



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:29 AM UTC

PDB ID : 4OGQ / pdb_00004ogq
Title : Internal Lipid Architecture of the Hetero-Oligomeric Cytochrome b6f Complex
Authors : Hasan, S.S.; Cramer, W.A.
Deposited on : 2014-01-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

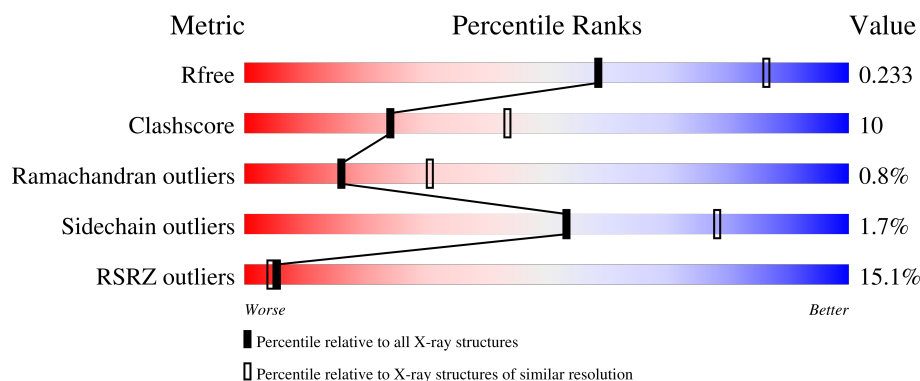
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



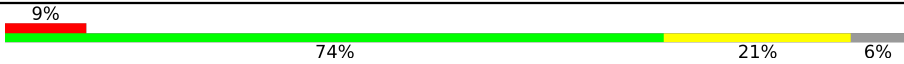
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	215	2% 91% 9%
2	B	160	8% 88% 11% .
3	C	333	13% 69% 14% . 16%
4	D	179	36% 72% 21% 7%
5	E	31	23% 77% 16% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	34	
7	G	37	
8	H	29	

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
14	CLA	B	204	X	-	-	-
24	1O2	F	103	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 8396 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1708	1139	271	288	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1232	825	194	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2137	1361	355	415	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1250	791	213	240	6			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			228	157	35	35	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			231	156	36	38	1			

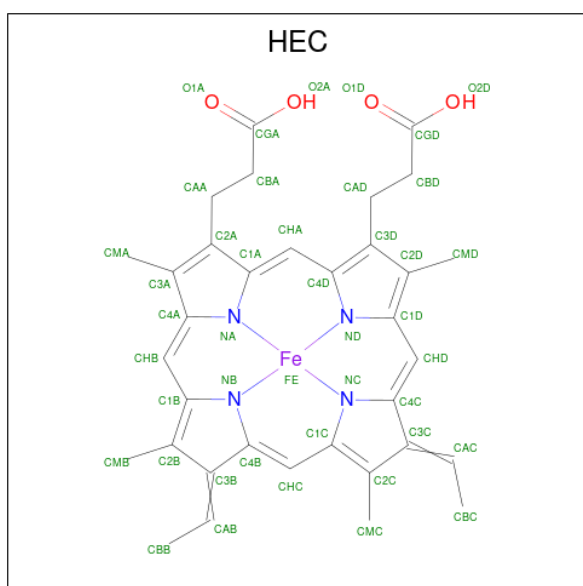
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			282	188	44	49	1			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

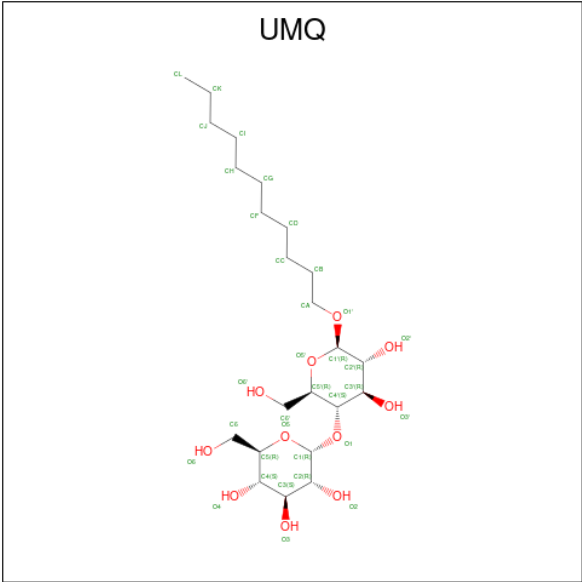
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			228	155	36	35	2			

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



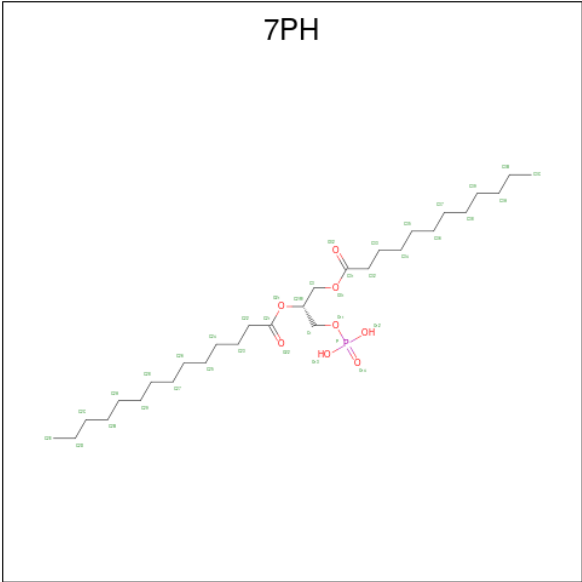
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



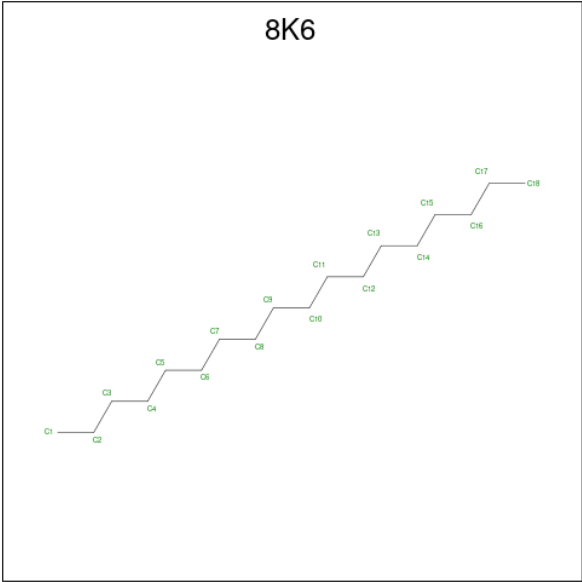
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	1
			34	23	11		
10	D	1	Total	C	O	0	0
			34	23	11		
10	G	1	Total	C	O	0	0
			34	23	11		

- Molecule 11 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



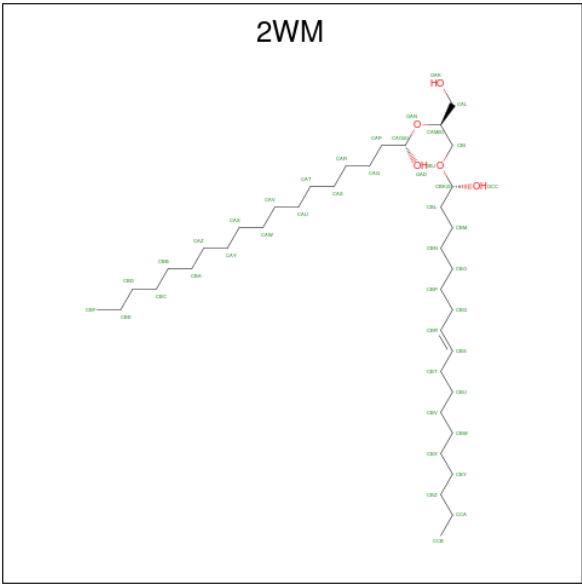
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			32	27	5		
11	B	1	Total	C	O	0	0
			32	27	5		
11	C	1	Total	C	O	0	0
			32	27	5		
11	D	1	Total	C	O	0	0
			32	27	5		
11	F	1	Total	C	O	0	0
			32	27	5		

- Molecule 12 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).



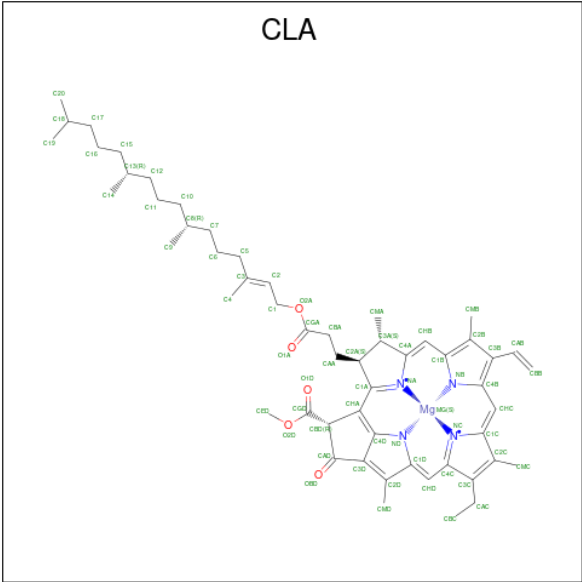
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C 18 18	0	0
12	A	1	Total C 18 18	0	0
12	A	1	Total C 14 14	0	0
12	B	1	Total C 18 18	0	1

- Molecule 13 is (1S,8E)-1-{[(2S)-3-hydroxy-2-{[(1S)-1-hydroxyoctadecyl]oxy}propyl]oxy}octadec-8-en-1-ol (CCD ID: 2WM) (formula: C₃₉H₇₈O₅).



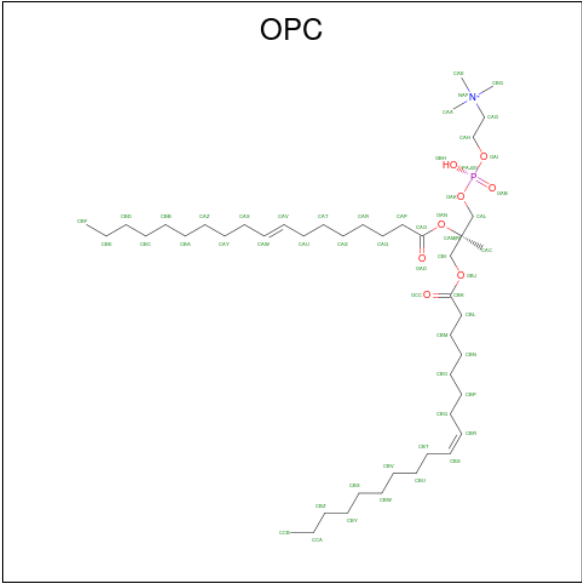
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 44 39 5	0	0

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C₄₅H₈₇NO₈P).

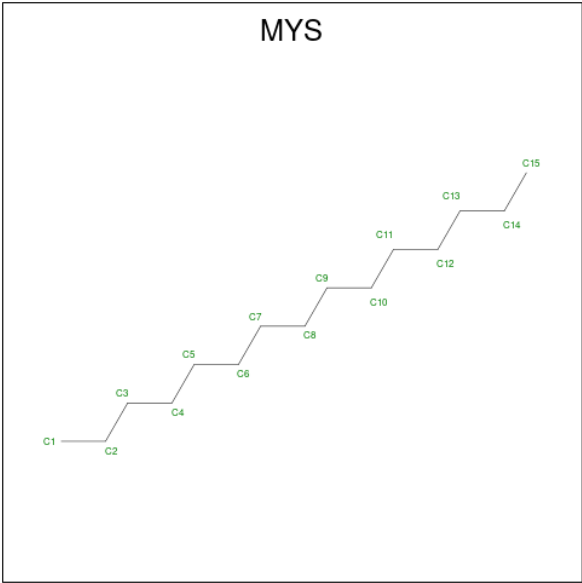


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 16 is CADMIUM ION (CCD ID: CD) (formula: Cd).

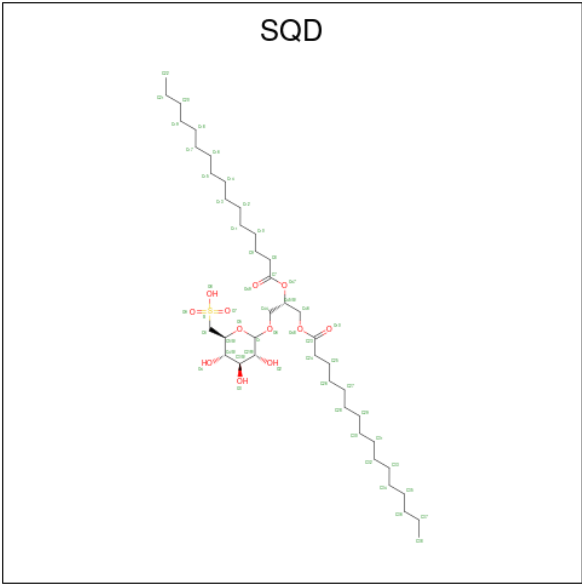
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	Cd	0	0
			1	1		

- Molecule 17 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



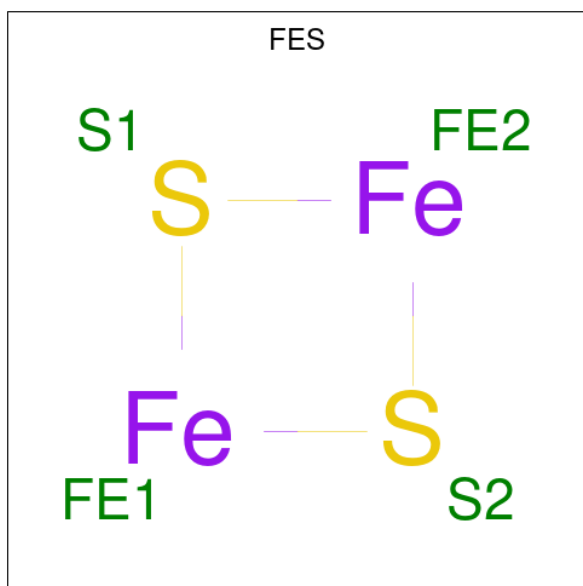
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total	C	0	0
			15	15		

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



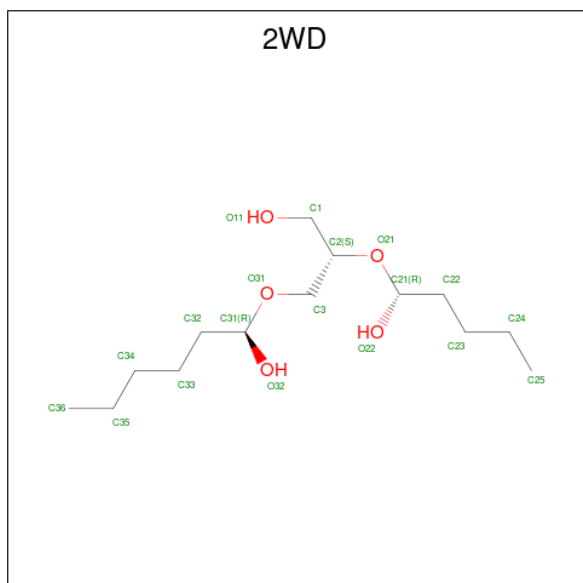
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



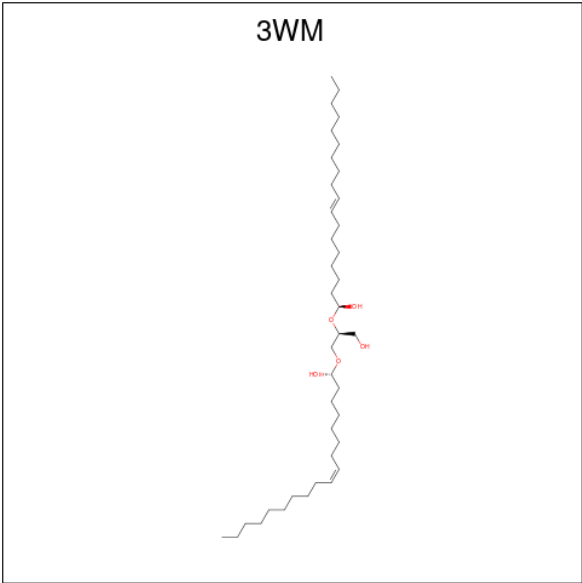
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is (1R)-1-{[(2S)-3-hydroxy-2-{[(1R)-1-hydroxypentyl]oxy}propyl]oxy}hexan-1-ol (CCD ID: 2WD) (formula: $\text{C}_{14}\text{H}_{30}\text{O}_5$).



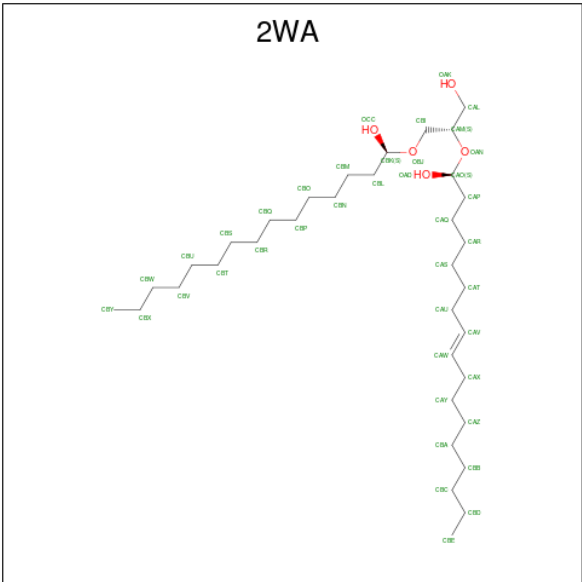
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			19	14	5		

- Molecule 21 is (1S,8E,1'R,8'Z)-1,1'-{[(2S)-3-hydroxypropane-1,2-diyl]bis(oxy)}bisooctadec-8-en-1-ol (CCD ID: 3WM) (formula: C₃₉H₇₆O₅).



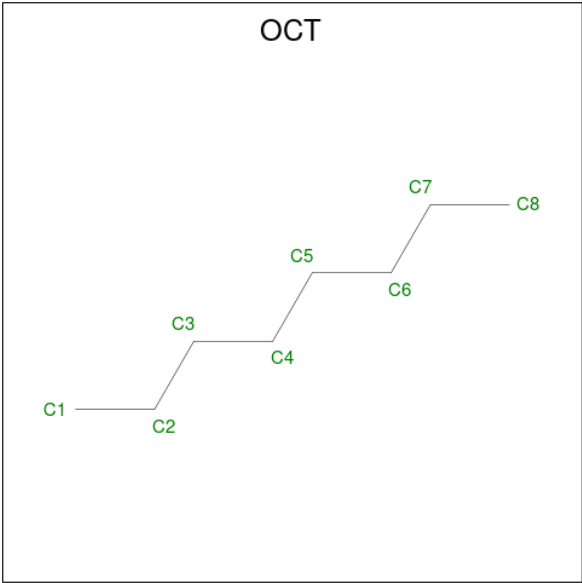
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			44	39	5		

- Molecule 22 is (1S,8E)-1-{[(2S)-1-hydroxy-3-{[(1S)-1-hydroxypentadecyl]oxy}propan-2-yl]oxy}heptadec-8-en-1-ol (CCD ID: 2WA) (formula: C₃₅H₇₀O₅).



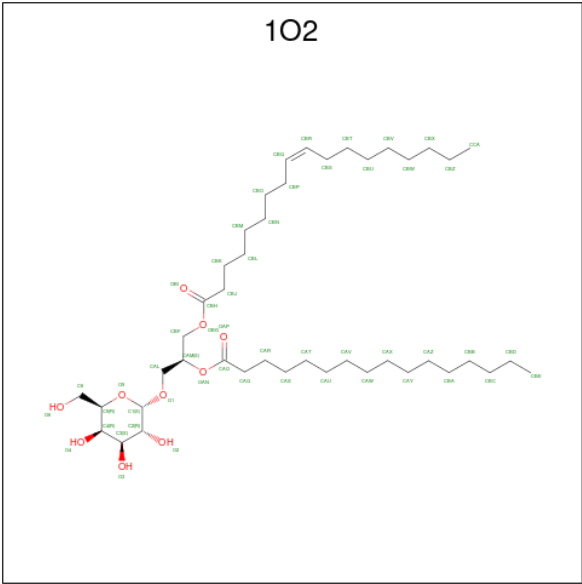
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	F	1	Total	C	O	0	0
			40	35	5		

- Molecule 23 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



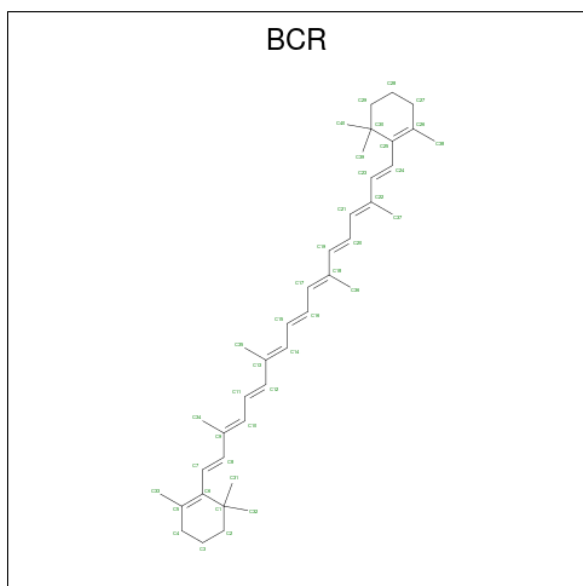
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	F	1	Total	C	0	0
			8	8		

- Molecule 24 is (2S)-3-(alpha-D-galactopyranosyloxy)-2-(hexadecanoyloxy)propyl (9Z)-octadec-9-enoate (CCD ID: 1O2) (formula: C₄₃H₈₀O₁₀).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	F	1	Total	C O	0	0
			49	39 10		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total	C	0	0
			40	40		

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	21	Total	O	0	0
			21	21		
26	B	25	Total	O	0	0
			25	25		
26	C	38	Total	O	0	0
			38	38		
26	D	1	Total	O	0	0
			1	1		
26	F	1	Total	O	0	0
			1	1		
26	G	7	Total	O	0	0
			7	7		

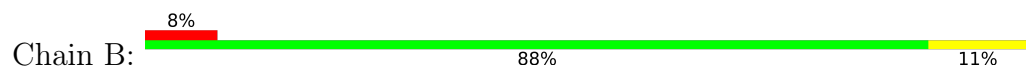
3 Residue-property plots [i](#)

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.

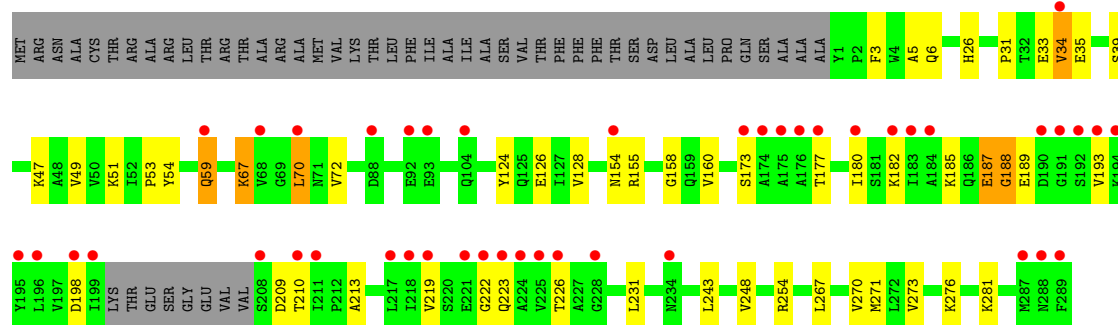
- Molecule 1: Cytochrome b6



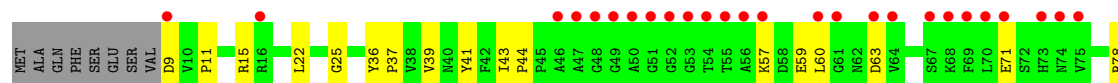
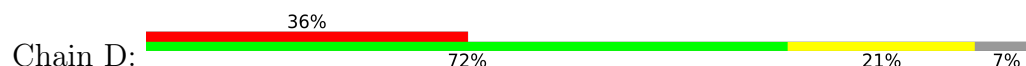
- Molecule 2: Cytochrome b6-f complex subunit 4

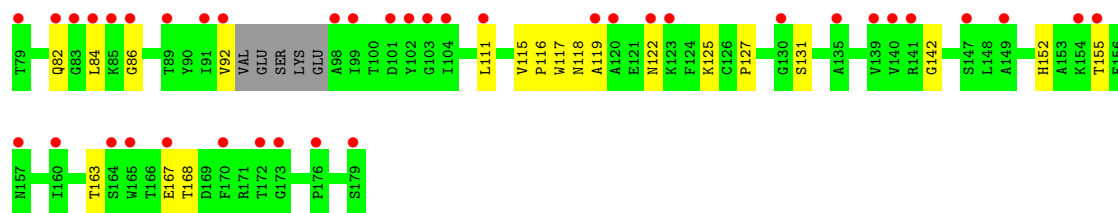


- Molecule 3: Apocytochrome f

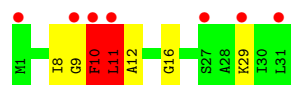
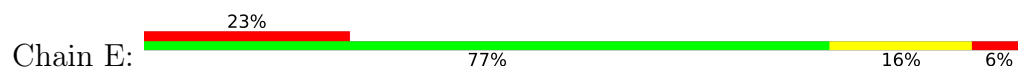


- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1

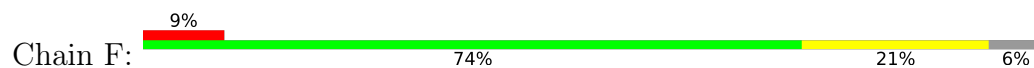




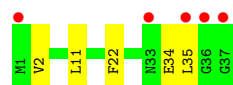
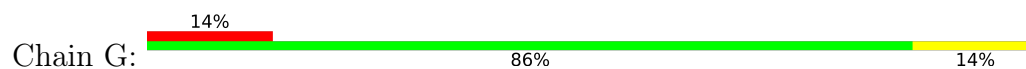
● Molecule 5: Cytochrome b6-f complex subunit 6



● Molecule 6: Cytochrome b6-f complex subunit 7



● Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.23Å 159.23Å 365.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.50) 89.3 (39.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.201 , 0.232 0.207 , 0.233	Depositor DCC
R_{free} test set	4694 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: FES, 1O2, OCT, 7PH, UMQ, SQD, HEC, CLA, 3WM, MYS, 2WD, 2WA, 2WM, CD, OPC, 8K6, BCR

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	0.33	0/1761	0.79	4/2401 (0.2%)
2	B	0.32	0/1271	0.75	1/1742 (0.1%)
3	C	0.28	0/2182	0.69	0/2972
4	D	0.28	0/1281	0.71	0/1745
5	E	0.36	0/231	1.08	3/309 (1.0%)
6	F	0.25	0/234	0.66	0/315
7	G	0.27	0/287	0.72	0/387
8	H	0.35	0/234	0.66	0/319
All	All	0.30	0/7481	0.74	8/10190 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	10	PHE	N-CA-C	8.31	123.90	113.43
5	E	10	PHE	CA-C-N	6.30	133.04	121.70
5	E	10	PHE	C-N-CA	6.30	133.04	121.70
1	A	158	ILE	CA-C-N	5.66	126.91	119.84
1	A	158	ILE	C-N-CA	5.66	126.91	119.84
1	A	26	VAL	CA-C-N	5.54	123.65	119.66
1	A	26	VAL	C-N-CA	5.54	123.65	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	VAL	CB-CA-C	-5.41	108.56	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1721	16	0
2	B	1232	0	1278	16	0
3	C	2137	0	2122	31	0
4	D	1250	0	1208	23	0
5	E	228	0	257	9	0
6	F	231	0	252	8	0
7	G	282	0	303	4	0
8	H	228	0	243	11	0
9	A	129	0	95	6	0
9	C	43	0	31	3	0
10	A	34	0	44	9	0
10	B	68	0	87	17	0
10	D	34	0	44	4	0
10	G	34	0	44	4	0
11	A	32	0	45	1	0
11	B	32	0	45	5	0
11	C	32	0	45	4	0
11	D	32	0	45	1	0
11	F	32	0	45	6	0
12	A	50	0	103	8	0
12	B	18	0	38	3	0
13	A	44	0	78	0	0
14	B	65	0	72	4	0
15	B	54	0	83	5	0
16	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	15	0	32	1	0
18	D	54	0	77	2	0
19	D	4	0	0	0	0
20	D	19	0	30	2	0
21	E	44	0	76	9	0
22	F	40	0	70	7	0
23	F	8	0	18	0	0
24	F	49	0	69	11	0
25	G	40	0	56	2	0
26	A	21	0	0	0	0
26	B	25	0	0	1	0
26	C	38	0	0	0	0
26	D	1	0	0	0	0
26	F	1	0	0	0	0
26	G	7	0	0	0	0
All	All	8396	0	8756	171	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 10.

All (171) 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)
10:G:101:UMQ:O5'	10:G:101:UMQ:C5'	1.63	1.46
10:A:304:UMQ:O5'	10:A:304:UMQ:C5'	1.63	1.45
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C5'	1.63	1.44
10:B:201:UMQ:C1'	10:B:201:UMQ:O5'	1.69	1.41
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C1'	1.69	1.38
10:D:201:UMQ:O5'	10:D:201:UMQ:C1'	1.69	1.38
10:A:304:UMQ:O5'	10:A:304:UMQ:C1'	1.69	1.38
10:G:101:UMQ:O5'	10:G:101:UMQ:C1'	1.69	1.37
10:D:201:UMQ:C1'	10:D:201:UMQ:C5'	2.46	0.93
10:G:101:UMQ:C5'	10:G:101:UMQ:C1'	2.47	0.93
10:B:203[B]:UMQ:C5'	10:B:203[B]:UMQ:C1'	2.47	0.92
10:A:304:UMQ:C5'	10:A:304:UMQ:C1'	2.48	0.92
10:B:201:UMQ:C1'	10:B:201:UMQ:C5'	2.48	0.92
10:A:304:UMQ:H6'2	10:A:304:UMQ:H11	1.59	0.83
3:C:34:VAL:HG23	3:C:243:LEU:HD23	1.70	0.73
11:C:303:7PH:H25	11:C:303:7PH:H35A	1.70	0.72
5:E:8:ILE:HD11	21:E:101:3WM:H11	1.71	0.71
2:B:41:PRO:HG3	12:B:202[A]:8K6:H92C	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:201:UMQ:H51	10:B:201:UMQ:H6'1	1.73	0.71
1:A:61:THR:HG22	1:A:63:ALA:H	1.56	0.70
8:H:26:ARG:HE	8:H:29:LEU:HD11	1.57	0.70
1:A:41:LEU:HD23	9:A:303:HEC:HBC3	1.74	0.70
3:C:31:PRO:O	3:C:155:ARG:NH2	2.26	0.69
1:A:4:VAL:HG13	11:A:305:7PH:H34	1.74	0.69
4:D:131:SER:HA	4:D:142:GLY:HA3	1.76	0.67
1:A:114:ARG:NH1	1:A:210:GLY:O	2.29	0.66
3:C:270:VAL:HA	8:H:21:MET:HE2	1.78	0.65
10:D:201:UMQ:H51	10:D:201:UMQ:H4'1	1.79	0.65
3:C:26:HIS:CG	3:C:154:ASN:HD21	2.14	0.64
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.81	0.62
10:D:201:UMQ:H4'1	10:D:201:UMQ:C5	2.30	0.62
3:C:281:LYS:NZ	4:D:9:ASP:O	2.29	0.61
24:F:103:1O2:HBSA	24:F:103:1O2:HAZA	1.82	0.60
21:E:101:3WM:H29	21:E:101:3WM:H44	1.83	0.60
24:F:103:1O2:HBQ	24:F:103:1O2:HAY	1.83	0.60
4:D:15:ARG:HH12	5:E:29:LYS:HE3	1.67	0.59
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C6'	2.47	0.58
24:F:103:1O2:HAY	24:F:103:1O2:CBQ	2.33	0.58
3:C:3:PHE:HA	3:C:6:GLN:HG2	1.84	0.58
2:B:32:TRP:CE2	10:B:201:UMQ:HC2	2.39	0.58
6:F:29:ILE:HG22	24:F:103:1O2:HAS	1.85	0.57
21:E:101:3WM:H53	8:H:12:LEU:HD21	1.86	0.57
10:B:203[B]:UMQ:H11	10:B:203[B]:UMQ:H6'1	1.85	0.57
11:B:206:7PH:H29A	11:B:206:7PH:H24	1.86	0.57
2:B:114:ILE:HD13	15:B:205:OPC:HAT2	1.88	0.56
10:A:304:UMQ:O5'	10:A:304:UMQ:C6'	2.47	0.55
6:F:13:PHE:CD2	22:F:101:2WA:H14	2.41	0.55
3:C:59:GLN:HB3	3:C:67:LYS:HG3	1.89	0.55
1:A:209:GLN:HA	2:B:22:MET:HE3	1.87	0.55
2:B:127:PRO:HD2	15:B:205:OPC:HAG1	1.88	0.55
10:G:101:UMQ:O5'	10:G:101:UMQ:C6'	2.48	0.54
3:C:180:ILE:HB	3:C:223:GLN:H	1.73	0.54
3:C:70:LEU:HD13	3:C:155:ARG:HB3	1.90	0.54
5:E:10:PHE:H	5:E:11:LEU:HB2	1.73	0.54
1:A:32:ILE:N	8:H:29:LEU:HD13	2.23	0.54
21:E:101:3WM:H1	24:F:103:1O2:HBEA	1.89	0.53
6:F:26:LEU:HD13	6:F:29:ILE:HD11	1.90	0.53
5:E:10:PHE:CD2	8:H:13:VAL:HG11	2.44	0.53
4:D:11:PRO:HA	4:D:15:ARG:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:308:8K6:H112	12:A:308:8K6:H72C	1.90	0.52
4:D:59:GLU:HG2	4:D:60:LEU:HD12	1.90	0.52
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.91	0.52
10:A:304:UMQ:HL3	10:B:201:UMQ:HK2	1.91	0.51
2:B:133:PHE:HA	14:B:204:CLA:HBB1	1.93	0.51
22:F:101:2WA:H2	11:F:104:7PH:H2B	1.92	0.51
12:A:308:8K6:H72C	12:A:308:8K6:C13	2.40	0.51
3:C:5:ALA:HB2	9:C:301:HEC:HHC	1.93	0.51
2:B:33:PRO:HG3	18:D:204:SQD:H4	1.91	0.51
1:A:92:MET:HB3	21:E:101:3WM:H76	1.93	0.50
11:C:303:7PH:H25	11:C:303:7PH:C35	2.39	0.50
21:E:101:3WM:H1	24:F:103:1O2:CBE	2.41	0.50
21:E:101:3WM:H65	8:H:15:PHE:CD1	2.46	0.50
3:C:180:ILE:HG13	3:C:219:VAL:HG11	1.92	0.50
8:H:23:VAL:HG13	8:H:28:GLY:HA2	1.93	0.50
4:D:78:ARG:HD3	4:D:92:VAL:HG22	1.93	0.50
3:C:158:GLY:H	9:C:301:HEC:C3D	2.25	0.50
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.47	0.49
3:C:273:VAL:HG21	8:H:21:MET:HE3	1.93	0.49
20:D:206:2WD:O22	20:D:206:2WD:H2	2.12	0.49
10:A:304:UMQ:HF2	10:A:304:UMQ:CJ	2.42	0.49
14:B:204:CLA:O1D	22:F:101:2WA:H66	2.13	0.48
11:B:206:7PH:H29A	11:B:206:7PH:C24	2.44	0.48
5:E:9:GLY:HA2	5:E:12:ALA:HB3	1.95	0.48
1:A:27:PRO:HG2	1:A:30:VAL:HG23	1.95	0.48
6:F:17:PHE:CE1	11:F:104:7PH:H29	2.49	0.47
12:A:306:8K6:H61C	12:A:306:8K6:H101	1.97	0.47
12:A:308:8K6:H72C	12:A:308:8K6:H131	1.97	0.47
24:F:103:1O2:HBQ	24:F:103:1O2:HAWA	1.97	0.47
1:A:129:VAL:HG21	14:B:204:CLA:H43	1.96	0.46
4:D:39:VAL:HG11	20:D:206:2WD:H19	1.97	0.46
4:D:57:LYS:NZ	4:D:63:ASP:OD1	2.49	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.96	0.46
6:F:5:LEU:HD21	7:G:11:LEU:HD12	1.98	0.46
1:A:66:TYR:OH	2:B:63:GLY:O	2.26	0.46
24:F:103:1O2:HBMA	24:F:103:1O2:HBJA	1.74	0.46
4:D:57:LYS:O	4:D:82:GLN:N	2.45	0.46
2:B:41:PRO:HG3	10:B:203[B]:UMQ:HF1	1.97	0.45
2:B:153:LYS:HG3	2:B:158:GLY:H	1.81	0.45
15:B:205:OPC:HAH2	15:B:205:OPC:HAA3	1.61	0.45
4:D:118:ASN:HD22	4:D:125:LYS:HE2	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:101:2WA:CBL	22:F:101:2WA:H34	2.46	0.45
24:F:103:1O2:HBSA	24:F:103:1O2:CAZ	2.45	0.45
4:D:25:GLY:HA2	18:D:204:SQD:H311	1.99	0.45
5:E:10:PHE:HD2	8:H:13:VAL:HG21	1.81	0.45
11:C:303:7PH:H33A	11:C:303:7PH:H36	1.74	0.45
3:C:209:ASP:OD1	3:C:210:THR:N	2.50	0.45
5:E:11:LEU:HD22	5:E:11:LEU:HA	1.78	0.45
1:A:53:ALA:HB1	4:D:41:TYR:CE1	2.52	0.45
2:B:131:THR:HG23	11:B:206:7PH:H25	1.98	0.45
6:F:27:LEU:HD21	8:H:27:ASN:HA	1.98	0.45
1:A:129:VAL:HG21	14:B:204:CLA:H11	1.99	0.45
3:C:160:VAL:O	9:C:301:HEC:HAC	2.17	0.45
9:A:303:HEC:C1A	10:B:203[B]:UMQ:H62	2.47	0.45
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.99	0.45
11:B:206:7PH:H35A	11:B:206:7PH:H38	1.68	0.44
4:D:117:TRP:HE1	4:D:119:ALA:HB2	1.83	0.44
6:F:20:TRP:CD2	11:F:104:7PH:H34A	2.52	0.44
9:A:303:HEC:HBA2	10:B:203[B]:UMQ:H41	2.00	0.44
3:C:182:LYS:HB2	3:C:198:ASP:H	1.82	0.44
11:F:104:7PH:H39A	11:F:104:7PH:H36	1.72	0.44
2:B:156:THR:HG22	2:B:159:LEU:H	1.81	0.44
10:A:304:UMQ:HB1	10:A:304:UMQ:H2'1	2.01	0.43
2:B:103:SER:OG	15:B:205:OPC:HBD2	2.18	0.43
3:C:54:TYR:HB3	3:C:155:ARG:HD3	1.99	0.43
3:C:193:VAL:HB	3:C:213:ALA:HB2	2.00	0.43
12:A:308:8K6:H171	12:A:308:8K6:H142	1.68	0.43
3:C:59:GLN:CB	3:C:67:LYS:HG3	2.49	0.43
11:F:104:7PH:H27A	25:G:102:BCR:C22	2.49	0.43
12:B:202[A]:8K6:H112	12:B:202[A]:8K6:H142	1.64	0.43
22:F:101:2WA:H44	7:G:2:VAL:HG11	2.00	0.42
25:G:102:BCR:H361	25:G:102:BCR:H20C	1.80	0.42
15:B:205:OPC:HBP1	15:B:205:OPC:HBS	1.79	0.42
5:E:16:GLY:CA	24:F:103:1O2:HBUA	2.49	0.42
4:D:116:PRO:HD2	4:D:127:PRO:HD3	2.01	0.42
12:A:308:8K6:H132	12:A:308:8K6:H62C	2.01	0.42
3:C:177:THR:HG23	3:C:226:THR:HA	2.01	0.42
4:D:167:GLU:HG2	4:D:168:THR:H	1.85	0.42
1:A:92:MET:SD	21:E:101:3WM:H71	2.60	0.42
3:C:51:LYS:HG2	3:C:126:GLU:HG2	2.01	0.42
3:C:53:PRO:HD2	3:C:155:ARG:HH21	1.85	0.42
4:D:84:LEU:C	4:D:86:GLY:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:303:HEC:HMD2	10:B:203[B]:UMQ:H6'2	2.00	0.41
11:B:206:7PH:H35	7:G:22:PHE:CD2	2.54	0.41
4:D:152:HIS:HB2	4:D:163:THR:OG1	2.21	0.41
12:A:307:8K6:H121	12:A:307:8K6:H152	1.84	0.41
2:B:32:TRP:NE1	10:B:201:UMQ:HA2	2.35	0.41
1:A:207:ARG:NH1	10:B:203[B]:UMQ:O2	2.54	0.41
21:E:101:3WM:H58	21:E:101:3WM:H55	1.74	0.41
12:A:306:8K6:H132	12:A:307:8K6:H81C	2.03	0.41
3:C:271:MET:HE2	4:D:22:LEU:HB3	2.02	0.41
4:D:122:ASN:O	4:D:122:ASN:ND2	2.54	0.41
6:F:5:LEU:HD22	22:F:101:2WA:H28	2.01	0.41
26:B:310:HOH:O	3:C:276:LYS:NZ	2.53	0.41
3:C:35:GLU:HB2	3:C:49:VAL:HB	2.03	0.41
3:C:39:SER:HB3	3:C:248:VAL:HB	2.02	0.41
3:C:187:GLU:HB2	3:C:188:GLY:H	1.72	0.41
22:F:101:2WA:H34	22:F:101:2WA:H42	2.03	0.41
1:A:114:ARG:NH2	2:B:21:GLY:O	2.54	0.41
3:C:72:VAL:HG21	3:C:124:TYR:O	2.21	0.41
3:C:254:ARG:HA	11:D:203:7PH:H25	2.03	0.41
11:C:303:7PH:O32	11:C:303:7PH:H34	2.15	0.41
10:A:304:UMQ:CL	10:B:201:UMQ:HI2	2.51	0.41
8:H:17:TRP:O	8:H:21:MET:HG2	2.21	0.41
9:A:303:HEC:HHD	9:A:303:HEC:CBC	2.51	0.40
1:A:107:THR:O	2:B:121:GLN:HB3	2.21	0.40
9:A:303:HEC:HBC2	12:B:202[A]:8K6:H151	2.02	0.40
5:E:16:GLY:HA3	24:F:103:1O2:HBUA	2.03	0.40
4:D:59:GLU:CD	4:D:59:GLU:H	2.29	0.40
17:D:202:MYS:H112	17:D:202:MYS:H82	1.64	0.40
4:D:43:ILE:HA	4:D:44:PRO:HD3	1.91	0.40
11:F:104:7PH:H29A	11:F:104:7PH:H2C	1.82	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	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	24	43
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	277/333 (83%)	249 (90%)	23 (8%)	5 (2%)	6	12
4	D	162/179 (90%)	147 (91%)	15 (9%)	0	100	100
5	E	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	4
6	F	30/34 (88%)	30 (100%)	0	0	100	100
7	G	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	929/1018 (91%)	865 (93%)	57 (6%)	7 (1%)	16	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	SER
1	A	3	ASN
3	C	185	LYS
5	E	11	LEU
3	C	189	GLU
3	C	222	GLY
3	C	188	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/184 (100%)	183 (100%)	0	100	100
2	B	133/134 (99%)	132 (99%)	1 (1%)	73	88
3	C	231/272 (85%)	224 (97%)	7 (3%)	36	64
4	D	133/145 (92%)	129 (97%)	4 (3%)	36	64
5	E	21/21 (100%)	20 (95%)	1 (5%)	23	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	22/24 (92%)	22 (100%)	0	100	100
7	G	29/29 (100%)	29 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
All	All	776/833 (93%)	763 (98%)	13 (2%)	53	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	155	LEU
3	C	34	VAL
3	C	59	GLN
3	C	67	LYS
3	C	70	LEU
3	C	187	GLU
3	C	231	LEU
3	C	267	LEU
4	D	71	GLU
4	D	111	LEU
4	D	115	VAL
4	D	155	THR
5	E	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	FES	D	205	4	0,4,4	-	-	-		
12	8K6	A	306	-	17,17,17	0.07	0	16,16,16	0.85	0
9	HEC	A	303	1,26	46,50,50	2.04	8 (17%)	58,82,82	1.23	3 (5%)
10	UMQ	B	203[B]	-	35,35,35	3.68	17 (48%)	46,46,46	2.11	8 (17%)
23	OCT	F	102	-	7,7,7	0.12	0	6,6,6	0.73	0
13	2WM	A	309	-	43,43,43	0.71	2 (4%)	41,45,45	0.50	0
10	UMQ	D	201	-	35,35,35	3.68	17 (48%)	46,46,46	2.14	9 (19%)
11	7PH	D	203	-	31,31,37	1.30	2 (6%)	33,33,42	1.14	2 (6%)
18	SQD	D	204	-	52,54,54	0.96	3 (5%)	62,65,65	1.41	9 (14%)
15	OPC	B	205	-	53,53,54	1.05	3 (5%)	59,61,64	1.01	2 (3%)
9	HEC	C	301	3	46,50,50	2.02	6 (13%)	58,82,82	1.11	2 (3%)
11	7PH	F	104	-	31,31,37	1.30	2 (6%)	33,33,42	1.20	2 (6%)
25	BCR	G	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
24	1O2	F	103	-	49,49,53	1.46	5 (10%)	57,57,61	1.11	5 (8%)
10	UMQ	A	304	-	35,35,35	3.67	17 (48%)	46,46,46	2.09	7 (15%)
9	HEC	A	301	1	46,50,50	2.03	7 (15%)	58,82,82	1.13	1 (1%)
17	MYS	D	202	-	14,14,14	0.08	0	13,13,13	0.85	0
10	UMQ	B	201	-	35,35,35	3.66	17 (48%)	46,46,46	2.12	6 (13%)
11	7PH	C	303	-	31,31,37	1.29	2 (6%)	33,33,42	1.22	2 (6%)
11	7PH	A	305	-	31,31,37	1.29	2 (6%)	33,33,42	1.20	2 (6%)
12	8K6	A	307	-	17,17,17	0.07	0	16,16,16	0.89	0
10	UMQ	G	101	-	35,35,35	3.67	17 (48%)	46,46,46	2.13	6 (13%)
12	8K6	A	308	-	13,13,17	0.09	0	12,12,16	0.79	0
20	2WD	D	206	-	18,18,18	1.18	1 (5%)	16,20,20	0.52	0
12	8K6	B	202[A]	-	17,17,17	0.07	0	16,16,16	0.86	0
21	3WM	E	101	-	43,43,43	0.79	1 (2%)	41,45,45	0.53	0
22	2WA	F	101	-	39,39,39	0.94	1 (2%)	37,41,41	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	7PH	B	206	-	31,31,37	1.30	2 (6%)	33,33,42	1.17	2 (6%)
9	HEC	A	302	1	46,50,50	2.03	7 (15%)	58,82,82	1.12	3 (5%)
14	CLA	B	204	26	69,73,73	1.19	7 (10%)	82,113,113	1.19	5 (6%)

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
19	FES	D	205	4	-	-	0/1/1/1
12	8K6	A	306	-	-	2/15/15/15	-
9	HEC	A	303	1,26	-	0/14/54/54	-
10	UMQ	B	203[B]	-	-	8/20/60/60	0/2/2/2
23	OCT	F	102	-	-	1/5/5/5	-
13	2WM	A	309	-	-	26/45/45/45	-
10	UMQ	D	201	-	-	7/20/60/60	0/2/2/2
11	7PH	D	203	-	-	13/33/33/39	-
18	SQD	D	204	-	-	16/49/69/69	0/1/1/1
15	OPC	B	205	-	-	19/57/57/60	-
9	HEC	C	301	3	-	2/14/54/54	-
11	7PH	F	104	-	-	12/33/33/39	-
25	BCR	G	102	-	-	7/29/63/63	0/2/2/2
24	1O2	F	103	-	1/1/8/10	25/44/64/68	0/1/1/1
10	UMQ	A	304	-	-	10/20/60/60	0/2/2/2
9	HEC	A	301	1	-	1/14/54/54	-
17	MYS	D	202	-	-	3/12/12/12	-
10	UMQ	B	201	-	-	3/20/60/60	0/2/2/2
11	7PH	C	303	-	-	21/33/33/39	-
11	7PH	A	305	-	-	14/33/33/39	-
12	8K6	A	307	-	-	3/15/15/15	-
10	UMQ	G	101	-	-	6/20/60/60	0/2/2/2
12	8K6	A	308	-	-	8/11/11/15	-
20	2WD	D	206	-	-	7/20/20/20	-
12	8K6	B	202[A]	-	-	5/15/15/15	-
21	3WM	E	101	-	-	24/45/45/45	-
22	2WA	F	101	-	-	21/41/41/41	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	7PH	B	206	-	-	15/33/33/39	-
9	HEC	A	302	1	-	3/14/54/54	-
14	CLA	B	204	26	1/1/15/20	9/39/115/115	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	O5'-C1'	10.69	1.69	1.41
10	D	201	UMQ	O5'-C1'	10.69	1.69	1.41
10	A	304	UMQ	O5'-C1'	10.69	1.69	1.41
10	G	101	UMQ	O5'-C1'	10.69	1.69	1.41
10	B	201	UMQ	O5'-C1'	10.65	1.69	1.41
10	B	201	UMQ	O3'-C3'	8.12	1.63	1.43
10	G	101	UMQ	O3'-C3'	8.09	1.63	1.43
10	B	203[B]	UMQ	O3'-C3'	8.06	1.62	1.43
10	A	304	UMQ	O3'-C3'	8.03	1.62	1.43
10	D	201	UMQ	O3'-C3'	8.01	1.62	1.43
10	A	304	UMQ	O5'-C5'	7.85	1.63	1.44
10	G	101	UMQ	O5'-C5'	7.83	1.63	1.44
10	B	203[B]	UMQ	O5'-C5'	7.82	1.63	1.44
10	D	201	UMQ	O5'-C5'	7.77	1.63	1.44
10	B	201	UMQ	O5'-C5'	7.70	1.63	1.44
9	A	301	HEC	CAB-C3B	6.41	1.55	1.35
9	A	301	HEC	CAC-C3C	6.41	1.55	1.35
9	A	303	HEC	CAB-C3B	6.38	1.55	1.35
9	A	302	HEC	CAB-C3B	6.35	1.55	1.35
9	C	301	HEC	CAC-C3C	6.34	1.55	1.35
9	A	302	HEC	CAC-C3C	6.34	1.55	1.35
9	C	301	HEC	CAB-C3B	6.33	1.55	1.35
9	A	303	HEC	CAC-C3C	6.26	1.55	1.35
10	D	201	UMQ	O5-C5	6.19	1.59	1.44
10	A	304	UMQ	O5-C5	6.01	1.59	1.44
10	B	203[B]	UMQ	O5-C5	6.01	1.59	1.44
10	B	201	UMQ	O5-C5	5.94	1.58	1.44
10	G	101	UMQ	O5-C5	5.93	1.58	1.44
10	B	203[B]	UMQ	C6-C5	-5.87	1.32	1.51
10	B	201	UMQ	C6-C5	-5.84	1.32	1.51
10	D	201	UMQ	C6-C5	-5.82	1.32	1.51
10	A	304	UMQ	C6-C5	-5.81	1.32	1.51
10	G	101	UMQ	C6-C5	-5.79	1.32	1.51
9	C	301	HEC	C3D-C2D	5.77	1.54	1.38
9	A	303	HEC	C3D-C2D	5.74	1.53	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEC	C3D-C2D	5.64	1.53	1.38
9	A	302	HEC	C3D-C2D	5.64	1.53	1.38
10	B	201	UMQ	O1'-C1'	-4.90	1.32	1.40
10	A	304	UMQ	O1'-C1'	-4.89	1.32	1.40
10	D	201	UMQ	O1'-C1'	-4.88	1.32	1.40
10	G	101	UMQ	O1'-C1'	-4.85	1.32	1.40
10	B	203[B]	UMQ	O1'-C1'	-4.82	1.32	1.40
10	A	304	UMQ	C3'-C4'	-4.57	1.39	1.52
10	B	201	UMQ	C3'-C4'	-4.54	1.39	1.52
10	G	101	UMQ	C3'-C4'	-4.52	1.40	1.52
10	D	201	UMQ	C3'-C4'	-4.51	1.40	1.52
10	B	203[B]	UMQ	C3'-C4'	-4.50	1.40	1.52
24	F	103	1O2	CBR-CBQ	4.46	1.57	1.31
24	F	103	1O2	OBG-CBH	4.39	1.46	1.33
10	D	201	UMQ	C3-C2	-4.30	1.41	1.52
10	A	304	UMQ	O2-C2	4.29	1.53	1.43
11	C	303	7PH	O31-C31	4.28	1.45	1.33
11	D	203	7PH	O31-C31	4.28	1.45	1.33
10	G	101	UMQ	C3-C2	-4.28	1.41	1.52
11	F	104	7PH	O31-C31	4.26	1.45	1.33
10	B	203[B]	UMQ	O2-C2	4.26	1.53	1.43
10	B	203[B]	UMQ	C3-C2	-4.25	1.41	1.52
10	D	201	UMQ	O2-C2	4.25	1.53	1.43
11	B	206	7PH	O31-C31	4.25	1.45	1.33
10	B	201	UMQ	O2-C2	4.23	1.53	1.43
10	G	101	UMQ	O2-C2	4.23	1.53	1.43
10	A	304	UMQ	C3-C2	-4.21	1.41	1.52
9	A	302	HEC	CBC-CAC	-4.20	1.33	1.49
11	A	305	7PH	O31-C31	4.20	1.45	1.33
10	B	201	UMQ	C3-C2	-4.19	1.41	1.52
24	F	103	1O2	OAN-CAO	4.18	1.46	1.34
9	A	303	HEC	CBC-CAC	-4.18	1.34	1.49
11	D	203	7PH	O21-C21	4.17	1.46	1.34
11	C	303	7PH	O21-C21	4.17	1.46	1.34
11	F	104	7PH	O21-C21	4.16	1.46	1.34
9	A	302	HEC	CBB-CAB	-4.16	1.34	1.49
11	B	206	7PH	O21-C21	4.15	1.46	1.34
11	A	305	7PH	O21-C21	4.14	1.46	1.34
9	A	301	HEC	CBB-CAB	-4.14	1.34	1.49
9	C	301	HEC	CBB-CAB	-4.14	1.34	1.49
9	A	303	HEC	CBB-CAB	-4.13	1.34	1.49
9	A	301	HEC	CBC-CAC	-4.10	1.34	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	301	HEC	CBC-CAC	-4.10	1.34	1.49
15	B	205	OPC	OBJ-CBK	3.80	1.44	1.33
20	D	206	2WD	O21-C2	-3.72	1.39	1.44
10	G	101	UMQ	C4-C5	3.69	1.60	1.53
10	D	201	UMQ	C4-C5	3.68	1.60	1.53
14	B	204	CLA	C1D-ND	3.66	1.42	1.37
10	B	201	UMQ	C4-C5	3.64	1.60	1.53
10	B	203[B]	UMQ	C4-C5	3.62	1.60	1.53
10	A	304	UMQ	C4-C5	3.62	1.60	1.53
10	A	304	UMQ	C3'-C2'	-3.60	1.43	1.52
25	G	102	BCR	C1-C6	-3.58	1.49	1.53
10	B	201	UMQ	C3'-C2'	-3.55	1.43	1.52
10	G	101	UMQ	C3'-C2'	-3.53	1.43	1.52
10	B	203[B]	UMQ	C3'-C2'	-3.52	1.43	1.52
10	D	201	UMQ	C3'-C2'	-3.49	1.43	1.52
24	F	103	1O2	O5-C1	3.33	1.50	1.41
13	A	309	2WM	CAV-CAW	-3.28	1.35	1.51
14	B	204	CLA	C4B-NB	3.28	1.42	1.37
18	D	204	SQD	O48-C23	3.23	1.42	1.33
10	B	203[B]	UMQ	O3-C3	3.22	1.50	1.43
10	G	101	UMQ	O3-C3	3.20	1.50	1.43
10	B	201	UMQ	O3-C3	3.19	1.50	1.43
10	D	201	UMQ	O3-C3	3.17	1.50	1.43
10	A	304	UMQ	O3-C3	3.16	1.50	1.43
15	B	205	OPC	OAN-CAO	3.06	1.42	1.34
10	B	203[B]	UMQ	C6'-C5'	-3.05	1.41	1.51
10	A	304	UMQ	O1-C4'	2.99	1.51	1.43
10	G	101	UMQ	C6'-C5'	-2.98	1.41	1.51
10	B	203[B]	UMQ	O1-C4'	2.97	1.51	1.43
10	D	201	UMQ	C6'-C5'	-2.96	1.41	1.51
10	B	201	UMQ	C6'-C5'	-2.96	1.41	1.51
25	G	102	BCR	C30-C25	-2.96	1.50	1.53
10	A	304	UMQ	C6'-C5'	-2.94	1.42	1.51
10	G	101	UMQ	O1-C4'	2.90	1.51	1.43
10	D	201	UMQ	O1-C4'	2.89	1.51	1.43
24	F	103	1O2	CAQ-CAO	2.88	1.59	1.50
18	D	204	SQD	O47-C7	2.85	1.42	1.34
10	B	201	UMQ	O1-C4'	2.81	1.51	1.43
14	B	204	CLA	C1B-C2B	2.62	1.49	1.43
10	B	203[B]	UMQ	C1-C2	-2.55	1.45	1.52
10	G	101	UMQ	C1-C2	-2.54	1.45	1.52
10	D	201	UMQ	C1-C2	-2.53	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	204	CLA	C3B-C4B	2.53	1.50	1.42
22	F	101	2WA	CBS-CBR	-2.52	1.39	1.51
13	A	309	2WM	OAN-CAM	-2.51	1.41	1.44
10	B	201	UMQ	C1-C2	-2.51	1.45	1.52
21	E	101	3WM	OAN-CAM	-2.48	1.41	1.44
10	A	304	UMQ	C1-C2	-2.43	1.45	1.52
10	G	101	UMQ	O2'-C2'	2.42	1.48	1.43
10	B	201	UMQ	O2'-C2'	2.42	1.48	1.43
10	D	201	UMQ	O2'-C2'	2.41	1.48	1.43
10	A	304	UMQ	O2'-C2'	2.36	1.48	1.43
14	B	204	CLA	CHC-C1C	2.35	1.43	1.38
10	B	203[B]	UMQ	O2'-C2'	2.33	1.48	1.43
10	D	201	UMQ	O5-C1	2.22	1.47	1.41
9	A	303	HEC	C3C-C2C	-2.20	1.33	1.41
9	A	303	HEC	CMB-C2B	2.20	1.55	1.50
9	A	301	HEC	CMC-C2C	2.17	1.55	1.50
10	A	304	UMQ	O5-C1	2.16	1.47	1.41
9	A	302	HEC	CMB-C2B	2.12	1.55	1.50
10	B	203[B]	UMQ	O5-C1	2.12	1.47	1.41
9	C	301	HEC	CMB-C2B	2.11	1.55	1.50
15	B	205	OPC	CAG-NAF	-2.10	1.45	1.51
10	G	101	UMQ	O5-C1	2.07	1.47	1.41
9	A	303	HEC	CMD-C2D	2.07	1.55	1.50
18	D	204	SQD	O2-C2	-2.05	1.37	1.43
9	A	301	HEC	CMB-C2B	2.05	1.55	1.50
14	B	204	CLA	CMB-C2B	-2.05	1.46	1.50
10	B	201	UMQ	O5-C1	2.03	1.47	1.41
9	A	302	HEC	CMC-C2C	2.02	1.54	1.50
14	B	204	CLA	CMD-C2D	-2.02	1.46	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	201	UMQ	C1'-O5'-C5'	-9.36	95.44	113.72
10	G	101	UMQ	C1'-O5'-C5'	-9.02	96.10	113.72
10	B	203[B]	UMQ	C1'-O5'-C5'	-8.87	96.41	113.72
10	A	304	UMQ	C1'-O5'-C5'	-8.82	96.50	113.72
10	B	201	UMQ	C1'-O5'-C5'	-8.78	96.57	113.72
10	B	203[B]	UMQ	C2'-C3'-C4'	7.01	125.58	109.68
10	D	201	UMQ	C2'-C3'-C4'	6.96	125.47	109.68
10	B	201	UMQ	C2'-C3'-C4'	6.84	125.20	109.68
10	A	304	UMQ	C2'-C3'-C4'	6.82	125.15	109.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	101	UMQ	C2'-C3'-C4'	6.80	125.12	109.68
14	B	204	CLA	C4A-NA-C1A	5.71	109.28	106.68
10	B	201	UMQ	O5-C5-C4	-4.21	102.11	109.70
10	G	101	UMQ	O5-C5-C4	-4.08	102.35	109.70
10	A	304	UMQ	O5-C5-C4	-4.05	102.40	109.70
24	F	103	1O2	OAN-CAO-CAQ	4.02	120.17	111.48
18	D	204	SQD	O9-S-O7	-3.94	101.02	113.82
10	B	201	UMQ	C1-O1-C4'	-3.94	108.65	117.98
10	G	101	UMQ	C1-O1-C4'	-3.88	108.79	117.98
11	C	303	7PH	O21-C21-C22	3.87	119.86	111.48
15	B	205	OPC	OAN-CAO-CAP	3.82	119.74	111.48
11	F	104	7PH	O21-C21-C22	3.76	119.62	111.48
11	A	305	7PH	O21-C21-C22	3.75	119.60	111.48
18	D	204	SQD	O47-C7-C8	3.68	119.44	111.48
9	A	303	HEC	C4D-ND-C1D	3.64	111.75	105.82
10	B	203[B]	UMQ	C1-O1-C4'	-3.58	109.50	117.98
9	C	301	HEC	C4D-ND-C1D	3.54	111.60	105.82
11	B	206	7PH	O21-C21-C22	3.52	119.10	111.48
9	A	301	HEC	C4D-ND-C1D	3.50	111.52	105.82
10	B	203[B]	UMQ	O5-C5-C4	-3.41	103.56	109.70
9	A	302	HEC	C4D-ND-C1D	3.36	111.30	105.82
10	A	304	UMQ	C1-O1-C4'	-3.28	110.21	117.98
18	D	204	SQD	O6-C1-C2	3.18	113.10	108.27
11	D	203	7PH	O21-C21-C22	3.13	118.26	111.48
18	D	204	SQD	O9-S-C6	3.12	111.42	106.76
10	D	201	UMQ	O5-C5-C4	-3.06	104.19	109.70
18	D	204	SQD	O7-S-C6	3.02	111.26	106.76
14	B	204	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	F	103	1O2	OBG-CBH-CBJ	2.74	120.20	111.83
14	B	204	CLA	C3B-C4B-NB	-2.74	108.08	110.53
10	D	201	UMQ	O5-C1-C2	2.72	115.97	110.37
25	G	102	BCR	C27-C26-C25	2.72	126.38	122.70
11	C	303	7PH	O31-C31-C32	2.69	120.05	111.83
15	B	205	OPC	OBJ-CBK-CBL	2.69	120.03	111.83
18	D	204	SQD	O48-C23-C24	2.67	119.99	111.83
11	B	206	7PH	O31-C31-C32	2.67	119.97	111.83
11	F	104	7PH	O31-C31-C32	2.66	119.95	111.83
9	A	303	HEC	C2A-C1A-NA	-2.64	107.77	110.32
25	G	102	BCR	C33-C5-C6	-2.62	121.62	124.48
11	A	305	7PH	O31-C31-C32	2.61	119.78	111.83
10	A	304	UMQ	C1-C2-C3	2.47	115.20	110.01
10	G	101	UMQ	C1-C2-C3	2.41	115.07	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	204	SQD	C44-O6-C1	2.40	118.95	113.80
10	D	201	UMQ	C1-C2-C3	2.39	115.04	110.01
10	D	201	UMQ	C1-O1-C4'	-2.38	112.34	117.98
11	D	203	7PH	O31-C31-C32	2.35	118.99	111.83
9	A	302	HEC	C2A-C1A-NA	-2.34	108.07	110.32
18	D	204	SQD	O8-S-C6	2.32	110.45	105.97
25	G	102	BCR	C7-C8-C9	-2.31	122.81	126.23
18	D	204	SQD	O5-C5-C4	2.28	113.81	109.70
10	B	203[B]	UMQ	O5-C5-C6	2.27	112.06	106.44
10	D	201	UMQ	C1-O5-C5	2.26	118.14	113.72
10	B	203[B]	UMQ	C1-C2-C3	2.24	114.72	110.01
10	B	203[B]	UMQ	O5'-C5'-C4'	2.22	114.31	109.72
25	G	102	BCR	C24-C23-C22	-2.22	122.95	126.23
14	B	204	CLA	CHB-C4A-NA	2.20	127.58	124.40
10	G	101	UMQ	C3-C4-C5	2.19	114.21	110.23
9	A	303	HEC	CBC-CAC-C3C	-2.15	123.14	127.43
9	C	301	HEC	C2A-C1A-NA	-2.14	108.26	110.32
24	F	103	1O2	O5-C1-C2	2.13	114.75	110.37
24	F	103	1O2	C1-C2-C3	2.12	114.46	110.01
24	F	103	1O2	C4-C3-C2	2.10	114.52	110.83
10	A	304	UMQ	O5-C1-C2	2.09	114.66	110.37
10	D	201	UMQ	O3'-C3'-C2'	-2.08	105.47	110.38
9	A	302	HEC	CBD-CAD-C3D	-2.05	106.85	112.53
10	B	201	UMQ	C1-C2-C3	2.05	114.32	110.01
10	D	201	UMQ	C3-C4-C5	2.02	113.89	110.23
10	B	201	UMQ	O3'-C3'-C2'	-2.01	105.63	110.38
10	A	304	UMQ	O5-C5-C6	2.01	111.43	106.44
10	B	203[B]	UMQ	C6'-C5'-C4'	-2.01	107.72	113.38
14	B	204	CLA	CAA-CBA-CGA	-2.00	107.53	113.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	B	204	CLA	ND
24	F	103	1O2	C1

All (291) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	301	HEC	C2C-C3C-CAC-CBC
9	C	301	HEC	C4C-C3C-CAC-CBC
10	A	304	UMQ	O5'-C1'-O1'-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	203[B]	UMQ	O5'-C1'-O1'-CA
11	A	305	7PH	O11-C1-C2-C3
11	A	305	7PH	O11-C1-C2-O21
11	B	206	7PH	O11-C1-C2-C3
11	B	206	7PH	O11-C1-C2-O21
11	C	303	7PH	O11-C1-C2-C3
11	C	303	7PH	O11-C1-C2-O21
11	C	303	7PH	O32-C31-O31-C3
11	C	303	7PH	C32-C31-O31-C3
11	D	203	7PH	O11-C1-C2-O21
11	D	203	7PH	C22-C21-O21-C2
11	F	104	7PH	O11-C1-C2-C3
11	F	104	7PH	O11-C1-C2-O21
13	A	309	2WM	OAD-CAO-OAN-CAM
13	A	309	2WM	OAK-CAL-CAM-OAN
13	A	309	2WM	OCC-CBK-CBL-CBM
18	D	204	SQD	O6-C44-C45-O47
18	D	204	SQD	O47-C45-C46-O48
20	D	206	2WD	O11-C1-C2-C3
20	D	206	2WD	O11-C1-C2-O21
20	D	206	2WD	C1-C2-O21-C21
21	E	101	3WM	OAD-CAO-OAN-CAM
21	E	101	3WM	OAK-CAL-CAM-OAN
21	E	101	3WM	OAK-CAL-CAM-CBI
21	E	101	3WM	OCC-CBK-OBJ-CBI
21	E	101	3WM	OCC-CBK-CBL-CBM
22	F	101	2WA	OAD-CAO-OAN-CAM
22	F	101	2WA	OAK-CAL-CAM-OAN
25	G	102	BCR	C22-C23-C24-C25
10	D	201	UMQ	O5-C1-O1-C4'
11	F	104	7PH	O22-C21-O21-C2
11	A	305	7PH	C32-C31-O31-C3
11	D	203	7PH	C32-C31-O31-C3
11	D	203	7PH	O22-C21-O21-C2
22	F	101	2WA	CBP-CBQ-CBR-CBS
11	A	305	7PH	O32-C31-O31-C3
24	F	103	1O2	OBI-CBH-OBG-CBF
24	F	103	1O2	O5-C5-C6-O6
11	A	305	7PH	C22-C21-O21-C2
11	B	206	7PH	C22-C21-O21-C2
11	F	104	7PH	C22-C21-O21-C2
15	B	205	OPC	CAP-CAO-OAN-CAM

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	F	103	1O2	CBJ-CBK-CBL-CBM
24	F	103	1O2	CBL-CBM-CBN-CBO
18	D	204	SQD	O5-C1-O6-C44
11	C	303	7PH	C31-C32-C33-C34
24	F	103	1O2	CBP-CBQ-CBR-CBS
11	A	305	7PH	C22-C23-C24-C25
22	F	101	2WA	CBR-CBS-CBT-CBU
11	D	203	7PH	O32-C31-O31-C3
11	B	206	7PH	C32-C31-O31-C3
11	F	104	7PH	C32-C31-O31-C3
24	F	103	1O2	CBJ-CBH-OBG-CBF
10	D	201	UMQ	C2'-C1'-O1'-CA
18	D	204	SQD	C2-C1-O6-C44
24	F	103	1O2	C2-C1-O1-CAL
11	B	206	7PH	O32-C31-O31-C3
25	G	102	BCR	C7-C8-C9-C34
13	A	309	2WM	CAU-CAV-CAW-CAX
24	F	103	1O2	C4-C5-C6-O6
15	B	205	OPC	CBK-CBL-CBM-CBN
14	B	204	CLA	C10-C11-C12-C13
24	F	103	1O2	O5-C1-O1-CAL
11	F	104	7PH	O32-C31-O31-C3
13	A	309	2WM	OAN-CAO-CAP-CAQ
11	A	305	7PH	O22-C21-O21-C2
11	B	206	7PH	O22-C21-O21-C2
15	B	205	OPC	OAD-CAO-OAN-CAM
13	A	309	2WM	CBN-CBO-CBP-CBQ
11	A	305	7PH	C32-C33-C34-C35
25	G	102	BCR	C11-C10-C9-C8
11	A	305	7PH	C31-C32-C33-C34
10	D	201	UMQ	O5-C5-C6-O6
11	D	203	7PH	C22-C23-C24-C25
10	B	203[B]	UMQ	O5-C5-C6-O6
10	G	101	UMQ	O5-C5-C6-O6
13	A	309	2WM	OAD-CAO-CAP-CAQ
20	D	206	2WD	O22-C21-C22-C23
21	E	101	3WM	CBL-CBM-CBN-CBO
24	F	103	1O2	CAS-CAT-CAU-CAV
11	A	305	7PH	C33-C34-C35-C36
12	A	307	8K6	C5-C6-C7-C8
18	D	204	SQD	C9-C10-C11-C12
24	F	103	1O2	CBH-CBJ-CBK-CBL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	201	UMQ	O5-C1-O1-C4'
14	B	204	CLA	C3A-C2A-CAA-CBA
12	A	308	8K6	C12-C13-C14-C15
13	A	309	2WM	CBM-CBN-CBO-CBP
24	F	103	1O2	CAY-CAZ-CBA-CBB
22	F	101	2WA	CAQ-CAR-CAS-CAT
24	F	103	1O2	CAT-CAU-CAV-CAW
15	B	205	OPC	CAS-CAT-CAU-CAV
21	E	101	3WM	CBM-CBN-CBO-CBP
17	D	202	MYS	C7-C8-C9-C10
10	B	203[B]	UMQ	CA-CB-CC-CD
13	A	309	2WM	CBT-CBU-CBV-CBW
18	D	204	SQD	C31-C32-C33-C34
22	F	101	2WA	CBN-CBO-CBP-CBQ
11	C	303	7PH	C22-C21-O21-C2
18	D	204	SQD	C8-C7-O47-C45
11	C	303	7PH	C21-C22-C23-C24
15	B	205	OPC	CBL-CBM-CBN-CBO
21	E	101	3WM	CAP-CAQ-CAR-CAS
10	A	304	UMQ	CG-CH-CI-CJ
12	A	308	8K6	C13-C14-C15-C16
11	B	206	7PH	C33-C34-C35-C36
11	B	206	7PH	C24-C25-C26-C27
13	A	309	2WM	CAY-CAZ-CBA-CBB
15	B	205	OPC	CAR-CAS-CAT-CAU
21	E	101	3WM	CBB-CBC-CBD-CBE
11	B	206	7PH	C25-C26-C27-C28
10	G	101	UMQ	O5'-C5'-C6'-O6'
20	D	206	2WD	O21-C2-C3-O31
21	E	101	3WM	CBS-CBT-CBU-CBV
13	A	309	2WM	CAS-CAT-CAU-CAV
10	B	203[B]	UMQ	O1'-CA-CB-CC
22	F	101	2WA	CBT-CBU-CBV-CBW
24	F	103	1O2	CBQ-CBR-CBS-CBT
24	F	103	1O2	CAW-CAX-CAY-CAZ
12	A	308	8K6	C11-C10-C9-C8
10	G	101	UMQ	CA-CB-CC-CD
14	B	204	CLA	C1A-C2A-CAA-CBA
21	E	101	3WM	CAW-CAX-CAY-CAZ
21	E	101	3WM	CBO-CBP-CBQ-CBR
22	F	101	2WA	CAW-CAX-CAY-CAZ
11	C	303	7PH	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	G	101	UMQ	C4-C5-C6-O6
10	A	304	UMQ	C5'-C4'-O1-C1
10	D	201	UMQ	O1'-CA-CB-CC
13	A	309	2WM	OBJ-CBK-CBL-CBM
20	D	206	2WD	O21-C21-C22-C23
12	A	306	8K6	C6-C7-C8-C9
22	F	101	2WA	CBA-CBB-CBC-CBD
24	F	103	1O2	CAV-CAW-CAX-CAY
12	B	202[A]	8K6	C9-C10-C11-C12
12	B	202[A]	8K6	C10-C11-C12-C13
18	D	204	SQD	O6-C44-C45-C46
20	D	206	2WD	C1-C2-C3-O31
24	F	103	1O2	O1-CAL-CAM-CBF
24	F	103	1O2	CBR-CBS-CBT-CBU
15	B	205	OPC	CBC-CBD-CBE-CBF
12	A	308	8K6	C9-C10-C11-C12
12	A	308	8K6	C10-C11-C12-C13
17	D	202	MYS	C11-C10-C9-C8
9	A	302	HEC	C2A-CAA-CBA-CGA
21	E	101	3WM	CAS-CAT-CAU-CAV
10	A	304	UMQ	C3'-C4'-O1-C1
22	F	101	2WA	CAY-CAZ-CBA-CBB
11	B	206	7PH	C32-C33-C34-C35
11	D	203	7PH	C2A-C2B-C2C-C2D
14	B	204	CLA	C16-C17-C18-C20
15	B	205	OPC	CBT-CBU-CBV-CBW
13	A	309	2WM	OAN-CAM-CBI-OBJ
15	B	205	OPC	CBU-CBV-CBW-CBX
10	A	304	UMQ	CB-CA-O1'-C1'
11	C	303	7PH	C27-C28-C29-C2A
10	A	304	UMQ	C2'-C1'-O1'-CA
10	B	203[B]	UMQ	C2'-C1'-O1'-CA
10	A	304	UMQ	CC-CD-CF-CG
10	D	201	UMQ	O5'-C1'-O1'-CA
10	A	304	UMQ	C2-C1-O1-C4'
10	D	201	UMQ	C4-C5-C6-O6
11	C	303	7PH	C1-C2-C3-O31
18	D	204	SQD	C44-C45-C46-O48
22	F	101	2WA	CAL-CAM-CBI-OBJ
10	D	201	UMQ	CA-CB-CC-CD
11	D	203	7PH	O11-C1-C2-C3
22	F	101	2WA	OAK-CAL-CAM-CBI

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	F	101	2WA	CAP-CAQ-CAR-CAS
15	B	205	OPC	CAX-CAY-CAZ-CBA
18	D	204	SQD	C11-C12-C13-C14
10	B	203[B]	UMQ	C4-C5-C6-O6
21	E	101	3WM	OBJ-CBK-CBL-CBM
14	B	204	CLA	C16-C17-C18-C19
18	D	204	SQD	C10-C11-C12-C13
21	E	101	3WM	CAX-CAY-CAZ-CBA
15	B	205	OPC	CAP-CAQ-CAR-CAS
11	D	203	7PH	C38-C39-C3A-C3B
10	A	304	UMQ	CH-CI-CJ-CK
12	A	306	8K6	C10-C11-C12-C13
9	A	301	HEC	C2A-CAA-CBA-CGA
22	F	101	2WA	CAM-CBI-OBJ-CBK
11	B	206	7PH	C3-C2-O21-C21
11	C	303	7PH	C3-C2-O21-C21
11	D	203	7PH	C1-C2-O21-C21
11	F	104	7PH	C3-C2-O21-C21
11	F	104	7PH	C1-C2-C3-O31
13	A	309	2WM	CAL-CAM-CBI-OBJ
21	E	101	3WM	CBQ-CBR-CBS-CBT
11	C	303	7PH	O21-C2-C3-O31
15	B	205	OPC	CAW-CAX-CAY-CAZ
12	B	202[A]	8K6	C3-C4-C5-C6
13	A	309	2WM	CBV-CBW-CBX-CBY
11	B	206	7PH	C35-C36-C37-C38
15	B	205	OPC	CBS-CBT-CBU-CBV
11	F	104	7PH	C31-C32-C33-C34
21	E	101	3WM	OAD-CAO-CAP-CAQ
13	A	309	2WM	CBL-CBK-OBJ-CBI
22	F	101	2WA	CBL-CBK-OBJ-CBI
11	F	104	7PH	O21-C21-C22-C23
11	B	206	7PH	C34-C35-C36-C37
14	B	204	CLA	C4-C3-C5-C6
21	E	101	3WM	OAN-CAO-CAP-CAQ
11	A	305	7PH	C34-C35-C36-C37
11	B	206	7PH	C23-C24-C25-C26
22	F	101	2WA	OAN-CAM-CBI-OBJ
24	F	103	1O2	O1-CAL-CAM-OAN
11	C	303	7PH	C26-C27-C28-C29
10	G	101	UMQ	CI-CJ-CK-CL
10	B	203[B]	UMQ	C5'-C4'-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	F	103	1O2	CAR-CAS-CAT-CAU
9	A	302	HEC	C1A-C2A-CAA-CBA
12	B	202[A]	8K6	C11-C12-C13-C14
13	A	309	2WM	CBY-CBZ-CCA-CCB
11	F	104	7PH	C29-C2A-C2B-C2C
11	A	305	7PH	C3-C2-O21-C21
13	A	309	2WM	CBR-CBS-CBT-CBU
13	A	309	2WM	CAZ-CBA-CBB-CBC
15	B	205	OPC	CBV-CBW-CBX-CBY
21	E	101	3WM	CAQ-CAR-CAS-CAT
18	D	204	SQD	C7-C8-C9-C10
12	A	307	8K6	C15-C16-C17-C18
12	A	307	8K6	C13-C14-C15-C16
25	G	102	BCR	C7-C8-C9-C10
10	B	201	UMQ	CB-CA-O1'-C1'
13	A	309	2WM	CBK-CBL-CBM-CBN
10	A	304	UMQ	O5-C1-O1-C4'
11	D	203	7PH	O21-C21-C22-C23
21	E	101	3WM	CAO-CAP-CAQ-CAR
15	B	205	OPC	CBN-CBO-CBP-CBQ
10	G	101	UMQ	O1'-CA-CB-CC
12	B	202[A]	8K6	C6-C7-C8-C9
24	F	103	1O2	OAN-CAM-CBF-OBG
24	F	103	1O2	CBA-CBB-CBC-CBD
14	B	204	CLA	C2-C3-C5-C6
11	D	203	7PH	C28-C29-C2A-C2B
10	B	201	UMQ	C2-C1-O1-C4'
21	E	101	3WM	CBT-CBU-CBV-CBW
12	A	308	8K6	C6-C7-C8-C9
18	D	204	SQD	C15-C16-C17-C18
13	A	309	2WM	CBL-CBM-CBN-CBO
25	G	102	BCR	C23-C24-C25-C30
11	C	303	7PH	C23-C24-C25-C26
10	B	203[B]	UMQ	C3'-C4'-O1-C1
24	F	103	1O2	OBG-CBH-CBJ-CBK
22	F	101	2WA	CBV-CBW-CBX-CBY
12	A	308	8K6	C14-C15-C16-C17
22	F	101	2WA	OBJ-CBK-CBL-CBM
22	F	101	2WA	CAO-CAP-CAQ-CAR
11	A	305	7PH	O21-C21-C22-C23
25	G	102	BCR	C11-C10-C9-C34
12	A	308	8K6	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	F	102	OCT	C1-C2-C3-C4
18	D	204	SQD	C12-C13-C14-C15
11	C	303	7PH	C25-C26-C27-C28
15	B	205	OPC	CAT-CAU-CAV-CAW
21	E	101	3WM	CAV-CAW-CAX-CAY
14	B	204	CLA	O2A-C1-C2-C3
15	B	205	OPC	CBR-CBS-CBT-CBU
22	F	101	2WA	CAT-CAU-CAV-CAW
17	D	202	MYS	C11-C12-C13-C14
25	G	102	BCR	C23-C24-C25-C26
11	C	303	7PH	C24-C25-C26-C27
11	D	203	7PH	C33-C34-C35-C36
13	A	309	2WM	CAW-CAX-CAY-CAZ
21	E	101	3WM	CAT-CAU-CAV-CAW
11	C	303	7PH	C33-C34-C35-C36
14	B	204	CLA	C4B-C3B-CAB-CBB
11	C	303	7PH	O21-C21-C22-C23
24	F	103	1O2	OAN-CAO-CAQ-CAR
13	A	309	2WM	CBA-CBB-CBC-CBD
21	E	101	3WM	CAZ-CBA-CBB-CBC
11	C	303	7PH	C2A-C2B-C2C-C2D
11	A	305	7PH	C21-C22-C23-C24
13	A	309	2WM	CBX-CBY-CBZ-CCA
15	B	205	OPC	OAK-CAL-CAM-OAN
13	A	309	2WM	CBW-CBX-CBY-CBZ
22	F	101	2WA	OCC-CBK-OBJ-CBI
24	F	103	1O2	OAP-CAO-CAQ-CAR
9	A	302	HEC	C3A-C2A-CAA-CBA
13	A	309	2WM	CAM-CBI-OBJ-CBK
11	F	104	7PH	O21-C2-C3-O31
18	D	204	SQD	O47-C7-C8-C9
11	C	303	7PH	O22-C21-C22-C23
11	C	303	7PH	C28-C29-C2A-C2B
15	B	205	OPC	OAK-CAL-CAM-CBI
18	D	204	SQD	C18-C19-C20-C21
11	B	206	7PH	O31-C31-C32-C33

There are no ring outliers.

25 monomers are involved in 103 short contacts:

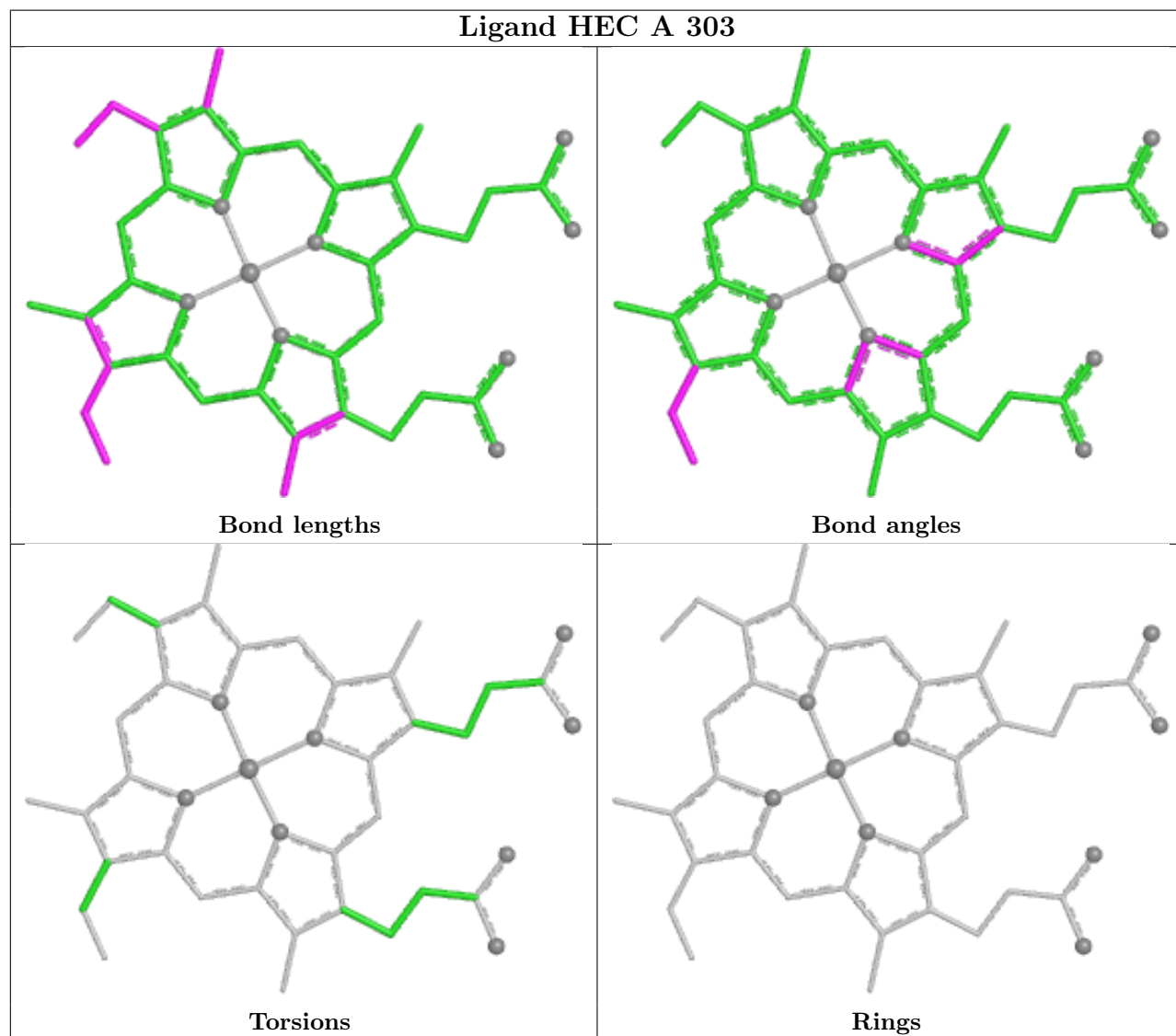
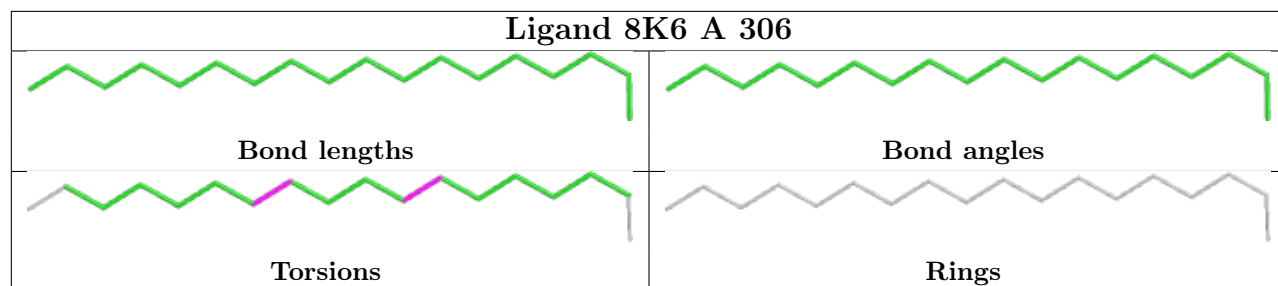
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	306	8K6	2	0

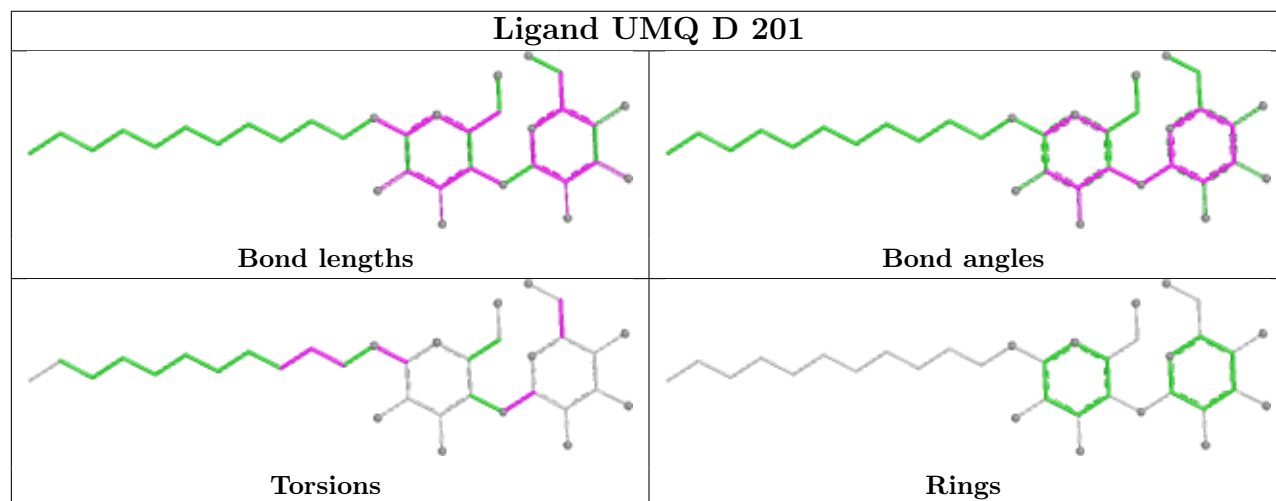
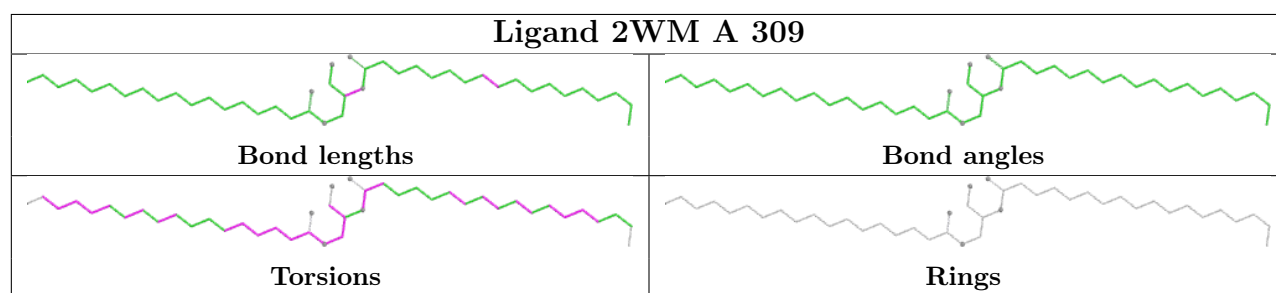
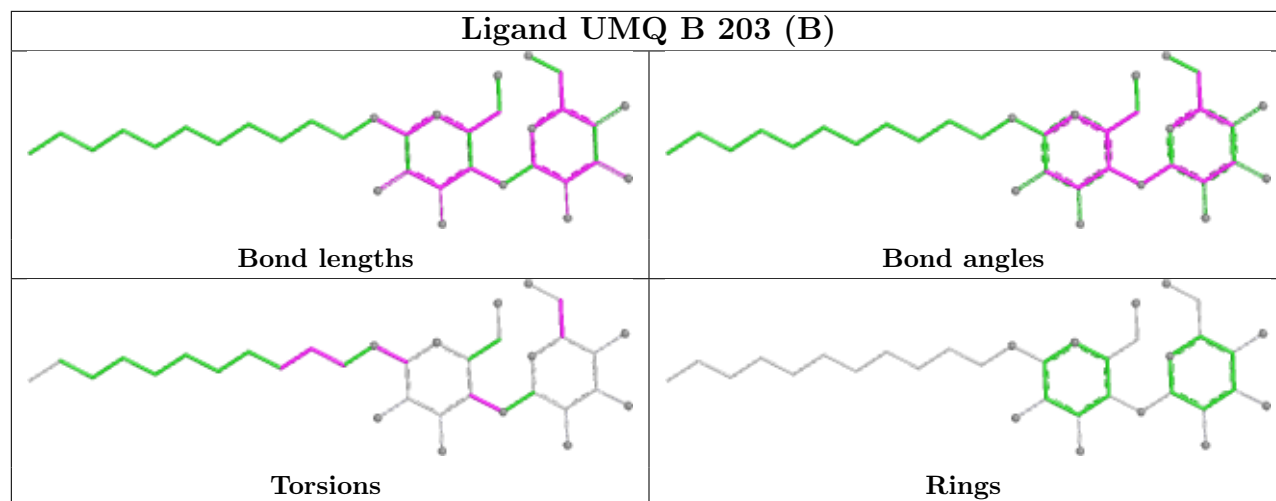
Continued on next page...

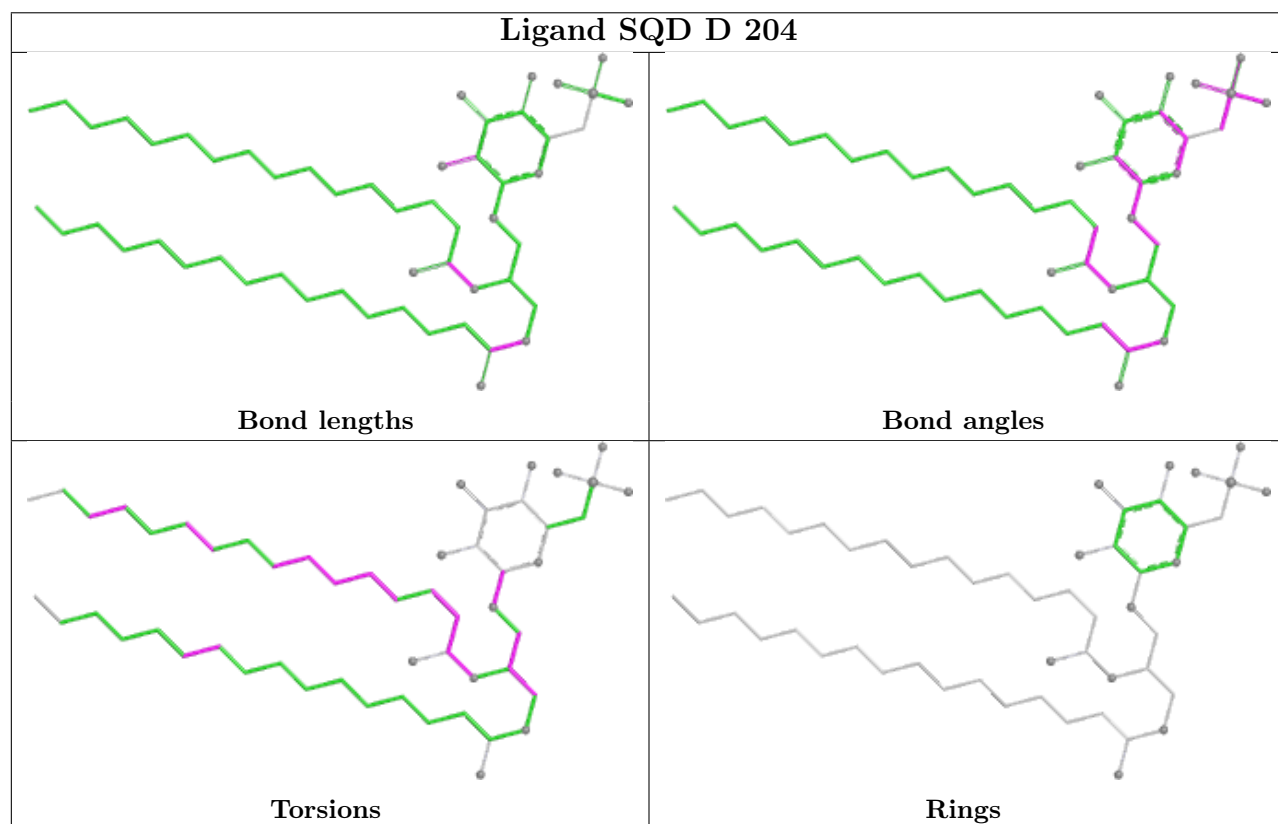
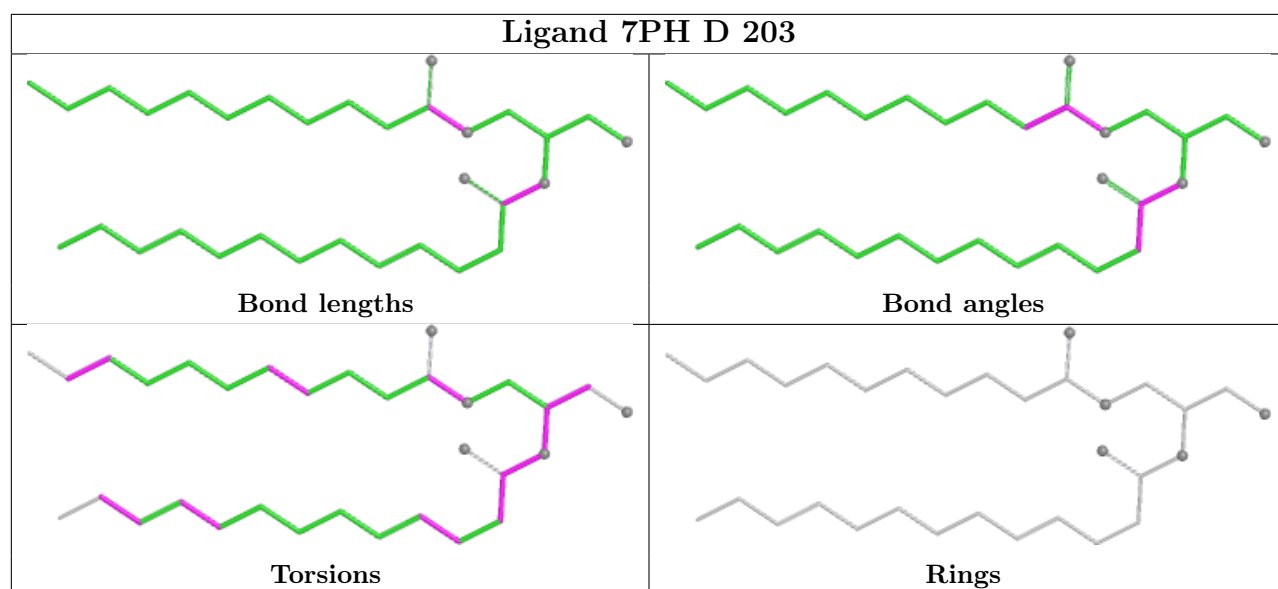
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	303	HEC	6	0
10	B	203[B]	UMQ	10	0
10	D	201	UMQ	4	0
11	D	203	7PH	1	0
18	D	204	SQD	2	0
15	B	205	OPC	5	0
9	C	301	HEC	3	0
11	F	104	7PH	6	0
25	G	102	BCR	2	0
24	F	103	1O2	11	0
10	A	304	UMQ	9	0
17	D	202	MYS	1	0
10	B	201	UMQ	7	0
11	C	303	7PH	4	0
11	A	305	7PH	1	0
12	A	307	8K6	2	0
10	G	101	UMQ	4	0
12	A	308	8K6	5	0
20	D	206	2WD	2	0
12	B	202[A]	8K6	3	0
21	E	101	3WM	9	0
22	F	101	2WA	7	0
11	B	206	7PH	5	0
14	B	204	CLA	4	0

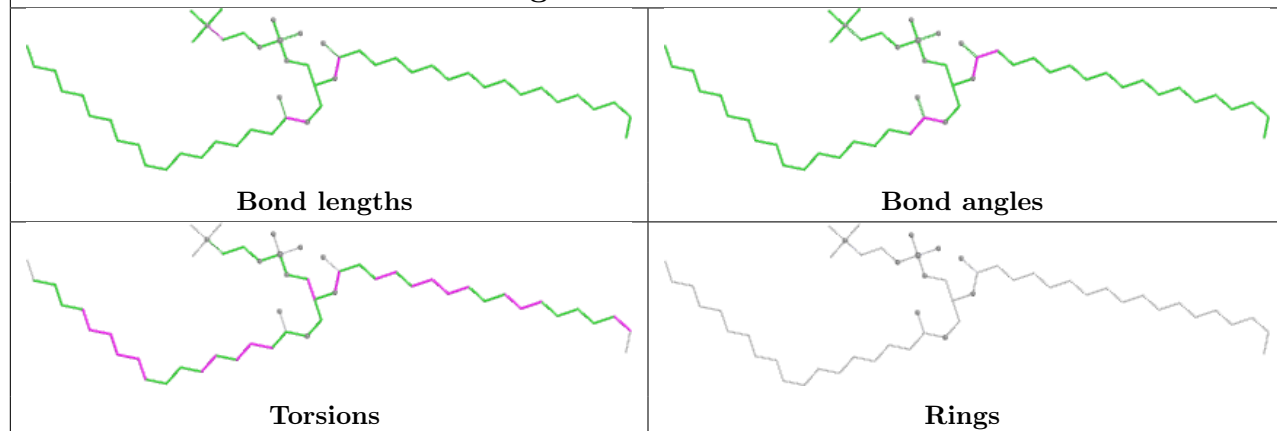
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



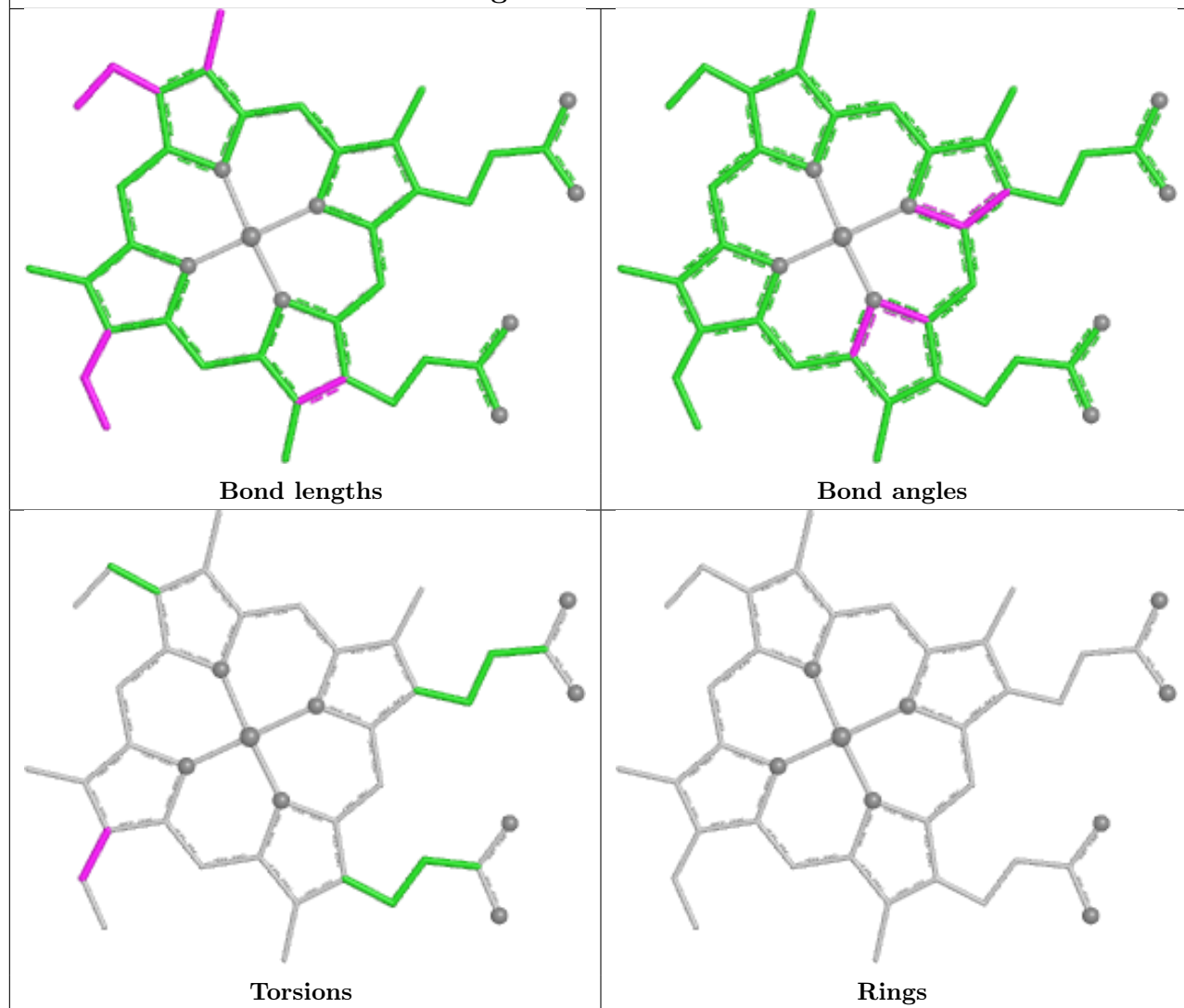


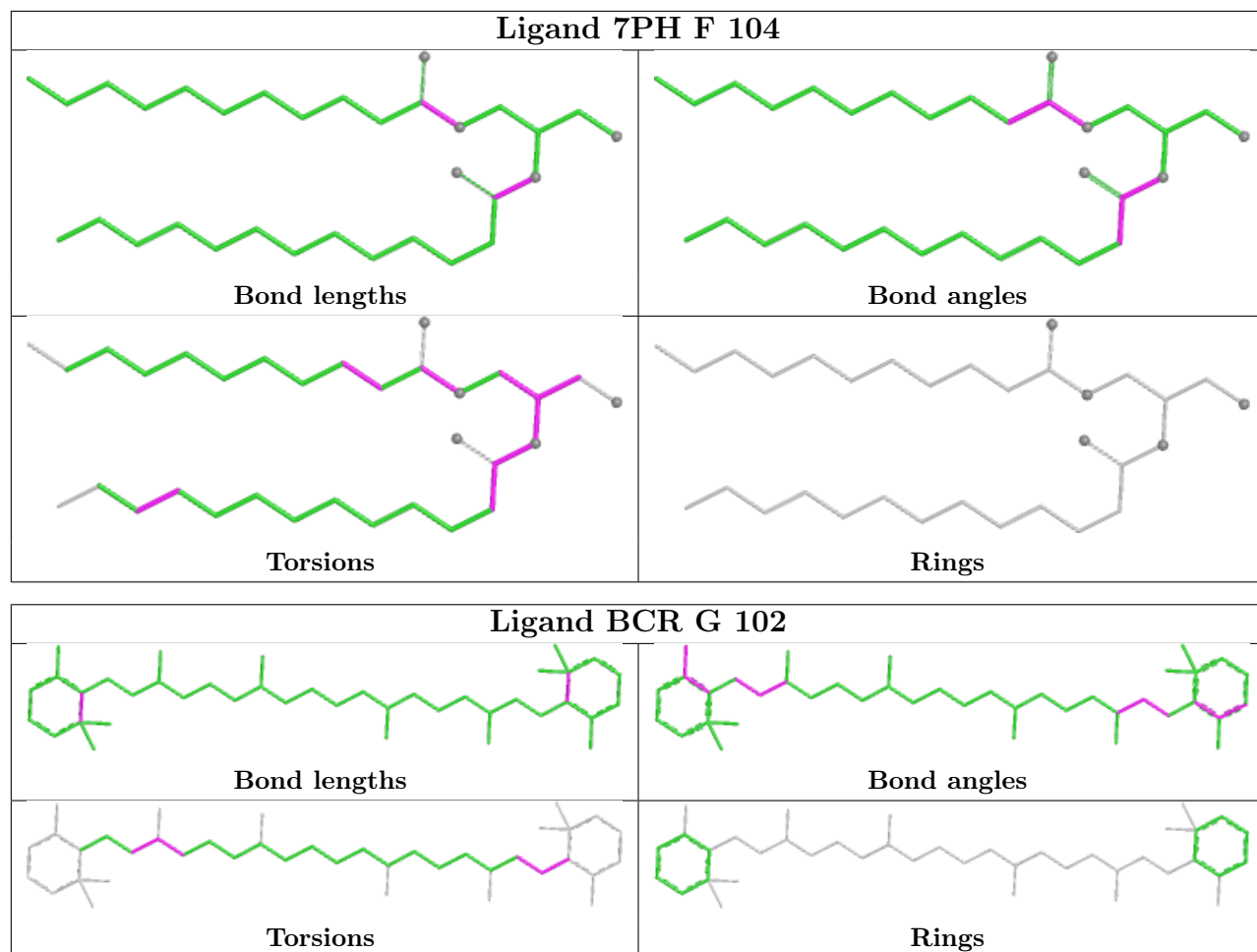


Ligand OPC B 205

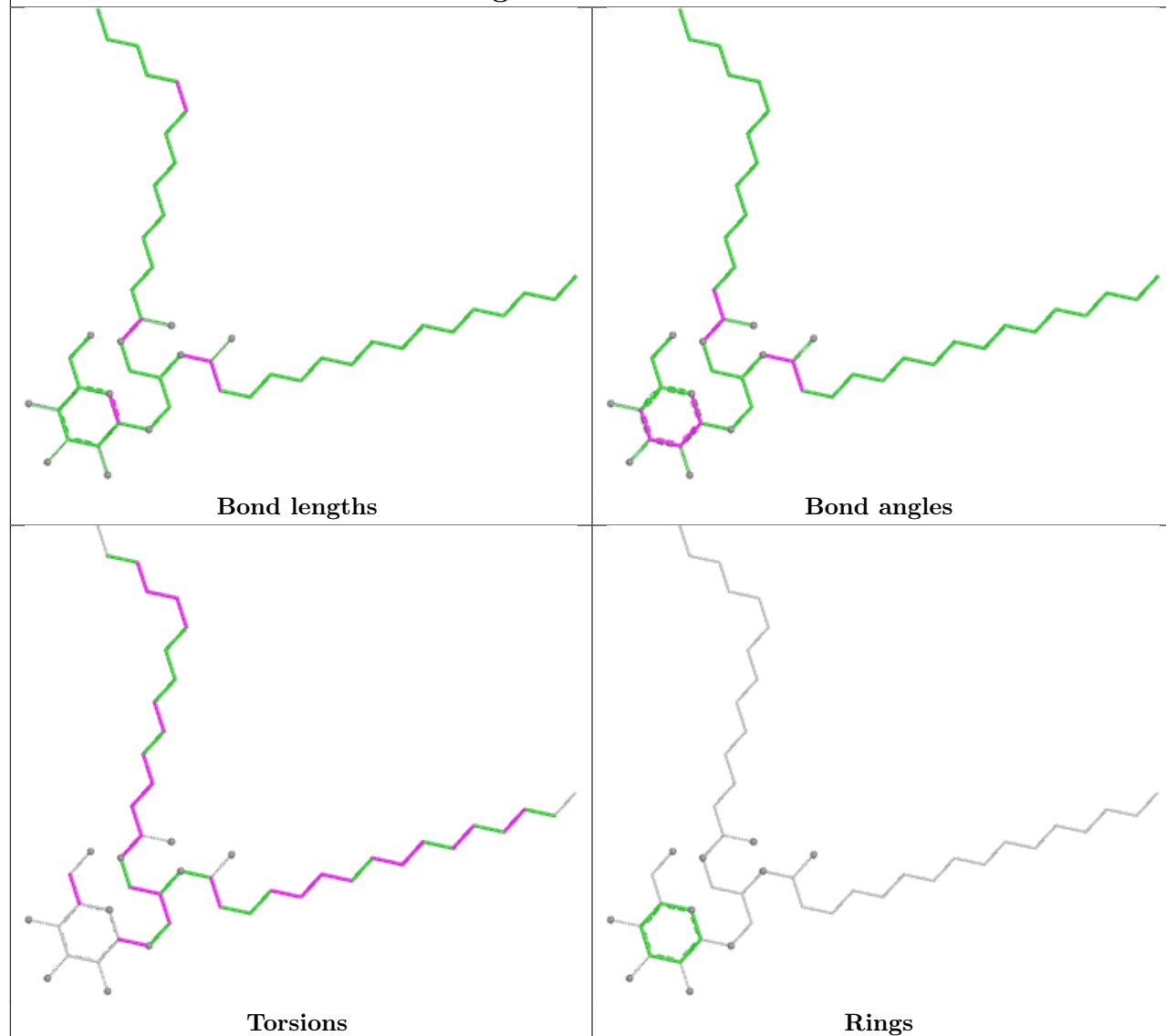


Ligand HEC C 301

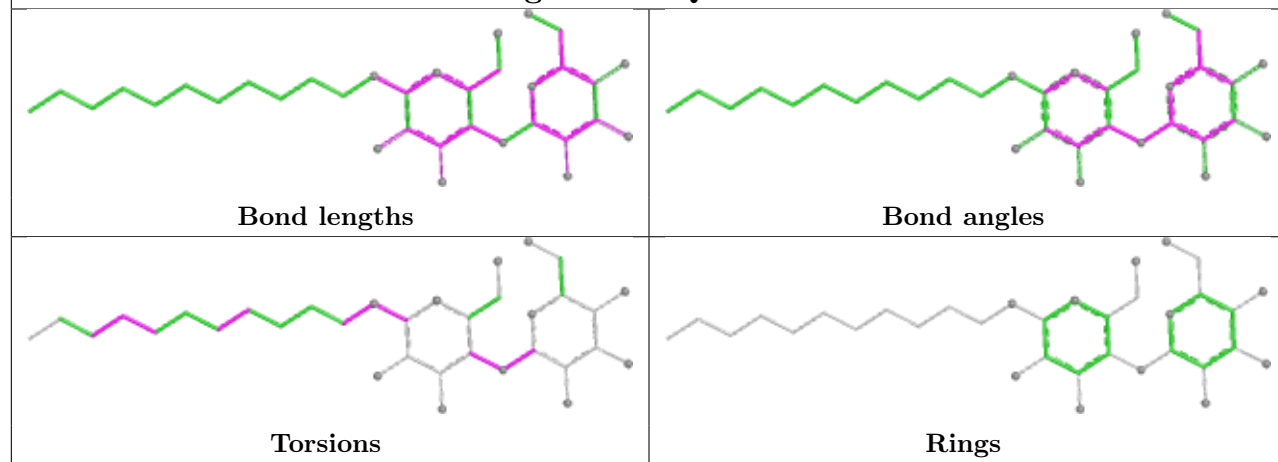




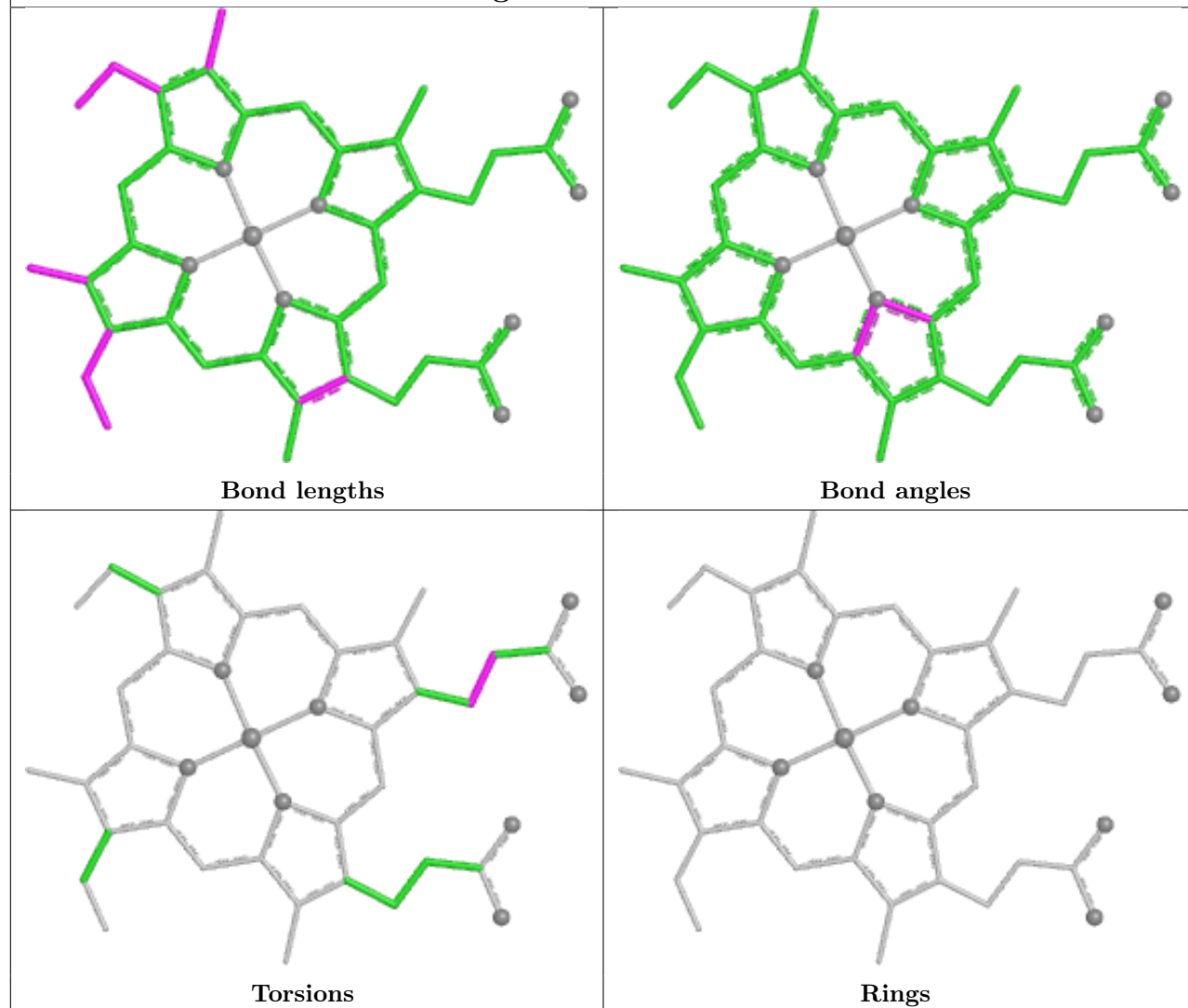
Ligand 1O2 F 103



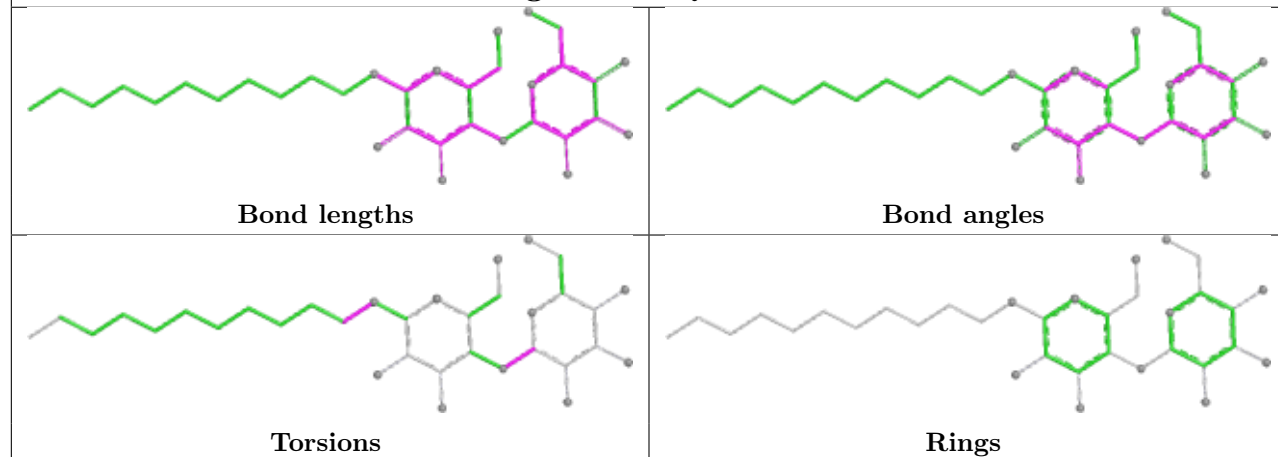
Ligand UMQ A 304

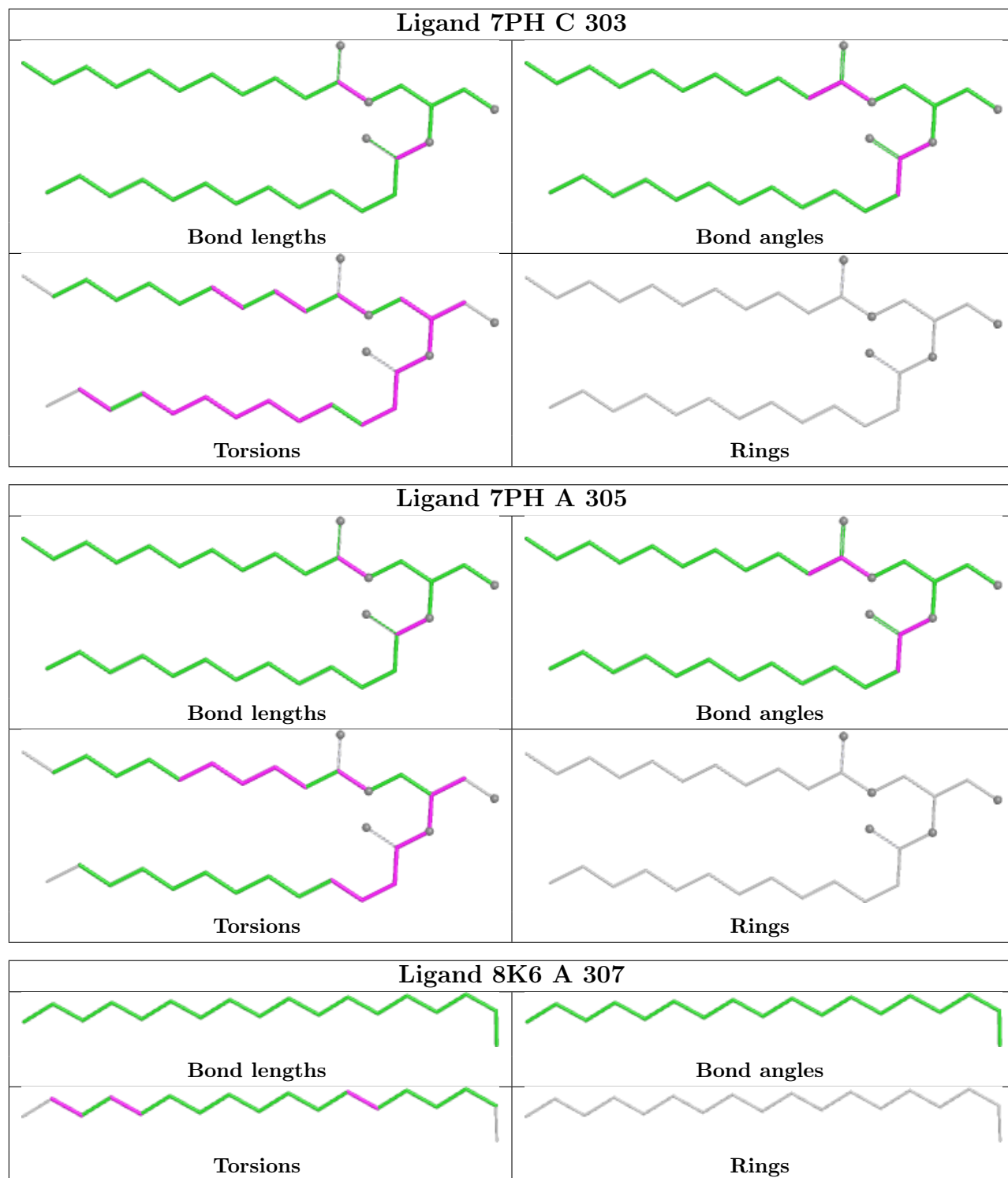


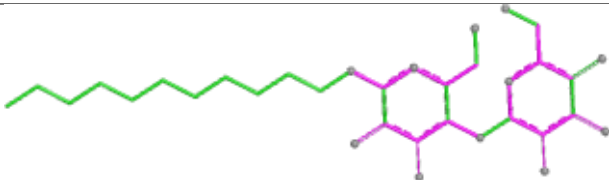
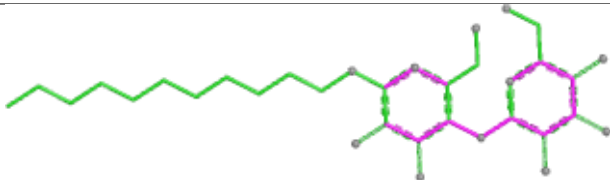
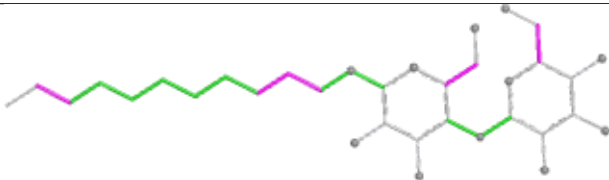
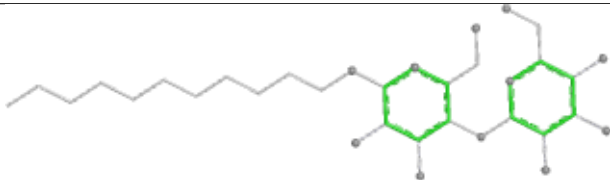
Ligand HEC A 301

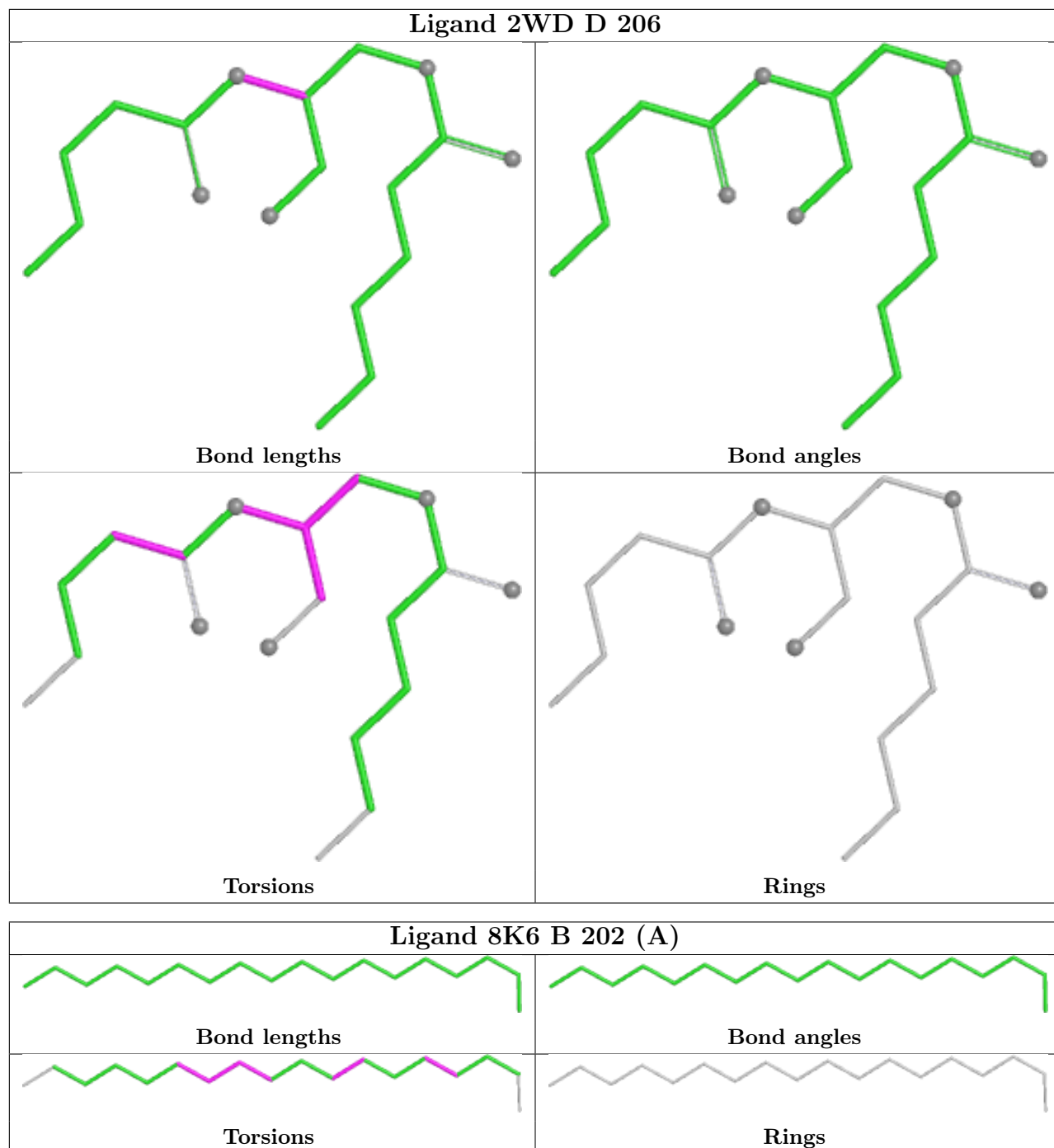


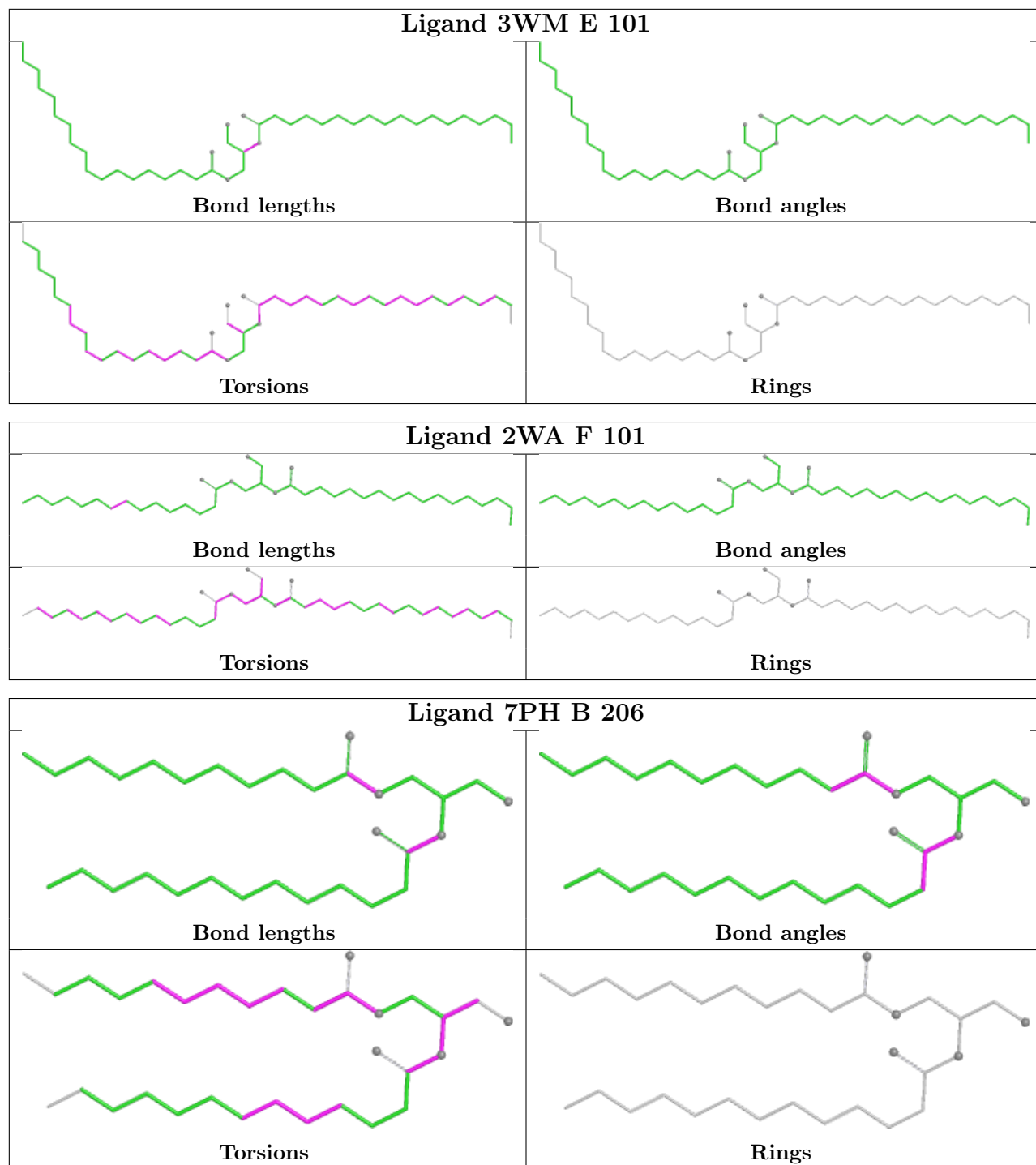
Ligand UMQ B 201



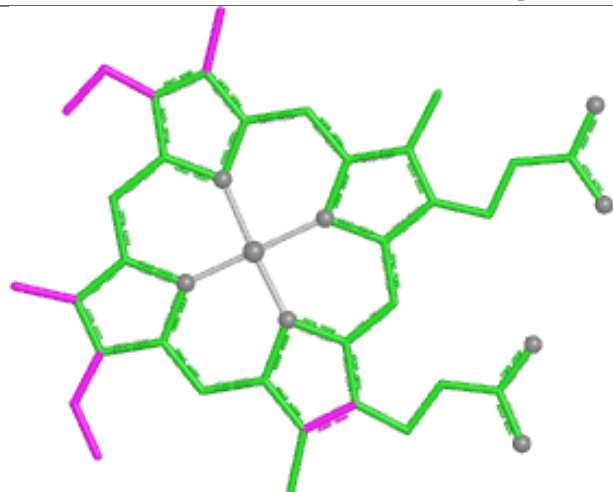


Ligand UMQ G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 8K6 A 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

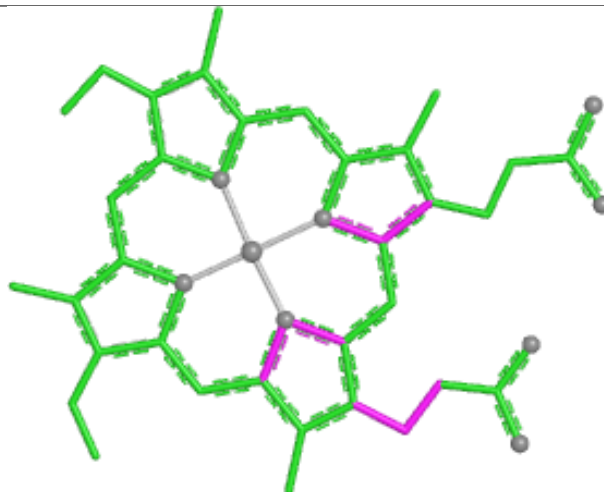




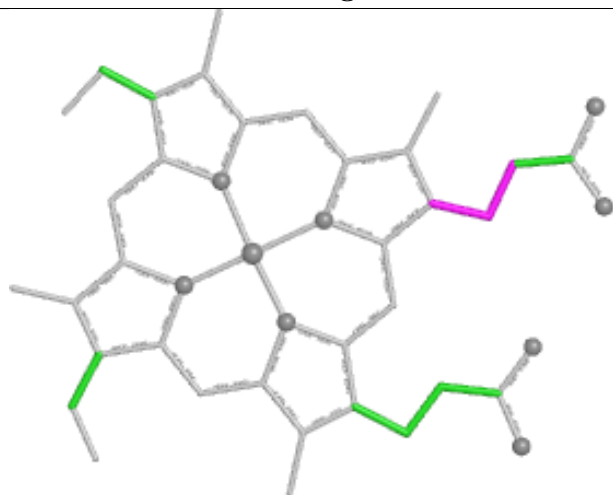
Ligand HEC A 302



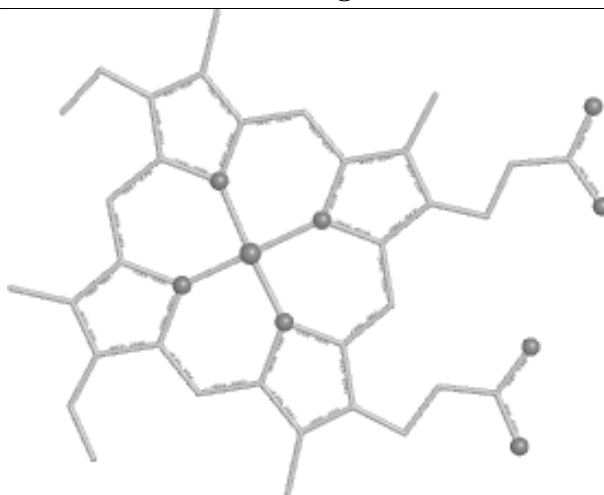
Bond lengths



Bond angles

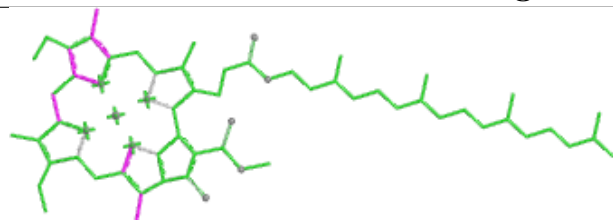


Torsions

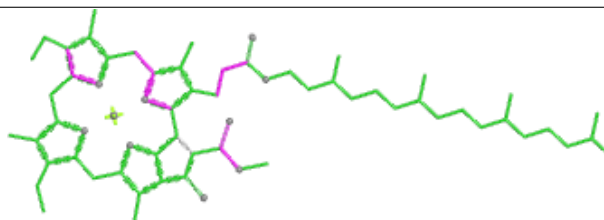


Rings

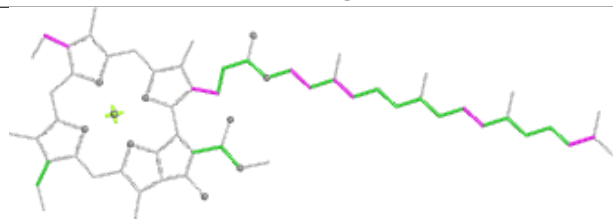
Ligand CLA B 204



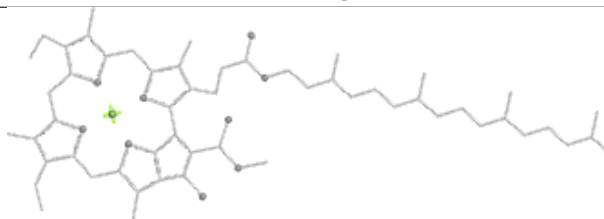
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/215 (99%)	-0.03	5 (2%) 61 57	43, 59, 97, 186	0
2	B	159/160 (99%)	0.30	12 (7%) 20 18	52, 77, 124, 195	0
3	C	281/333 (84%)	0.76	44 (15%) 5 4	57, 85, 191, 249	0
4	D	166/179 (92%)	1.92	65 (39%) 1 0	50, 145, 205, 239	0
5	E	31/31 (100%)	1.11	7 (22%) 2 2	81, 98, 123, 153	0
6	F	32/34 (94%)	0.72	3 (9%) 14 12	69, 87, 131, 169	0
7	G	37/37 (100%)	0.64	5 (13%) 7 5	57, 74, 144, 155	0
8	H	29/29 (100%)	0.29	2 (6%) 23 20	59, 71, 100, 144	0
All	All	949/1018 (93%)	0.70	143 (15%) 5 4	43, 81, 185, 249	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	98	ALA	11.5
4	D	50	ALA	9.1
4	D	99	ILE	7.7
3	C	192	SER	6.6
5	E	10	PHE	6.5
3	C	199	ILE	6.4
3	C	191	GLY	5.8
2	B	160	PHE	5.6
4	D	49	GLY	5.3
4	D	55	THR	5.3
4	D	155	THR	5.2
3	C	224	ALA	5.1
4	D	92	VAL	5.0
3	C	68	VAL	4.9
4	D	56	ALA	4.8
4	D	86	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	48	GLY	4.5
2	B	159	LEU	4.5
3	C	194	LYS	4.5
6	F	1	MET	4.4
3	C	287	MET	4.4
4	D	70	LEU	4.3
4	D	75	VAL	4.3
4	D	84	LEU	4.3
7	G	37	GLY	4.2
4	D	135	ALA	4.2
3	C	183	ILE	4.1
1	A	151	VAL	4.0
4	D	74	ASN	4.0
4	D	71	GLU	3.9
2	B	153	LYS	3.9
3	C	196	LEU	3.8
3	C	288	ASN	3.8
4	D	69	PHE	3.8
4	D	73	HIS	3.7
3	C	198	ASP	3.7
3	C	174	ALA	3.7
3	C	190	ASP	3.7
4	D	173	GLY	3.7
1	A	2	ALA	3.6
7	G	36	GLY	3.6
4	D	57	LYS	3.5
4	D	47	ALA	3.5
3	C	59	GLN	3.5
4	D	85	LYS	3.5
4	D	60	LEU	3.5
3	C	208	SER	3.5
4	D	51	GLY	3.4
8	H	28	GLY	3.4
3	C	226	THR	3.4
3	C	228	GLY	3.4
4	D	172	THR	3.3
4	D	52	GLY	3.3
5	E	9	GLY	3.3
6	F	32	ALA	3.3
1	A	149	LYS	3.2
4	D	61	GLY	3.2
4	D	64	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	184	ALA	3.2
2	B	152	ASP	3.2
4	D	63	ASP	3.2
5	E	29	LYS	3.2
4	D	82	GLN	3.1
4	D	154	LYS	3.1
4	D	139	VAL	3.1
4	D	68	LYS	3.0
3	C	92	GLU	3.0
4	D	147	SER	3.0
4	D	176	PRO	3.0
3	C	217	LEU	3.0
2	B	155	LEU	3.0
2	B	62	THR	3.0
1	A	150	ILE	2.9
3	C	175	ALA	2.9
7	G	1	MET	2.9
1	A	159	PRO	2.9
4	D	179	SER	2.8
3	C	193	VAL	2.8
3	C	177	THR	2.8
4	D	101	ASP	2.8
5	E	27	SER	2.8
4	D	79	THR	2.8
3	C	176	ALA	2.8
3	C	88	ASP	2.8
4	D	122	ASN	2.7
7	G	35	LEU	2.7
8	H	29	LEU	2.7
4	D	167	GLU	2.7
3	C	222	GLY	2.7
6	F	29	ILE	2.7
2	B	142	TRP	2.7
2	B	157	LEU	2.7
3	C	182	LYS	2.7
4	D	165	TRP	2.7
3	C	93	GLU	2.7
4	D	53	GLY	2.6
4	D	103	GLY	2.6
4	D	83	GLY	2.6
7	G	33	ASN	2.6
4	D	46	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	89	THR	2.6
4	D	91	ILE	2.6
3	C	104	GLN	2.6
3	C	218	ILE	2.5
4	D	111	LEU	2.5
2	B	26	TYR	2.5
3	C	34	VAL	2.5
4	D	67	SER	2.5
4	D	16	ARG	2.5
2	B	92	PRO	2.5
4	D	104	ILE	2.5
3	C	173	SER	2.5
4	D	54	THR	2.5
3	C	225	VAL	2.4
3	C	154	ASN	2.4
4	D	123	LYS	2.4
3	C	211	ILE	2.4
4	D	141	ARG	2.4
5	E	31	LEU	2.4
3	C	210	THR	2.3
3	C	219	VAL	2.3
3	C	195	TYR	2.3
2	B	74	GLU	2.3
4	D	102	TYR	2.3
2	B	154	SER	2.2
3	C	70	LEU	2.2
4	D	160	ILE	2.2
4	D	140	VAL	2.2
4	D	119	ALA	2.2
4	D	157	ASN	2.2
5	E	11	LEU	2.2
4	D	170	PHE	2.2
3	C	221	GLU	2.1
4	D	9	ASP	2.1
4	D	120	ALA	2.1
4	D	164	SER	2.1
5	E	1	MET	2.1
3	C	223	GLN	2.0
4	D	130	GLY	2.0
3	C	289	PHE	2.0
4	D	149	ALA	2.0
3	C	234	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	180	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	UMQ	A	304	34/34	0.68	0.25	127,146,201,254	0
10	UMQ	G	101	34/34	0.72	0.20	81,173,199,284	0
20	2WD	D	206	19/19	0.72	0.26	75,123,142,145	0
23	OCT	F	102	8/8	0.74	0.29	101,106,110,116	0
10	UMQ	D	201	34/34	0.78	0.22	102,210,248,264	0
11	7PH	B	206	32/38	0.81	0.23	77,132,182,184	0
11	7PH	C	303	32/38	0.81	0.26	73,117,149,150	0
24	1O2	F	103	49/53	0.81	0.20	80,127,216,220	0
12	8K6	A	306	18/18	0.82	0.23	93,113,147,148	0
13	2WM	A	309	44/44	0.83	0.22	70,96,152,158	0
12	8K6	A	307	18/18	0.84	0.21	76,108,124,127	0
12	8K6	B	202[A]	18/18	0.84	0.24	47,102,122,122	18
11	7PH	F	104	32/38	0.84	0.21	81,101,172,175	0
12	8K6	A	308	14/18	0.85	0.21	62,82,95,99	0
11	7PH	A	305	32/38	0.85	0.24	93,126,189,190	0
10	UMQ	B	201	34/34	0.85	0.18	64,114,151,224	0
18	SQD	D	204	54/54	0.86	0.20	73,116,159,177	0
10	UMQ	B	203[B]	34/34	0.86	0.28	80,103,132,144	34
17	MYS	D	202	15/15	0.88	0.22	93,107,121,126	0
16	CD	C	302	1/1	0.89	0.11	136,136,136,136	1
11	7PH	D	203	32/38	0.89	0.16	54,81,153,157	0
22	2WA	F	101	40/40	0.90	0.20	70,111,169,182	0

Continued on next page...

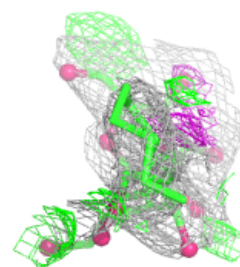
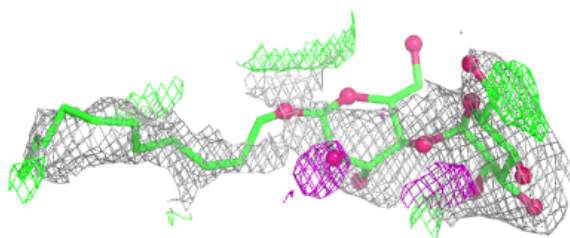
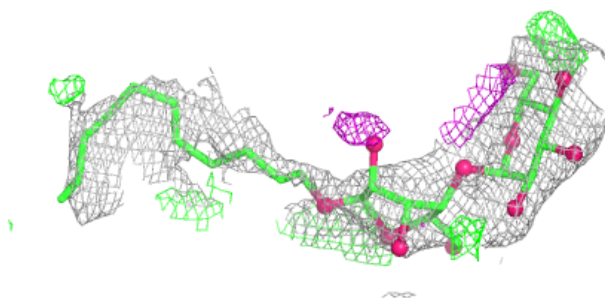
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	OPC	B	205	54/55	0.92	0.17	55,92,121,137	0
25	BCR	G	102	40/40	0.92	0.15	49,74,116,122	0
21	3WM	E	101	44/44	0.93	0.17	60,97,122,125	0
14	CLA	B	204	65/65	0.94	0.12	59,79,107,117	0
9	HEC	C	301	43/43	0.98	0.12	46,69,96,113	0
9	HEC	A	302	43/43	0.98	0.09	34,57,71,76	0
9	HEC	A	303	43/43	0.98	0.09	47,66,85,95	0
9	HEC	A	301	43/43	0.99	0.09	31,50,65,78	0
19	FES	D	205	4/4	0.99	0.07	96,97,100,102	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.

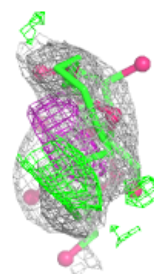
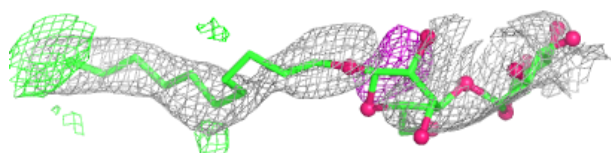
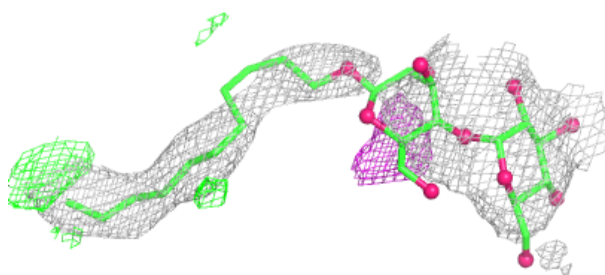
Electron density around UMQ A 304:

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

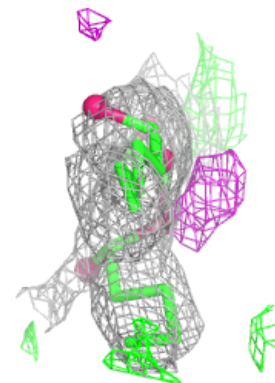
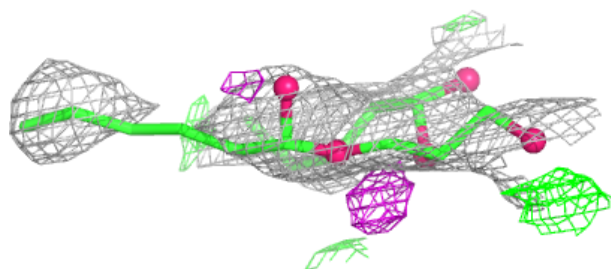
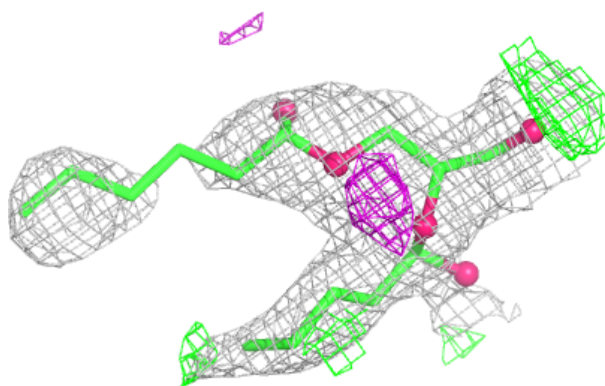


Electron density around UMQ G 101:

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

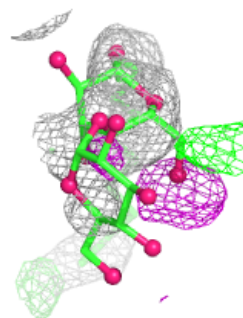
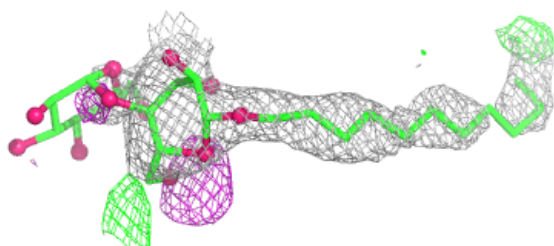
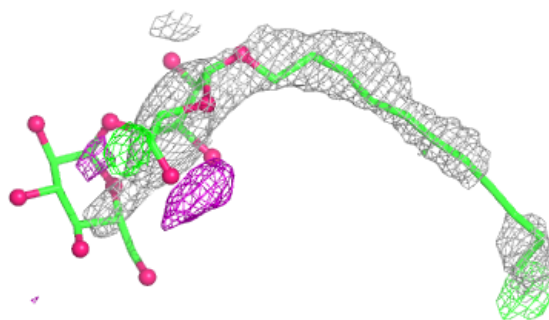
**Electron density around 2WD D 206:**

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



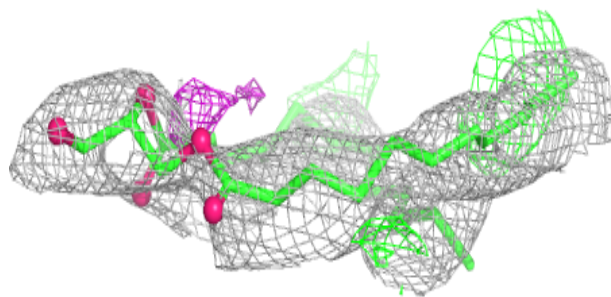
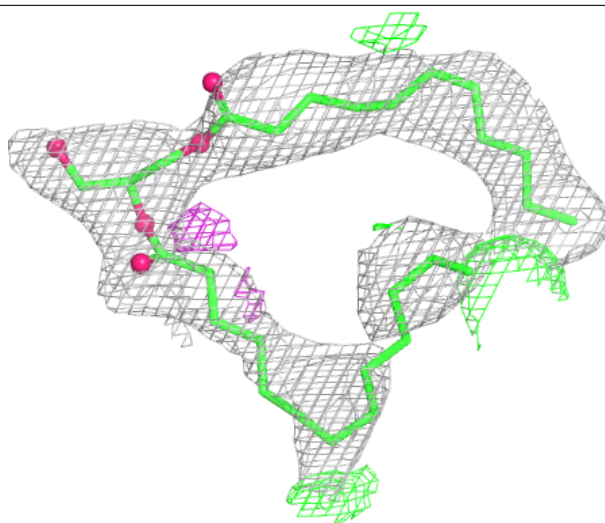
Electron density around UMQ D 201:

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



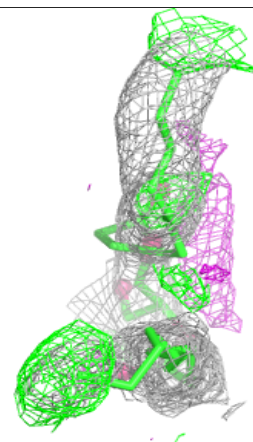
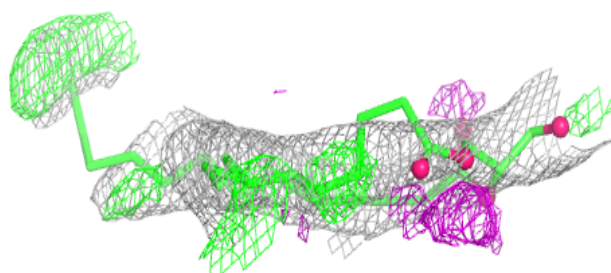
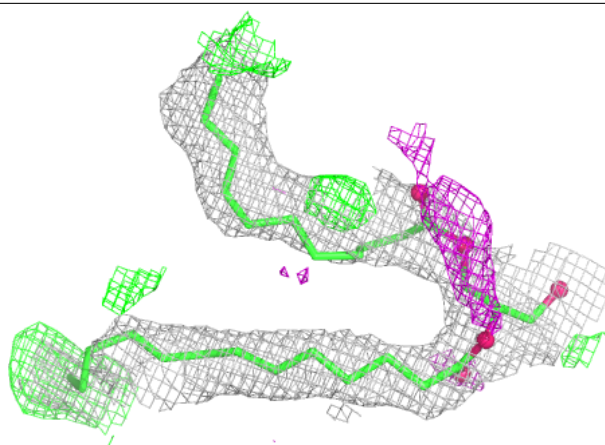
Electron density around 7PH B 206:

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

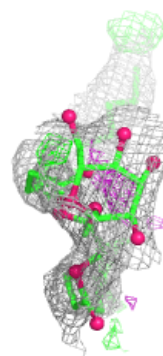
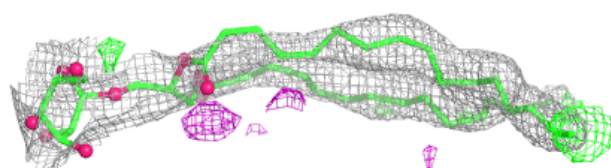
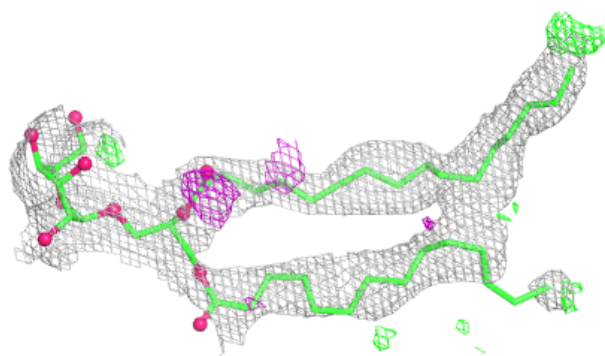


Electron density around 7PH C 303:

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

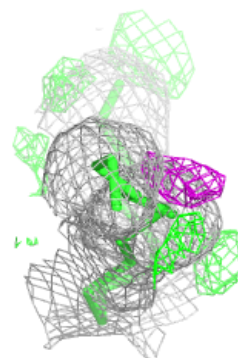
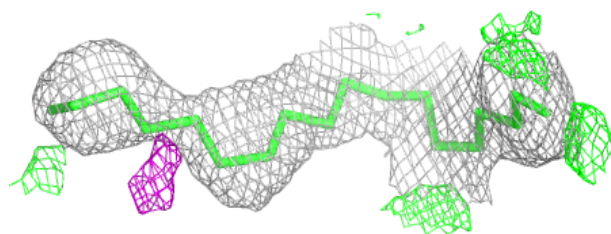
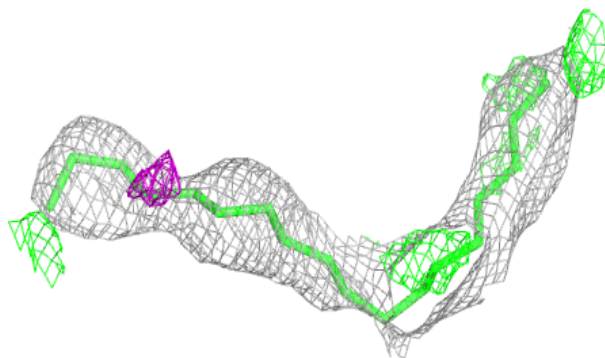
**Electron density around 1O2 F 103:**

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

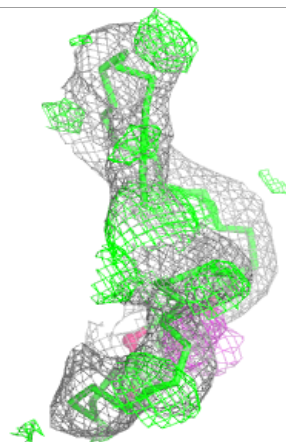
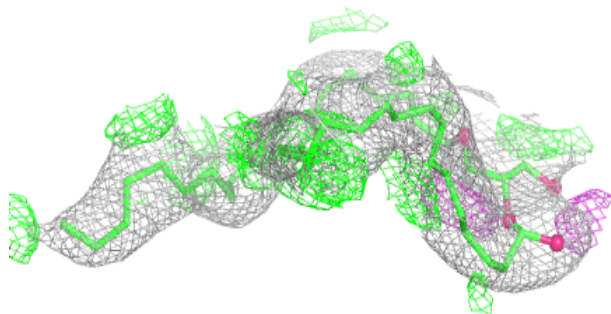
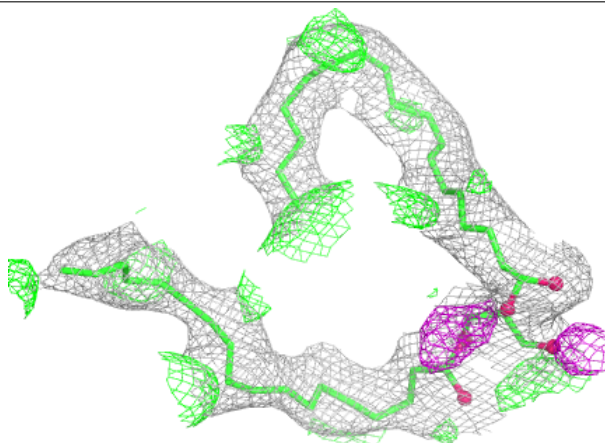


Electron density around 8K6 A 306:

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

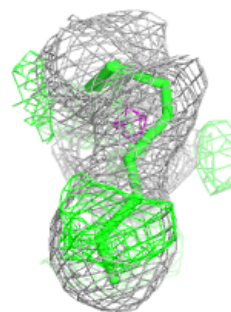
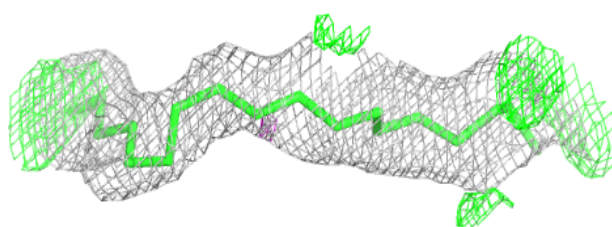
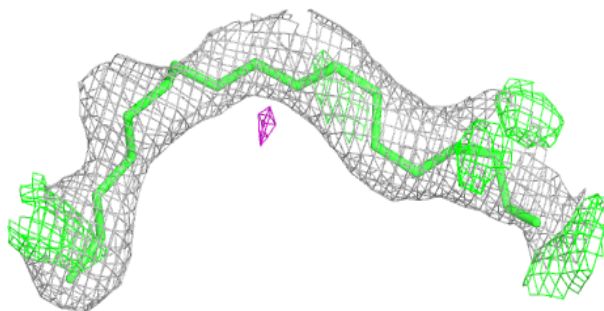
**Electron density around 2WM A 309:**

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

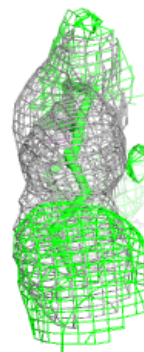
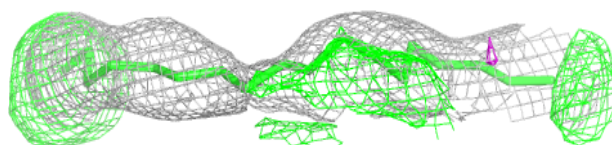
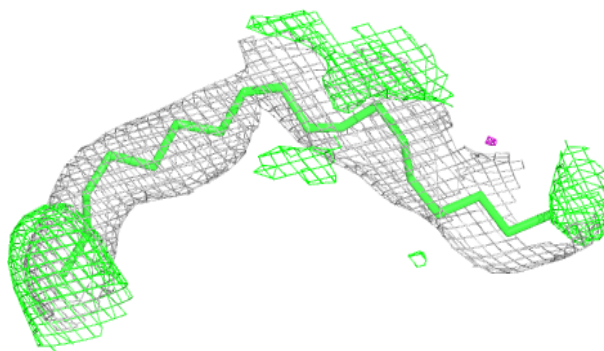


Electron density around 8K6 A 307:

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

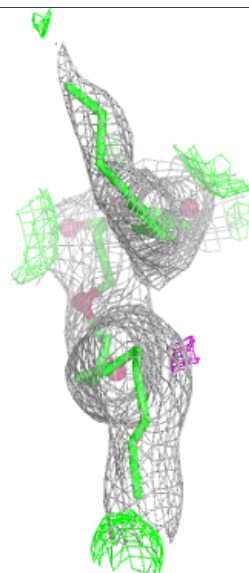
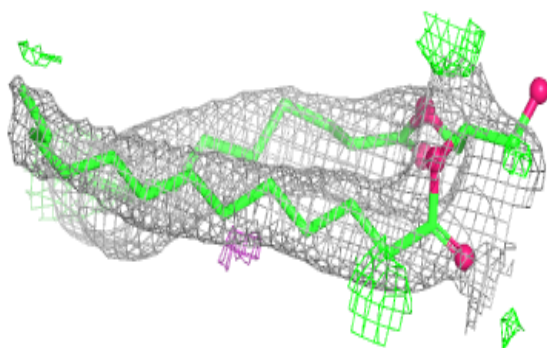
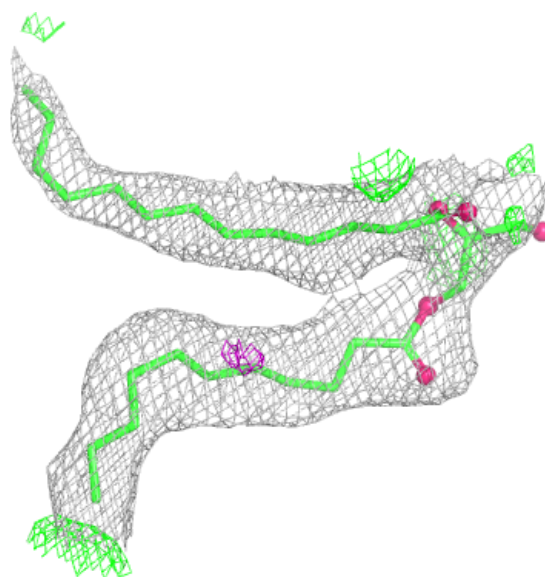
**Electron density around 8K6 B 202 (A):**

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



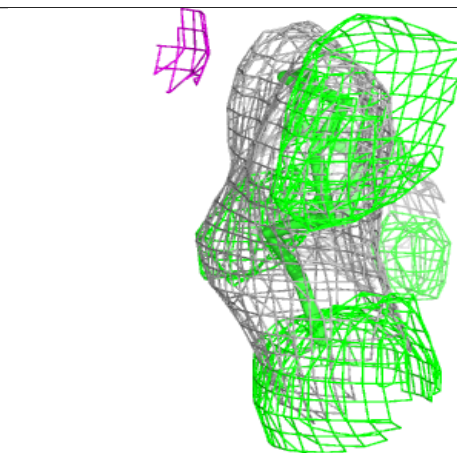
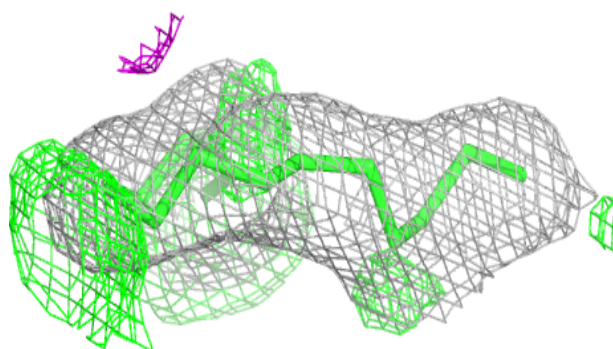
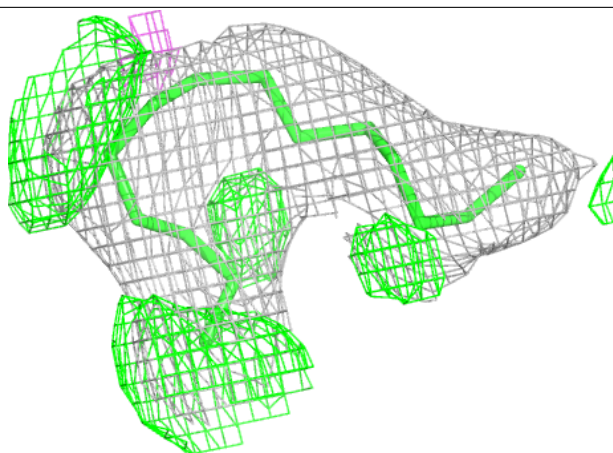
Electron density around 7PH F 104:

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

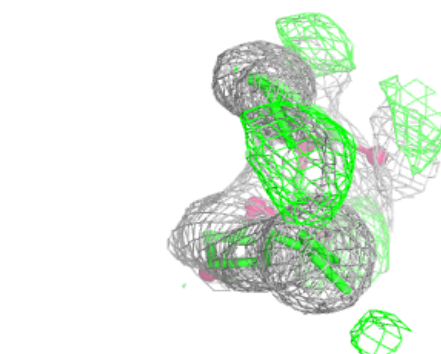
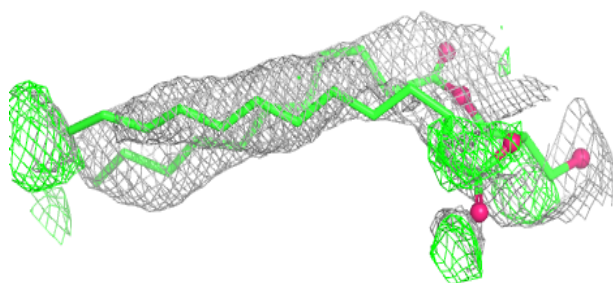
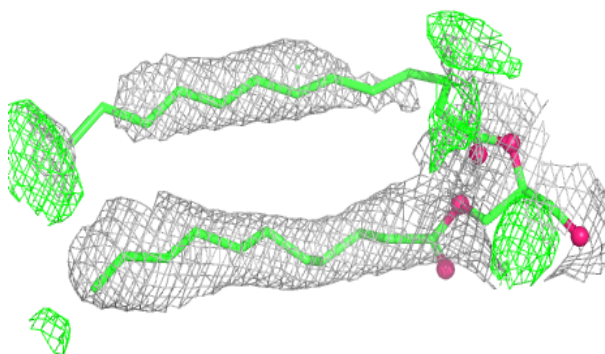


Electron density around 8K6 A 308:

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

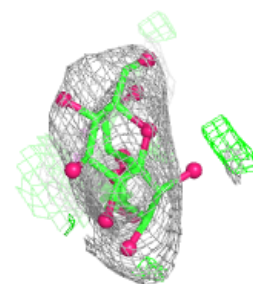
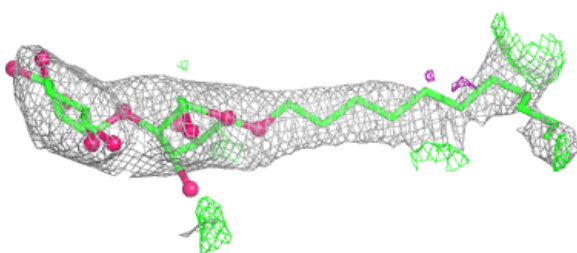
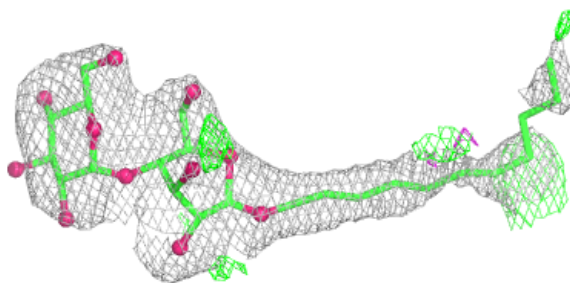
**Electron density around 7PH A 305:**

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

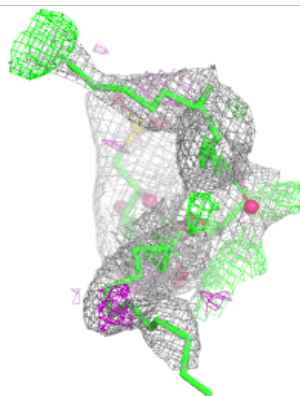
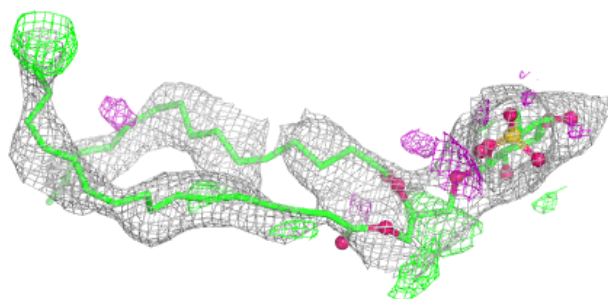
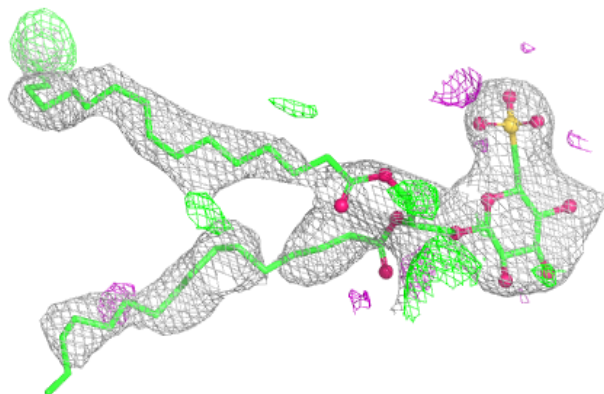


Electron density around UMQ B 201:

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

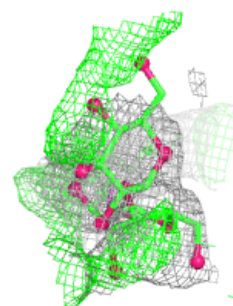
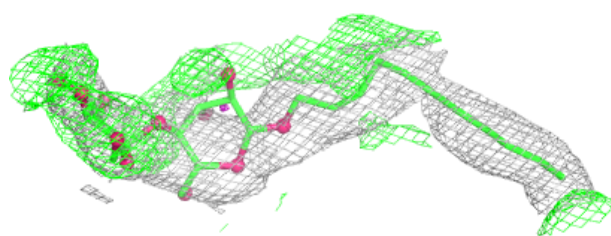
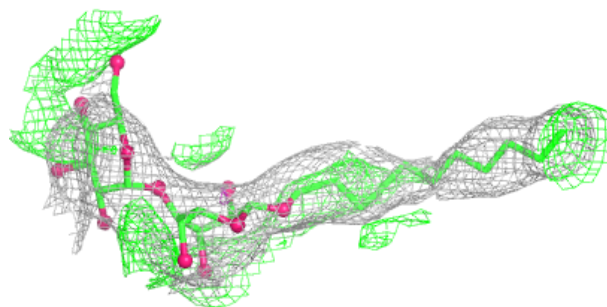
**Electron density around SQD D 204:**

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

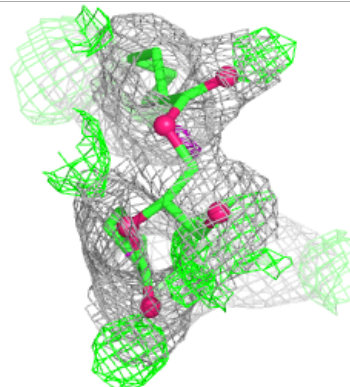
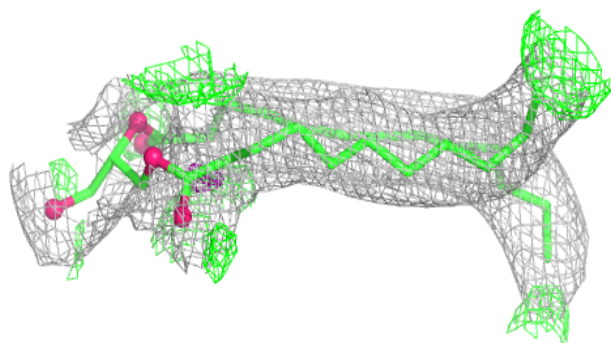
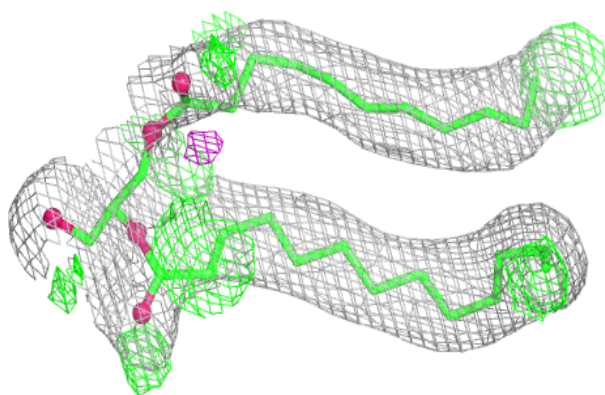


Electron density around UMQ B 203 (B):

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

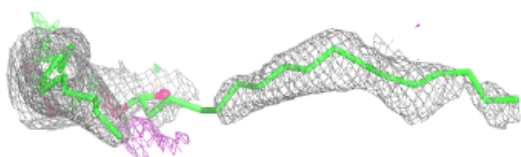
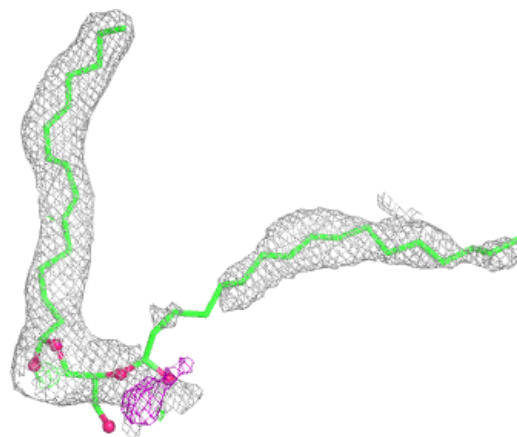
**Electron density around 7PH D 203:**

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

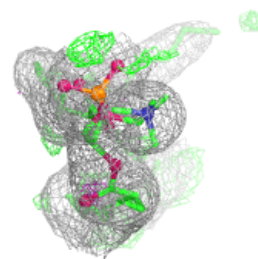
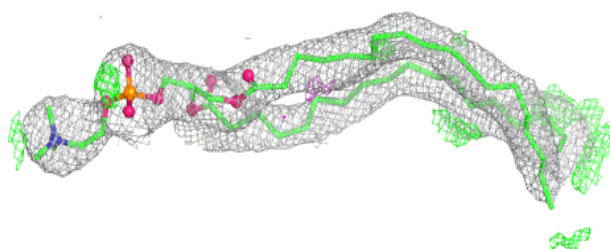
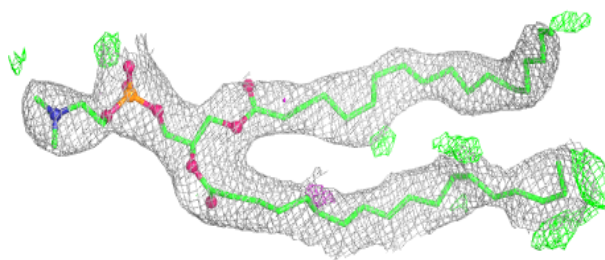


Electron density around 2WA F 101:

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

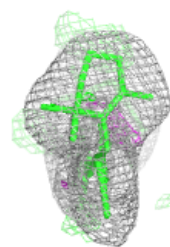
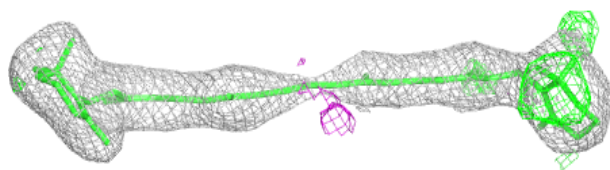
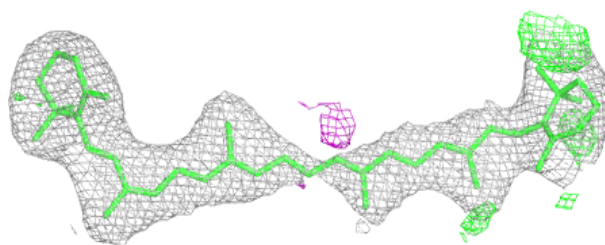
**Electron density around OPC B 205:**

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



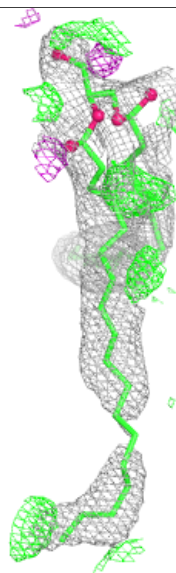
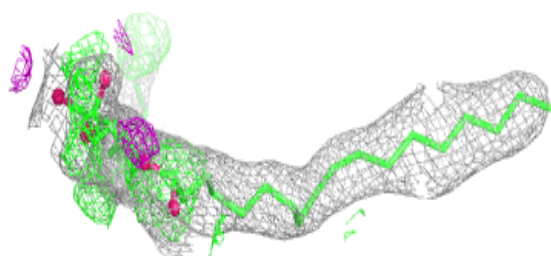
Electron density around BCR G 102:

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



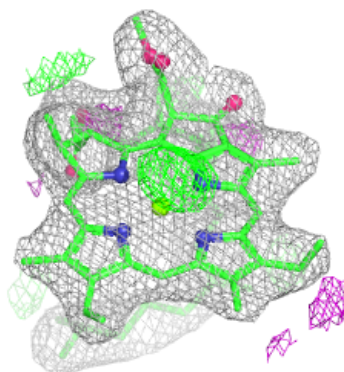
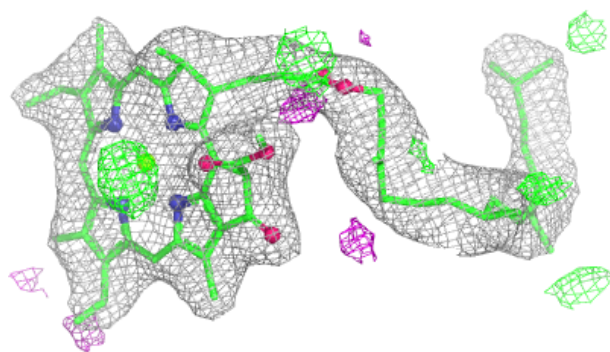
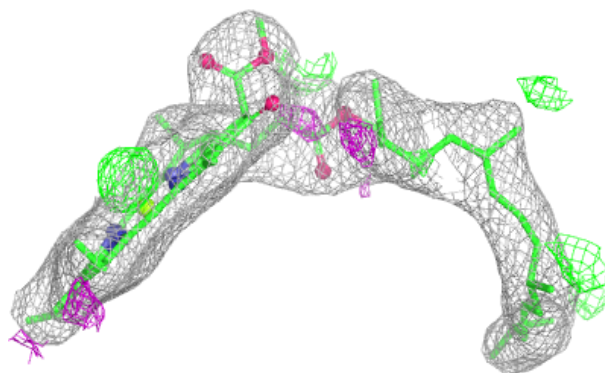
Electron density around 3WM E 101:

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



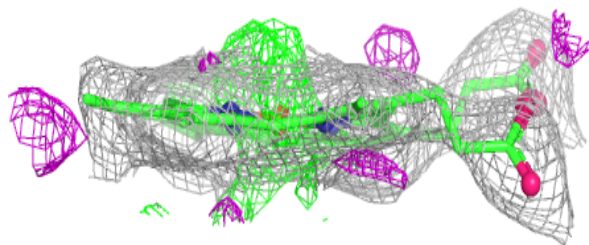
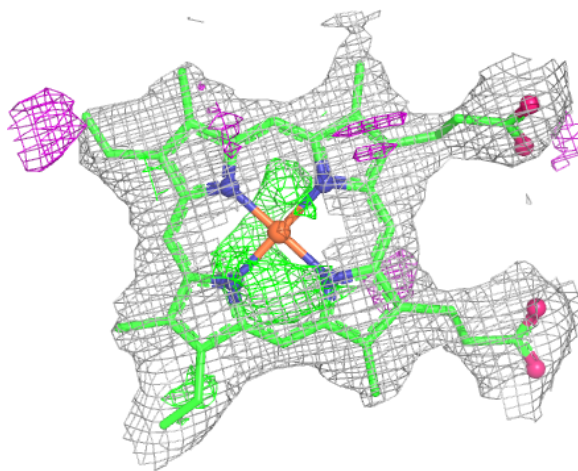
Electron density around CLA B 204:

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



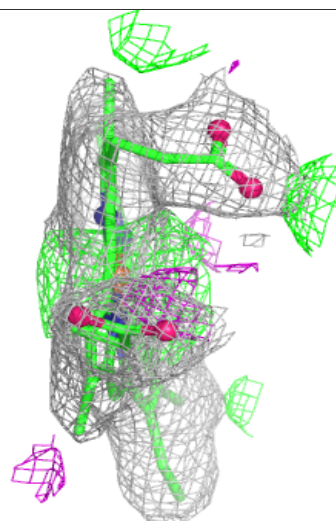
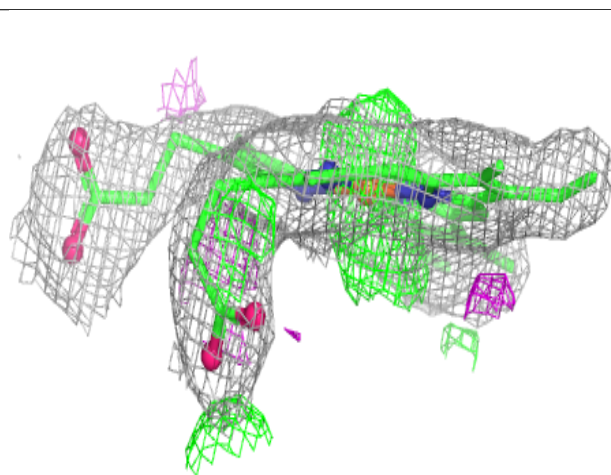
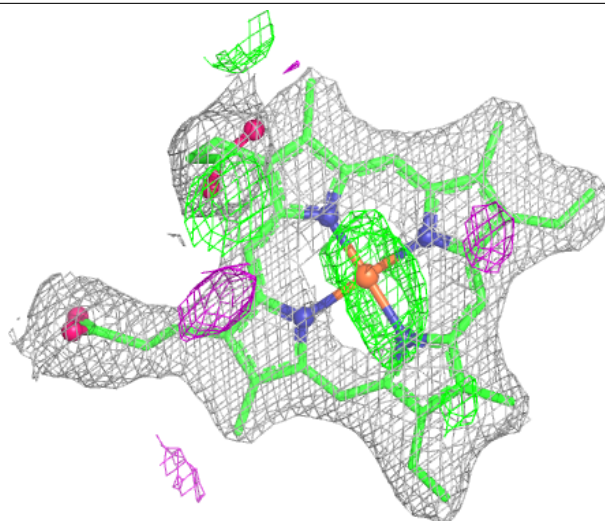
Electron density around HEC C 301:

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



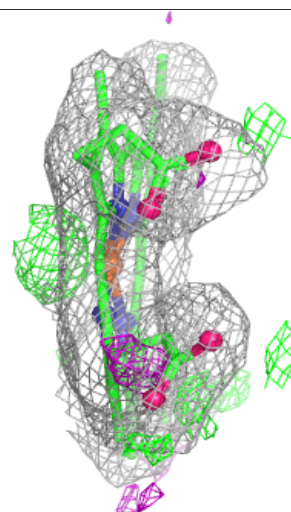
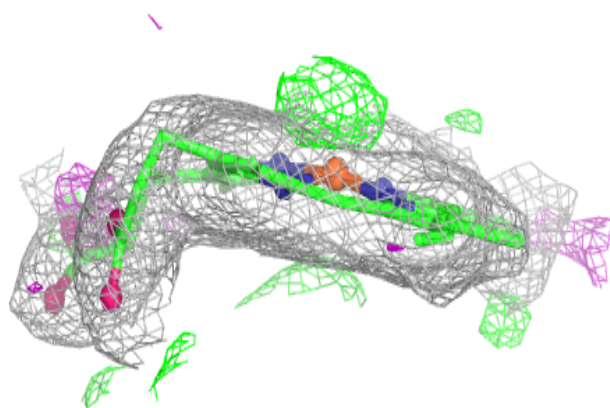
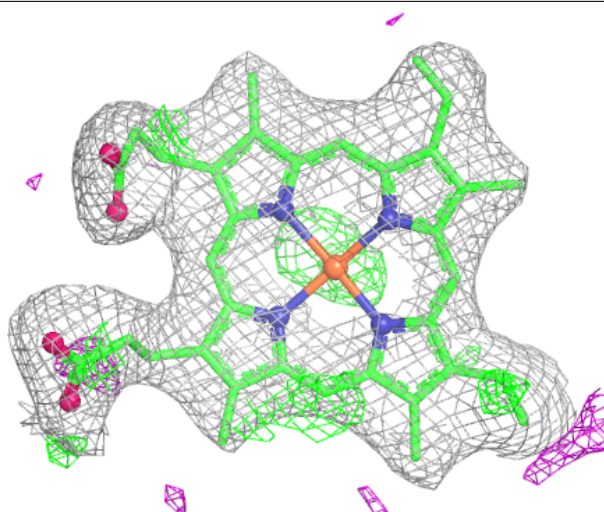
Electron density around HEC A 302:

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



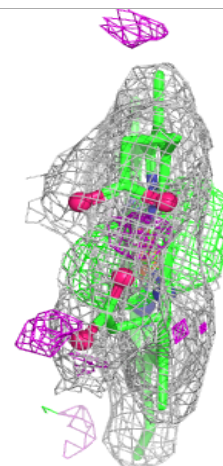
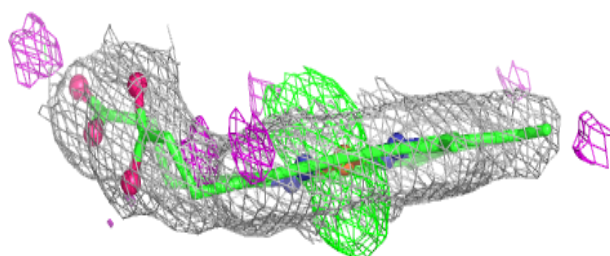
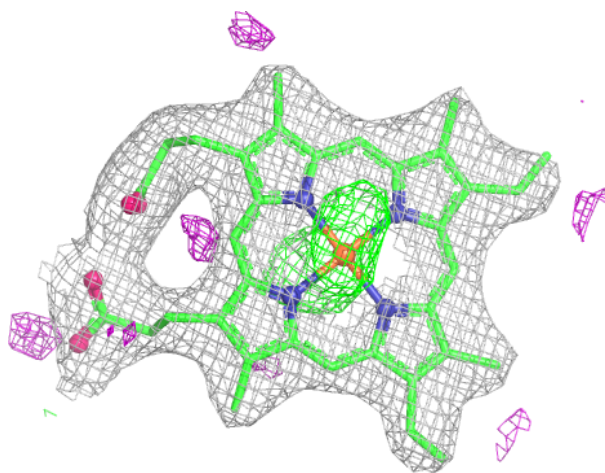
Electron density around HEC A 303:

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



Electron density around HEC A 301:

$2mF_o-DF_c$ (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.