



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:24 PM UTC

PDB ID : 4H44 / pdb_00004h44
Title : 2.70 Å Cytochrome b6f Complex Structure From Nostoc PCC 7120
Authors : Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on : 2012-09-16
Resolution : 2.70 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

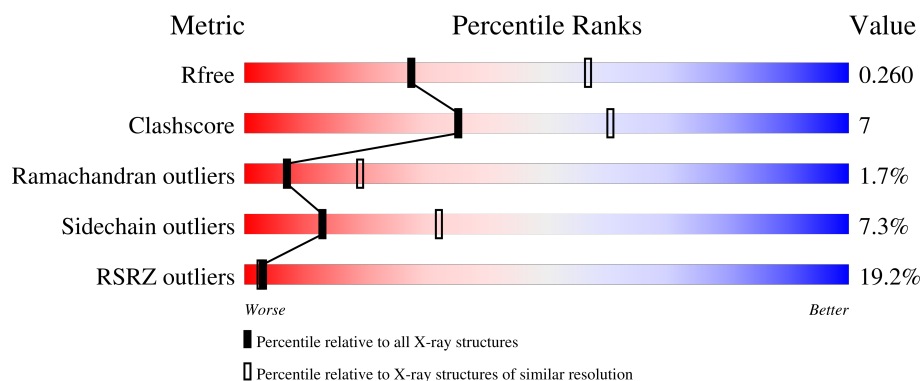
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



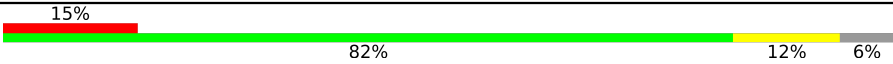
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	4% 80% 18% .
2	B	160	7% 78% 19% .
3	C	289	25% 79% 19% .
4	D	179	43% 82% 10% 7%
5	E	31	10% 90% 10%

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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
10	UMQ	A	304	X	-	-	-
10	UMQ	A	305	X	-	-	-
10	UMQ	A	307	X	-	-	-
10	UMQ	A	309	X	-	-	-
10	UMQ	F	101	X	-	-	-
13	CLA	B	201	X	-	-	-
16	CD	C	304	-	-	-	X

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 16386 atoms, of which 8258 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	215	Total	C	H	N	O	S	0	0	0
			3451	1144	1736	272	288	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	160	Total	C	H	N	O	S	0	0	0
			2531	830	1292	195	208	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	289	Total	C	H	N	O	S	0	0	0
			4379	1396	2184	364	429	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	H	N	O	S	0	0	0
			2459	791	1210	213	239	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	H	N	O	S	0	0	0
			484	157	257	35	34	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	H	N	O	S	0	0	0
			483	156	252	36	38	1			

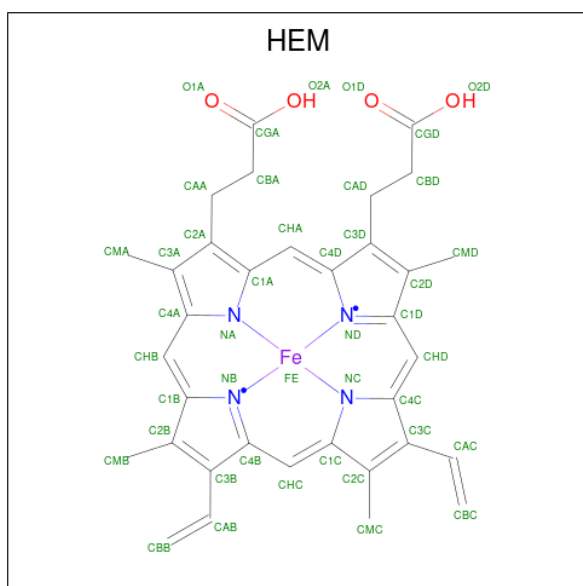
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	37	Total	C	H	N	O	S	0	0	0
			584	188	303	44	48	1			

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

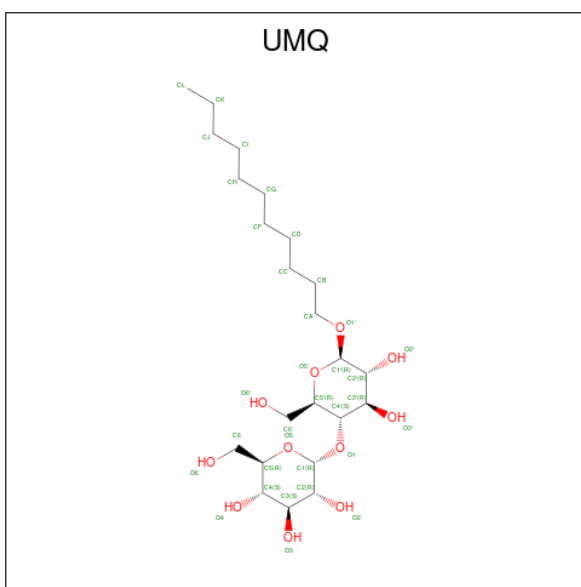
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	29	Total	C	H	N	O	S	0	0	0
			470	155	243	36	34	2			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



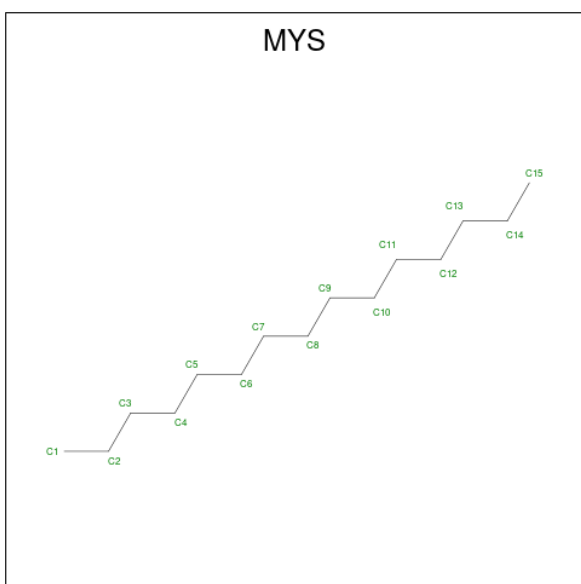
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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



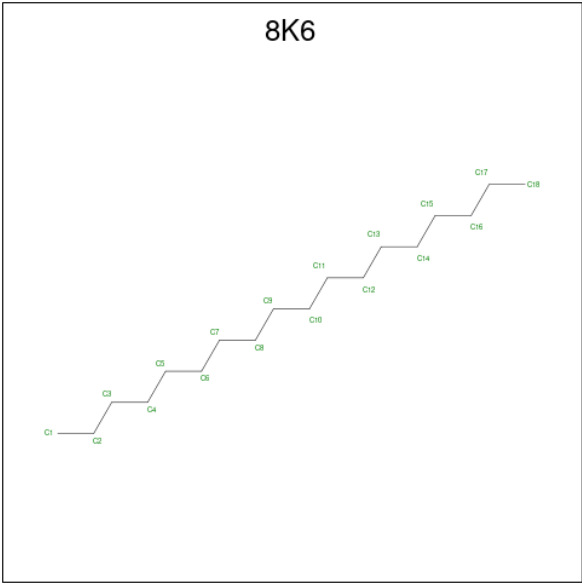
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total 77	C 23	H 43	O 11	0	0
10	A	1	Total 77	C 23	H 43	O 11	0	0
10	A	1	Total 78	C 23	H 44	O 11	0	0
10	A	1	Total 77	C 23	H 43	O 11	0	0
10	F	1	Total 77	C 23	H 43	O 11	0	0

- Molecule 11 is PENTADECANE (CCD ID: MYS) (formula: $C_{15}H_{32}$).



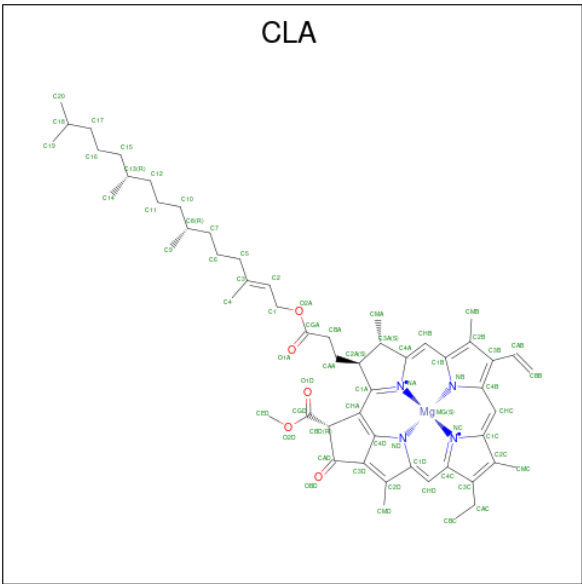
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	H	0	0
			47	15	32		

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



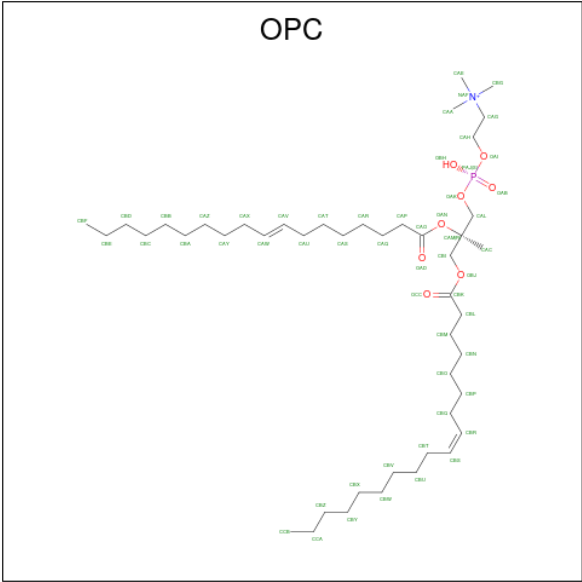
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



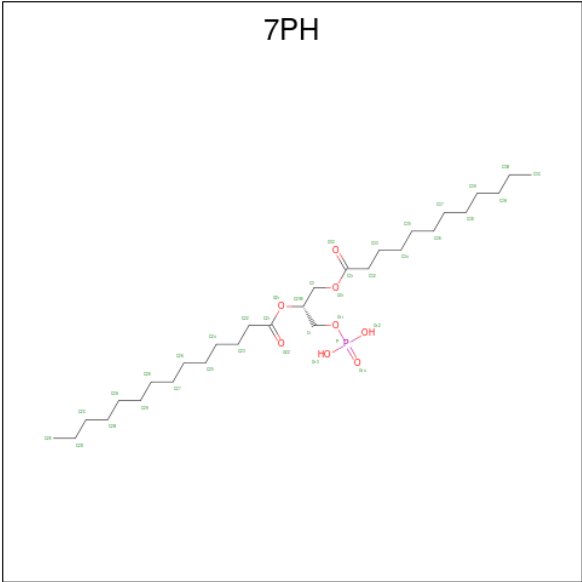
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 14 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
14	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
14	C	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 15 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).

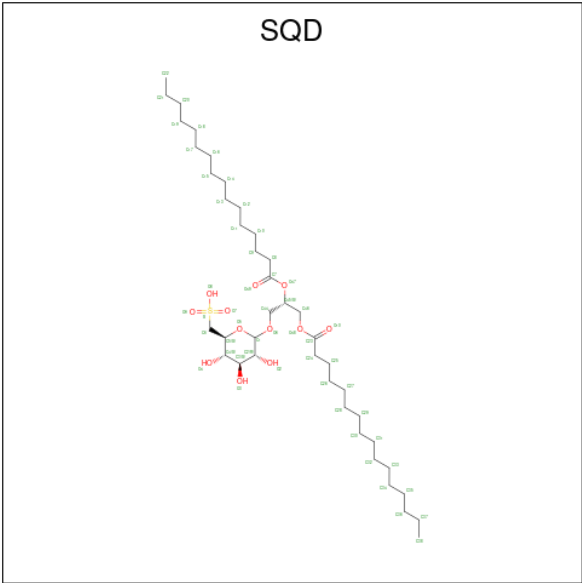


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	H	O	0	0
			81	27	49	5		

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

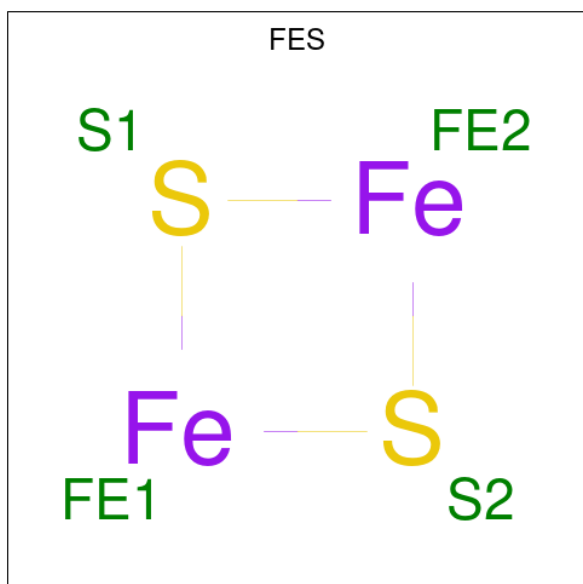
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	Cd	0	0
			1	1		

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



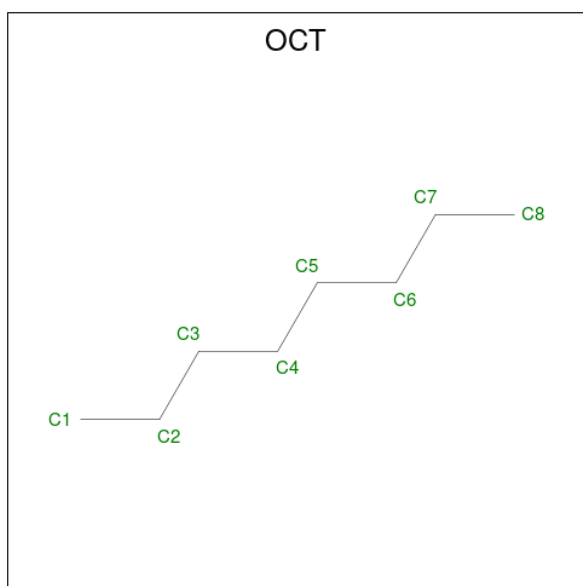
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	H	O	S	0	0
			53	16	24	12	1		

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



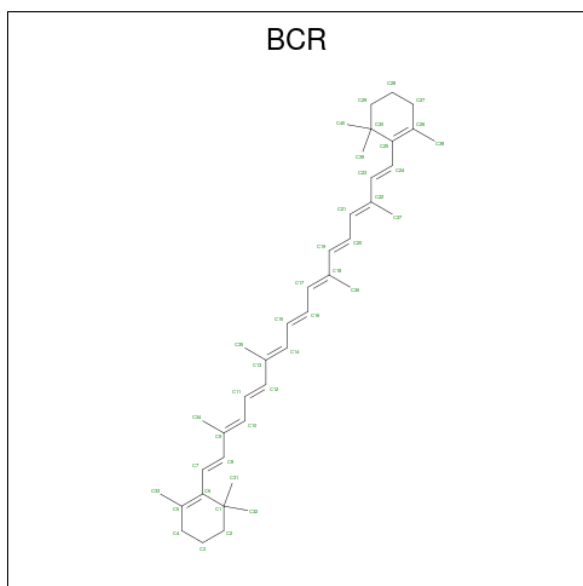
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 19 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total	C	H	0	0
			26	8	18		

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total	C	H	0	0
			96	40	56		

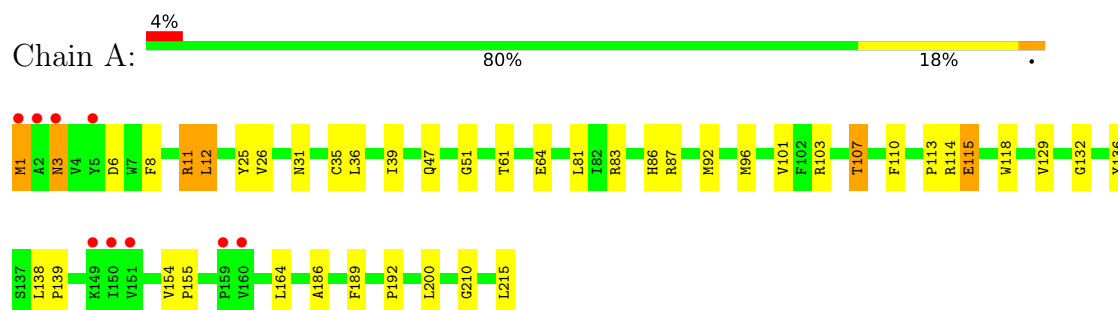
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	26	Total	O	0	0
			26	26		
21	B	22	Total	O	0	0
			22	22		
21	C	45	Total	O	0	0
			45	45		
21	D	1	Total	O	0	0
			1	1		
21	G	5	Total	O	0	0
			5	5		
21	H	3	Total	O	0	0
			3	3		

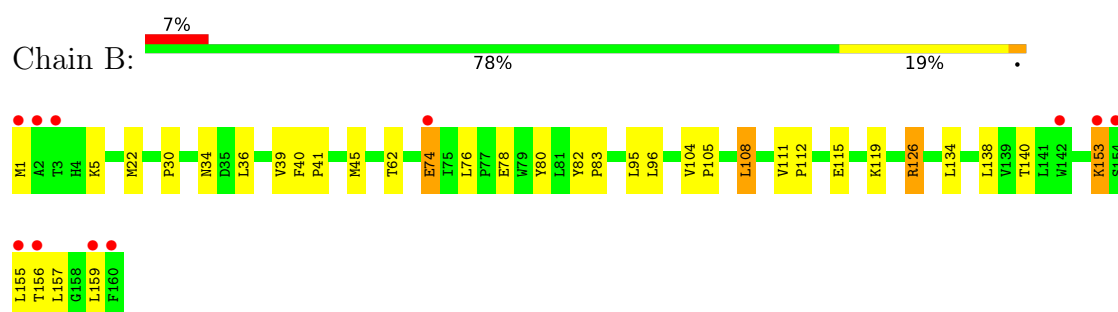
3 Residue-property plots [i](#)

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.

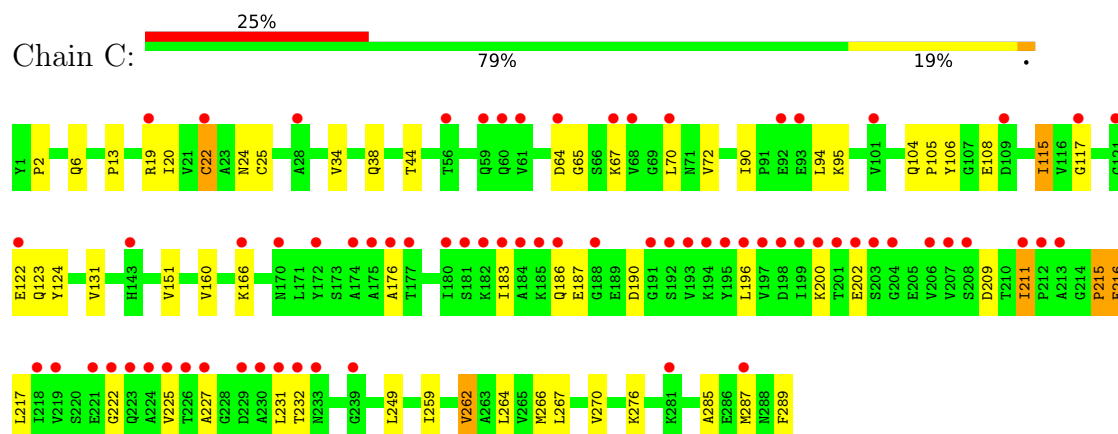
• Molecule 1: Cytochrome b6



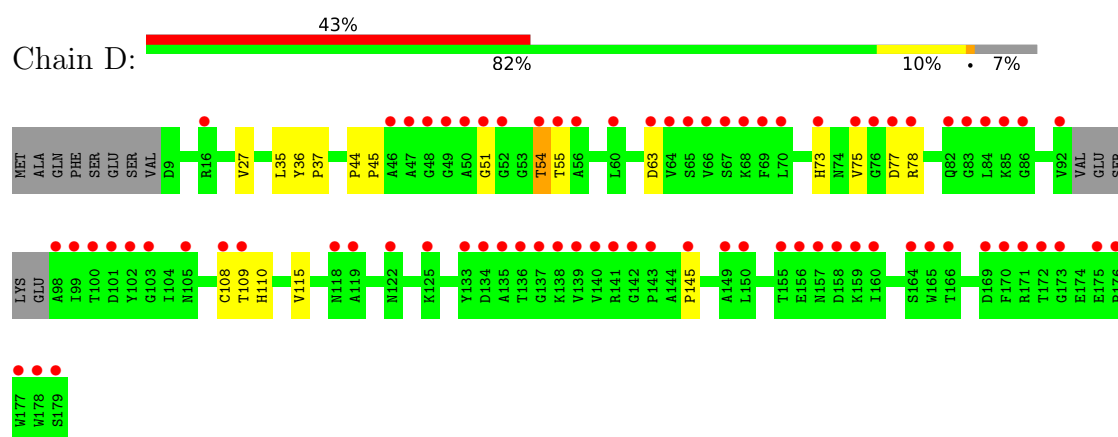
• Molecule 2: Cytochrome b6-f complex subunit 4



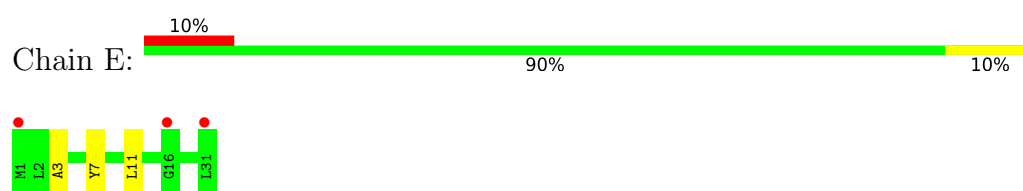
• Molecule 3: Apocytochrome f



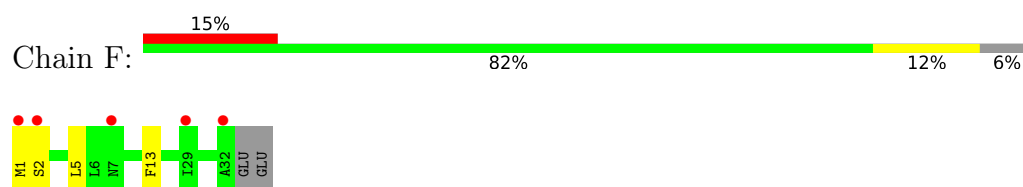
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1



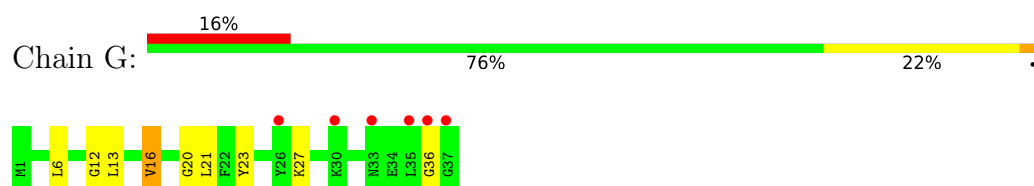
- Molecule 5: Cytochrome b6-f complex subunit 6



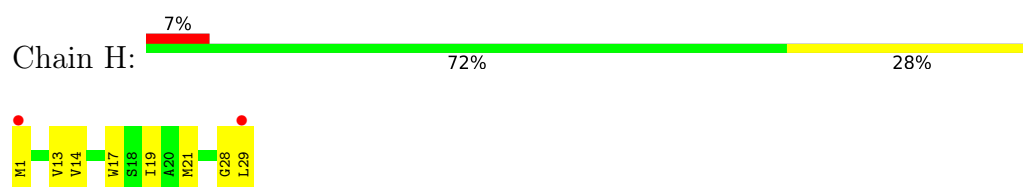
- Molecule 6: Cytochrome b6-f complex subunit 7



- 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	159.13Å 159.13Å 364.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.55 – 2.70 39.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.55-2.70) 98.0 (39.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.220 , 0.246 (Not available) , 0.260	Depositor DCC
R_{free} test set	3733 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16386	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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: UMQ, OCT, 7PH, MYS, 8K6, CLA, HEM, OPC, FES, BCR, SQD, CD

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	0.31	0/1768	0.70	0/2411
2	B	0.31	0/1278	0.73	2/1752 (0.1%)
3	C	0.29	0/2241	0.66	0/3053
4	D	0.28	0/1280	0.67	1/1745 (0.1%)
5	E	0.28	0/230	0.71	0/309
6	F	0.30	0/234	0.67	0/315
7	G	0.30	0/286	0.79	0/387
8	H	0.32	0/233	0.73	0/319
All	All	0.30	0/7550	0.69	3/10291 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	ARG	CA-C-N	5.58	125.11	119.19
2	B	126	ARG	C-N-CA	5.58	125.11	119.19
4	D	75	VAL	N-CA-C	-5.41	107.47	112.83

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	1715	1736	1734	34	1
2	B	1239	1292	1290	24	0
3	C	2195	2184	2183	32	0
4	D	1249	1210	1208	9	0
5	E	227	257	257	2	0
6	F	231	252	252	4	0
7	G	281	303	303	6	0
8	H	227	243	243	11	0
9	A	129	90	90	19	0
9	C	43	30	30	7	0
10	A	136	173	166	5	0
10	F	34	43	42	1	0
11	A	15	32	32	1	0
12	A	18	38	38	0	0
13	B	65	62	72	3	0
14	B	54	83	83	0	0
14	C	54	83	83	3	0
15	C	32	49	45	0	0
16	C	1	0	0	0	0
17	D	29	24	22	0	0
18	D	4	0	0	1	0
19	F	8	18	18	0	0
20	G	40	56	56	5	0
21	A	26	0	0	5	0
21	B	22	0	0	4	0
21	C	45	0	0	3	0
21	D	1	0	0	0	0
21	G	5	0	0	0	0
21	H	3	0	0	0	0
All	All	8128	8258	8247	120	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (120) 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)
2:B:126:ARG:NH1	21:B:319:HOH:O	2.04	0.90
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.65	0.84
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.70	0.80
9:A:303:HEM:O1A	21:A:425:HOH:O	2.03	0.77
1:A:3:ASN:ND2	1:A:6:ASP:OD2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:307:UMQ:H51	2:B:36:LEU:HD21	1.71	0.73
1:A:47:GLN:O	21:A:422:HOH:O	2.06	0.72
7:G:23:TYR:CE1	20:G:101:BCR:H23C	2.25	0.71
3:C:151:VAL:O	21:C:417:HOH:O	2.07	0.70
13:B:201:CLA:HBB1	13:B:201:CLA:HHC	1.75	0.67
3:C:22:CYS:SG	9:C:301:HEM:CAB	2.83	0.67
9:C:301:HEM:HMB1	9:C:301:HEM:HBB2	1.76	0.67
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.28	0.66
2:B:115:GLU:OE1	21:B:319:HOH:O	2.15	0.64
1:A:114:ARG:NH1	1:A:210:GLY:O	2.31	0.64
9:A:303:HEM:HBC2	9:A:303:HEM:HHD	1.80	0.64
1:A:35:CYS:SG	9:A:303:HEM:CBB	2.86	0.63
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.81	0.63
3:C:25:CYS:SG	9:C:301:HEM:CBC	2.87	0.62
3:C:270:VAL:HA	8:H:21:MET:HE2	1.81	0.61
1:A:35:CYS:HG	9:A:303:HEM:CAB	2.12	0.61
3:C:64:ASP:OD2	3:C:65:GLY:N	2.34	0.61
3:C:262:VAL:HG13	8:H:14:VAL:HG13	1.81	0.61
1:A:39:ILE:HD11	20:G:101:BCR:H312	1.84	0.59
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.86	0.58
3:C:262:VAL:HG13	8:H:14:VAL:CG1	2.34	0.57
1:A:1:MET:SD	1:A:1:MET:N	2.78	0.56
3:C:215:PRO:O	3:C:216:GLU:HB3	2.05	0.56
1:A:86:HIS:CE1	9:A:301:HEM:C4D	2.94	0.54
1:A:86:HIS:CD2	21:A:422:HOH:O	2.59	0.54
6:F:13:PHE:CD1	7:G:16:VAL:HG13	2.43	0.54
3:C:44:THR:HG21	8:H:1:MET:HE2	1.91	0.53
2:B:140:THR:OG1	21:B:318:HOH:O	2.08	0.53
1:A:215:LEU:O	21:A:406:HOH:O	2.19	0.53
5:E:7:TYR:CZ	5:E:11:LEU:HD11	2.43	0.53
3:C:270:VAL:HA	8:H:21:MET:CE	2.39	0.53
3:C:215:PRO:O	3:C:216:GLU:CB	2.55	0.53
8:H:28:GLY:O	8:H:29:LEU:HB2	2.09	0.52
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	1.92	0.52
2:B:104:VAL:HB	2:B:105:PRO:CD	2.40	0.52
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.92	0.52
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.51
2:B:36:LEU:O	2:B:40:PHE:HB2	2.11	0.51
7:G:20:GLY:N	20:G:101:BCR:H363	2.26	0.51
14:C:302:OPC:HAR1	5:E:3:ALA:HB1	1.93	0.51
8:H:17:TRP:O	8:H:21:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PRO:HG3	2:B:22:MET:HE2	1.93	0.51
3:C:183:ILE:HG22	3:C:183:ILE:O	2.11	0.50
9:A:303:HEM:C2A	10:A:307:UMQ:H62	2.45	0.50
9:A:303:HEM:CBA	10:A:307:UMQ:H41	2.42	0.50
3:C:160:VAL:O	9:C:301:HEM:HMD1	2.10	0.50
4:D:108:CYS:SG	4:D:115:VAL:HG22	2.51	0.50
1:A:136:TYR:CE1	2:B:78:GLU:CG	2.94	0.50
9:A:303:HEM:HBB2	9:A:303:HEM:HMB1	1.94	0.50
7:G:13:LEU:HA	7:G:16:VAL:HG23	1.93	0.49
9:A:302:HEM:HMB1	9:A:302:HEM:HBB2	1.95	0.49
2:B:30:PRO:O	2:B:34:ASN:HB2	2.13	0.49
13:B:201:CLA:HHC	13:B:201:CLA:CBB	2.40	0.49
9:A:301:HEM:HMB1	9:A:301:HEM:HBB2	1.93	0.49
3:C:19:ARG:NH1	3:C:24:ASN:OD1	2.46	0.49
9:C:301:HEM:HMC2	9:C:301:HEM:HBC2	1.95	0.48
1:A:86:HIS:HE1	9:A:301:HEM:C4D	2.16	0.48
3:C:22:CYS:SG	9:C:301:HEM:CBB	3.02	0.47
1:A:31:ASN:HA	8:H:29:LEU:HD13	1.96	0.47
2:B:45:MET:CE	4:D:27:VAL:HG13	2.45	0.47
4:D:73:HIS:O	4:D:73:HIS:ND1	2.48	0.47
1:A:92:MET:O	1:A:96:MET:HG2	2.15	0.47
1:A:107:THR:O	1:A:107:THR:HG23	2.14	0.46
1:A:186:ALA:HB2	11:A:306:MYS:H81	1.96	0.46
14:C:302:OPC:CAE	8:H:1:MET:HE3	2.45	0.46
4:D:77:ASP:OD2	4:D:77:ASP:N	2.47	0.46
1:A:35:CYS:SG	9:A:303:HEM:C3B	3.07	0.46
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.96	0.46
3:C:115:ILE:HG21	21:C:413:HOH:O	2.16	0.46
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.97	0.45
2:B:111:VAL:N	2:B:112:PRO:HD2	2.32	0.45
2:B:153:LYS:O	2:B:157:LEU:N	2.50	0.45
3:C:72:VAL:HG21	3:C:124:TYR:O	2.17	0.45
3:C:211:ILE:O	3:C:211:ILE:HG13	2.15	0.45
1:A:154:VAL:N	1:A:155:PRO:CD	2.80	0.44
3:C:2:PRO:HG2	3:C:117:GLY:HA2	1.98	0.44
6:F:13:PHE:C	6:F:13:PHE:CD2	2.96	0.44
1:A:103:ARG:C	1:A:103:ARG:HD2	2.41	0.44
3:C:38:GLN:N	14:C:302:OPC:OAB	2.50	0.44
1:A:25:TYR:OH	3:C:289:PHE:O	2.27	0.44
1:A:101:VAL:CG2	9:A:302:HEM:HMC3	2.47	0.44
1:A:8:PHE:O	1:A:12:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TYR:CE1	2:B:78:GLU:HG2	2.53	0.44
3:C:231:LEU:HD12	3:C:232:THR:HG23	1.99	0.44
7:G:12:GLY:O	7:G:16:VAL:HG22	2.18	0.43
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.53	0.43
3:C:217:LEU:HD23	3:C:232:THR:HG22	2.00	0.43
20:G:101:BCR:C32	8:H:19:ILE:HD13	2.48	0.43
21:B:308:HOH:O	3:C:276:LYS:NZ	2.52	0.43
3:C:186:GLN:OE1	3:C:187:GLU:N	2.52	0.43
1:A:118:TRP:CE3	9:A:302:HEM:HAC	2.54	0.43
1:A:51:GLY:HA3	21:A:422:HOH:O	2.19	0.43
3:C:6:GLN:NE2	21:C:413:HOH:O	2.51	0.42
3:C:266:MET:SD	8:H:13:VAL:HG12	2.59	0.42
2:B:45:MET:HE1	4:D:27:VAL:HA	2.02	0.42
4:D:110:HIS:HB3	18:D:202:FES:S2	2.59	0.42
6:F:5:LEU:C	6:F:5:LEU:HD23	2.45	0.42
10:A:307:UMQ:H31	2:B:36:LEU:HD11	2.01	0.42
3:C:90:ILE:O	3:C:95:LYS:NZ	2.49	0.42
1:A:129:VAL:HG21	13:B:201:CLA:H11	2.02	0.42
2:B:119:LYS:O	2:B:119:LYS:HG2	2.20	0.42
3:C:176:ALA:HA	3:C:227:ALA:HB2	2.02	0.42
1:A:25:TYR:CZ	2:B:5:LYS:HD3	2.55	0.41
1:A:132:GLY:HA3	2:B:80:TYR:OH	2.20	0.41
7:G:23:TYR:CD2	20:G:101:BCR:H19C	2.56	0.41
1:A:110:PHE:HB3	1:A:118:TRP:CE3	2.56	0.41
10:A:307:UMQ:O3'	10:A:307:UMQ:O2	2.29	0.41
1:A:189:PHE:C	1:A:192:PRO:HD2	2.46	0.41
2:B:108:LEU:HD13	2:B:108:LEU:HA	1.94	0.41
2:B:82:TYR:N	2:B:83:PRO:CD	2.84	0.41
2:B:40:PHE:HB2	2:B:41:PRO:HD3	2.02	0.40
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.97	0.40
4:D:44:PRO:HA	4:D:45:PRO:HD3	1.98	0.40
6:F:1:MET:O	10:F:101:UMQ:O6'	2.20	0.40
2:B:45:MET:HE3	4:D:27:VAL:HG13	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH1	1:A:115:GLU:OE1[12_565]	2.04	0.16

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	213/215 (99%)	206 (97%)	6 (3%)	1 (0%)	24	48
2	B	158/160 (99%)	149 (94%)	8 (5%)	1 (1%)	21	44
3	C	287/289 (99%)	252 (88%)	27 (9%)	8 (3%)	4	9
4	D	162/179 (90%)	136 (84%)	22 (14%)	4 (2%)	4	11
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	7
7	G	35/37 (95%)	34 (97%)	0	1 (3%)	3	9
8	H	27/29 (93%)	27 (100%)	0	0	100	100
All	All	941/974 (97%)	860 (91%)	65 (7%)	16 (2%)	7	19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	190	ASP
3	C	216	GLU
4	D	78	ARG
3	C	200	LYS
3	C	222	GLY
3	C	287	MET
4	D	145	PRO
7	G	36	GLY
1	A	3	ASN
3	C	202	GLU
3	C	285	ALA
4	D	54	THR
2	B	74	GLU
3	C	215	PRO
6	F	2	SER
4	D	51	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	184/184 (100%)	171 (93%)	13 (7%)	13	33
2	B	134/134 (100%)	120 (90%)	14 (10%)	7	17
3	C	238/238 (100%)	217 (91%)	21 (9%)	9	23
4	D	133/145 (92%)	128 (96%)	5 (4%)	29	58
5	E	21/21 (100%)	21 (100%)	0	100	100
6	F	22/24 (92%)	22 (100%)	0	100	100
7	G	29/29 (100%)	25 (86%)	4 (14%)	3	9
8	H	24/24 (100%)	24 (100%)	0	100	100
All	All	785/799 (98%)	728 (93%)	57 (7%)	13	32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	12	LEU
1	A	26	VAL
1	A	36	LEU
1	A	61	THR
1	A	64	GLU
1	A	81	LEU
1	A	87	ARG
1	A	107	THR
1	A	115	GLU
1	A	164	LEU
1	A	200	LEU
2	B	1	MET
2	B	39	VAL
2	B	62	THR
2	B	74	GLU
2	B	76	LEU
2	B	95	LEU

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Mol	Chain	Res	Type
2	B	96	LEU
2	B	108	LEU
2	B	134	LEU
2	B	138	LEU
2	B	153	LYS
2	B	155	LEU
2	B	156	THR
2	B	159	LEU
3	C	20	ILE
3	C	22	CYS
3	C	34	VAL
3	C	67	LYS
3	C	70	LEU
3	C	94	LEU
3	C	108	GLU
3	C	115	ILE
3	C	122	GLU
3	C	123	GLN
3	C	131	VAL
3	C	166	LYS
3	C	196	LEU
3	C	209	ASP
3	C	211	ILE
3	C	225	VAL
3	C	249	LEU
3	C	259	ILE
3	C	262	VAL
3	C	264	LEU
3	C	267	LEU
4	D	35	LEU
4	D	54	THR
4	D	55	THR
4	D	63	ASP
4	D	109	THR
7	G	6	LEU
7	G	16	VAL
7	G	21	LEU
7	G	27	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	86	HIS
3	C	123	GLN
3	C	138	ASN
3	C	143	HIS
4	D	74	ASN
6	F	7	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
18	FES	D	202	4	0,4,4	-	-	-		
15	7PH	C	303	-	31,31,37	1.00	2 (6%)	33,33,42	1.20	3 (9%)
10	UMQ	A	307	-	35,35,35	1.28	5 (14%)	46,46,46	2.02	11 (23%)
14	OPC	C	302	-	53,53,54	1.01	4 (7%)	59,61,64	0.99	2 (3%)
10	UMQ	F	101	-	35,35,35	1.31	6 (17%)	46,46,46	2.03	13 (28%)
10	UMQ	A	305	-	35,35,35	1.35	6 (17%)	46,46,46	2.11	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SQD	D	201	-	27,29,54	1.87	8 (29%)	37,40,65	4.81	9 (24%)
11	MYS	A	306	-	14,14,14	0.38	0	13,13,13	0.81	0
9	HEM	A	302	1	50,50,50	1.88	9 (18%)	67,82,82	1.23	3 (4%)
12	8K6	A	308	-	17,17,17	0.24	0	16,16,16	0.57	0
9	HEM	A	303	-	50,50,50	2.01	9 (18%)	67,82,82	1.42	6 (8%)
10	UMQ	A	309	-	35,35,35	1.27	5 (14%)	46,46,46	2.04	12 (26%)
9	HEM	C	301	3	50,50,50	1.82	8 (16%)	67,82,82	1.22	3 (4%)
13	CLA	B	201	21	69,73,73	1.19	6 (8%)	82,113,113	1.21	6 (7%)
19	OCT	F	102	-	7,7,7	0.33	0	6,6,6	0.70	0
14	OPC	B	202	-	53,53,54	0.99	4 (7%)	59,61,64	1.01	1 (1%)
9	HEM	A	301	1	50,50,50	2.01	7 (14%)	67,82,82	1.36	5 (7%)
20	BCR	G	101	-	41,41,41	2.16	20 (48%)	56,56,56	2.20	19 (33%)
10	UMQ	A	304	-	35,35,35	1.28	6 (17%)	46,46,46	2.06	10 (21%)

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
18	FES	D	202	4	-	-	0/1/1/1
15	7PH	C	303	-	-	13/33/33/39	-
10	UMQ	A	307	-	2/2/10/10	13/20/60/60	0/2/2/2
14	OPC	C	302	-	-	28/57/57/60	-
10	UMQ	F	101	-	2/2/10/10	6/20/60/60	0/2/2/2
10	UMQ	A	305	-	2/2/10/10	5/20/60/60	0/2/2/2
17	SQD	D	201	-	-	6/23/43/69	0/1/1/1
11	MYS	A	306	-	-	3/12/12/12	-
9	HEM	A	302	1	-	1/14/54/54	-
12	8K6	A	308	-	-	7/15/15/15	-
9	HEM	A	303	-	-	4/14/54/54	-
10	UMQ	A	309	-	2/2/10/10	12/20/60/60	0/2/2/2
9	HEM	C	301	3	-	3/14/54/54	-
13	CLA	B	201	21	1/1/17/20	8/39/115/115	-
19	OCT	F	102	-	-	0/5/5/5	-
14	OPC	B	202	-	-	25/57/57/60	-
9	HEM	A	301	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	G	101	-	-	19/29/63/63	0/2/2/2
10	UMQ	A	304	-	2/2/10/10	12/20/60/60	0/2/2/2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	301	HEM	C3D-C2D	8.03	1.54	1.36
9	A	303	HEM	C3D-C2D	7.91	1.53	1.36
9	A	301	HEM	C3D-C2D	7.90	1.53	1.36
9	A	302	HEM	C3D-C2D	7.66	1.53	1.36
9	A	301	HEM	FE-ND	6.89	2.16	1.94
9	A	302	HEM	FE-ND	5.43	2.11	1.94
9	A	303	HEM	FE-ND	5.38	2.11	1.94
17	D	201	SQD	O47-C45	-5.06	1.34	1.46
9	A	303	HEM	FE-NB	4.49	2.08	1.94
9	C	301	HEM	FE-ND	4.18	2.07	1.94
9	A	303	HEM	FE-NC	4.06	2.08	1.95
9	A	301	HEM	FE-NC	4.03	2.08	1.95
9	A	302	HEM	FE-NC	3.72	2.07	1.95
9	A	303	HEM	FE-NA	3.62	2.07	1.95
9	C	301	HEM	FE-NC	3.59	2.07	1.95
15	C	303	7PH	O21-C2	-3.54	1.38	1.46
13	B	201	CLA	C1D-ND	3.52	1.42	1.37
20	G	101	BCR	C20-C21	3.49	1.54	1.43
14	C	302	OPC	OAN-CAO	3.46	1.44	1.34
17	D	201	SQD	C3-C2	-3.45	1.43	1.52
9	A	301	HEM	FE-NA	3.42	2.06	1.95
9	A	302	HEM	FE-NB	3.39	2.05	1.94
10	A	307	UMQ	C4-C5	-3.37	1.45	1.53
14	B	202	OPC	OAN-CAO	3.35	1.43	1.34
20	G	101	BCR	C23-C22	3.33	1.53	1.46
20	G	101	BCR	C16-C17	3.30	1.53	1.43
20	G	101	BCR	C15-C14	3.30	1.53	1.43
13	B	201	CLA	C4B-NB	3.27	1.42	1.37
10	A	305	UMQ	C4-C5	-3.26	1.46	1.53
20	G	101	BCR	C11-C10	3.24	1.53	1.43
9	C	301	HEM	FE-NB	3.24	2.04	1.94
17	D	201	SQD	O48-C23	3.16	1.42	1.33
20	G	101	BCR	C12-C13	3.16	1.52	1.46
20	G	101	BCR	C19-C18	3.15	1.52	1.46
20	G	101	BCR	C8-C9	3.14	1.52	1.46
9	A	303	HEM	CAC-C3C	3.12	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	101	BCR	C26-C25	3.10	1.39	1.34
9	A	301	HEM	CAC-C3C	3.09	1.55	1.47
9	A	301	HEM	CAB-C3B	3.06	1.55	1.47
10	A	304	UMQ	C4-C5	-3.03	1.46	1.53
9	A	303	HEM	CAB-C3B	3.02	1.55	1.47
9	A	302	HEM	CAC-C3C	3.02	1.55	1.47
9	C	301	HEM	CAB-C3B	2.98	1.55	1.47
9	A	302	HEM	CAB-C3B	2.98	1.55	1.47
9	C	301	HEM	CAC-C3C	2.98	1.55	1.47
10	A	309	UMQ	C4-C5	-2.93	1.46	1.53
15	C	303	7PH	O31-C3	-2.90	1.38	1.45
9	A	301	HEM	FE-NB	2.85	2.03	1.94
20	G	101	BCR	C32-C1	-2.81	1.48	1.53
10	A	307	UMQ	C3-C4	-2.77	1.45	1.52
10	F	101	UMQ	C4-C5	-2.74	1.47	1.53
10	A	304	UMQ	C3-C4	-2.70	1.45	1.52
17	D	201	SQD	O47-C7	2.69	1.41	1.35
13	B	201	CLA	C1B-C2B	2.66	1.49	1.43
10	F	101	UMQ	O5'-C5'	-2.65	1.37	1.44
10	F	101	UMQ	O2'-C2'	-2.60	1.36	1.43
10	A	305	UMQ	C3-C4	-2.58	1.45	1.52
14	C	302	OPC	OBJ-CBK	2.58	1.40	1.33
10	A	305	UMQ	O2'-C2'	-2.56	1.36	1.43
10	A	309	UMQ	O2'-C2'	-2.56	1.36	1.43
13	B	201	CLA	C3B-C4B	2.54	1.50	1.42
10	A	307	UMQ	O2'-C2'	-2.52	1.36	1.43
20	G	101	BCR	C40-C30	-2.51	1.49	1.53
17	D	201	SQD	C1-C2	-2.46	1.45	1.52
13	B	201	CLA	CHC-C1C	2.45	1.43	1.38
9	A	302	HEM	FE-NA	2.41	2.03	1.95
10	A	309	UMQ	C3-C4	-2.40	1.46	1.52
10	A	304	UMQ	O3'-C3'	-2.40	1.37	1.43
14	B	202	OPC	OBJ-CBI	-2.36	1.39	1.45
10	A	309	UMQ	O5'-C5'	-2.35	1.38	1.44
20	G	101	BCR	C5-C6	2.35	1.38	1.34
10	A	305	UMQ	O3'-C3'	-2.35	1.37	1.43
10	F	101	UMQ	C3-C4	-2.33	1.46	1.52
10	A	309	UMQ	O3'-C3'	-2.32	1.37	1.43
20	G	101	BCR	C39-C30	-2.32	1.49	1.53
10	F	101	UMQ	O3'-C3'	-2.31	1.37	1.43
20	G	101	BCR	C31-C1	-2.30	1.49	1.53
20	G	101	BCR	C24-C23	2.29	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	305	UMQ	O5'-C5'	-2.28	1.38	1.44
14	B	202	OPC	OBJ-CBK	2.28	1.40	1.33
17	D	201	SQD	O5-C5	2.27	1.49	1.44
20	G	101	BCR	C24-C25	2.26	1.52	1.45
17	D	201	SQD	O4-C4	-2.23	1.37	1.43
10	A	304	UMQ	O2'-C2'	-2.23	1.37	1.43
17	D	201	SQD	C4-C3	-2.21	1.46	1.52
10	A	304	UMQ	O1-C1	-2.21	1.35	1.41
14	C	302	OPC	OBJ-CBI	-2.20	1.40	1.45
20	G	101	BCR	C29-C28	-2.18	1.47	1.52
20	G	101	BCR	C7-C6	2.16	1.52	1.45
14	C	302	OPC	CAV-CAW	2.16	1.44	1.31
14	B	202	OPC	CAV-CAW	2.12	1.43	1.31
20	G	101	BCR	C20-C19	2.10	1.40	1.34
10	F	101	UMQ	O1-C1	-2.08	1.35	1.41
10	A	307	UMQ	O3'-C3'	-2.08	1.37	1.43
9	A	302	HEM	CMC-C2C	2.07	1.55	1.50
9	C	301	HEM	CMB-C2B	2.07	1.55	1.50
10	A	304	UMQ	O5'-C5'	-2.07	1.39	1.44
9	A	302	HEM	CMD-C2D	2.07	1.55	1.50
9	A	303	HEM	CMC-C2C	2.06	1.55	1.50
20	G	101	BCR	C11-C12	2.06	1.40	1.34
10	A	307	UMQ	O5'-C5'	-2.05	1.39	1.44
9	C	301	HEM	CMD-C2D	2.05	1.55	1.50
9	A	303	HEM	CMA-C3A	2.04	1.55	1.50
13	B	201	CLA	CMD-C2D	-2.03	1.46	1.50
10	A	305	UMQ	O1-C1	-2.01	1.36	1.41

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	SQD	O7-S-C6	20.20	136.92	106.76
17	D	201	SQD	O9-S-C6	-16.23	82.53	106.76
17	D	201	SQD	O9-S-O7	-9.75	82.10	113.82
10	A	305	UMQ	O1'-C1'-C2'	7.44	119.57	108.27
10	F	101	UMQ	O5-C5-C4	6.36	121.17	109.70
10	A	305	UMQ	O5'-C5'-C4'	5.97	122.06	109.72
9	A	301	HEM	C4D-ND-C1D	5.90	112.20	105.21
10	A	307	UMQ	C1-C2-C3	5.74	122.08	110.01
9	A	303	HEM	C4D-ND-C1D	5.69	111.94	105.21
13	B	201	CLA	C4A-NA-C1A	5.67	109.26	106.68
9	C	301	HEM	C4D-ND-C1D	5.55	111.78	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	302	HEM	C4D-ND-C1D	5.42	111.63	105.21
10	A	309	UMQ	O1-C1-C2	5.34	121.24	108.09
10	A	304	UMQ	O1-C4'-C5'	5.25	123.26	109.48
17	D	201	SQD	O47-C7-C8	5.16	120.29	111.09
10	A	309	UMQ	CA-O1'-C1'	5.14	122.46	113.68
10	A	305	UMQ	O5'-C1'-C2'	5.04	120.72	110.37
10	A	304	UMQ	O5'-C5'-C6'	4.90	118.58	106.44
10	A	304	UMQ	O5'-C5'-C4'	4.85	119.75	109.72
10	A	305	UMQ	O5'-C5'-C6'	4.82	118.39	106.44
10	A	304	UMQ	O1-C4'-C3'	4.81	119.45	107.23
10	F	101	UMQ	O5-C5-C6	4.79	118.32	106.44
10	A	309	UMQ	O2-C2-C1	4.65	121.15	110.08
20	G	101	BCR	C2-C1-C6	4.64	117.19	110.44
20	G	101	BCR	C16-C17-C18	-4.64	120.77	127.28
20	G	101	BCR	C15-C14-C13	-4.54	120.91	127.28
10	A	309	UMQ	O2-C2-C3	4.53	121.06	110.38
10	A	307	UMQ	O3'-C3'-C2'	4.53	121.04	110.38
10	A	304	UMQ	O2'-C2'-C1'	4.44	120.67	110.08
10	A	307	UMQ	O3'-C3'-C4'	4.39	121.20	109.94
10	A	307	UMQ	CA-O1'-C1'	4.39	121.18	113.68
20	G	101	BCR	C20-C21-C22	-4.39	121.12	127.28
10	F	101	UMQ	C1-C2-C3	4.27	118.98	110.01
20	G	101	BCR	C7-C8-C9	-4.26	119.93	126.23
10	A	304	UMQ	O2'-C2'-C3'	4.25	120.40	110.38
10	F	101	UMQ	O2-C2-C3	4.22	120.33	110.38
10	A	309	UMQ	O1-C1-O5	4.22	121.79	110.69
10	F	101	UMQ	O2-C2-C1	4.12	119.89	110.08
14	C	302	OPC	OAN-CAO-CAP	4.05	120.24	111.48
10	A	305	UMQ	O5'-C1'-O1'	4.04	119.58	110.04
14	B	202	OPC	OAN-CAO-CAP	4.00	120.14	111.48
10	A	309	UMQ	O5'-C5'-C4'	3.88	117.75	109.72
20	G	101	BCR	C11-C10-C9	-3.87	121.85	127.28
10	A	304	UMQ	C1'-C2'-C3'	3.86	118.13	110.01
10	A	305	UMQ	CA-O1'-C1'	3.84	120.25	113.68
20	G	101	BCR	C38-C26-C25	-3.81	120.33	124.48
10	A	307	UMQ	O2-C2-C1	3.61	118.68	110.08
20	G	101	BCR	C33-C5-C6	-3.61	120.55	124.48
10	A	307	UMQ	O2-C2-C3	3.46	118.54	110.38
10	A	309	UMQ	C1-C2-C3	3.44	117.26	110.01
20	G	101	BCR	C23-C24-C25	-3.33	118.10	127.00
9	A	303	HEM	CAD-C3D-C4D	3.33	130.50	124.70
10	A	307	UMQ	C2'-C3'-C4'	3.28	117.12	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	305	UMQ	C1-O1-C4'	-3.22	110.34	117.98
15	C	303	7PH	O21-C21-C22	3.17	118.33	111.48
20	G	101	BCR	C33-C5-C4	3.15	120.32	113.60
10	A	307	UMQ	C1-O1-C4'	-3.13	110.55	117.98
20	G	101	BCR	C29-C30-C25	3.13	114.98	110.44
10	A	309	UMQ	O5-C1-C2	3.12	116.78	110.37
10	A	307	UMQ	O5'-C5'-C4'	3.01	115.94	109.72
20	G	101	BCR	C24-C23-C22	-3.00	121.80	126.23
10	A	309	UMQ	C1-O1-C4'	-3.00	110.88	117.98
9	A	303	HEM	CHD-C1D-ND	2.98	127.64	124.42
13	B	201	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
20	G	101	BCR	C38-C26-C27	2.89	119.76	113.60
13	B	201	CLA	C3B-C4B-NB	-2.88	107.95	110.53
10	F	101	UMQ	CA-O1'-C1'	2.85	118.54	113.68
17	D	201	SQD	O8-S-C6	2.84	111.45	105.97
17	D	201	SQD	O48-C46-C45	2.83	116.56	108.40
17	D	201	SQD	C44-O6-C1	2.77	119.74	113.80
10	F	101	UMQ	C6-C5-C4	2.76	119.80	113.02
10	F	101	UMQ	C1'-O5'-C5'	-2.70	108.45	113.72
10	F	101	UMQ	C1-O1-C4'	-2.68	111.64	117.98
14	C	302	OPC	OBJ-CBK-CBL	2.67	119.96	111.83
20	G	101	BCR	C4-C5-C6	-2.64	119.14	122.70
20	G	101	BCR	C8-C7-C6	-2.58	120.09	127.00
17	D	201	SQD	O48-C23-C24	2.57	119.68	111.83
9	A	301	HEM	C1B-NB-C4B	2.56	108.24	105.21
15	C	303	7PH	O21-C21-O22	-2.54	117.77	123.70
20	G	101	BCR	C32-C1-C6	-2.47	106.36	110.24
10	A	304	UMQ	C6'-C5'-C4'	2.44	120.24	113.38
20	G	101	BCR	C34-C9-C10	-2.43	118.88	122.82
10	F	101	UMQ	C1-O5-C5	-2.41	109.01	113.72
9	A	301	HEM	C2A-C1A-NA	-2.38	107.51	110.15
9	C	301	HEM	C1B-NB-C4B	2.37	108.02	105.21
10	A	309	UMQ	C1-O5-C5	-2.37	109.10	113.72
10	A	304	UMQ	CA-O1'-C1'	2.36	117.71	113.68
10	F	101	UMQ	O5'-C5'-C4'	2.33	114.54	109.72
20	G	101	BCR	C1-C6-C5	-2.27	119.54	122.64
15	C	303	7PH	O31-C31-C32	2.26	118.72	111.83
9	A	303	HEM	C2A-C1A-NA	-2.23	107.68	110.15
10	A	309	UMQ	C3'-C4'-C5'	2.22	115.84	110.93
9	A	303	HEM	CAC-C3C-C4C	2.21	130.10	124.82
13	B	201	CLA	CHB-C4A-NA	2.21	127.58	124.40
10	F	101	UMQ	O5'-C1'-C2'	-2.20	105.85	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	SQD	O6-C44-C45	2.20	116.16	110.82
10	A	307	UMQ	O5-C5-C6	2.19	111.87	106.44
10	F	101	UMQ	C6'-C5'-C4'	-2.17	107.28	113.38
10	A	305	UMQ	C1-O5-C5	-2.16	109.50	113.72
9	A	302	HEM	C1B-NB-C4B	2.13	107.72	105.21
9	A	301	HEM	CHA-C4D-ND	2.12	127.00	124.37
13	B	201	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
10	A	304	UMQ	C4-C3-C2	-2.07	107.20	110.83
20	G	101	BCR	C27-C26-C25	-2.06	119.92	122.70
9	A	302	HEM	CMD-C2D-C1D	2.06	128.25	125.03
9	C	301	HEM	C2A-C1A-NA	-2.05	107.88	110.15
9	A	301	HEM	C3B-C2B-C1B	2.04	107.94	106.41
10	A	307	UMQ	C1'-O5'-C5'	2.01	117.65	113.72
9	A	303	HEM	C1B-NB-C4B	2.01	107.59	105.21
13	B	201	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
10	A	309	UMQ	C6'-C5'-C4'	-2.00	107.74	113.38

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	304	UMQ	C5'
10	A	304	UMQ	C2'
10	A	305	UMQ	C5'
10	A	305	UMQ	C1'
10	A	307	UMQ	C3'
10	A	307	UMQ	C2
10	A	309	UMQ	C1
10	A	309	UMQ	C2
10	F	101	UMQ	C5
10	F	101	UMQ	C2
13	B	201	CLA	ND

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	307	UMQ	O5'-C1'-O1'-CA
10	F	101	UMQ	O5'-C1'-O1'-CA
13	B	201	CLA	C1A-C2A-CAA-CBA
13	B	201	CLA	C3A-C2A-CAA-CBA
14	B	202	OPC	CAL-OAK-PAJ-OAB
14	B	202	OPC	CAL-OAK-PAJ-OAI
14	B	202	OPC	CAH-OAI-PAJ-OAK

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Mol	Chain	Res	Type	Atoms
14	B	202	OPC	CAH-OAI-PAJ-OBH
14	B	202	OPC	CAH-OAI-PAJ-OAB
14	C	302	OPC	CAM-CAL-OAK-PAJ
14	C	302	OPC	NAF-CAG-CAH-OAI
15	C	303	7PH	O11-C1-C2-C3
15	C	303	7PH	O11-C1-C2-O21
15	C	303	7PH	O22-C21-O21-C2
15	C	303	7PH	C22-C21-O21-C2
17	D	201	SQD	O49-C7-O47-C45
17	D	201	SQD	C8-C7-O47-C45
17	D	201	SQD	C5-C6-S-O8
17	D	201	SQD	C5-C6-S-O9
20	G	101	BCR	C7-C8-C9-C10
20	G	101	BCR	C7-C8-C9-C34
20	G	101	BCR	C21-C22-C23-C24
20	G	101	BCR	C22-C23-C24-C25
10	A	309	UMQ	O5-C1-O1-C4'
17	D	201	SQD	O10-C23-O48-C46
17	D	201	SQD	C24-C23-O48-C46
10	A	305	UMQ	O5-C5-C6-O6
10	A	309	UMQ	O5-C5-C6-O6
10	A	305	UMQ	C4'-C5'-C6'-O6'
10	A	309	UMQ	C4'-C5'-C6'-O6'
14	C	302	OPC	CAP-CAO-OAN-CAM
10	A	305	UMQ	C4-C5-C6-O6
10	F	101	UMQ	O5-C5-C6-O6
10	A	309	UMQ	C4-C5-C6-O6
10	A	305	UMQ	O5'-C1'-O1'-CA
10	A	304	UMQ	O5'-C5'-C6'-O6'
9	A	303	HEM	C4D-C3D-CAD-CBD
10	F	101	UMQ	C2'-C1'-O1'-CA
20	G	101	BCR	C11-C12-C13-C35
20	G	101	BCR	C36-C18-C19-C20
20	G	101	BCR	C37-C22-C23-C24
20	G	101	BCR	C11-C12-C13-C14
20	G	101	BCR	C17-C18-C19-C20
10	A	309	UMQ	O5'-C5'-C6'-O6'
13	B	201	CLA	C8-C10-C11-C12
13	B	201	CLA	C10-C11-C12-C13
10	A	307	UMQ	O5-C5-C6-O6
10	A	307	UMQ	C2-C1-O1-C4'
14	C	302	OPC	OAD-CAO-OAN-CAM

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Mol	Chain	Res	Type	Atoms
14	B	202	OPC	CBL-CBK-OBJ-CBI
9	A	303	HEM	C2D-C3D-CAD-CBD
10	A	307	UMQ	O5-C1-O1-C4'
10	A	307	UMQ	O1'-CA-CB-CC
20	G	101	BCR	C16-C17-C18-C19
10	A	309	UMQ	O5'-C1'-O1'-CA
14	B	202	OPC	CBA-CBB-CBC-CBD
10	A	307	UMQ	CB-CA-O1'-C1'
14	B	202	OPC	CAR-CAS-CAT-CAU
10	A	307	UMQ	CG-CH-CI-CJ
11	A	306	MYS	C6-C7-C8-C9
14	B	202	OPC	CAQ-CAR-CAS-CAT
10	A	309	UMQ	CA-CB-CC-CD
10	A	304	UMQ	C4-C5-C6-O6
20	G	101	BCR	C19-C20-C21-C22
15	C	303	7PH	C36-C37-C38-C39
14	C	302	OPC	CBW-CBX-CBY-CBZ
20	G	101	BCR	C23-C24-C25-C30
14	C	302	OPC	CBX-CBY-CBZ-CCA
11	A	306	MYS	C4-C5-C6-C7
15	C	303	7PH	C21-C22-C23-C24
10	A	307	UMQ	CA-CB-CC-CD
14	B	202	OPC	CBM-CBN-CBO-CBP
12	A	308	8K6	C5-C6-C7-C8
14	C	302	OPC	CAS-CAT-CAU-CAV
14	C	302	OPC	CBO-CBP-CBQ-CBR
14	C	302	OPC	CBB-CBC-CBD-CBE
10	A	304	UMQ	C4'-C5'-C6'-O6'
15	C	303	7PH	C29-C2A-C2B-C2C
14	C	302	OPC	CBT-CBU-CBV-CBW
10	F	101	UMQ	CD-CF-CG-CH
10	A	309	UMQ	CH-CI-CJ-CK
14	C	302	OPC	CBV-CBW-CBX-CBY
14	C	302	OPC	CAQ-CAR-CAS-CAT
10	F	101	UMQ	CH-CI-CJ-CK
10	A	304	UMQ	C5'-C4'-O1-C1
12	A	308	8K6	C14-C15-C16-C17
10	A	304	UMQ	C2'-C1'-O1'-CA
14	B	202	OPC	CBO-CBP-CBQ-CBR
14	B	202	OPC	CBS-CBT-CBU-CBV
14	C	302	OPC	CAW-CAX-CAY-CAZ
15	C	303	7PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
10	A	309	UMQ	CI-CJ-CK-CL
14	C	302	OPC	CAP-CAQ-CAR-CAS
13	B	201	CLA	C4-C3-C5-C6
14	B	202	OPC	OAD-CAO-OAN-CAM
9	A	301	HEM	C2A-CAA-CBA-CGA
10	A	307	UMQ	C2'-C1'-O1'-CA
10	A	304	UMQ	CC-CD-CF-CG
14	B	202	OPC	CAP-CAQ-CAR-CAS
13	B	201	CLA	C2-C3-C5-C6
15	C	303	7PH	C1-C2-C3-O31
10	A	304	UMQ	CA-CB-CC-CD
20	G	101	BCR	C1-C6-C7-C8
14	B	202	OPC	OAN-CAM-CBI-OBJ
14	B	202	OPC	CBN-CBO-CBP-CBQ
14	C	302	OPC	CBM-CBN-CBO-CBP
14	B	202	OPC	CBK-CBL-CBM-CBN
20	G	101	BCR	C16-C17-C18-C36
14	C	302	OPC	OAK-CAL-CAM-CBI
14	B	202	OPC	CBB-CBC-CBD-CBE
13	B	201	CLA	O2A-C1-C2-C3
10	A	305	UMQ	CC-CD-CF-CG
15	C	303	7PH	C23-C24-C25-C26
14	C	302	OPC	OAK-CAL-CAM-OAN
10	A	304	UMQ	O5'-C1'-O1'-CA
14	B	202	OPC	CAL-CAM-CBI-OBJ
9	A	303	HEM	C4C-C3C-CAC-CBC
14	B	202	OPC	CBC-CBD-CBE-CBF
14	C	302	OPC	CBQ-CBR-CBS-CBT
14	C	302	OPC	CAY-CAZ-CBA-CBB
14	B	202	OPC	NAF-CAG-CAH-OAI
14	C	302	OPC	CBU-CBV-CBW-CBX
9	C	301	HEM	C2D-C3D-CAD-CBD
14	B	202	OPC	CAS-CAT-CAU-CAV
10	A	307	UMQ	CB-CC-CD-CF
15	C	303	7PH	O21-C2-C3-O31
14	C	302	OPC	CAH-OAI-PAJ-OAB
9	A	302	HEM	C2A-CAA-CBA-CGA
14	C	302	OPC	CBI-CAM-OAN-CAO
14	B	202	OPC	CBV-CBW-CBX-CBY
9	C	301	HEM	C4D-C3D-CAD-CBD
10	A	304	UMQ	O5-C1-O1-C4'
10	A	304	UMQ	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	F	101	UMQ	CF-CG-CH-CI
10	A	304	UMQ	CF-CG-CH-CI
10	A	307	UMQ	C4-C5-C6-O6
15	C	303	7PH	C27-C28-C29-C2A
10	A	307	UMQ	CH-CI-CJ-CK
20	G	101	BCR	C11-C10-C9-C34
20	G	101	BCR	C9-C10-C11-C12
12	A	308	8K6	C1-C2-C3-C4
13	B	201	CLA	C13-C15-C16-C17
20	G	101	BCR	C11-C10-C9-C8
20	G	101	BCR	C5-C6-C7-C8
20	G	101	BCR	C23-C24-C25-C26
12	A	308	8K6	C7-C8-C9-C10
10	A	304	UMQ	C2-C1-O1-C4'
10	A	309	UMQ	CD-CF-CG-CH
12	A	308	8K6	C12-C13-C14-C15
14	C	302	OPC	CBR-CBS-CBT-CBU
10	A	309	UMQ	CF-CG-CH-CI
14	C	302	OPC	OBJ-CBK-CBL-CBM
14	C	302	OPC	OCC-CBK-OBJ-CBI
14	C	302	OPC	CBP-CBQ-CBR-CBS
12	A	308	8K6	C15-C16-C17-C18
14	C	302	OPC	CBL-CBK-OBJ-CBI
10	A	309	UMQ	O1'-CA-CB-CC
15	C	303	7PH	C31-C32-C33-C34
9	A	301	HEM	C2D-C3D-CAD-CBD
10	A	307	UMQ	O5'-C5'-C6'-O6'
14	C	302	OPC	CBN-CBO-CBP-CBQ
11	A	306	MYS	C5-C6-C7-C8
14	B	202	OPC	OCC-CBK-OBJ-CBI
12	A	308	8K6	C13-C14-C15-C16
9	A	303	HEM	CAD-CBD-CGD-O2D
14	B	202	OPC	CBL-CBM-CBN-CBO
9	C	301	HEM	CAD-CBD-CGD-O2D
9	A	301	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

11 monomers are involved in 43 short contacts:

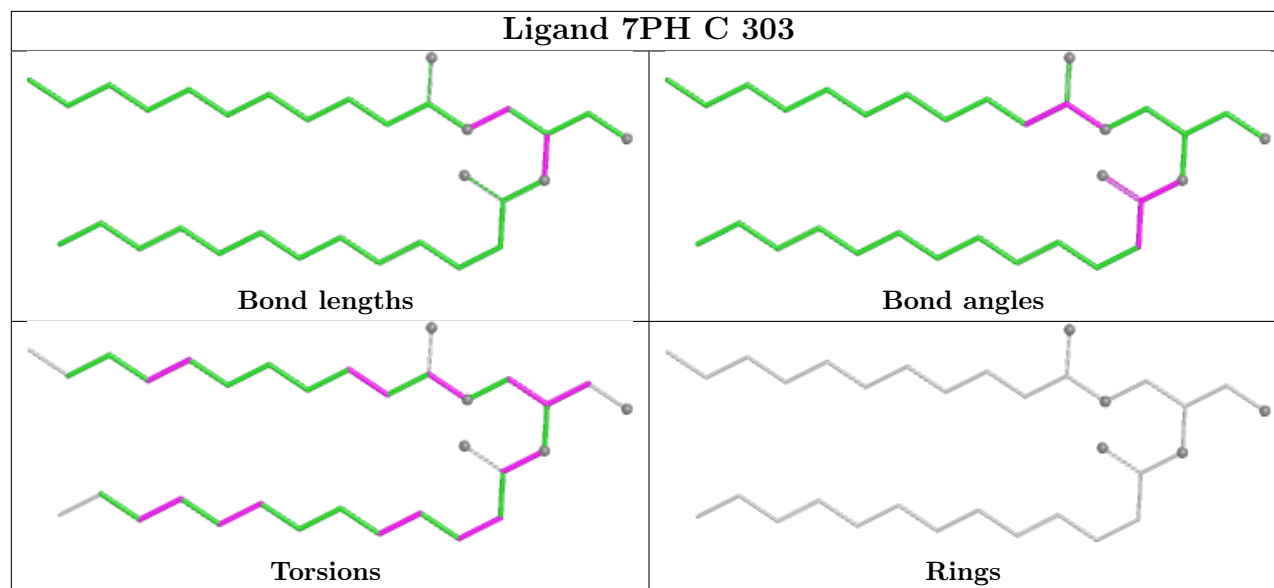
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	202	FES	1	0
10	A	307	UMQ	5	0

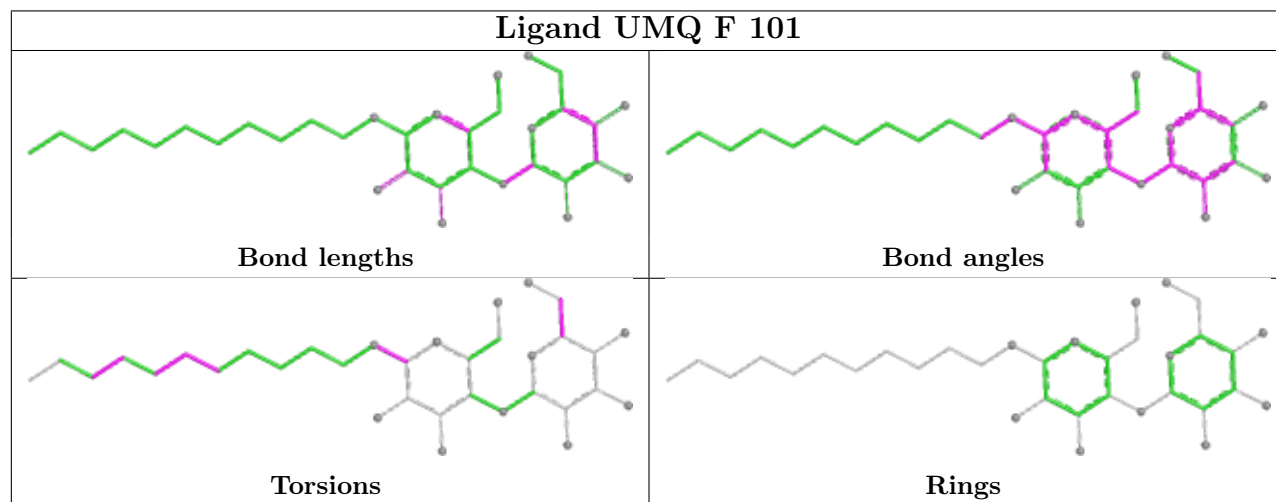
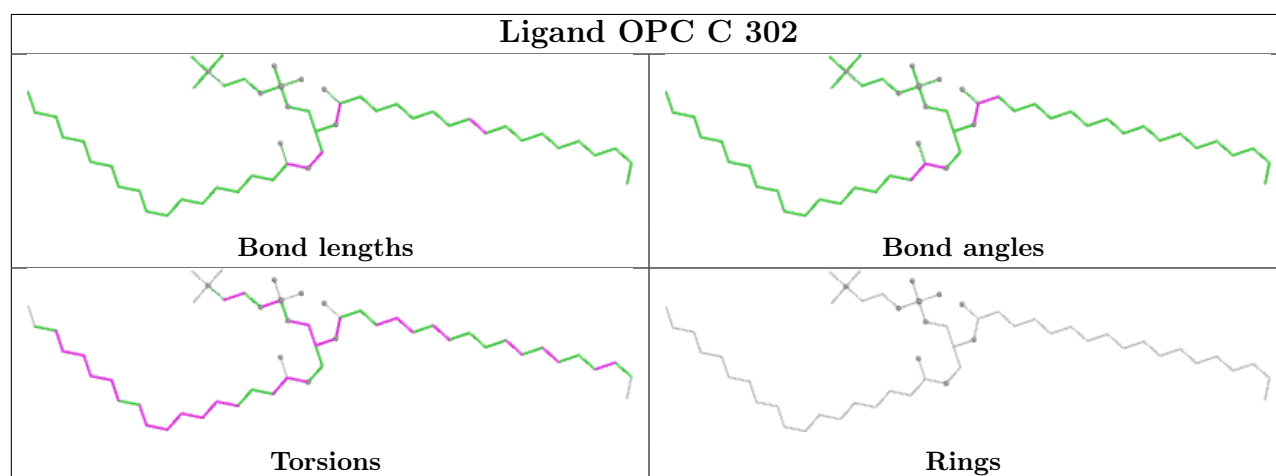
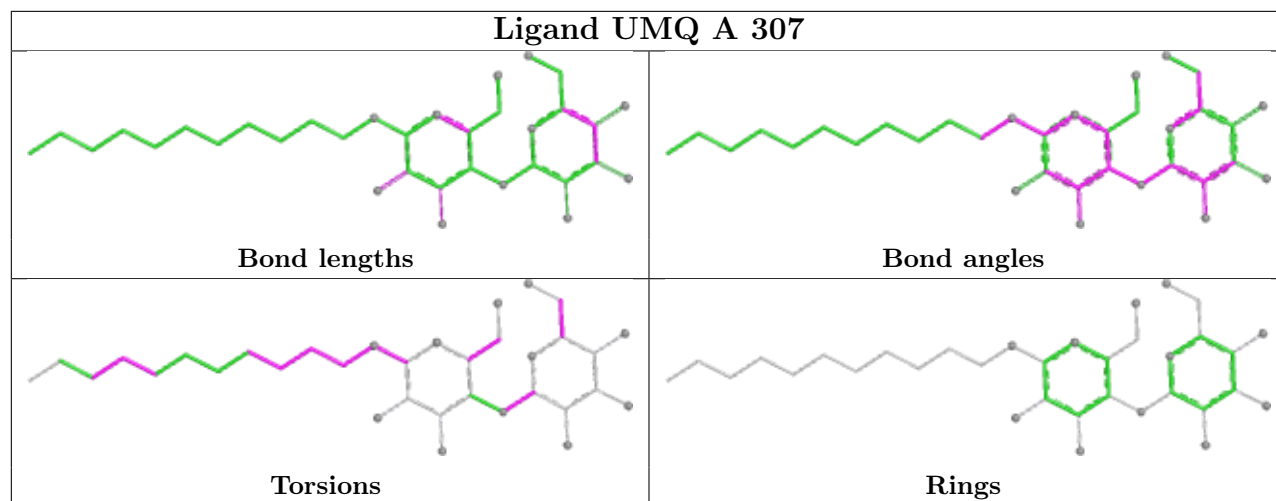
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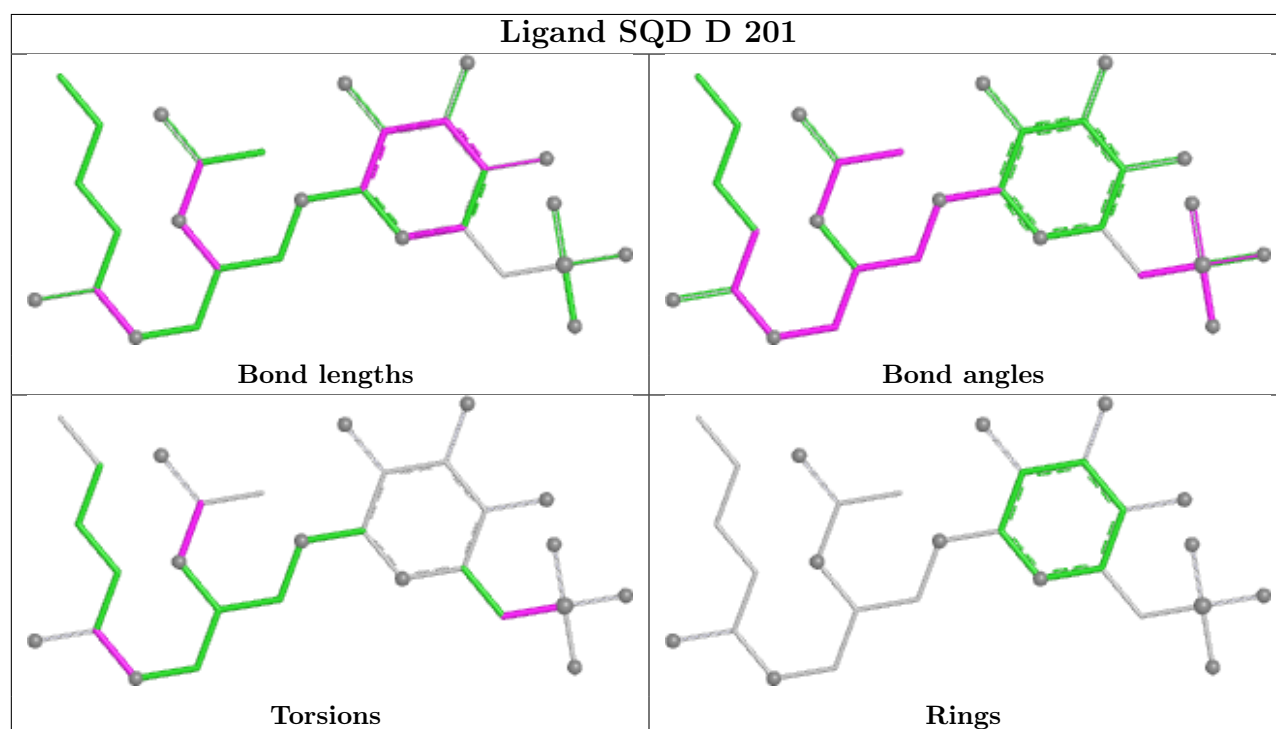
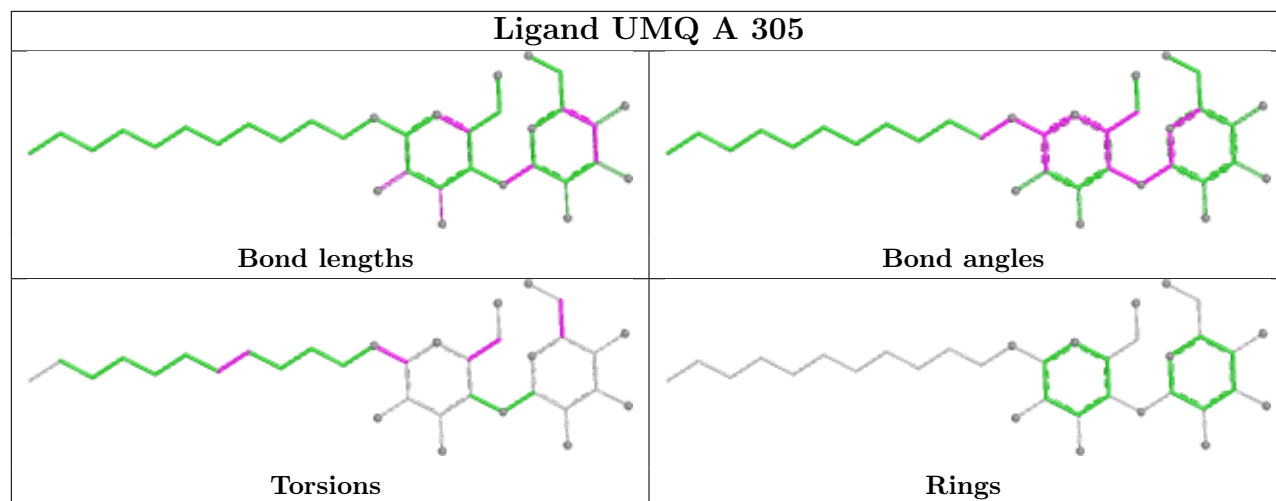
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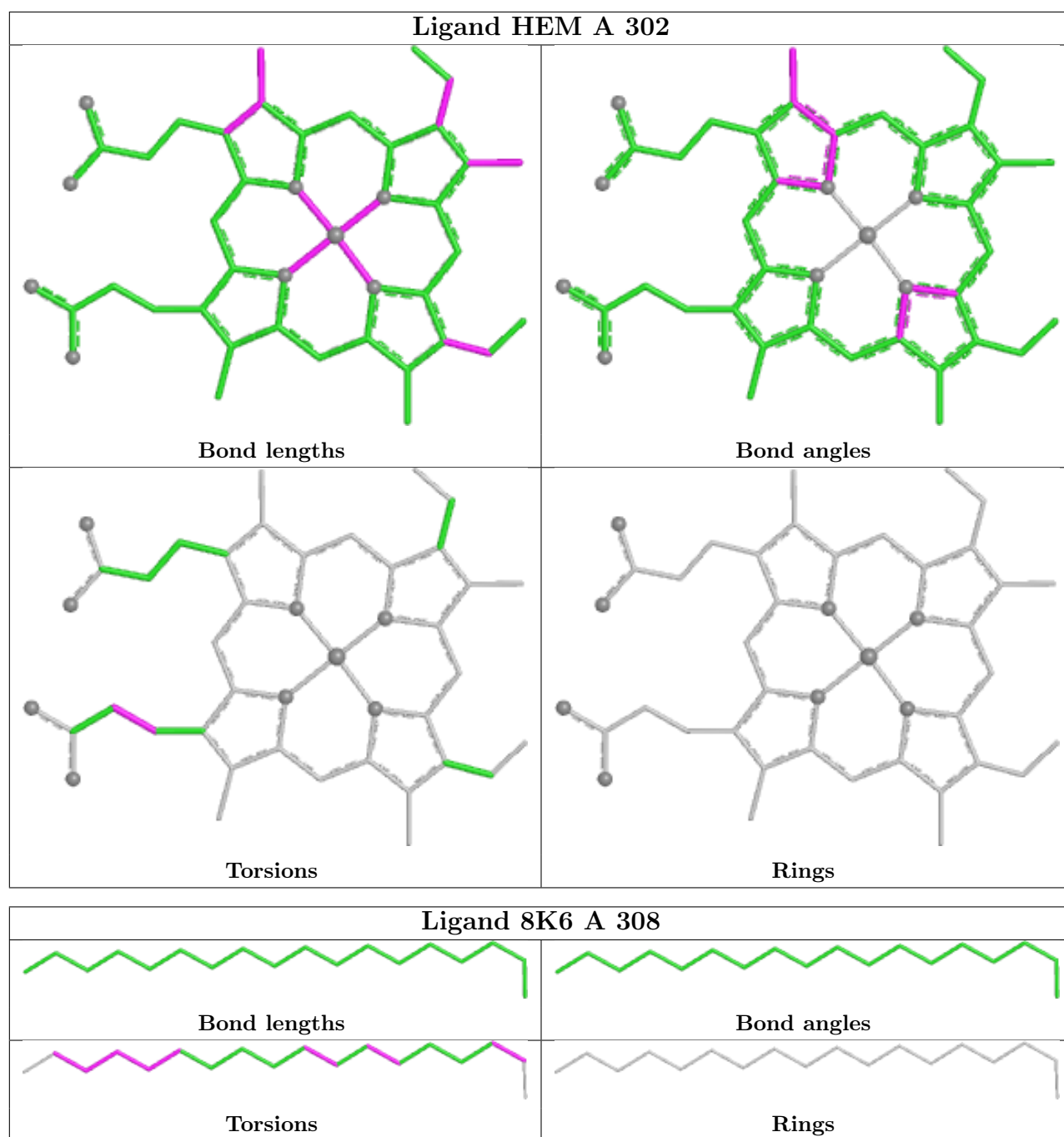
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	302	OPC	3	0
10	F	101	UMQ	1	0
11	A	306	MYS	1	0
9	A	302	HEM	4	0
9	A	303	HEM	10	0
9	C	301	HEM	7	0
13	B	201	CLA	3	0
9	A	301	HEM	5	0
20	G	101	BCR	5	0

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.

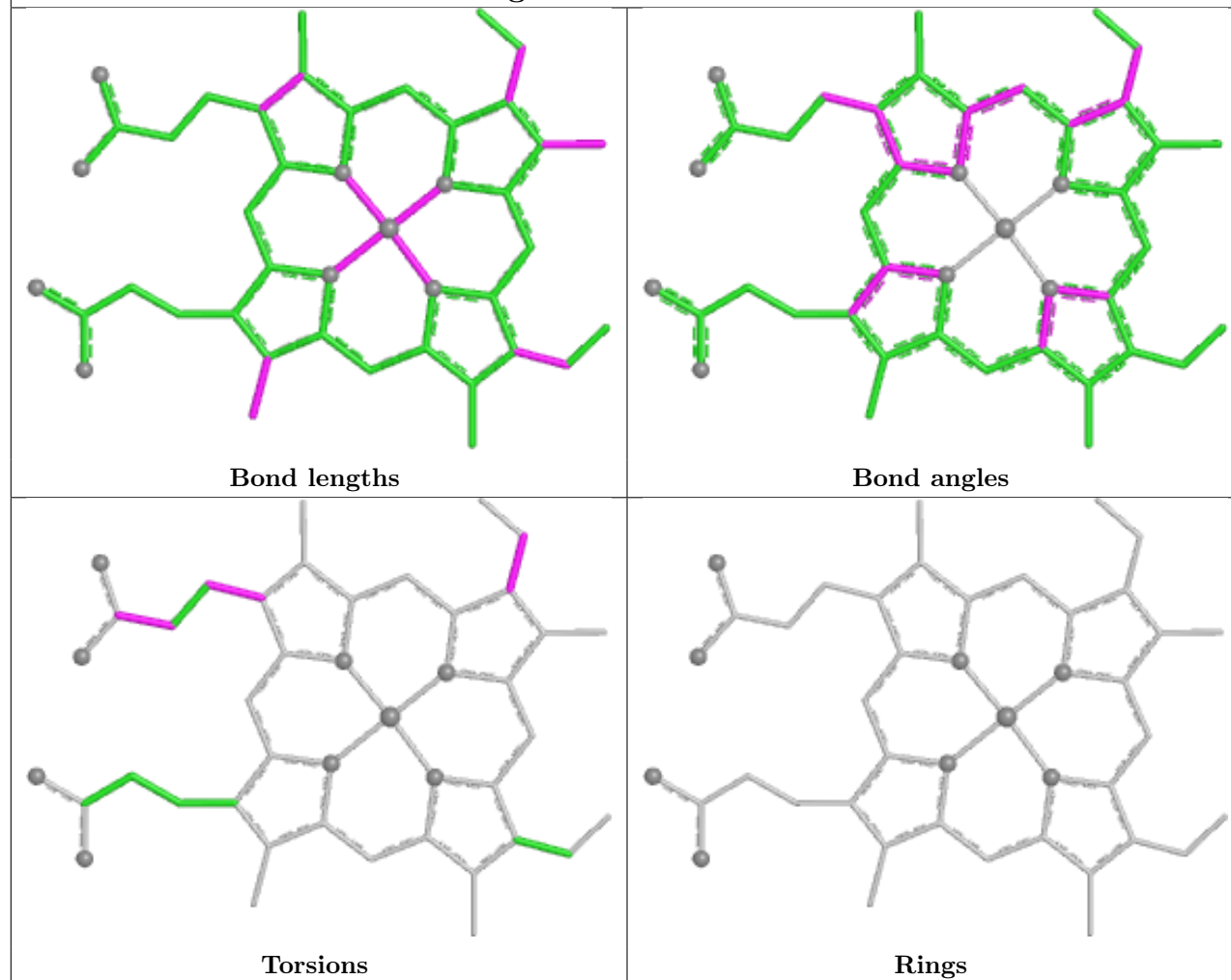




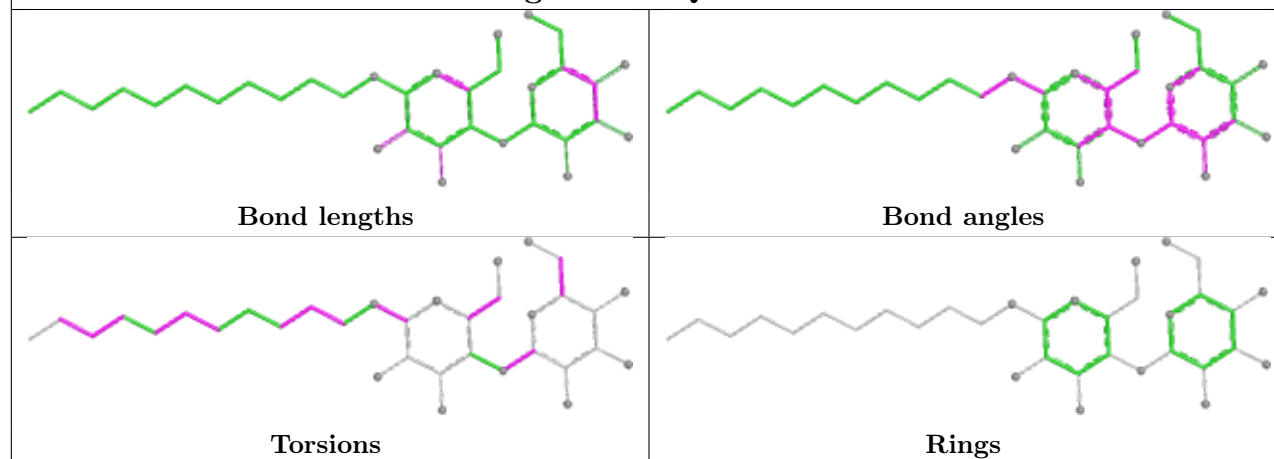


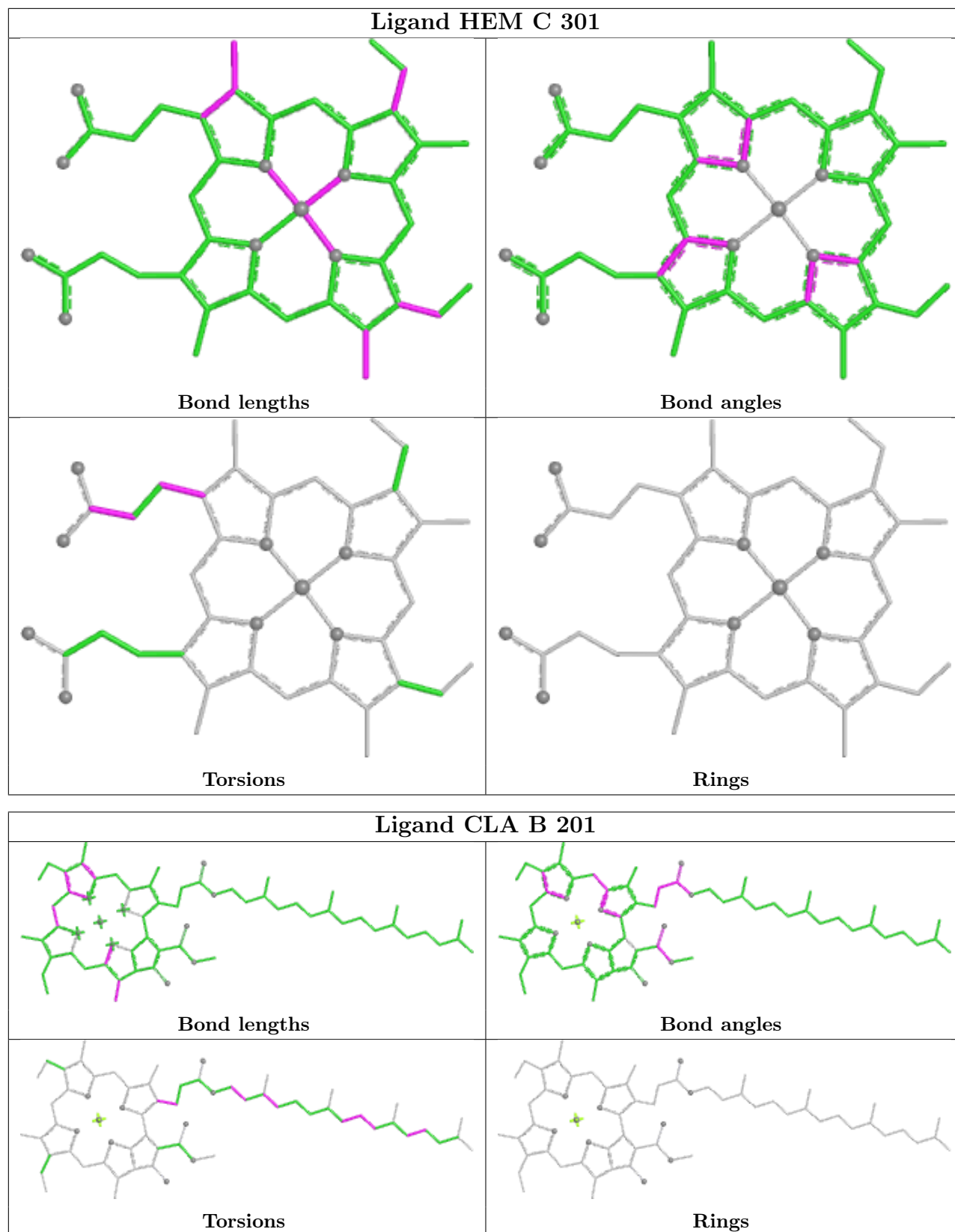


Ligand HEM A 303

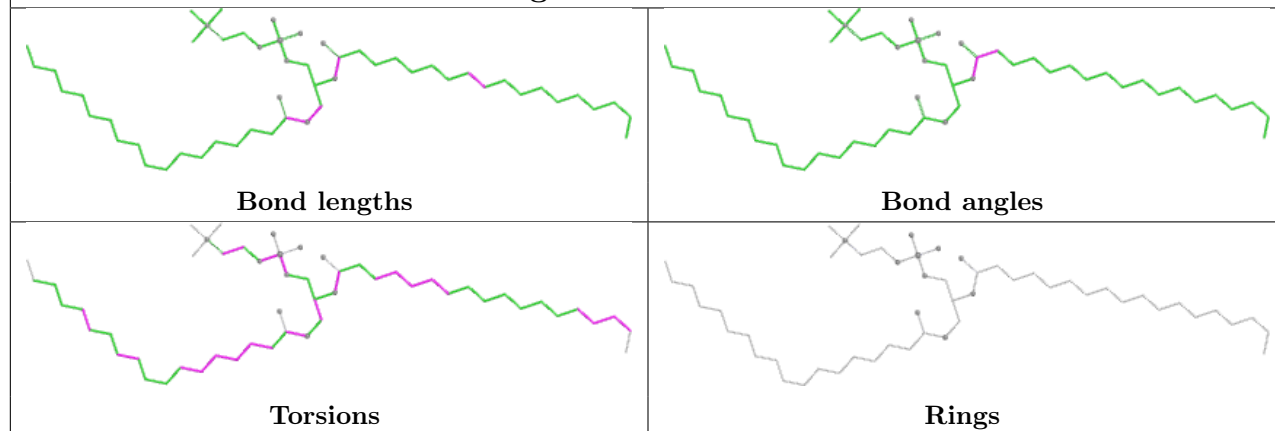


Ligand UMQ A 309

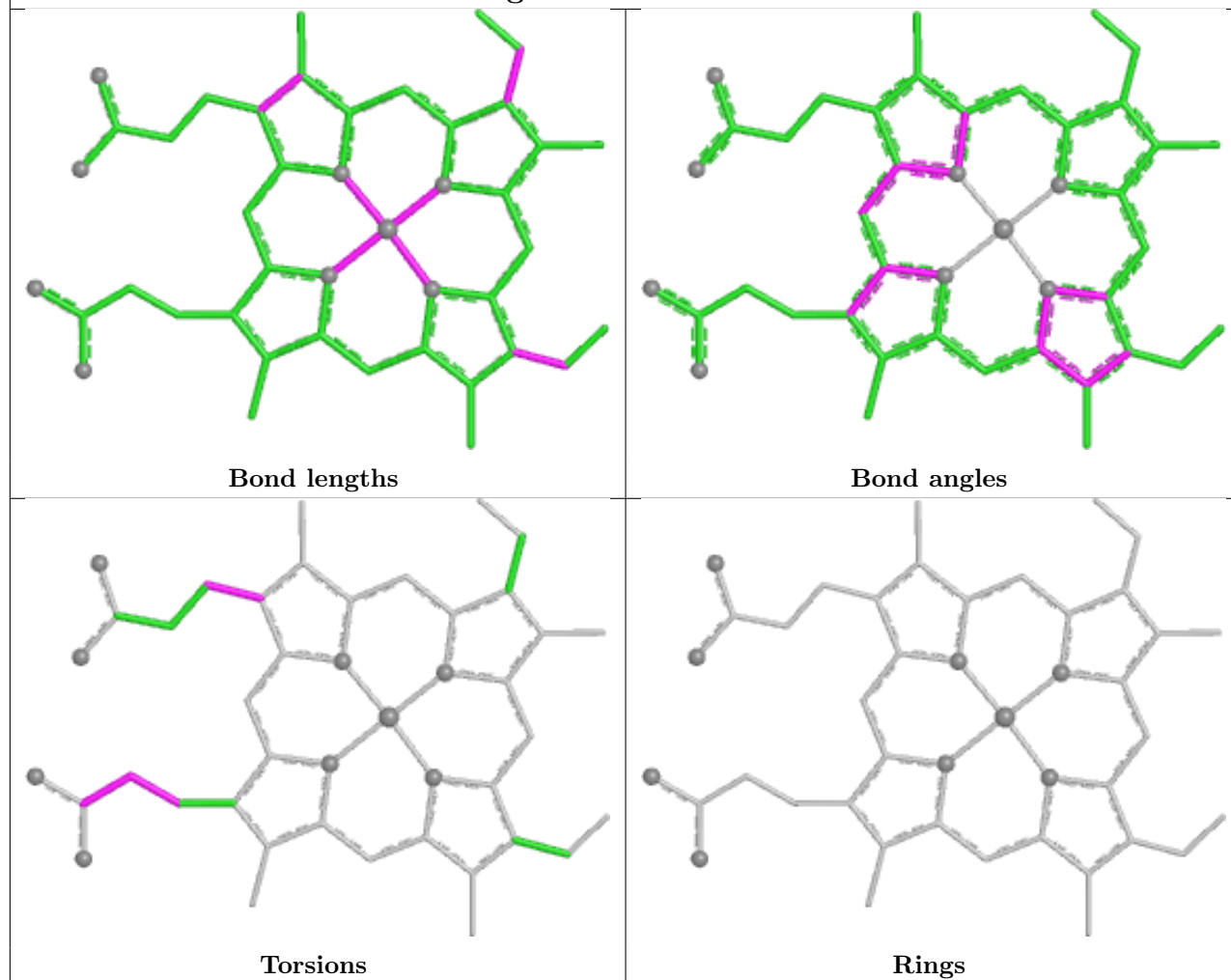


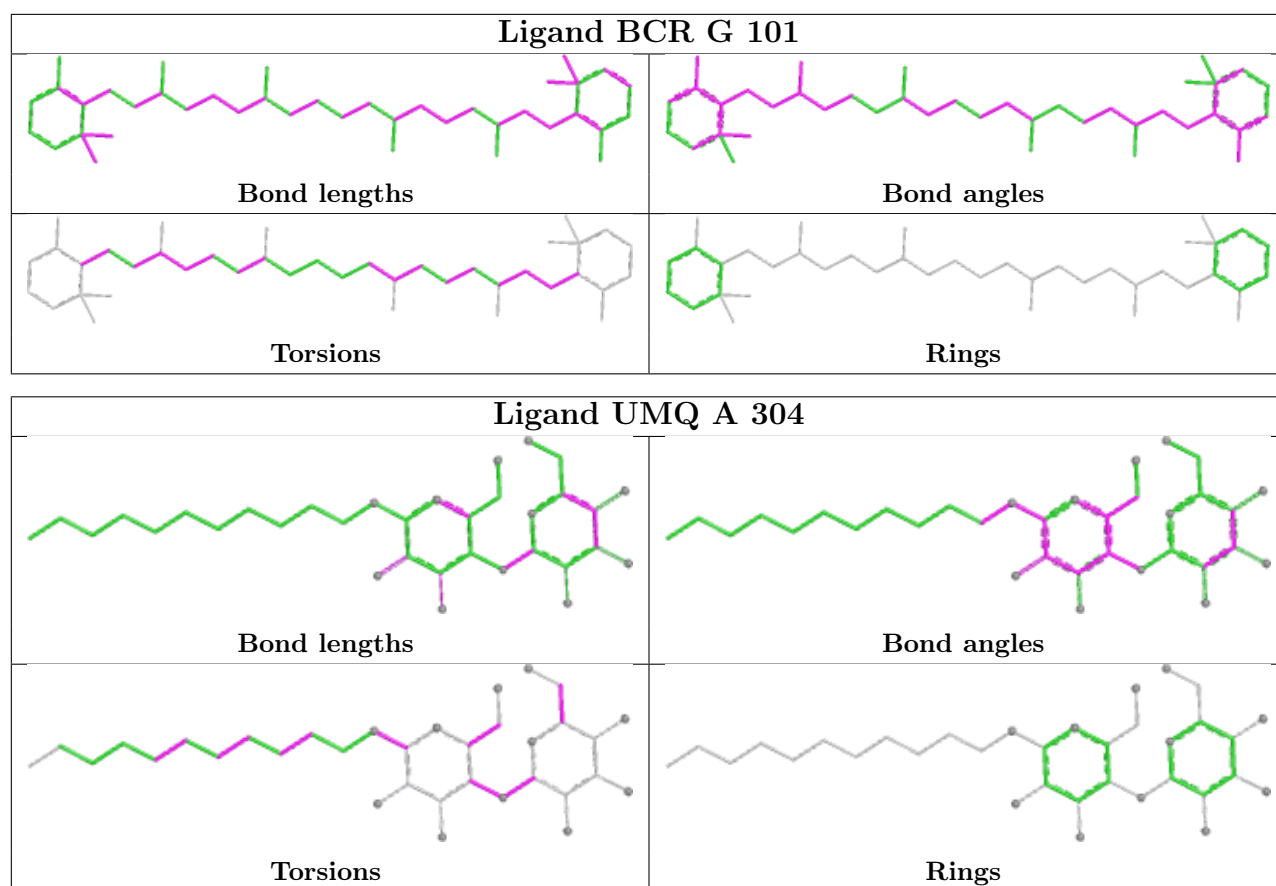


Ligand OPC B 202



Ligand HEM A 301





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	215/215 (100%)	-0.08	9 (4%) 40 37	31, 47, 82, 181	0
2	B	160/160 (100%)	0.47	11 (6%) 23 20	43, 64, 111, 138	0
3	C	289/289 (100%)	1.20	71 (24%) 2 1	44, 73, 182, 204	0
4	D	166/179 (92%)	2.02	77 (46%) 0 0	38, 131, 181, 193	0
5	E	31/31 (100%)	0.82	3 (9%) 13 11	66, 81, 112, 130	0
6	F	32/34 (94%)	0.88	5 (15%) 5 4	57, 72, 116, 137	0
7	G	37/37 (100%)	1.10	6 (16%) 4 4	48, 61, 115, 126	0
8	H	29/29 (100%)	0.35	2 (6%) 23 20	51, 62, 71, 101	0
All	All	959/974 (98%)	0.88	184 (19%) 3 3	31, 68, 174, 204	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	98	ALA	11.0
7	G	37	GLY	11.0
4	D	50	ALA	9.0
4	D	70	LEU	7.8
4	D	75	VAL	6.6
3	C	143	HIS	6.4
1	A	2	ALA	6.2
4	D	170	PHE	6.1
3	C	201	THR	5.9
3	C	224	ALA	5.8
3	C	191	GLY	5.8
4	D	99	ILE	5.7
3	C	199	ILE	5.6
4	D	179	SER	5.5
3	C	200	LYS	5.4
4	D	51	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	206	VAL	5.3
3	C	192	SER	5.1
3	C	222	GLY	5.0
3	C	175	ALA	5.0
1	A	1	MET	5.0
2	B	160	PHE	4.9
4	D	92	VAL	4.7
6	F	1	MET	4.6
3	C	203	SER	4.3
3	C	176	ALA	4.3
3	C	170	ASN	4.3
3	C	117	GLY	4.3
4	D	137	GLY	4.2
3	C	177	THR	4.1
4	D	49	GLY	4.0
4	D	172	THR	4.0
7	G	36	GLY	4.0
4	D	134	ASP	3.9
2	B	155	LEU	3.9
4	D	69	PHE	3.9
4	D	149	ALA	3.9
4	D	108	CYS	3.9
3	C	226	THR	3.8
3	C	223	GLN	3.8
3	C	181	SER	3.8
4	D	67	SER	3.8
3	C	218	ILE	3.8
7	G	35	LEU	3.8
4	D	135	ALA	3.7
3	C	212	PRO	3.7
3	C	225	VAL	3.7
4	D	55	THR	3.7
3	C	213	ALA	3.7
4	D	171	ARG	3.6
3	C	188	GLY	3.6
3	C	230	ALA	3.6
3	C	202	GLU	3.6
4	D	176	PRO	3.5
4	D	140	VAL	3.5
4	D	84	LEU	3.5
4	D	109	THR	3.5
4	D	155	THR	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	219	VAL	3.5
4	D	173	GLY	3.5
3	C	184	ALA	3.4
3	C	93	GLU	3.4
3	C	56	THR	3.4
3	C	194	LYS	3.4
3	C	207	VAL	3.4
4	D	66	VAL	3.4
3	C	183	ILE	3.3
4	D	139	VAL	3.3
4	D	133	TYR	3.3
4	D	160	ILE	3.3
4	D	54	THR	3.3
3	C	281	LYS	3.3
4	D	169	ASP	3.3
4	D	102	TYR	3.2
4	D	68	LYS	3.1
6	F	32	ALA	3.1
4	D	119	ALA	3.1
2	B	2	ALA	3.0
3	C	180	ILE	3.0
4	D	76	GLY	3.0
3	C	198	ASP	3.0
4	D	48	GLY	3.0
4	D	138	LYS	2.9
3	C	239	GLY	2.9
4	D	52	GLY	2.9
3	C	227	ALA	2.9
4	D	150	LEU	2.9
3	C	28	ALA	2.9
3	C	109	ASP	2.9
4	D	86	GLY	2.9
4	D	82	GLN	2.8
1	A	3	ASN	2.8
4	D	122	ASN	2.8
4	D	60	LEU	2.8
3	C	221	GLU	2.8
4	D	63	ASP	2.8
4	D	56	ALA	2.8
3	C	68	VAL	2.8
3	C	60	GLN	2.8
4	D	85	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	46	ALA	2.8
4	D	175	GLU	2.8
3	C	231	LEU	2.7
3	C	195	TYR	2.7
2	B	159	LEU	2.7
3	C	204	GLY	2.7
4	D	156	GLU	2.7
4	D	47	ALA	2.7
3	C	211	ILE	2.7
4	D	164	SER	2.7
4	D	136	THR	2.7
3	C	229	ASP	2.7
3	C	186	GLN	2.6
3	C	172	TYR	2.6
4	D	125	LYS	2.6
3	C	174	ALA	2.6
4	D	178	TRP	2.6
4	D	77	ASP	2.6
3	C	208	SER	2.6
4	D	158	ASP	2.6
6	F	2	SER	2.6
2	B	153	LYS	2.6
3	C	232	THR	2.5
8	H	1	MET	2.5
3	C	121	GLY	2.5
1	A	151	VAL	2.5
3	C	19	ARG	2.5
4	D	73	HIS	2.5
4	D	105	ASN	2.5
4	D	157	ASN	2.5
4	D	159	LYS	2.5
1	A	159	PRO	2.4
5	E	1	MET	2.4
3	C	59	GLN	2.4
3	C	101	VAL	2.4
3	C	193	VAL	2.4
4	D	78	ARG	2.4
6	F	29	ILE	2.4
3	C	92	GLU	2.4
3	C	182	LYS	2.4
4	D	64	VAL	2.4
4	D	166	THR	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	29	LEU	2.4
7	G	33	ASN	2.4
2	B	154	SER	2.4
2	B	142	TRP	2.4
4	D	103	GLY	2.4
3	C	61	VAL	2.4
1	A	150	ILE	2.4
4	D	101	ASP	2.4
4	D	177	TRP	2.4
3	C	166	LYS	2.4
7	G	30	LYS	2.4
2	B	74	GLU	2.3
3	C	122	GLU	2.3
4	D	165	TRP	2.3
4	D	143	PRO	2.3
4	D	142	GLY	2.3
3	C	70	LEU	2.3
4	D	118	ASN	2.3
3	C	22	CYS	2.3
5	E	31	LEU	2.3
3	C	67	LYS	2.3
3	C	64	ASP	2.3
3	C	196	LEU	2.3
4	D	141	ARG	2.2
4	D	65	SER	2.2
1	A	160	VAL	2.2
2	B	3	THR	2.2
2	B	1	MET	2.2
1	A	5	TYR	2.2
3	C	287	MET	2.2
4	D	16	ARG	2.1
4	D	100	THR	2.1
6	F	7	ASN	2.1
3	C	197	VAL	2.1
2	B	156	THR	2.1
1	A	149	LYS	2.1
3	C	233	ASN	2.1
4	D	83	GLY	2.1
5	E	16	GLY	2.1
3	C	185	LYS	2.0
4	D	145	PRO	2.0
7	G	26	TYR	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](#)

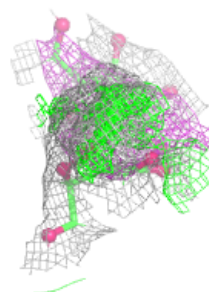
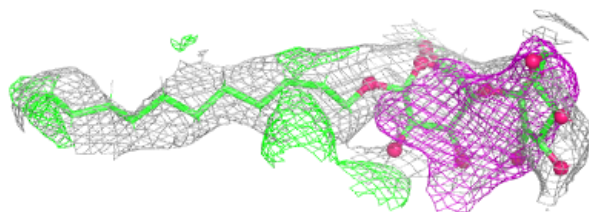
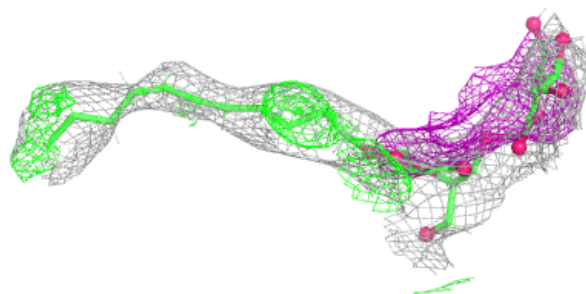
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	CD	C	304	1/1	0.06	0.48	206,206,206,206	0
10	UMQ	A	307	34/34	0.66	0.27	72,111,140,165	0
10	UMQ	A	304	34/34	0.66	0.25	78,129,162,173	0
10	UMQ	A	309	34/34	0.71	0.21	57,121,187,208	0
10	UMQ	F	101	34/34	0.78	0.21	63,128,205,215	0
19	OCT	F	102	8/8	0.78	0.21	61,76,90,99	0
10	UMQ	A	305	34/34	0.83	0.17	58,110,148,166	0
11	MYS	A	306	15/15	0.85	0.20	50,68,96,98	0
15	7PH	C	303	32/38	0.85	0.18	49,72,135,154	0
17	SQD	D	201	29/54	0.87	0.18	63,90,129,145	0
14	OPC	C	302	54/55	0.87	0.22	47,96,152,167	0
14	OPC	B	202	54/55	0.89	0.21	52,93,137,149	0
12	8K6	A	308	18/18	0.91	0.12	50,71,84,87	0
20	BCR	G	101	40/40	0.91	0.17	40,73,127,138	0
13	CLA	B	201	65/65	0.92	0.14	47,73,127,132	0
18	FES	D	202	4/4	0.95	0.09	79,81,82,95	0
9	HEM	A	303	43/43	0.97	0.09	40,60,72,79	0
9	HEM	C	301	43/43	0.97	0.13	34,61,83,89	0
9	HEM	A	301	43/43	0.98	0.09	29,39,55,66	0
9	HEM	A	302	43/43	0.98	0.09	23,42,53,56	0

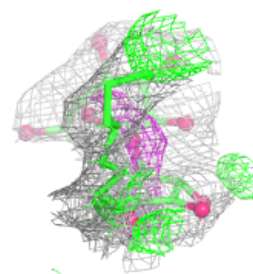
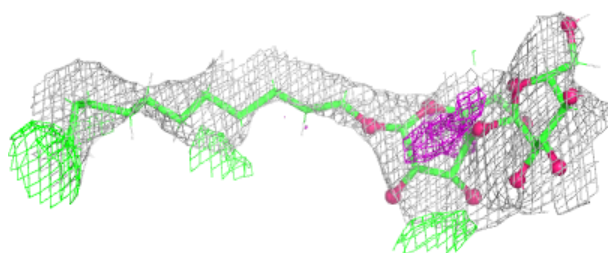
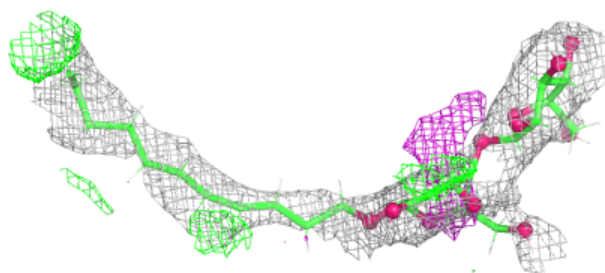
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UMQ A 307:

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

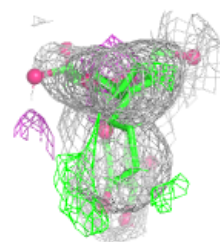
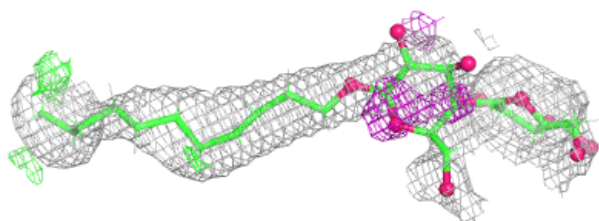
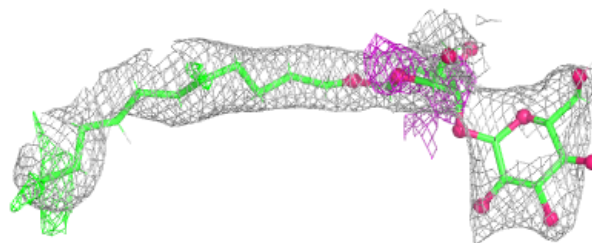
**Electron density around UMQ A 304:**

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

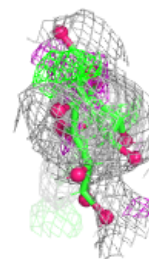
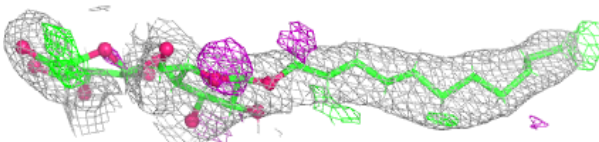
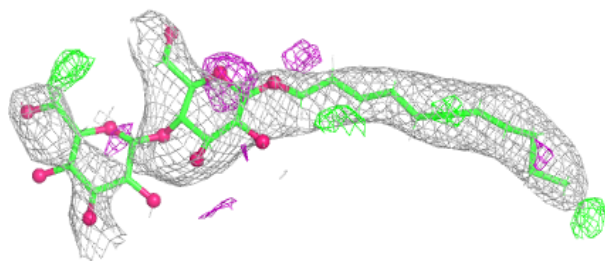


Electron density around UMQ A 309:

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

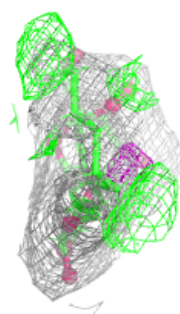
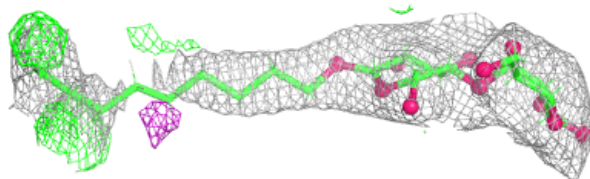
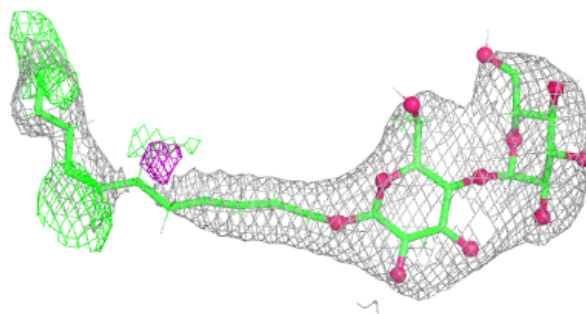
**Electron density around UMQ F 101:**

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

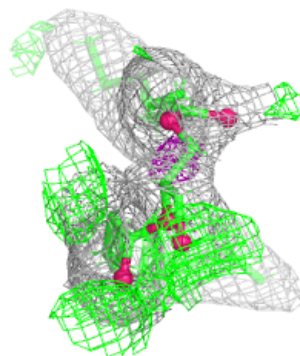
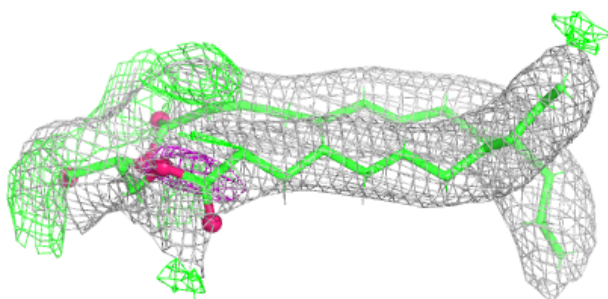
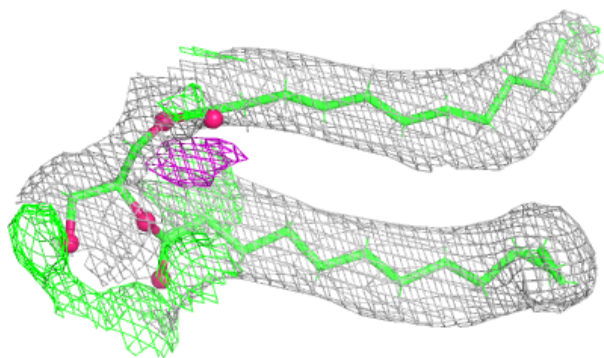


Electron density around UMQ A 305:

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

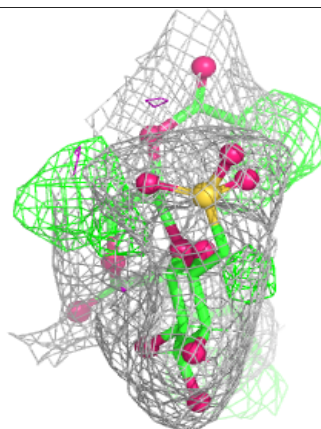
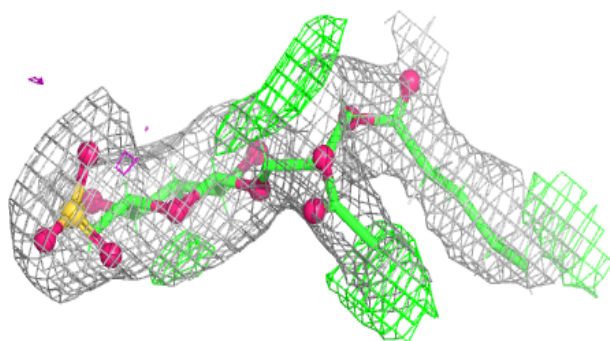
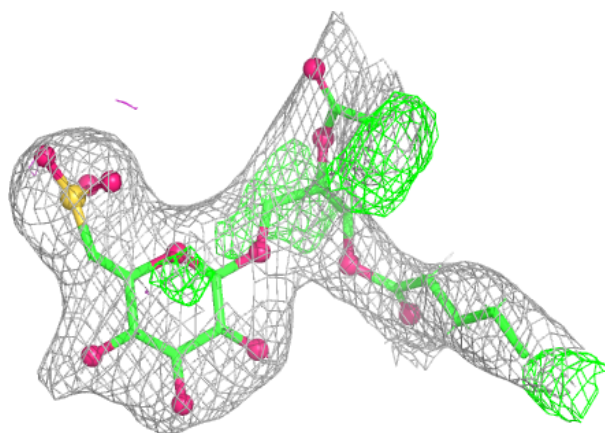
**Electron density around 7PH C 303:**

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



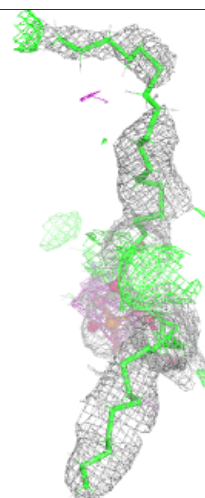
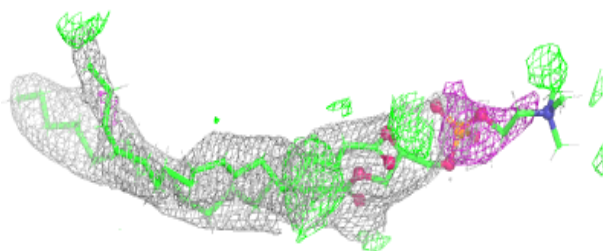
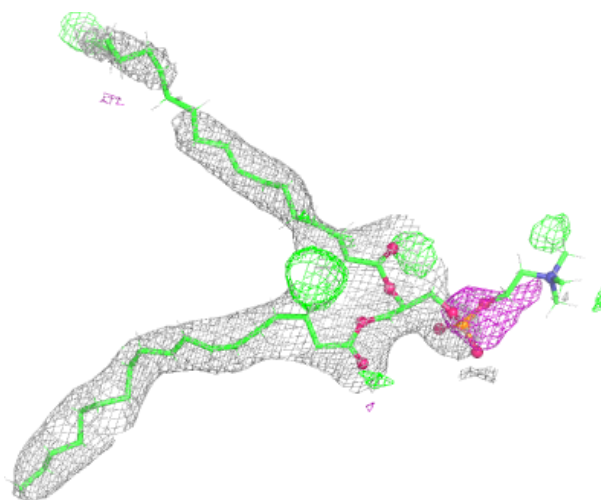
Electron density around SQD D 201:

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



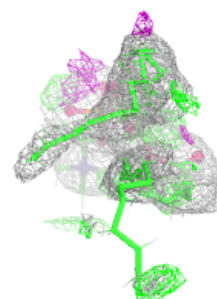
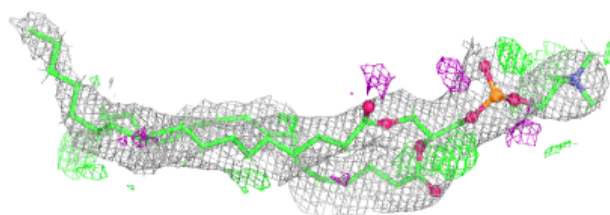
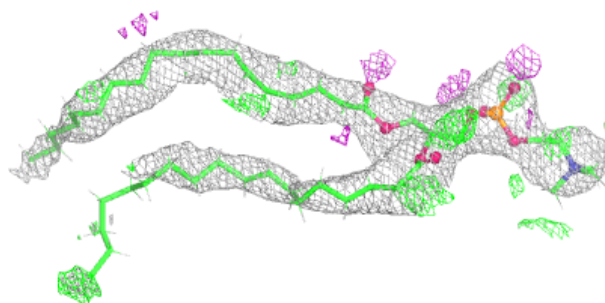
Electron density around OPC C 302:

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

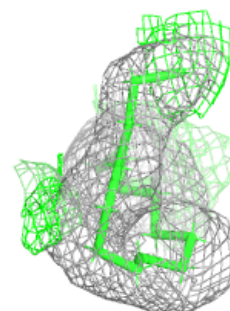
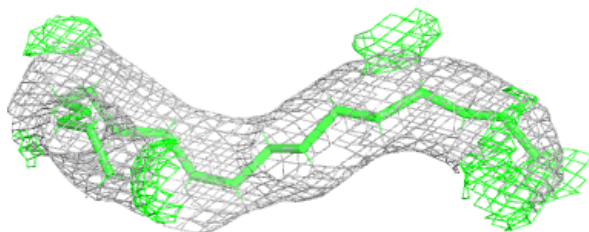
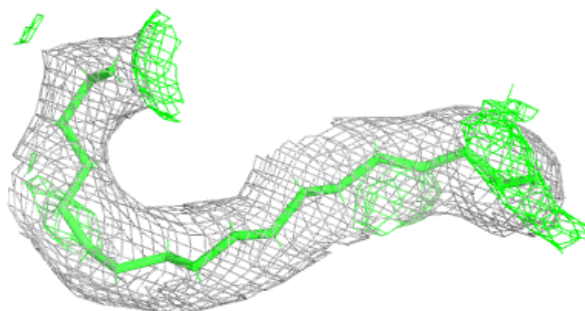


Electron density around OPC B 202:

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

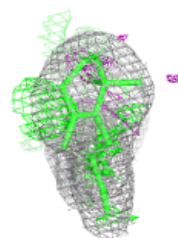
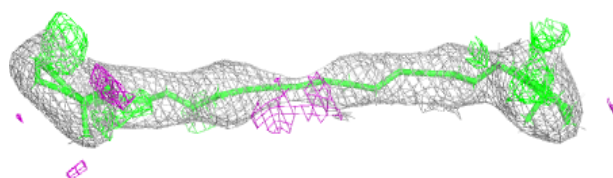
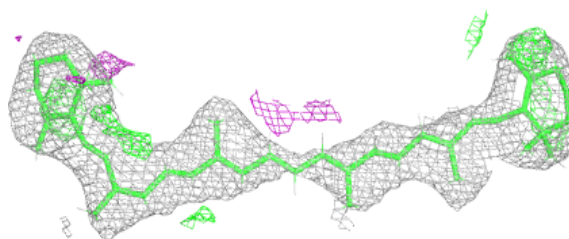
**Electron density around 8K6 A 308:**

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

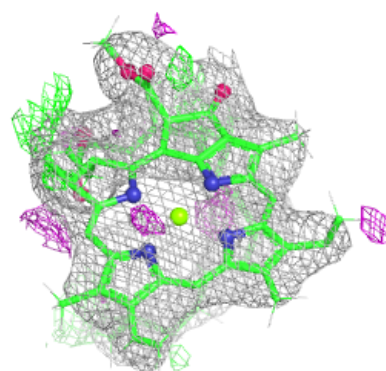
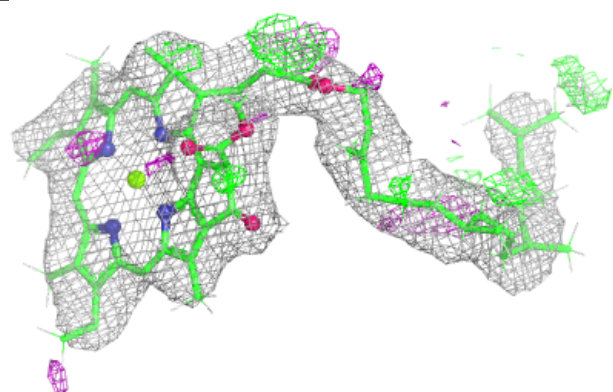
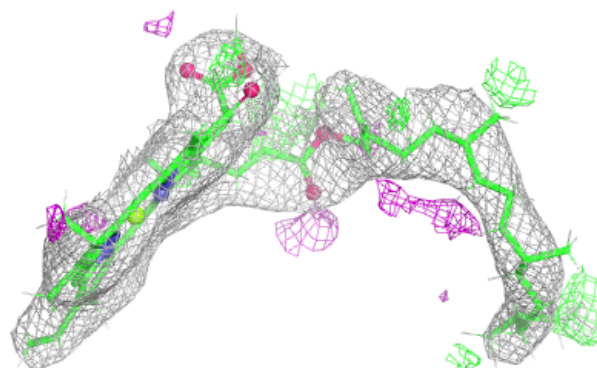


Electron density around BCR G 101:

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

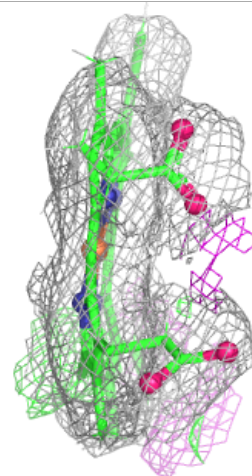
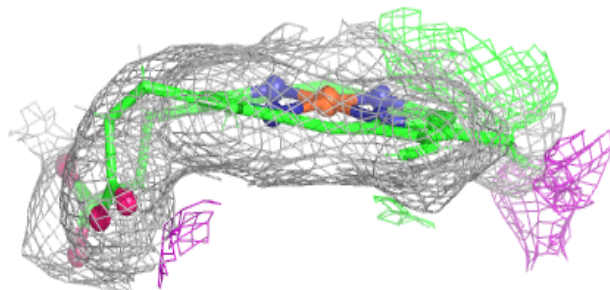
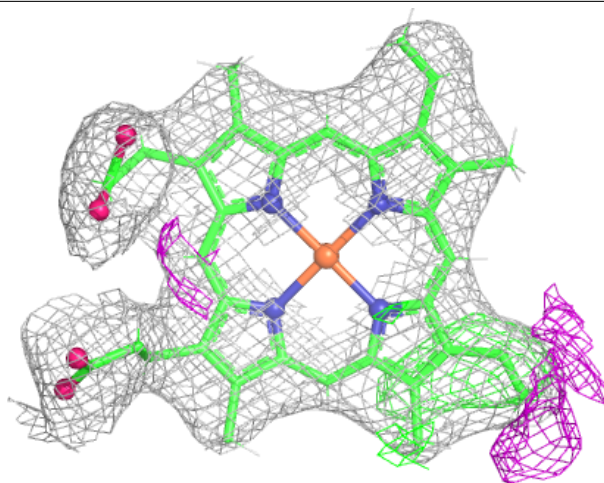
**Electron density around CLA B 201:**

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



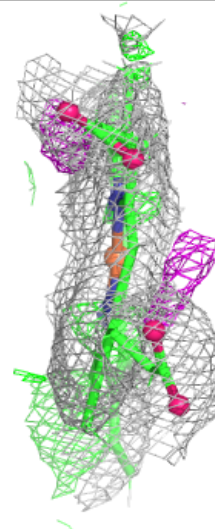
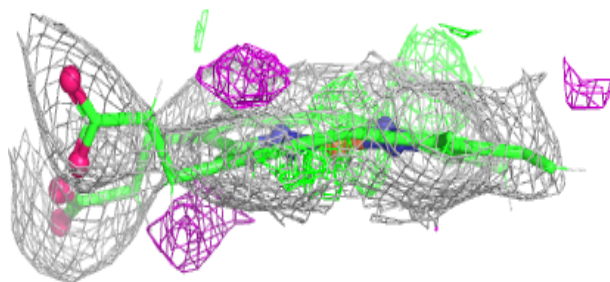
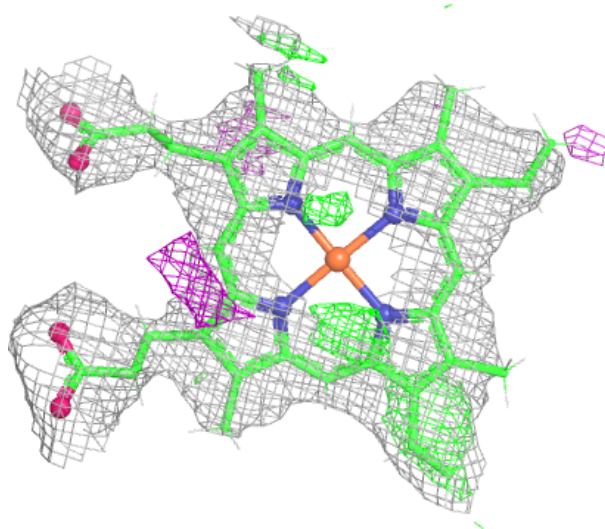
Electron density around HEM A 303:

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



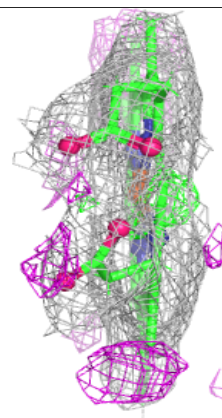
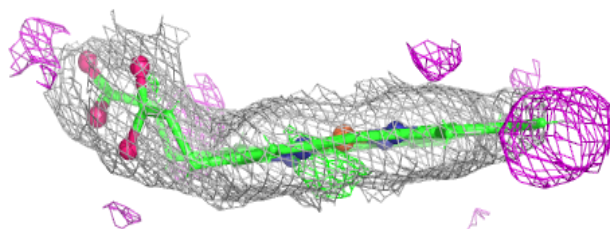
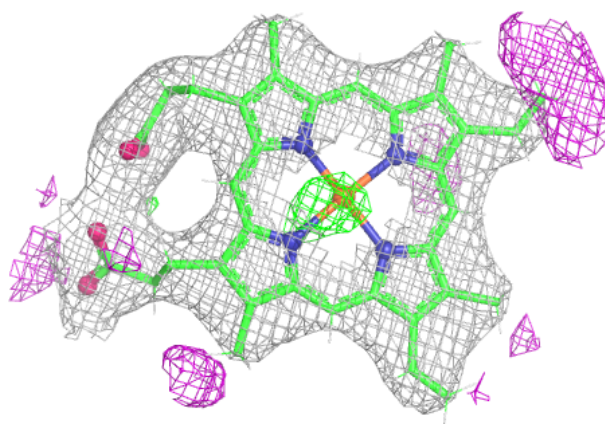
Electron density around HEM C 301:

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



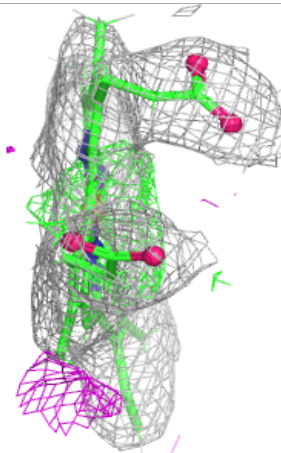
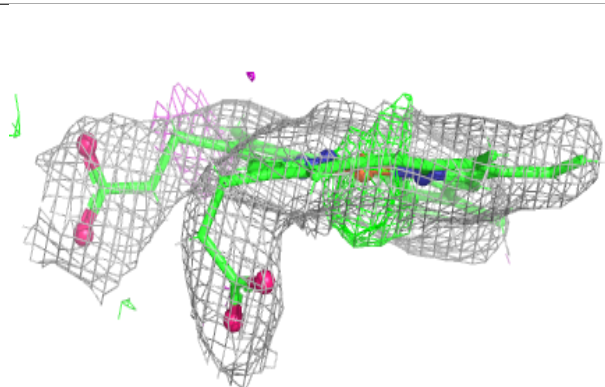
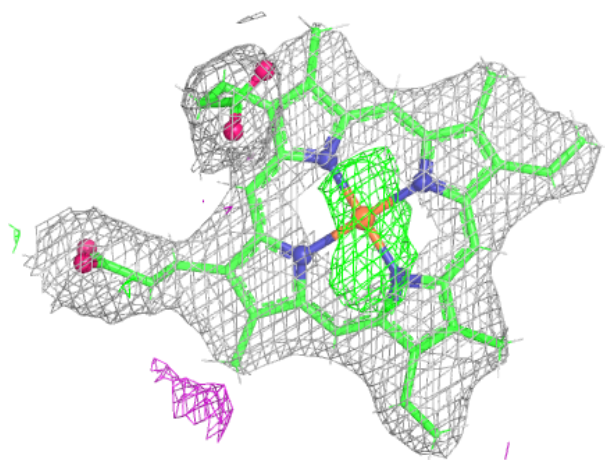
Electron density around HEM A 301:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.