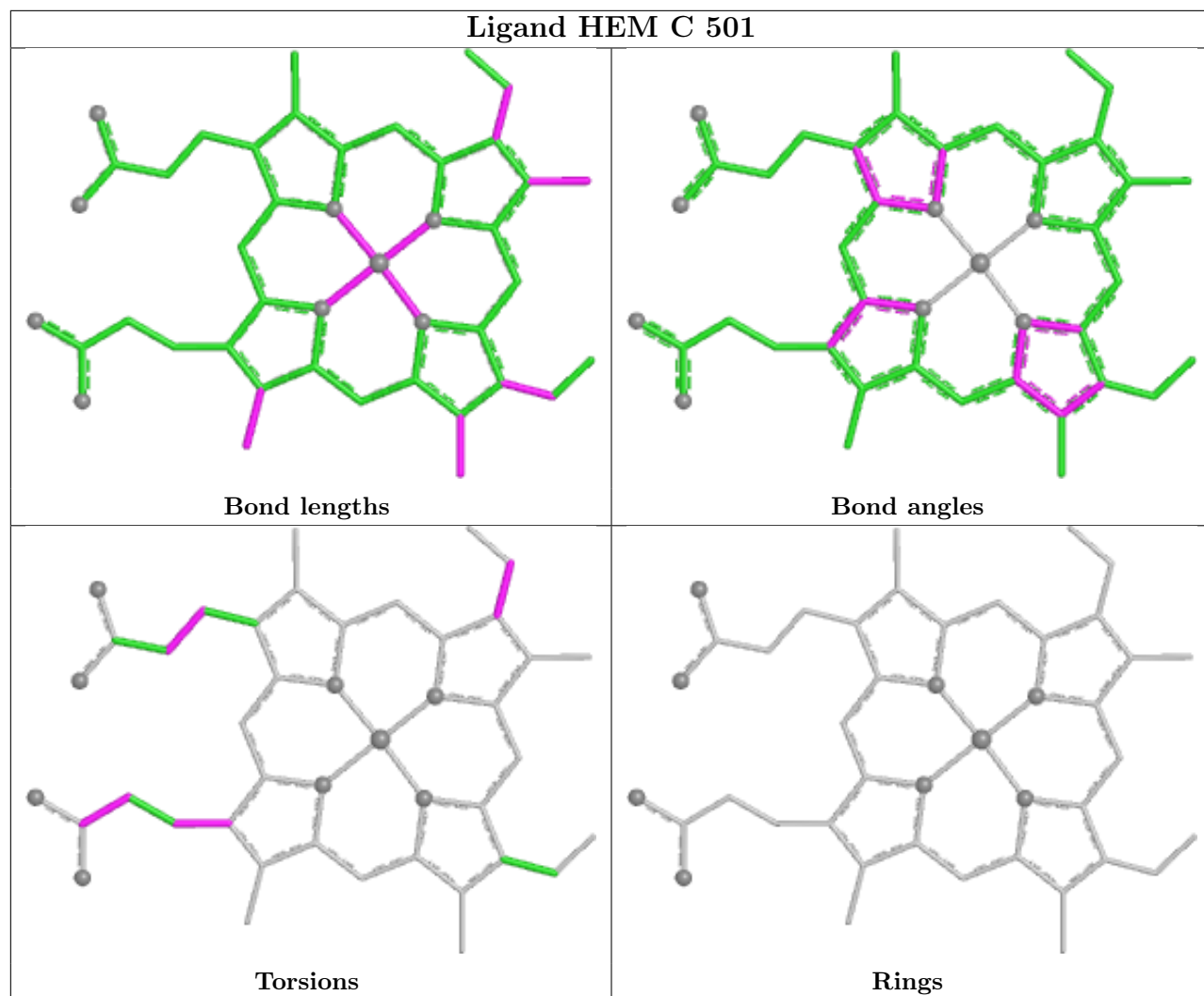


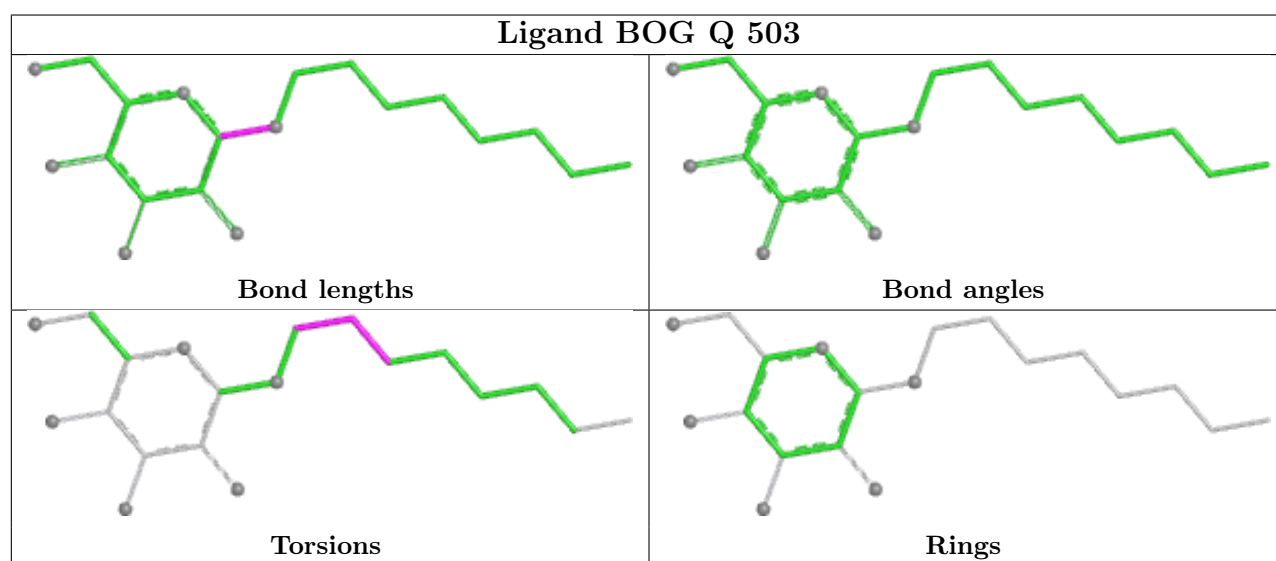
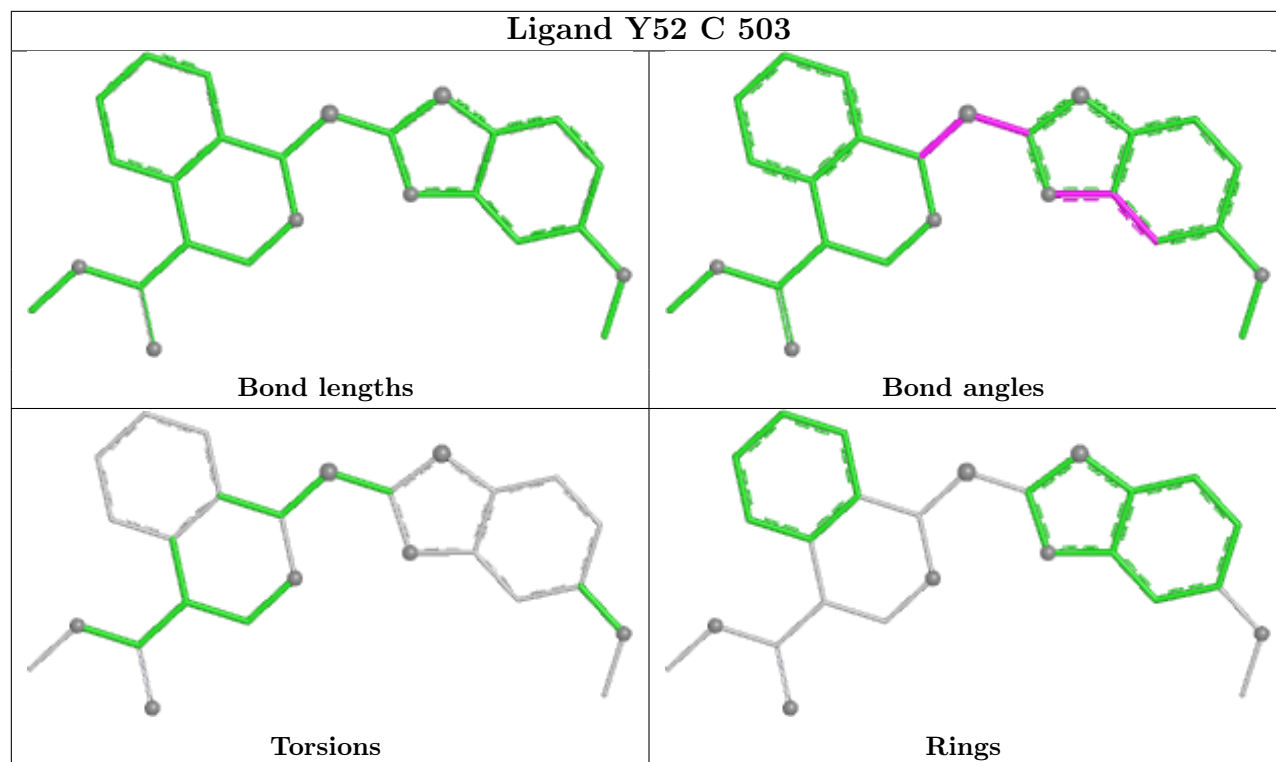
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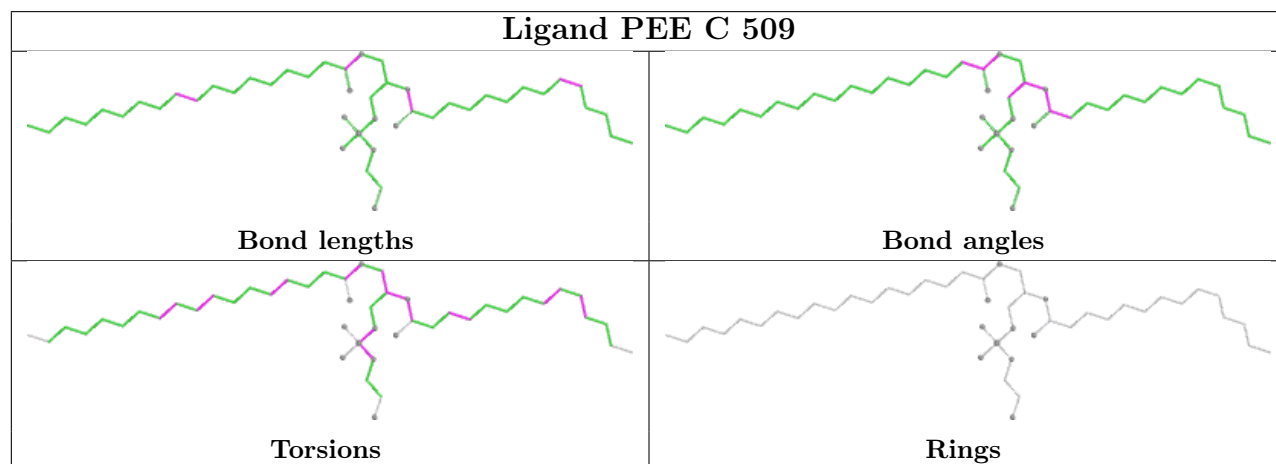
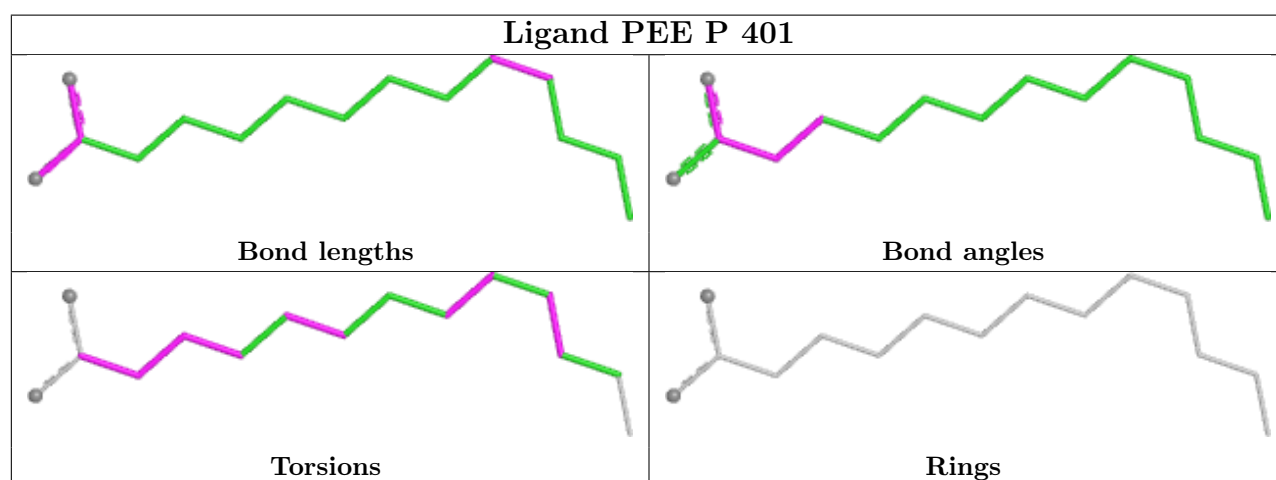
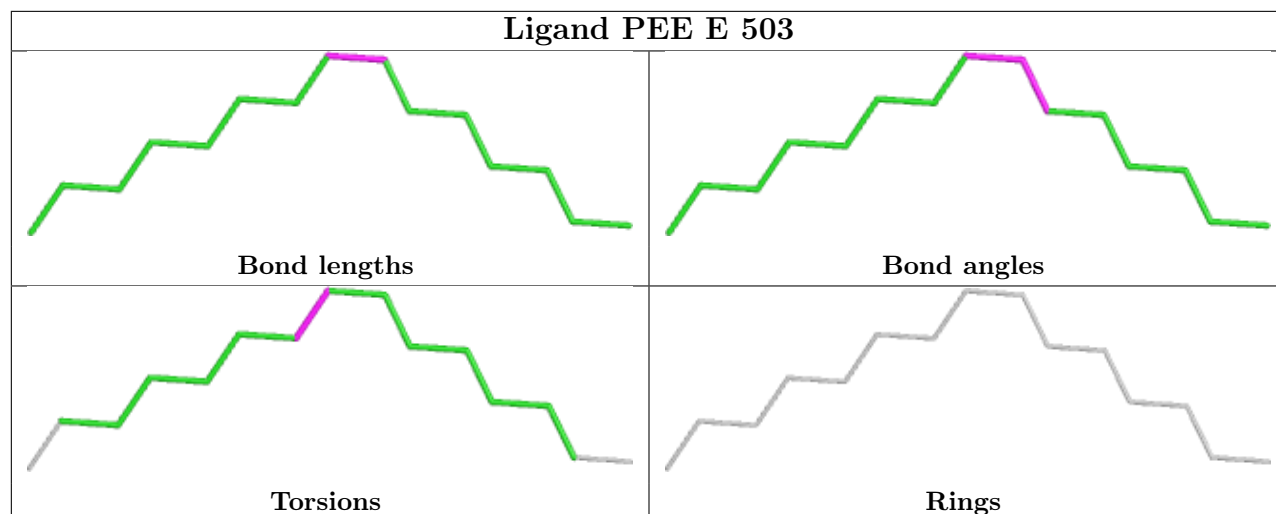


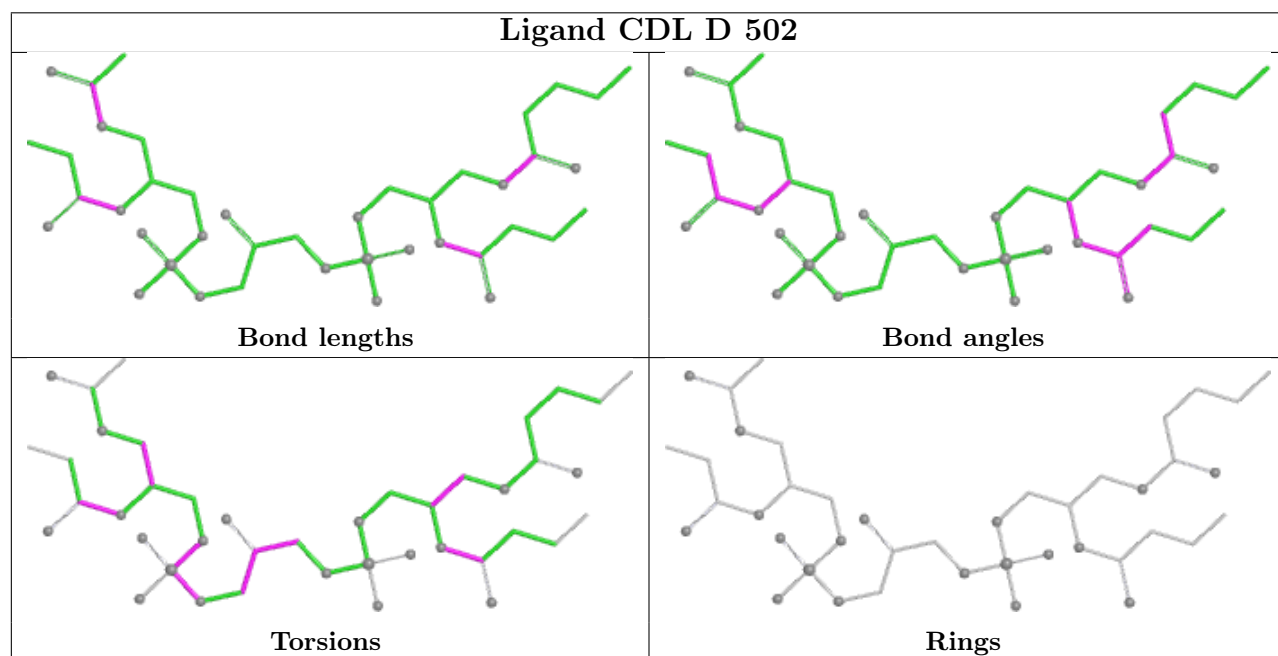
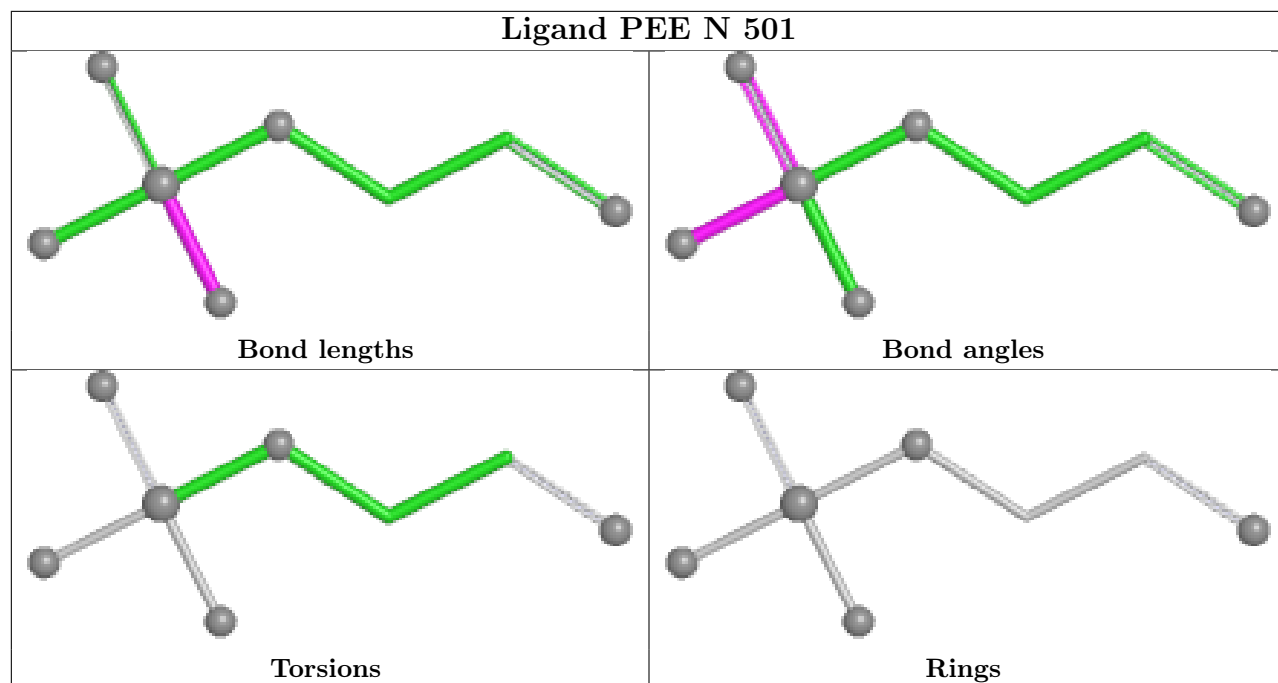
Ligand PEE P 407

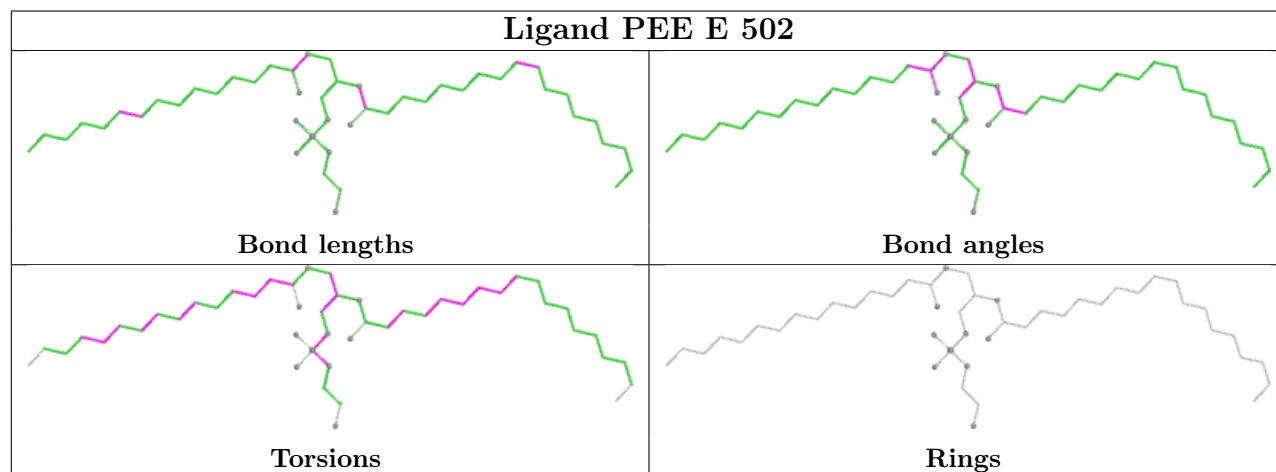
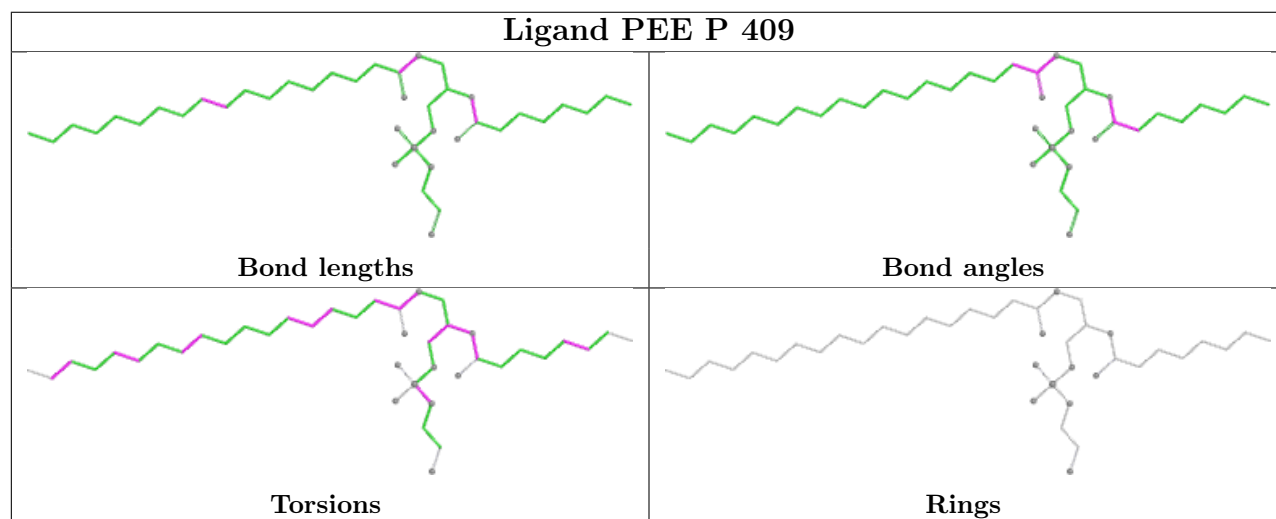
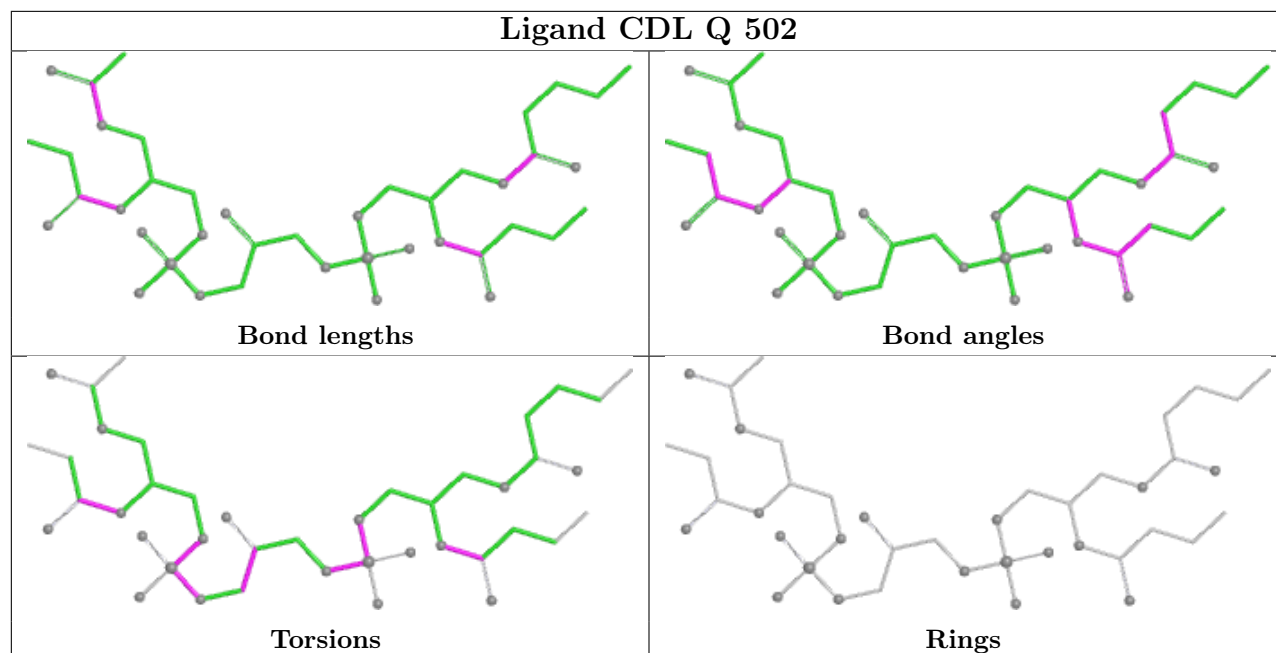




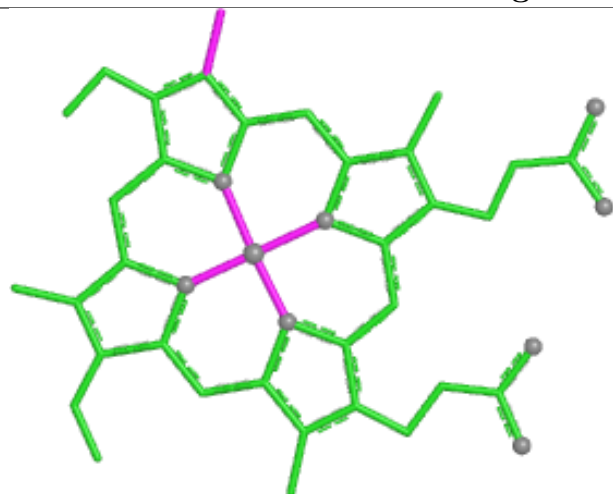




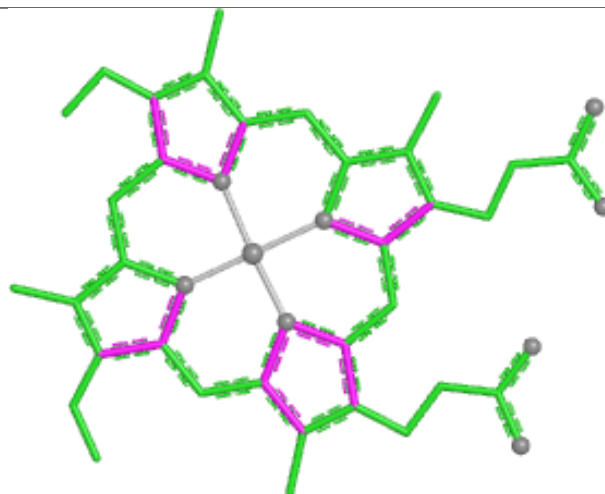




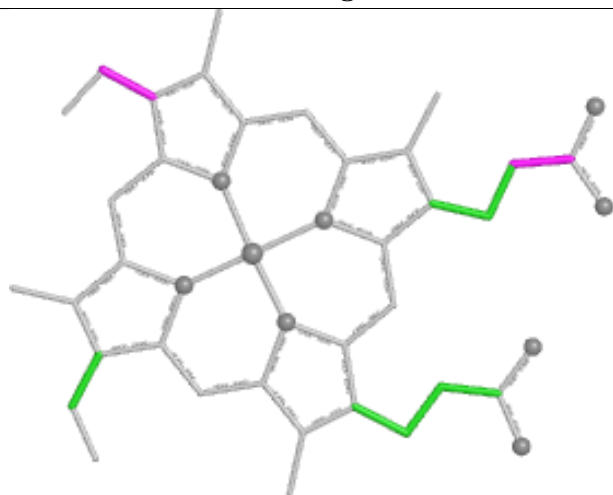
Ligand HEC D 501



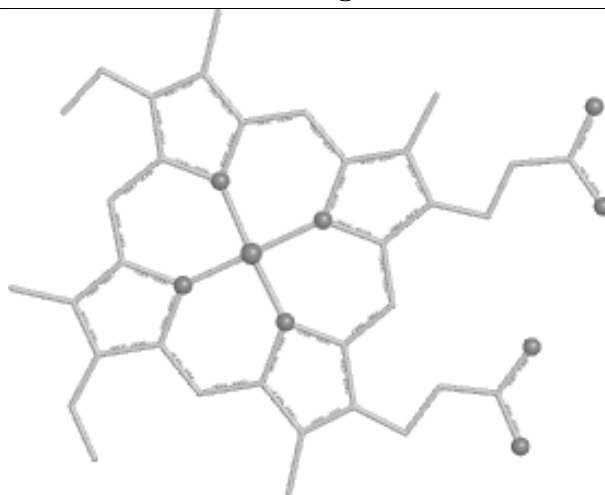
Bond lengths



Bond angles

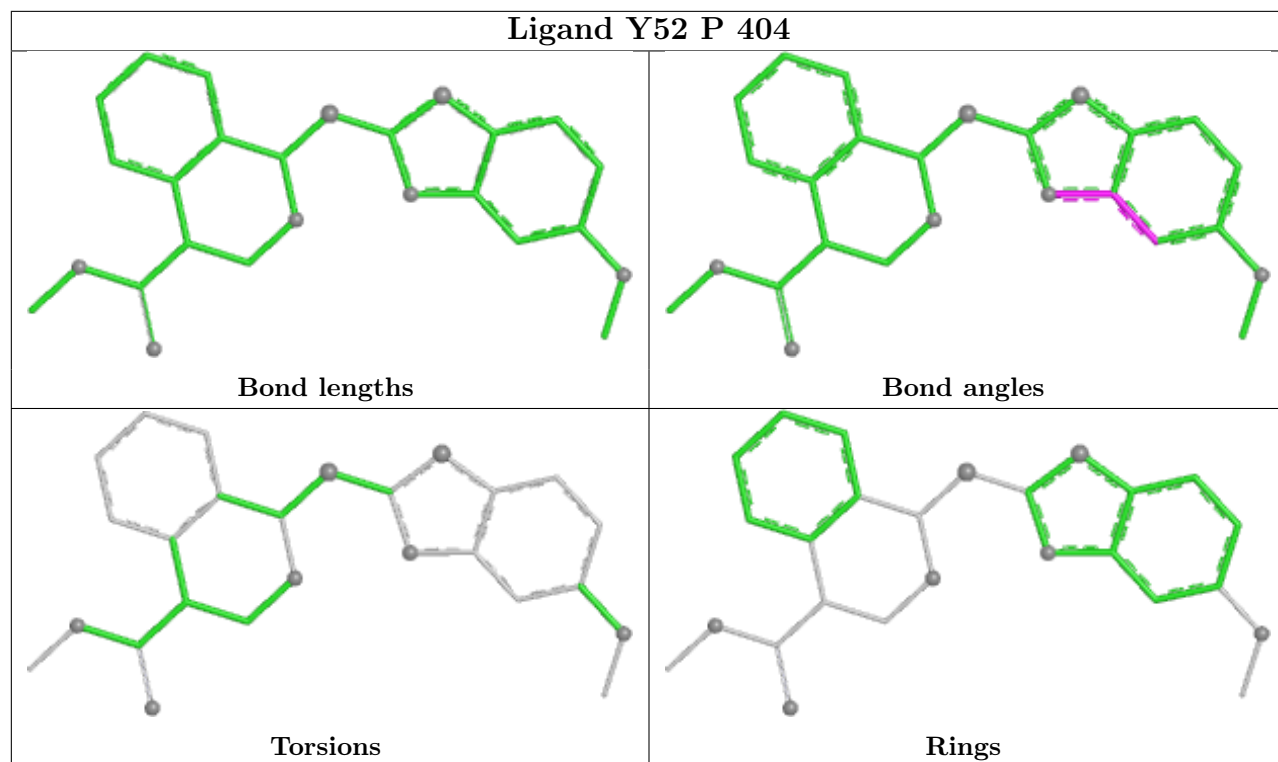


Torsions

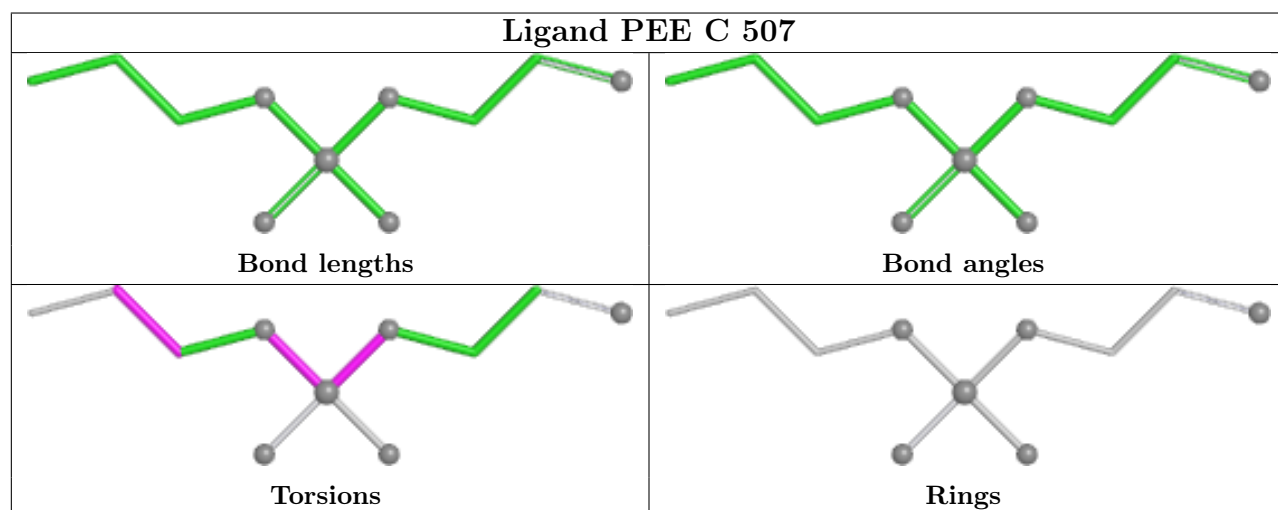


Rings

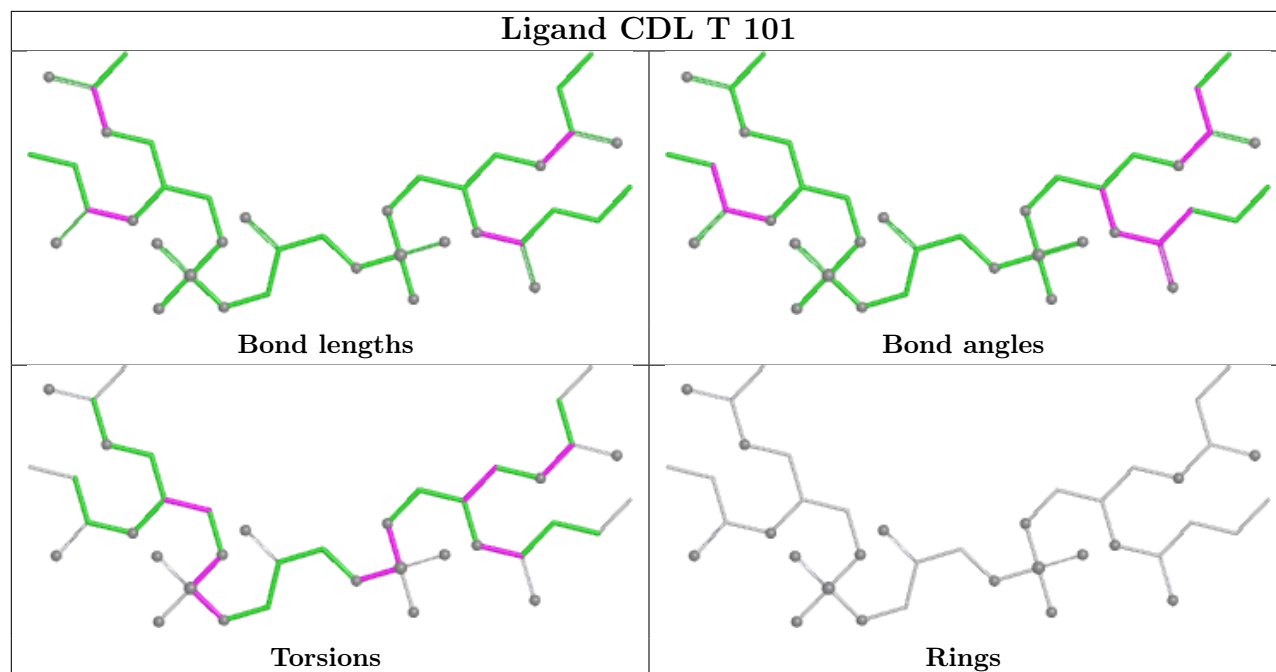
Ligand Y52 P 404



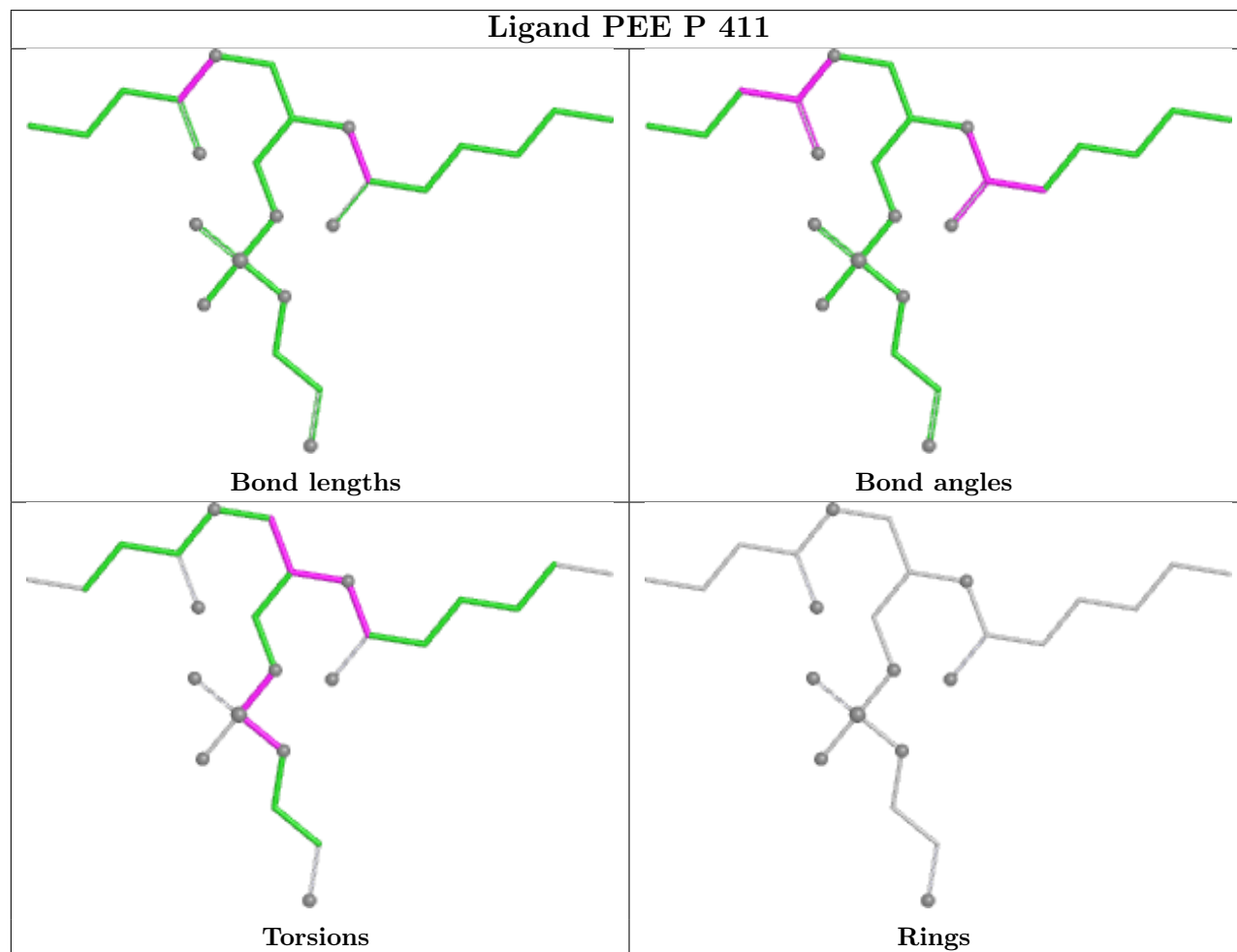
Ligand PEE C 507

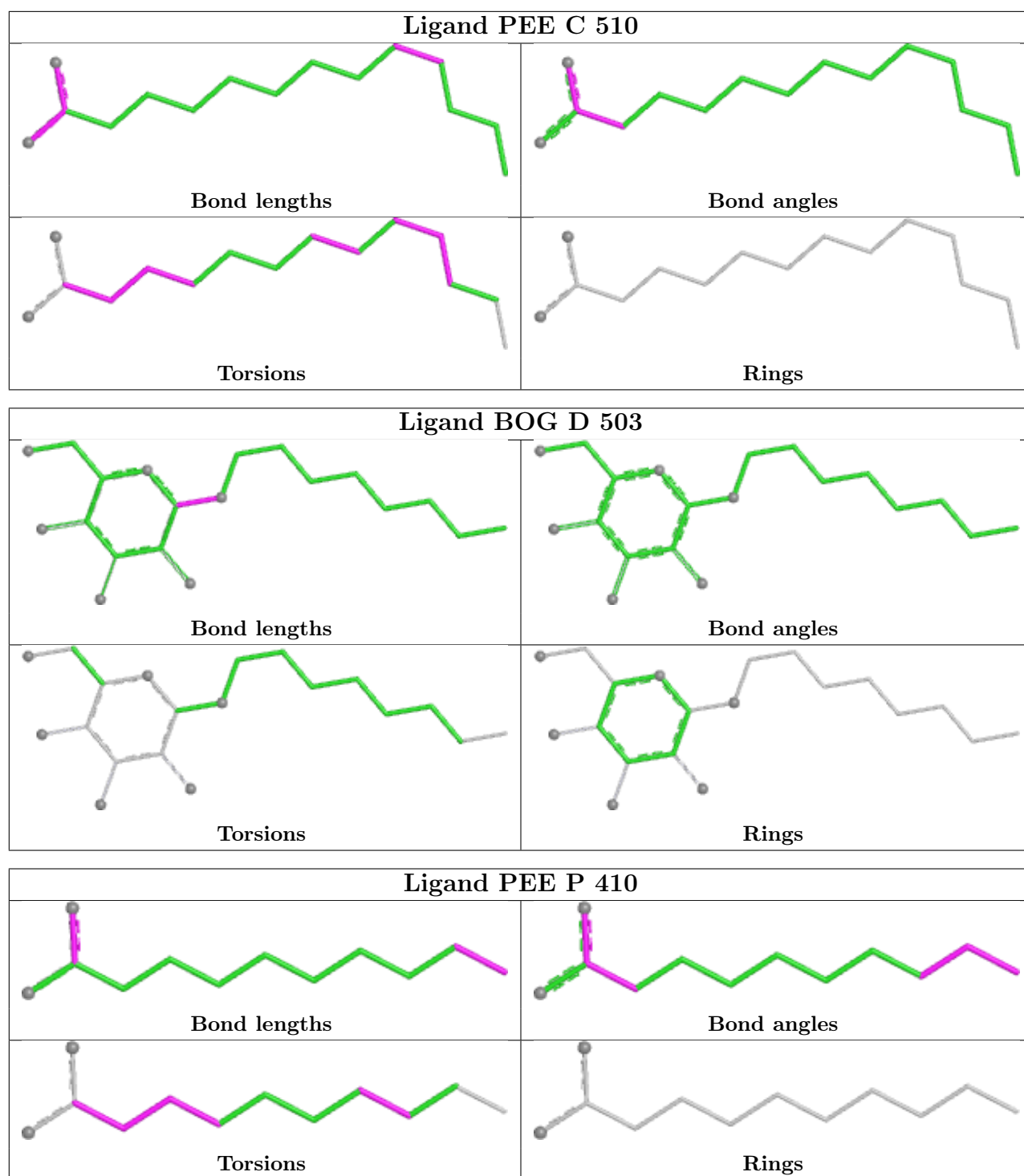


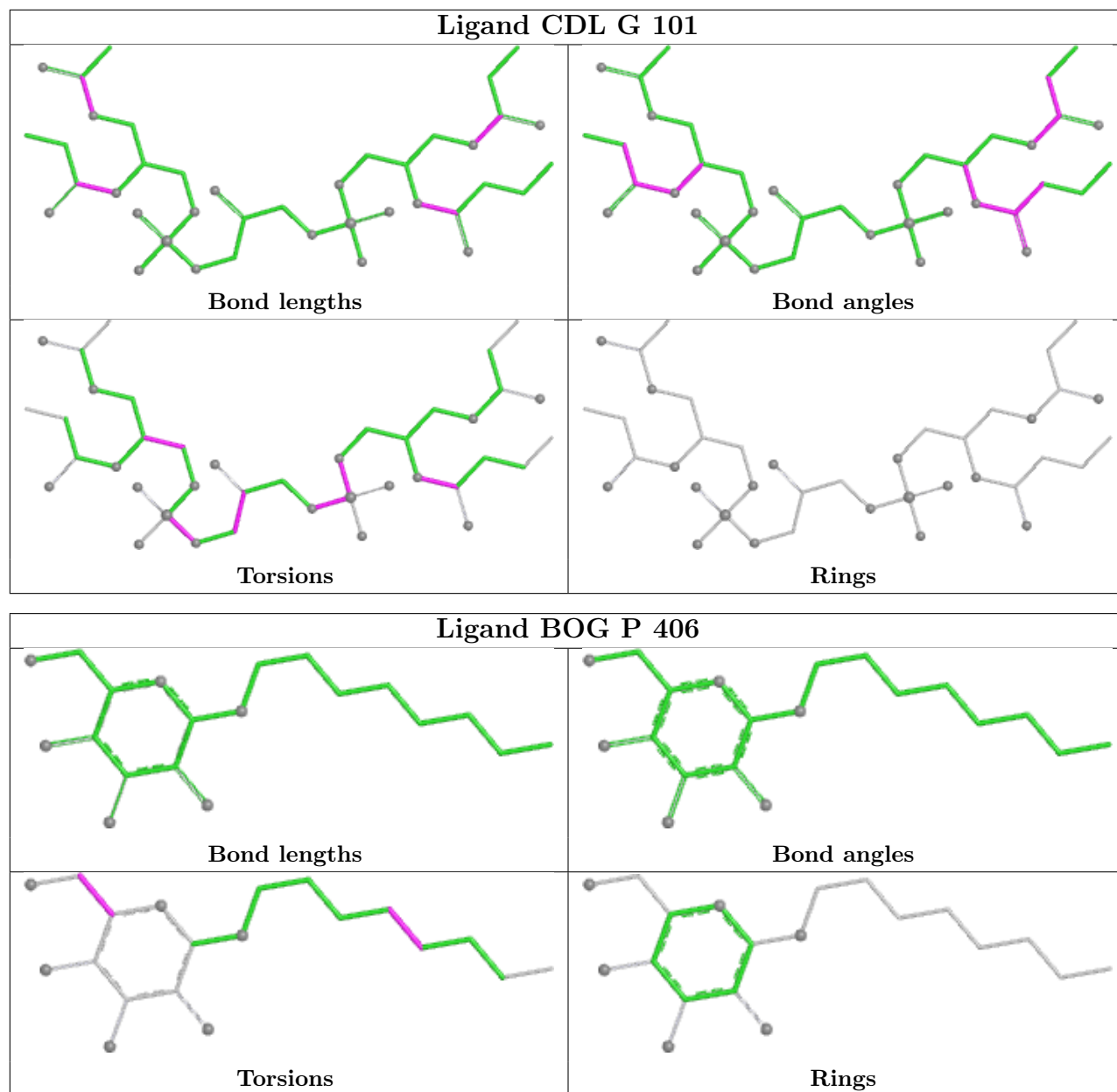
Ligand CDL T 101

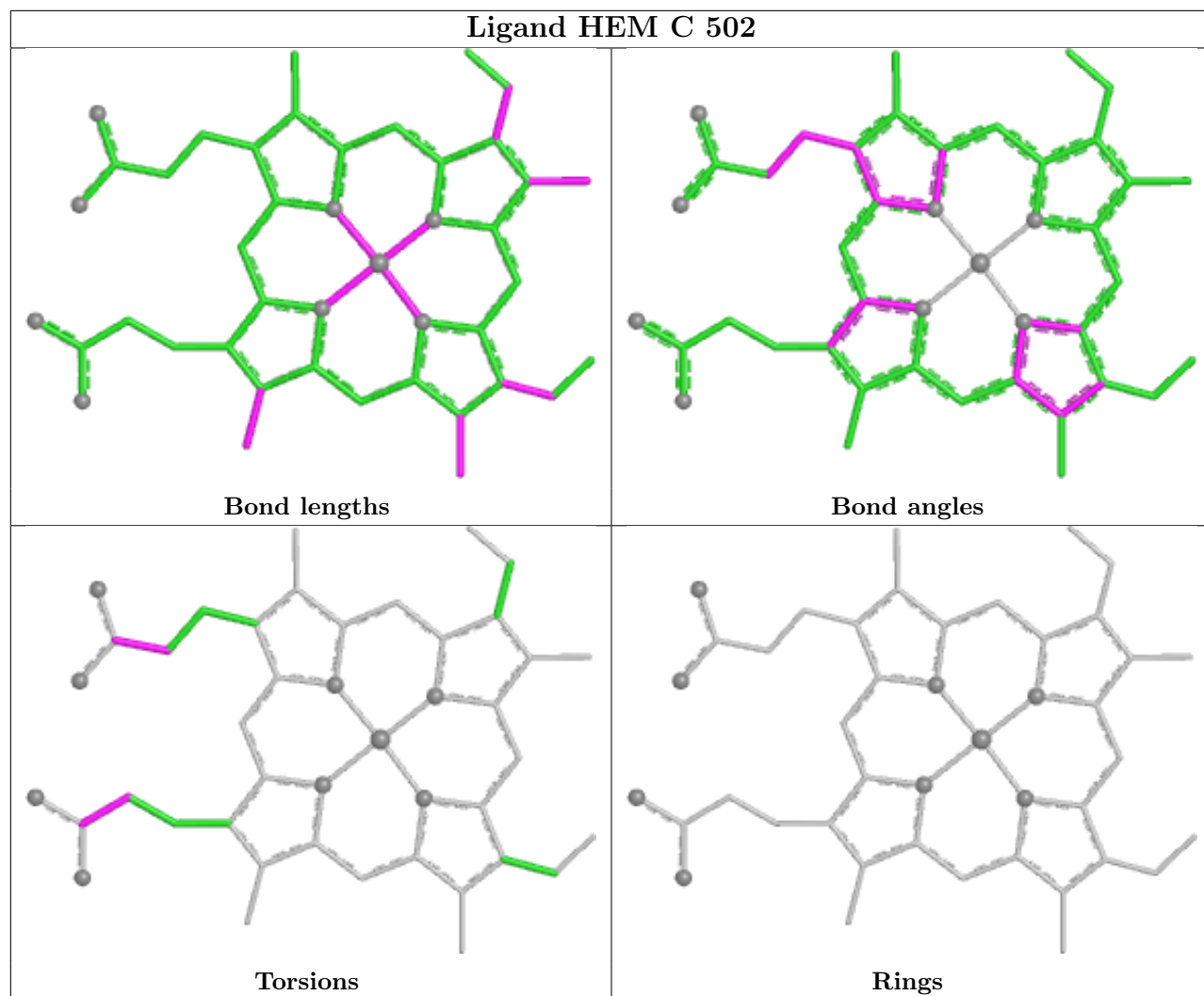


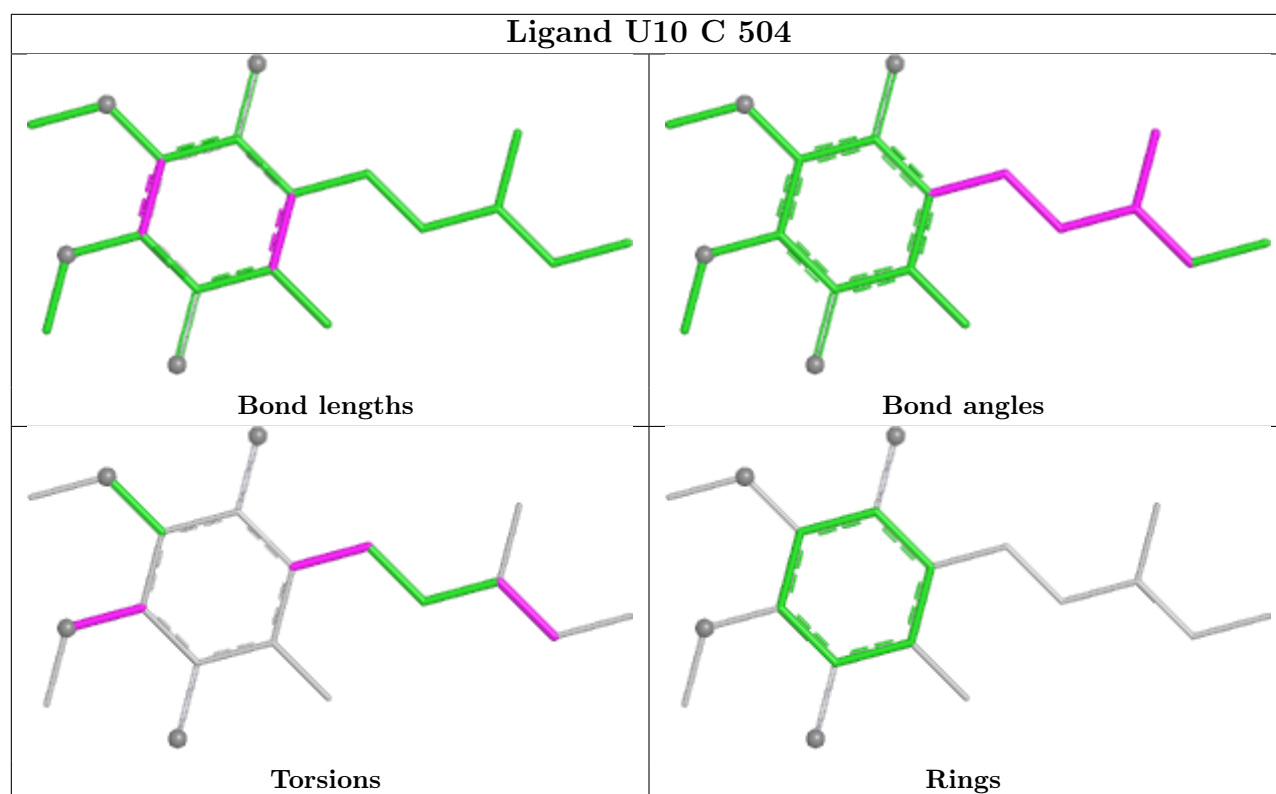
Ligand PEE P 411

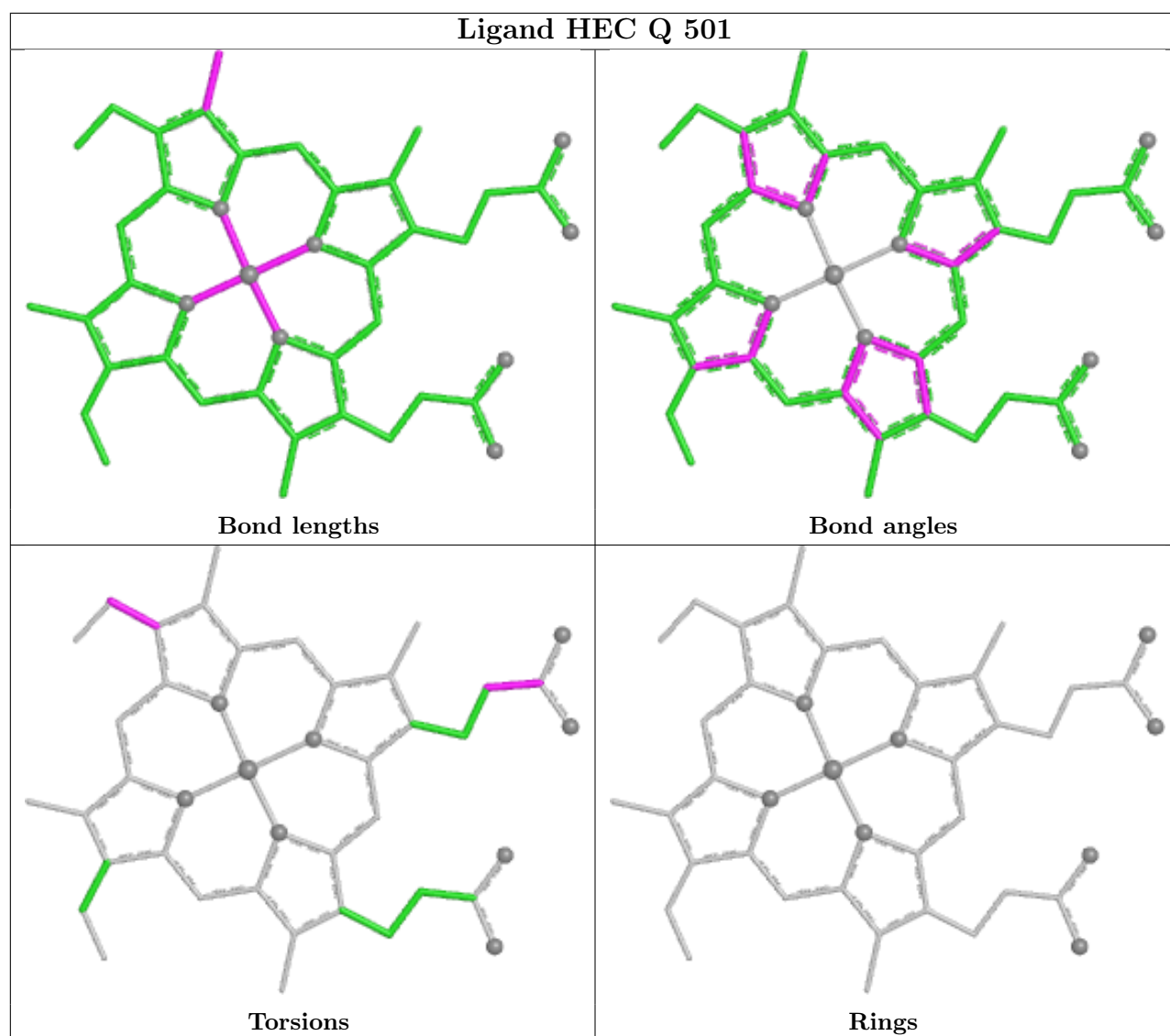












5.7 Other polymers [i](#)

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	443/446 (99%)	0.03	6 (1%) 73 54	28, 53, 78, 101	0
1	N	442/446 (99%)	0.19	1 (0%) 91 85	36, 57, 81, 99	0
2	B	421/441 (95%)	0.36	8 (1%) 66 46	47, 67, 102, 123	0
2	O	422/441 (95%)	0.28	2 (0%) 87 76	35, 63, 86, 104	0
3	C	379/380 (99%)	-0.26	2 (0%) 87 76	22, 33, 70, 102	0
3	P	379/380 (99%)	0.03	2 (0%) 87 76	18, 51, 78, 104	1 (0%)
4	D	241/241 (100%)	-0.16	1 (0%) 88 79	25, 37, 73, 95	0
4	Q	241/241 (100%)	0.18	0 100 100	39, 59, 85, 117	0
5	E	196/196 (100%)	1.14	55 (28%) 1 1	28, 111, 166, 182	9 (4%)
5	R	196/196 (100%)	0.60	17 (8%) 16 11	36, 81, 128, 141	8 (4%)
6	F	101/110 (91%)	-0.29	0 100 100	25, 37, 53, 78	0
6	S	101/110 (91%)	0.08	1 (0%) 79 63	46, 59, 86, 102	0
7	G	80/81 (98%)	0.02	2 (2%) 58 39	28, 45, 73, 89	0
7	T	79/81 (97%)	0.50	2 (2%) 58 39	40, 70, 122, 127	0
8	H	68/77 (88%)	0.01	2 (2%) 53 35	35, 50, 68, 101	0
8	U	68/77 (88%)	0.81	3 (4%) 39 25	66, 91, 113, 117	0
9	I	30/76 (39%)	1.44	7 (23%) 2 2	55, 77, 116, 120	0
9	V	30/76 (39%)	1.58	9 (30%) 1 1	47, 78, 119, 130	0
10	J	61/61 (100%)	0.02	2 (3%) 49 31	34, 46, 79, 129	0
10	W	60/61 (98%)	0.21	1 (1%) 69 49	41, 55, 92, 117	0
All	All	4038/4218 (95%)	0.20	123 (3%) 52 34	18, 56, 106, 182	18 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	7.9
5	E	162	GLY	7.1
9	I	57	GLY	6.2
3	P	69[G]	HIS	6.1
5	E	176	ALA	5.8
5	E	120	PRO	5.6
5	R	114	VAL	4.9
5	E	102	THR	4.9
9	V	57	GLY	4.6
5	E	117	LEU	4.5
9	V	50	LEU	4.3
9	I	48	PRO	4.3
10	J	62	SER	4.2
5	E	112	VAL	4.0
5	E	127	VAL	3.9
5	E	85	LYS	3.9
2	O	296	TYR	3.9
5	R	143	GLY	3.7
9	V	61	ARG	3.6
9	V	54	SER	3.6
5	E	121	GLN	3.5
5	E	124	LEU	3.5
5	R	124	LEU	3.5
9	V	49	LEU	3.5
5	E	172	ARG	3.4
1	A	219	VAL	3.3
5	E	115	SER	3.3
5	E	192	LEU	3.3
5	E	157	TYR	3.2
5	E	82	PRO	3.2
3	C	14	MET	3.2
9	I	51	CYS	3.1
5	E	188	VAL	3.1
9	V	51	CYS	3.1
5	E	106	ILE	3.0
5	E	150	SER	3.0
5	E	146	PRO	3.0
5	E	100	HIS	2.9
2	B	226	ILE	2.9
9	I	54	SER	2.9
5	E	185	TYR	2.8
5	E	107	ASN	2.8
2	B	282	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	180	LEU	2.8
5	E	122	HIS	2.8
5	E	110	ALA	2.8
5	E	191	ASP	2.8
5	R	125	ASP	2.7
5	E	156	TYR	2.7
5	R	158	CYS	2.7
5	R	163	SER	2.7
7	G	2	ILE	2.7
5	E	114	VAL	2.7
9	I	50	LEU	2.7
5	E	186	GLN	2.7
5	R	105	GLU	2.7
8	U	11	GLU	2.7
2	B	296	TYR	2.7
8	U	13	LEU	2.7
1	N	9	GLN	2.7
5	E	165	TYR	2.7
5	E	164	HIS	2.6
5	R	109	GLU	2.6
9	I	49	LEU	2.6
5	E	119	ASP	2.6
5	E	152	ASP	2.6
2	B	31	ASN	2.6
5	R	112	VAL	2.6
5	E	168	SER	2.6
5	E	126	ARG	2.6
5	R	127	VAL	2.6
10	W	61	ALA	2.5
5	R	82	PRO	2.5
9	V	59	SER	2.5
5	E	179	ASN	2.5
2	B	223	PHE	2.5
5	E	167	ALA	2.4
10	J	61	ALA	2.4
5	E	81	ILE	2.4
7	T	2	ILE	2.4
5	R	150	SER	2.4
5	E	147	ILE	2.4
6	S	13	MET	2.4
5	E	118	ARG	2.4
5	E	189	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	3	THR	2.3
2	B	227	ARG	2.3
5	R	102	THR	2.3
5	E	178	TYR	2.3
5	E	153	PHE	2.3
5	R	122	HIS	2.3
8	H	40	CYS	2.3
5	E	187	PHE	2.3
5	E	175	PRO	2.3
1	A	145	MET	2.3
2	B	388	LEU	2.3
1	A	444	ILE	2.2
9	V	48	PRO	2.2
5	E	171	ILE	2.2
5	E	177	PRO	2.2
5	E	174	GLY	2.2
1	A	69	LYS	2.2
8	H	11	GLU	2.2
5	R	104	ALA	2.2
7	T	74	PRO	2.2
5	E	125	ASP	2.2
9	V	63	ASP	2.2
5	E	130	PRO	2.1
5	R	120	PRO	2.1
5	E	184	THR	2.1
2	B	230	ALA	2.1
4	D	80	LEU	2.1
9	I	56	SER	2.1
5	E	128	LYS	2.1
2	O	387	LEU	2.1
8	U	50	THR	2.1
1	A	2	ALA	2.1
5	R	148	ALA	2.1
7	G	80	ASP	2.1
5	E	78	LEU	2.0
3	C	5	ILE	2.0
5	E	190	ASP	2.0
3	P	151	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	FME	C	1	9/11	0.57	0.19	72,88,96,99	0

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
11	PEE	A	501	26/51	0.52	0.19	27,87,106,123	0
11	PEE	P	409	41/51	0.54	0.20	54,69,112,128	0
18	CDL	Q	502	42/100	0.56	0.20	40,99,121,136	0
19	BOG	P	406	20/20	0.61	0.14	39,74,96,98	0
11	PEE	P	411	25/51	0.63	0.20	36,60,75,80	25
11	PEE	C	507	11/51	0.64	0.26	25,51,62,63	11
15	MES	C	506	12/12	0.65	0.15	45,69,109,122	0
11	PEE	E	503	15/51	0.66	0.18	22,49,63,68	0
11	PEE	C	509	47/51	0.68	0.17	22,48,88,107	0
11	PEE	N	501	8/51	0.69	0.17	57,79,96,112	0
18	CDL	D	502	42/100	0.69	0.17	46,80,99,127	0
14	U10	P	405	19/63	0.70	0.20	60,75,88,91	0
11	PEE	E	502	48/51	0.75	0.16	36,55,80,86	0
14	U10	C	504	19/63	0.76	0.21	45,59,67,70	0
18	CDL	T	101	40/100	0.77	0.17	44,85,97,98	0
11	PEE	R	502	49/51	0.79	0.16	33,64,79,88	0
11	PEE	P	401	15/51	0.81	0.21	41,58,88,89	0
11	PEE	P	407	49/51	0.82	0.14	45,68,84,89	0
18	CDL	G	101	40/100	0.84	0.14	24,56,69,73	0
11	PEE	C	510	15/51	0.86	0.13	25,54,81,84	0
19	BOG	D	503	20/20	0.86	0.12	29,46,54,57	0

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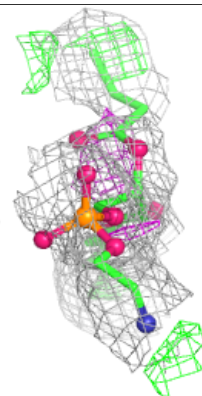
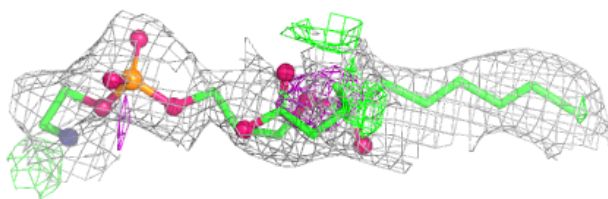
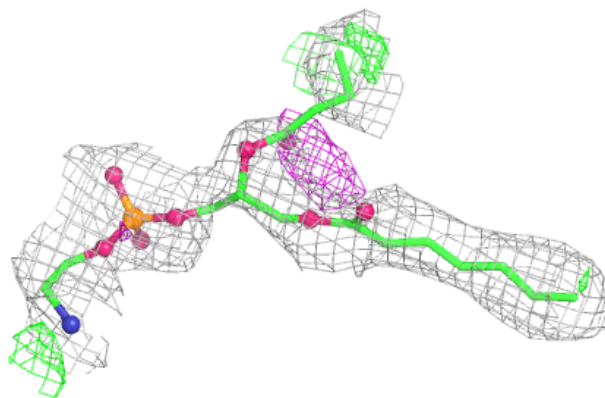
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	PEE	P	410	12/51	0.86	0.10	30,37,46,47	0
19	BOG	Q	503	20/20	0.87	0.10	34,54,62,63	0
11	PEE	C	505	49/51	0.88	0.12	22,43,54,57	0
13	Y52	P	404	27/27	0.93	0.10	38,46,58,63	0
16	GOL	P	408	6/6	0.94	0.09	42,43,49,51	0
17	HEC	Q	501	43/43	0.95	0.10	44,51,63,71	0
16	GOL	C	508	6/6	0.95	0.10	34,35,38,43	0
13	Y52	C	503	27/27	0.96	0.07	25,33,45,51	0
20	FES	R	501	4/4	0.96	0.06	71,84,92,107	0
12	HEM	P	403	43/43	0.97	0.10	27,33,50,53	0
12	HEM	C	501	43/43	0.97	0.10	18,24,32,35	0
17	HEC	D	501	43/43	0.97	0.08	26,34,40,42	0
20	FES	E	501	4/4	0.97	0.06	92,103,103,106	4
12	HEM	P	402	43/43	0.97	0.10	26,32,43,53	0
12	HEM	C	502	43/43	0.98	0.09	19,24,32,37	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.

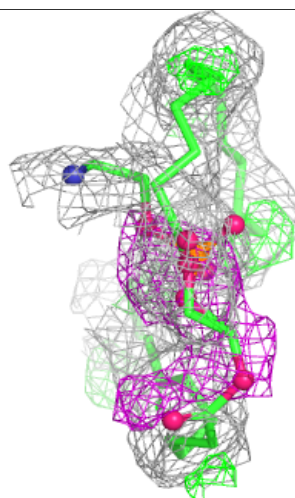
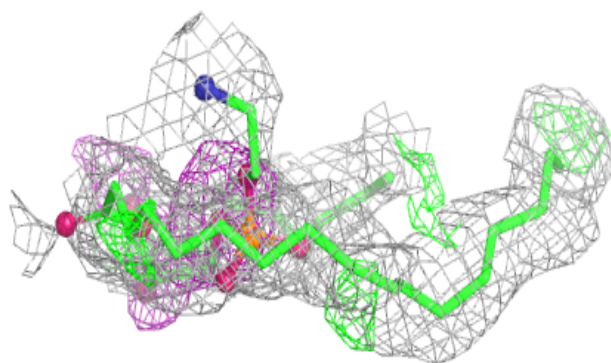
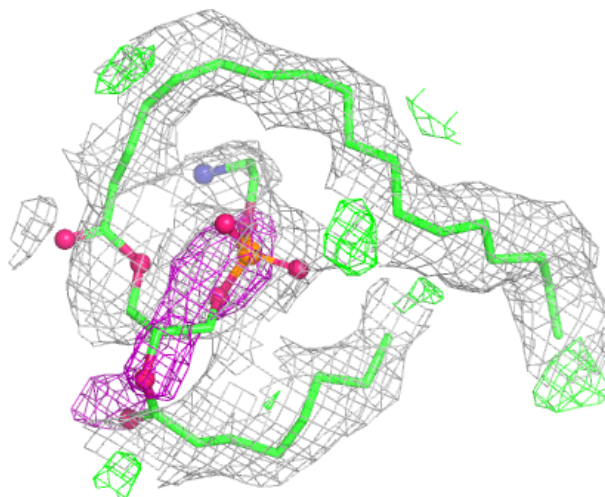
Electron density around PEE A 501:

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



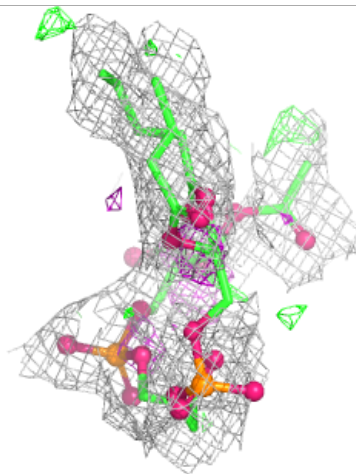
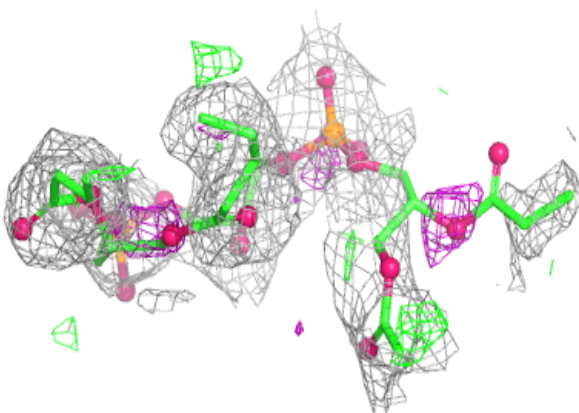
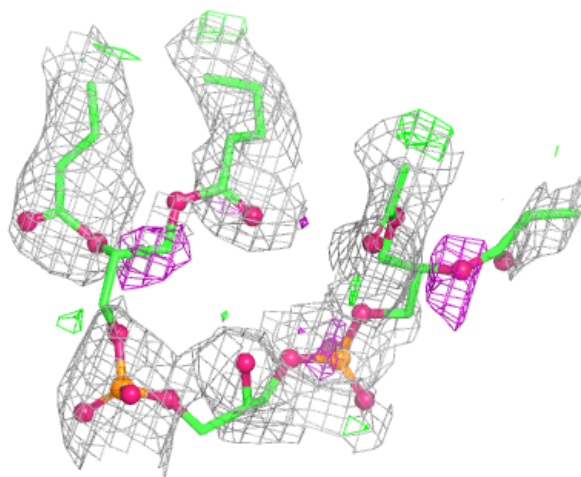
Electron density around PEE P 409:

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



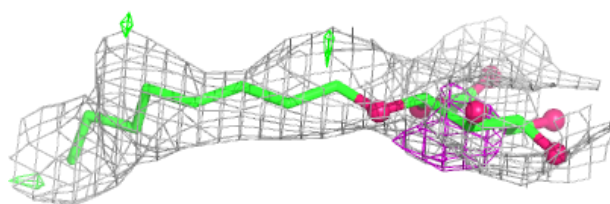
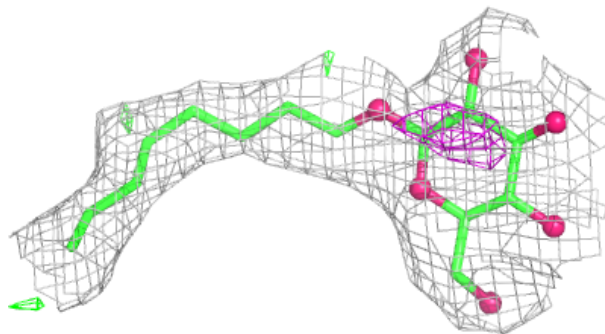
Electron density around CDL Q 502:

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



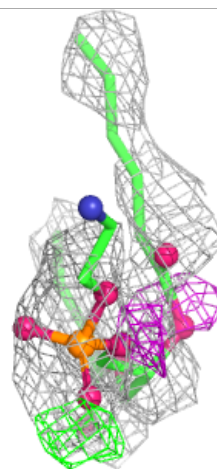
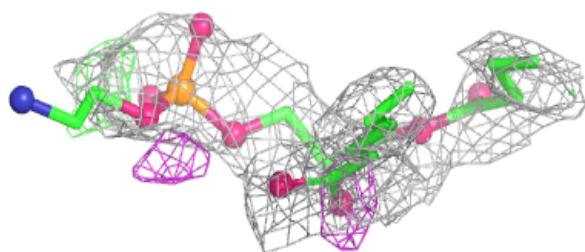
Electron density around BOG P 406:

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



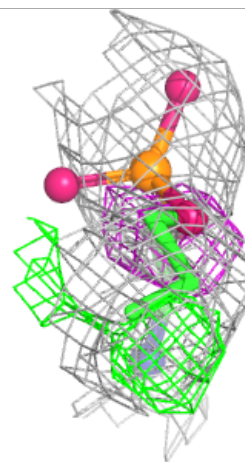
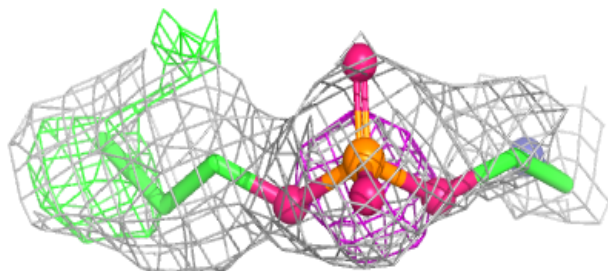
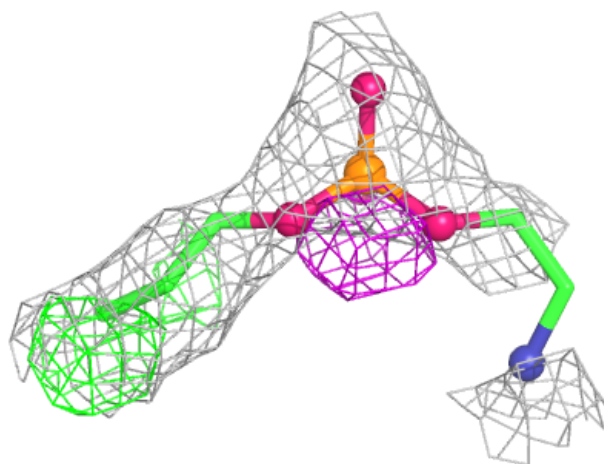
Electron density around PEE P 411:

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



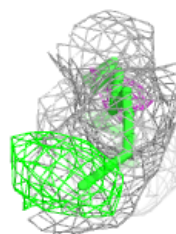
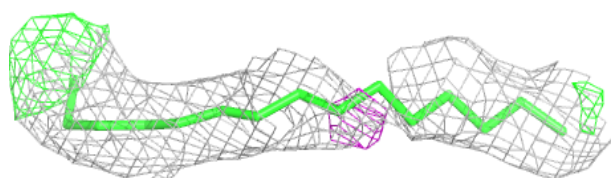
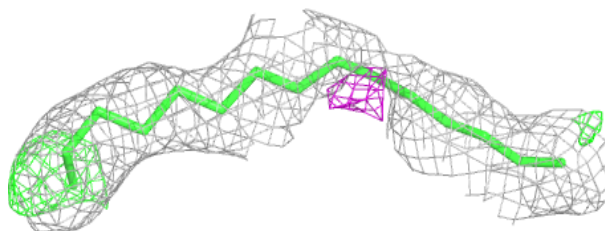
Electron density around PEE C 507:

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

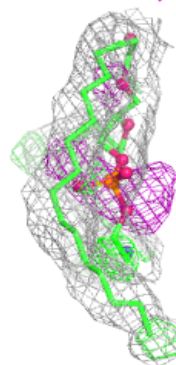
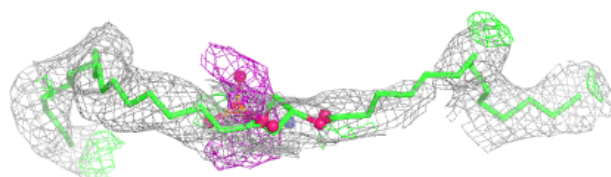
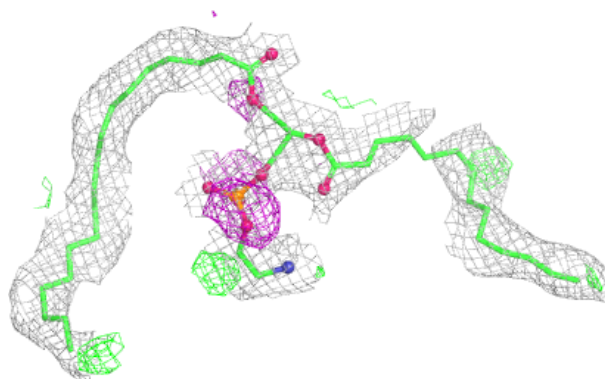


Electron density around PEE E 503:

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and green (positive)

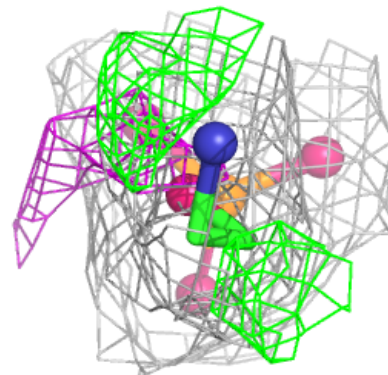
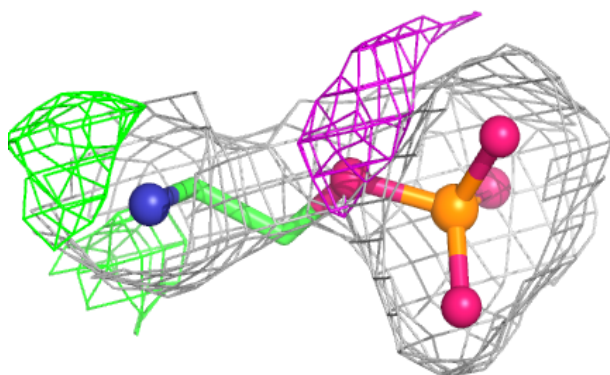
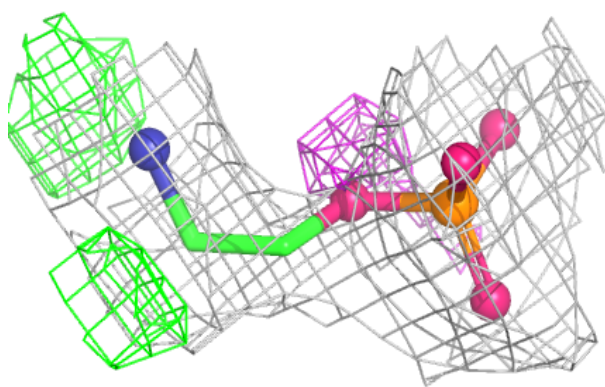
**Electron density around PEE C 509:**

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and green (positive)

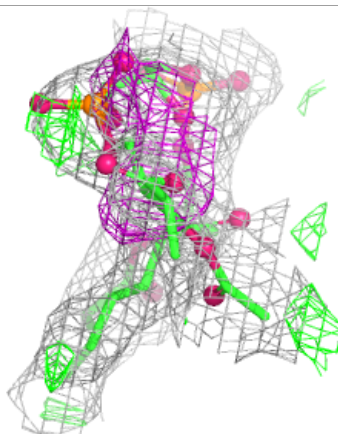
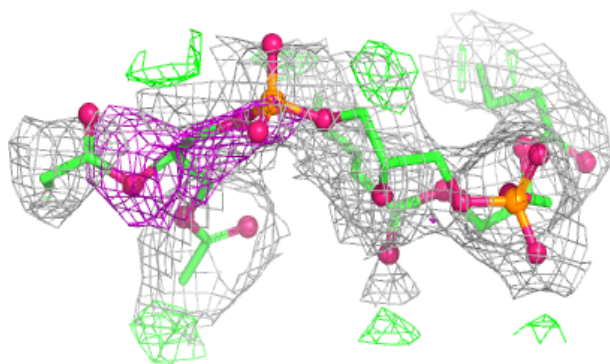
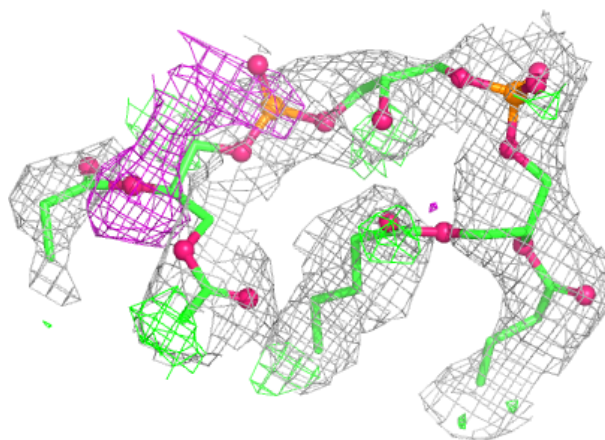


Electron density around PEE N 501:

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

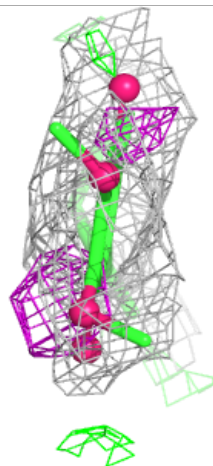
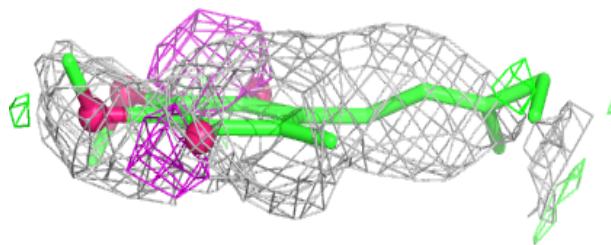
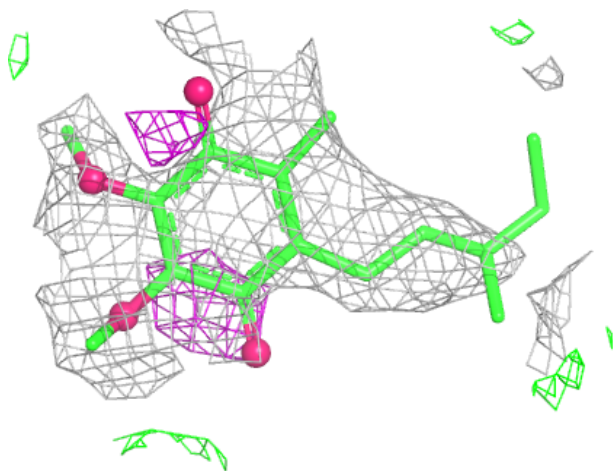
**Electron density around CDL D 502:**

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



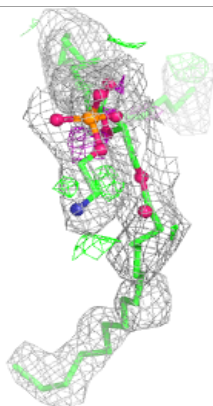
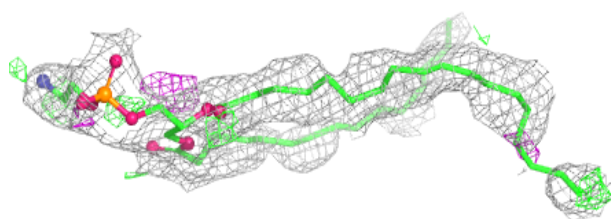
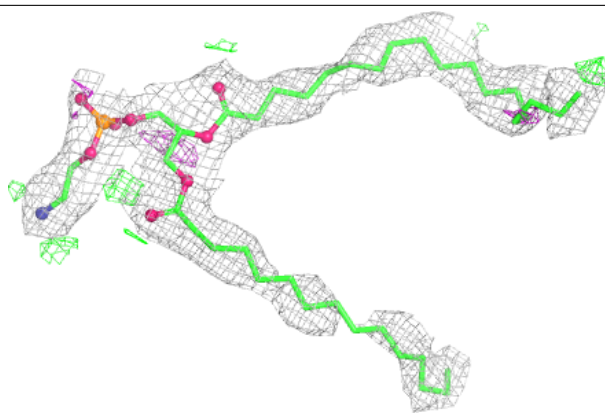
Electron density around U10 P 405:

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

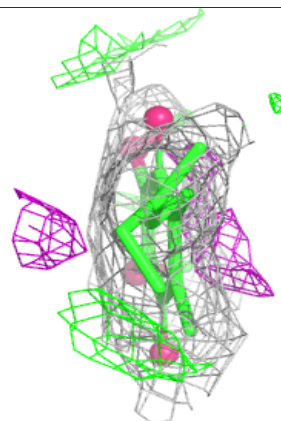
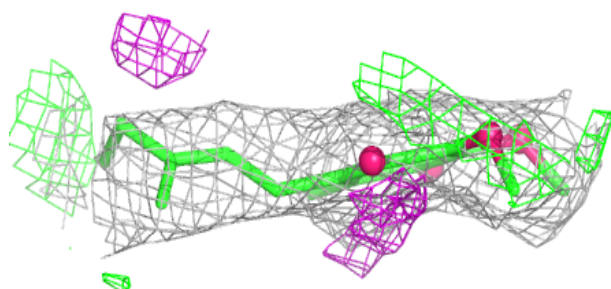
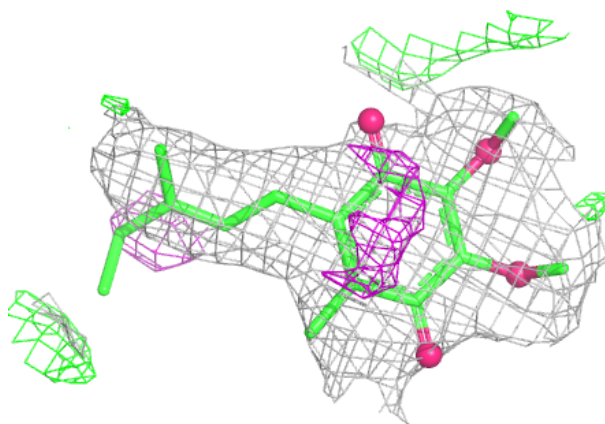


Electron density around PEE E 502:

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

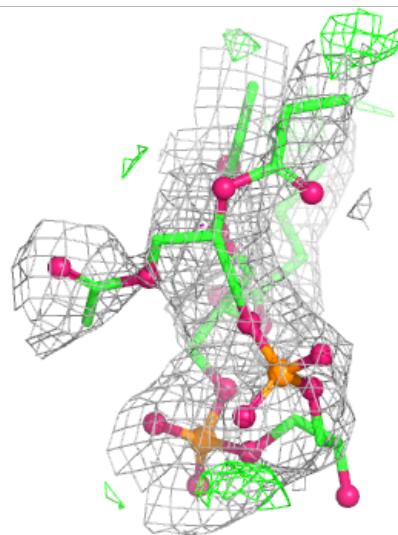
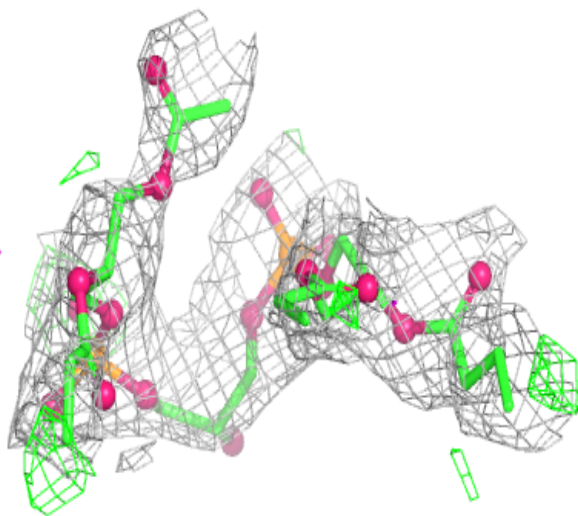
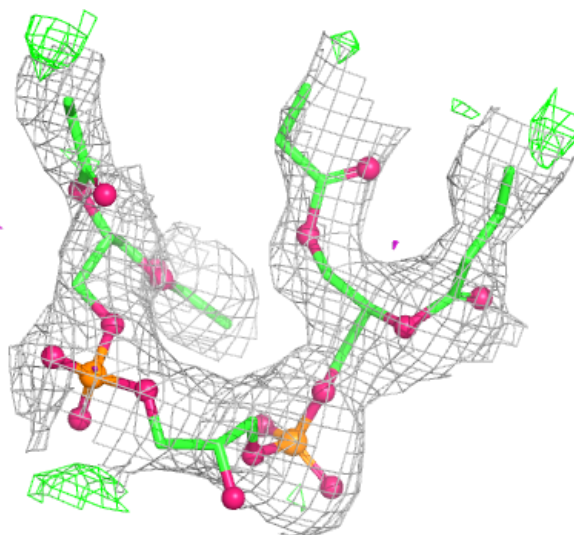
**Electron density around U10 C 504:**

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



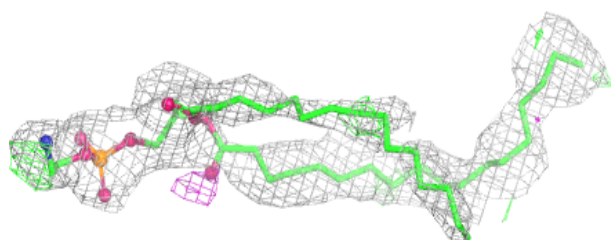
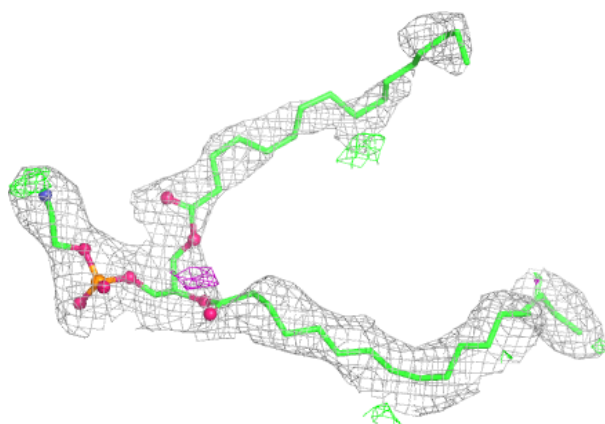
Electron density around CDL T 101:

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

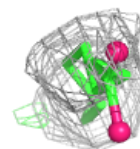
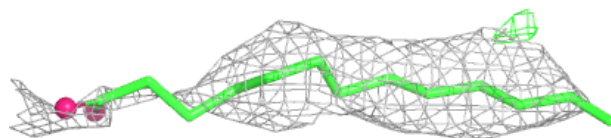
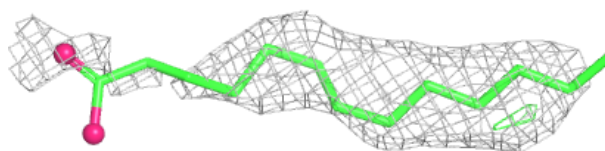


Electron density around PEE R 502:

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

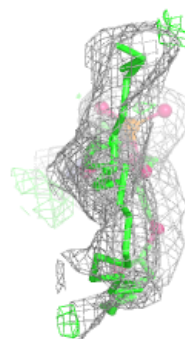
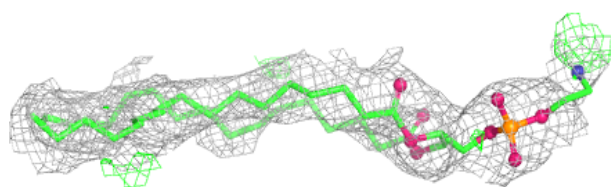
**Electron density around PEE P 401:**

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



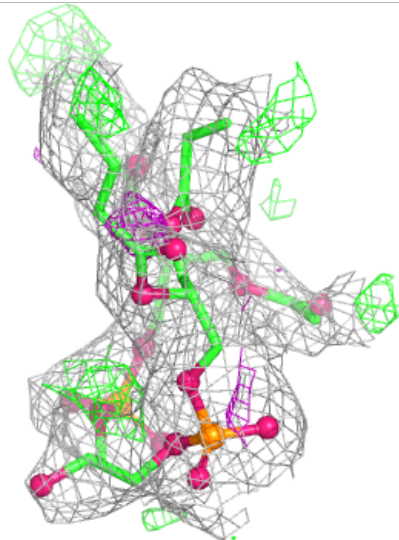
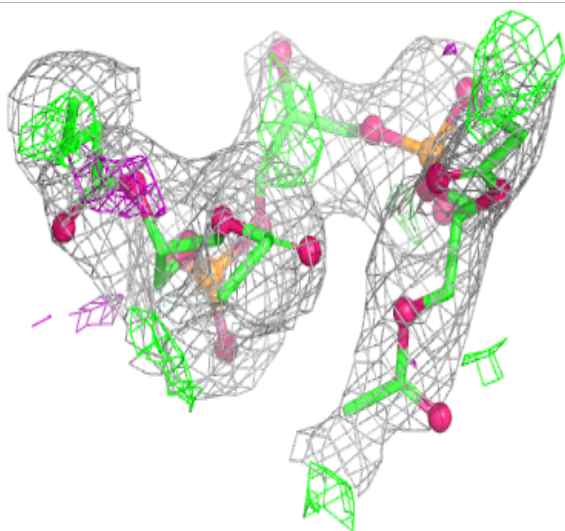
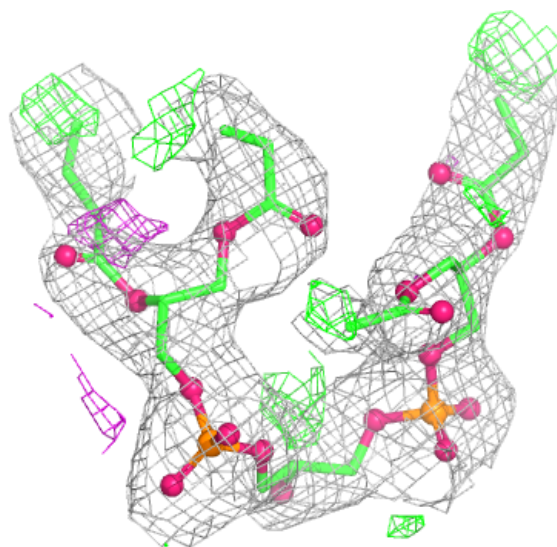
Electron density around PEE P 407:

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



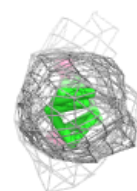
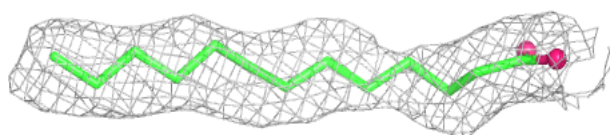
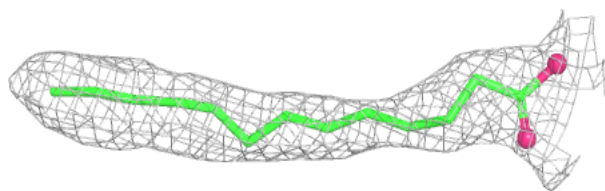
Electron density around CDL G 101:

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

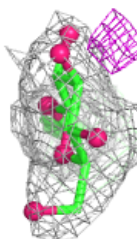
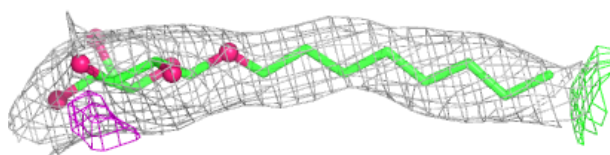
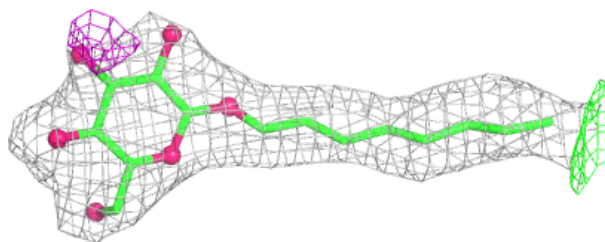


Electron density around PEE C 510:

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

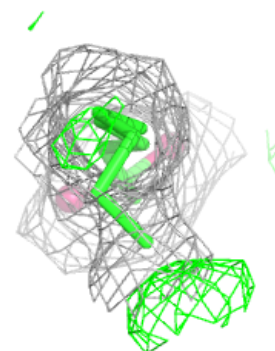
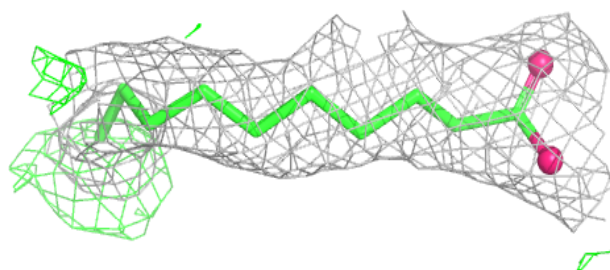
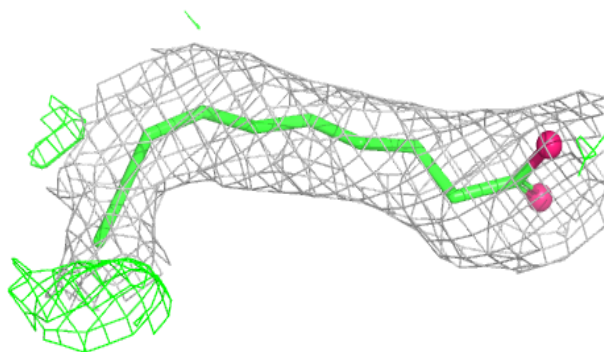
**Electron density around BOG D 503:**

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

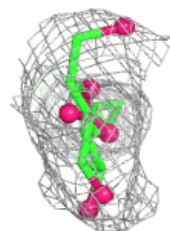
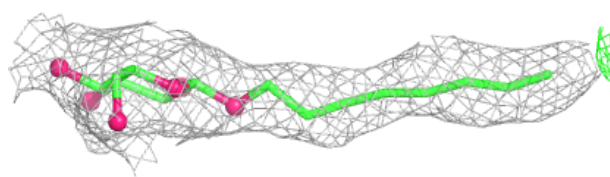
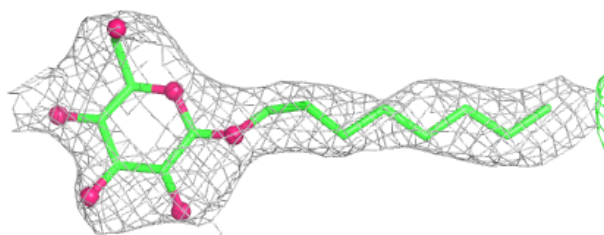


Electron density around PEE P 410:

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

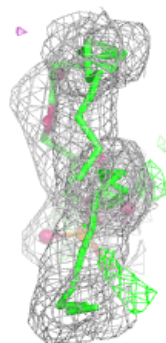
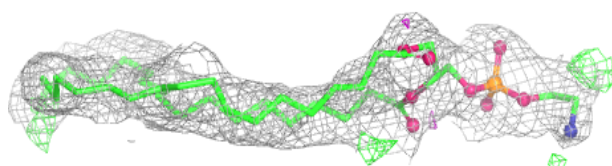
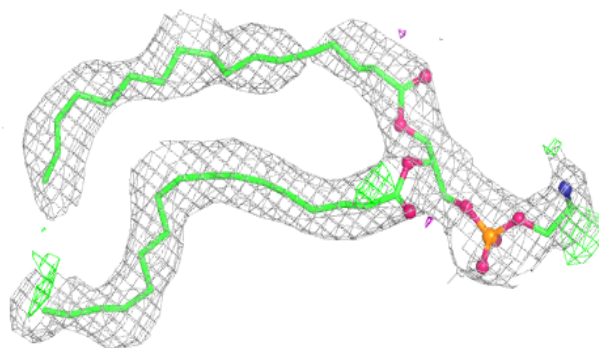
**Electron density around BOG Q 503:**

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

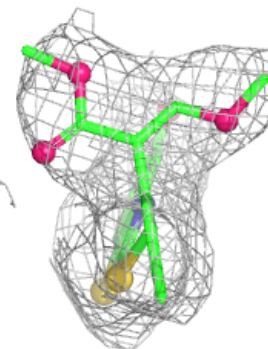
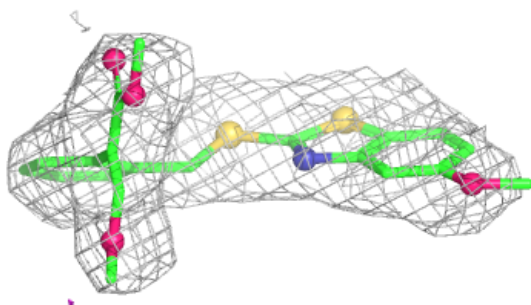
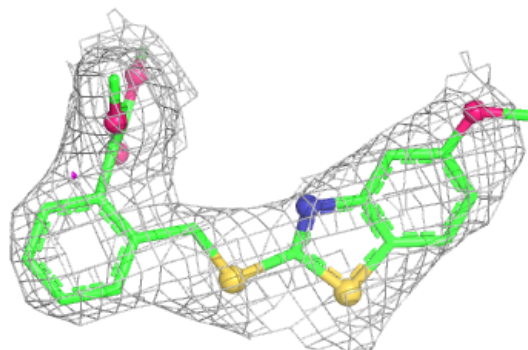


Electron density around PEE C 505:

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

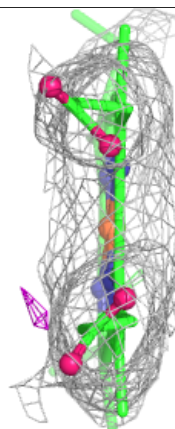
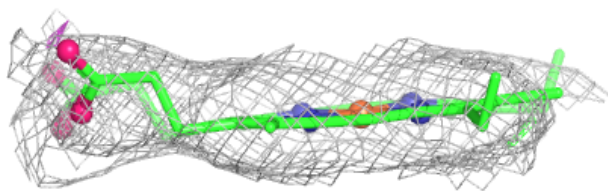
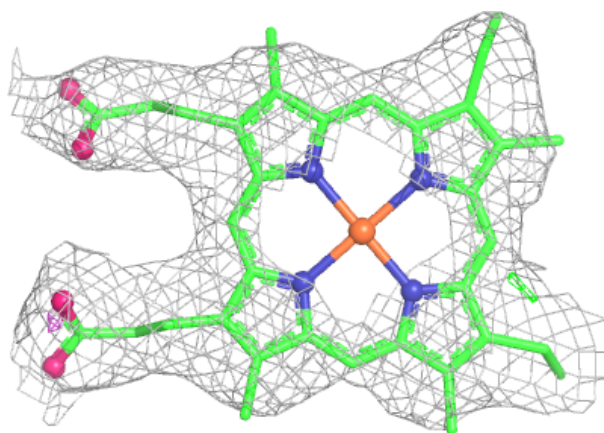
**Electron density around Y52 P 404:**

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

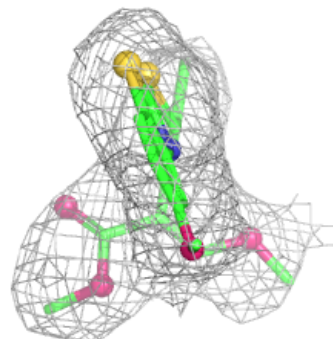
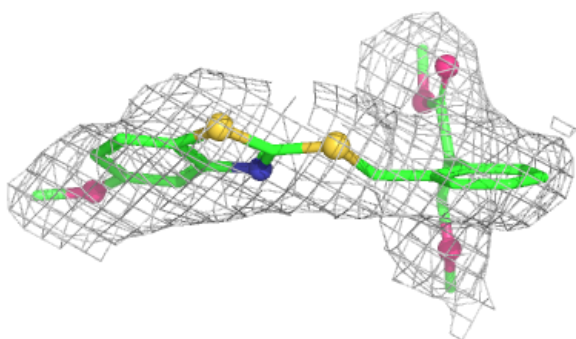
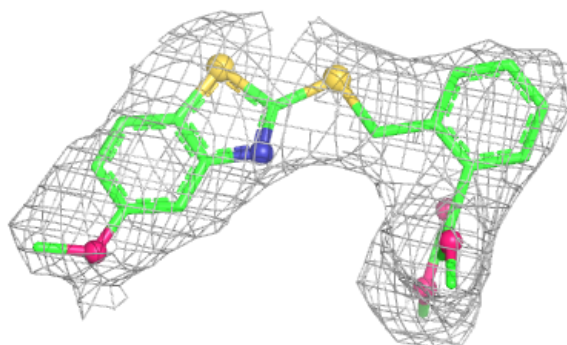


Electron density around HEC Q 501:

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

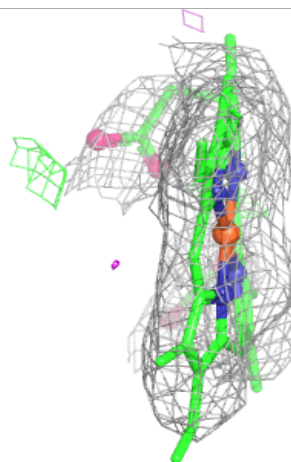
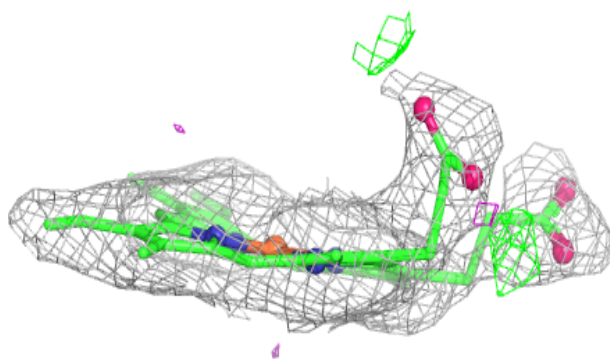
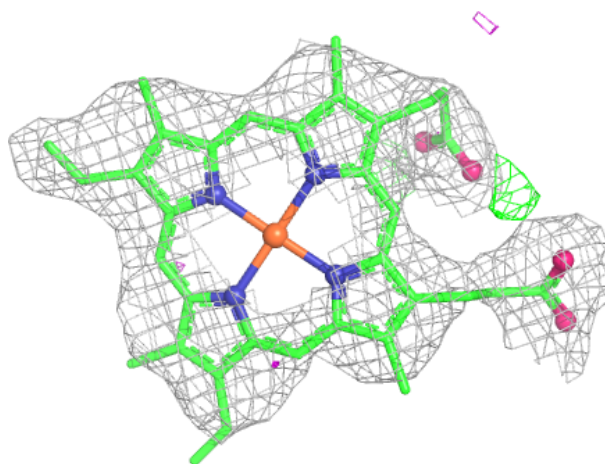
**Electron density around Y52 C 503:**

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



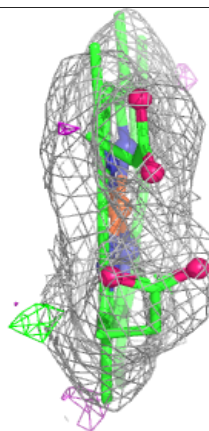
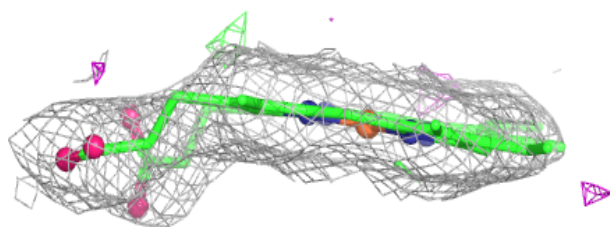
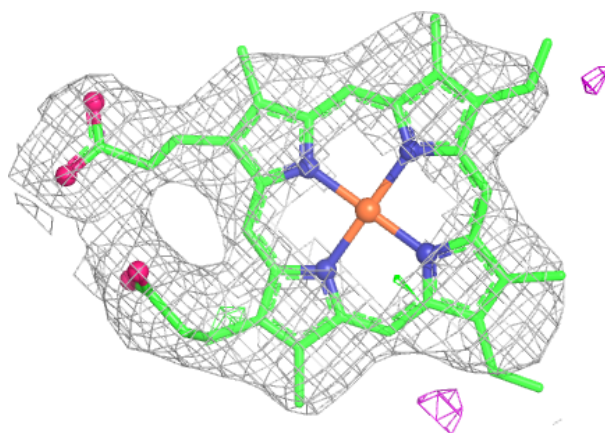
Electron density around HEM P 403:

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



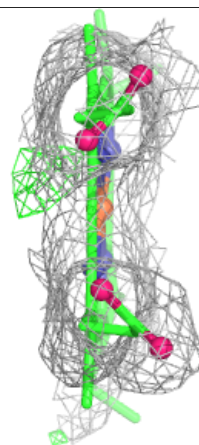
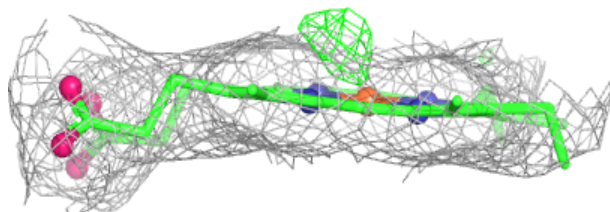
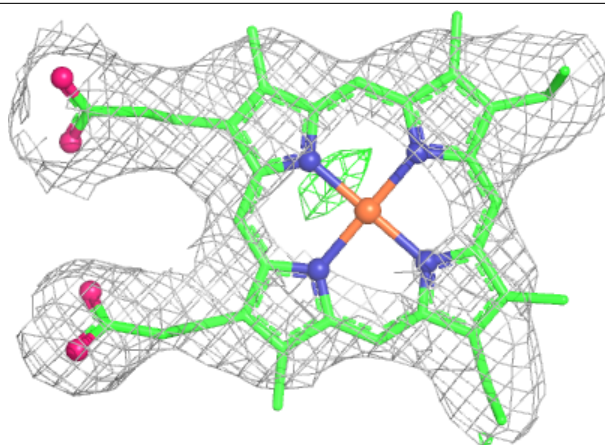
Electron density around HEM C 501:

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



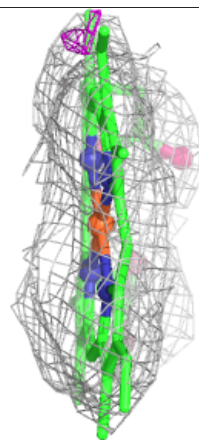
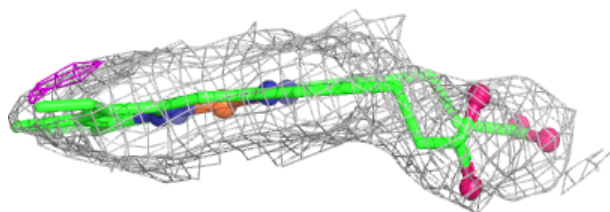
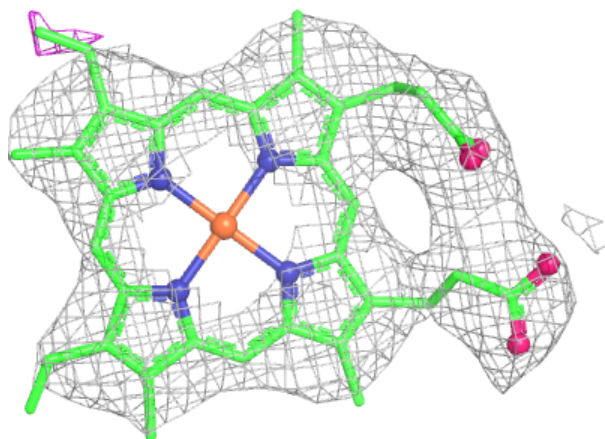
Electron density around HEC D 501:

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



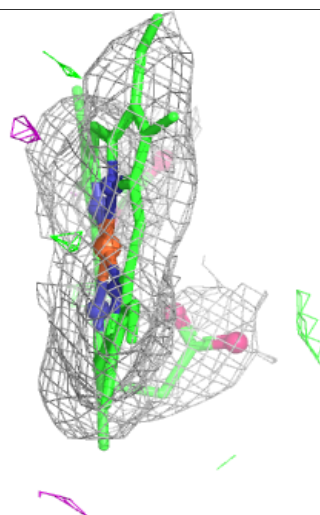
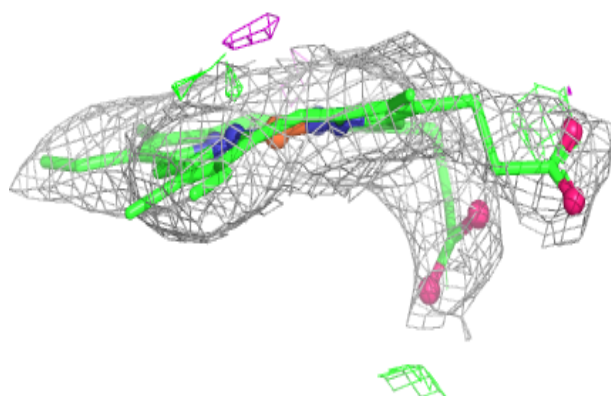
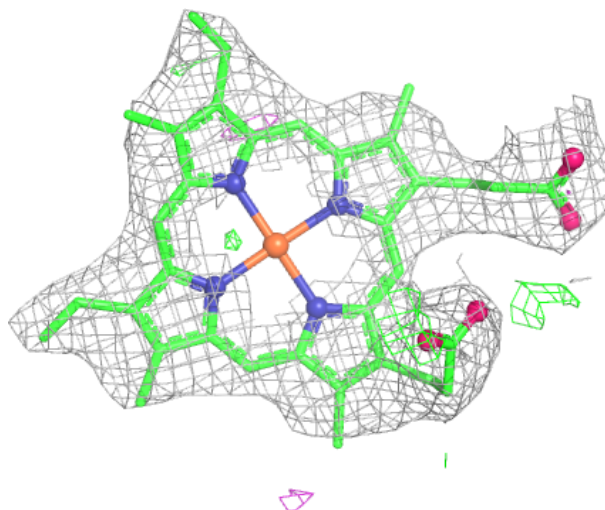
Electron density around HEM P 402:

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



Electron density around HEM C 502:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.