



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2026 – 08:32 am BST

PDB ID : 6HAW / pdb_00006haw
Title : Crystal structure of bovine cytochrome bc1 in complex with 2-pyrazolyl quinolone inhibitor WDH2G7
Authors : Amporndanai, K.; Hong, W.D.; O'Neill, P.M.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on : 2018-08-08
Resolution : 3.45 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	:	1.8.4, CSD as541be (2020)
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

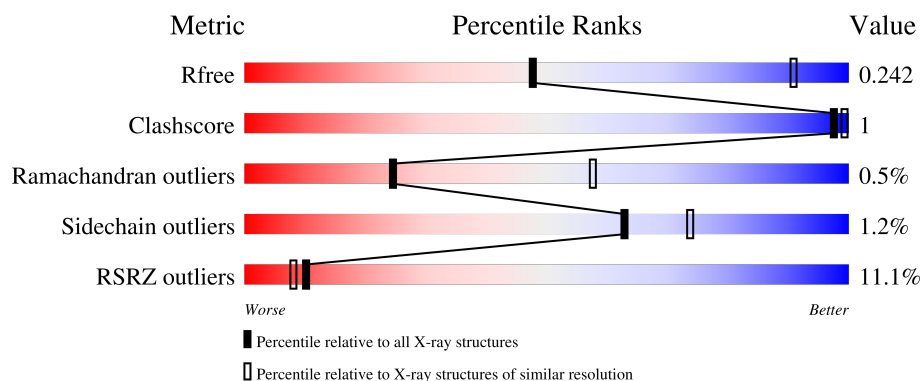
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	438	9% 96% .
2	B	413	8% 98% .
3	C	378	8% 95% 5%
4	D	239	8% 96% .
5	E	196	24% 98% .

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Mol	Chain	Length	Quality of chain
6	F	99	
7	G	74	
8	H	64	
9	I	46	
10	J	59	

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
19	PEE	C	405	X	-	-	-
19	PEE	E	204	X	-	-	-
20	FX2	C	406	X	-	-	-
21	HEC	D	501	X	-	-	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 16062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3331	2081	590	640	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P31800
A	?	-	TYR	deletion	UNP P31800
A	?	-	ASP	deletion	UNP P31800
A	?	-	GLU	deletion	UNP P31800
A	?	-	ASP	deletion	UNP P31800
A	?	-	ALA	deletion	UNP P31800

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3073	1931	538	597	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P23004
B	?	-	LEU	deletion	UNP P23004
B	?	-	GLY	deletion	UNP P23004
B	?	-	LEU	deletion	UNP P23004
B	?	-	SER	deletion	UNP P23004

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			2996	2007	471	500	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1851	1181	322	333	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1450	907	254	282	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			853	542	153	156	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			612	400	113	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			490	297	84	104	5			

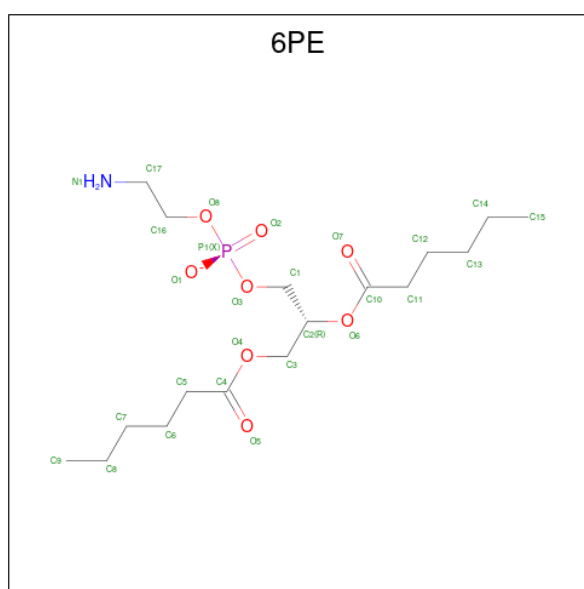
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			322	201	63	57	1			

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

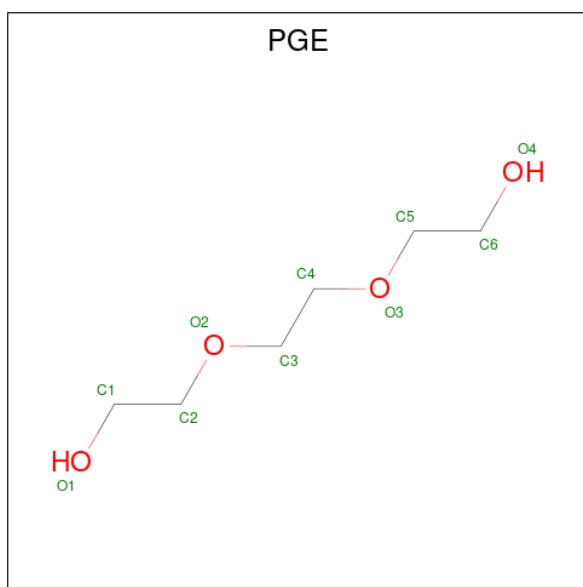
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O		0	0	0
			487	320	84	83				

- Molecule 11 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: 6PE) (formula: $C_{17}H_{33}NO_8P$).



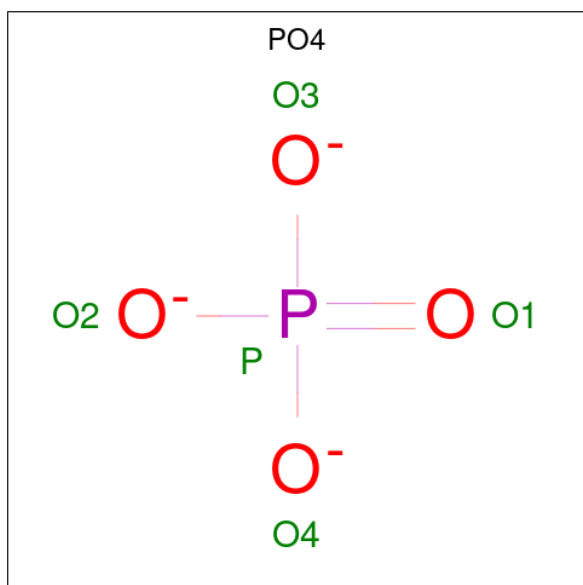
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



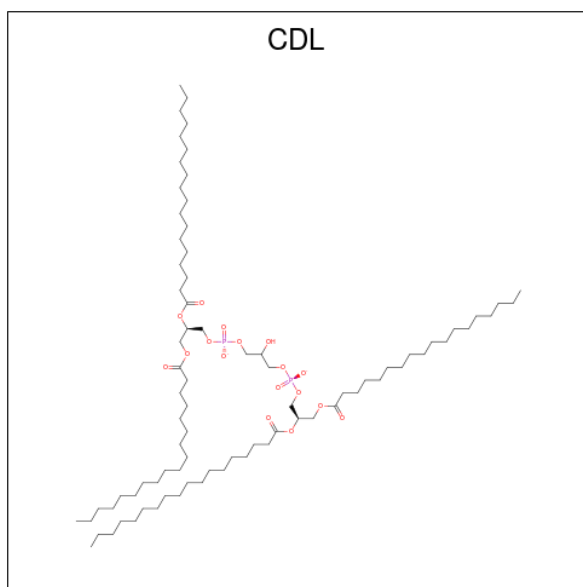
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total O P 5 4 1	0	0
13	A	1	Total O P 5 4 1	0	0
13	A	1	Total O P 5 4 1	0	0
13	B	1	Total O P 5 4 1	0	0
13	D	1	Total O P 5 4 1	0	0
13	E	1	Total O P 5 4 1	0	0
13	F	1	Total O P 5 4 1	0	0
13	F	1	Total O P 5 4 1	0	0
13	G	1	Total O P 5 4 1	0	0
13	G	1	Total O P 5 4 1	0	0
13	G	1	Total O P 5 4 1	0	0

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



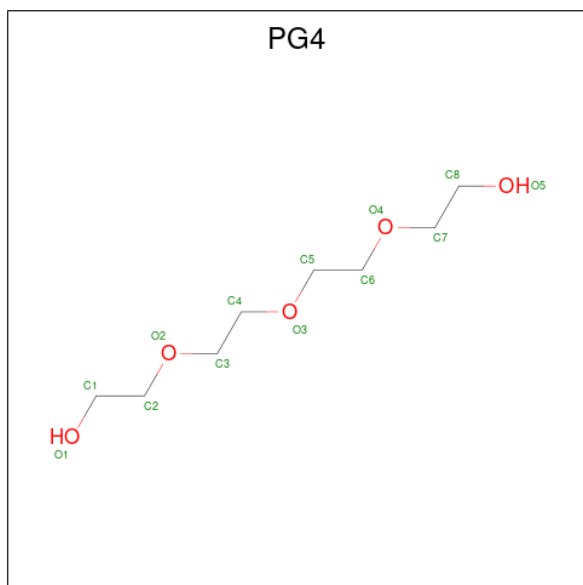
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C O P 34 17 15 2	0	0

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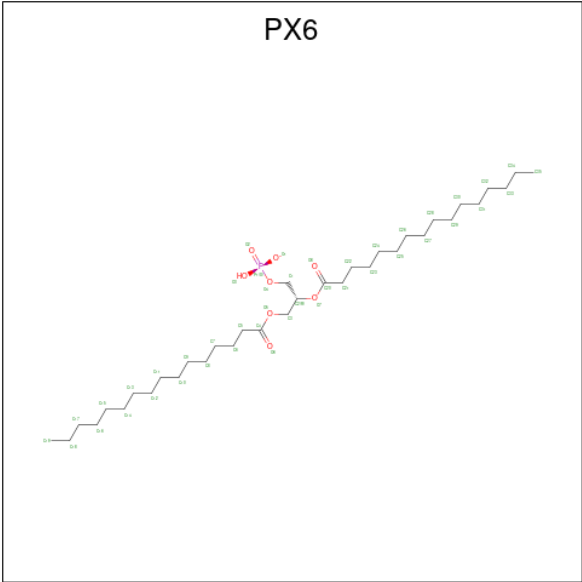
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			38	19	17	2		
14	D	1	Total	C	O	P	0	0
			27	12	13	2		
14	E	1	Total	C	O	P	0	0
			28	13	13	2		

- Molecule 15 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



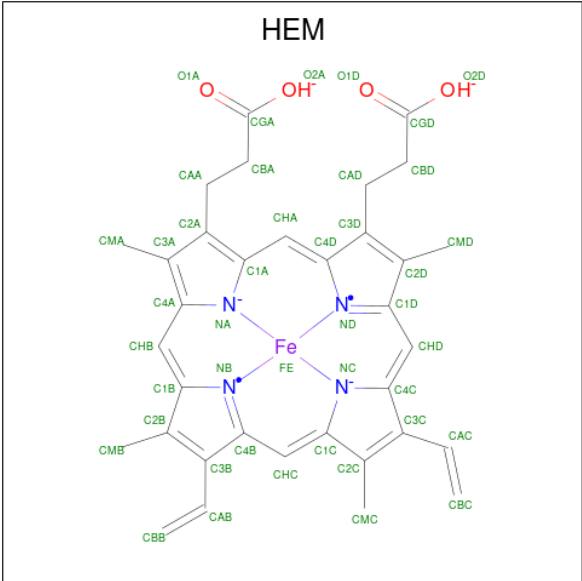
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 16 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX6) (formula: $C_{35}H_{68}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	O	P	0	0
			17	9	7	1		
16	C	1	Total	C	O	P	0	0
			14	6	7	1		

- Molecule 17 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



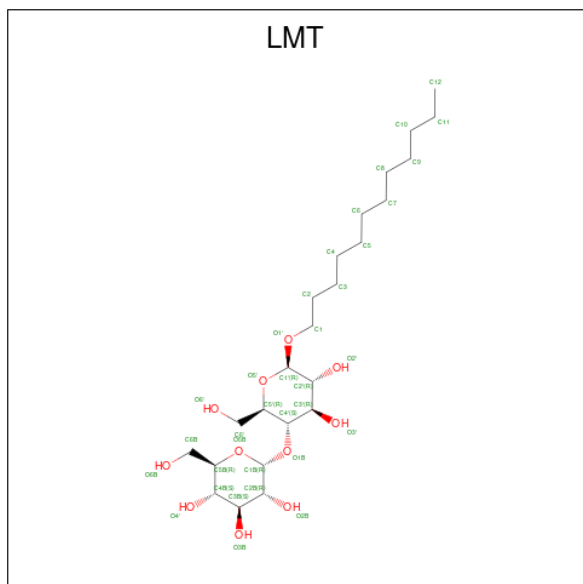
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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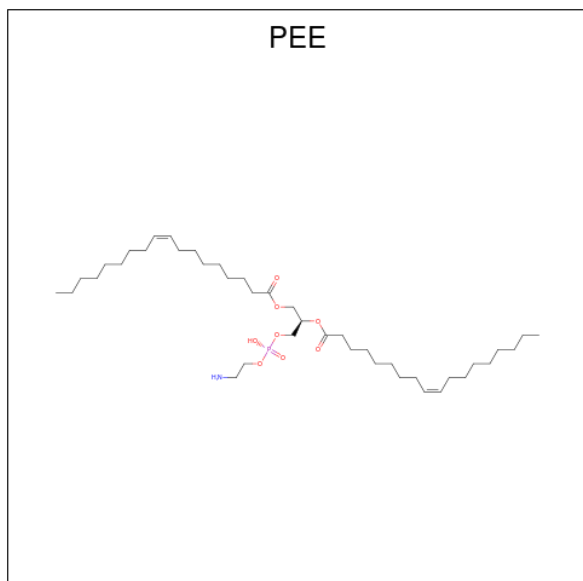
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 18 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



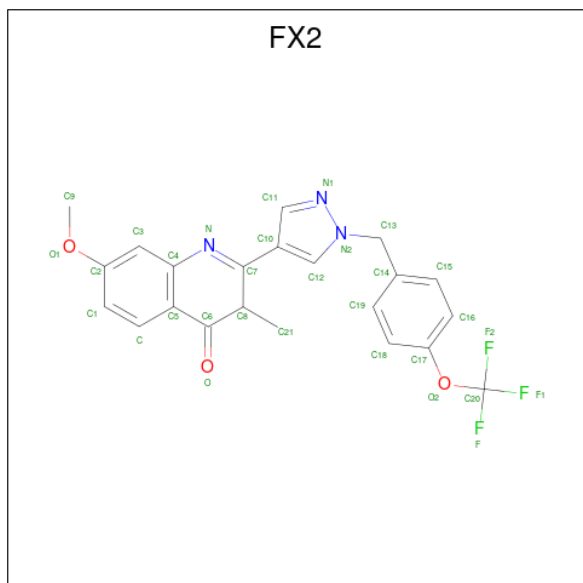
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	C O		
			35	24 11	0	0

- Molecule 19 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



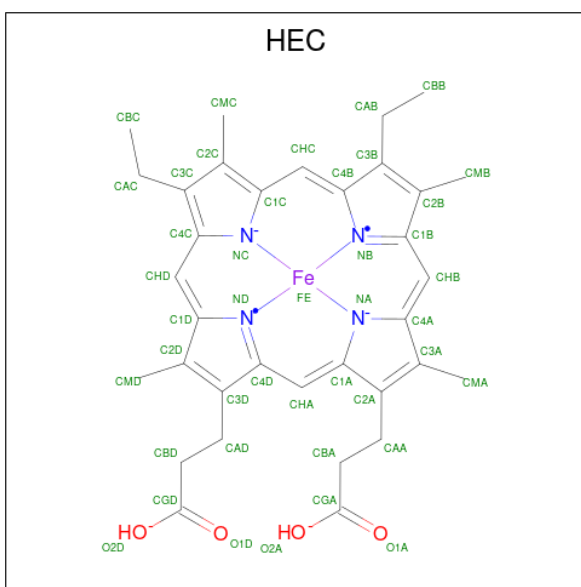
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
19	E	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 20 is 7-methoxy-3-methyl-2-[1-[[4-(trifluoromethoxy)phenyl]methyl]pyrazol-4-yl]-3 {H}-quinolin-4-one (CCD ID: FX2) (formula: C₂₂H₁₈F₃N₃O₃) (labeled as "Ligand of Interest" by depositor).



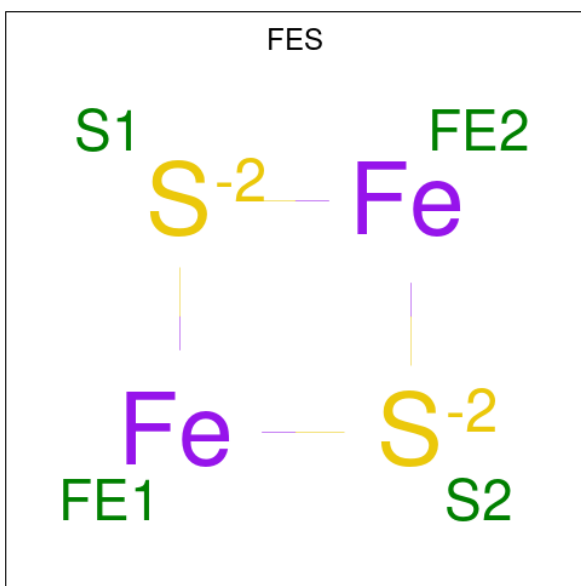
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total	C	F	N	O	0	0
			31	22	3	3	3		

- Molecule 21 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



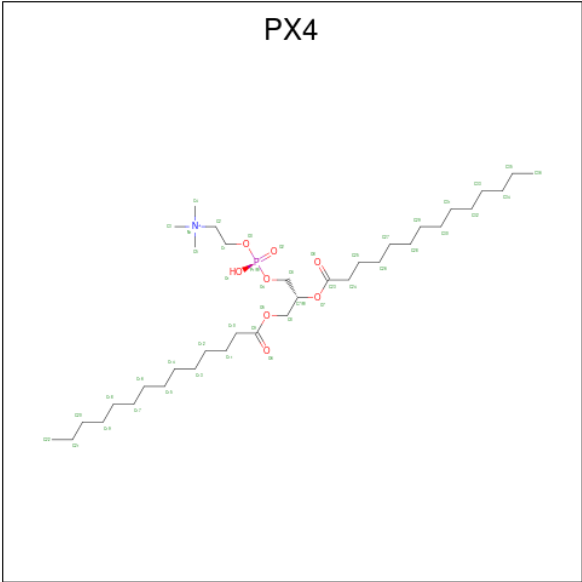
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 23 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: $\text{C}_{36}\text{H}_{73}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	E	1	Total	C	N	O	P	0	0
			28	18	1	8	1		

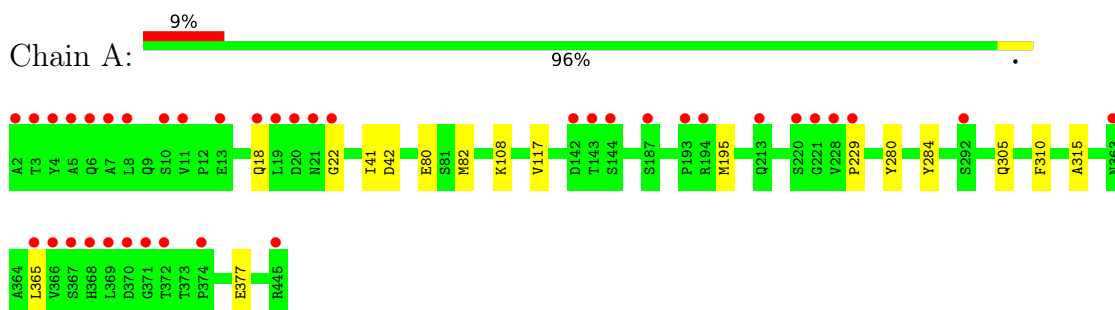
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	10	Total	O	0	0
			10	10		
24	B	4	Total	O	0	0
			4	4		
24	C	8	Total	O	0	0
			8	8		
24	D	4	Total	O	0	0
			4	4		
24	E	2	Total	O	0	0
			2	2		
24	H	1	Total	O	0	0
			1	1		
24	J	1	Total	O	0	0
			1	1		

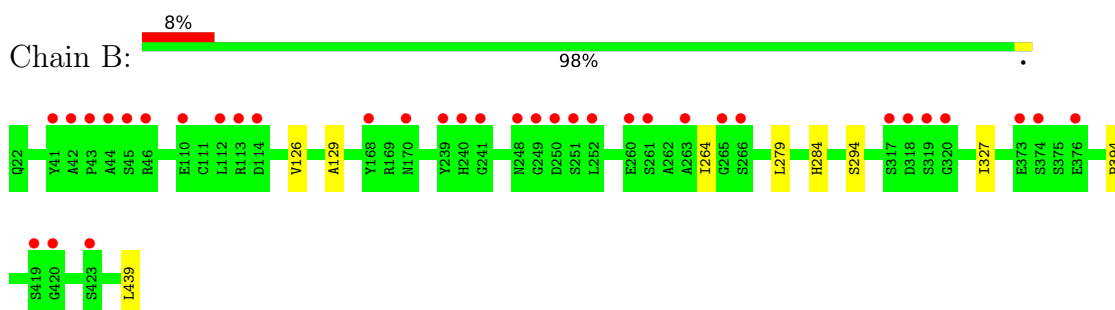
3 Residue-property plots [i](#)

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

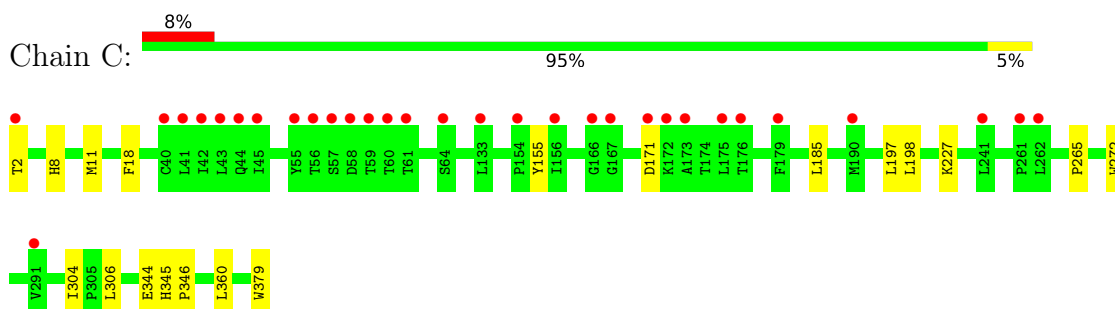
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



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

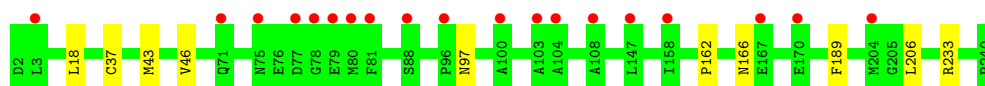


- Molecule 3: Cytochrome b

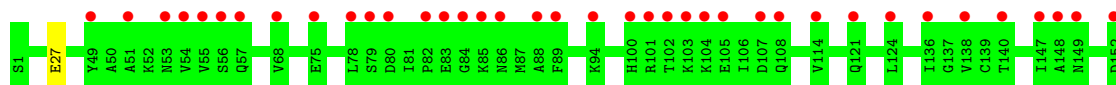


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

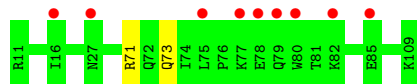




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



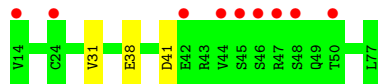
- Molecule 6: Cytochrome b-c1 complex subunit 7



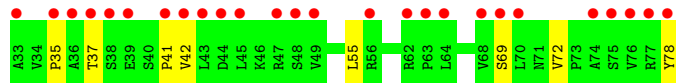
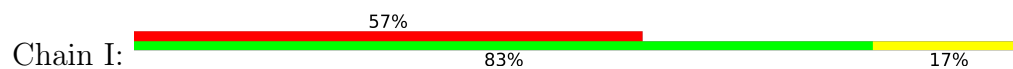
- Molecule 7: Cytochrome b-c1 complex subunit 8



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

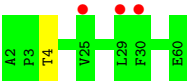


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 9





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	212.69Å 212.69Å 347.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.10 – 3.45 92.10 – 3.45	Depositor EDS
% Data completeness (in resolution range)	89.2 (92.10-3.45) 89.2 (92.10-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.210 , 0.242 0.209 , 0.242	Depositor DCC
R_{free} test set	2762 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16062	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: PG4, PX6, PEE, LMT, HEC, PX4, FES, FX2, PO4, HEM, PGE, CDL, 6PE

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	0.60	0/3400	1.01	1/4620 (0.0%)
2	B	0.61	1/3128 (0.0%)	1.00	1/4248 (0.0%)
3	C	0.62	1/3092 (0.0%)	1.05	2/4231 (0.0%)
4	D	0.62	0/1910	1.00	2/2601 (0.1%)
5	E	0.64	0/1482	0.99	0/2014
6	F	0.53	0/872	1.03	0/1174
7	G	0.66	0/633	1.07	2/859 (0.2%)
8	H	0.54	0/495	1.07	0/670
9	I	0.89	0/326	1.29	4/445 (0.9%)
10	J	0.59	0/500	1.04	0/675
All	All	0.62	2/15838 (0.0%)	1.03	12/21537 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	304	ILE	CA-CB	6.34	1.57	1.54
2	B	394	PRO	CA-C	5.25	1.54	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	35	PRO	CA-C-N	-6.45	112.49	122.87
9	I	35	PRO	C-N-CA	-6.45	112.49	122.87
7	G	50	PRO	N-CA-C	6.13	118.18	110.70
1	A	310	PHE	N-CA-C	6.08	123.74	110.80
4	D	233	ARG	N-CA-C	5.91	117.92	110.24
2	B	129	ALA	N-CA-C	5.88	118.05	109.30
9	I	72	VAL	N-CA-C	5.86	114.69	108.95
7	G	29	TYR	N-CA-C	5.75	117.22	111.07
9	I	69	SER	N-CA-C	5.71	115.81	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	97	ASN	N-CA-C	5.25	112.75	108.07
3	C	265	PRO	O-C-N	5.04	123.52	121.15
3	C	272	TRP	N-CA-C	5.04	117.43	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3331	0	3189	7	0
2	B	3073	0	3020	3	0
3	C	2996	0	3058	3	0
4	D	1851	0	1749	7	0
5	E	1450	0	1357	0	0
6	F	853	0	825	1	0
7	G	612	0	601	0	0
8	H	490	0	433	1	0
9	I	322	0	317	2	0
10	J	487	0	487	0	0
11	A	23	0	19	2	0
12	A	7	0	9	0	0
12	C	30	0	42	0	0
13	A	15	0	0	0	0
13	B	5	0	0	0	0
13	D	5	0	0	0	0
13	E	5	0	0	0	0
13	F	10	0	0	0	0
13	G	15	0	0	0	0
14	A	34	0	24	2	0
14	C	38	0	20	0	0
14	D	27	0	15	0	0
14	E	28	0	17	0	0
15	B	13	0	18	0	0
16	B	17	0	14	0	0
16	C	14	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	86	0	60	2	0
18	C	35	0	46	0	0
19	C	34	0	42	0	0
19	E	20	0	14	0	0
20	C	31	0	0	0	0
21	D	43	0	32	3	0
22	E	4	0	0	0	0
23	E	28	0	30	0	0
24	A	10	0	0	0	0
24	B	4	0	0	0	0
24	C	8	0	0	0	0
24	D	4	0	0	0	0
24	E	2	0	0	0	0
24	H	1	0	0	0	0
24	J	1	0	0	0	0
All	All	16062	0	15446	24	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 1.

All (24) 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)
4:D:37:CYS:SG	21:D:501:HEC:CAB	2.88	0.61
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.68	0.58
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.83	0.58
4:D:37:CYS:SG	21:D:501:HEC:HBB3	2.44	0.58
17:C:401:HEM:HMC1	17:C:401:HEM:HBC2	1.88	0.56
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.89	0.55
11:A:501:6PE:H28	14:A:506:CDL:HB31	1.94	0.49
3:C:8:HIS:HB3	3:C:11:MET:HB2	1.96	0.47
6:F:71:ARG:HB3	6:F:73:GLN:HG3	1.96	0.47
4:D:37:CYS:SG	21:D:501:HEC:CBB	3.04	0.45
1:A:82:MET:HE1	1:A:108:LYS:HB3	1.98	0.44
4:D:166:ASN:H	4:D:166:ASN:HD22	1.65	0.44
3:C:197:LEU:HD21	17:C:402:HEM:HMA3	2.00	0.44
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.54	0.43
11:A:501:6PE:H6	14:A:506:CDL:H712	2.00	0.43
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.53	0.43
3:C:345:HIS:HA	3:C:346:PRO:HA	1.75	0.42
1:A:80:GLU:HG2	2:B:284:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLN:NE2	9:I:42:VAL:HG12	2.34	0.42
2:B:279:LEU:HA	2:B:294:SER:HB3	2.01	0.42
2:B:327:ILE:HG21	9:I:55:LEU:HD11	2.00	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.02	0.41
4:D:18:LEU:HD22	4:D:206:LEU:HB2	2.04	0.40
8:H:38:GLU:HA	8:H:41:ASP:HB2	2.04	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	434/438 (99%)	420 (97%)	12 (3%)	2 (0%)	24	57
2	B	409/413 (99%)	396 (97%)	13 (3%)	0	100	100
3	C	376/378 (100%)	362 (96%)	13 (4%)	1 (0%)	36	67
4	D	237/239 (99%)	227 (96%)	9 (4%)	1 (0%)	30	62
5	E	194/196 (99%)	184 (95%)	7 (4%)	3 (2%)	8	37
6	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
7	G	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
8	H	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
9	I	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	17
10	J	57/59 (97%)	54 (95%)	2 (4%)	1 (2%)	6	34
All	All	1982/2006 (99%)	1905 (96%)	67 (3%)	10 (0%)	24	57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	37	THR

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Mol	Chain	Res	Type
9	I	41	PRO
1	A	315	ALA
3	C	155	TYR
5	E	177	PRO
4	D	162	PRO
1	A	229	PRO
5	E	155	GLY
5	E	162	GLY
10	J	4	THR

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	347/363 (96%)	344 (99%)	3 (1%)	70	76
2	B	318/324 (98%)	315 (99%)	3 (1%)	70	76
3	C	325/326 (100%)	315 (97%)	10 (3%)	35	61
4	D	190/204 (93%)	190 (100%)	0	100	100
5	E	149/168 (89%)	148 (99%)	1 (1%)	76	78
6	F	87/91 (96%)	87 (100%)	0	100	100
7	G	63/66 (96%)	63 (100%)	0	100	100
8	H	53/61 (87%)	52 (98%)	1 (2%)	50	68
9	I	30/38 (79%)	29 (97%)	1 (3%)	33	59
10	J	49/49 (100%)	49 (100%)	0	100	100
All	All	1611/1690 (95%)	1592 (99%)	19 (1%)	63	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	365	LEU
1	A	377	GLU
2	B	126	VAL

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Mol	Chain	Res	Type
2	B	264	ILE
2	B	439	LEU
3	C	2	THR
3	C	18	PHE
3	C	171	ASP
3	C	185	LEU
3	C	198	LEU
3	C	227	LYS
3	C	306	LEU
3	C	344	GLU
3	C	360	LEU
3	C	379	TRP
5	E	27	GLU
8	H	31	VAL
9	I	78	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	213	GLN
1	A	240	GLN
1	A	252	HIS
1	A	328	HIS
1	A	339	GLN
1	A	368	HIS
2	B	158	HIS
2	B	343	GLN
3	C	54	HIS
3	C	159	ASN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	6	HIS
4	D	71	GLN
4	D	105	ASN
4	D	121	HIS
4	D	166	ASN
4	D	225	HIS
5	E	57	GLN
5	E	100	HIS

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Mol	Chain	Res	Type
5	E	122	HIS
6	F	27	ASN
6	F	38	HIS
6	F	79	GLN
7	G	12	HIS
10	J	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	$\# Z > 2$
13	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.51	0
13	PO4	G	101	-	4,4,4	0.91	0	6,6,6	0.27	0
17	HEM	C	401	3	50,50,50	1.56	6 (12%)	66,82,82	1.37	12 (18%)
23	PX4	E	202	-	27,27,45	1.40	2 (7%)	33,35,53	1.31	4 (12%)
13	PO4	F	502	-	4,4,4	0.99	0	6,6,6	0.35	0
17	HEM	C	402	3	50,50,50	1.54	6 (12%)	66,82,82	1.31	8 (12%)
12	PGE	C	407	-	9,9,9	0.50	0	8,8,8	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CDL	C	404	-	37,37,99	1.65	4 (10%)	43,49,111	1.39	4 (9%)
18	LMT	C	403	-	36,36,36	0.66	1 (2%)	47,47,47	0.86	1 (2%)
21	HEC	D	501	4	50,50,50	2.96	28 (56%)	68,82,82	2.65	29 (42%)
20	FX2	C	406	-	32,34,34	1.73	7 (21%)	43,50,50	1.75	9 (20%)
14	CDL	E	205	-	27,27,99	1.20	2 (7%)	32,36,111	1.44	6 (18%)
12	PGE	C	408	-	9,9,9	0.44	0	8,8,8	0.29	0
16	PX6	B	503	-	16,16,43	1.25	1 (6%)	19,20,48	1.43	2 (10%)
16	PX6	C	410	-	13,13,43	1.27	1 (7%)	16,17,48	1.26	2 (12%)
13	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.39	0
19	PEE	C	405	-	33,33,50	1.38	3 (9%)	36,38,55	1.17	2 (5%)
13	PO4	E	203	-	4,4,4	0.97	0	6,6,6	0.57	0
13	PO4	A	504	-	4,4,4	0.97	0	6,6,6	0.42	0
12	PGE	C	409	-	9,9,9	0.47	0	8,8,8	0.23	0
13	PO4	D	502	-	4,4,4	0.92	0	6,6,6	0.34	0
12	PGE	A	502	-	6,6,9	0.55	0	5,5,8	0.31	0
13	PO4	G	102	-	4,4,4	0.89	0	6,6,6	0.46	0
14	CDL	A	506	-	33,33,99	1.23	2 (6%)	37,43,111	1.20	3 (8%)
13	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.46	0
13	PO4	A	505	-	4,4,4	0.98	0	6,6,6	0.43	0
14	CDL	D	503	-	26,26,99	1.45	2 (7%)	31,35,111	1.31	4 (12%)
11	6PE	A	501	-	22,22,26	1.54	2 (9%)	25,27,31	1.35	3 (12%)
13	PO4	B	501	-	4,4,4	0.90	0	6,6,6	0.50	0
15	PG4	B	502	-	12,12,12	0.50	0	11,11,11	0.18	0
22	FES	E	201	-	0,4,4	-	-	-	-	-
19	PEE	E	204	-	19,19,50	1.42	2 (10%)	22,24,55	1.36	2 (9%)

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
17	HEM	C	401	3	-	5/14/54/54	-
23	PX4	E	202	-	-	17/31/31/49	-
17	HEM	C	402	3	-	2/14/54/54	-
12	PGE	C	407	-	-	5/7/7/7	-
14	CDL	C	404	-	-	19/46/46/110	-
18	LMT	C	403	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	HEC	D	501	4	1/1/3/7	6/14/54/54	-
20	FX2	C	406	-	1/1/4/4	1/11/31/31	0/3/4/4
14	CDL	E	205	-	-	19/31/31/110	-
12	PGE	C	408	-	-	3/7/7/7	-
16	PX6	B	503	-	-	7/17/17/45	-
16	PX6	C	410	-	-	9/13/13/45	-
19	PEE	C	405	-	1/1/4/8	14/37/37/54	-
12	PGE	C	409	-	-	4/7/7/7	-
12	PGE	A	502	-	-	3/4/4/7	-
14	CDL	A	506	-	-	15/41/41/110	-
14	CDL	D	503	-	-	18/31/31/110	-
11	6PE	A	501	-	-	11/26/26/30	-
15	PG4	B	502	-	-	7/10/10/10	-
22	FES	E	201	-	-	-	0/1/1/1
19	PEE	E	204	-	1/1/4/8	13/22/22/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	406	FX2	C5-C4	6.99	1.49	1.40
21	D	501	HEC	FE-ND	5.57	2.12	1.94
21	D	501	HEC	C2A-C3A	5.36	1.48	1.36
14	C	404	CDL	OA6-CA5	5.32	1.47	1.35
17	C	402	HEM	FE-NB	5.28	2.11	1.94
17	C	401	HEM	FE-NB	5.27	2.11	1.94
21	D	501	HEC	C3D-C2D	5.17	1.47	1.36
14	C	404	CDL	OB6-CB5	5.10	1.48	1.34
21	D	501	HEC	C3B-C2B	5.07	1.47	1.36
21	D	501	HEC	FE-NB	5.06	2.10	1.94
14	C	404	CDL	OB8-CB7	5.03	1.48	1.33
19	E	204	PEE	O2-C10	4.94	1.48	1.34
21	D	501	HEC	CHA-C1A	4.91	1.47	1.38
21	D	501	HEC	CHB-C4A	4.91	1.47	1.38
11	A	501	6PE	O6-C10	4.83	1.47	1.34
19	C	405	PEE	O3-C30	4.78	1.47	1.33
21	D	501	HEC	FE-NC	4.69	2.11	1.95
11	A	501	6PE	O4-C4	4.68	1.47	1.33
21	D	501	HEC	CHC-C4B	4.67	1.48	1.38
14	D	503	CDL	OA8-CA7	4.66	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	503	CDL	OA6-CA5	4.64	1.47	1.34
14	A	506	CDL	OB8-CB7	4.57	1.46	1.33
23	E	202	PX4	O7-C23	4.51	1.47	1.34
21	D	501	HEC	FE-NA	4.49	2.10	1.95
16	B	503	PX6	O7-C20	4.46	1.46	1.34
14	E	205	CDL	OB6-CB5	4.45	1.46	1.34
23	E	202	PX4	O5-C9	4.43	1.46	1.33
14	A	506	CDL	OB6-CB5	4.39	1.46	1.34
21	D	501	HEC	CHD-C1D	4.37	1.47	1.38
16	C	410	PX6	O5-C4	4.19	1.45	1.33
17	C	401	HEM	FE-NC	4.18	2.09	1.95
19	C	405	PEE	O2-C10	4.17	1.46	1.34
21	D	501	HEC	CHC-C1C	4.08	1.48	1.39
17	C	402	HEM	FE-NC	4.07	2.08	1.95
19	C	405	PEE	C18-C19	3.75	1.53	1.31
21	D	501	HEC	CHA-C4D	3.73	1.47	1.39
21	D	501	HEC	CHD-C4C	3.68	1.47	1.39
21	D	501	HEC	C3C-C2C	3.67	1.48	1.38
21	D	501	HEC	CHB-C1B	3.58	1.47	1.39
17	C	401	HEM	C1B-NB	-3.37	1.34	1.40
17	C	402	HEM	C1B-NB	-3.35	1.34	1.40
21	D	501	HEC	C4B-NB	-3.10	1.35	1.40
21	D	501	HEC	C1C-C2C	3.02	1.50	1.43
17	C	401	HEM	C4D-ND	-2.92	1.35	1.40
21	D	501	HEC	C4D-C3D	2.77	1.49	1.45
14	C	404	CDL	OA8-CA7	2.71	1.46	1.33
14	E	205	CDL	OB8-CB7	2.68	1.46	1.33
17	C	402	HEM	C4D-ND	-2.66	1.35	1.40
21	D	501	HEC	C1D-ND	-2.63	1.35	1.40
20	C	406	FX2	C4-N	-2.58	1.34	1.39
19	E	204	PEE	O3-C30	2.55	1.46	1.33
21	D	501	HEC	C1B-C2B	2.51	1.49	1.44
20	C	406	FX2	O-C6	2.50	1.25	1.22
20	C	406	FX2	C10-C7	2.48	1.50	1.46
17	C	401	HEM	C3B-C4B	2.48	1.49	1.44
21	D	501	HEC	C1A-C2A	2.43	1.49	1.45
21	D	501	HEC	C4A-NA	-2.40	1.35	1.39
21	D	501	HEC	C1D-C2D	2.37	1.49	1.44
21	D	501	HEC	C4B-C3B	2.35	1.49	1.45
17	C	402	HEM	C4B-NB	-2.31	1.34	1.38
20	C	406	FX2	C7-N	2.28	1.35	1.30
21	D	501	HEC	C4A-C3A	2.25	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	403	LMT	O1'-C1'	2.23	1.44	1.40
20	C	406	FX2	N2-N1	2.22	1.40	1.36
17	C	401	HEM	C4D-C3D	2.15	1.48	1.45
20	C	406	FX2	O2-C20	2.14	1.43	1.31
21	D	501	HEC	C1A-NA	-2.08	1.35	1.39
21	D	501	HEC	C4C-NC	-2.06	1.35	1.39
17	C	402	HEM	C3B-C4B	2.03	1.48	1.44

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	406	FX2	C4-N-C7	6.15	124.89	117.77
21	D	501	HEC	C1B-C2B-C3B	-5.94	100.71	106.96
21	D	501	HEC	C3D-C4D-ND	5.76	115.94	110.36
21	D	501	HEC	C2B-C1B-NB	5.63	116.63	109.88
21	D	501	HEC	C2A-C1A-NA	5.42	115.60	110.32
21	D	501	HEC	C2D-C1D-ND	5.34	116.16	109.84
23	E	202	PX4	O7-C23-C24	5.06	122.40	111.50
21	D	501	HEC	CBC-CAC-C3C	5.02	126.26	112.43
21	D	501	HEC	C1C-C2C-C3C	-4.88	101.13	106.83
21	D	501	HEC	CBB-CAB-C3B	4.84	125.78	112.43
14	C	404	CDL	OA6-CA5-C11	4.71	119.76	111.09
14	A	506	CDL	OB6-CB5-C51	4.57	121.35	111.50
11	A	501	6PE	O6-C10-C11	4.37	120.92	111.50
16	B	503	PX6	O7-C20-C21	4.24	120.64	111.50
19	C	405	PEE	O3-C30-C31	4.17	122.32	111.38
19	E	204	PEE	O2-C10-C11	4.13	122.31	110.80
21	D	501	HEC	C1D-C2D-C3D	-4.10	102.64	106.96
21	D	501	HEC	C3C-C4C-NC	4.10	114.73	110.15
20	C	406	FX2	C10-C11-N1	-4.09	108.95	112.14
20	C	406	FX2	C12-C10-C11	4.07	107.72	104.05
17	C	402	HEM	CHC-C4B-NB	3.93	128.69	124.42
21	D	501	HEC	C2C-C1C-NC	3.78	115.84	110.08
17	C	401	HEM	CHC-C4B-NB	3.78	128.53	124.42
14	E	205	CDL	OB6-CB5-C51	3.74	119.56	111.50
14	E	205	CDL	CB6-OB8-CB7	3.71	126.42	117.10
21	D	501	HEC	C1A-C2A-C3A	-3.67	102.34	107.13
21	D	501	HEC	C3B-C4B-NB	3.65	114.23	110.17
14	D	503	CDL	OA6-CA5-C11	3.53	120.65	110.80
14	A	506	CDL	OB8-CB7-C71	3.53	120.63	111.38
14	D	503	CDL	OA8-CA7-C31	3.50	120.56	111.38
14	C	404	CDL	OB8-CB7-C71	3.41	120.32	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	501	HEC	CAC-C3C-C2C	3.33	132.20	126.86
16	C	410	PX6	O5-C4-C5	3.32	120.10	111.38
14	C	404	CDL	OB6-CB5-C51	3.28	119.95	110.80
21	D	501	HEC	C4D-C3D-C2D	-3.11	102.36	106.90
21	D	501	HEC	C3A-C4A-NA	3.08	115.38	109.69
20	C	406	FX2	C9-O1-C2	3.06	124.15	117.51
17	C	401	HEM	C1B-NB-C4B	3.06	108.23	105.07
17	C	402	HEM	C1B-NB-C4B	3.03	108.20	105.07
20	C	406	FX2	C13-N2-N1	-2.97	115.61	121.02
14	E	205	CDL	PA1-OA2-CA2	2.93	126.36	118.30
17	C	402	HEM	CHD-C1D-ND	2.91	127.58	124.42
23	E	202	PX4	O7-C23-O8	-2.89	116.71	123.70
21	D	501	HEC	C4A-C3A-C2A	-2.85	102.78	106.94
21	D	501	HEC	CHB-C1B-NB	-2.77	121.41	124.42
21	D	501	HEC	CAD-C3D-C4D	2.76	129.49	124.66
23	E	202	PX4	O5-C9-C10	2.76	120.58	111.91
17	C	401	HEM	CHD-C1D-ND	2.68	127.33	124.42
19	C	405	PEE	O2-C10-C11	2.68	117.28	111.50
21	D	501	HEC	CMC-C2C-C3C	2.67	131.39	125.61
20	C	406	FX2	C13-N2-C12	2.67	132.69	128.64
17	C	402	HEM	C4C-NC-C1C	2.66	107.96	105.35
11	A	501	6PE	O4-C4-C5	2.65	120.21	111.91
17	C	402	HEM	O2D-CGD-CBD	2.57	122.28	114.03
17	C	401	HEM	CHD-C1D-C2D	-2.54	121.01	124.98
17	C	401	HEM	C4C-NC-C1C	2.50	107.80	105.35
21	D	501	HEC	CHB-C4A-NA	-2.50	121.73	124.44
20	C	406	FX2	C8-C7-C10	2.48	123.96	119.71
21	D	501	HEC	CAA-CBA-CGA	-2.43	108.37	113.60
21	D	501	HEC	CMD-C2D-C1D	2.33	128.59	125.04
21	D	501	HEC	CMA-C3A-C4A	2.33	128.81	124.71
17	C	402	HEM	CHA-C4D-ND	2.28	127.19	124.37
14	E	205	CDL	OA4-PA1-OA3	2.27	119.56	110.68
21	D	501	HEC	CHA-C4D-ND	-2.27	121.95	124.42
14	C	404	CDL	CA6-OA8-CA7	2.25	122.75	117.10
17	C	402	HEM	O2A-CGA-CBA	2.25	121.25	114.03
17	C	401	HEM	CHD-C4C-NC	2.24	126.86	124.44
16	B	503	PX6	O7-C2-C3	2.22	116.34	108.36
17	C	401	HEM	C4B-C3B-C2B	-2.21	105.36	107.11
21	D	501	HEC	CMB-C2B-C1B	2.21	128.40	125.04
14	E	205	CDL	OB8-CB6-CB4	2.20	114.85	108.43
14	D	503	CDL	PB2-OB2-CB2	2.18	124.31	118.30
20	C	406	FX2	C20-O2-C17	2.18	125.21	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	501	HEC	C1D-ND-C4D	-2.12	102.88	105.07
17	C	401	HEM	CBA-CAA-C2A	-2.12	106.74	112.63
11	A	501	6PE	O6-C10-O7	-2.12	118.59	123.70
17	C	401	HEM	CAD-C3D-C4D	2.12	128.35	124.66
17	C	402	HEM	CHD-C1D-C2D	-2.11	121.68	124.98
23	E	202	PX4	O5-C9-O6	-2.08	118.33	123.59
14	A	506	CDL	OB6-CB5-OB7	-2.08	118.68	123.70
18	C	403	LMT	C1B-O1B-C4'	-2.07	112.83	117.96
17	C	401	HEM	O2D-CGD-CBD	2.07	120.68	114.03
19	E	204	PEE	C3-O3-C30	2.06	122.28	117.10
14	D	503	CDL	OB4-PB2-OB3	2.05	118.69	110.68
16	C	410	PX6	O5-C4-O6	-2.04	118.44	123.59
17	C	401	HEM	CHA-C4D-ND	2.03	126.88	124.37
21	D	501	HEC	CHA-C1A-C2A	-2.03	121.65	124.94
17	C	401	HEM	CHB-C1B-NB	2.02	126.86	124.37
21	D	501	HEC	CAA-C2A-C1A	2.01	128.68	124.89
20	C	406	FX2	C-C5-C6	2.01	122.80	119.80
14	E	205	CDL	OA5-PA1-OA2	-2.01	101.40	106.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	C	405	PEE	C2
19	E	204	PEE	C2
20	C	406	FX2	C8
21	D	501	HEC	NA

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	6PE	C1-O3-P1-O1
11	A	501	6PE	C11-C10-O6-C2
11	A	501	6PE	O8-C16-C17-N1
14	A	506	CDL	C51-CB5-OB6-CB4
14	C	404	CDL	CA3-OA5-PA1-OA4
14	C	404	CDL	C11-CA5-OA6-CA4
14	D	503	CDL	CA2-OA2-PA1-OA3
14	D	503	CDL	CA2-OA2-PA1-OA4
14	D	503	CDL	CA3-OA5-PA1-OA3
14	D	503	CDL	CB2-OB2-PB2-OB3
14	D	503	CDL	CB2-OB2-PB2-OB4
14	D	503	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
14	E	205	CDL	C1-CA2-OA2-PA1
14	E	205	CDL	CA2-OA2-PA1-OA4
14	E	205	CDL	CA2-OA2-PA1-OA5
14	E	205	CDL	C1-CB2-OB2-PB2
14	E	205	CDL	CB4-CB6-OB8-CB7
16	C	410	PX6	C1-O4-P1-O1
16	C	410	PX6	C1-O4-P1-O3
19	C	405	PEE	C4-O4P-P-O3P
19	C	405	PEE	C4-O4P-P-O2P
19	C	405	PEE	C4-O4P-P-O1P
19	E	204	PEE	C4-O4P-P-O1P
19	E	204	PEE	O4P-C4-C5-N
23	E	202	PX4	C1-O3-P1-O2
23	E	202	PX4	C24-C23-O7-C7
21	D	501	HEC	C2B-C3B-CAB-CBB
21	D	501	HEC	C4B-C3B-CAB-CBB
21	D	501	HEC	C4C-C3C-CAC-CBC
21	D	501	HEC	C2C-C3C-CAC-CBC
11	A	501	6PE	O7-C10-O6-C2
14	A	506	CDL	OB7-CB5-OB6-CB4
23	E	202	PX4	O8-C23-O7-C7
14	C	404	CDL	OA7-CA5-OA6-CA4
14	E	205	CDL	C71-CB7-OB8-CB6
19	E	204	PEE	C31-C30-O3-C3
19	C	405	PEE	C17-C18-C19-C20
14	D	503	CDL	O1-C1-CA2-OA2
16	C	410	PX6	O4-C1-C2-O7
23	E	202	PX4	C10-C9-O5-C8
23	E	202	PX4	O6-C9-O5-C8
14	E	205	CDL	C51-CB5-OB6-CB4
16	B	503	PX6	C21-C20-O7-C2
14	C	404	CDL	C31-CA7-OA8-CA6
14	D	503	CDL	CB2-C1-CA2-OA2
16	B	503	PX6	O8-C20-O7-C2
14	D	503	CDL	C31-CA7-OA8-CA6
16	C	410	PX6	C5-C4-O5-C3
19	C	405	PEE	C31-C30-O3-C3
12	C	409	PGE	O2-C3-C4-O3
14	A	506	CDL	O1-C1-CB2-OB2
14	E	205	CDL	O1-C1-CB2-OB2
14	E	205	CDL	OB9-CB7-OB8-CB6
14	D	503	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	C	410	PX6	O6-C4-O5-C3
19	C	405	PEE	O5-C30-O3-C3
14	C	404	CDL	OA9-CA7-OA8-CA6
19	E	204	PEE	O5-C30-O3-C3
16	B	503	PX6	C20-C21-C22-C23
14	E	205	CDL	OB7-CB5-OB6-CB4
14	A	506	CDL	CB5-C51-C52-C53
14	A	506	CDL	OA5-CA3-CA4-OA6
14	E	205	CDL	O1-C1-CA2-OA2
16	C	410	PX6	O7-C2-C3-O5
11	A	501	6PE	C1-O3-P1-O8
14	A	506	CDL	CA3-OA5-PA1-OA2
14	C	404	CDL	CA3-OA5-PA1-OA2
14	D	503	CDL	CA2-OA2-PA1-OA5
14	D	503	CDL	CA3-OA5-PA1-OA2
14	E	205	CDL	CB2-OB2-PB2-OB5
19	E	204	PEE	C1-O3P-P-O4P
23	E	202	PX4	C1-O3-P1-O4
14	A	506	CDL	OA5-CA3-CA4-CA6
12	C	407	PGE	O3-C5-C6-O4
15	B	502	PG4	O3-C5-C6-O4
19	C	405	PEE	C14-C15-C16-C17
18	C	403	LMT	C11-C10-C9-C8
16	B	503	PX6	C21-C22-C23-C24
19	C	405	PEE	C13-C14-C15-C16
18	C	403	LMT	O1'-C1-C2-C3
14	E	205	CDL	CB2-C1-CA2-OA2
12	A	502	PGE	O1-C1-C2-O2
23	E	202	PX4	C9-C10-C11-C12
18	C	403	LMT	C7-C8-C9-C10
12	C	407	PGE	O2-C3-C4-O3
19	E	204	PEE	O4-C10-O2-C2
19	C	405	PEE	C11-C12-C13-C14
14	C	404	CDL	C51-CB5-OB6-CB4
19	E	204	PEE	C11-C10-O2-C2
14	C	404	CDL	OB7-CB5-OB6-CB4
19	E	204	PEE	O2-C2-C3-O3
11	A	501	6PE	C2-C1-O3-P1
14	A	506	CDL	OB5-CB3-CB4-CB6
14	A	506	CDL	CA2-C1-CB2-OB2
18	C	403	LMT	C4-C5-C6-C7
19	C	405	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	C	405	PEE	C10-C11-C12-C13
18	C	403	LMT	O5B-C5B-C6B-O6B
16	B	503	PX6	C3-C2-O7-C20
14	E	205	CDL	CA2-OA2-PA1-OA3
16	C	410	PX6	C1-O4-P1-O2
14	E	205	CDL	C51-C52-C53-C54
19	C	405	PEE	C22-C23-C24-C25
14	E	205	CDL	CB5-C51-C52-C53
23	E	202	PX4	C10-C11-C12-C13
23	E	202	PX4	C24-C25-C26-C27
12	C	409	PGE	O1-C1-C2-O2
14	C	404	CDL	C71-CB7-OB8-CB6
16	B	503	PX6	C2-C1-O4-P1
17	C	401	HEM	C3D-CAD-CBD-CGD
19	E	204	PEE	C1-C2-C3-O3
14	A	506	CDL	OB5-CB3-CB4-OB6
14	A	506	CDL	CA4-CA3-OA5-PA1
14	E	205	CDL	CB4-CB3-OB5-PB2
14	A	506	CDL	C51-C52-C53-C54
14	C	404	CDL	OB5-CB3-CB4-CB6
19	C	405	PEE	O3P-C1-C2-C3
15	B	502	PG4	O2-C3-C4-O3
15	B	502	PG4	C6-C5-O3-C4
12	C	408	PGE	C1-C2-O2-C3
18	C	403	LMT	O5'-C5'-C6'-O6'
19	C	405	PEE	O3P-C1-C2-O2
14	E	205	CDL	CA2-C1-CB2-OB2
16	C	410	PX6	O4-C1-C2-C3
14	C	404	CDL	OB9-CB7-OB8-CB6
11	A	501	6PE	O6-C2-C3-O4
15	B	502	PG4	C8-C7-O4-C6
14	C	404	CDL	CB4-CB3-OB5-PB2
14	A	506	CDL	CA3-OA5-PA1-OA3
14	C	404	CDL	CB2-OB2-PB2-OB3
14	D	503	CDL	CA3-OA5-PA1-OA4
14	E	205	CDL	CB2-OB2-PB2-OB3
19	E	204	PEE	C1-O3P-P-O2P
23	E	202	PX4	C1-O3-P1-O1
19	E	204	PEE	O3P-C1-C2-C3
12	A	502	PGE	O2-C3-C4-O3
14	C	404	CDL	OB5-CB3-CB4-OB6
14	D	503	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
23	E	202	PX4	O3-C1-C2-N1
14	C	404	CDL	OB6-CB4-CB6-OB8
14	D	503	CDL	OA6-CA4-CA6-OA8
12	C	407	PGE	C6-C5-O3-C4
12	C	409	PGE	C1-C2-O2-C3
12	C	408	PGE	O2-C3-C4-O3
15	B	502	PG4	C3-C4-O3-C5
23	E	202	PX4	C23-C24-C25-C26
12	C	407	PGE	C3-C4-O3-C5
15	B	502	PG4	C5-C6-O4-C7
14	C	404	CDL	CB2-OB2-PB2-OB5
12	C	407	PGE	C1-C2-O2-C3
15	B	502	PG4	O4-C7-C8-O5
12	C	408	PGE	C3-C4-O3-C5
14	D	503	CDL	OA5-CA3-CA4-OA6
17	C	402	HEM	CAA-CBA-CGA-O2A
11	A	501	6PE	C5-C4-O4-C3
17	C	402	HEM	CAA-CBA-CGA-O1A
16	C	410	PX6	C1-C2-C3-O5
19	E	204	PEE	C3-C2-O2-C10
23	E	202	PX4	O4-C6-C7-O7
18	C	403	LMT	C3-C4-C5-C6
11	A	501	6PE	O5-C4-O4-C3
11	A	501	6PE	C1-C2-C3-O4
17	C	401	HEM	CAA-CBA-CGA-O2A
17	C	401	HEM	CAA-CBA-CGA-O1A
12	A	502	PGE	C4-C3-O2-C2
14	C	404	CDL	C52-C51-CB5-OB6
23	E	202	PX4	C11-C10-C9-O5
14	C	404	CDL	C52-C51-CB5-OB7
14	D	503	CDL	OA7-CA5-OA6-CA4
21	D	501	HEC	CAA-CBA-CGA-O2A
17	C	401	HEM	CAD-CBD-CGD-O2D
20	C	406	FX2	C16-C17-O2-C20
17	C	401	HEM	CAD-CBD-CGD-O1D
12	C	409	PGE	C6-C5-O3-C4
14	D	503	CDL	C11-CA5-OA6-CA4
21	D	501	HEC	CAA-CBA-CGA-O1A
23	E	202	PX4	C11-C10-C9-O6
14	C	404	CDL	CB3-CB4-CB6-OB8
23	E	202	PX4	O7-C23-C24-C25
19	E	204	PEE	C5-C4-O4P-P

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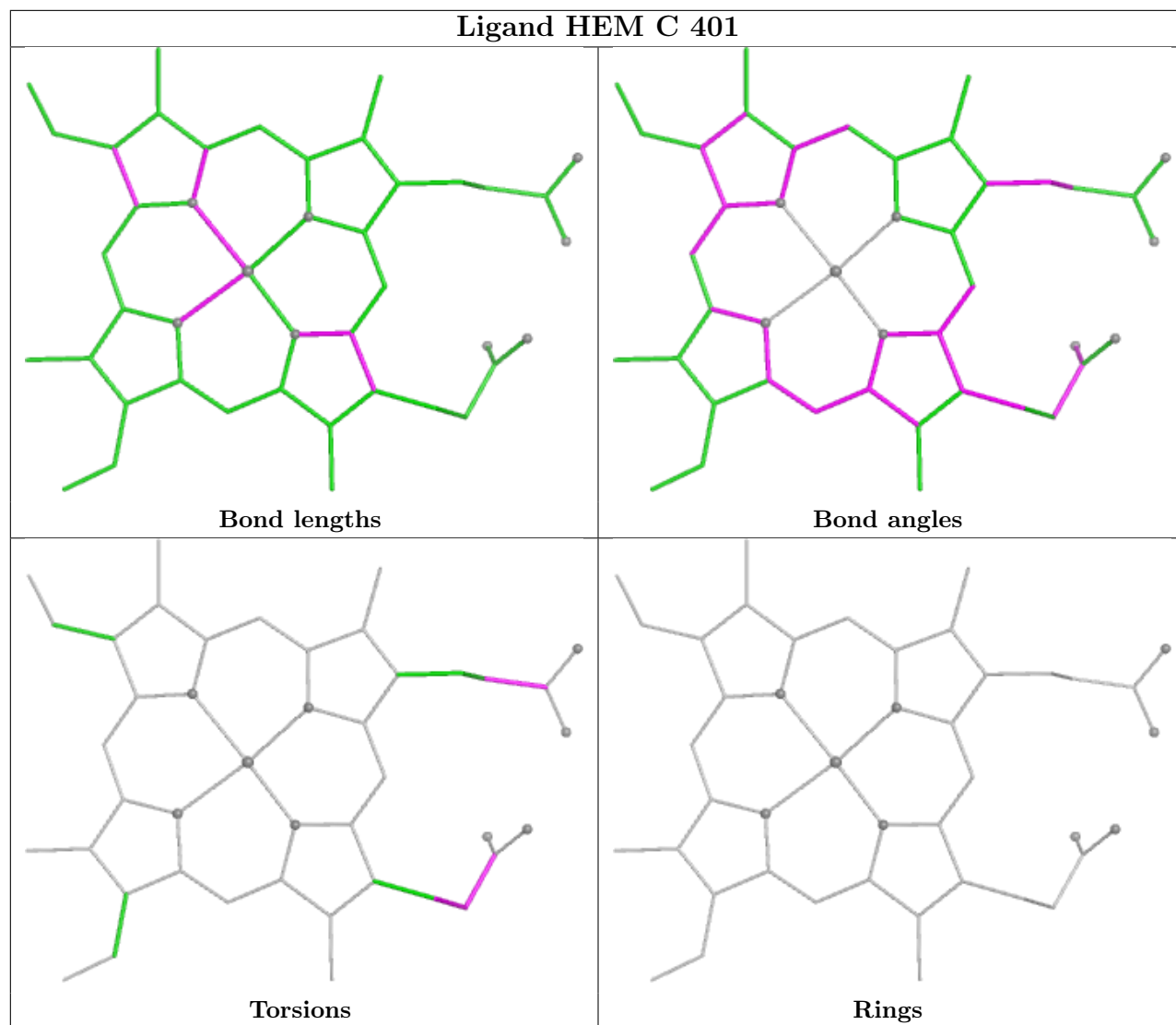
Mol	Chain	Res	Type	Atoms
14	A	506	CDL	C52-C51-CB5-OB6
18	C	403	LMT	C5-C6-C7-C8
14	A	506	CDL	C52-C51-CB5-OB7
11	A	501	6PE	O4-C4-C5-C6
23	E	202	PX4	O8-C23-C24-C25
16	B	503	PX6	O7-C20-C21-C22

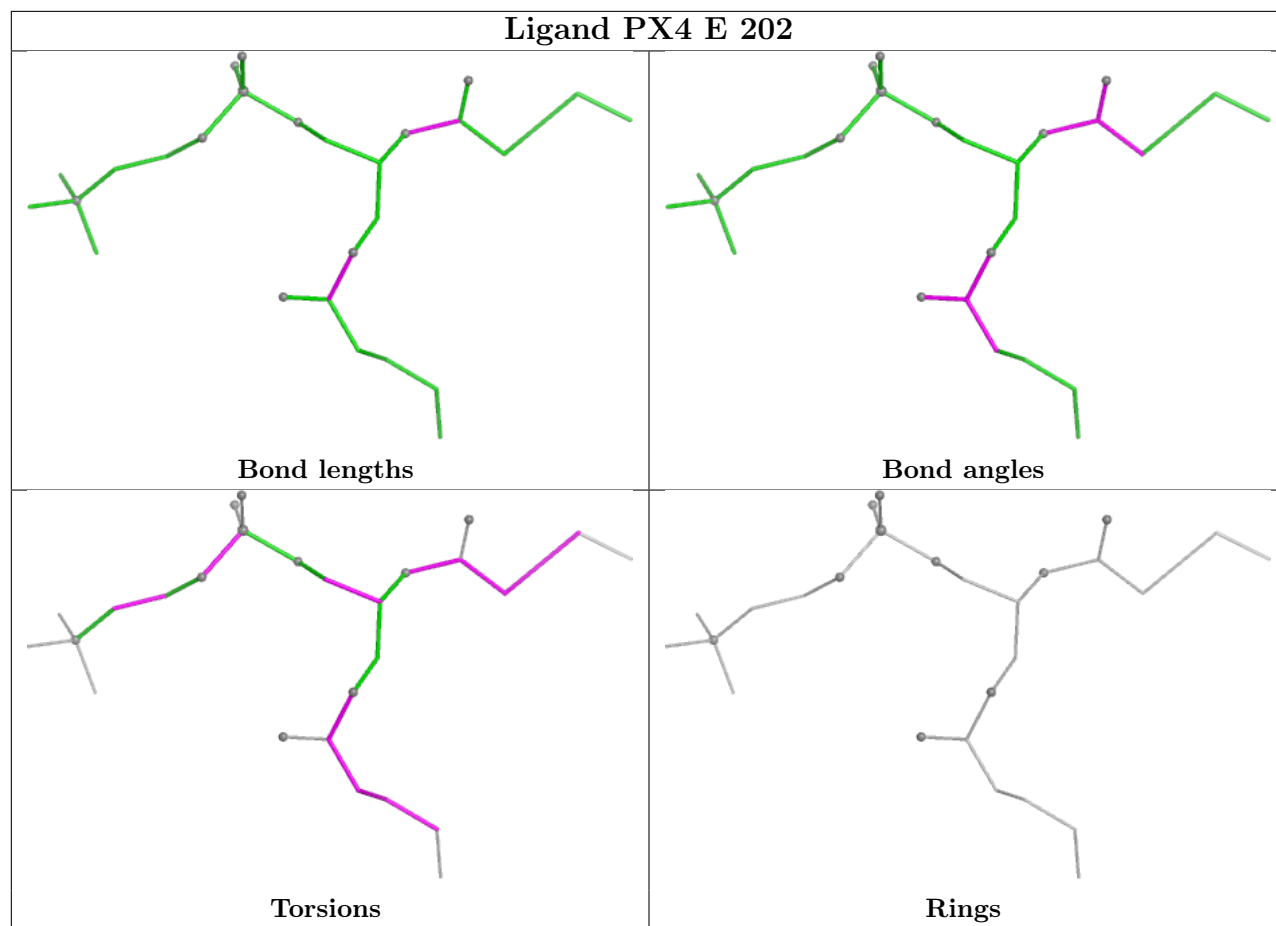
There are no ring outliers.

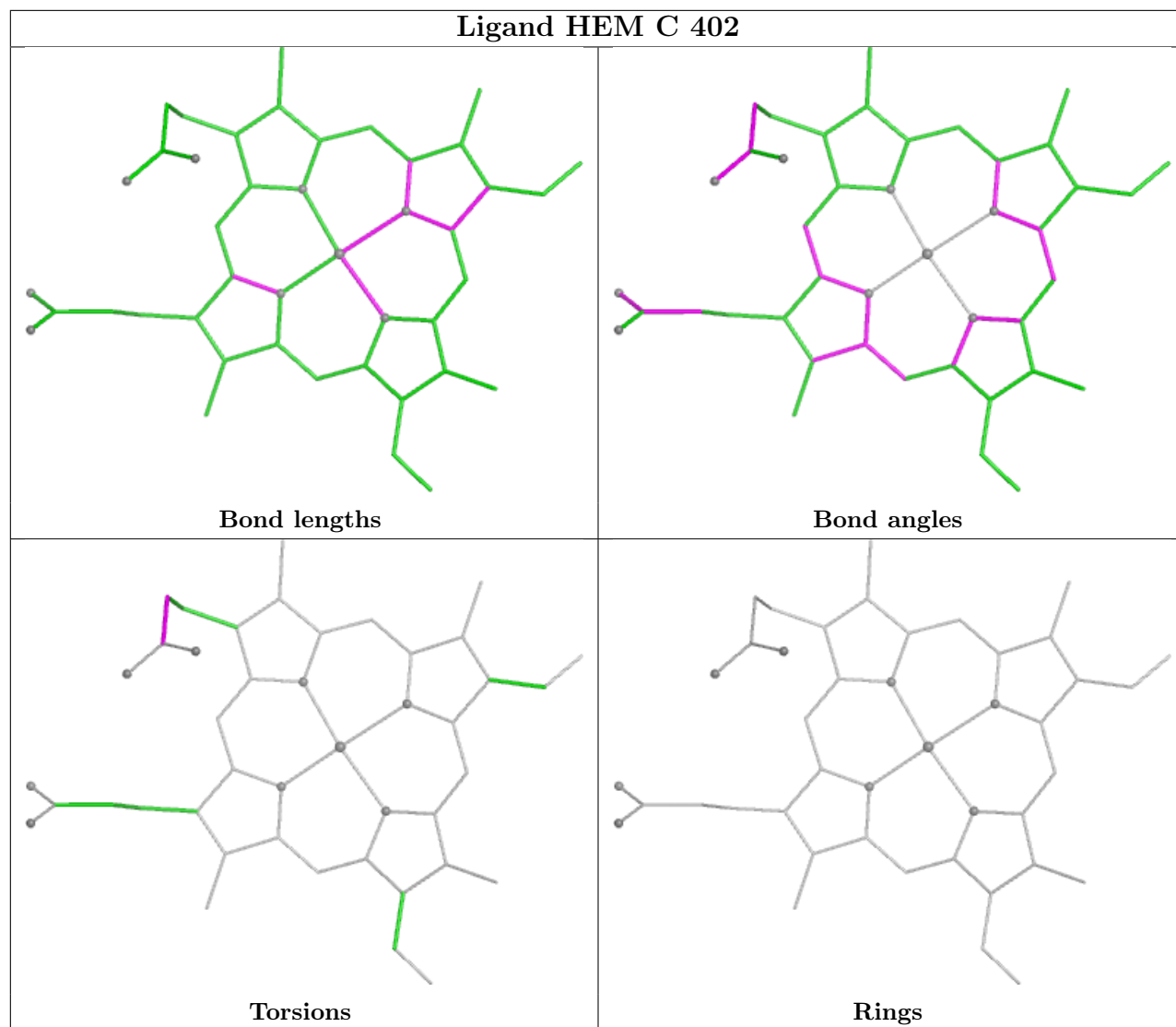
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	401	HEM	1	0
17	C	402	HEM	1	0
21	D	501	HEC	3	0
14	A	506	CDL	2	0
11	A	501	6PE	2	0

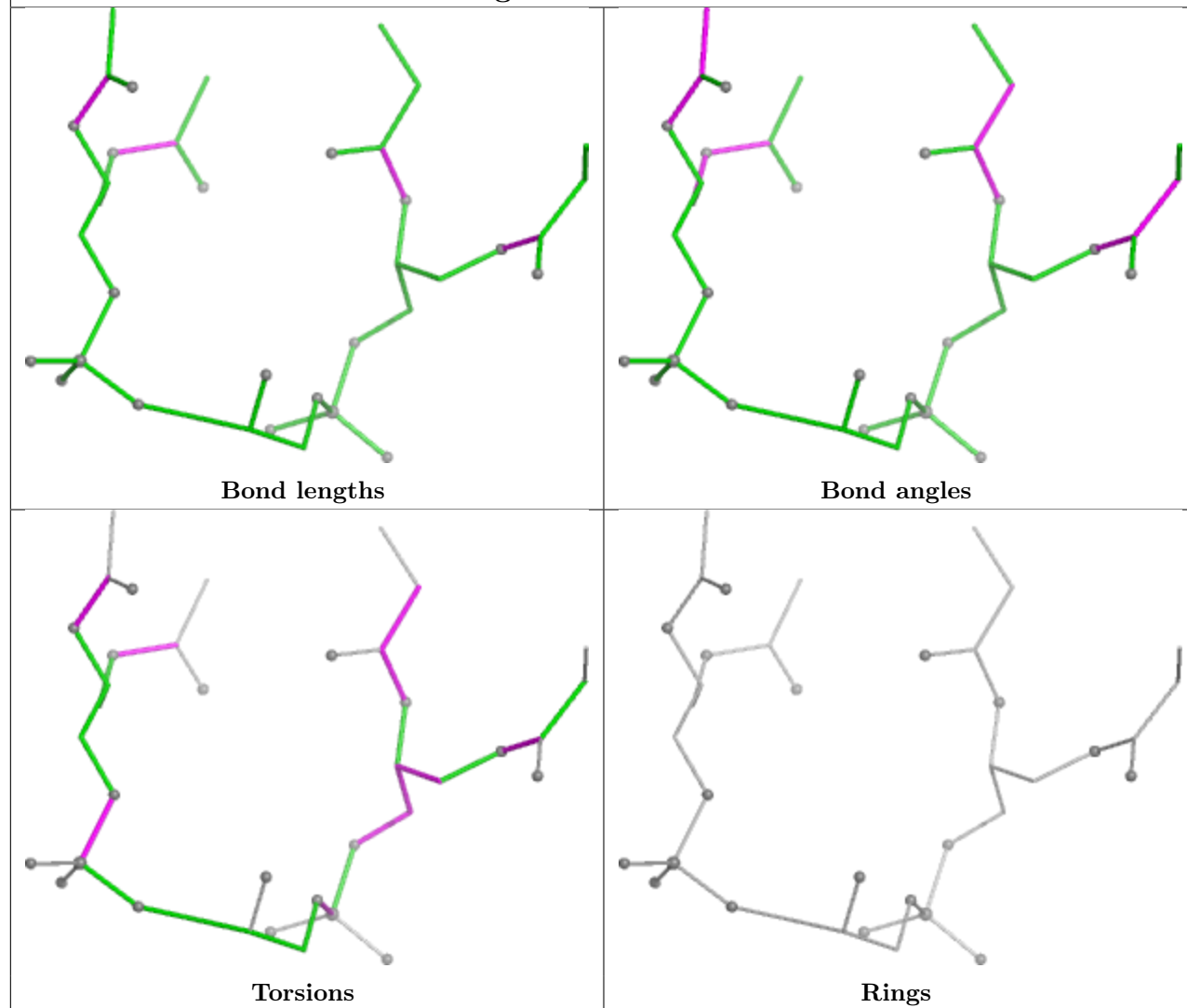
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



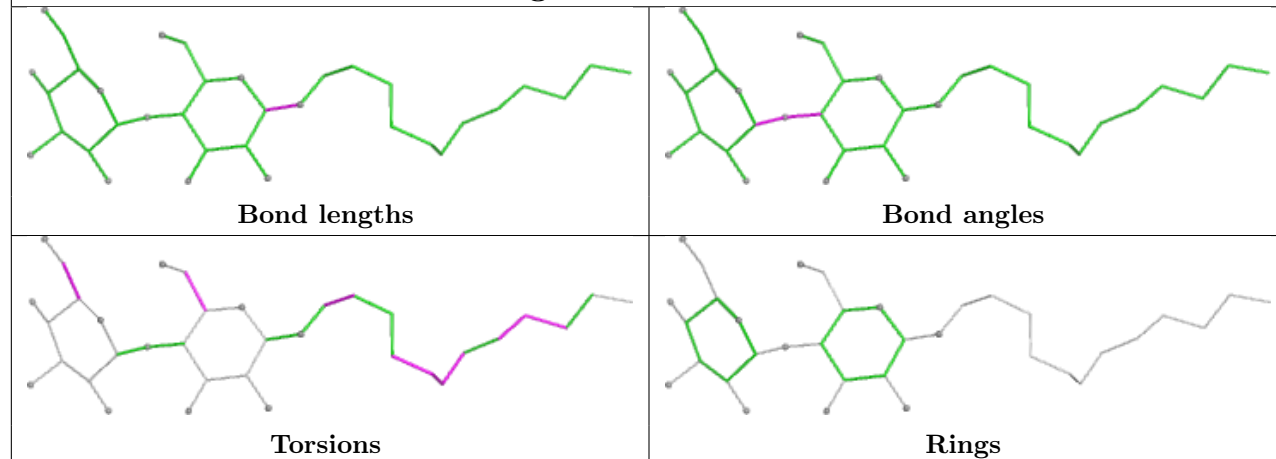


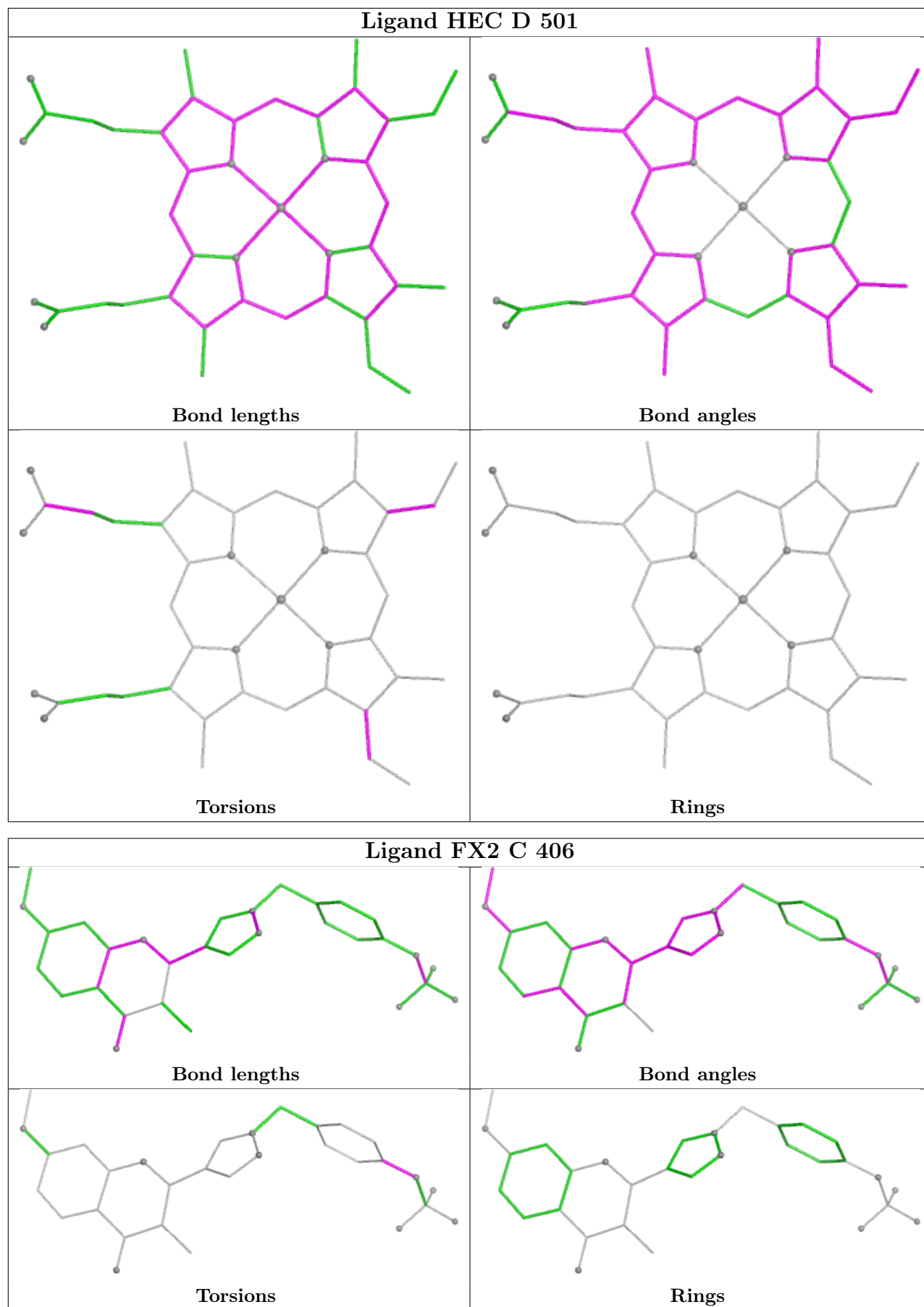


Ligand CDL C 404

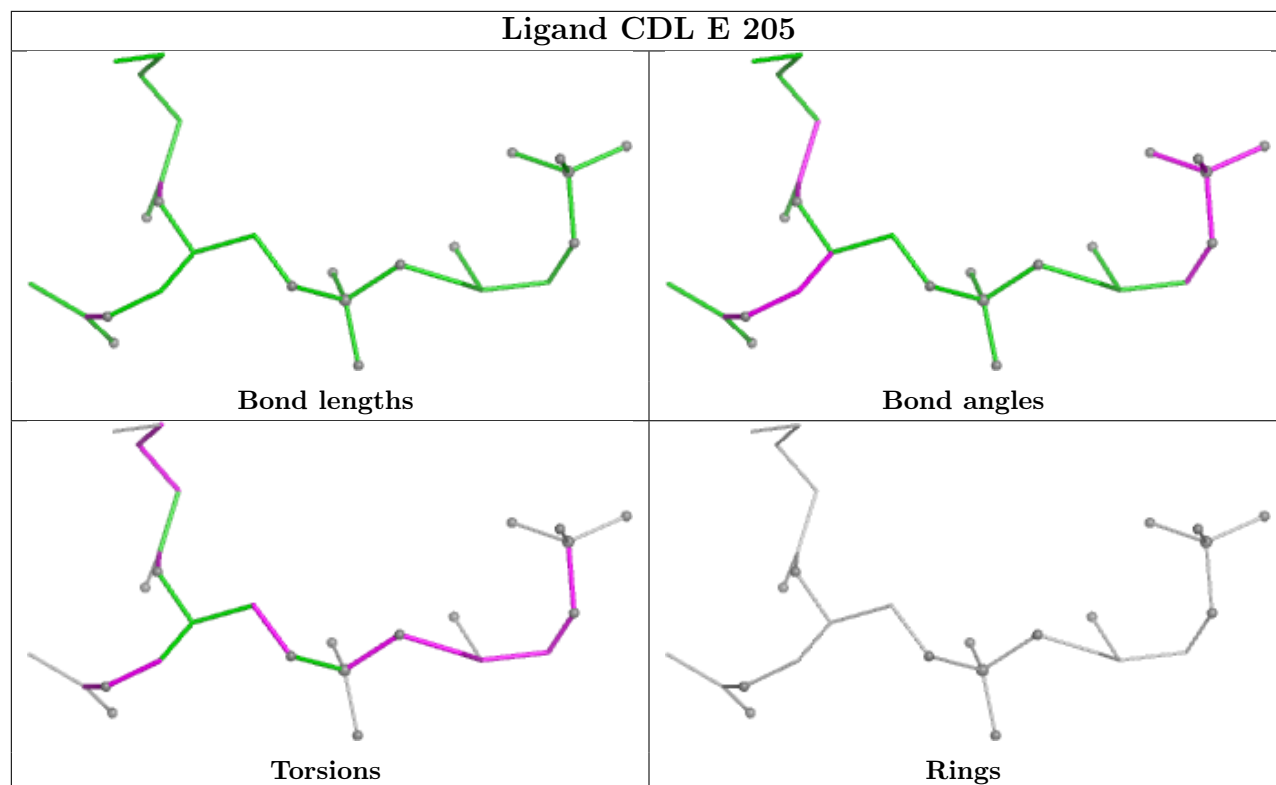


Ligand LMT C 403

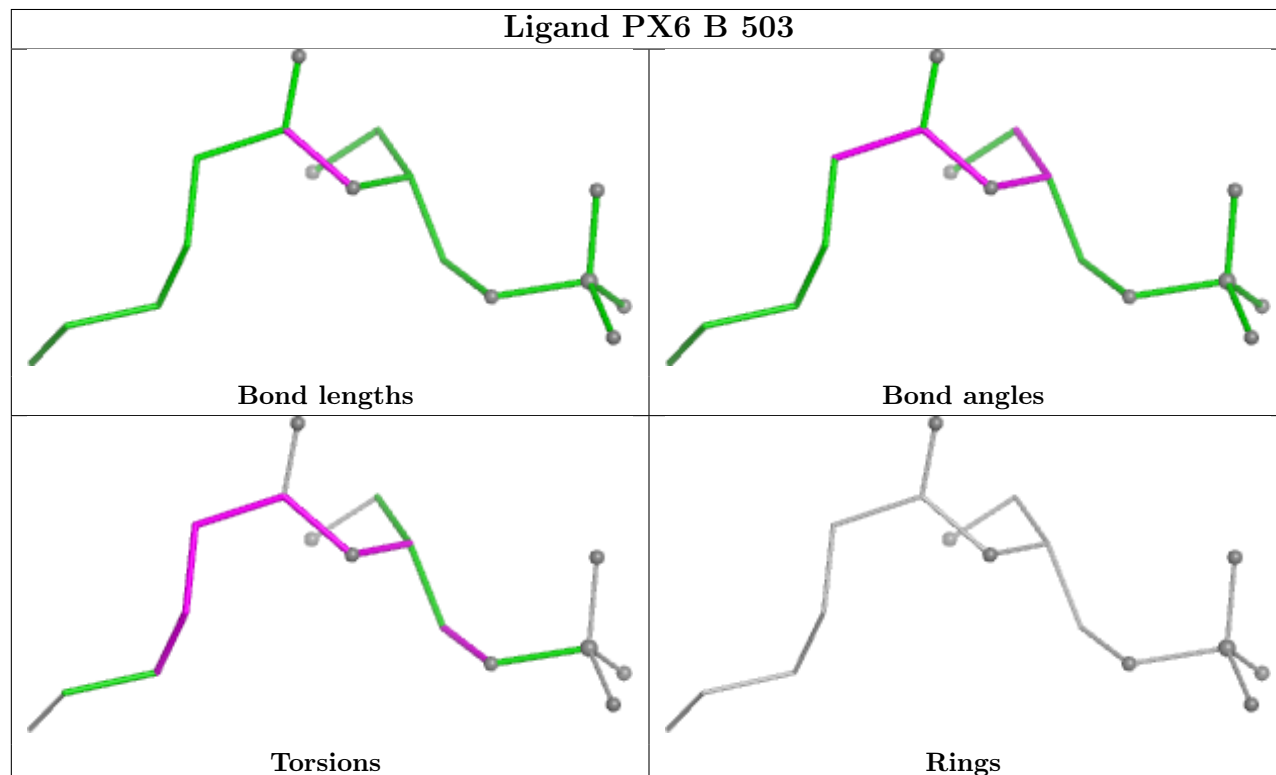


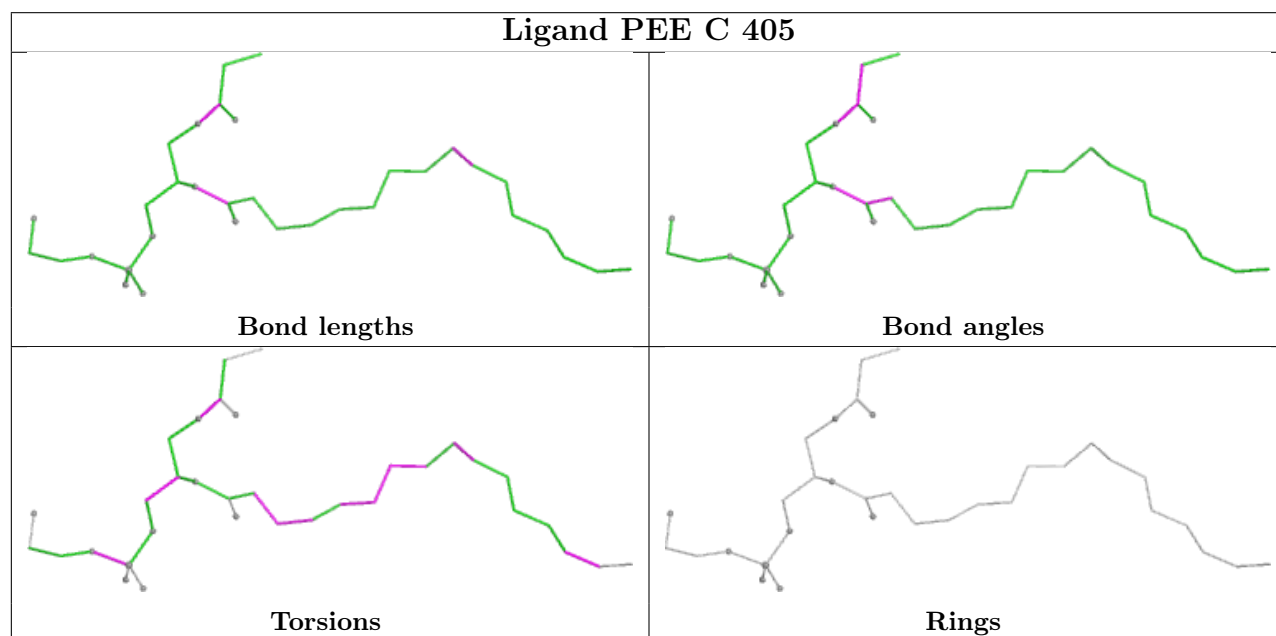
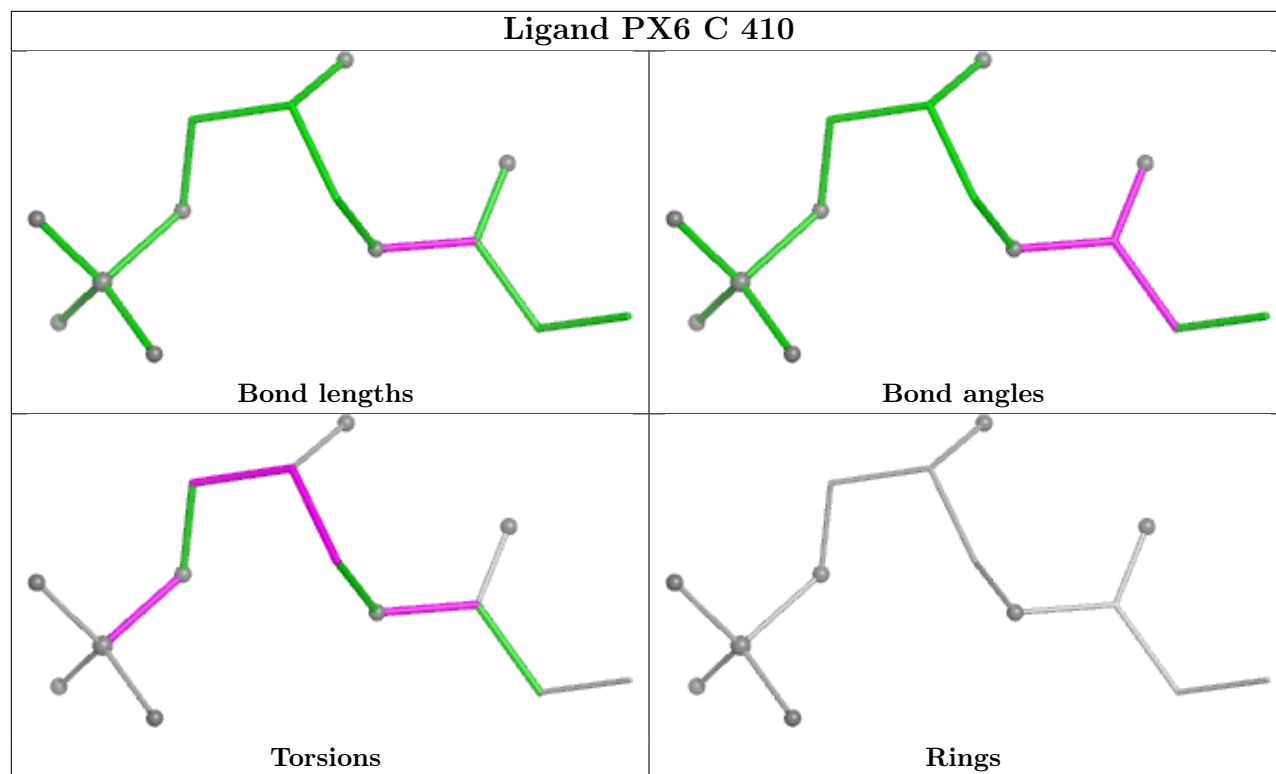


Ligand CDL E 205

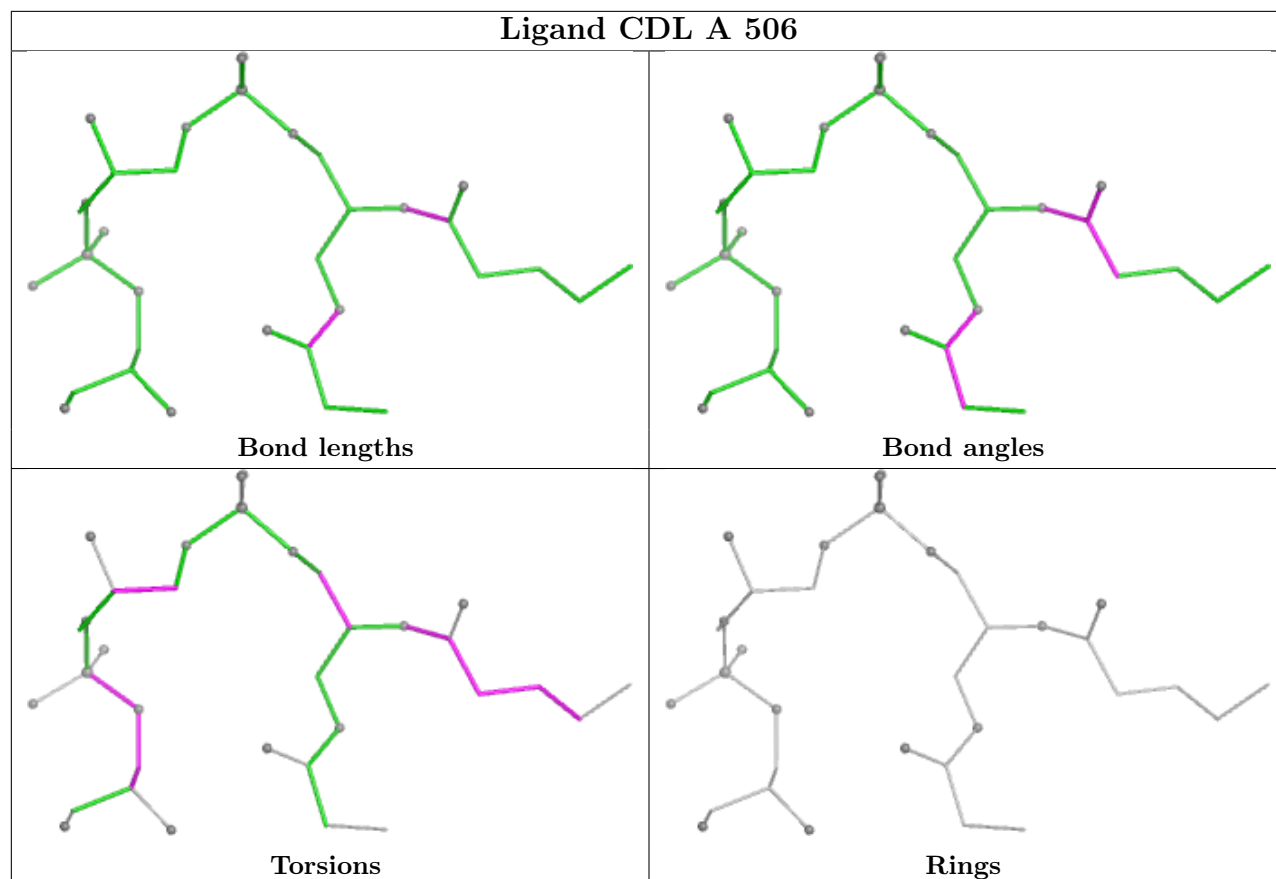


Ligand PX6 B 503

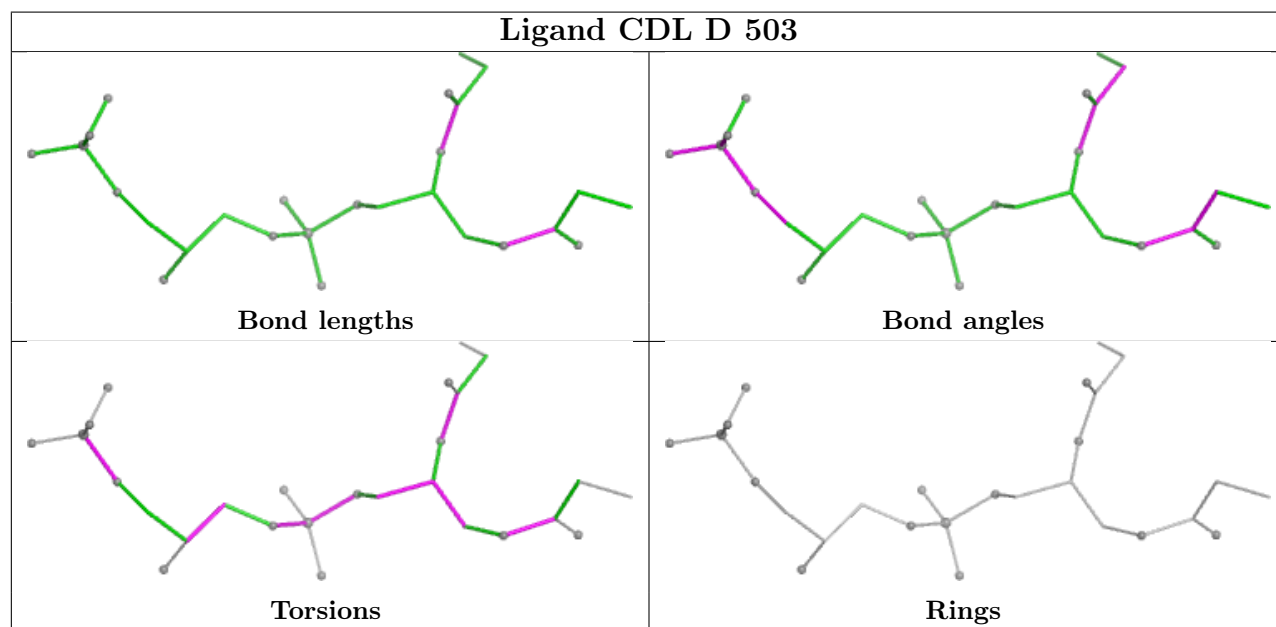


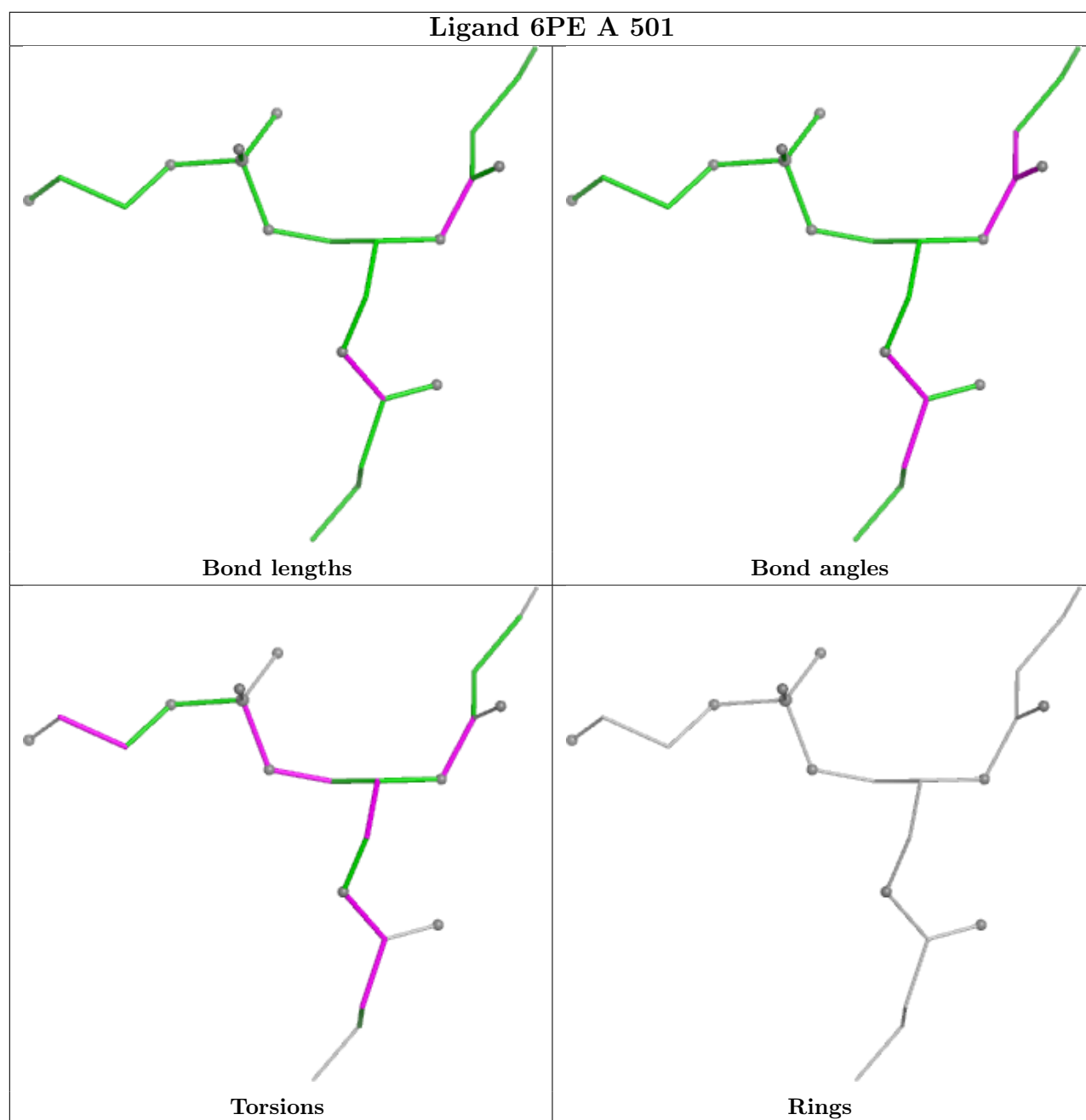


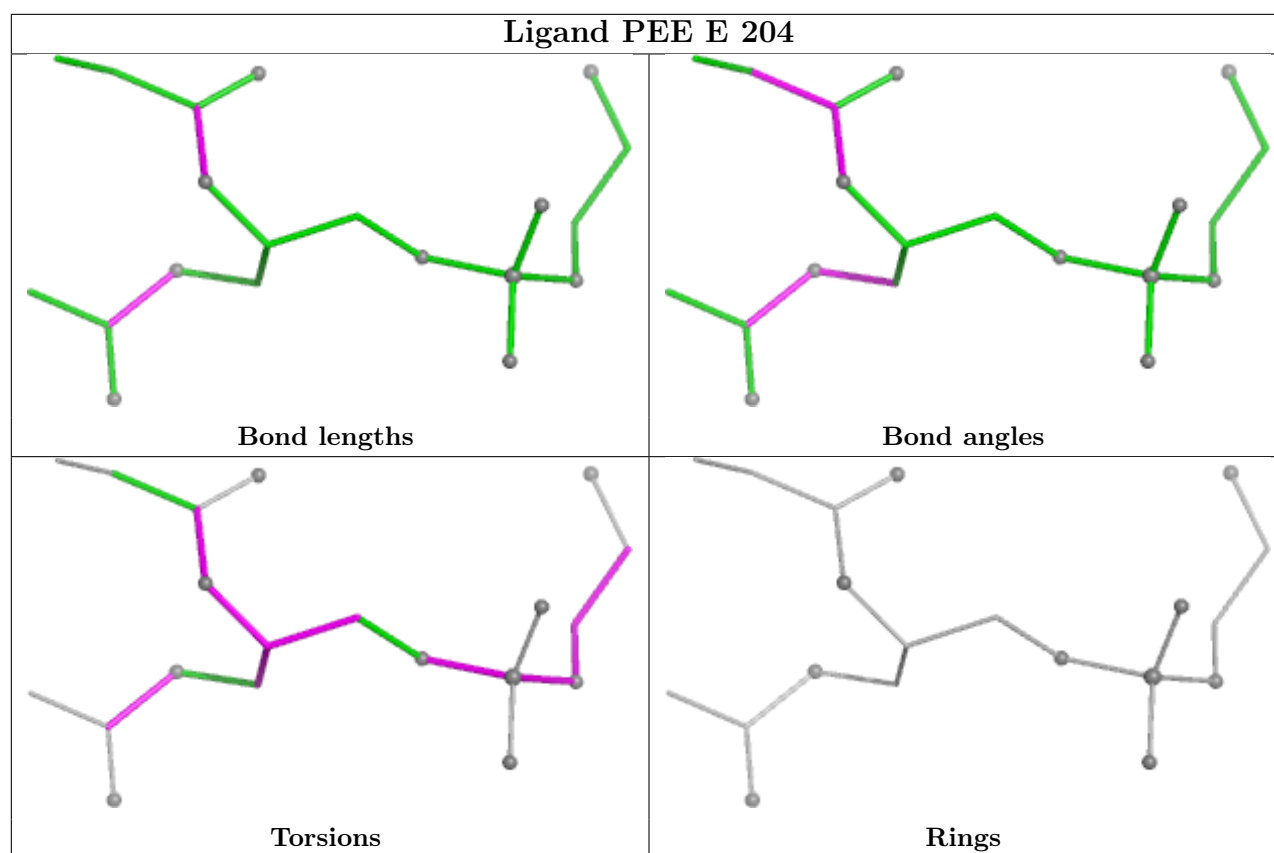
Ligand CDL A 506



Ligand CDL D 503







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	229:GLY	C	235:ALA	N	11.37
1	A	221:GLY	C	228:VAL	N	9.55

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(Å²)	Q<0.9
1	A	438/438 (100%)	0.21	38 (8%)	16	11	60, 93, 119, 131	0
2	B	413/413 (100%)	0.19	35 (8%)	16	12	71, 96, 122, 143	0
3	C	378/378 (100%)	0.27	31 (8%)	17	13	63, 84, 117, 146	0
4	D	239/239 (100%)	0.32	19 (7%)	18	13	73, 116, 143, 153	0
5	E	196/196 (100%)	1.07	48 (24%)	2	2	68, 138, 182, 215	0
6	F	99/99 (100%)	0.22	9 (9%)	15	11	67, 87, 120, 166	0
7	G	74/74 (100%)	0.14	5 (6%)	23	16	68, 93, 135, 142	0
8	H	64/64 (100%)	0.49	9 (14%)	6	6	111, 138, 151, 159	0
9	I	46/46 (100%)	2.68	26 (56%)	0	1	116, 128, 149, 154	0
10	J	59/59 (100%)	0.06	3 (5%)	33	20	79, 101, 139, 158	0
All	All	2006/2006 (100%)	0.37	223 (11%)	10	8	60, 98, 148, 215	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	43	LEU	10.5
1	A	367	SER	8.0
2	B	376	GLU	7.8
5	E	82	PRO	7.1
8	H	48	SER	7.0
4	D	77	ASP	6.9
5	E	53	ASN	6.8
5	E	104	LYS	6.7
1	A	370	ASP	6.6
1	A	20	ASP	6.4
9	I	37	THR	6.1
3	C	58	ASP	5.8
1	A	18	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
9	I	70	LEU	5.7
1	A	365	LEU	5.5
2	B	318	ASP	5.4
4	D	78	GLY	5.4
8	H	45	SER	5.4
9	I	42	VAL	5.1
3	C	57	SER	5.0
1	A	369	LEU	4.9
5	E	108	GLN	4.8
9	I	38	SER	4.8
5	E	83	GLU	4.8
8	H	46	SER	4.8
5	E	84	GLY	4.8
2	B	240	HIS	4.7
1	A	371	GLY	4.7
2	B	419	SER	4.7
2	B	239	TYR	4.7
2	B	110	GLU	4.7
5	E	57	GLN	4.6
1	A	363	ASN	4.6
3	C	172	LYS	4.6
6	F	78	GLU	4.6
4	D	81	PHE	4.6
2	B	41	TYR	4.5
1	A	220	SER	4.5
5	E	103	LYS	4.5
9	I	39	GLU	4.5
2	B	260	GLU	4.4
1	A	143	THR	4.4
1	A	2	ALA	4.3
9	I	48	SER	4.3
1	A	4	TYR	4.3
9	I	74	ALA	4.2
5	E	85	LYS	4.2
5	E	49	TYR	4.2
2	B	251	SER	4.2
3	C	56	THR	4.2
1	A	366	VAL	4.1
5	E	55	VAL	4.1
2	B	374	SER	4.0
1	A	22	GLY	4.0
5	E	154	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
5	E	138	VAL	4.0
5	E	51	ALA	4.0
1	A	144	SER	4.0
5	E	152	ASP	3.9
5	E	89	PHE	3.9
2	B	250	ASP	3.9
2	B	265	GLY	3.8
9	I	36	ALA	3.8
1	A	228	VAL	3.8
7	G	75	ALA	3.8
8	H	14	VAL	3.8
1	A	6	GLN	3.8
9	I	76	VAL	3.8
1	A	374	PRO	3.8
3	C	2	THR	3.7
5	E	107	ASP	3.7
5	E	80	ASP	3.7
1	A	21	ASN	3.7
4	D	167	GLU	3.7
9	I	75	SER	3.6
9	I	47	ARG	3.6
9	I	78	TYR	3.5
9	I	77	ARG	3.5
9	I	45	LEU	3.5
9	I	44	ASP	3.5
9	I	41	PRO	3.5
4	D	80	MET	3.5
3	C	61	THR	3.4
4	D	79	GLU	3.4
1	A	221	GLY	3.4
4	D	204	MET	3.4
5	E	100	HIS	3.4
1	A	11	VAL	3.3
3	C	40	CYS	3.3
2	B	249	GLY	3.3
5	E	88	ALA	3.3
9	I	68	VAL	3.3
5	E	136	ILE	3.3
6	F	80	TRP	3.2
3	C	173	ALA	3.2
2	B	241	GLY	3.2
3	C	176	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	373	GLU	3.2
2	B	44	ALA	3.2
5	E	102	THR	3.2
1	A	229	PRO	3.1
5	E	159	PRO	3.1
2	B	319	SER	3.1
2	B	168	TYR	3.1
2	B	170	ASN	3.1
9	I	69	SER	3.1
5	E	149	ASN	3.1
5	E	140	THR	3.1
5	E	68	VAL	3.1
5	E	79	SER	3.0
1	A	7	ALA	3.0
3	C	59	THR	3.0
10	J	29	LEU	3.0
3	C	60	THR	3.0
2	B	42	ALA	2.9
3	C	156	ILE	2.9
2	B	46	ARG	2.9
4	D	170	GLU	2.9
2	B	423	SER	2.9
2	B	420	GLY	2.9
1	A	368	HIS	2.9
3	C	262	LEU	2.9
1	A	193	PRO	2.9
2	B	252	LEU	2.9
3	C	166	GLY	2.9
8	H	44	VAL	2.9
1	A	187	SER	2.8
2	B	114	ASP	2.8
4	D	100	ALA	2.8
1	A	8	LEU	2.8
3	C	43	LEU	2.8
5	E	148	ALA	2.8
6	F	77	LYS	2.8
9	I	33	ALA	2.8
2	B	266	SER	2.8
1	A	194	ARG	2.7
4	D	75	ASN	2.7
5	E	94	LYS	2.7
6	F	75	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	121	GLN	2.7
9	I	35	PRO	2.7
4	D	3	LEU	2.7
5	E	178	LEU	2.7
5	E	114	VAL	2.7
5	E	171	ILE	2.6
2	B	263	ALA	2.6
3	C	41	LEU	2.6
2	B	43	PRO	2.6
1	A	3	THR	2.6
7	G	56	TYR	2.6
5	E	160	CYS	2.6
2	B	317	SER	2.6
6	F	79	GLN	2.6
5	E	101	ARG	2.6
9	I	49	VAL	2.6
6	F	82	LYS	2.6
5	E	157	TYR	2.5
2	B	113	ARG	2.5
7	G	70	LYS	2.5
4	D	103	ALA	2.5
3	C	175	LEU	2.5
2	B	45	SER	2.4
4	D	88	SER	2.4
1	A	19	LEU	2.4
9	I	64	LEU	2.4
7	G	74	PRO	2.4
1	A	5	ALA	2.4
10	J	25	VAL	2.4
3	C	44	GLN	2.4
5	E	147	ILE	2.4
5	E	161	HIS	2.4
9	I	56	ARG	2.4
1	A	10	SER	2.4
5	E	86	ASN	2.4
1	A	13	GLU	2.4
6	F	85	GLU	2.4
5	E	56	SER	2.4
2	B	261	SER	2.3
1	A	372	THR	2.3
4	D	108	ALA	2.3
3	C	190	MET	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	57	LEU	2.3
3	C	261	PRO	2.3
3	C	42	ILE	2.3
3	C	133	LEU	2.3
4	D	147	LEU	2.3
5	E	54	VAL	2.3
5	E	75	GLU	2.2
3	C	241	LEU	2.2
3	C	171	ASP	2.2
4	D	96	PRO	2.2
5	E	124	LEU	2.2
4	D	71	GLN	2.2
4	D	158	ILE	2.2
5	E	105	GLU	2.2
4	D	104	ALA	2.2
6	F	16	ILE	2.2
8	H	24	CYS	2.2
5	E	190	ASP	2.2
5	E	187	PHE	2.2
9	I	62	ARG	2.2
3	C	45	ILE	2.2
6	F	27	ASN	2.2
2	B	112	LEU	2.1
10	J	30	PHE	2.1
3	C	291	VAL	2.1
8	H	50	THR	2.1
3	C	179	PHE	2.1
1	A	213	GLN	2.1
3	C	167	GLY	2.1
1	A	292	SER	2.1
1	A	142	ASP	2.1
2	B	320	GLY	2.1
9	I	63	PRO	2.1
3	C	64	SER	2.0
2	B	248	ASN	2.0
8	H	47	ARG	2.0
3	C	55	TYR	2.0
8	H	42	GLU	2.0
1	A	445	ARG	2.0
5	E	78	LEU	2.0
5	E	164	HIS	2.0
3	C	154	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

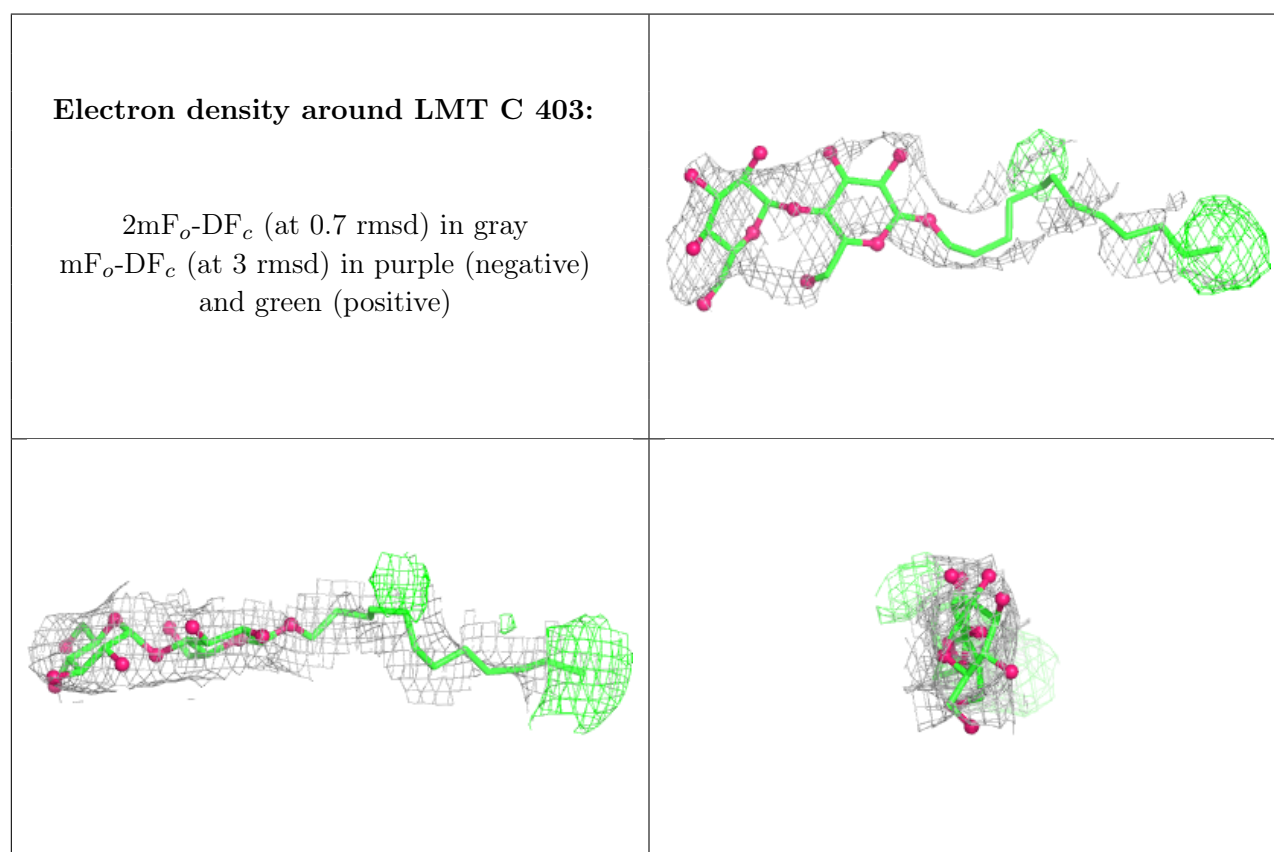
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	LMT	C	403	35/35	-0.00	0.23	147,181,189,191	0
16	PX6	B	503	17/44	0.45	0.20	110,152,160,160	0
14	CDL	E	205	28/100	0.71	0.17	147,195,219,228	0
13	PO4	E	203	5/5	0.73	0.14	164,165,170,170	0
16	PX6	C	410	14/44	0.76	0.18	128,153,171,175	0
20	FX2	C	406	31/31	0.76	0.26	120,124,143,147	0
12	PGE	C	407	10/10	0.79	0.20	105,119,128,128	0
12	PGE	A	502	7/10	0.81	0.12	90,91,93,94	0
13	PO4	G	102	5/5	0.82	0.09	169,170,172,179	0
13	PO4	A	503	5/5	0.82	0.16	144,147,149,150	0
13	PO4	D	502	5/5	0.83	0.11	185,185,186,187	0
13	PO4	B	501	5/5	0.83	0.12	162,162,164,168	0
15	PG4	B	502	13/13	0.84	0.15	73,85,87,88	0
13	PO4	F	501	5/5	0.88	0.26	145,150,152,153	0
13	PO4	G	103	5/5	0.88	0.16	156,157,158,160	0
11	6PE	A	501	23/27	0.90	0.18	102,127,141,143	0
14	CDL	A	506	34/100	0.90	0.17	122,151,159,160	0
19	PEE	E	204	20/51	0.90	0.14	93,103,109,113	0
14	CDL	D	503	27/100	0.90	0.12	96,108,145,147	0
13	PO4	G	101	5/5	0.91	0.09	122,124,128,128	0
13	PO4	A	505	5/5	0.92	0.15	129,131,132,138	0
23	PX4	E	202	28/46	0.93	0.20	107,122,133,135	0
12	PGE	C	409	10/10	0.94	0.14	87,94,99,99	0
13	PO4	F	502	5/5	0.94	0.19	137,140,141,143	0
19	PEE	C	405	34/51	0.94	0.11	75,80,89,92	0
12	PGE	C	408	10/10	0.95	0.18	69,74,78,78	0
13	PO4	A	504	5/5	0.95	0.14	148,149,151,151	0

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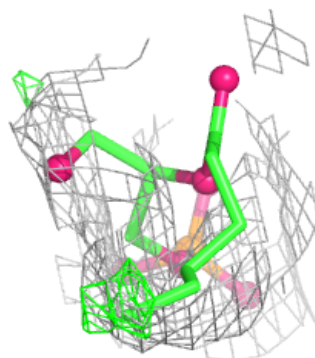
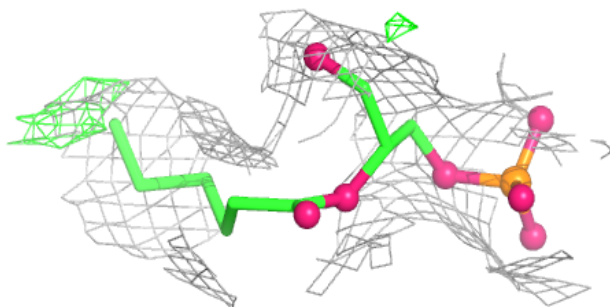
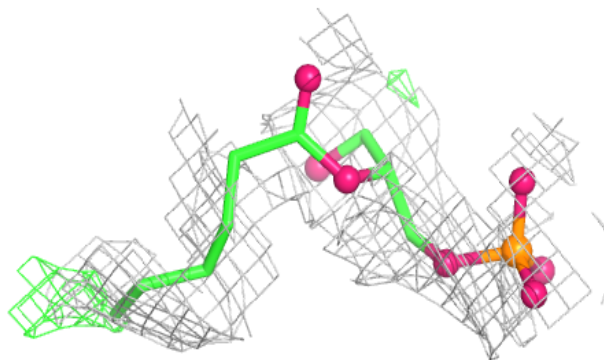
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	FES	E	201	4/4	0.96	0.05	241,242,245,246	0
14	CDL	C	404	38/100	0.96	0.10	84,95,107,110	0
17	HEM	C	401	43/43	0.97	0.10	71,73,80,82	0
21	HEC	D	501	43/43	0.97	0.10	114,121,128,132	0
17	HEM	C	402	43/43	0.98	0.08	64,67,70,72	0

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.

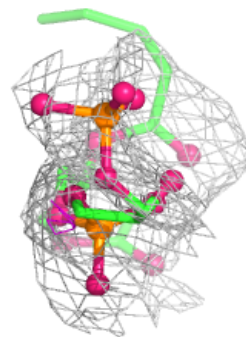
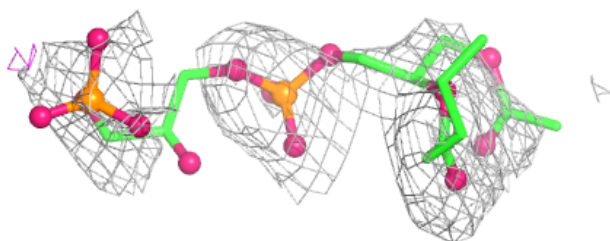
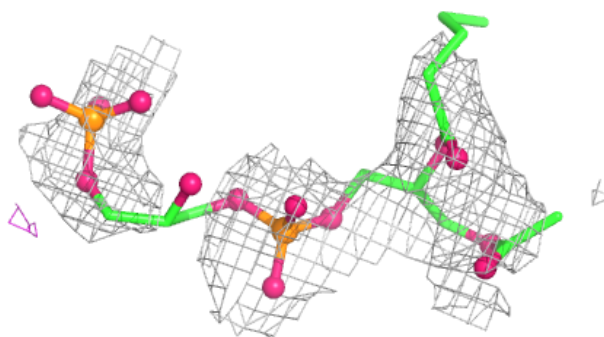


Electron density around PX6 B 503:

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

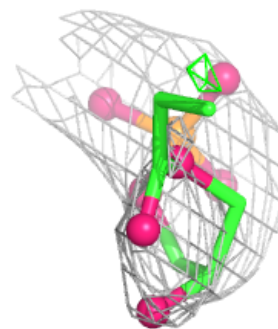
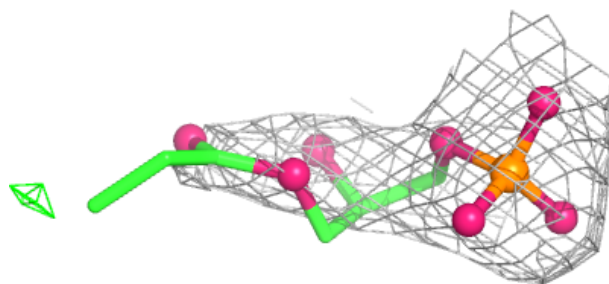
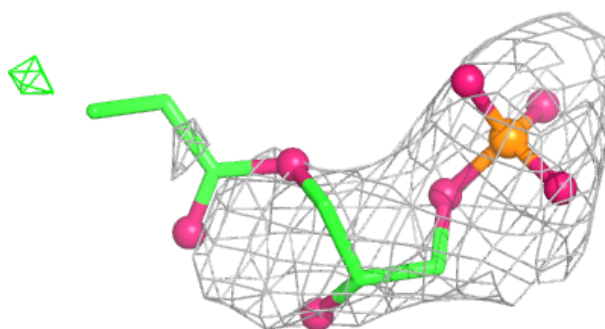
**Electron density around CDL E 205:**

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

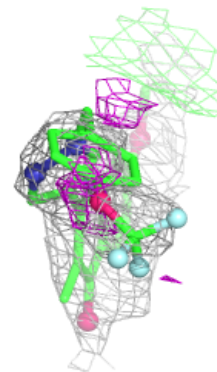
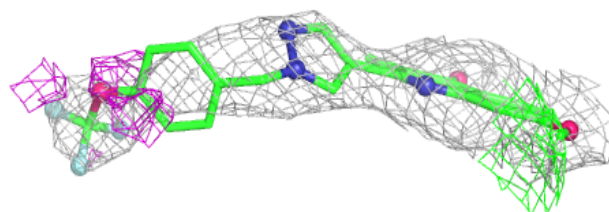
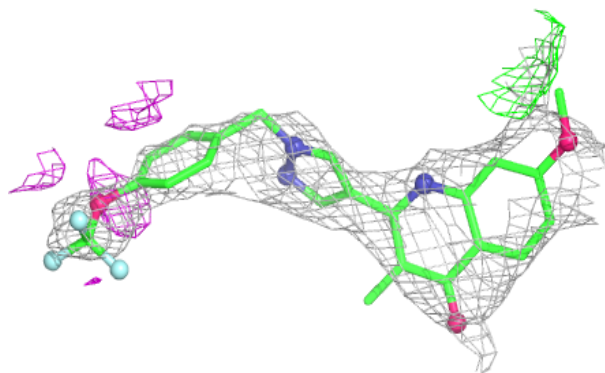


Electron density around PX6 C 410:

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

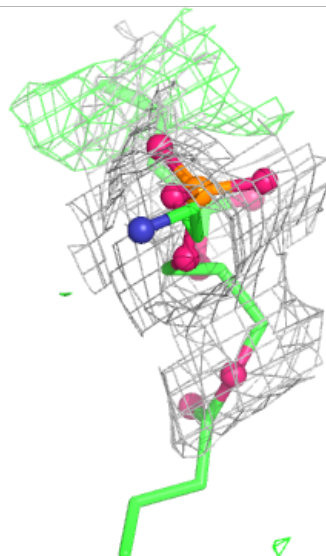
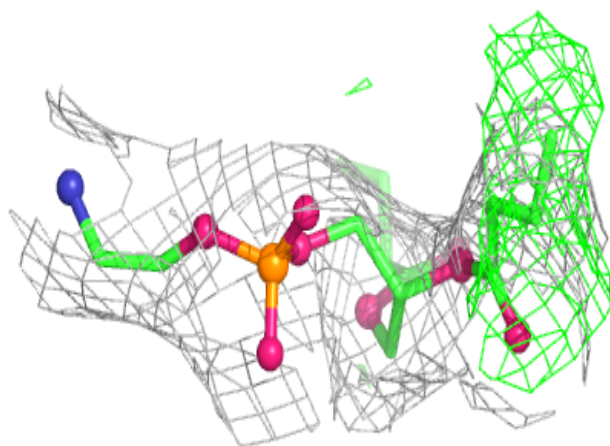
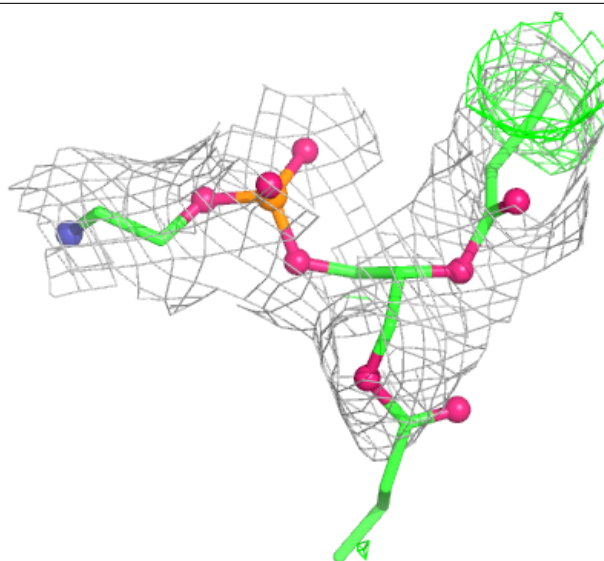
**Electron density around FX2 C 406:**

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



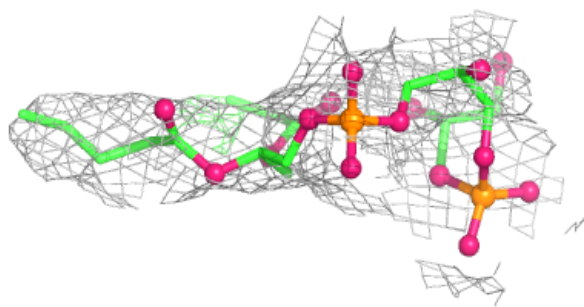
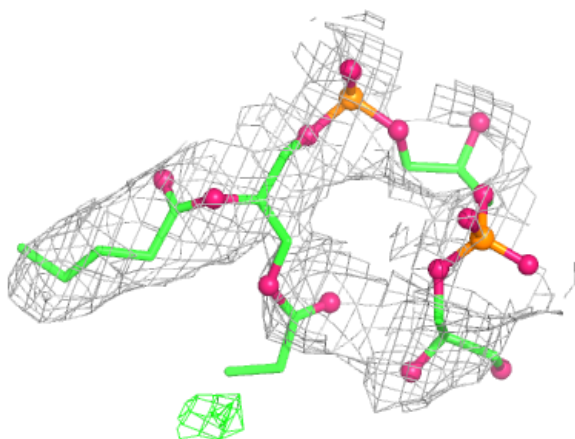
Electron density around 6PE A 501:

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



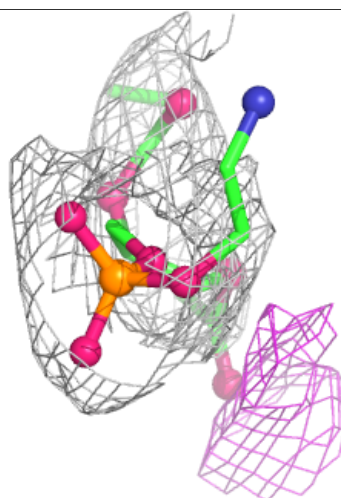
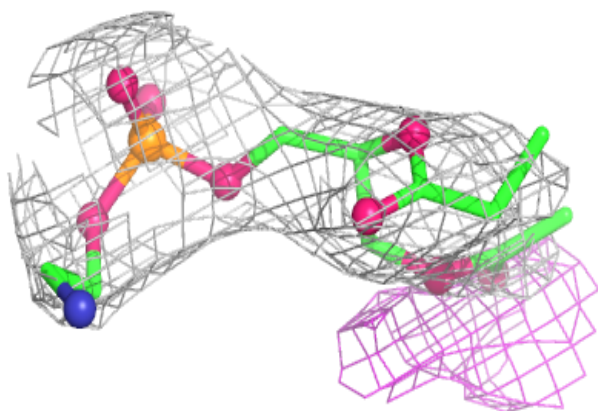
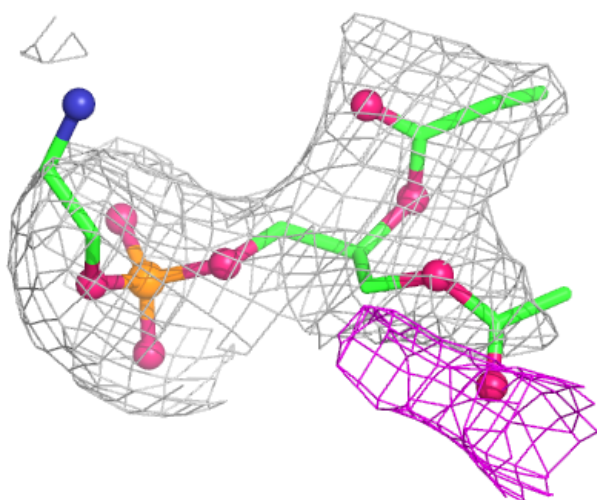
Electron density around CDL A 506:

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



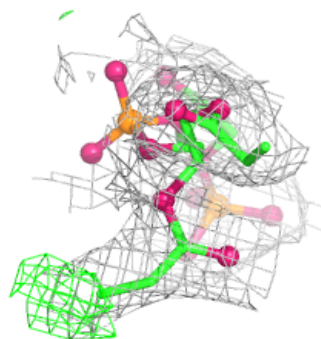
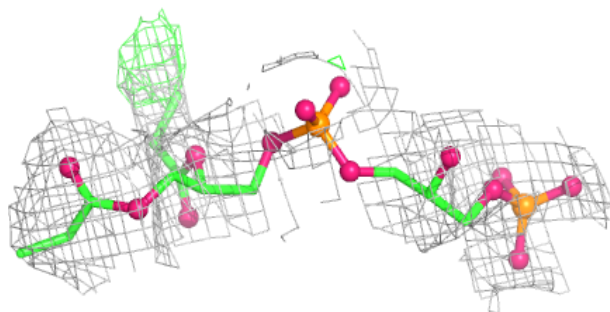
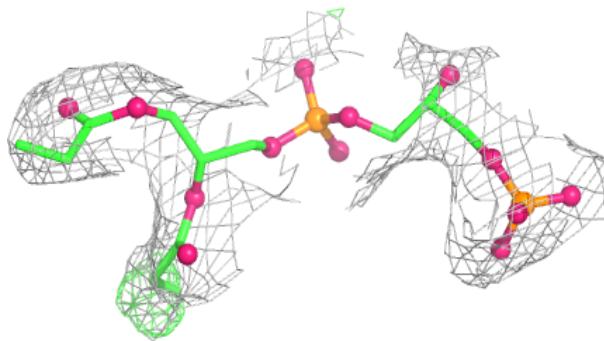
Electron density around PEE E 204:

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

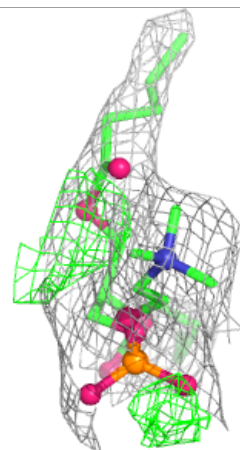
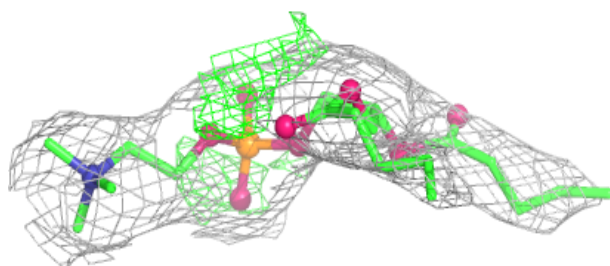
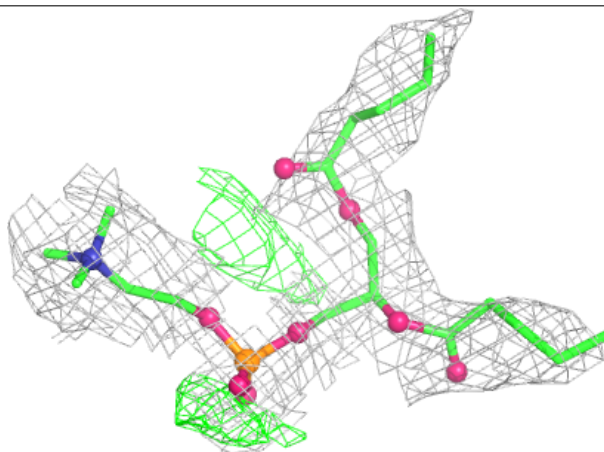


Electron density around CDL D 503:

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

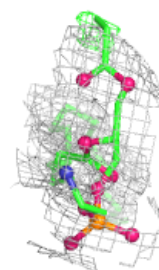
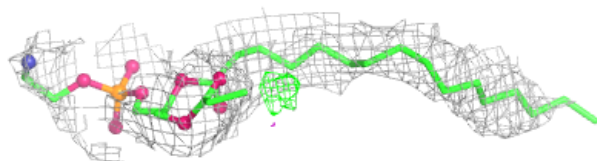
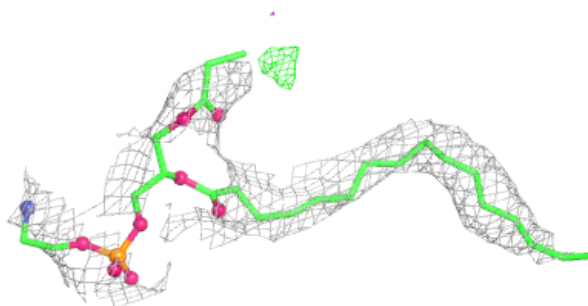
**Electron density around PX4 E 202:**

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



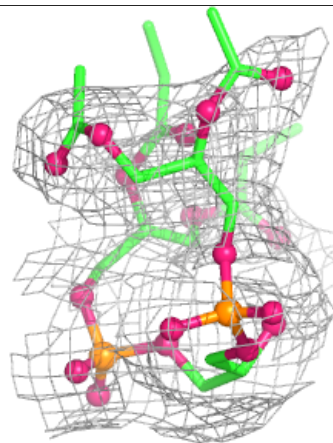
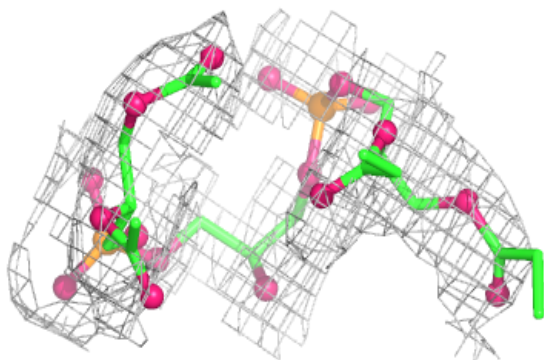
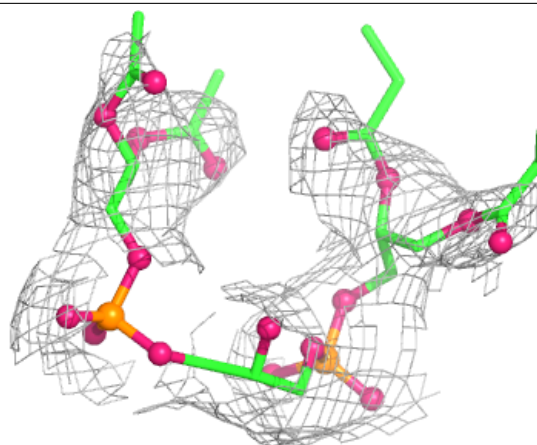
Electron density around PEE C 405:

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



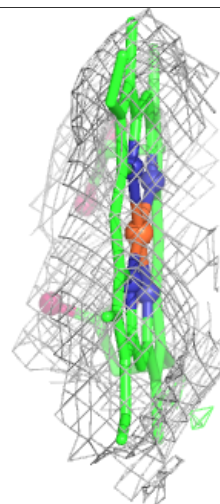
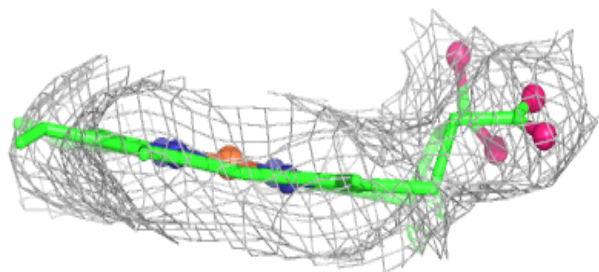
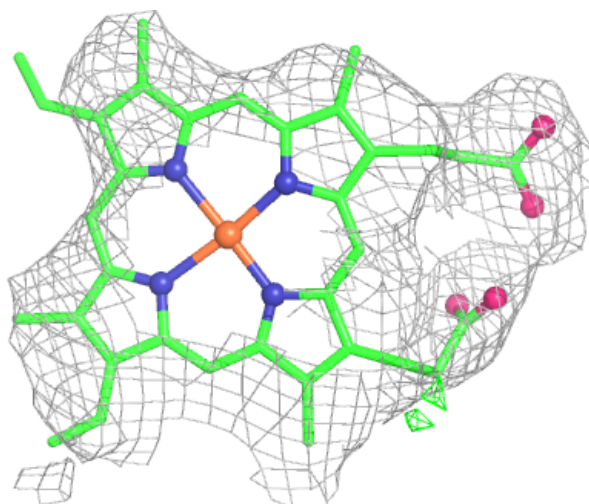
Electron density around CDL C 404:

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



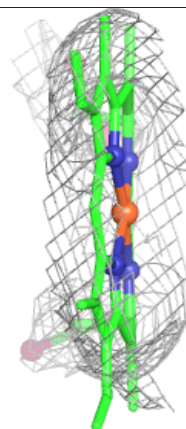
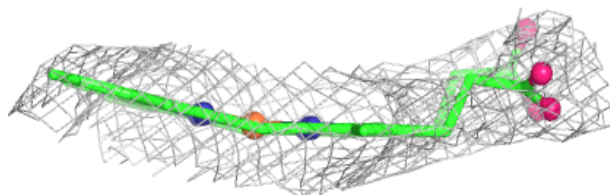
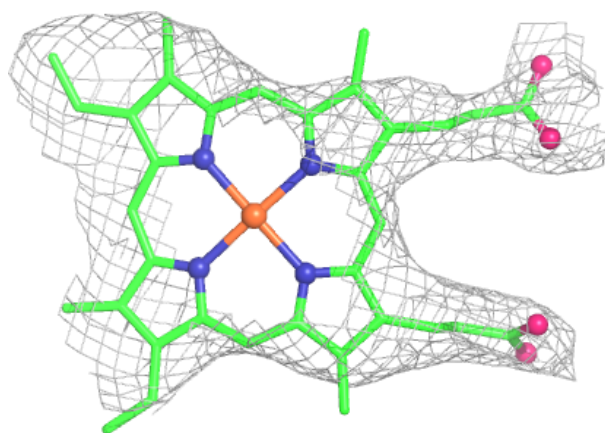
Electron density around HEM C 401:

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



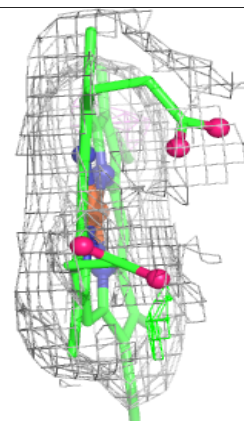
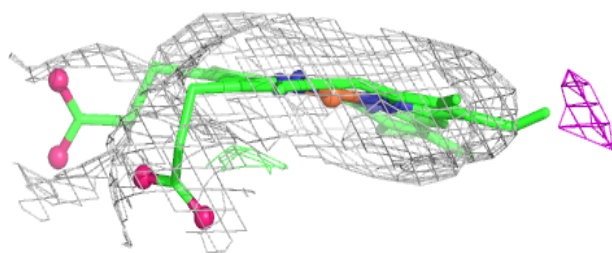
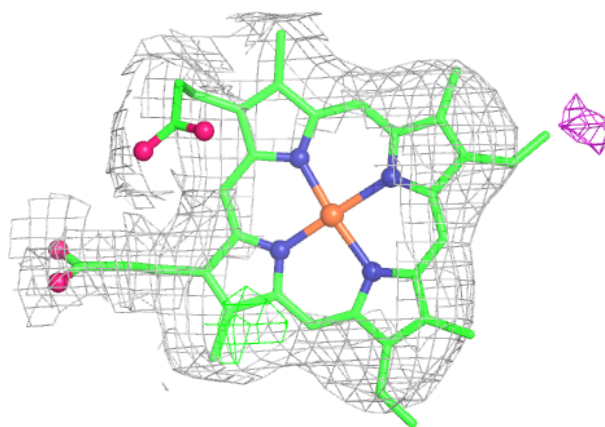
Electron density around HEC D 501:

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



Electron density around HEM C 402:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.