Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:23 PM BST

PDB ID	:	3EJD
Title	:	Crystal Structure of P450BioI in complex with hexadec-9Z-enoic acid ligated Acyl Carrier Protein
Authors	:	Cryle, M.J.; Schlichting, I.
Deposited on	:	2008-09-18
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

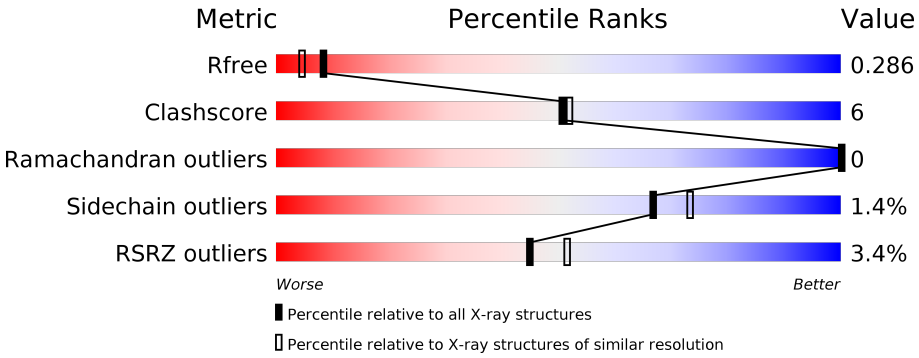
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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 <=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	97	3% 75% 5% 20%
1	C	97	7% 76% • 21%
1	E	97	3% 77% • 20%
1	G	97	2% 75% • 21%
2	B	404	2% 83% 11% 5%
2	D	404	4% 80% 14% • 5%

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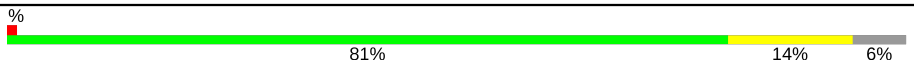
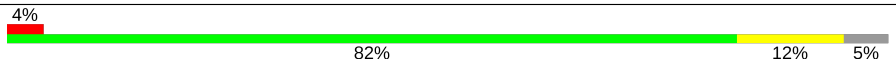
Mol	Chain	Length	Quality of chain
2	F	404	
2	H	404	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16057 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 Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			606	374	95	135	2			
1	C	77	Total	C	N	O	S	0	0	0
			596	368	92	134	2			
1	E	78	Total	C	N	O	S	0	0	0
			606	374	95	135	2			
1	G	77	Total	C	N	O	S	0	0	0
			596	368	92	134	2			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0A6A8
A	2	SER	-	expression tag	UNP P0A6A8
A	3	SER	-	expression tag	UNP P0A6A8
A	4	HIS	-	expression tag	UNP P0A6A8
A	5	HIS	-	expression tag	UNP P0A6A8
A	6	HIS	-	expression tag	UNP P0A6A8
A	7	HIS	-	expression tag	UNP P0A6A8
A	8	HIS	-	expression tag	UNP P0A6A8
A	9	HIS	-	expression tag	UNP P0A6A8
A	10	SER	-	expression tag	UNP P0A6A8
A	11	SER	-	expression tag	UNP P0A6A8
A	12	GLY	-	expression tag	UNP P0A6A8
A	13	LEU	-	expression tag	UNP P0A6A8
A	14	VAL	-	expression tag	UNP P0A6A8
A	15	PRO	-	expression tag	UNP P0A6A8
A	16	ARG	-	expression tag	UNP P0A6A8
A	17	GLY	-	expression tag	UNP P0A6A8
A	18	SER	-	expression tag	UNP P0A6A8
A	19	HIS	-	expression tag	UNP P0A6A8
C	1	GLY	-	expression tag	UNP P0A6A8
C	2	SER	-	expression tag	UNP P0A6A8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	SER	-	expression tag	UNP P0A6A8
C	4	HIS	-	expression tag	UNP P0A6A8
C	5	HIS	-	expression tag	UNP P0A6A8
C	6	HIS	-	expression tag	UNP P0A6A8
C	7	HIS	-	expression tag	UNP P0A6A8
C	8	HIS	-	expression tag	UNP P0A6A8
C	9	HIS	-	expression tag	UNP P0A6A8
C	10	SER	-	expression tag	UNP P0A6A8
C	11	SER	-	expression tag	UNP P0A6A8
C	12	GLY	-	expression tag	UNP P0A6A8
C	13	LEU	-	expression tag	UNP P0A6A8
C	14	VAL	-	expression tag	UNP P0A6A8
C	15	PRO	-	expression tag	UNP P0A6A8
C	16	ARG	-	expression tag	UNP P0A6A8
C	17	GLY	-	expression tag	UNP P0A6A8
C	18	SER	-	expression tag	UNP P0A6A8
C	19	HIS	-	expression tag	UNP P0A6A8
E	1	GLY	-	expression tag	UNP P0A6A8
E	2	SER	-	expression tag	UNP P0A6A8
E	3	SER	-	expression tag	UNP P0A6A8
E	4	HIS	-	expression tag	UNP P0A6A8
E	5	HIS	-	expression tag	UNP P0A6A8
E	6	HIS	-	expression tag	UNP P0A6A8
E	7	HIS	-	expression tag	UNP P0A6A8
E	8	HIS	-	expression tag	UNP P0A6A8
E	9	HIS	-	expression tag	UNP P0A6A8
E	10	SER	-	expression tag	UNP P0A6A8
E	11	SER	-	expression tag	UNP P0A6A8
E	12	GLY	-	expression tag	UNP P0A6A8
E	13	LEU	-	expression tag	UNP P0A6A8
E	14	VAL	-	expression tag	UNP P0A6A8
E	15	PRO	-	expression tag	UNP P0A6A8
E	16	ARG	-	expression tag	UNP P0A6A8
E	17	GLY	-	expression tag	UNP P0A6A8
E	18	SER	-	expression tag	UNP P0A6A8
E	19	HIS	-	expression tag	UNP P0A6A8
G	1	GLY	-	expression tag	UNP P0A6A8
G	2	SER	-	expression tag	UNP P0A6A8
G	3	SER	-	expression tag	UNP P0A6A8
G	4	HIS	-	expression tag	UNP P0A6A8
G	5	HIS	-	expression tag	UNP P0A6A8
G	6	HIS	-	expression tag	UNP P0A6A8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	7	HIS	-	expression tag	UNP P0A6A8
G	8	HIS	-	expression tag	UNP P0A6A8
G	9	HIS	-	expression tag	UNP P0A6A8
G	10	SER	-	expression tag	UNP P0A6A8
G	11	SER	-	expression tag	UNP P0A6A8
G	12	GLY	-	expression tag	UNP P0A6A8
G	13	LEU	-	expression tag	UNP P0A6A8
G	14	VAL	-	expression tag	UNP P0A6A8
G	15	PRO	-	expression tag	UNP P0A6A8
G	16	ARG	-	expression tag	UNP P0A6A8
G	17	GLY	-	expression tag	UNP P0A6A8
G	18	SER	-	expression tag	UNP P0A6A8
G	19	HIS	-	expression tag	UNP P0A6A8

- Molecule 2 is a protein called Biotin biosynthesis cytochrome P450-like enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	382	Total	C	N	O	S	0	0	0
			3056	1945	529	568	14			
2	D	385	Total	C	N	O	S	0	0	0
			3080	1958	535	573	14			
2	F	381	Total	C	N	O	S	0	0	0
			3053	1943	531	565	14			
2	H	382	Total	C	N	O	S	0	0	0
			3052	1942	529	567	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	395	ALA	-	expression tag	UNP P53554
B	396	SER	-	expression tag	UNP P53554
B	397	TRP	-	expression tag	UNP P53554
B	398	SER	-	expression tag	UNP P53554
B	399	HIS	-	expression tag	UNP P53554
B	400	PRO	-	expression tag	UNP P53554
B	401	GLN	-	expression tag	UNP P53554
B	402	PHE	-	expression tag	UNP P53554
B	403	GLU	-	expression tag	UNP P53554
B	404	LYS	-	expression tag	UNP P53554
D	395	ALA	-	expression tag	UNP P53554
D	396	SER	-	expression tag	UNP P53554
D	397	TRP	-	expression tag	UNP P53554

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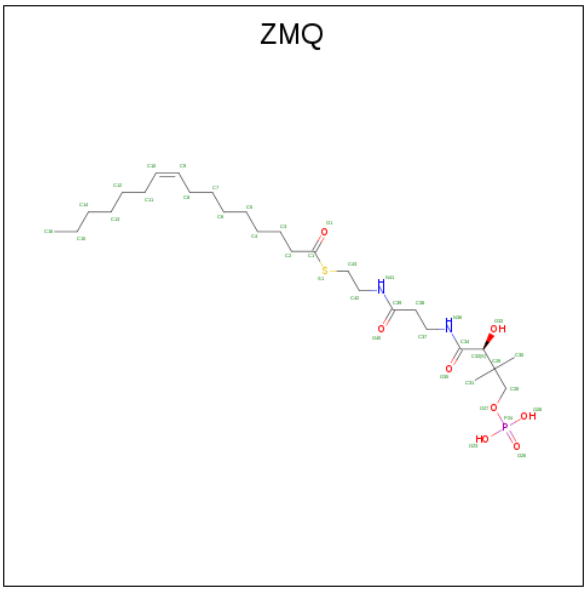
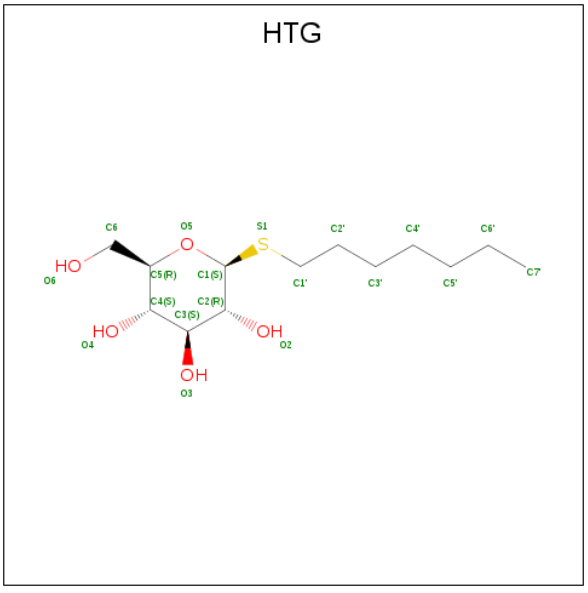
Chain	Residue	Modelled	Actual	Comment	Reference
D	398	SER	-	expression tag	UNP P53554
D	399	HIS	-	expression tag	UNP P53554
D	400	PRO	-	expression tag	UNP P53554
D	401	GLN	-	expression tag	UNP P53554
D	402	PHE	-	expression tag	UNP P53554
D	403	GLU	-	expression tag	UNP P53554
D	404	LYS	-	expression tag	UNP P53554
F	395	ALA	-	expression tag	UNP P53554
F	396	SER	-	expression tag	UNP P53554
F	397	TRP	-	expression tag	UNP P53554
F	398	SER	-	expression tag	UNP P53554
F	399	HIS	-	expression tag	UNP P53554
F	400	PRO	-	expression tag	UNP P53554
F	401	GLN	-	expression tag	UNP P53554
F	402	PHE	-	expression tag	UNP P53554
F	403	GLU	-	expression tag	UNP P53554
F	404	LYS	-	expression tag	UNP P53554
H	395	ALA	-	expression tag	UNP P53554
H	396	SER	-	expression tag	UNP P53554
H	397	TRP	-	expression tag	UNP P53554
H	398	SER	-	expression tag	UNP P53554
H	399	HIS	-	expression tag	UNP P53554
H	400	PRO	-	expression tag	UNP P53554
H	401	GLN	-	expression tag	UNP P53554
H	402	PHE	-	expression tag	UNP P53554
H	403	GLU	-	expression tag	UNP P53554
H	404	LYS	-	expression tag	UNP P53554

- Molecule 3 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] (9Z)-hexadec-9-enethioate (three-letter code: ZMQ) (formula: $C_{27}H_{51}N_2O_8PS$).



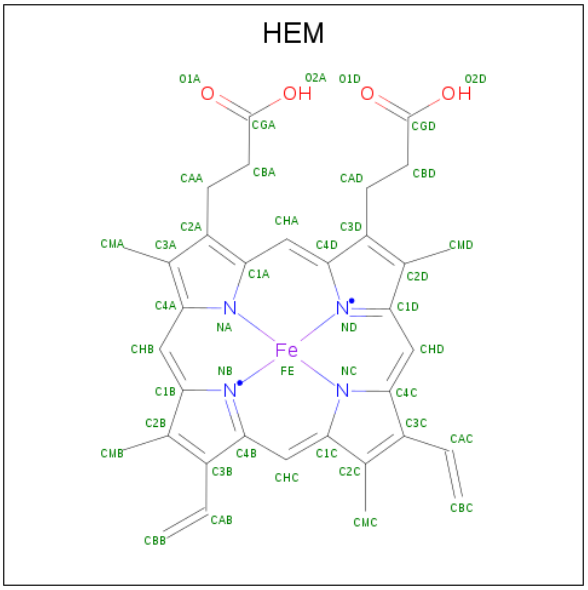
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			38	27	2	7	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			38	27	2	7	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			38	27	2	7	1	1		
3	G	1	Total	C	N	O	P	S	0	0
			38	27	2	7	1	1		

- Molecule 4 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 15 9 5 1	0	0
4	A	1	Total C 7 7	0	0
4	C	1	Total C O S 12 6 5 1	0	0
4	D	1	Total C 5 5	0	0
4	E	1	Total C O S 12 6 5 1	0	0
4	F	1	Total C 6 6	0	0
4	G	1	Total C O S 12 6 5 1	0	0
4	H	1	Total C S 7 6 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

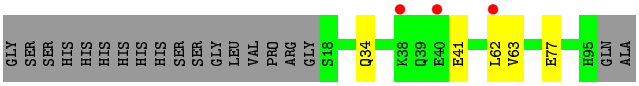
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	219	Total	O	0	0
			219	219		
7	C	45	Total	O	0	0
			45	45		
7	D	189	Total	O	0	0
			189	189		
7	E	71	Total	O	0	0
			71	71		
7	F	223	Total	O	0	0
			223	223		
7	G	51	Total	O	0	0
			51	51		
7	H	159	Total	O	0	0
			159	159		

3 Residue-property plots

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

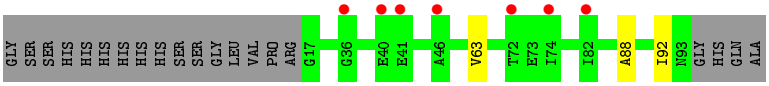
- Molecule 1: Acyl carrier protein

Chain A:



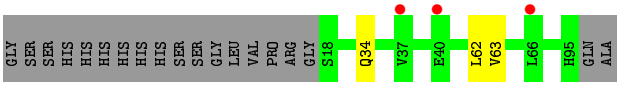
- Molecule 1: Acyl carrier protein

Chain C:



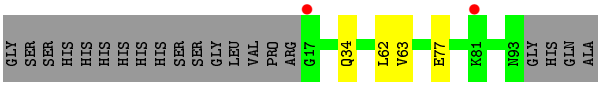
- Molecule 1: Acyl carrier protein

Chain E:



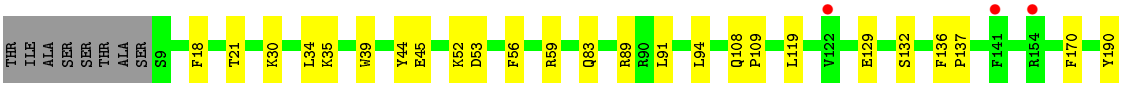
- Molecule 1: Acyl carrier protein

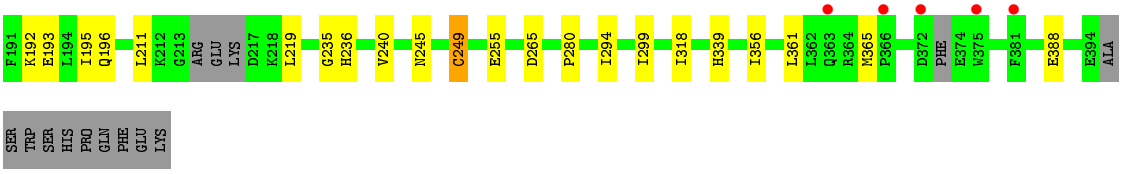
Chain G:



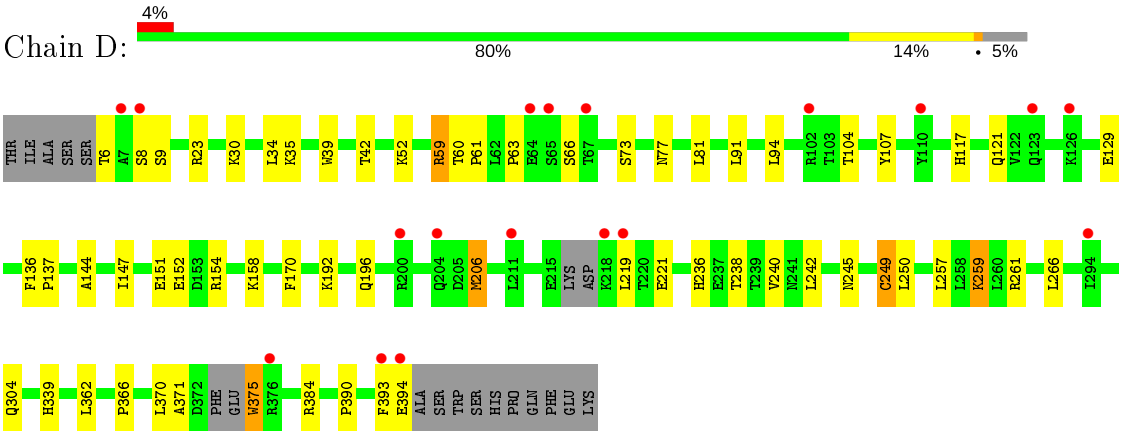
- Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme

Chain B:

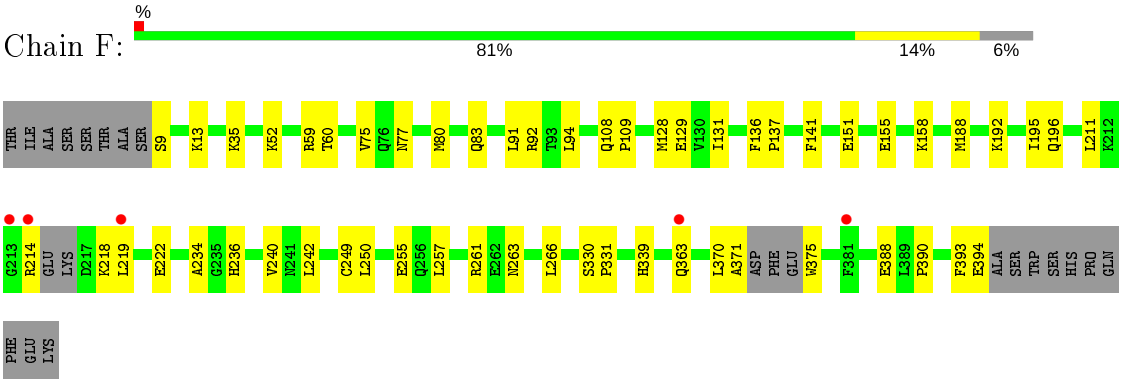




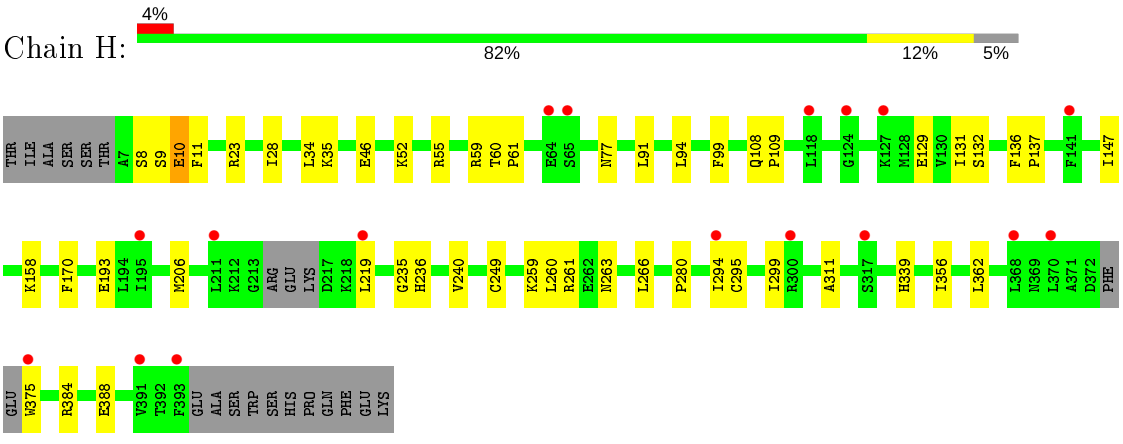
• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme



• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme



• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.30Å 92.10Å 107.70Å 109.00° 89.20° 90.10°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.10) 92.9 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.241 , 0.285 0.242 , 0.286	Depositor DCC
R_{free} test set	6319 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.267 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16057	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HTG, HEM, ZMQ, CL

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	0.24	0/611	0.37	0/826
1	C	0.25	0/600	0.35	0/811
1	E	0.23	0/611	0.37	0/826
1	G	0.24	0/600	0.36	0/811
2	B	0.26	0/3122	0.39	0/4231
2	D	0.24	0/3146	0.38	0/4263
2	F	0.24	0/3119	0.38	0/4226
2	H	0.25	0/3118	0.39	1/4226 (0.0%)
All	All	0.25	0/14927	0.38	1/20220 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	260	LEU	N-CA-C	-5.21	96.92	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	259	LYS	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	606	0	578	4	0
1	C	596	0	571	2	0
1	E	606	0	578	2	0
1	G	596	0	571	2	0
2	B	3056	0	3049	32	0
2	D	3080	0	3077	44	0
2	F	3053	0	3054	42	0
2	H	3052	0	3049	40	0
3	A	38	0	47	3	0
3	C	38	0	47	5	0
3	E	38	0	48	4	0
3	G	38	0	47	2	0
4	A	22	0	28	2	0
4	C	12	0	11	0	0
4	D	5	0	9	1	0
4	E	12	0	11	0	0
4	F	6	0	11	0	0
4	G	12	0	11	0	0
4	H	7	0	10	1	0
5	B	43	0	30	2	0
5	D	43	0	30	1	0
5	F	43	0	30	4	0
5	H	43	0	30	2	0
6	B	1	0	0	1	0
6	F	1	0	0	1	0
7	A	53	0	0	1	0
7	B	219	0	0	1	0
7	C	45	0	0	0	0
7	D	189	0	0	2	0
7	E	71	0	0	0	0
7	F	223	0	0	4	0
7	G	51	0	0	0	0
7	H	159	0	0	1	0
All	All	16057	0	14927	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 6.

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)
2:H:8:SER:HA	2:H:10:GLU:H	1.27	0.99
2:D:60:THR:HG21	2:D:77:ASN:OD1	1.66	0.95
2:D:94:LEU:HD13	2:D:219:LEU:HD13	1.49	0.94
2:F:9:SER:O	2:F:13:LYS:HG2	1.76	0.85
2:F:393:PHE:HD1	2:F:394:GLU:HG2	1.44	0.83
2:F:255:GLU:HB2	6:F:418:CL:CL	2.23	0.76
3:E:99:ZMQ:H37	3:E:99:ZMQ:O33	1.87	0.75
3:E:99:ZMQ:H9	2:F:234:ALA:HB2	1.67	0.74
3:E:99:ZMQ:C37	3:E:99:ZMQ:O33	2.37	0.73
2:H:8:SER:HA	2:H:10:GLU:N	2.02	0.72
3:G:99:ZMQ:O35	3:G:99:ZMQ:H30A	1.88	0.71
2:F:60:THR:OG1	7:F:502:HOH:O	2.09	0.71
2:H:23:ARG:NH2	2:H:311:ALA:O	2.23	0.71
2:B:192:LYS:O	2:B:196:GLN:HG2	1.91	0.71
2:H:8:SER:CA	2:H:10:GLU:H	2.04	0.70
2:D:94:LEU:CD1	2:D:219:LEU:HD13	2.22	0.68
2:D:192:LYS:O	2:D:196:GLN:HG2	1.93	0.68
2:H:129:GLU:OE1	2:H:388:GLU:HB2	1.92	0.68
2:F:257:LEU:HD21	2:F:261:ARG:HH21	1.59	0.67
3:A:99:ZMQ:C37	3:A:99:ZMQ:O33	2.42	0.67
2:F:94:LEU:HD13	2:F:219:LEU:HG	1.77	0.67
2:H:94:LEU:HD13	2:H:219:LEU:HG	1.76	0.66
2:D:34:LEU:HD12	2:D:170:PHE:HB3	1.80	0.63
2:H:91:LEU:HD23	2:H:219:LEU:HD21	1.81	0.63
2:F:263:ASN:OD1	2:F:266:LEU:HG	2.00	0.61
2:B:236:HIS:O	2:B:240:VAL:HG23	2.00	0.61
2:D:6:THR:HG23	2:D:9:SER:H	1.66	0.61
2:F:75:VAL:HG22	2:F:188:MET:HE3	1.82	0.61
2:D:23:ARG:NH1	2:D:42:THR:O	2.34	0.61
2:F:131:ILE:HD12	2:F:388:GLU:HA	1.81	0.60
2:F:242:LEU:HD22	5:F:405:HEM:HBB1	1.84	0.59
2:F:363:GLN:HB3	7:F:486:HOH:O	2.01	0.59
2:F:80:MET:HE1	2:F:92:ARG:HG3	1.84	0.59
2:B:34:LEU:HD12	2:B:170:PHE:HB3	1.83	0.59
2:H:8:SER:HA	2:H:9:SER:HB3	1.84	0.59
2:D:136:PHE:CZ	2:D:158:LYS:HG3	2.37	0.59
2:D:52:LYS:HG3	2:D:339:HIS:CD2	2.38	0.58
2:D:370:LEU:HD13	2:D:375:TRP:CH2	2.38	0.58
2:H:52:LYS:HE3	2:H:339:HIS:NE2	2.19	0.58
2:B:91:LEU:HD23	2:B:219:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:PRO:O	2:F:141:PHE:HD2	1.86	0.57
2:H:129:GLU:HG2	2:H:132:SER:HB2	1.87	0.57
2:H:136:PHE:CZ	2:H:158:LYS:HG3	2.39	0.57
2:F:151:GLU:HG2	7:F:619:HOH:O	2.05	0.57
1:C:63:VAL:HG11	2:D:35:LYS:HE2	1.87	0.57
1:E:34:GLN:HG2	1:E:62:LEU:HG	1.87	0.56
2:D:370:LEU:HD13	2:D:375:TRP:CZ3	2.40	0.56
2:H:60:THR:HG21	2:H:77:ASN:CG	2.26	0.56
2:H:8:SER:CA	2:H:9:SER:HB3	2.36	0.56
1:G:34:GLN:HG2	1:G:62:LEU:HG	1.86	0.56
2:B:94:LEU:HD13	2:B:219:LEU:HG	1.89	0.55
1:A:41:GLU:HA	7:A:151:HOH:O	2.04	0.55
2:H:236:HIS:O	2:H:240:VAL:HG23	2.07	0.54
2:B:52:LYS:HE2	2:B:339:HIS:NE2	2.22	0.54
2:F:91:LEU:HD23	2:F:219:LEU:CD2	2.38	0.54
3:G:99:ZMQ:C30	3:G:99:ZMQ:O35	2.56	0.54
2:B:18:PHE:O	2:B:21:THR:HG22	2.07	0.54
2:F:80:MET:HE2	5:F:405:HEM:HBD2	1.88	0.54
1:A:77:GLU:HG2	4:A:101:HTG:H7'1	1.88	0.54
2:H:99:PHE:CE2	2:H:206:MET:HE1	2.42	0.54
2:B:235:GLY:HA2	5:B:405:HEM:CBB	2.38	0.54
2:B:89:ARG:HD2	7:B:555:HOH:O	2.08	0.53
2:F:236:HIS:O	2:F:240:VAL:HG23	2.08	0.53
2:F:192:LYS:HE2	2:F:222:GLU:HG2	1.90	0.53
2:F:91:LEU:HD23	2:F:219:LEU:HD21	1.91	0.53
2:D:236:HIS:O	2:D:240:VAL:HG23	2.08	0.53
2:B:265:ASP:OD2	2:D:259:LYS:HE3	2.09	0.52
2:F:192:LYS:O	2:F:196:GLN:HG2	2.09	0.52
3:C:99:ZMQ:O40	2:D:59:ARG:NH2	2.40	0.52
2:F:80:MET:HE2	5:F:405:HEM:CBD	2.39	0.52
1:E:63:VAL:HG11	2:F:35:LYS:HE2	1.90	0.52
2:H:91:LEU:HD23	2:H:219:LEU:CD2	2.39	0.52
2:H:261:ARG:NH1	2:H:362:LEU:O	2.43	0.52
2:F:370:LEU:HD22	2:F:375:TRP:CH2	2.45	0.52
2:D:393:PHE:HD1	2:D:394:GLU:HB2	1.75	0.51
2:F:393:PHE:CD1	2:F:394:GLU:HG2	2.35	0.51
2:H:34:LEU:HD22	2:H:170:PHE:HB3	1.93	0.50
2:D:261:ARG:NH1	2:D:362:LEU:O	2.44	0.50
2:B:255:GLU:HB2	6:B:416:CL:CL	2.49	0.50
2:B:190:TYR:O	2:B:193:GLU:HG2	2.11	0.50
2:D:250:LEU:HB3	2:D:257:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:SER:HA	4:D:417:HTG:H4'2	1.94	0.50
2:F:94:LEU:CD2	2:F:214:ARG:H	2.24	0.49
3:C:99:ZMQ:H31	3:C:99:ZMQ:O35	2.12	0.49
2:D:242:LEU:HD22	5:D:405:HEM:HBB1	1.95	0.49
2:F:136:PHE:HB3	2:F:137:PRO:HD3	1.95	0.48
2:F:94:LEU:HD23	2:F:214:ARG:H	1.77	0.48
3:C:99:ZMQ:H9	2:D:238:THR:HG21	1.95	0.48
1:G:63:VAL:HG11	2:H:35:LYS:HE2	1.95	0.48
2:F:195:ILE:HG23	2:F:211:LEU:HD21	1.96	0.47
2:B:129:GLU:OE1	2:B:388:GLU:HB2	2.14	0.47
2:H:147:ILE:HA	2:H:206:MET:HB3	1.96	0.47
2:H:263:ASN:OD1	2:H:266:LEU:HG	2.14	0.47
2:F:257:LEU:HD21	2:F:261:ARG:NH2	2.26	0.47
2:D:91:LEU:HD23	2:D:219:LEU:HD11	1.96	0.46
2:F:371:ALA:HB3	2:F:390:PRO:HB2	1.98	0.46
2:D:375:TRP:HA	7:D:590:HOH:O	2.16	0.45
2:D:59:ARG:NH1	2:D:304:GLN:OE1	2.50	0.45
2:B:136:PHE:HB3	2:B:137:PRO:HD3	1.97	0.45
2:B:129:GLU:HG3	2:B:132:SER:OG	2.16	0.45
3:C:99:ZMQ:C31	3:C:99:ZMQ:O35	2.63	0.45
2:D:73:SER:O	2:D:77:ASN:ND2	2.49	0.45
2:B:91:LEU:HD23	2:B:219:LEU:HD22	1.99	0.45
2:F:218:LYS:HA	7:F:605:HOH:O	2.17	0.45
2:H:11:PHE:CE2	4:H:417:HTG:H3'1	2.51	0.45
2:B:52:LYS:NZ	2:D:52:LYS:HD3	2.32	0.45
2:D:52:LYS:HE3	7:D:470:HOH:O	2.16	0.45
2:F:370:LEU:HB3	2:F:375:TRP:HH2	1.81	0.45
2:H:294:ILE:HD11	2:H:299:ILE:HD12	1.99	0.45
2:H:52:LYS:HG3	2:H:339:HIS:CD2	2.52	0.45
2:B:195:ILE:HG23	2:B:211:LEU:HD21	1.99	0.44
2:D:151:GLU:HG2	2:D:154:ARG:NH2	2.33	0.44
2:D:245:ASN:O	2:D:249:CYS:HB2	2.17	0.44
2:B:30:LYS:HB2	2:B:39:TRP:CZ3	2.53	0.44
2:H:129:GLU:HG3	2:H:129:GLU:O	2.18	0.44
2:H:108:GLN:HB3	2:H:109:PRO:HD3	2.00	0.44
2:B:294:ILE:HD11	2:B:299:ILE:HD12	2.00	0.43
2:D:144:ALA:HB3	2:D:154:ARG:HD3	2.00	0.43
2:H:280:PRO:HD2	5:H:405:HEM:HBC1	1.99	0.43
2:D:371:ALA:HB3	2:D:390:PRO:HB2	2.00	0.43
2:F:330:SER:HA	2:F:331:PRO:HA	1.83	0.43
2:B:44:TYR:CG	2:B:318:ILE:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:LEU:O	2:B:35:LYS:HB2	2.18	0.43
2:F:250:LEU:HB3	2:F:257:LEU:HD12	2.00	0.43
2:F:80:MET:HE2	5:F:405:HEM:CGD	2.49	0.43
2:D:104:THR:HA	2:D:107:TYR:CD2	2.54	0.43
2:H:55:ARG:NH2	7:H:545:HOH:O	2.52	0.43
2:B:119:LEU:HD22	2:B:365:MET:CE	2.49	0.42
2:F:52:LYS:HG3	2:F:339:HIS:CD2	2.54	0.42
2:H:8:SER:N	2:H:9:SER:HB3	2.34	0.42
2:D:147:ILE:HA	2:D:206:MET:HB3	2.02	0.42
2:F:137:PRO:O	2:F:141:PHE:CD2	2.71	0.42
3:E:99:ZMQ:H9	2:F:234:ALA:CB	2.42	0.42
2:F:77:ASN:O	2:F:83:GLN:NE2	2.43	0.42
2:H:129:GLU:CG	2:H:132:SER:HB2	2.49	0.42
2:D:144:ALA:CB	2:D:154:ARG:HD3	2.49	0.42
2:F:108:GLN:HB3	2:F:109:PRO:HD3	2.02	0.42
2:D:60:THR:HA	2:D:61:PRO:HD3	1.88	0.42
2:B:53:ASP:HB3	2:B:56:PHE:HD2	1.85	0.42
3:A:99:ZMQ:H37A	3:A:99:ZMQ:O33	2.19	0.42
2:H:8:SER:CA	2:H:9:SER:CB	2.98	0.42
2:D:261:ARG:NH1	2:D:366:PRO:HA	2.35	0.41
2:B:45:GLU:OE1	2:B:45:GLU:HA	2.20	0.41
2:H:131:ILE:HD12	2:H:388:GLU:HA	2.03	0.41
2:B:108:GLN:HB3	2:B:109:PRO:HD3	2.03	0.41
2:D:196:GLN:NE2	2:D:221:GLU:OE1	2.52	0.41
2:H:129:GLU:HG3	2:H:132:SER:H	1.85	0.41
2:H:235:GLY:HA2	5:H:405:HEM:HAB	2.02	0.41
4:A:100:HTG:H1	4:A:100:HTG:H2'1	1.87	0.41
2:B:361:LEU:O	2:B:365:MET:HG2	2.20	0.41
2:B:265:ASP:HB3	2:D:266:LEU:HD21	2.03	0.41
2:D:151:GLU:H	2:D:151:GLU:HG3	1.64	0.41
2:D:30:LYS:HB2	2:D:39:TRP:CZ3	2.56	0.41
1:A:63:VAL:HG11	2:B:35:LYS:HE2	2.03	0.41
2:H:60:THR:HA	2:H:61:PRO:HD3	1.87	0.41
3:A:99:ZMQ:H37	3:A:99:ZMQ:O33	2.18	0.41
2:B:280:PRO:HD2	5:B:405:HEM:HBC1	2.01	0.41
1:C:88:ALA:O	1:C:92:ILE:HG12	2.20	0.41
2:D:117:HIS:O	2:D:121:GLN:HG2	2.21	0.41
2:B:108:GLN:HG3	2:B:356:ILE:HD11	2.03	0.41
2:D:63:PRO:HB2	2:D:66:SER:HB2	2.02	0.41
1:A:34:GLN:HG2	1:A:62:LEU:HG	2.02	0.40
2:F:155:GLU:HA	2:F:158:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:PHE:HE2	2:H:206:MET:HE1	1.86	0.40
2:H:28:ILE:HD12	2:H:295:CYS:HB3	2.03	0.40
2:D:136:PHE:HB3	2:D:137:PRO:HD3	2.02	0.40
3:C:99:ZMQ:H3A	2:D:81:LEU:HD21	2.04	0.40
2:B:245:ASN:O	2:B:249:CYS:HB2	2.21	0.40
2:H:136:PHE:HB3	2:H:137:PRO:HD3	2.03	0.40
2:H:46:GLU:N	2:H:46:GLU:OE1	2.43	0.40
2:H:108:GLN:HG3	2:H:356:ILE:HD11	2.02	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	76/97 (78%)	76 (100%)	0	0	100	100
1	C	75/97 (77%)	75 (100%)	0	0	100	100
1	E	76/97 (78%)	76 (100%)	0	0	100	100
1	G	75/97 (77%)	75 (100%)	0	0	100	100
2	B	376/404 (93%)	368 (98%)	8 (2%)	0	100	100
2	D	379/404 (94%)	370 (98%)	9 (2%)	0	100	100
2	F	375/404 (93%)	367 (98%)	8 (2%)	0	100	100
2	H	376/404 (93%)	363 (96%)	13 (4%)	0	100	100
All	All	1808/2004 (90%)	1770 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	68/83 (82%)	68 (100%)	0	100	100
1	C	67/83 (81%)	67 (100%)	0	100	100
1	E	68/83 (82%)	68 (100%)	0	100	100
1	G	67/83 (81%)	66 (98%)	1 (2%)	65	71
2	B	335/355 (94%)	332 (99%)	3 (1%)	78	84
2	D	338/355 (95%)	330 (98%)	8 (2%)	49	53
2	F	335/355 (94%)	331 (99%)	4 (1%)	71	77
2	H	335/355 (94%)	329 (98%)	6 (2%)	59	65
All	All	1613/1752 (92%)	1591 (99%)	22 (1%)	67	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	ARG
2	B	83	GLN
2	B	249	CYS
2	D	59	ARG
2	D	129	GLU
2	D	152	GLU
2	D	206	MET
2	D	249	CYS
2	D	259	LYS
2	D	375	TRP
2	D	384	ARG
2	F	59	ARG
2	F	128	MET
2	F	129	GLU
2	F	249	CYS
1	G	77	GLU
2	H	10	GLU
2	H	59	ARG
2	H	193	GLU

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Mol	Chain	Res	Type
2	H	249	CYS
2	H	375	TRP
2	H	384	ARG

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

Mol	Chain	Res	Type
1	G	39	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	HTG	A	100	-	15,15,19	3.69	2 (13%)	18,20,24	1.28	1 (5%)
4	HTG	C	100	-	11,12,19	0.31	0	15,17,24	0.77	0
4	HTG	E	100	-	11,12,19	0.32	0	15,17,24	0.76	0
4	HTG	G	100	-	11,12,19	0.30	0	15,17,24	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HTG	A	101	-	6,6,19	0.55	0	5,5,24	0.64	0
4	HTG	H	417	-	6,6,19	1.75	1 (16%)	5,5,24	1.19	1 (20%)
5	HEM	D	405	2	27,50,50	2.15	6 (22%)	17,82,82	1.41	3 (17%)
5	HEM	F	405	2	27,50,50	2.17	6 (22%)	17,82,82	1.49	2 (11%)
5	HEM	H	405	2	27,50,50	2.16	5 (18%)	17,82,82	1.29	1 (5%)
3	ZMQ	E	99	1	31,37,38	2.08	6 (19%)	36,44,47	1.64	5 (13%)
4	HTG	D	417	-	4,4,19	0.47	0	3,3,24	0.55	0
4	HTG	F	417	-	5,5,19	0.53	0	4,4,24	0.56	0
3	ZMQ	C	99	1	31,37,38	2.10	6 (19%)	36,44,47	1.74	8 (22%)
5	HEM	B	405	2	27,50,50	2.12	6 (22%)	17,82,82	1.42	3 (17%)
3	ZMQ	G	99	1	31,37,38	2.12	6 (19%)	36,44,47	1.87	9 (25%)
3	ZMQ	A	99	1	31,37,38	2.09	6 (19%)	36,44,47	1.83	10 (27%)

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
4	HTG	A	100	-	-	1/6/26/30	0/1/1/1
4	HTG	C	100	-	-	0/2/22/30	0/1/1/1
4	HTG	E	100	-	-	0/2/22/30	0/1/1/1
4	HTG	G	100	-	-	0/2/22/30	0/1/1/1
4	HTG	A	101	-	-	3/4/4/30	-
4	HTG	H	417	-	-	2/4/4/30	-
5	HEM	D	405	2	-	0/6/54/54	-
5	HEM	F	405	2	-	0/6/54/54	-
5	HEM	H	405	2	-	0/6/54/54	-
3	ZMQ	E	99	1	-	16/42/44/45	-
4	HTG	D	417	-	-	0/2/2/30	-
4	HTG	F	417	-	-	3/3/3/30	-
3	ZMQ	C	99	1	-	16/42/44/45	-
5	HEM	B	405	2	-	0/6/54/54	-
3	ZMQ	G	99	1	-	24/42/44/45	-
3	ZMQ	A	99	1	-	16/42/44/45	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	100	HTG	C1'-S1	-11.40	1.66	1.81
4	A	100	HTG	C1-S1	-8.54	1.67	1.80
3	C	99	ZMQ	O1-C1	7.62	1.33	1.21
3	E	99	ZMQ	O1-C1	7.61	1.33	1.21
3	A	99	ZMQ	O1-C1	7.58	1.33	1.21
3	G	99	ZMQ	O1-C1	7.58	1.33	1.21
5	B	405	HEM	C3D-C2D	5.40	1.53	1.37
5	D	405	HEM	C3D-C2D	5.39	1.53	1.37
5	F	405	HEM	C3D-C2D	5.37	1.53	1.37
5	H	405	HEM	C3D-C2D	5.36	1.53	1.37
3	E	99	ZMQ	O35-C34	5.22	1.33	1.23
3	A	99	ZMQ	O35-C34	5.18	1.33	1.23
3	G	99	ZMQ	O35-C34	5.18	1.33	1.23
3	C	99	ZMQ	O35-C34	5.14	1.33	1.23
3	G	99	ZMQ	O40-C39	5.08	1.33	1.23
3	C	99	ZMQ	O40-C39	4.97	1.33	1.23
3	A	99	ZMQ	O40-C39	4.97	1.33	1.23
3	E	99	ZMQ	O40-C39	4.91	1.33	1.23
5	F	405	HEM	C3C-C2C	-4.69	1.33	1.40
5	H	405	HEM	C3B-C2B	-4.54	1.34	1.40
5	H	405	HEM	C3C-C2C	-4.39	1.34	1.40
5	D	405	HEM	C3C-C2C	-4.34	1.34	1.40
5	F	405	HEM	C3B-C2B	-4.26	1.34	1.40
5	B	405	HEM	C3B-C2B	-4.18	1.34	1.40
5	B	405	HEM	C3C-C2C	-4.13	1.34	1.40
5	D	405	HEM	C3B-C2B	-4.11	1.34	1.40
4	H	417	HTG	C1'-S1	-4.04	1.66	1.80
5	D	405	HEM	C3B-CAB	3.60	1.55	1.47
5	B	405	HEM	C3C-CAC	3.56	1.55	1.47
5	D	405	HEM	C3C-CAC	3.54	1.55	1.47
5	F	405	HEM	C3B-CAB	3.52	1.55	1.47
5	B	405	HEM	C3B-CAB	3.48	1.55	1.47
5	H	405	HEM	C3C-CAC	3.46	1.54	1.47
5	F	405	HEM	C3C-CAC	3.40	1.54	1.47
5	H	405	HEM	C3B-CAB	3.36	1.54	1.47
3	G	99	ZMQ	C34-N36	-3.30	1.26	1.33
3	C	99	ZMQ	C34-N36	-3.20	1.26	1.33
3	G	99	ZMQ	C39-N41	-3.04	1.26	1.33
3	C	99	ZMQ	C39-N41	-3.03	1.26	1.33
3	A	99	ZMQ	C34-N36	-2.91	1.27	1.33
3	E	99	ZMQ	C34-N36	-2.88	1.27	1.33
3	A	99	ZMQ	C39-N41	-2.84	1.26	1.33
3	E	99	ZMQ	C39-N41	-2.77	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	405	HEM	CAA-C2A	2.28	1.55	1.52
3	A	99	ZMQ	C2-C1	2.26	1.53	1.50
5	D	405	HEM	CAA-C2A	2.17	1.55	1.52
3	G	99	ZMQ	C2-C1	2.12	1.53	1.50
3	E	99	ZMQ	C2-C1	2.09	1.53	1.50
5	F	405	HEM	CAA-C2A	2.06	1.55	1.52
3	C	99	ZMQ	C2-C1	2.05	1.53	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	99	ZMQ	C2-C1-S1	5.61	119.98	113.46
3	A	99	ZMQ	C2-C1-S1	5.44	119.78	113.46
3	G	99	ZMQ	C2-C1-S1	5.10	119.40	113.46
4	A	100	HTG	C1'-S1-C1	4.70	108.88	100.09
3	G	99	ZMQ	O1-C1-C2	-4.63	118.53	123.99
3	A	99	ZMQ	O1-C1-C2	-4.56	118.61	123.99
3	C	99	ZMQ	C43-C42-N41	-4.03	103.95	112.42
3	C	99	ZMQ	C2-C1-S1	4.01	118.12	113.46
3	C	99	ZMQ	O1-C1-S1	-3.69	117.81	122.61
3	E	99	ZMQ	O1-C1-C2	-3.65	119.68	123.99
3	E	99	ZMQ	C42-N41-C39	3.62	129.55	122.84
3	G	99	ZMQ	C37-N36-C34	3.61	129.02	122.59
3	C	99	ZMQ	O1-C1-C2	-3.57	119.78	123.99
3	G	99	ZMQ	C43-C42-N41	-3.53	104.99	112.42
3	C	99	ZMQ	C37-N36-C34	3.49	128.81	122.59
3	G	99	ZMQ	C38-C37-N36	-3.48	104.88	111.90
3	G	99	ZMQ	O1-C1-S1	-2.96	118.78	122.61
3	A	99	ZMQ	C43-S1-C1	2.95	111.06	101.87
3	A	99	ZMQ	C37-N36-C34	2.94	127.83	122.59
5	F	405	HEM	CBD-CAD-C3D	-2.90	107.14	112.48
3	E	99	ZMQ	O1-C1-S1	-2.86	118.91	122.61
3	A	99	ZMQ	C43-C42-N41	-2.85	106.44	112.42
3	A	99	ZMQ	C42-N41-C39	2.82	128.08	122.84
3	A	99	ZMQ	O1-C1-S1	-2.76	119.02	122.61
3	C	99	ZMQ	C38-C37-N36	-2.75	106.34	111.90
5	F	405	HEM	C1D-C2D-C3D	-2.69	105.13	107.00
3	G	99	ZMQ	C43-S1-C1	2.57	109.86	101.87
3	C	99	ZMQ	C42-N41-C39	2.54	127.55	122.84
5	D	405	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
5	B	405	HEM	C1D-C2D-C3D	-2.42	105.31	107.00
3	C	99	ZMQ	C43-S1-C1	2.41	109.37	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	99	ZMQ	C38-C37-N36	-2.35	107.15	111.90
5	D	405	HEM	CBD-CAD-C3D	-2.31	108.23	112.48
5	B	405	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
4	H	417	HTG	C3'-C2'-C1'	-2.26	109.06	113.09
3	E	99	ZMQ	C43-S1-C1	2.26	108.90	101.87
3	A	99	ZMQ	C32-C34-N36	2.25	121.05	116.58
5	B	405	HEM	CAD-CBD-CGD	-2.22	108.95	112.67
3	A	99	ZMQ	C38-C39-N41	2.18	120.09	116.42
3	G	99	ZMQ	C42-N41-C39	2.15	126.82	122.84
5	H	405	HEM	C1D-C2D-C3D	-2.14	105.51	107.00
3	G	99	ZMQ	C30-C29-C32	2.07	112.42	108.82
5	D	405	HEM	CAA-CBA-CGA	-2.04	109.25	112.67

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	99	ZMQ	C28-C29-C32-O33
3	E	99	ZMQ	C28-C29-C32-C34
3	E	99	ZMQ	C31-C29-C32-O33
3	E	99	ZMQ	C31-C29-C32-C34
3	E	99	ZMQ	C30-C29-C32-O33
3	E	99	ZMQ	C30-C29-C32-C34
3	E	99	ZMQ	C32-C34-N36-C37
3	C	99	ZMQ	C28-C29-C32-O33
3	C	99	ZMQ	C31-C29-C32-O33
3	C	99	ZMQ	O1-C1-S1-C43
3	G	99	ZMQ	O27-C28-C29-C30
3	G	99	ZMQ	O27-C28-C29-C32
3	G	99	ZMQ	C28-C29-C32-O33
3	G	99	ZMQ	C28-C29-C32-C34
3	G	99	ZMQ	C31-C29-C32-O33
3	G	99	ZMQ	C31-C29-C32-C34
3	G	99	ZMQ	C30-C29-C32-O33
3	G	99	ZMQ	C30-C29-C32-C34
3	G	99	ZMQ	O33-C32-C34-O35
3	G	99	ZMQ	O33-C32-C34-N36
3	G	99	ZMQ	O1-C1-S1-C43
3	A	99	ZMQ	C28-C29-C32-O33
3	A	99	ZMQ	C32-C34-N36-C37
3	A	99	ZMQ	O1-C1-C2-C3
3	A	99	ZMQ	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	E	99	ZMQ	O35-C34-N36-C37
3	A	99	ZMQ	O35-C34-N36-C37
3	G	99	ZMQ	C6-C7-C8-C9
3	E	99	ZMQ	C2-C3-C4-C5
3	E	99	ZMQ	C4-C5-C6-C7
3	G	99	ZMQ	O27-C28-C29-C31
3	A	99	ZMQ	C3-C4-C5-C6
3	A	99	ZMQ	C5-C6-C7-C8
3	G	99	ZMQ	C4-C5-C6-C7
4	F	417	HTG	C3'-C4'-C5'-C6'
3	C	99	ZMQ	C3-C4-C5-C6
3	C	99	ZMQ	C4-C5-C6-C7
3	A	99	ZMQ	C2-C3-C4-C5
4	A	101	HTG	C2'-C3'-C4'-C5'
3	C	99	ZMQ	C6-C7-C8-C9
4	A	101	HTG	C3'-C4'-C5'-C6'
3	A	99	ZMQ	C12-C13-C14-C15
3	C	99	ZMQ	C2-C3-C4-C5
3	G	99	ZMQ	C5-C6-C7-C8
4	A	101	HTG	C1'-C2'-C3'-C4'
3	C	99	ZMQ	O33-C32-C34-O35
4	F	417	HTG	C4'-C5'-C6'-C7'
3	C	99	ZMQ	C30-C29-C32-O33
3	C	99	ZMQ	C11-C12-C13-C14
3	G	99	ZMQ	C29-C32-C34-O35
3	G	99	ZMQ	C2-C3-C4-C5
3	G	99	ZMQ	C29-C32-C34-N36
3	E	99	ZMQ	C13-C14-C15-C16
4	F	417	HTG	C2'-C3'-C4'-C5'
4	H	417	HTG	C2'-C3'-C4'-C5'
3	E	99	ZMQ	O1-C1-S1-C43
3	G	99	ZMQ	S1-C1-C2-C3
3	G	99	ZMQ	O1-C1-C2-C3
3	A	99	ZMQ	S1-C1-C2-C3
3	C	99	ZMQ	C1-C2-C3-C4
4	A	100	HTG	C2'-C1'-S1-C1
3	E	99	ZMQ	C12-C13-C14-C15
3	C	99	ZMQ	C2-C1-S1-C43
3	G	99	ZMQ	C2-C1-S1-C43
3	C	99	ZMQ	C31-C29-C32-C34
3	E	99	ZMQ	C6-C7-C8-C9
3	E	99	ZMQ	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	H	417	HTG	C3'-C4'-C5'-C6'
3	A	99	ZMQ	C31-C29-C32-O33
3	A	99	ZMQ	C30-C29-C32-O33
3	E	99	ZMQ	C10-C11-C12-C13
3	A	99	ZMQ	C9-C10-C11-C12
3	G	99	ZMQ	C12-C13-C14-C15
3	G	99	ZMQ	C13-C14-C15-C16
3	C	99	ZMQ	O33-C32-C34-N36
3	A	99	ZMQ	N41-C42-C43-S1
3	A	99	ZMQ	N36-C37-C38-C39
3	G	99	ZMQ	C9-C10-C11-C12
3	C	99	ZMQ	C30-C29-C32-C34
3	A	99	ZMQ	C11-C12-C13-C14
3	C	99	ZMQ	C28-C29-C32-C34

There are no ring outliers.

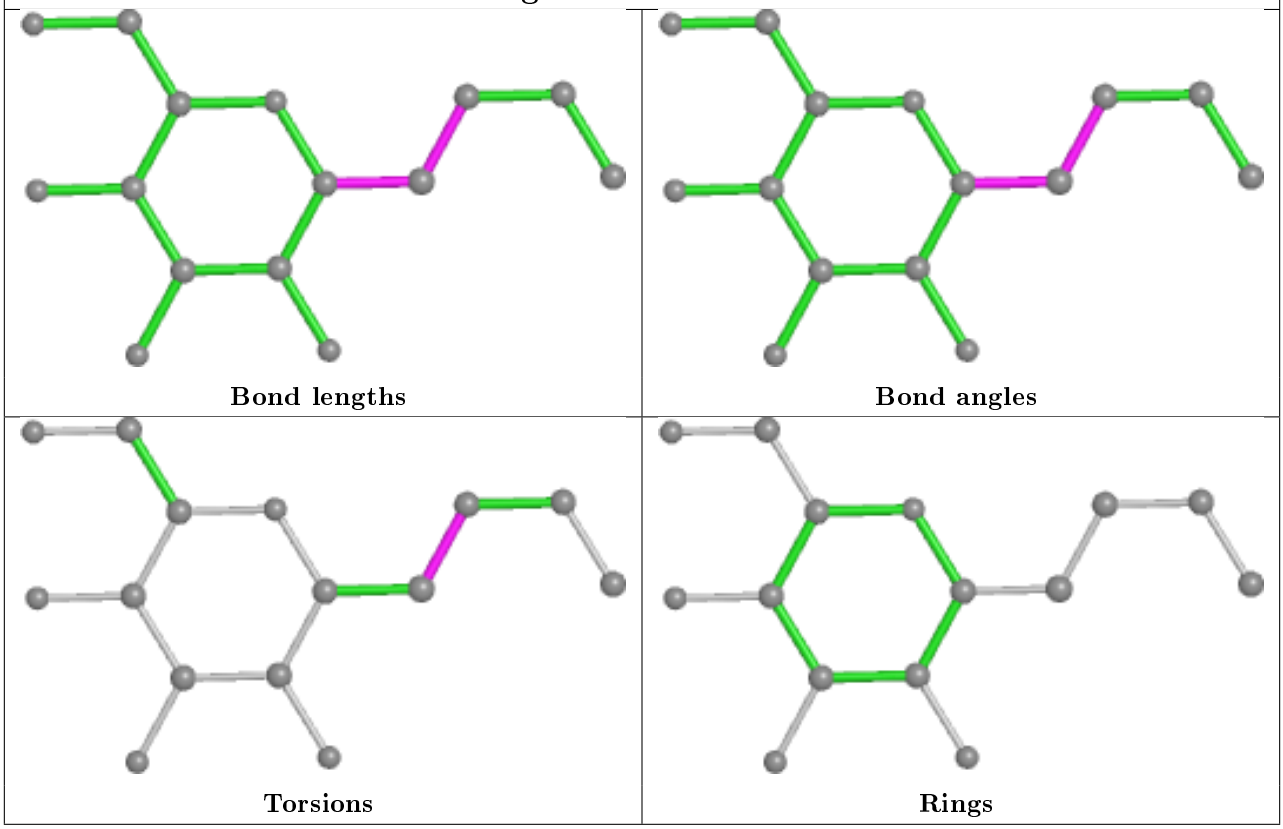
12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	100	HTG	1	0
4	A	101	HTG	1	0
4	H	417	HTG	1	0
5	D	405	HEM	1	0
5	F	405	HEM	4	0
5	H	405	HEM	2	0
3	E	99	ZMQ	4	0
4	D	417	HTG	1	0
3	C	99	ZMQ	5	0
5	B	405	HEM	2	0
3	G	99	ZMQ	2	0
3	A	99	ZMQ	3	0

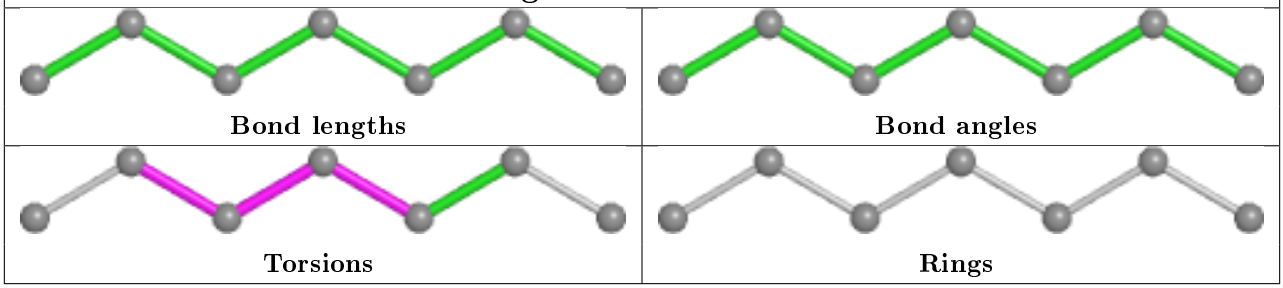
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

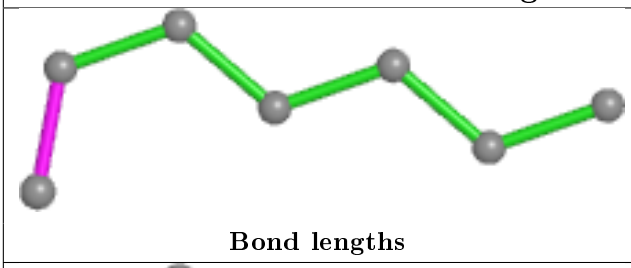
Ligand HTG A 100



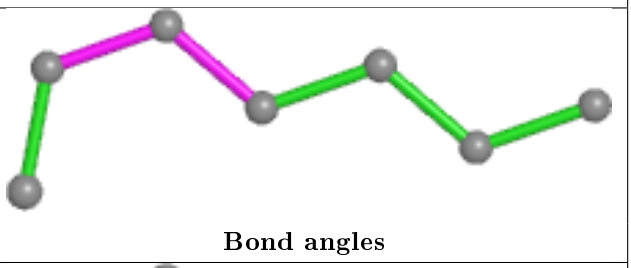
Ligand HTG A 101



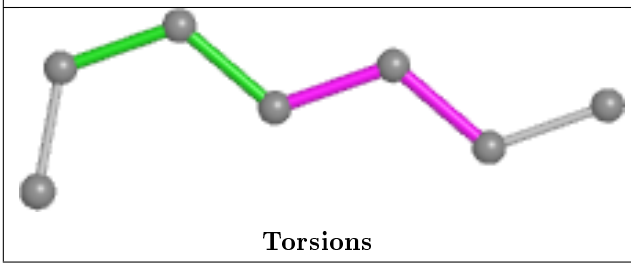
Ligand HTG H 417



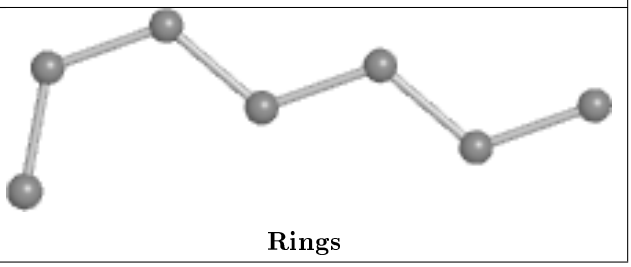
Bond lengths



Bond angles

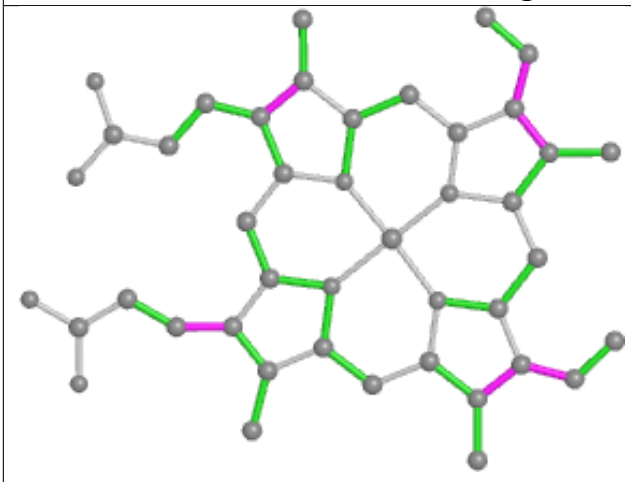


Torsions

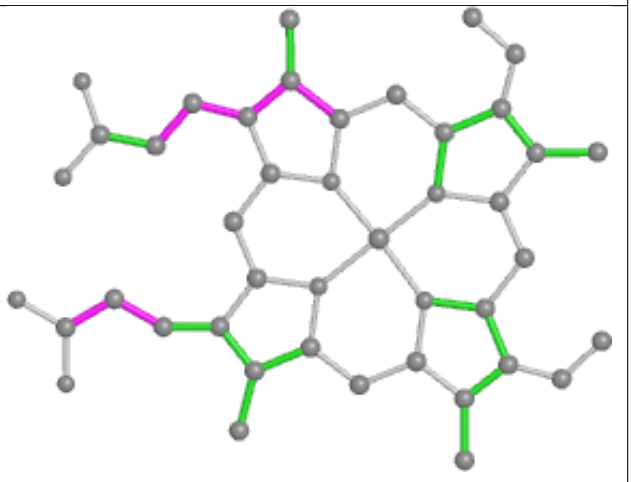


Rings

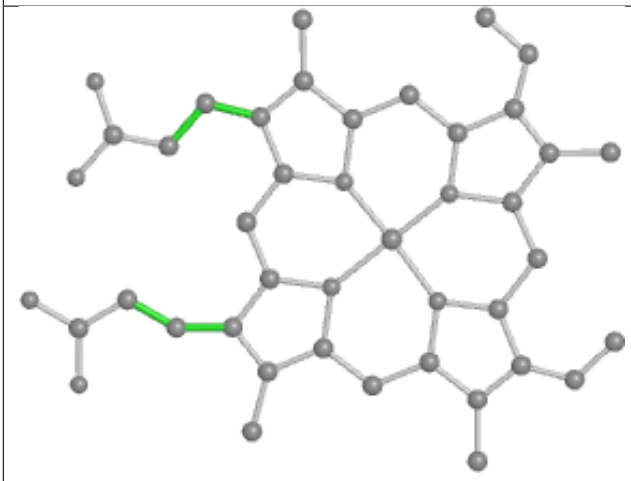
Ligand HEM D 405



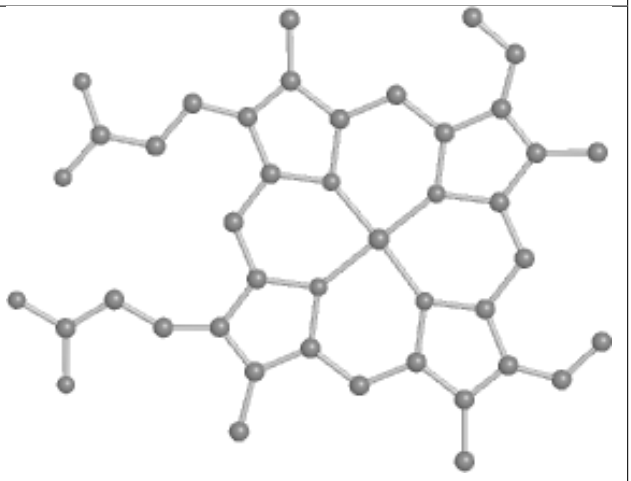
Bond lengths



Bond angles

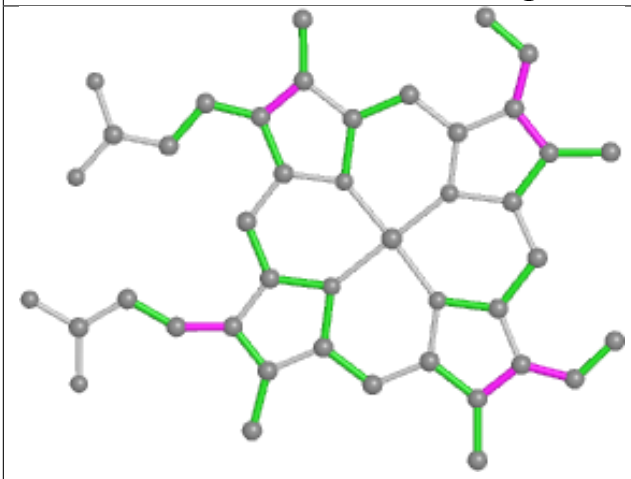


Torsions

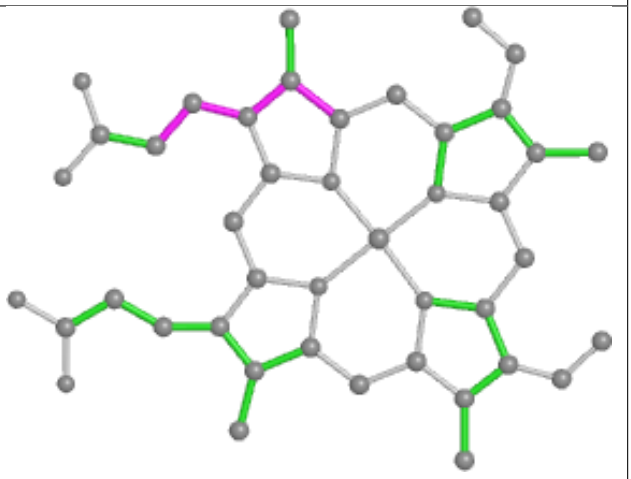


Rings

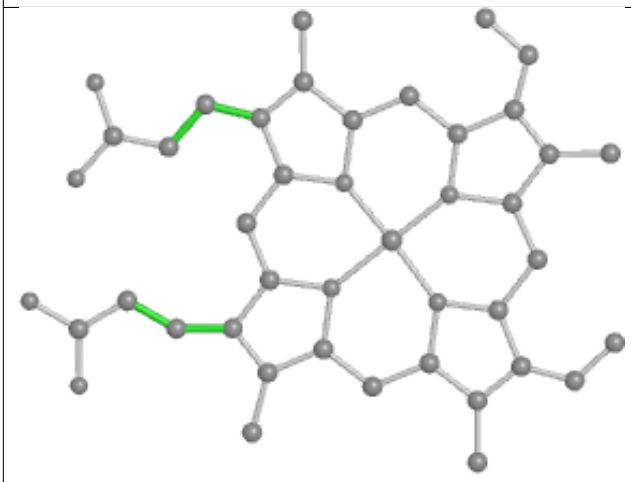
Ligand HEM F 405



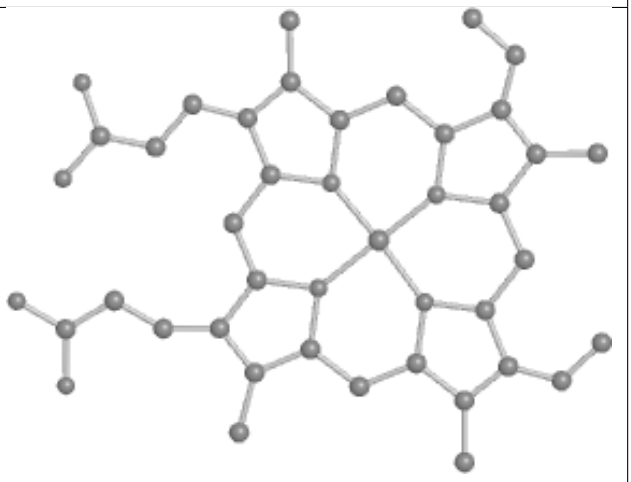
Bond lengths



Bond angles

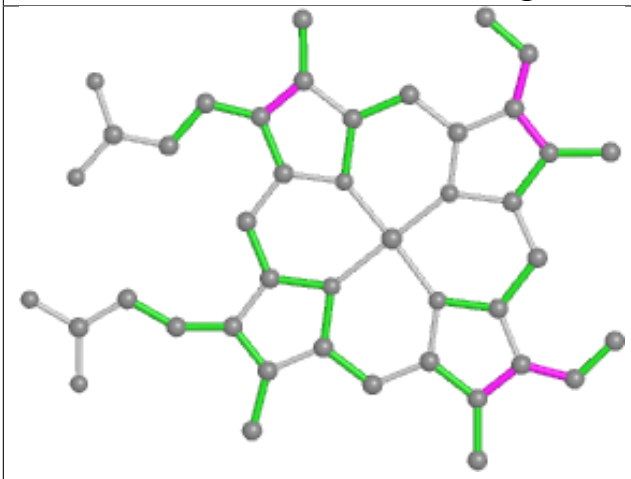


Torsions

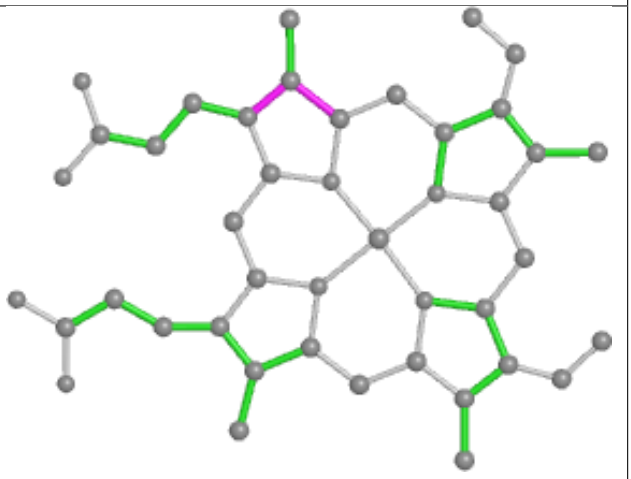


Rings

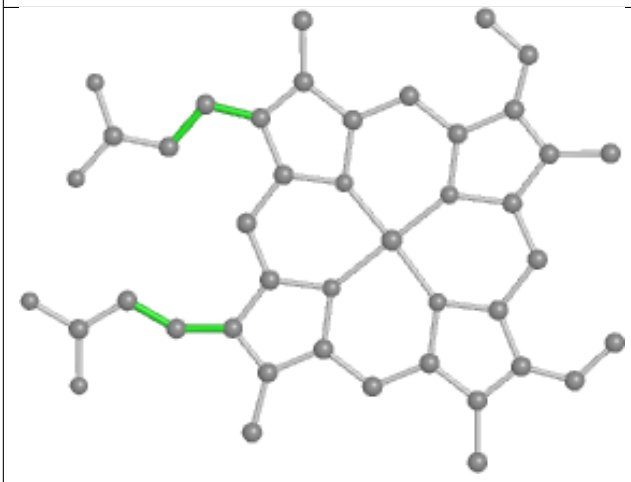
Ligand HEM H 405



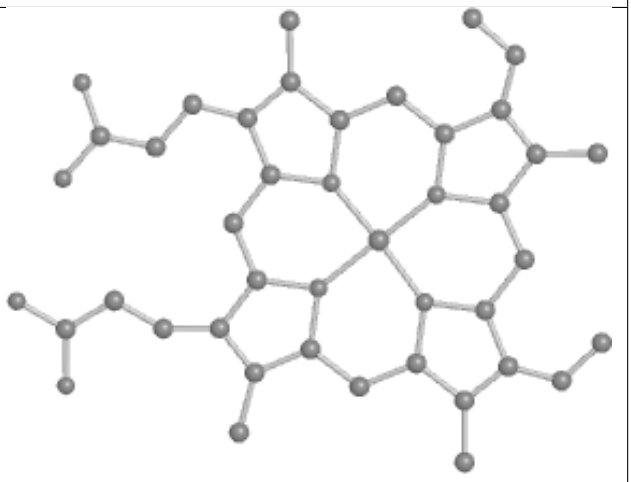
Bond lengths



Bond angles

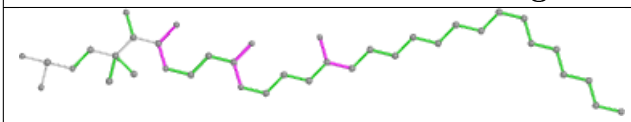


Torsions

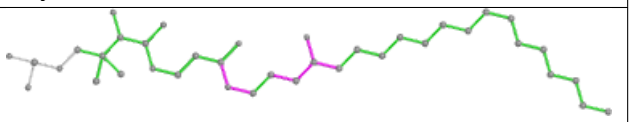


Rings

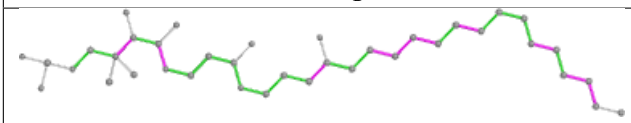
Ligand ZMQ E 99



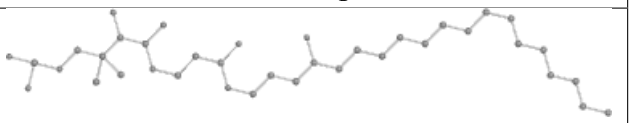
Bond lengths



Bond angles

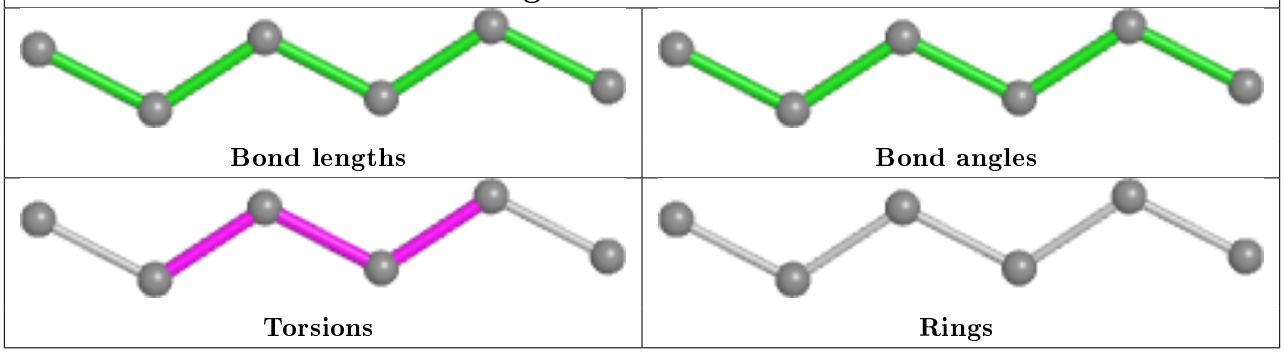


Torsions

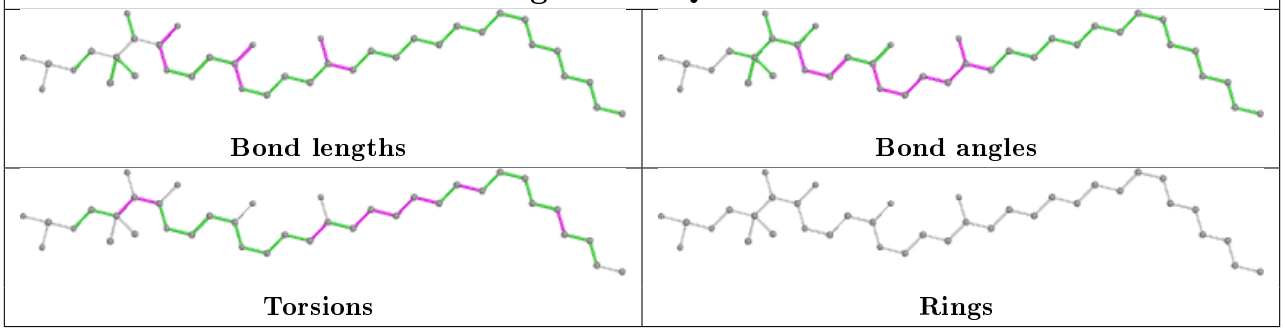


Rings

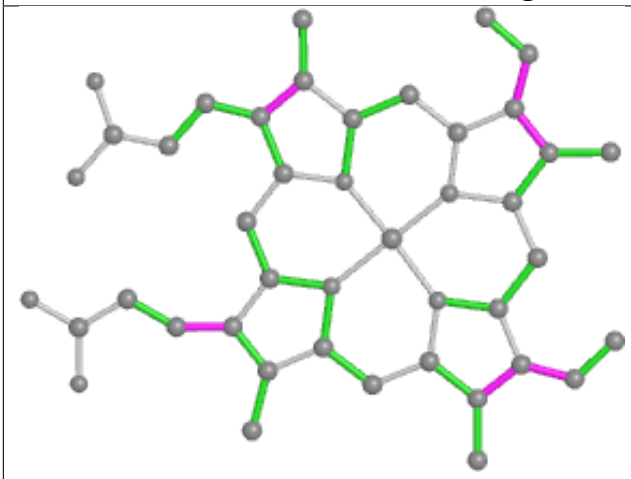
Ligand HTG F 417



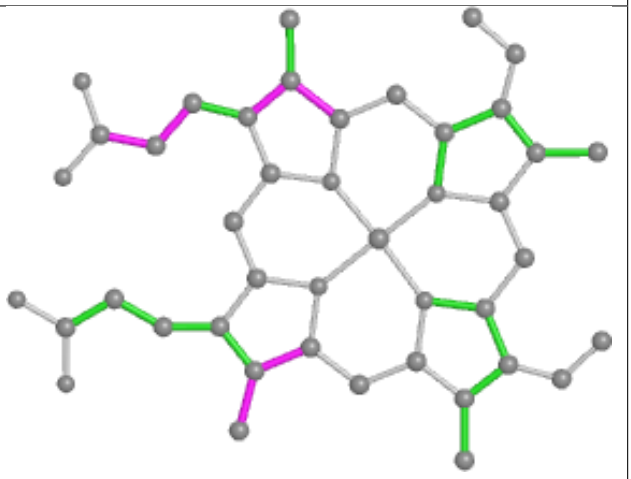
Ligand ZMQ C 99



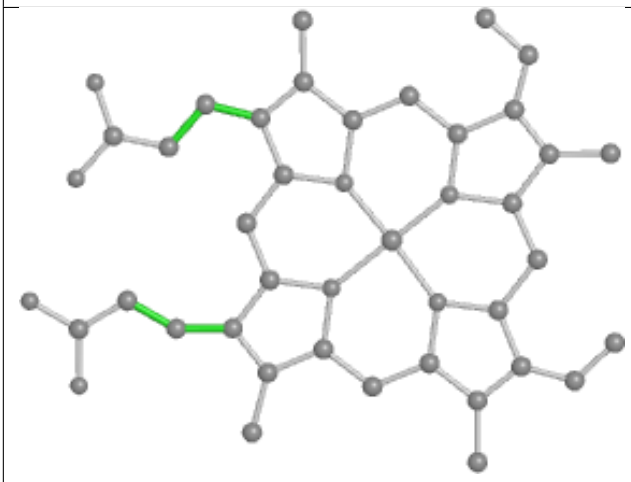
Ligand HEM B 405



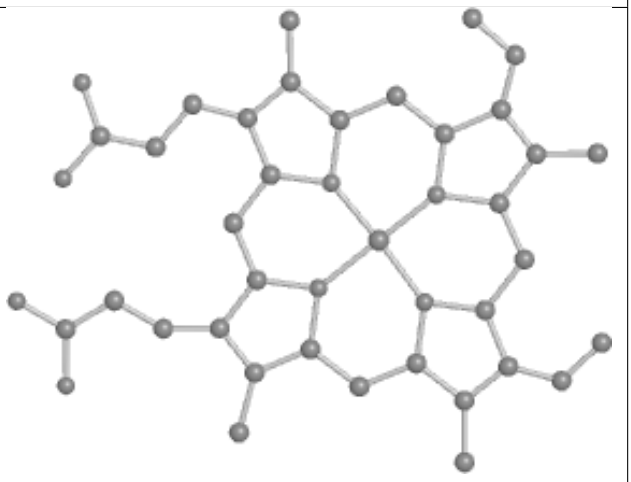
Bond lengths



Bond angles

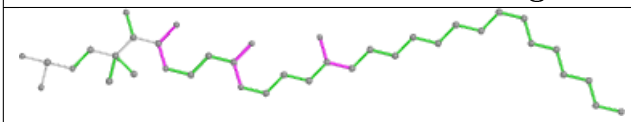


Torsions

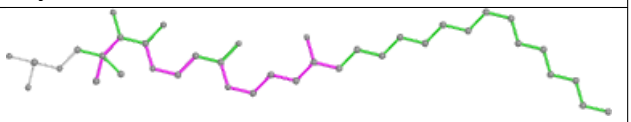


Rings

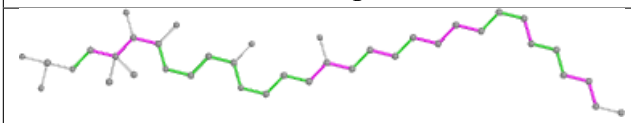
Ligand ZMQ G 99



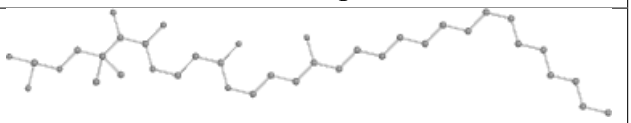
Bond lengths



Bond angles

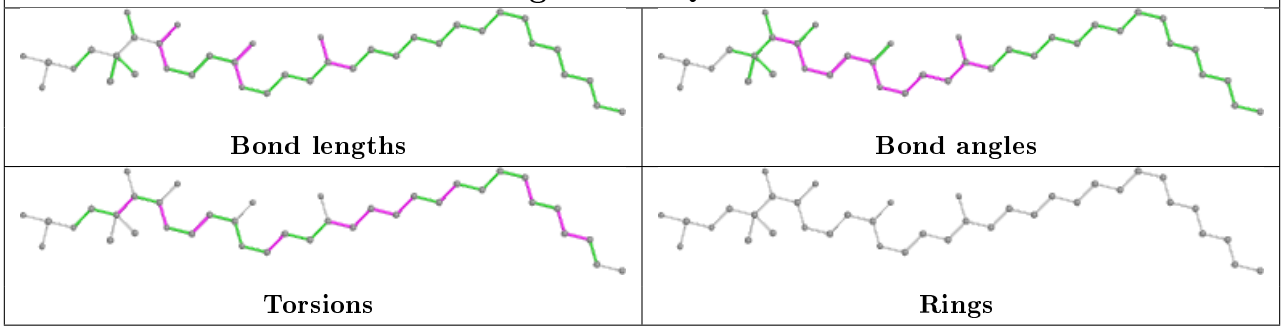


Torsions



Rings

Ligand ZMQ A 99



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	78/97 (80%)	0.49	3 (3%)	40	46	26, 39, 56, 60	0
1	C	77/97 (79%)	0.67	7 (9%)	9	12	27, 39, 56, 60	0
1	E	78/97 (80%)	0.51	3 (3%)	40	46	26, 39, 56, 60	0
1	G	77/97 (79%)	0.36	2 (2%)	56	61	26, 38, 56, 60	0
2	B	382/404 (94%)	0.36	8 (2%)	63	68	19, 32, 48, 56	0
2	D	385/404 (95%)	0.33	18 (4%)	31	37	19, 32, 48, 58	0
2	F	381/404 (94%)	0.31	5 (1%)	77	80	19, 32, 48, 58	0
2	H	382/404 (94%)	0.43	17 (4%)	33	38	19, 32, 48, 56	0
All	All	1840/2004 (91%)	0.38	63 (3%)	45	51	19, 33, 49, 60	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	214	ARG	7.1
1	G	17	GLY	5.3
2	D	65	SER	4.6
2	D	123	GLN	4.4
1	C	46	ALA	4.0
1	A	38	LYS	4.0
2	B	372	ASP	3.9
1	C	41	GLU	3.9
2	B	366	PRO	3.6
2	H	118	LEU	3.5
2	H	65	SER	3.4
2	H	375	TRP	3.3
2	H	294	ILE	3.3
2	D	211	LEU	3.2
2	D	204	GLN	3.1
1	A	40	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	40	GLU	3.0
2	F	381	PHE	2.9
2	D	64	GLU	2.9
2	H	393	PHE	2.8
2	H	317	SER	2.8
2	D	218	LYS	2.8
2	H	195	ILE	2.7
2	D	393	PHE	2.7
2	D	294	ILE	2.7
2	H	368	LEU	2.7
2	H	141	PHE	2.7
2	F	213	GLY	2.7
2	H	211	LEU	2.7
1	C	72	THR	2.6
2	H	64	GLU	2.6
2	H	124	GLY	2.6
2	B	381	PHE	2.5
2	D	8	SER	2.5
2	H	127	LYS	2.4
1	C	40	GLU	2.3
2	D	110	TYR	2.3
2	B	363	GLN	2.3
2	H	391	VAL	2.3
2	H	300	ARG	2.3
2	D	102	ARG	2.2
2	F	219	LEU	2.2
1	C	36	GLY	2.2
1	G	81	LYS	2.2
1	E	66	LEU	2.1
2	B	375	TRP	2.1
1	C	74	ILE	2.1
1	C	82	ILE	2.1
2	B	154	ARG	2.1
2	H	219	LEU	2.1
2	D	394	GLU	2.1
1	E	37	VAL	2.1
2	D	126	LYS	2.1
2	D	7	ALA	2.1
2	D	376	ARG	2.1
2	F	363	GLN	2.1
2	D	219	LEU	2.1
2	B	141	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	370	LEU	2.0
2	D	67	THR	2.0
2	D	200	ARG	2.0
1	A	62	LEU	2.0
2	B	122	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

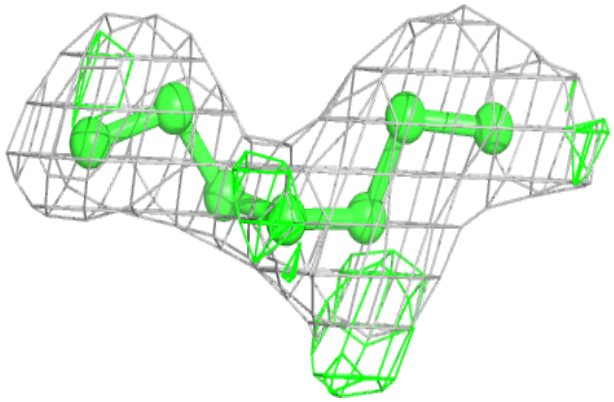
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

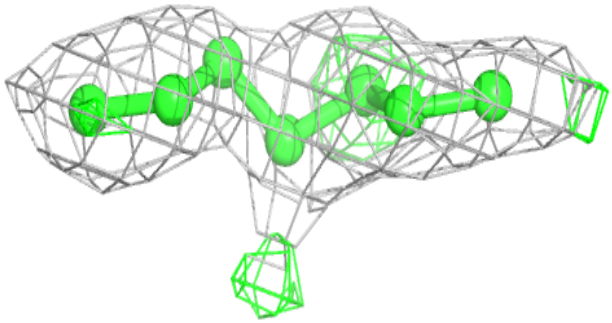
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	B	416	1/1	0.53	0.17	60,60,60,60	0
4	HTG	A	101	7/19	0.77	0.17	36,37,37,38	0
4	HTG	H	417	7/19	0.80	0.20	51,51,51,51	0
4	HTG	F	417	6/19	0.83	0.25	48,49,49,49	0
4	HTG	D	417	5/19	0.84	0.16	33,33,34,34	0
4	HTG	C	100	12/19	0.85	0.16	49,50,51,51	0
4	HTG	E	100	12/19	0.87	0.13	34,36,37,37	0
6	CL	F	418	1/1	0.87	0.06	45,45,45,45	0
3	ZMQ	E	99	38/39	0.89	0.17	26,31,37,39	0
3	ZMQ	G	99	38/39	0.90	0.15	32,35,40,40	0
4	HTG	G	100	12/19	0.90	0.14	37,40,40,41	0
4	HTG	A	100	15/19	0.91	0.15	35,39,40,40	0
3	ZMQ	C	99	38/39	0.91	0.15	30,34,40,41	0
3	ZMQ	A	99	38/39	0.91	0.15	26,32,39,39	0
5	HEM	H	405	43/43	0.96	0.13	16,17,20,22	0
5	HEM	D	405	43/43	0.96	0.13	15,16,19,20	0
5	HEM	B	405	43/43	0.97	0.12	13,15,16,19	0
5	HEM	F	405	43/43	0.97	0.12	16,20,22,25	0

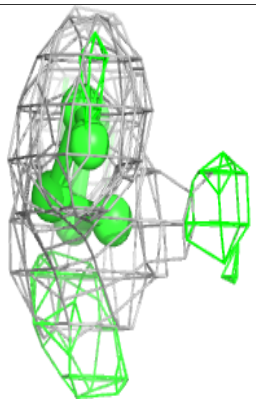
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG A 101:

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

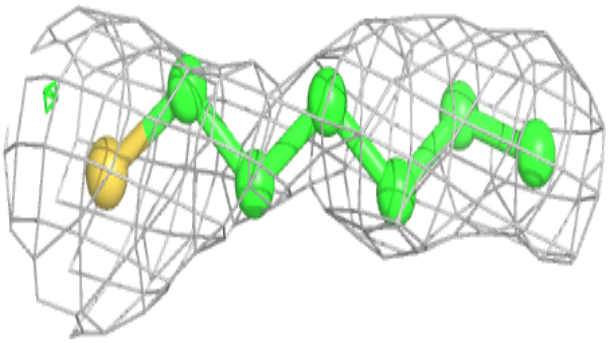


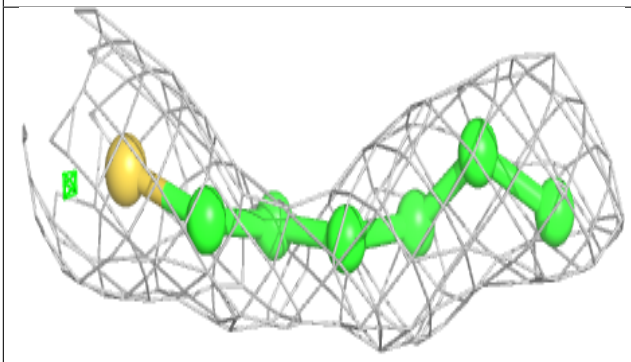


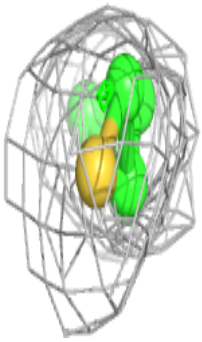


Electron density around HTG H 417:

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

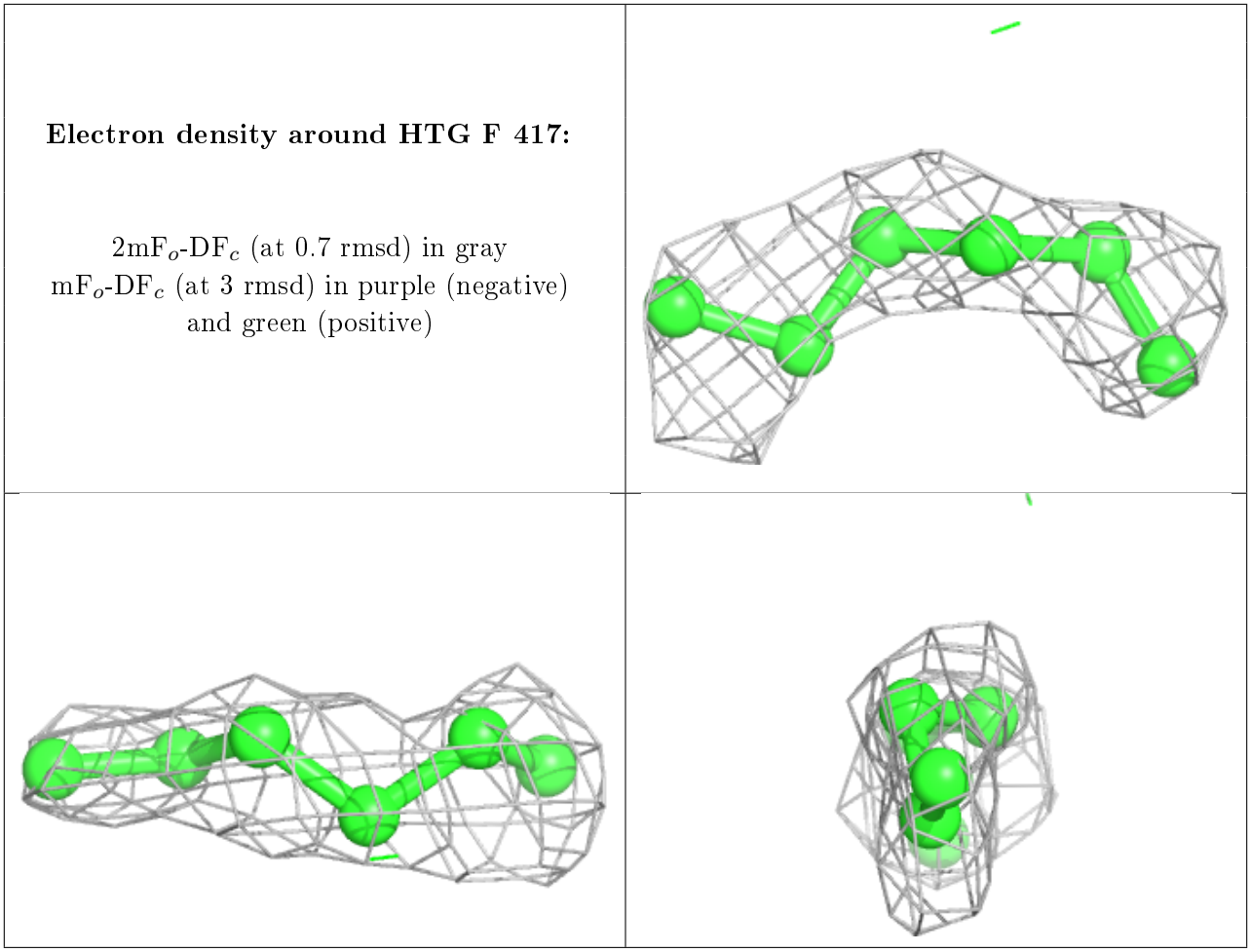






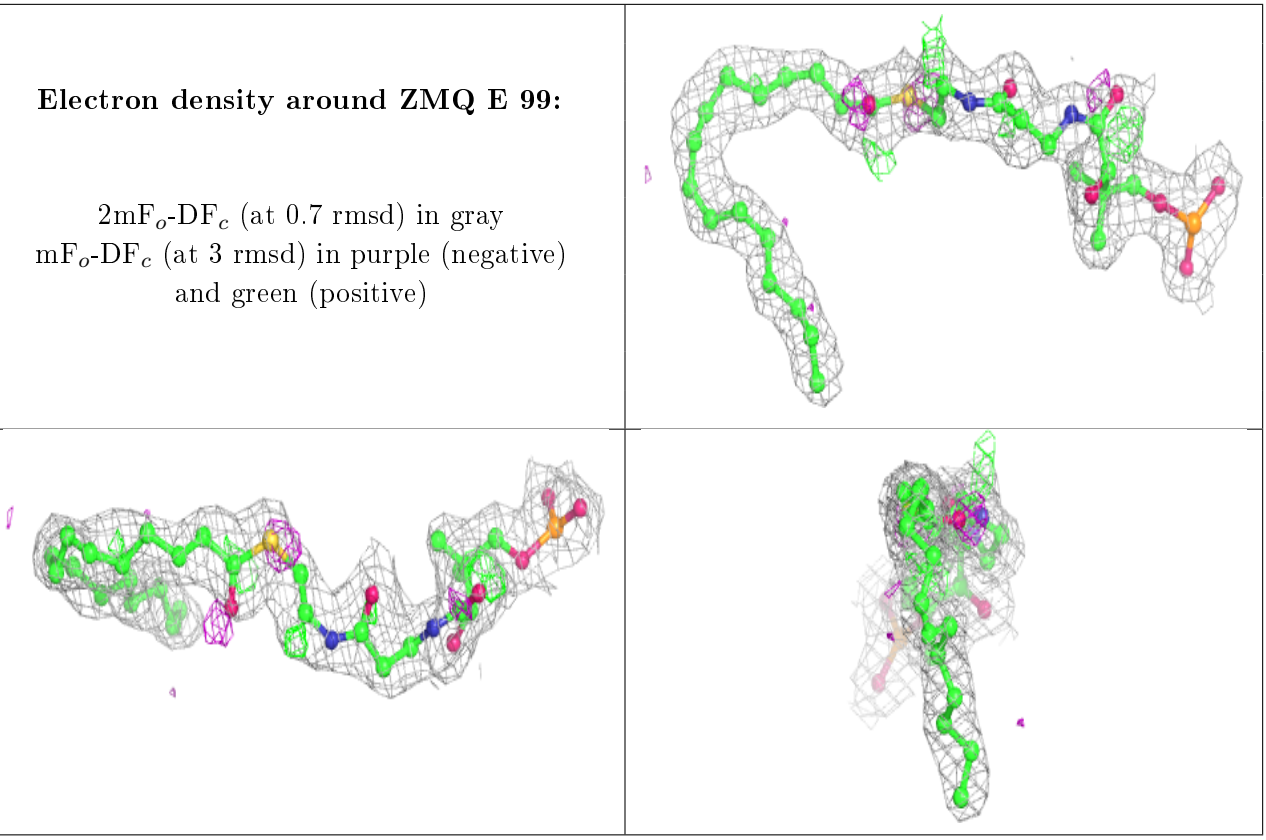
Electron density around HTG F 417:

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



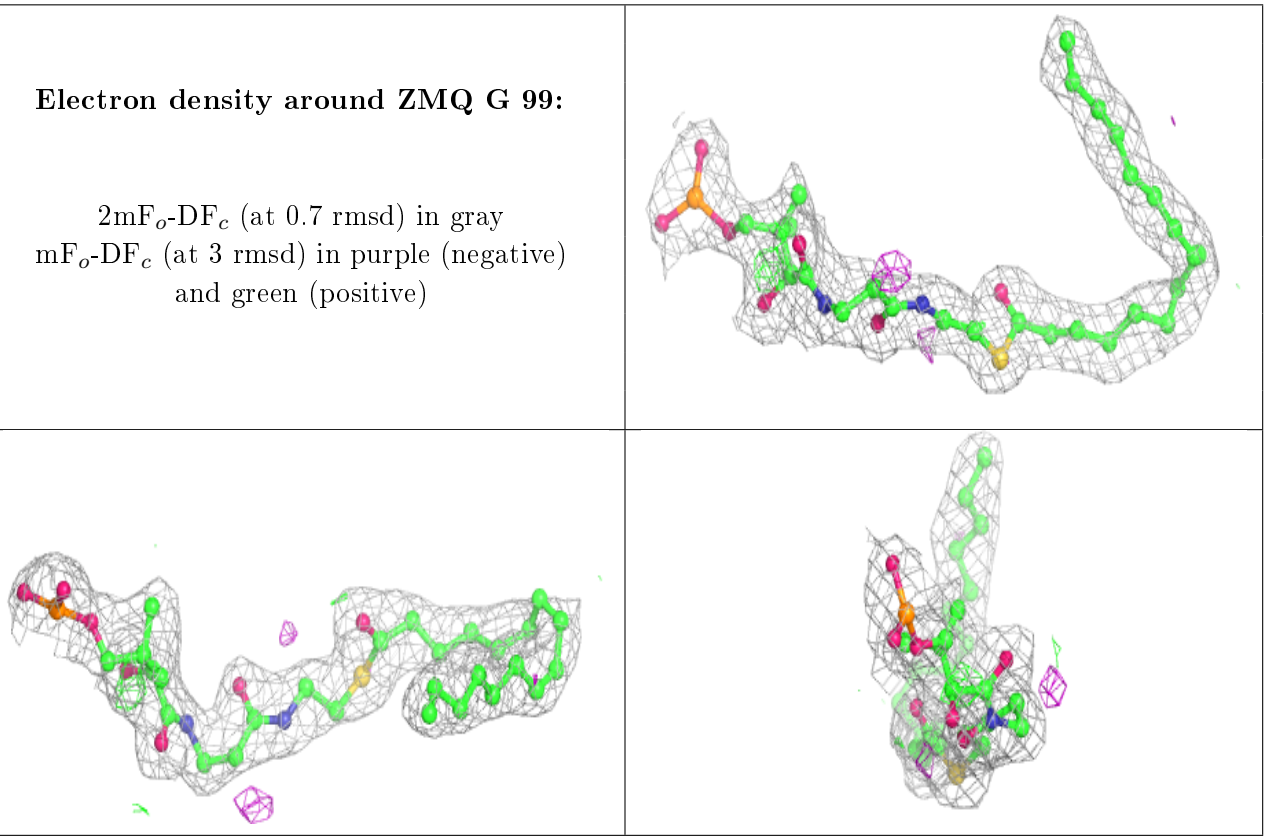
Electron density around ZMQ E 99:

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



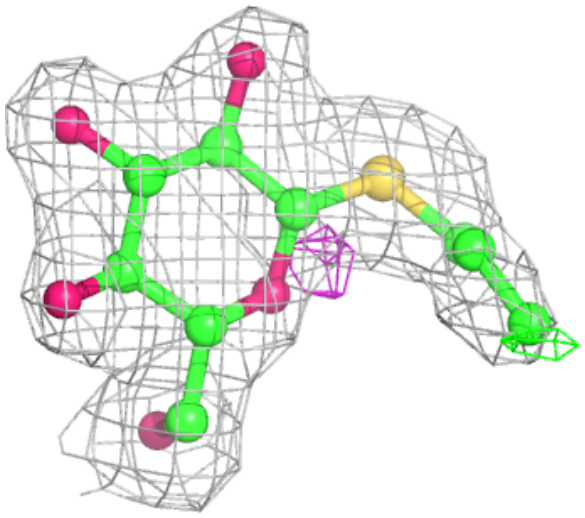
Electron density around ZMQ G 99:

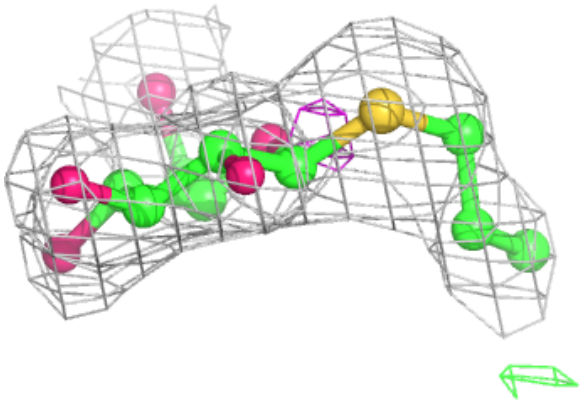
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

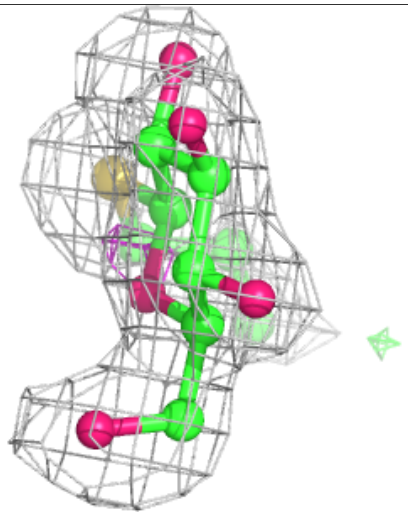


Electron density around HTG A 100:

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

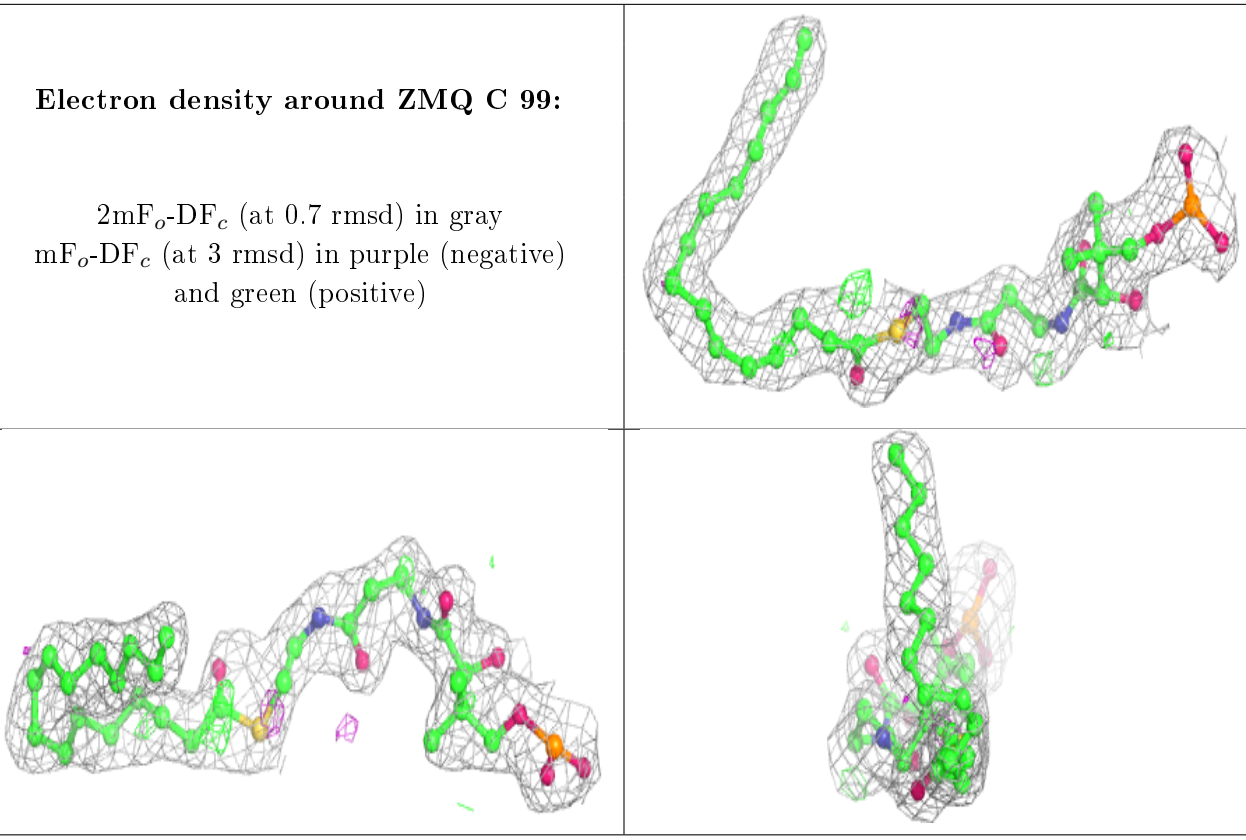






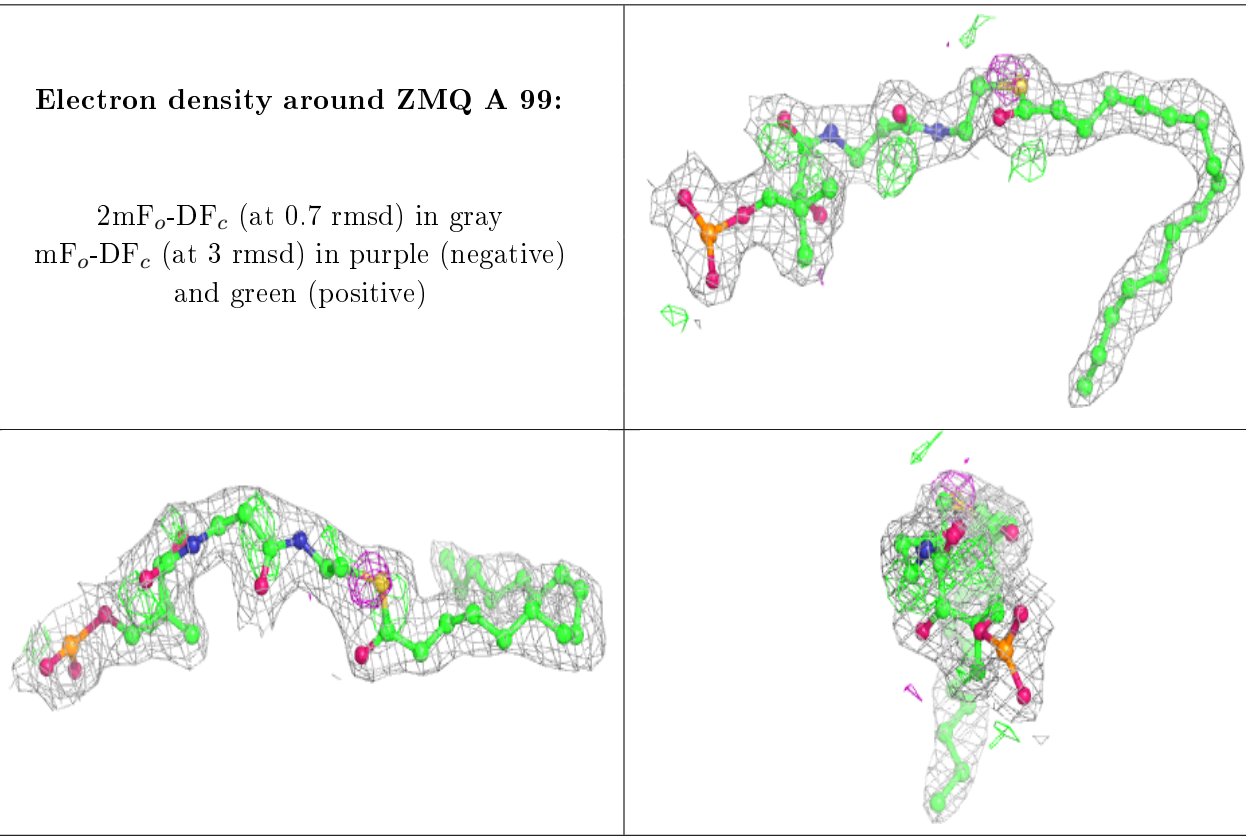
Electron density around ZMQ C 99:

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



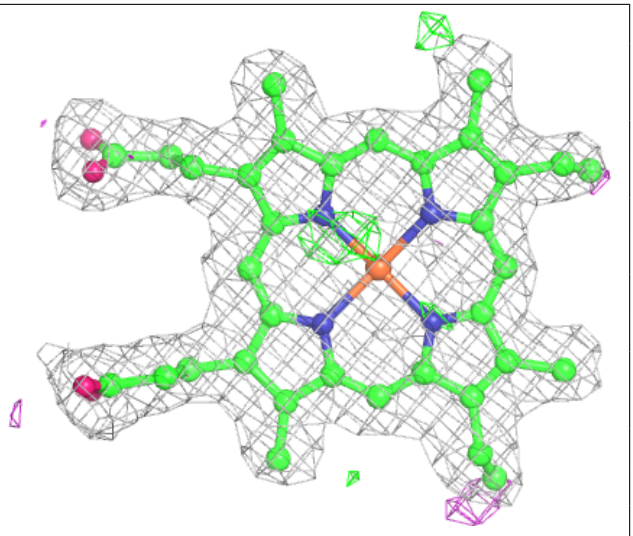
Electron density around ZMQ A 99:

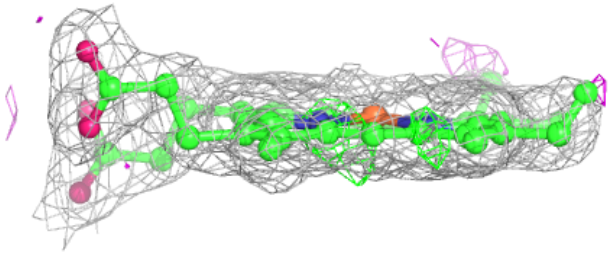
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

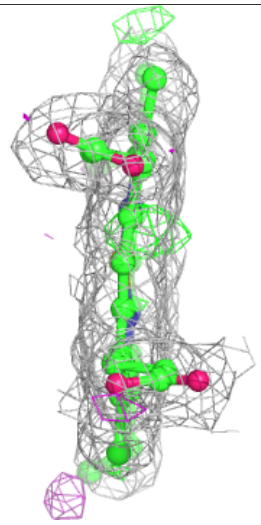


Electron density around HEM H 405:

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

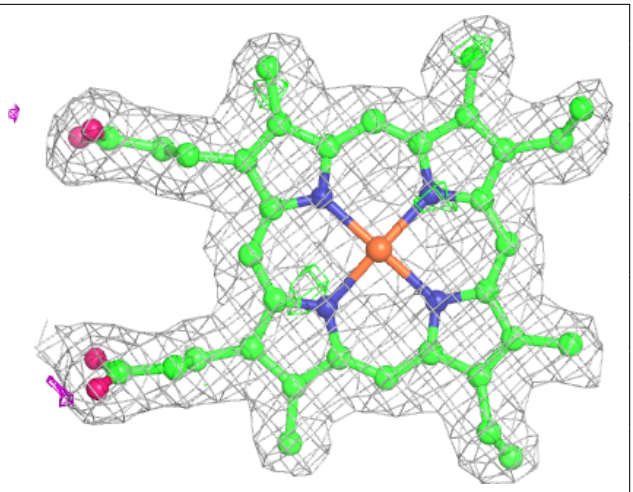


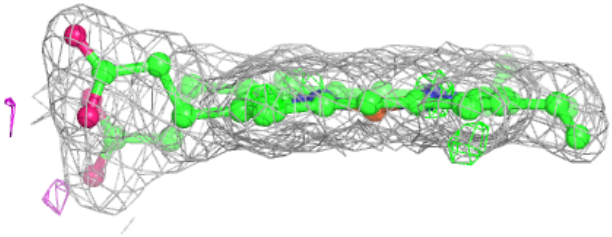


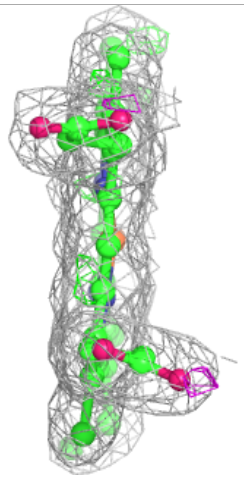


Electron density around HEM D 405:

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

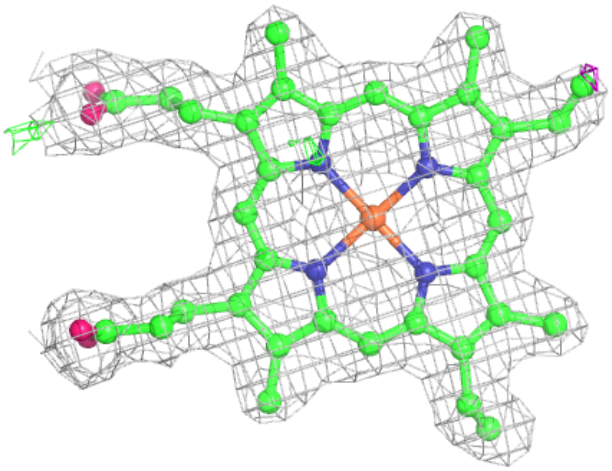


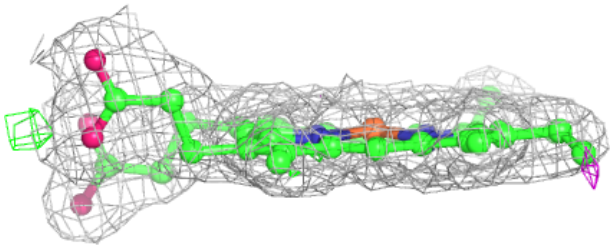


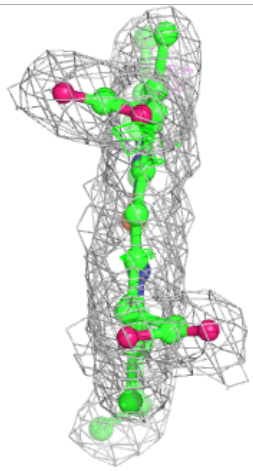


Electron density around HEM B 405:

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

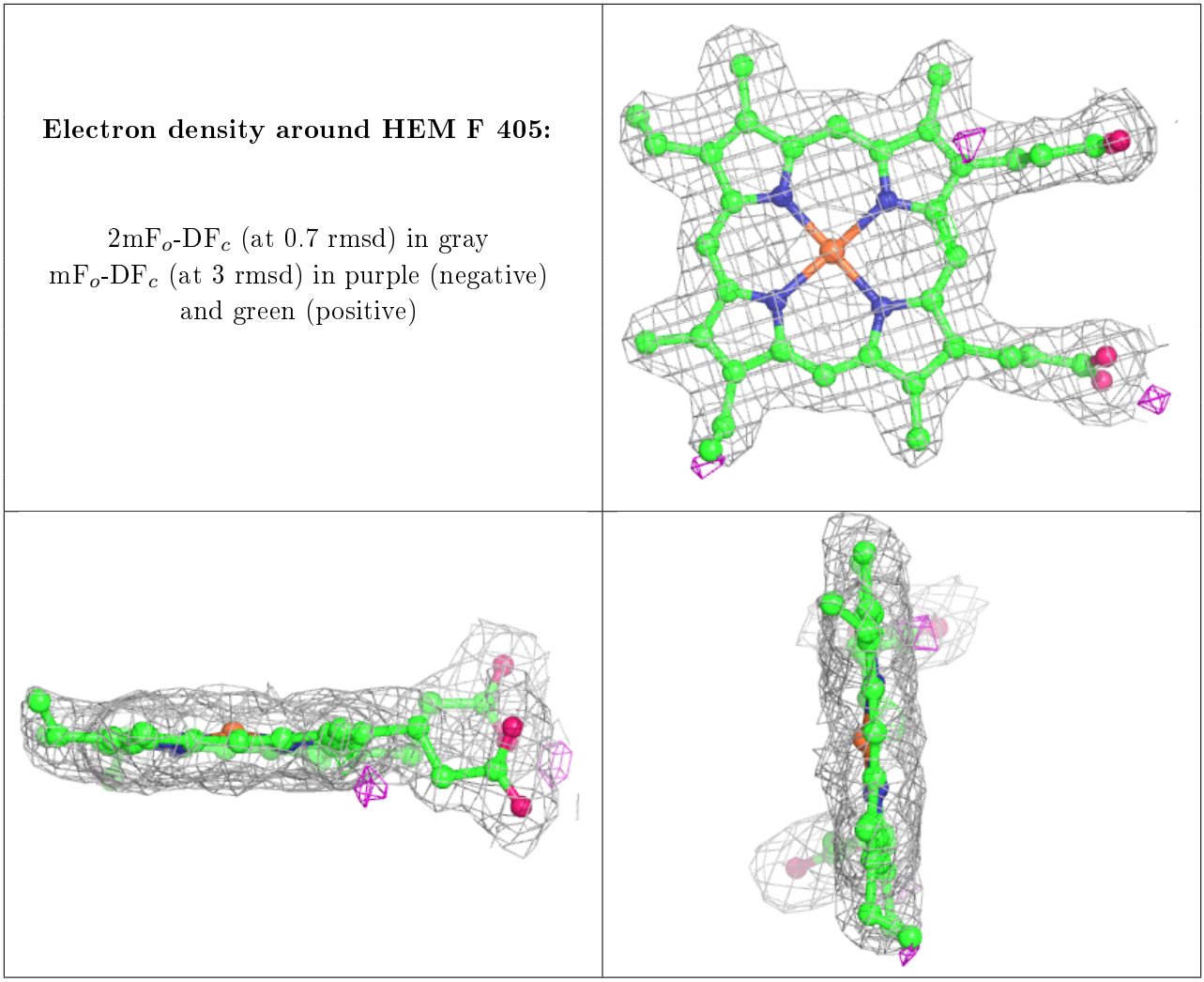






Electron density around HEM F 405:

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



6.5 Other polymers

There are no such residues in this entry.