



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:17 PM EDT

PDB ID : 6NHG / pdb_00006nhg
Title : Rhodobacter sphaeroides Mitochondrial respiratory chain complex
Authors : Xia, D.; Zhou, F.; Esser, L.
Deposited on : 2018-12-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

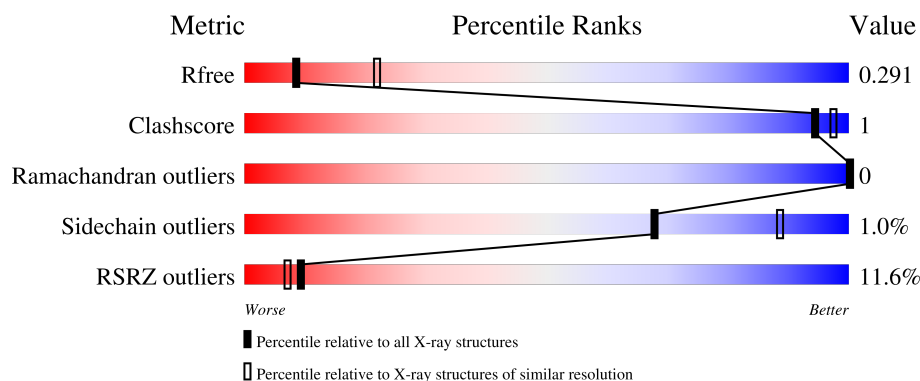
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	3% 97% .
2	B	439	3% 95% ..
3	C	379	4% 94% 6%
4	D	241	10% 95% 5%
5	E	196	62% 96% .

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Mol	Chain	Length	Quality of chain
6	F	110	
7	G	80	
8	H	78	
9	I	78	
10	J	63	
11	K	55	

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	1001	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 33542 atoms, of which 16676 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	446	Total	C	H	N	O	S	0	0	0
			6799	2161	3341	609	668	20			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	0	0
			6328	1998	3147	564	612	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	378	Total	C	H	N	O	S	0	0	0
			6056	2013	3053	471	501	18			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	241	Total	C	H	N	O	S	0	0	0
			3778	1225	1859	330	349	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	H	N	O	S	0	0	0
			3015	957	1497	263	290	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	105	Total	C	H	N	O	S	0	0	0
			1816	576	905	166	167	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0	0
			1261	410	633	118	99	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0	0
			1075	332	527	99	112	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	34	Total	C	H	N	O	S	0	0	0
			509	149	265	51	43	1			

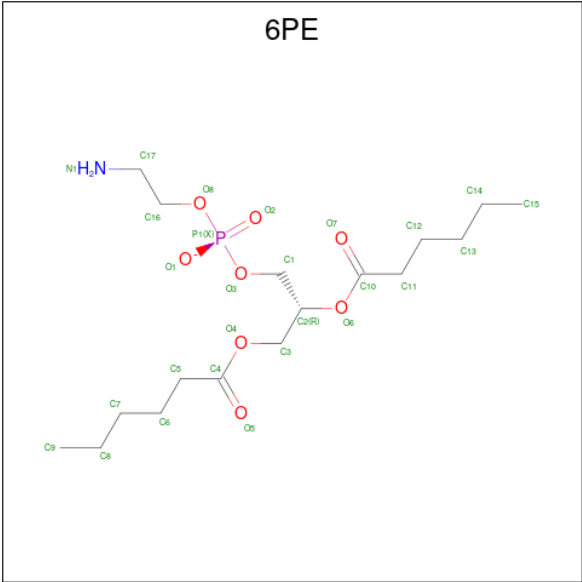
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	J	61	Total	C	H	N	O		0	0	0
			1004	329	502	87	86				

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

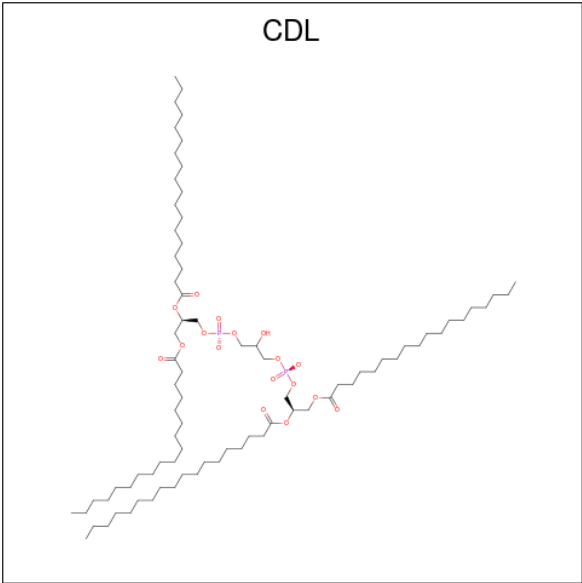
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	K	52	Total	C	H	N	O		0	0	0
			865	288	435	77	65				

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: 6PE) (formula: C₁₇H₃₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
12	A	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0
12	K	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



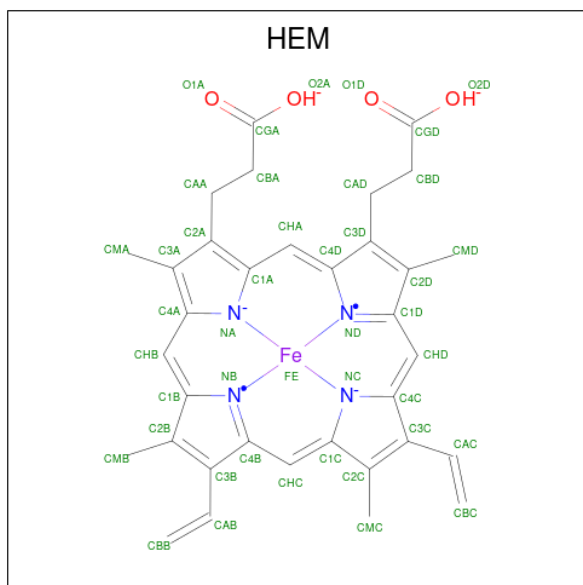
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	O	P	0	0
			124	41	64	17	2		
13	D	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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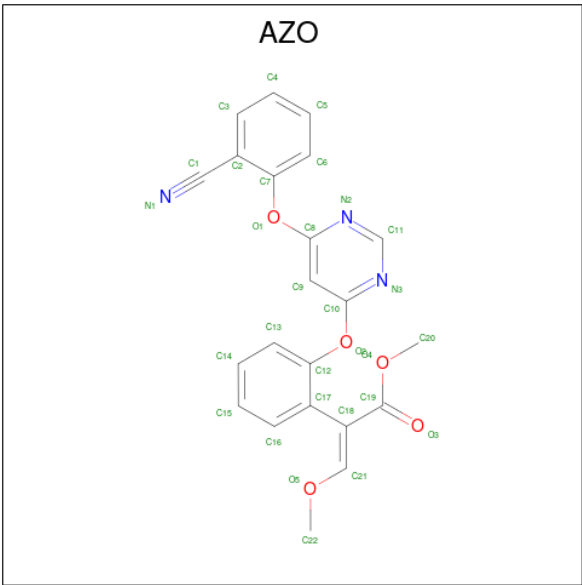
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	G	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



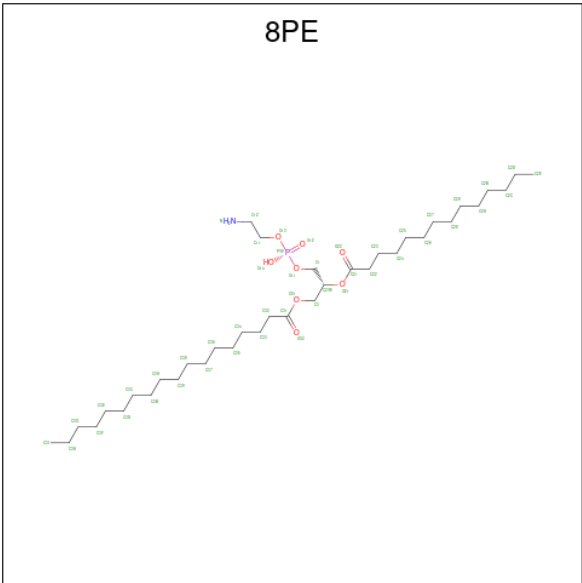
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
14	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 15 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (CCD ID: AZO) (formula: $C_{22}H_{17}N_3O_5$).



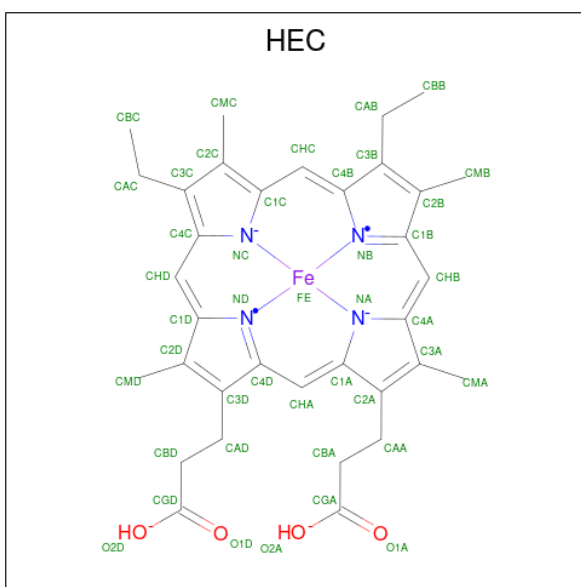
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	H	N	O	0	0
			47	22	17	3	5		

- Molecule 16 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



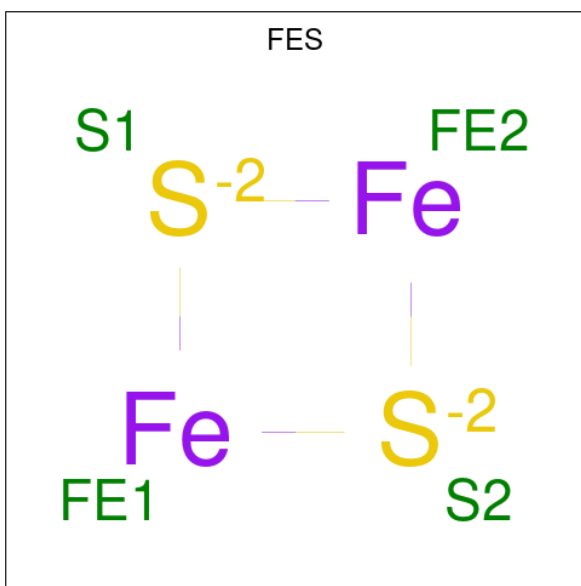
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	0	0
			120	37	73	1	8		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



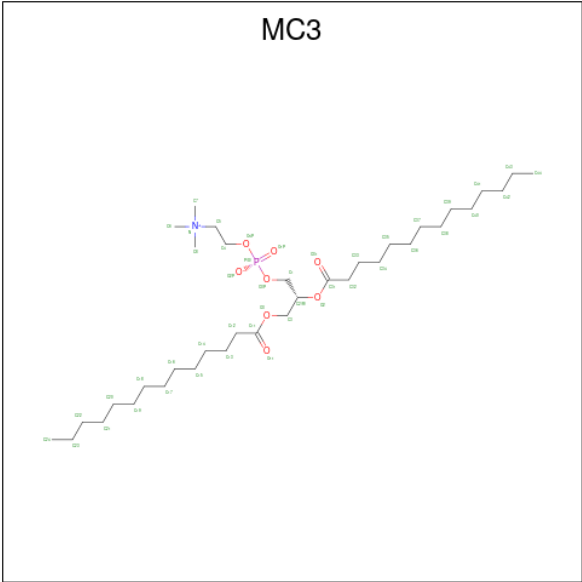
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 19 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: $C_{36}H_{72}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
19	J	1	Total	C	H	N	O	P	0	0
			118	36	72	1	8	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	O	0	0
			1	1		
20	B	23	Total	O	0	0
			23	23		
20	C	1	Total	O	0	0
			1	1		
20	F	6	Total	O	0	0
			6	6		
20	G	2	Total	O	0	0
			2	2		
20	I	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.

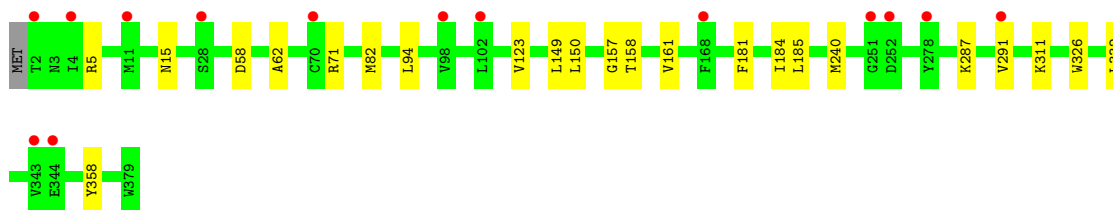
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



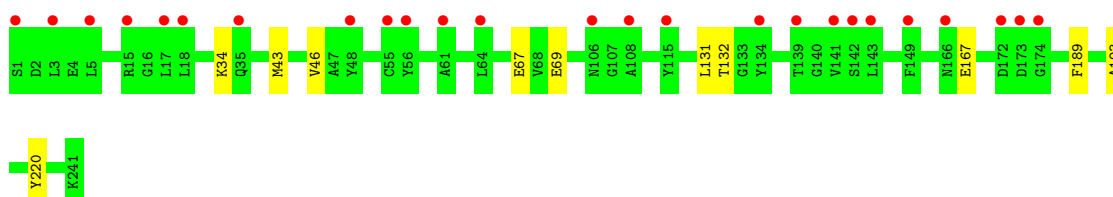
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



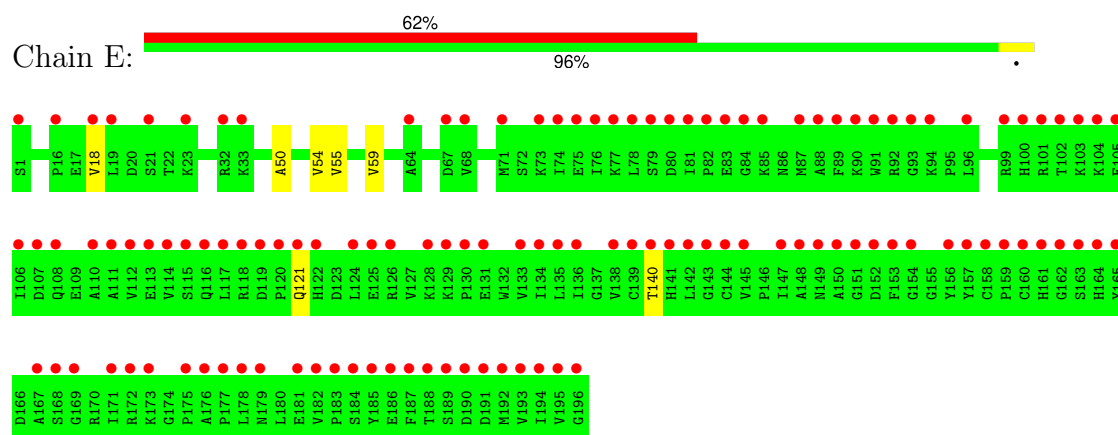
- Molecule 3: Cytochrome b



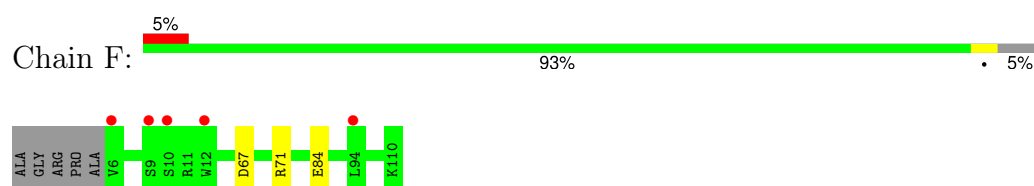
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



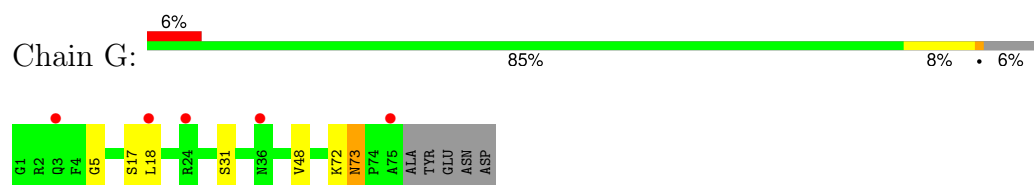
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



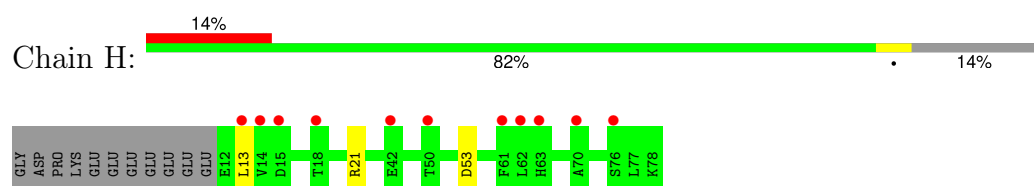
- Molecule 6: Cytochrome b-c1 complex subunit 7



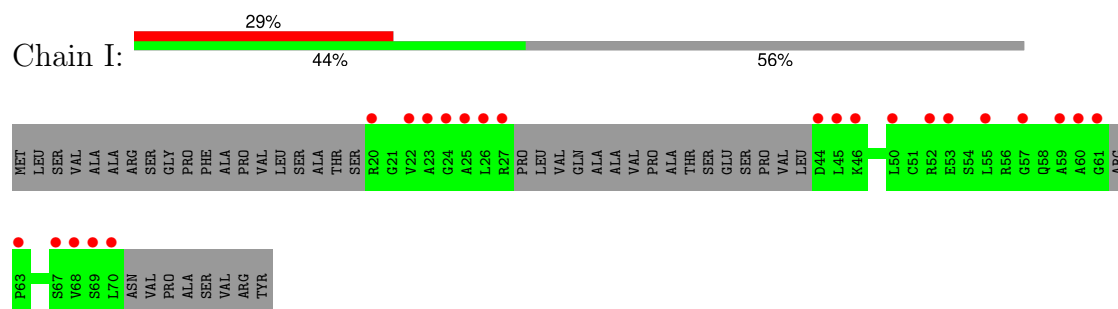
- Molecule 7: Cytochrome b-c1 complex subunit 8



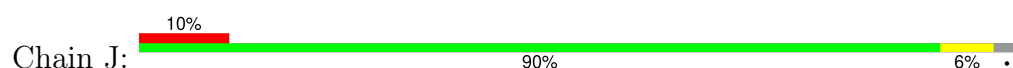
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

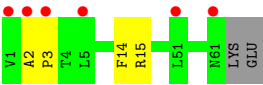


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

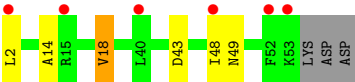
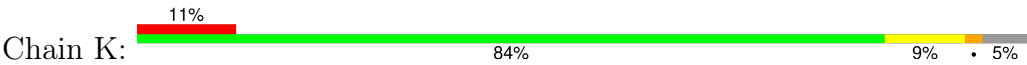


- Molecule 10: Cytochrome b-c1 complex subunit 9





● Molecule 11: Cytochrome b-c1 complex subunit 10



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.18Å 154.18Å 598.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80 29.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.87-2.80) 84.5 (29.87-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.289 0.255 , 0.291	Depositor DCC
R_{free} test set	1999 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	33542	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: HEM, AZO, MC3, 8PE, FES, 6PE, HEC, CDL

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	0.14	0/3531	0.30	0/4792
2	B	0.15	0/3241	0.32	0/4398
3	C	0.14	0/3100	0.31	0/4242
4	D	0.19	0/1978	0.43	0/2684
5	E	0.13	0/1552	0.25	0/2100
6	F	0.14	0/930	0.28	0/1246
7	G	0.17	0/649	0.35	0/878
8	H	0.16	0/553	0.29	0/741
9	I	0.20	0/242	0.38	0/319
10	J	0.14	0/515	0.27	0/696
11	K	0.17	0/446	0.29	0/611
All	All	0.15	0/16737	0.32	0/22707

There are no bond length outliers.

There are no bond angle outliers.

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	3458	3341	3356	7	0
2	B	3181	3147	3160	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3003	3053	3065	12	0
4	D	1919	1859	1868	9	0
5	E	1518	1497	1503	3	0
6	F	911	905	906	2	0
7	G	628	633	636	4	0
8	H	548	527	530	3	0
9	I	244	265	265	0	0
10	J	502	502	505	3	0
11	K	430	435	435	3	0
12	A	27	33	33	1	0
12	K	27	33	33	0	0
13	A	60	64	64	0	0
13	D	60	64	64	1	0
13	G	60	64	64	0	0
14	C	86	60	60	1	0
15	C	30	17	17	0	0
16	C	47	73	73	0	0
17	D	43	32	30	2	0
18	E	4	0	0	0	0
19	J	46	72	72	1	0
20	A	1	0	0	0	0
20	B	23	0	0	0	0
20	C	1	0	0	0	0
20	F	6	0	0	0	0
20	G	2	0	0	0	0
20	I	1	0	0	0	0
All	All	16866	16676	16739	45	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 (45) 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)
3:C:287:LYS:NZ	5:E:140:THR:O	2.25	0.66
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.38	0.59
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.35	0.58
10:J:14:PHE:O	19:J:101:MC3:H71	2.04	0.58
4:D:131:LEU:HD11	17:D:1001:HEC:HMB2	1.88	0.56
17:D:1001:HEC:HBC3	17:D:1001:HEC:HMC1	1.89	0.55
7:G:73:ASN:N	7:G:73:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LEU:HB2	3:C:161:VAL:HG22	1.88	0.54
1:A:412:SER:O	10:J:15:ARG:NH2	2.40	0.53
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.42	0.53
10:J:2:ALA:HB1	10:J:3:PRO:HD2	1.91	0.52
11:K:43:ASP:O	11:K:49:ASN:ND2	2.43	0.51
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.93	0.51
6:F:67:ASP:OD2	6:F:71:ARG:NH2	2.45	0.49
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.96	0.47
1:A:221:GLY:O	1:A:222:THR:OG1	2.25	0.47
1:A:429:GLU:OE1	7:G:5:GLY:N	2.44	0.47
7:G:72:LYS:NZ	8:H:53:ASP:O	2.46	0.47
5:E:50:ALA:O	5:E:54:VAL:HG23	2.15	0.47
3:C:58:ASP:O	3:C:62:ALA:N	2.46	0.47
1:A:271:GLN:HB3	1:A:361:LEU:HD11	1.96	0.46
2:B:47:ILE:HD13	2:B:120:MET:CE	2.44	0.46
3:C:157:GLY:O	3:C:161:VAL:HG23	2.15	0.46
11:K:14:ALA:O	11:K:18:VAL:HG23	2.16	0.46
4:D:132:THR:O	8:H:21:ARG:NH2	2.48	0.46
11:K:48:ILE:O	11:K:48:ILE:HG22	2.15	0.46
14:C:1002:HEM:HBC2	14:C:1002:HEM:HMC2	1.98	0.46
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.50	0.46
6:F:84:GLU:OE1	6:F:84:GLU:N	2.49	0.45
3:C:94:LEU:HD11	3:C:123:VAL:HG11	1.99	0.45
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.32	0.44
3:C:181:PHE:HA	3:C:184:ILE:HG22	2.00	0.44
3:C:149:LEU:HB3	3:C:291:VAL:HG22	2.01	0.43
3:C:5:ARG:NH1	3:C:15:ASN:OD1	2.47	0.43
2:B:33:LEU:HD23	2:B:220:ALA:HB1	2.00	0.43
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.00	0.43
4:D:167:GLU:HG3	8:H:13:LEU:HD12	2.01	0.42
2:B:109:VAL:HG22	2:B:119:LEU:HD23	2.02	0.41
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.56	0.41
3:C:82:MET:HE2	3:C:240:MET:HE1	2.03	0.41
4:D:220:TYR:OH	13:D:1002:CDL:OA4	2.36	0.41
3:C:71:ARG:NH2	4:D:193:ALA:O	2.50	0.41
1:A:87:ASN:OD1	1:A:88:ALA:N	2.48	0.40
5:E:55:VAL:O	5:E:59:VAL:HG23	2.21	0.40
1:A:442:PHE:O	12:A:501:6PE:N1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	434 (98%)	10 (2%)	0	100	100
2	B	423/439 (96%)	413 (98%)	10 (2%)	0	100	100
3	C	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
6	F	103/110 (94%)	103 (100%)	0	0	100	100
7	G	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
8	H	65/78 (83%)	64 (98%)	1 (2%)	0	100	100
9	I	28/78 (36%)	25 (89%)	3 (11%)	0	100	100
10	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
11	K	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
All	All	2054/2165 (95%)	2000 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	370/370 (100%)	367 (99%)	3 (1%)	73	90
2	B	332/343 (97%)	330 (99%)	2 (1%)	78	92
3	C	326/327 (100%)	323 (99%)	3 (1%)	70	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	205 (100%)	1 (0%)	81	93
5	E	168/168 (100%)	166 (99%)	2 (1%)	63	87
6	F	96/98 (98%)	96 (100%)	0	100	100
7	G	66/70 (94%)	62 (94%)	4 (6%)	17	46
8	H	64/74 (86%)	64 (100%)	0	100	100
9	I	25/60 (42%)	25 (100%)	0	100	100
10	J	51/53 (96%)	51 (100%)	0	100	100
11	K	42/45 (93%)	40 (95%)	2 (5%)	23	56
All	All	1746/1814 (96%)	1729 (99%)	17 (1%)	68	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	LEU
1	A	245	GLU
1	A	325	VAL
2	B	109	VAL
2	B	258	VAL
3	C	158	THR
3	C	185	LEU
3	C	311	LYS
4	D	69	GLU
5	E	18	VAL
5	E	121	GLN
7	G	17	SER
7	G	18	LEU
7	G	31	SER
7	G	73	ASN
11	K	2	LEU
11	K	18	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	15	GLN
1	A	94	HIS
1	A	118	GLN

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Mol	Chain	Res	Type
1	A	240	GLN
1	A	328	HIS
2	B	104	ASN
2	B	125	ASN
2	B	277	HIS
2	B	343	GLN
3	C	68	HIS
7	G	64	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
16	8PE	C	1004	-	46,46,46	1.67	6 (13%)	49,51,51	1.09	4 (8%)
13	CDL	G	101	-	59,59,99	1.30	6 (10%)	65,71,111	1.02	4 (6%)
13	CDL	A	502	-	59,59,99	1.28	8 (13%)	65,71,111	1.10	4 (6%)
12	6PE	A	501	-	26,26,26	1.76	8 (30%)	29,31,31	1.12	3 (10%)
17	HEC	D	1001	4	50,50,50	1.84	8 (16%)	68,82,82	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEM	C	1001	3	50,50,50	1.46	10 (20%)	67,82,82	1.11	4 (5%)
15	AZO	C	1003	-	32,32,32	0.67	0	42,42,42	1.63	9 (21%)
14	HEM	C	1002	3	50,50,50	1.48	10 (20%)	67,82,82	1.10	5 (7%)
12	6PE	K	101	-	26,26,26	1.79	8 (30%)	29,31,31	1.15	2 (6%)
19	MC3	J	101	-	45,45,45	1.41	5 (11%)	51,53,53	0.99	5 (9%)
18	FES	E	1001	5	0,4,4	-	-	-	-	-
13	CDL	D	1002	-	59,59,99	1.28	6 (10%)	65,71,111	1.20	6 (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
16	8PE	C	1004	-	-	21/50/50/50	-
13	CDL	G	101	-	-	16/70/70/110	-
13	CDL	A	502	-	-	24/70/70/110	-
12	6PE	A	501	-	-	13/30/30/30	-
17	HEC	D	1001	4	1/1/7/7	6/14/54/54	-
14	HEM	C	1001	3	-	4/14/54/54	-
15	AZO	C	1003	-	-	2/23/23/23	0/3/3/3
14	HEM	C	1002	3	-	3/14/54/54	-
12	6PE	K	101	-	-	11/30/30/30	-
19	MC3	J	101	-	-	24/49/49/49	-
18	FES	E	1001	5	-	-	0/1/1/1
13	CDL	D	1002	-	-	32/70/70/110	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	1001	HEC	C3D-C2D	7.87	1.53	1.36
19	J	101	MC3	P-O4P	5.01	1.79	1.59
16	C	1004	8PE	P-O11	4.94	1.78	1.59
17	D	1001	HEC	FE-ND	4.64	2.09	1.94
14	C	1002	HEM	FE-NB	4.26	2.08	1.94
12	K	101	6PE	P1-O3	4.20	1.75	1.59
13	G	101	CDL	OA8-CA7	4.14	1.45	1.33
13	D	1002	CDL	OA6-CA5	4.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	101	CDL	OA6-CA5	4.03	1.45	1.34
13	A	502	CDL	OA6-CA5	4.02	1.45	1.34
13	D	1002	CDL	OA8-CA7	4.01	1.45	1.33
13	A	502	CDL	OA8-CA7	3.98	1.44	1.33
17	D	1001	HEC	FE-NA	3.73	2.07	1.95
12	A	501	6PE	P1-O8	3.71	1.73	1.59
17	D	1001	HEC	FE-NB	3.70	2.06	1.94
14	C	1002	HEM	FE-NC	3.68	2.07	1.95
12	A	501	6PE	P1-O3	3.66	1.73	1.59
14	C	1001	HEM	FE-NC	3.63	2.07	1.95
13	G	101	CDL	OB8-CB7	3.57	1.43	1.33
14	C	1001	HEM	FE-NB	3.49	2.05	1.94
13	D	1002	CDL	OB8-CB7	3.48	1.43	1.33
13	A	502	CDL	OB8-CB7	3.47	1.43	1.33
12	K	101	6PE	P1-O8	3.44	1.72	1.59
16	C	1004	8PE	P-O13	3.42	1.72	1.59
16	C	1004	8PE	C3-C2	3.37	1.61	1.50
17	D	1001	HEC	FE-NC	3.37	2.06	1.95
14	C	1001	HEM	FE-ND	3.37	2.05	1.94
14	C	1002	HEM	FE-NA	3.31	2.06	1.95
12	A	501	6PE	C3-C2	3.26	1.61	1.50
13	D	1002	CDL	OB6-CB5	3.23	1.43	1.34
13	G	101	CDL	OB6-CB5	3.23	1.43	1.34
16	C	1004	8PE	C1-C2	3.18	1.60	1.50
12	K	101	6PE	C3-C2	3.13	1.60	1.50
13	A	502	CDL	OB6-CB5	3.11	1.43	1.34
14	C	1001	HEM	CAB-C3B	3.06	1.55	1.47
14	C	1002	HEM	CAB-C3B	3.04	1.55	1.47
14	C	1001	HEM	FE-NA	3.02	2.05	1.95
14	C	1001	HEM	CAC-C3C	2.94	1.55	1.47
14	C	1002	HEM	CAC-C3C	2.90	1.55	1.47
19	J	101	MC3	C1-C2	2.69	1.59	1.50
16	C	1004	8PE	C32-C31	2.54	1.58	1.50
12	A	501	6PE	C5-C4	2.47	1.57	1.50
12	K	101	6PE	O4-C4	2.47	1.40	1.33
16	C	1004	8PE	C33-C32	2.43	1.61	1.52
12	K	101	6PE	C5-C4	2.43	1.57	1.50
13	A	502	CDL	OA6-CA4	-2.42	1.40	1.46
13	G	101	CDL	OA6-CA4	-2.41	1.40	1.46
12	A	501	6PE	O4-C4	2.38	1.40	1.33
12	K	101	6PE	C11-C10	2.36	1.57	1.50
19	J	101	MC3	P-O3P	2.36	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	101	6PE	O6-C10	2.33	1.40	1.34
17	D	1001	HEC	CMC-C2C	2.32	1.55	1.50
14	C	1002	HEM	FE-ND	2.30	2.02	1.94
12	K	101	6PE	C1-C2	2.27	1.57	1.50
12	A	501	6PE	C11-C10	2.24	1.57	1.50
14	C	1002	HEM	CMB-C2B	2.22	1.55	1.50
14	C	1001	HEM	CMC-C2C	2.21	1.55	1.50
12	A	501	6PE	C1-C2	2.15	1.57	1.50
12	A	501	6PE	O6-C10	2.15	1.40	1.34
13	D	1002	CDL	C11-CA5	2.14	1.56	1.50
14	C	1001	HEM	CMB-C2B	2.12	1.55	1.50
14	C	1002	HEM	CMC-C2C	2.09	1.55	1.50
14	C	1001	HEM	CMD-C2D	2.09	1.55	1.50
13	A	502	CDL	OB6-CB4	-2.08	1.41	1.46
14	C	1002	HEM	CMA-C3A	2.07	1.55	1.50
13	A	502	CDL	C11-CA5	2.06	1.56	1.50
19	J	101	MC3	O4P-C4	-2.04	1.36	1.44
14	C	1001	HEM	CMA-C3A	2.04	1.55	1.50
17	D	1001	HEC	CMB-C2B	2.04	1.55	1.50
13	G	101	CDL	C11-CA5	2.04	1.56	1.50
13	A	502	CDL	C31-CA7	2.03	1.56	1.50
17	D	1001	HEC	CMA-C3A	2.02	1.54	1.50
14	C	1002	HEM	CMD-C2D	2.02	1.54	1.50
19	J	101	MC3	C5-C4	2.01	1.57	1.51
13	D	1002	CDL	C31-CA7	2.01	1.56	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	1003	AZO	C11-N3-C10	5.73	118.86	114.50
17	D	1001	HEC	C1D-ND-C4D	5.72	111.98	105.21
13	D	1002	CDL	OA6-CA5-C11	4.55	121.32	111.48
13	A	502	CDL	OB6-CB5-C51	4.13	120.42	111.48
13	G	101	CDL	OB6-CB5-C51	3.88	119.87	111.48
16	C	1004	8PE	O21-C21-C22	3.81	119.72	111.48
13	D	1002	CDL	OB6-CB5-C51	3.64	119.36	111.48
13	A	502	CDL	OA6-CA5-C11	3.49	119.03	111.48
19	J	101	MC3	O2P-P-O1P	3.44	128.46	112.44
12	K	101	6PE	O6-C10-C11	3.31	118.65	111.48
13	G	101	CDL	OA6-CA5-C11	3.29	118.59	111.48
15	C	1003	AZO	C11-N2-C8	3.28	117.00	114.50
16	C	1004	8PE	O31-C31-C32	3.16	121.48	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	1003	AZO	C9-C10-N3	-3.15	120.01	124.47
15	C	1003	AZO	C20-O4-C19	3.07	121.53	115.85
16	C	1004	8PE	O31-C31-O32	-2.76	116.71	123.63
13	D	1002	CDL	OA8-CA7-C31	2.75	120.21	111.83
15	C	1003	AZO	N2-C11-N3	-2.74	124.43	128.58
13	A	502	CDL	OA8-CA7-C31	2.64	119.89	111.83
13	D	1002	CDL	OB8-CB7-C71	2.61	119.80	111.83
14	C	1002	HEM	C4D-ND-C1D	2.59	108.27	105.21
12	A	501	6PE	O6-C10-C11	2.56	117.02	111.48
14	C	1002	HEM	CBD-CAD-C3D	-2.52	105.57	112.53
13	A	502	CDL	OB8-CB7-C71	2.49	119.43	111.83
14	C	1001	HEM	C4D-ND-C1D	2.49	108.15	105.21
13	G	101	CDL	OB8-CB7-C71	2.48	119.41	111.83
13	G	101	CDL	OA8-CA7-C31	2.42	119.21	111.83
15	C	1003	AZO	C21-C18-C19	2.39	121.44	117.16
14	C	1001	HEM	C1B-NB-C4B	2.37	108.02	105.21
15	C	1003	AZO	C7-C2-C1	2.37	121.91	119.60
17	D	1001	HEC	C4B-NB-C1B	2.36	108.01	105.21
12	A	501	6PE	O4-C3-C2	2.35	115.18	108.40
17	D	1001	HEC	C2A-C1A-NA	-2.34	108.06	110.32
14	C	1001	HEM	C2A-C1A-NA	-2.34	107.56	110.15
12	K	101	6PE	O4-C3-C2	2.29	114.98	108.40
19	J	101	MC3	O2-C31-O31	-2.26	118.41	123.70
14	C	1001	HEM	C3D-C4D-ND	-2.25	107.71	110.17
14	C	1002	HEM	C3D-C4D-ND	-2.25	107.71	110.17
15	C	1003	AZO	O2-C10-N3	2.24	123.95	118.47
16	C	1004	8PE	O31-C3-C2	2.22	114.78	108.40
19	J	101	MC3	O3-C11-O11	-2.17	118.20	123.63
17	D	1001	HEC	CHA-C4D-ND	2.12	126.70	124.42
14	C	1002	HEM	C2A-C1A-NA	-2.11	107.81	110.15
12	A	501	6PE	O4-C4-C5	2.07	118.16	111.83
14	C	1002	HEM	C1B-NB-C4B	2.07	107.66	105.21
13	D	1002	CDL	OA6-CA4-CA6	2.06	115.73	108.34
19	J	101	MC3	O4P-P-O1P	-2.06	100.79	108.94
19	J	101	MC3	O2-C31-C32	2.05	115.92	111.48
13	D	1002	CDL	OA6-CA5-OA7	-2.02	118.97	123.70
17	D	1001	HEC	C3B-C4B-NB	-2.02	107.96	110.17
15	C	1003	AZO	C10-C9-C8	2.01	116.94	115.20

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
17	D	1001	HEC	NA

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	C1-O3-P1-O8
12	A	501	6PE	C11-C10-O6-C2
12	K	101	6PE	C16-O8-P1-O1
12	K	101	6PE	C16-O8-P1-O2
12	K	101	6PE	C16-O8-P1-O3
12	K	101	6PE	O8-C16-C17-N1
13	A	502	CDL	CB2-OB2-PB2-OB3
13	A	502	CDL	CB2-OB2-PB2-OB5
13	A	502	CDL	C51-CB5-OB6-CB4
13	D	1002	CDL	O1-C1-CA2-OA2
13	D	1002	CDL	CA3-OA5-PA1-OA2
13	D	1002	CDL	CA3-OA5-PA1-OA3
13	D	1002	CDL	OA7-CA5-OA6-CA4
13	D	1002	CDL	CB2-OB2-PB2-OB3
13	D	1002	CDL	CB3-OB5-PB2-OB2
13	D	1002	CDL	CB3-OB5-PB2-OB4
13	G	101	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	CB2-OB2-PB2-OB4
13	G	101	CDL	CB2-OB2-PB2-OB5
16	C	1004	8PE	C1-O11-P-O13
16	C	1004	8PE	C1-O11-P-O14
16	C	1004	8PE	O13-C11-C12-N
17	D	1001	HEC	C2C-C3C-CAC-CBC
19	J	101	MC3	C1-O3P-P-O1P
16	C	1004	8PE	O32-C31-O31-C3
17	D	1001	HEC	C4C-C3C-CAC-CBC
12	K	101	6PE	C5-C4-O4-C3
12	K	101	6PE	O5-C4-O4-C3
13	A	502	CDL	OB7-CB5-OB6-CB4
13	D	1002	CDL	C31-CA7-OA8-CA6
16	C	1004	8PE	C32-C31-O31-C3
13	D	1002	CDL	C11-CA5-OA6-CA4
19	J	101	MC3	C12-C11-O3-C3
13	D	1002	CDL	OB9-CB7-OB8-CB6
12	A	501	6PE	O7-C10-O6-C2

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Mol	Chain	Res	Type	Atoms
13	A	502	CDL	O1-C1-CB2-OB2
13	D	1002	CDL	O1-C1-CB2-OB2
13	D	1002	CDL	C71-CB7-OB8-CB6
13	D	1002	CDL	OA9-CA7-OA8-CA6
19	J	101	MC3	O11-C11-O3-C3
13	A	502	CDL	CA2-C1-CB2-OB2
13	D	1002	CDL	CB2-C1-CA2-OA2
13	A	502	CDL	C31-CA7-OA8-CA6
12	A	501	6PE	C10-C11-C12-C13
13	G	101	CDL	CA7-C31-C32-C33
12	A	501	6PE	O5-C4-O4-C3
13	A	502	CDL	OA9-CA7-OA8-CA6
19	J	101	MC3	C32-C31-O2-C2
13	D	1002	CDL	C51-CB5-OB6-CB4
13	D	1002	CDL	OB7-CB5-OB6-CB4
13	G	101	CDL	O1-C1-CB2-OB2
19	J	101	MC3	C13-C14-C15-C16
13	A	502	CDL	C12-C13-C14-C15
19	J	101	MC3	C32-C33-C34-C35
19	J	101	MC3	C36-C37-C38-C39
12	A	501	6PE	C4-C5-C6-C7
13	A	502	CDL	CB7-C71-C72-C73
16	C	1004	8PE	C3B-C3C-C3D-C3E
13	G	101	CDL	C52-C53-C54-C55
12	K	101	6PE	O7-C10-O6-C2
12	A	501	6PE	C5-C4-O4-C3
16	C	1004	8PE	C38-C39-C3A-C3B
12	K	101	6PE	C11-C10-O6-C2
13	A	502	CDL	C11-CA5-OA6-CA4
16	C	1004	8PE	C22-C21-O21-C2
13	A	502	CDL	OA7-CA5-OA6-CA4
13	D	1002	CDL	C72-C73-C74-C75
16	C	1004	8PE	C2-C3-O31-C31
13	D	1002	CDL	CB5-C51-C52-C53
13	D	1002	CDL	C51-C52-C53-C54
12	A	501	6PE	O6-C2-C3-O4
13	D	1002	CDL	CA2-C1-CB2-OB2
13	G	101	CDL	C12-C13-C14-C15
19	J	101	MC3	C41-C42-C43-C44
16	C	1004	8PE	C26-C27-C28-C29
19	J	101	MC3	C35-C36-C37-C38
19	J	101	MC3	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
17	D	1001	HEC	C2B-C3B-CAB-CBB
13	D	1002	CDL	C31-C32-C33-C34
19	J	101	MC3	C31-C32-C33-C34
13	A	502	CDL	C51-C52-C53-C54
13	D	1002	CDL	C12-C13-C14-C15
16	C	1004	8PE	C3A-C3B-C3C-C3D
16	C	1004	8PE	C35-C36-C37-C38
19	J	101	MC3	C14-C15-C16-C17
13	A	502	CDL	C14-C15-C16-C17
19	J	101	MC3	C37-C38-C39-C40
13	A	502	CDL	OB5-CB3-CB4-CB6
19	J	101	MC3	C34-C35-C36-C37
13	A	502	CDL	C74-C75-C76-C77
16	C	1004	8PE	C3D-C3E-C3F-C3G
19	J	101	MC3	C33-C34-C35-C36
16	C	1004	8PE	C1-C2-C3-O31
19	J	101	MC3	O3P-C1-C2-O2
14	C	1001	HEM	C3D-CAD-CBD-CGD
13	G	101	CDL	C51-CB5-OB6-CB4
19	J	101	MC3	O3P-C1-C2-C3
13	G	101	CDL	C11-C12-C13-C14
16	C	1004	8PE	C25-C26-C27-C28
12	A	501	6PE	C1-C2-C3-O4
13	G	101	CDL	CA3-CA4-CA6-OA8
13	G	101	CDL	C14-C15-C16-C17
13	G	101	CDL	OB7-CB5-OB6-CB4
19	J	101	MC3	O4P-C4-C5-N
16	C	1004	8PE	C24-C25-C26-C27
12	K	101	6PE	C2-C1-O3-P1
13	A	502	CDL	OB5-CB3-CB4-OB6
16	C	1004	8PE	O21-C2-C3-O31
16	C	1004	8PE	C3E-C3F-C3G-C3H
19	J	101	MC3	C38-C39-C40-C41
17	D	1001	HEC	C4B-C3B-CAB-CBB
13	A	502	CDL	CB2-OB2-PB2-OB4
13	D	1002	CDL	CA3-OA5-PA1-OA4
13	D	1002	CDL	CB2-OB2-PB2-OB4
13	D	1002	CDL	CB2-OB2-PB2-OB5
13	D	1002	CDL	CB3-OB5-PB2-OB3
16	C	1004	8PE	C1-O11-P-O12
16	C	1004	8PE	C11-O13-P-O12
19	J	101	MC3	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
19	J	101	MC3	C1-O3P-P-O4P
12	A	501	6PE	C2-C1-O3-P1
13	D	1002	CDL	CA6-CA4-OA6-CA5
13	D	1002	CDL	CB6-CB4-OB6-CB5
19	J	101	MC3	O2-C2-C3-O3
19	J	101	MC3	C1-C2-C3-O3
13	A	502	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	C73-C74-C75-C76
13	D	1002	CDL	OA5-CA3-CA4-OA6
12	K	101	6PE	O6-C2-C3-O4
12	K	101	6PE	C1-C2-C3-O4
13	A	502	CDL	CA3-CA4-CA6-OA8
13	D	1002	CDL	CA3-CA4-CA6-OA8
13	G	101	CDL	OB9-CB7-OB8-CB6
13	A	502	CDL	OA5-CA3-CA4-CA6
17	D	1001	HEC	CAA-CBA-CGA-O2A
15	C	1003	AZO	N1-C1-C2-C7
13	A	502	CDL	C71-C72-C73-C74
13	G	101	CDL	C71-CB7-OB8-CB6
14	C	1002	HEM	CAA-CBA-CGA-O1A
17	D	1001	HEC	CAA-CBA-CGA-O1A
12	A	501	6PE	O3-C1-C2-C3
15	C	1003	AZO	C12-C17-C18-C21
13	A	502	CDL	C52-C51-CB5-OB6
13	D	1002	CDL	C14-C15-C16-C17
14	C	1001	HEM	CAD-CBD-CGD-O1D
14	C	1002	HEM	CAA-CBA-CGA-O2A
16	C	1004	8PE	C29-C2A-C2B-C2C
14	C	1001	HEM	CAA-CBA-CGA-O2A
12	A	501	6PE	O7-C10-C11-C12
13	G	101	CDL	OA7-CA5-OA6-CA4
19	J	101	MC3	O2-C31-C32-C33
13	A	502	CDL	C52-C51-CB5-OB7
14	C	1002	HEM	CAD-CBD-CGD-O2D
13	D	1002	CDL	C52-C51-CB5-OB6
14	C	1001	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

5 monomers are involved in 6 short contacts:

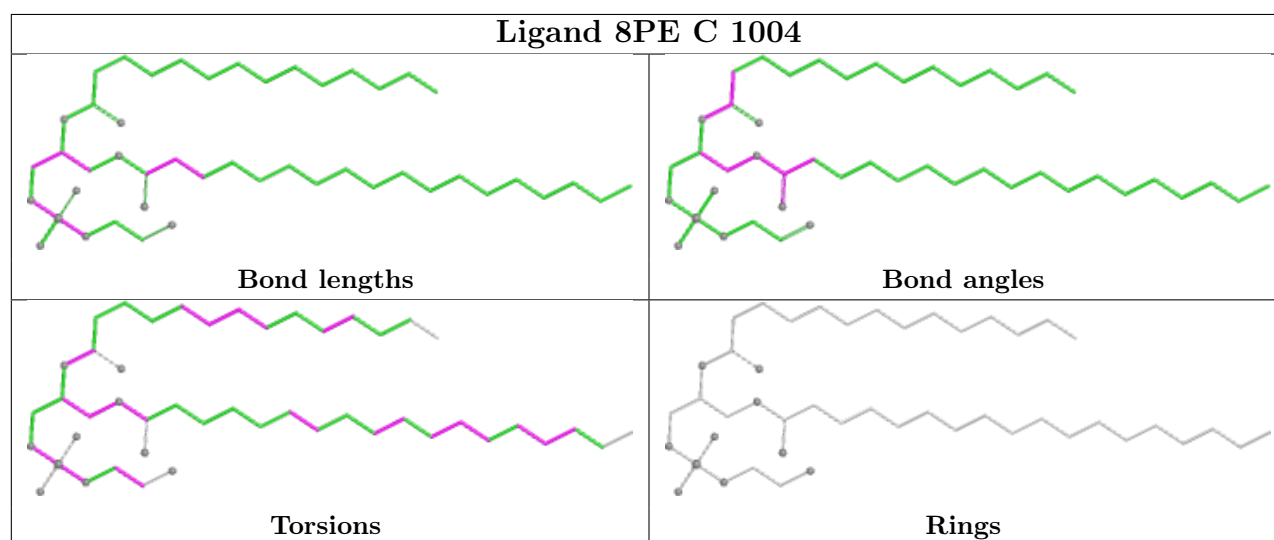
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	501	6PE	1	0

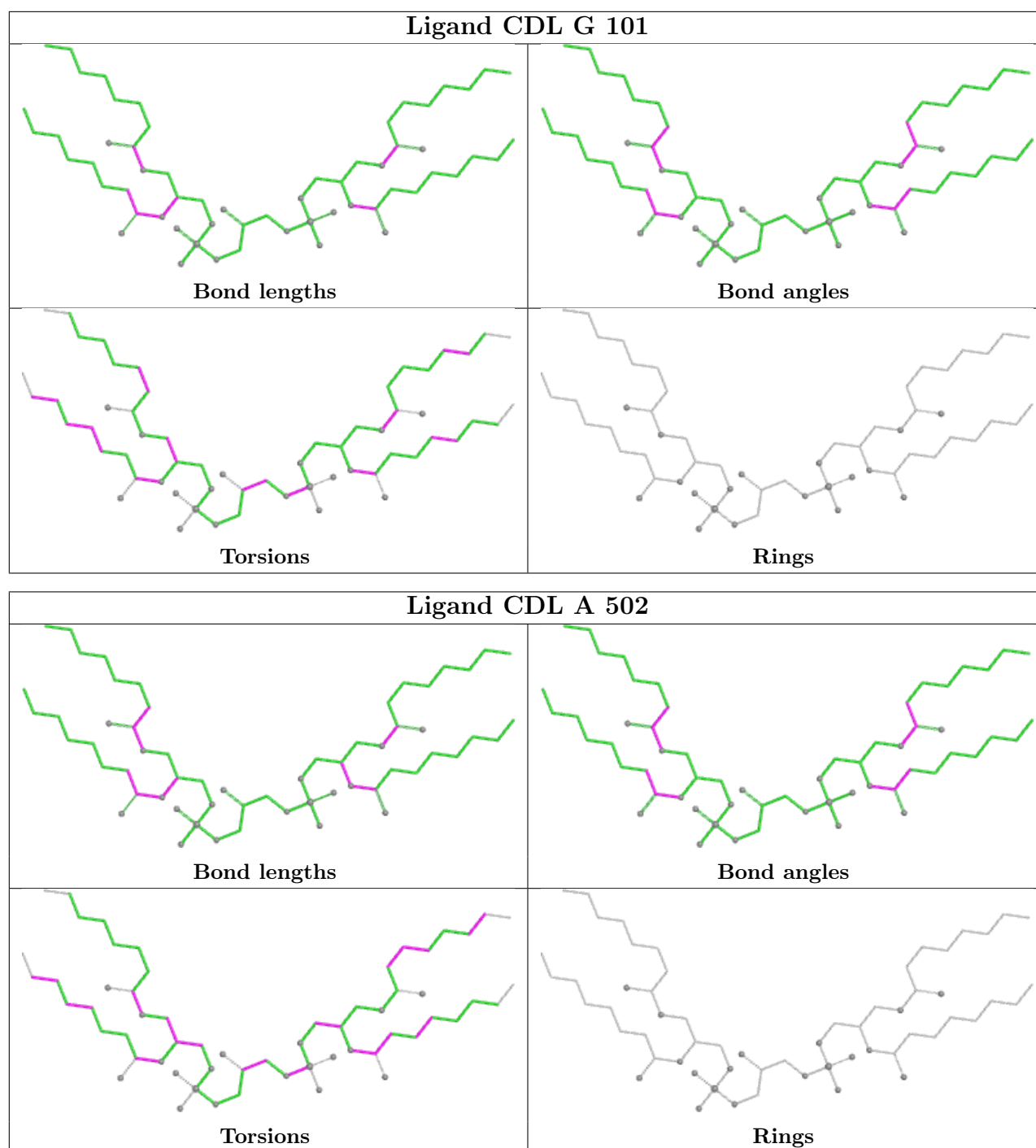
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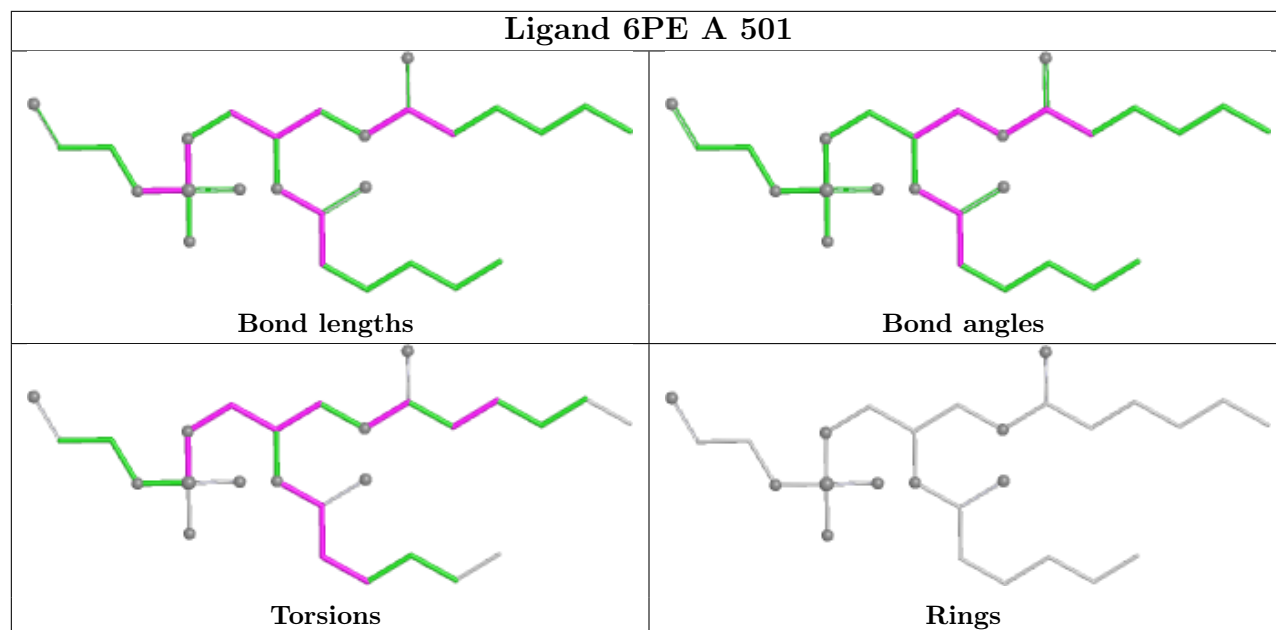
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	1001	HEC	2	0
14	C	1002	HEM	1	0
19	J	101	MC3	1	0
13	D	1002	CDL	1	0

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.

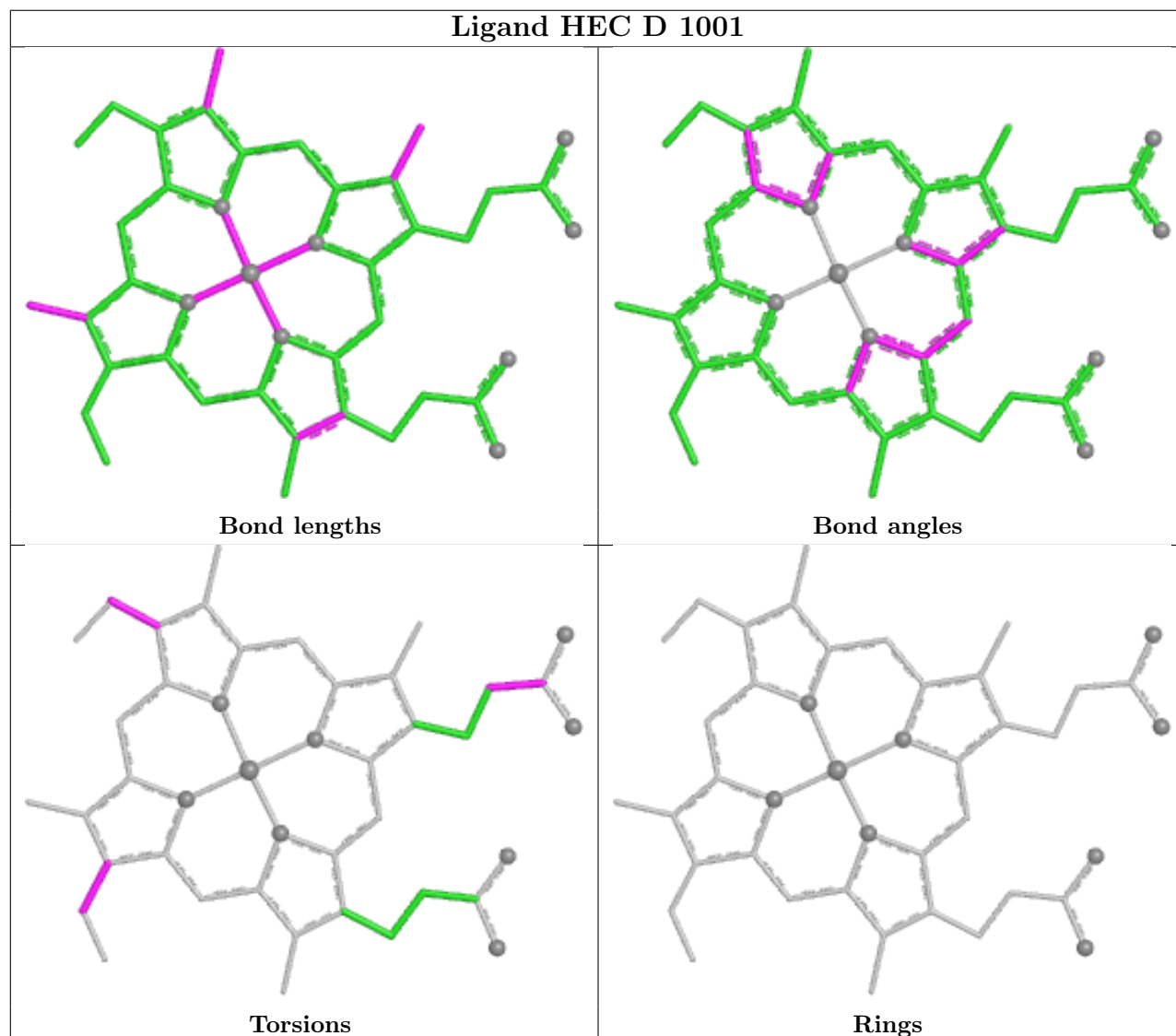




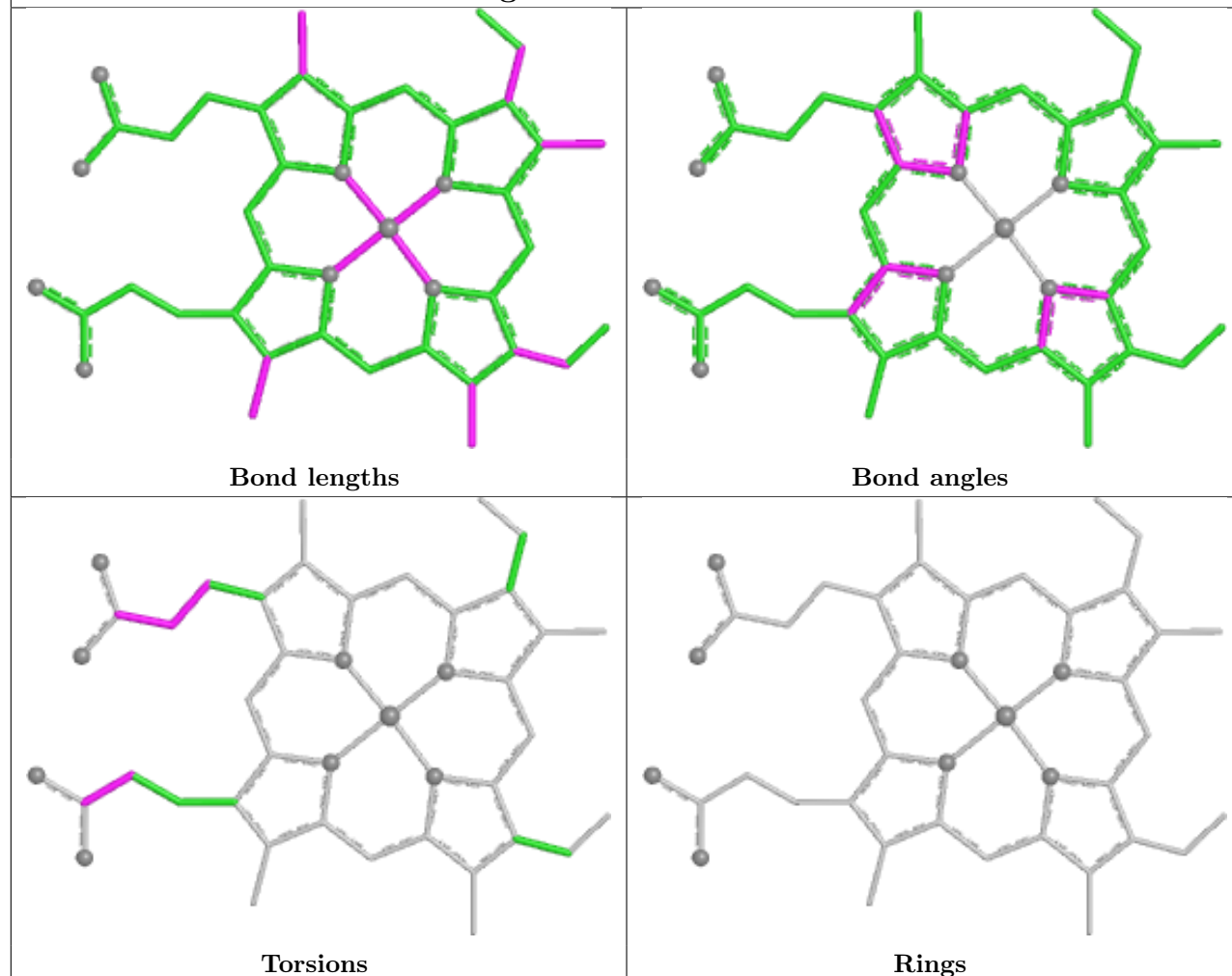
Ligand 6PE A 501



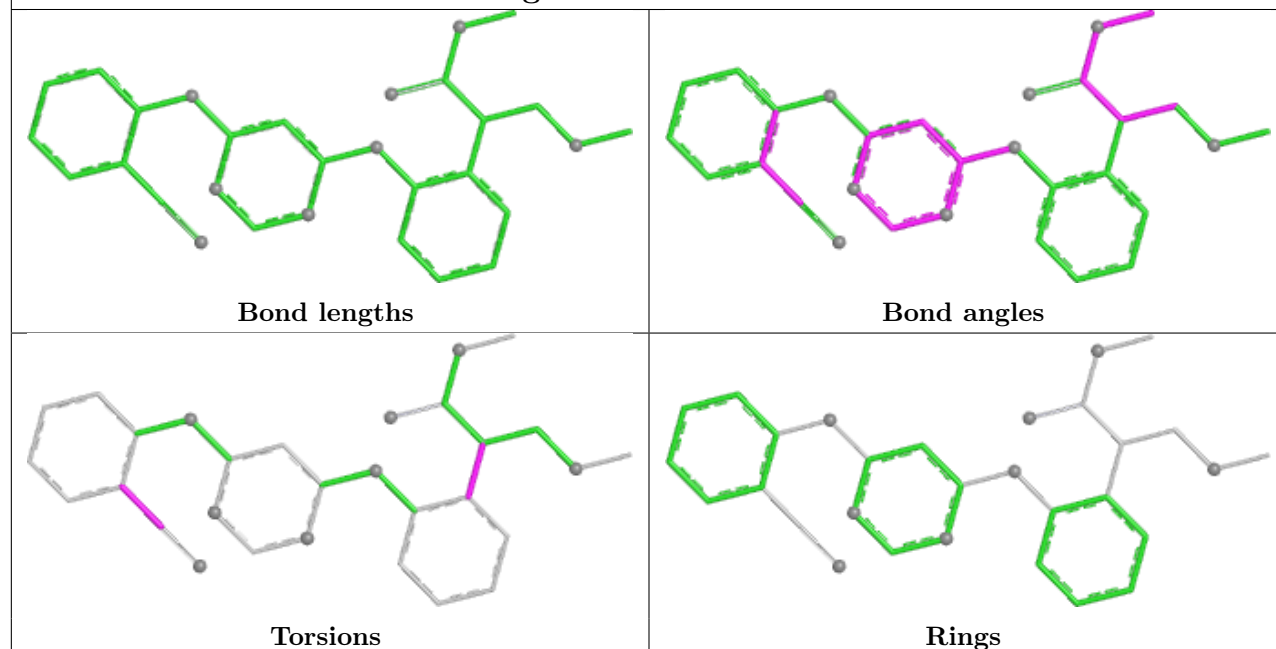
Ligand HEC D 1001



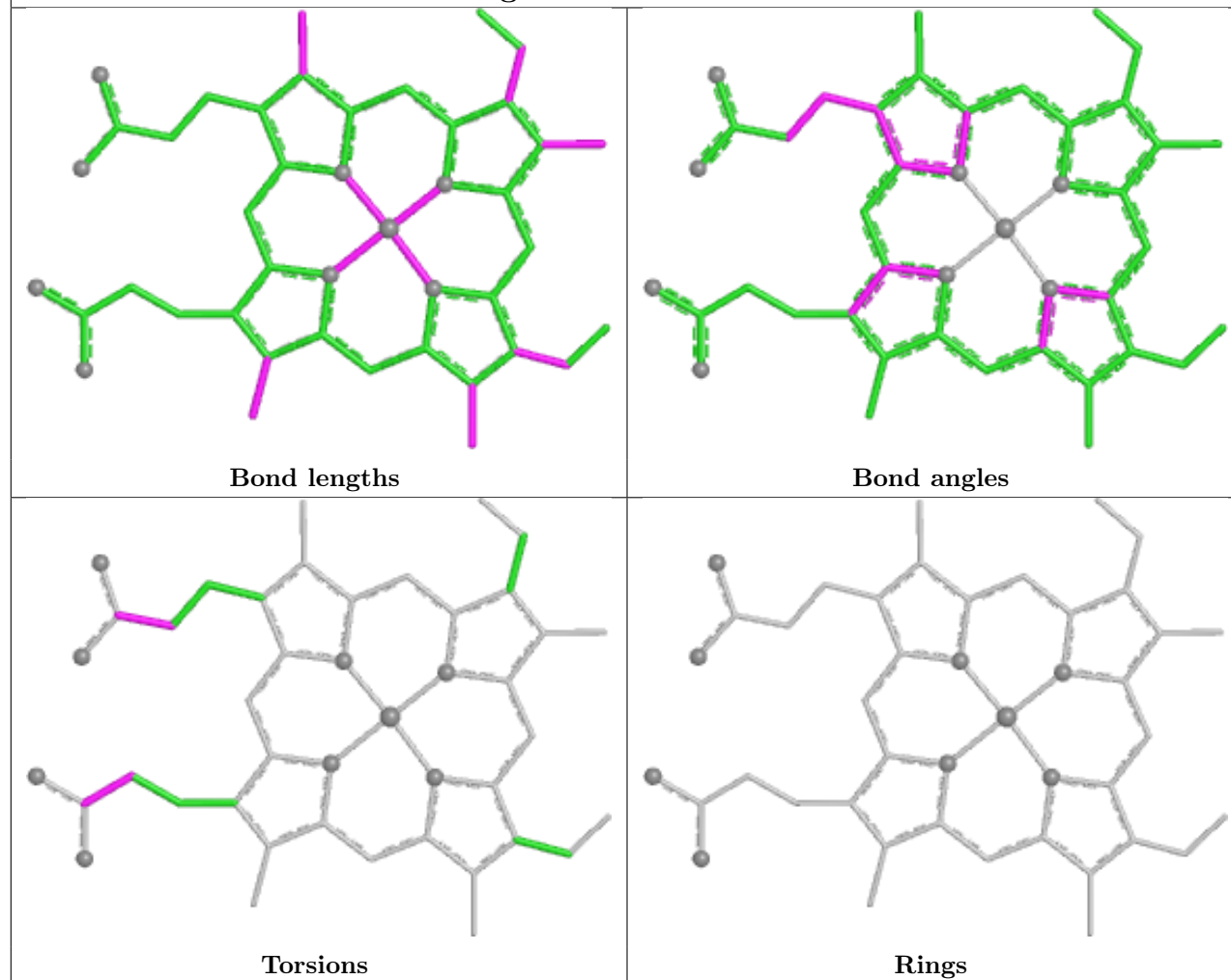
Ligand HEM C 1001



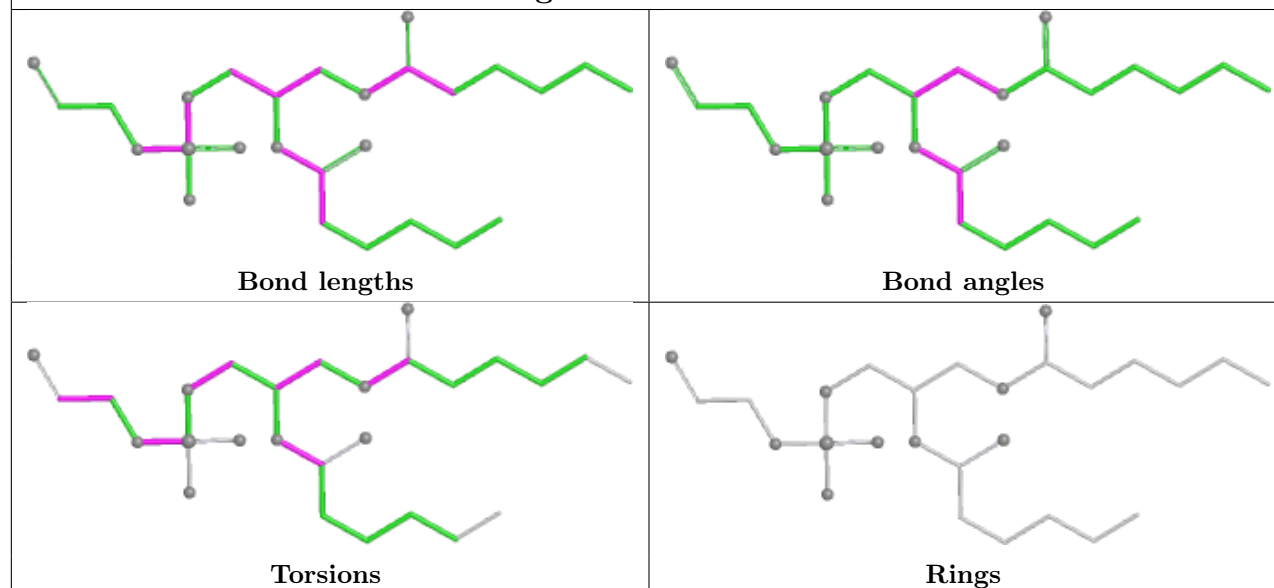
Ligand AZO C 1003



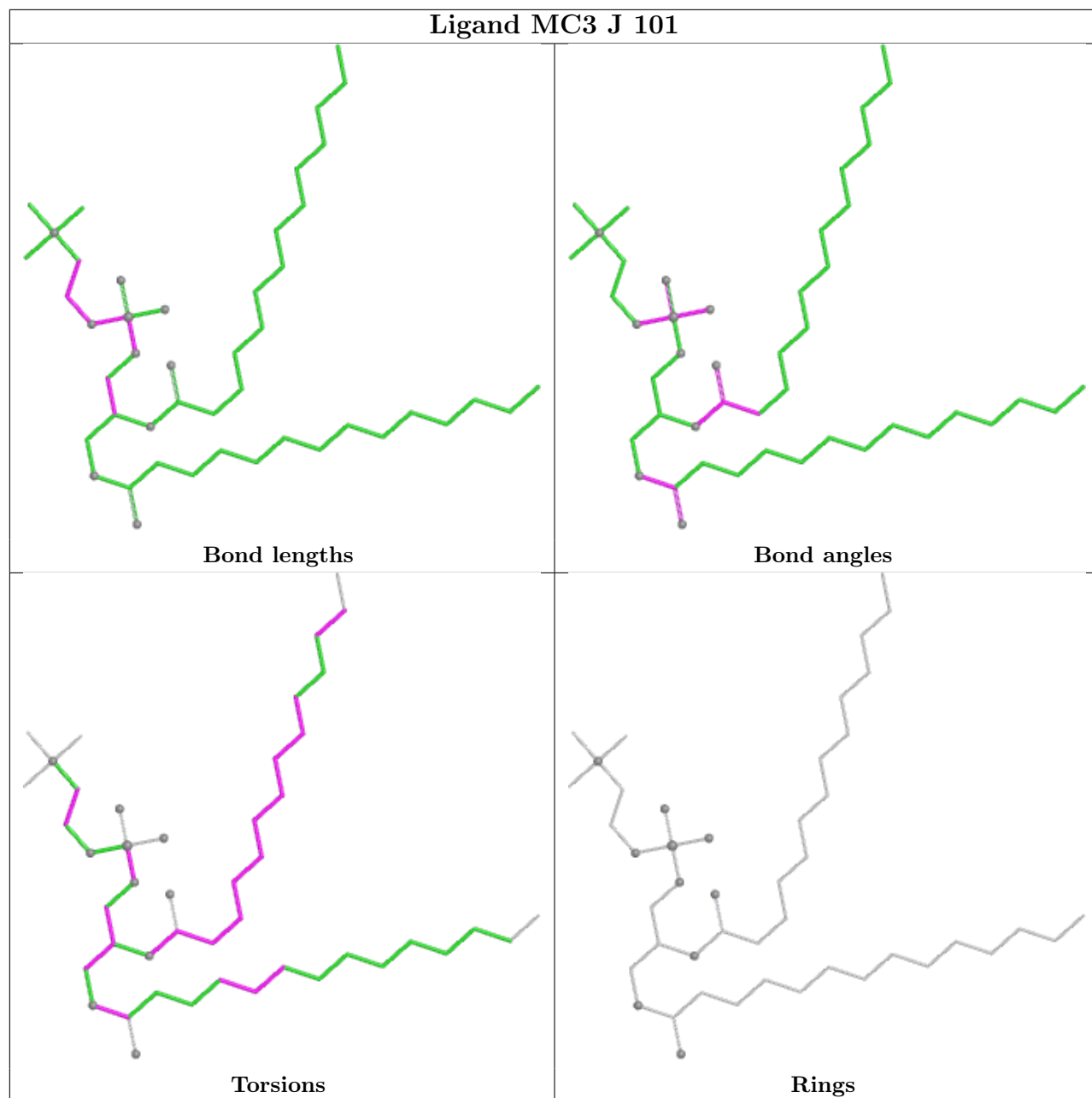
Ligand HEM C 1002

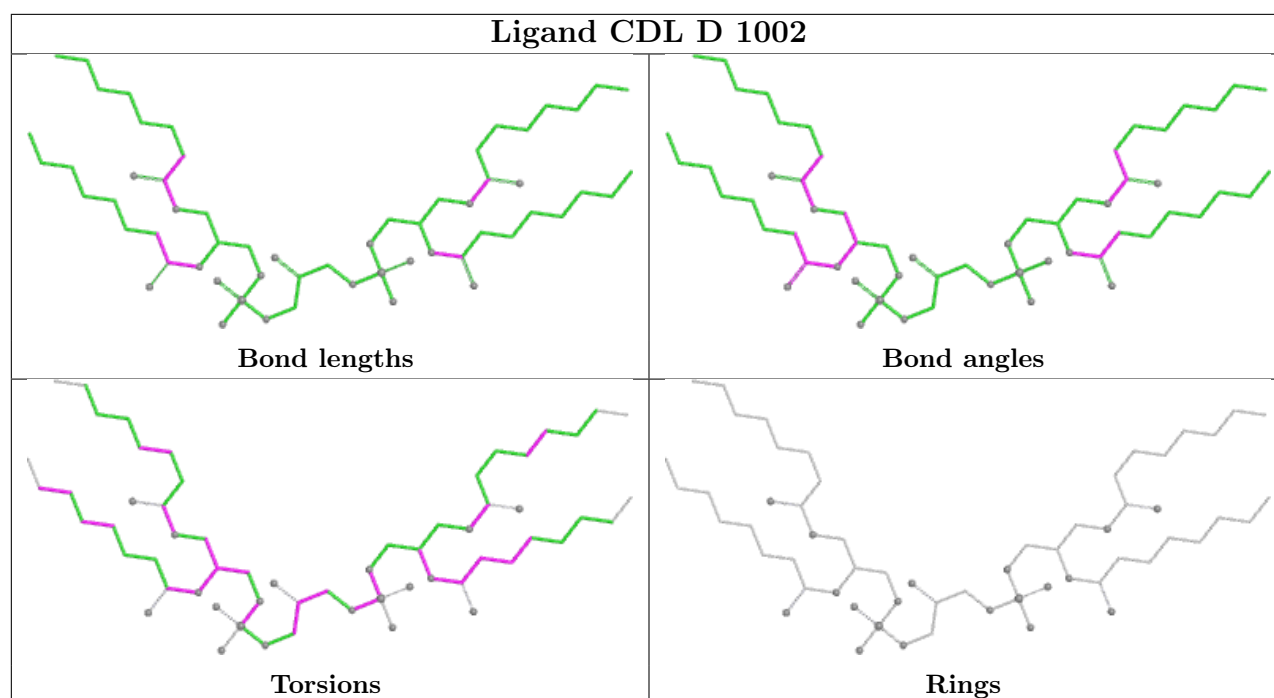


Ligand 6PE K 101



Ligand MC3 J 101





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	446/446 (100%)	0.40	12 (2%) 56 46	63, 92, 121, 199	0
2	B	425/439 (96%)	0.22	14 (3%) 49 39	54, 72, 102, 179	0
3	C	378/379 (99%)	0.47	14 (3%) 45 36	73, 107, 144, 165	0
4	D	241/241 (100%)	1.00	25 (10%) 11 8	78, 160, 183, 199	0
5	E	196/196 (100%)	3.85	121 (61%) 0 0	17, 20, 139, 177	124 (63%)
6	F	105/110 (95%)	0.45	5 (4%) 35 28	69, 92, 139, 154	0
7	G	75/80 (93%)	0.52	5 (6%) 24 17	73, 113, 156, 181	0
8	H	67/78 (85%)	1.27	11 (16%) 4 3	155, 172, 194, 198	0
9	I	34/78 (43%)	2.75	23 (67%) 0 0	81, 131, 162, 173	0
10	J	61/63 (96%)	0.89	6 (9%) 13 9	104, 143, 169, 187	0
11	K	52/55 (94%)	0.70	6 (11%) 9 7	104, 131, 166, 182	0
All	All	2080/2165 (96%)	0.86	242 (11%) 9 7	17, 97, 172, 199	124 (5%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	142	LEU	22.6
5	E	116	GLN	16.3
5	E	93	GLY	14.4
5	E	103	LYS	14.2
5	E	115	SER	13.0
5	E	161	HIS	12.2
5	E	73	LYS	12.1
5	E	160	CYS	11.7
5	E	111	ALA	11.7
5	E	143	GLY	11.6
5	E	104	LYS	10.9
5	E	159	PRO	10.5

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Mol	Chain	Res	Type	RSRZ
5	E	189	SER	10.4
5	E	90	LYS	10.3
5	E	80	ASP	9.9
5	E	77	LYS	9.7
5	E	124	LEU	9.5
9	I	70	LEU	9.3
5	E	92	ARG	9.2
5	E	107	ASP	8.7
5	E	188	THR	8.7
5	E	152	ASP	8.2
5	E	191	ASP	8.2
5	E	82	PRO	8.1
5	E	156	TYR	8.1
5	E	196	GLY	8.0
5	E	175	PRO	8.0
5	E	117	LEU	7.7
5	E	113	GLU	7.7
5	E	177	PRO	7.5
5	E	141	HIS	7.4
9	I	69	SER	7.2
5	E	184	SER	7.2
5	E	74	ILE	7.1
5	E	120	PRO	7.0
5	E	79	SER	6.9
5	E	144	CYS	6.8
5	E	114	VAL	6.7
5	E	128	LYS	6.7
5	E	91	TRP	6.5
5	E	110	ALA	6.5
5	E	176	ALA	6.4
5	E	190	ASP	6.3
5	E	195	VAL	6.1
5	E	130	PRO	6.0
5	E	102	THR	5.9
2	B	17	VAL	5.9
5	E	194	ILE	5.8
5	E	83	GLU	5.7
5	E	193	VAL	5.5
5	E	186	GLU	5.3
5	E	192	MET	5.2
5	E	122	HIS	5.2
5	E	108	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
5	E	178	LEU	5.1
5	E	183	PRO	5.1
5	E	164	HIS	5.0
5	E	147	ILE	5.0
5	E	153	PHE	5.0
5	E	96	LEU	4.9
5	E	125	GLU	4.8
8	H	13	LEU	4.7
5	E	162	GLY	4.6
5	E	173	LYS	4.5
9	I	68	VAL	4.5
5	E	94	LYS	4.5
4	D	17	LEU	4.5
5	E	106	ILE	4.5
5	E	157	TYR	4.4
5	E	118	ARG	4.4
5	E	67	ASP	4.4
5	E	169	GLY	4.3
5	E	134	ILE	4.3
5	E	126	ARG	4.3
4	D	106	ASN	4.2
5	E	133	VAL	4.2
4	D	56	TYR	4.2
2	B	16	GLY	4.2
5	E	154	GLY	4.2
5	E	185	TYR	4.1
10	J	1	VAL	4.1
5	E	16	PRO	4.0
9	I	25	ALA	4.0
5	E	85	LYS	4.0
5	E	149	ASN	4.0
6	F	12	TRP	4.0
5	E	181	GLU	4.0
5	E	1	SER	4.0
5	E	121	GLN	4.0
5	E	187	PHE	3.9
2	B	233	SER	3.9
5	E	84	GLY	3.8
5	E	151	GLY	3.8
5	E	71	MET	3.8
11	K	2	LEU	3.8
5	E	87	MET	3.8

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Mol	Chain	Res	Type	RSRZ
9	I	57	GLY	3.8
4	D	3	LEU	3.7
5	E	119	ASP	3.7
11	K	52	PHE	3.7
9	I	24	GLY	3.7
5	E	100	HIS	3.7
4	D	55	CYS	3.7
5	E	75	GLU	3.7
5	E	129	LYS	3.6
9	I	23	ALA	3.6
2	B	15	ALA	3.5
5	E	145	VAL	3.5
1	A	222	THR	3.5
9	I	45	LEU	3.5
4	D	61	ALA	3.5
5	E	139	CYS	3.4
5	E	168	SER	3.4
3	C	11	MET	3.3
5	E	76	ILE	3.3
9	I	26	LEU	3.3
4	D	1	SER	3.3
9	I	59	ALA	3.3
5	E	171	ILE	3.2
10	J	2	ALA	3.2
2	B	232	LEU	3.2
5	E	150	ALA	3.2
5	E	163	SER	3.1
6	F	10	SER	3.1
5	E	179	ASN	3.1
3	C	344	GLU	3.1
5	E	112	VAL	3.1
2	B	230	LEU	3.0
7	G	18	LEU	3.0
11	K	15	ARG	3.0
3	C	291	VAL	3.0
1	A	223	TYR	3.0
4	D	143	LEU	3.0
2	B	161	GLU	3.0
9	I	50	LEU	2.9
3	C	70	CYS	2.9
5	E	140	THR	2.9
5	E	138	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	182	VAL	2.9
5	E	81	ILE	2.9
9	I	52	ARG	2.8
4	D	108	ALA	2.8
7	G	75	ALA	2.8
5	E	78	LEU	2.8
9	I	27	ARG	2.7
4	D	141	VAL	2.7
1	A	220	SER	2.7
6	F	9	SER	2.7
8	H	14	VAL	2.7
5	E	32	ARG	2.7
5	E	148	ALA	2.7
2	B	228	GLY	2.7
4	D	174	GLY	2.7
3	C	28	SER	2.7
5	E	167	ALA	2.6
2	B	421	ARG	2.6
8	H	62	LEU	2.6
10	J	61	ASN	2.6
4	D	172	ASP	2.6
5	E	88	ALA	2.6
9	I	44	ASP	2.6
4	D	48	TYR	2.6
4	D	115	TYR	2.6
8	H	42	GLU	2.6
9	I	60	ALA	2.6
4	D	173	ASP	2.6
4	D	15	ARG	2.5
9	I	67	SER	2.5
3	C	168	PHE	2.5
9	I	63	PRO	2.5
9	I	61	GLY	2.5
2	B	19	PRO	2.5
9	I	55	LEU	2.5
5	E	105	GLU	2.5
5	E	131	GLU	2.5
4	D	18	LEU	2.5
5	E	135	LEU	2.5
5	E	165	TYR	2.5
11	K	40	LEU	2.4
4	D	149	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	172	ARG	2.4
8	H	61	PHE	2.4
10	J	3	PRO	2.4
5	E	136	ILE	2.4
6	F	6	VAL	2.4
2	B	173	ALA	2.4
1	A	120	CYS	2.4
3	C	2	THR	2.4
8	H	63	HIS	2.4
10	J	5	LEU	2.4
10	J	51	LEU	2.4
3	C	251	GLY	2.3
5	E	99	ARG	2.3
7	G	24	ARG	2.3
4	D	166	ASN	2.3
5	E	89	PHE	2.3
5	E	19	LEU	2.3
5	E	68	VAL	2.3
2	B	234	GLY	2.3
6	F	94	LEU	2.3
9	I	20	ARG	2.3
3	C	343	VAL	2.3
1	A	1	THR	2.2
3	C	252	ASP	2.2
5	E	158	CYS	2.2
5	E	33	LYS	2.2
9	I	53	GLU	2.2
5	E	101	ARG	2.2
2	B	95	LYS	2.2
5	E	64	ALA	2.2
8	H	18	THR	2.2
4	D	134	TYR	2.2
4	D	142	SER	2.2
8	H	76	SER	2.2
9	I	22	VAL	2.1
11	K	53	LYS	2.1
8	H	70	ALA	2.1
3	C	98	VAL	2.1
5	E	23	LYS	2.1
3	C	278	TYR	2.1
5	E	21	SER	2.1
1	A	72	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	50	THR	2.1
3	C	4	ILE	2.1
4	D	35	GLN	2.1
2	B	20	HIS	2.1
3	C	102	LEU	2.1
4	D	64	LEU	2.1
8	H	15	ASP	2.1
1	A	18	GLN	2.0
7	G	3	GLN	2.0
9	I	46	LYS	2.0
1	A	73	ASN	2.0
4	D	5	LEU	2.0
11	K	48	ILE	2.0
1	A	416	TYR	2.0
1	A	62	LEU	2.0
1	A	381	ARG	2.0
7	G	36	ASN	2.0
1	A	221	GLY	2.0
4	D	139	THR	2.0
5	E	18	VAL	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
12	6PE	K	101	27/27	0.57	0.28	132,162,168,168	0
18	FES	E	1001	4/4	0.66	0.22	75,76,76,76	4
13	CDL	G	101	60/100	0.74	0.23	94,115,138,139	0

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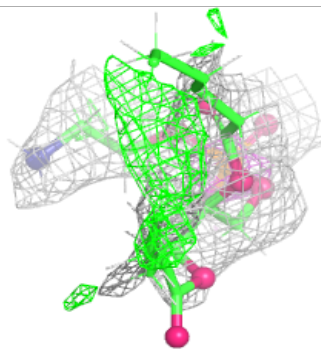
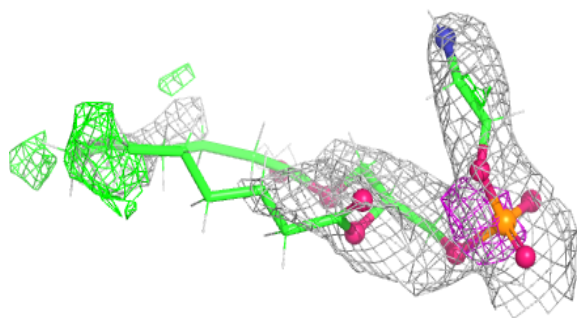
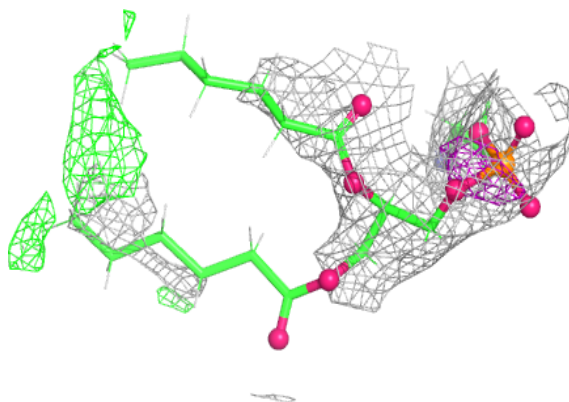
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CDL	D	1002	60/100	0.78	0.22	96,117,139,142	0
13	CDL	A	502	60/100	0.80	0.16	96,117,140,143	0
12	6PE	A	501	27/27	0.84	0.17	91,114,138,138	0
19	MC3	J	101	46/46	0.87	0.20	96,119,143,144	0
16	8PE	C	1004	47/47	0.89	0.20	74,98,129,132	0
17	HEC	D	1001	43/43	0.92	0.15	135,156,179,191	0
15	AZO	C	1003	30/30	0.93	0.14	99,113,137,157	0
14	HEM	C	1001	43/43	0.95	0.17	105,115,130,147	0
14	HEM	C	1002	43/43	0.97	0.12	70,86,111,117	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.

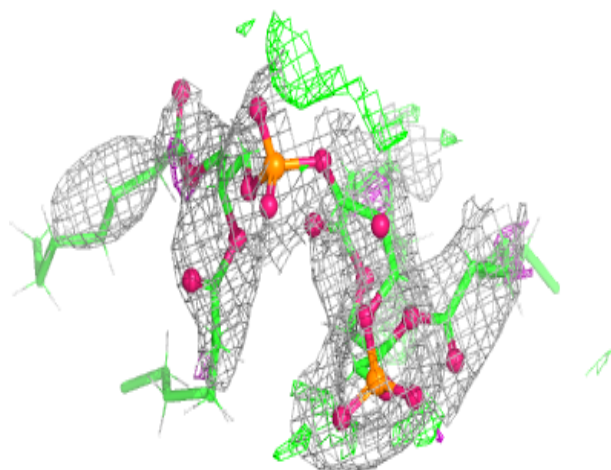
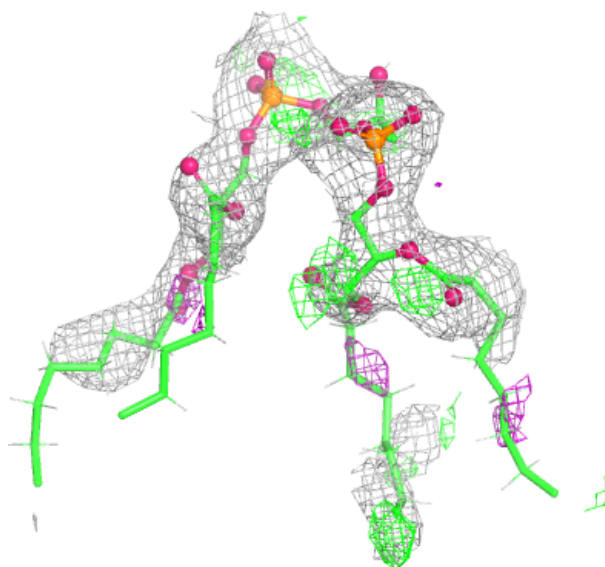
Electron density around 6PE K 101:

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



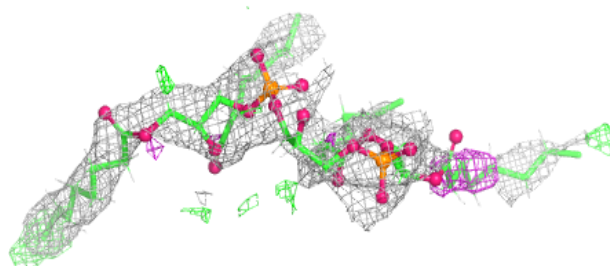
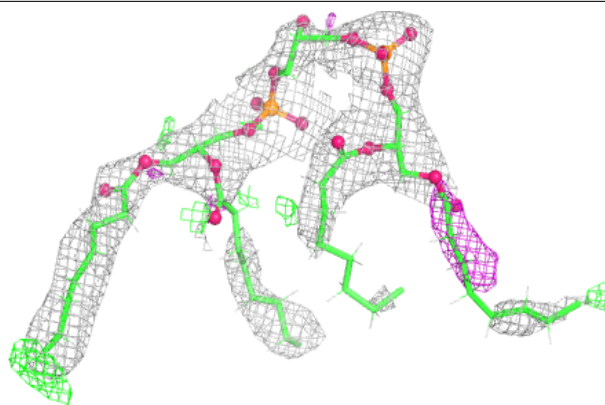
Electron density around CDL G 101:

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



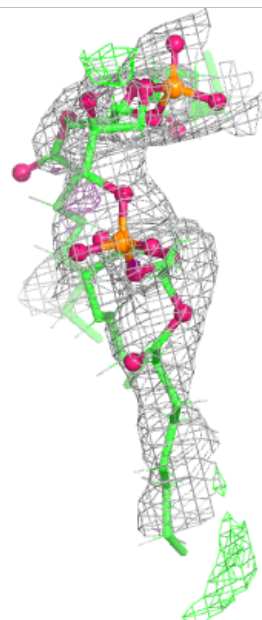
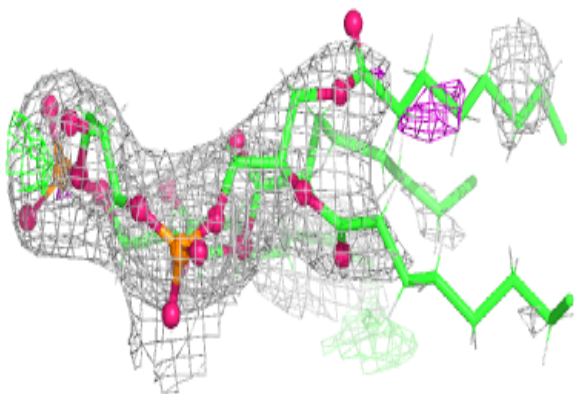
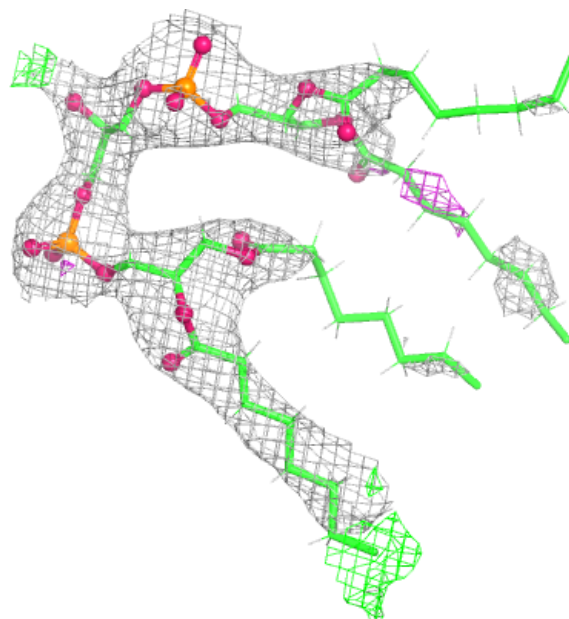
Electron density around CDL D 1002:

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



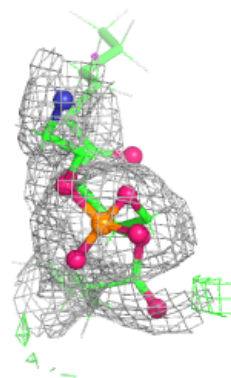
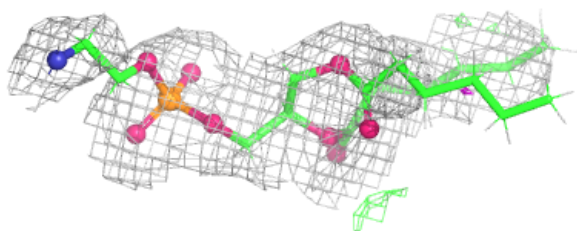
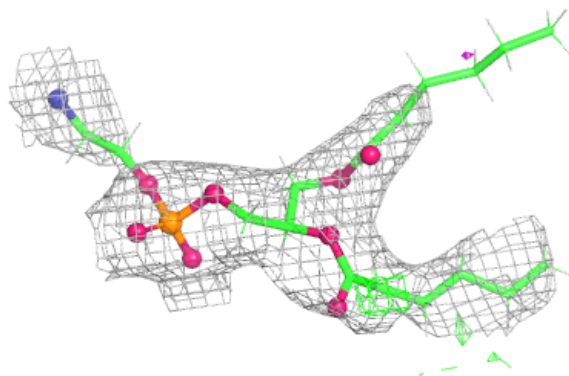
Electron density around CDL A 502:

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



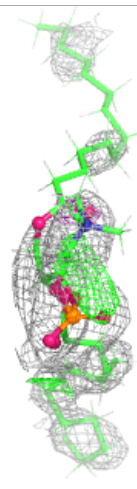
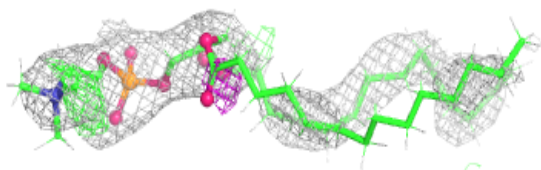
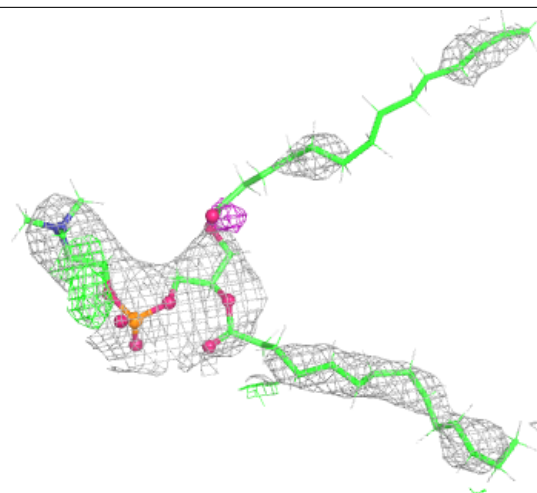
Electron density around 6PE A 501:

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



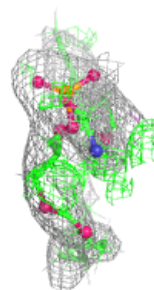
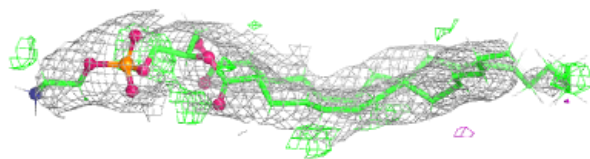
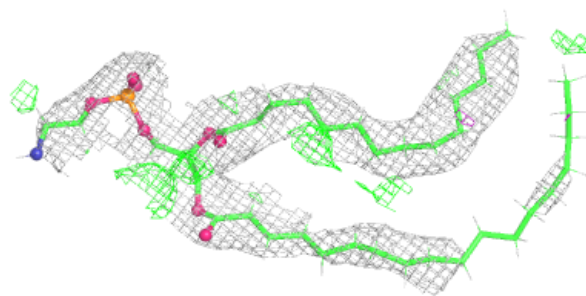
Electron density around MC3 J 101:

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



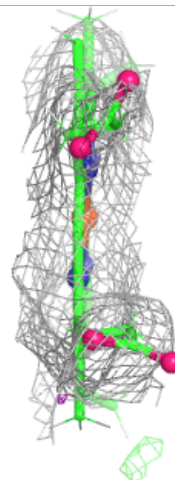
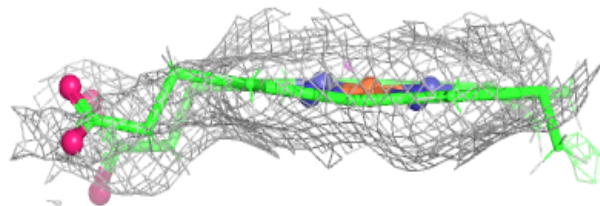
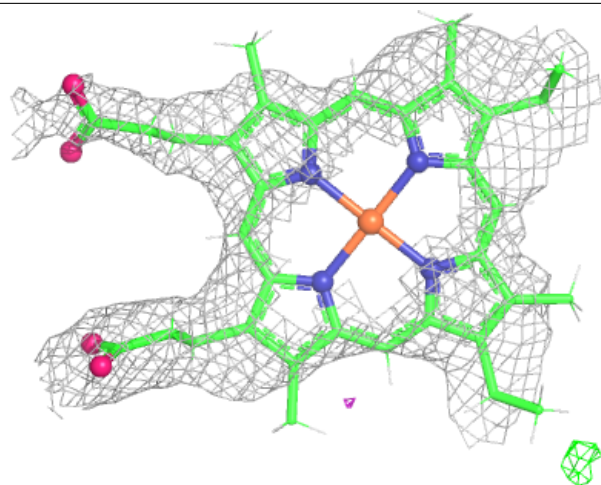
Electron density around 8PE C 1004:

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



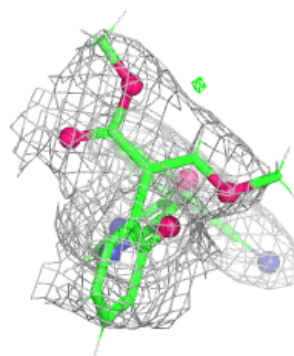
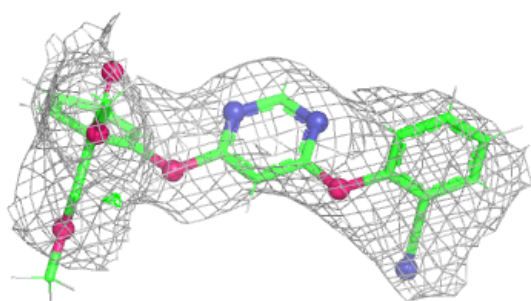
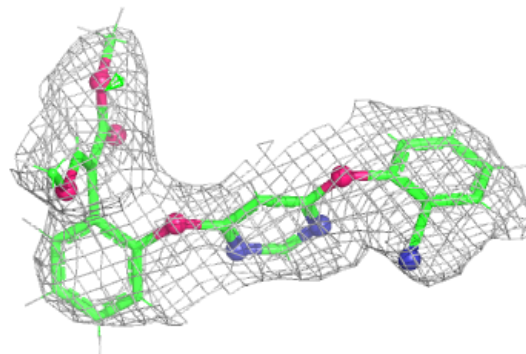
Electron density around HEC D 1001:

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



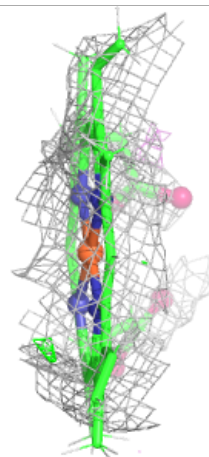
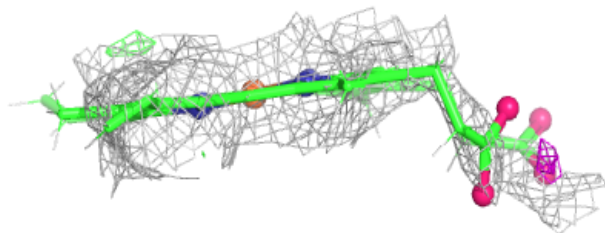
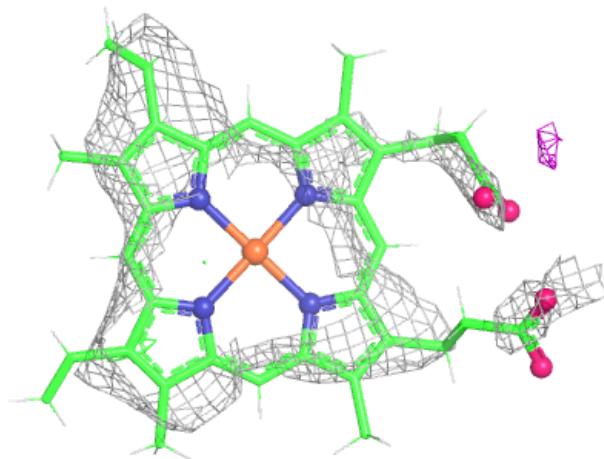
Electron density around AZO C 1003:

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



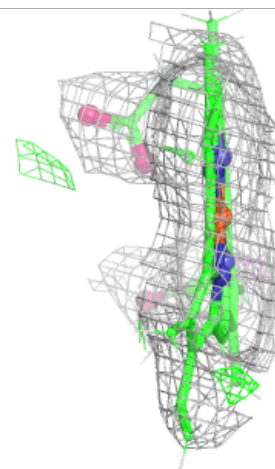
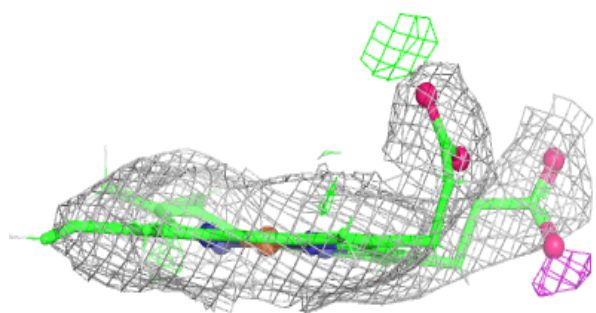
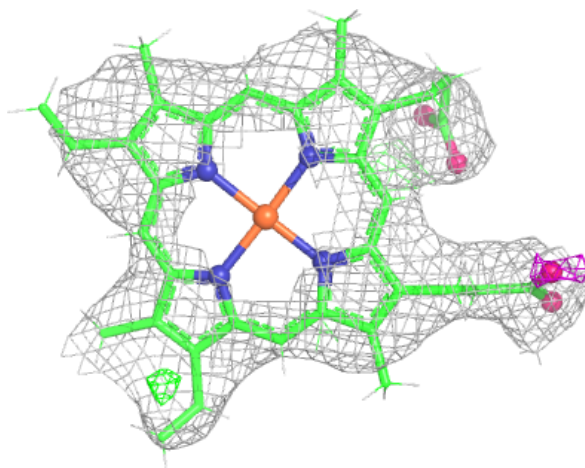
Electron density around HEM C 1001:

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



Electron density around HEM C 1002:

$2mF_o-DF_c$ (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.