wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2026 – 08:45 AM EDT

PDB ID	:	5JQU / pdb_00005jqu
Title	:	Crystal structure of Cytochrome P450 BM3 heme domain G265F/T269V/L272W/L322I/F405M/A406S (WIVS-FM) variant with iron(III) deuteroporphyrin IX bound
Authors	:	Reynolds, E.W.; McHenry, M.W.; Cannac, F.; Gober, J.G.; Snow, C.D.; Brustad, E.M.
Deposited on	:	2016-05-05
Resolution	:	2.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

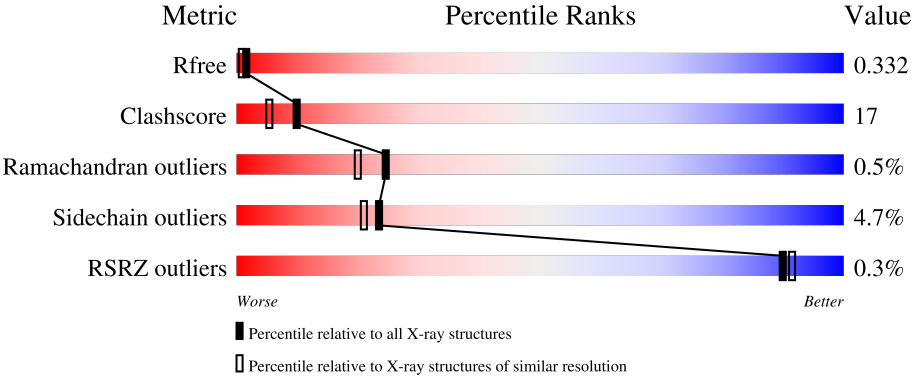
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 <=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	471	63% 31% • •
1	B	471	63% 31% • •
1	C	471	62% 32% • •
1	D	471	60% 35% • •
1	E	471	68% 25% • •

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Mol	Chain	Length	Quality of chain
1	F	471	59% 35%
1	G	471	% 59% 34%
1	H	471	61% 33%

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
2	FDE	A	501	X	-	-	-
2	FDE	B	501	X	-	-	-
2	FDE	C	501	X	-	-	-
2	FDE	D	501	X	-	-	-
2	FDE	E	501	X	-	-	-
2	FDE	F	501	X	-	-	-
2	FDE	G	501	X	-	-	-
2	FDE	H	501	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29916 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 Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3554	2284	606	646	18	0	0	0
1	B	453	3578	2293	607	660	18	0	0	0
1	C	453	3552	2281	604	650	17	0	0	0
1	D	454	3485	2243	591	633	18	0	0	0
1	E	451	3579	2299	606	656	18	0	1	0
1	F	455	3543	2275	602	648	18	0	0	0
1	G	451	3546	2274	600	655	17	0	2	0
1	H	450	3571	2294	605	654	18	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	PHE	GLY	engineered mutation	UNP P14779
A	269	VAL	THR	engineered mutation	UNP P14779
A	272	TRP	LEU	engineered mutation	UNP P14779
A	322	ILE	LEU	engineered mutation	UNP P14779
A	405	MET	PHE	engineered mutation	UNP P14779
A	406	SER	ALA	engineered mutation	UNP P14779
A	464	LEU	-	expression tag	UNP P14779
A	465	GLU	-	expression tag	UNP P14779
A	466	HIS	-	expression tag	UNP P14779
A	467	HIS	-	expression tag	UNP P14779
A	468	HIS	-	expression tag	UNP P14779
A	469	HIS	-	expression tag	UNP P14779
A	470	HIS	-	expression tag	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
A	471	HIS	-	expression tag	UNP P14779
B	265	PHE	GLY	engineered mutation	UNP P14779
B	269	VAL	THR	engineered mutation	UNP P14779
B	272	TRP	LEU	engineered mutation	UNP P14779
B	322	ILE	LEU	engineered mutation	UNP P14779
B	405	MET	PHE	engineered mutation	UNP P14779
B	406	SER	ALA	engineered mutation	UNP P14779
B	464	LEU	-	expression tag	UNP P14779
B	465	GLU	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	HIS	-	expression tag	UNP P14779
B	468	HIS	-	expression tag	UNP P14779
B	469	HIS	-	expression tag	UNP P14779
B	470	HIS	-	expression tag	UNP P14779
B	471	HIS	-	expression tag	UNP P14779
C	265	PHE	GLY	engineered mutation	UNP P14779
C	269	VAL	THR	engineered mutation	UNP P14779
C	272	TRP	LEU	engineered mutation	UNP P14779
C	322	ILE	LEU	engineered mutation	UNP P14779
C	405	MET	PHE	engineered mutation	UNP P14779
C	406	SER	ALA	engineered mutation	UNP P14779
C	464	LEU	-	expression tag	UNP P14779
C	465	GLU	-	expression tag	UNP P14779
C	466	HIS	-	expression tag	UNP P14779
C	467	HIS	-	expression tag	UNP P14779
C	468	HIS	-	expression tag	UNP P14779
C	469	HIS	-	expression tag	UNP P14779
C	470	HIS	-	expression tag	UNP P14779
C	471	HIS	-	expression tag	UNP P14779
D	265	PHE	GLY	engineered mutation	UNP P14779
D	269	VAL	THR	engineered mutation	UNP P14779
D	272	TRP	LEU	engineered mutation	UNP P14779
D	322	ILE	LEU	engineered mutation	UNP P14779
D	405	MET	PHE	engineered mutation	UNP P14779
D	406	SER	ALA	engineered mutation	UNP P14779
D	464	LEU	-	expression tag	UNP P14779
D	465	GLU	-	expression tag	UNP P14779
D	466	HIS	-	expression tag	UNP P14779
D	467	HIS	-	expression tag	UNP P14779
D	468	HIS	-	expression tag	UNP P14779
D	469	HIS	-	expression tag	UNP P14779
D	470	HIS	-	expression tag	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
D	471	HIS	-	expression tag	UNP P14779
E	265	PHE	GLY	engineered mutation	UNP P14779
E	269	VAL	THR	engineered mutation	UNP P14779
E	272	TRP	LEU	engineered mutation	UNP P14779
E	322	ILE	LEU	engineered mutation	UNP P14779
E	405	MET	PHE	engineered mutation	UNP P14779
E	406	SER	ALA	engineered mutation	UNP P14779
E	464	LEU	-	expression tag	UNP P14779
E	465	GLU	-	expression tag	UNP P14779
E	466	HIS	-	expression tag	UNP P14779
E	467	HIS	-	expression tag	UNP P14779
E	468	HIS	-	expression tag	UNP P14779
E	469	HIS	-	expression tag	UNP P14779
E	470	HIS	-	expression tag	UNP P14779
E	471	HIS	-	expression tag	UNP P14779
F	265	PHE	GLY	engineered mutation	UNP P14779
F	269	VAL	THR	engineered mutation	UNP P14779
F	272	TRP	LEU	engineered mutation	UNP P14779
F	322	ILE	LEU	engineered mutation	UNP P14779
F	405	MET	PHE	engineered mutation	UNP P14779
F	406	SER	ALA	engineered mutation	UNP P14779
F	464	LEU	-	expression tag	UNP P14779
F	465	GLU	-	expression tag	UNP P14779
F	466	HIS	-	expression tag	UNP P14779
F	467	HIS	-	expression tag	UNP P14779
F	468	HIS	-	expression tag	UNP P14779
F	469	HIS	-	expression tag	UNP P14779
F	470	HIS	-	expression tag	UNP P14779
F	471	HIS	-	expression tag	UNP P14779
G	265	PHE	GLY	engineered mutation	UNP P14779
G	269	VAL	THR	engineered mutation	UNP P14779
G	272	TRP	LEU	engineered mutation	UNP P14779
G	322	ILE	LEU	engineered mutation	UNP P14779
G	405	MET	PHE	engineered mutation	UNP P14779
G	406	SER	ALA	engineered mutation	UNP P14779
G	464	LEU	-	expression tag	UNP P14779
G	465	GLU	-	expression tag	UNP P14779
G	466	HIS	-	expression tag	UNP P14779
G	467	HIS	-	expression tag	UNP P14779
G	468	HIS	-	expression tag	UNP P14779
G	469	HIS	-	expression tag	UNP P14779
G	470	HIS	-	expression tag	UNP P14779

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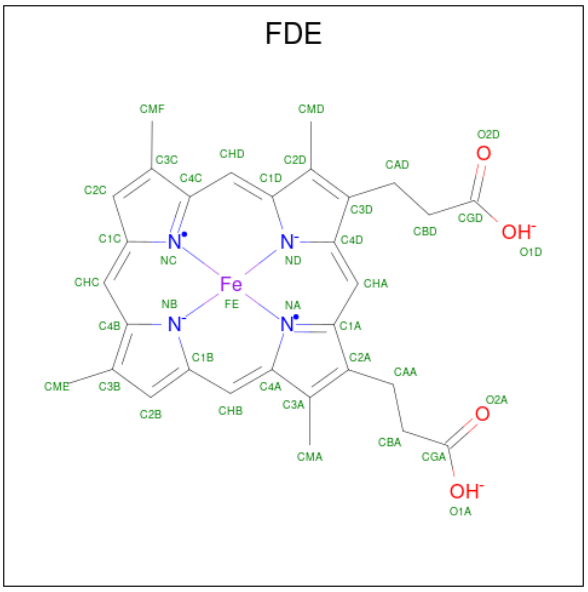
Chain	Residue	Modelled	Actual	Comment	Reference
G	471	HIS	-	expression tag	UNP P14779
H	265	PHE	GLY	engineered mutation	UNP P14779
H	269	VAL	THR	engineered mutation	UNP P14779
H	272	TRP	LEU	engineered mutation	UNP P14779
H	322	ILE	LEU	engineered mutation	UNP P14779
H	405	MET	PHE	engineered mutation	UNP P14779
H	406	SER	ALA	engineered mutation	UNP P14779
H	464	LEU	-	expression tag	UNP P14779
H	465	GLU	-	expression tag	UNP P14779
H	466	HIS	-	expression tag	UNP P14779
H	467	HIS	-	expression tag	UNP P14779
H	468	HIS	-	expression tag	UNP P14779
H	469	HIS	-	expression tag	UNP P14779
H	470	HIS	-	expression tag	UNP P14779
H	471	HIS	-	expression tag	UNP P14779

- Molecule 2 is FE(III) DEUTEROPORPHYRIN IX (CCD ID: FDE) (formula: $C_{30}H_{28}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	39	30	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	39	30	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	39	30	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	39	30	1	4	4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	E	1	39	30	1	4	4	0	0
2	F	1	39	30	1	4	4	0	0
2	G	1	39	30	1	4	4	0	0
2	H	1	39	30	1	4	4	0	0

- Molecule 3 is water.

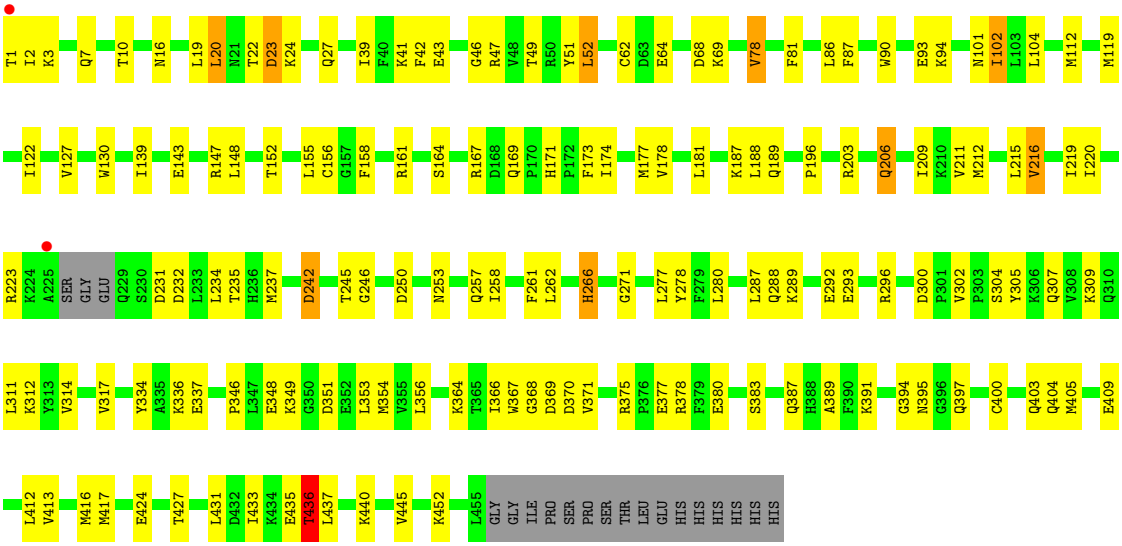
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	149	149	149	0	0
3	B	189	189	189	0	0
3	C	165	165	165	0	0
3	D	112	112	112	0	0
3	E	155	155	155	0	0
3	F	117	117	117	0	0
3	G	138	138	138	0	0
3	H	171	171	171	0	0

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.

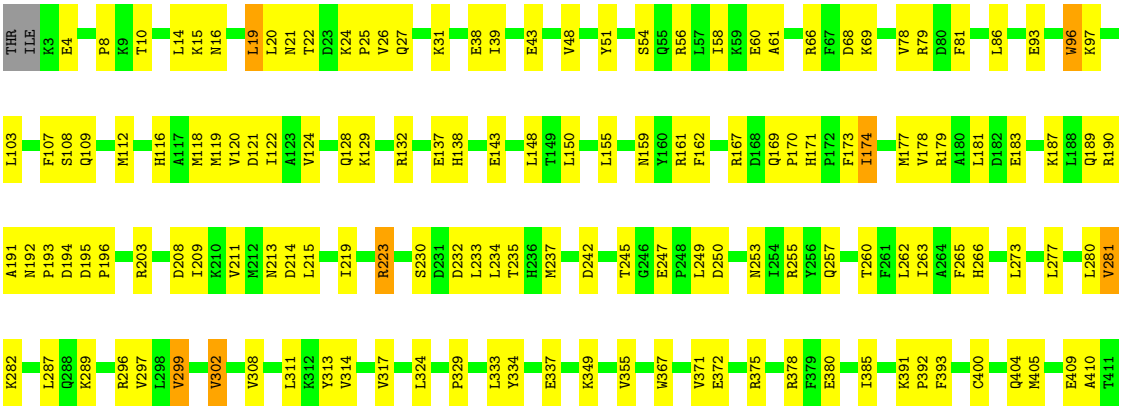
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

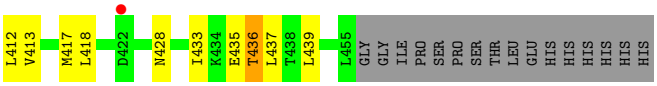
Chain A:



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

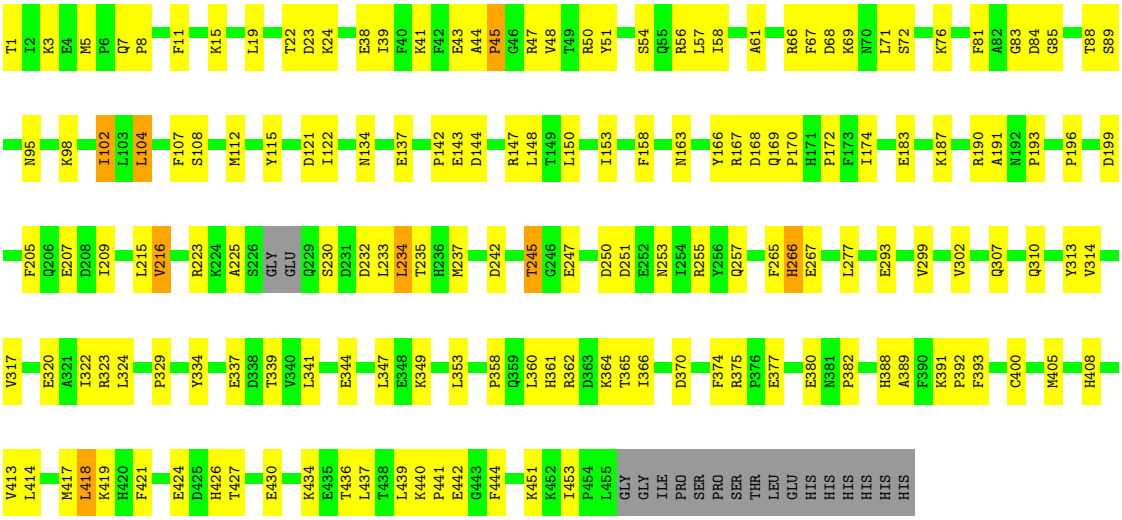
Chain B:





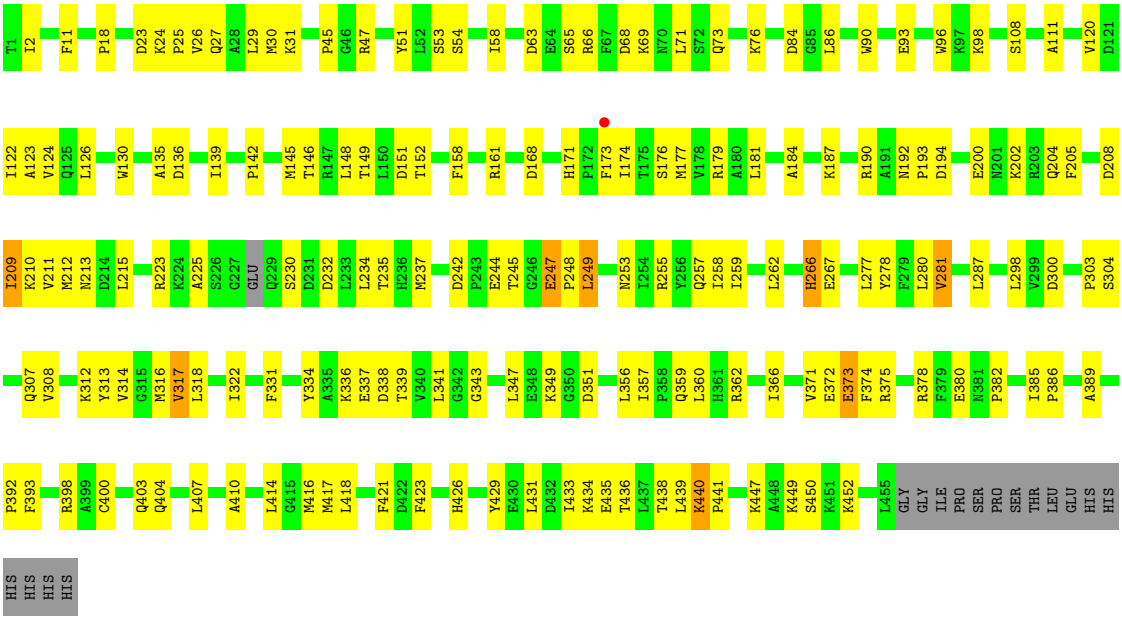
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain C:



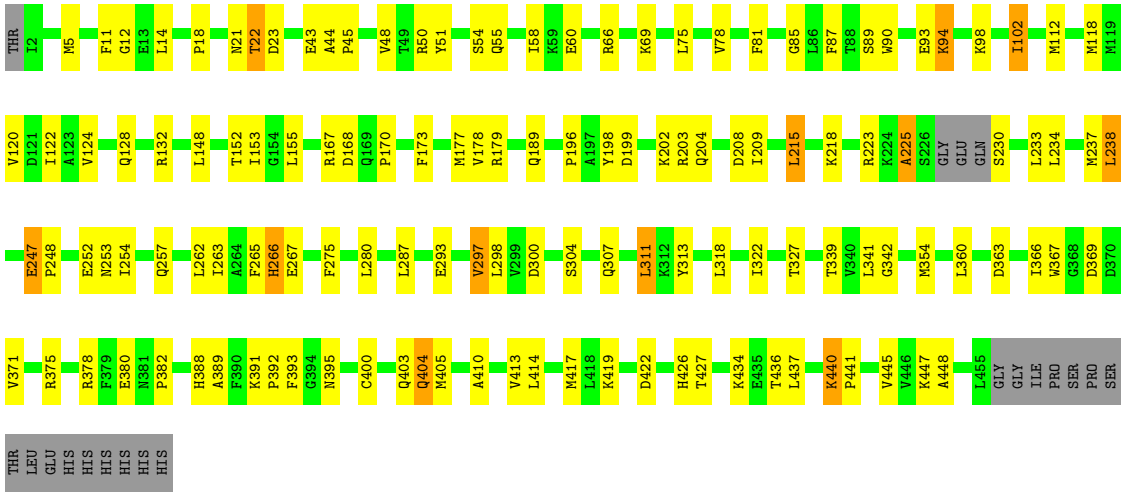
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain D:



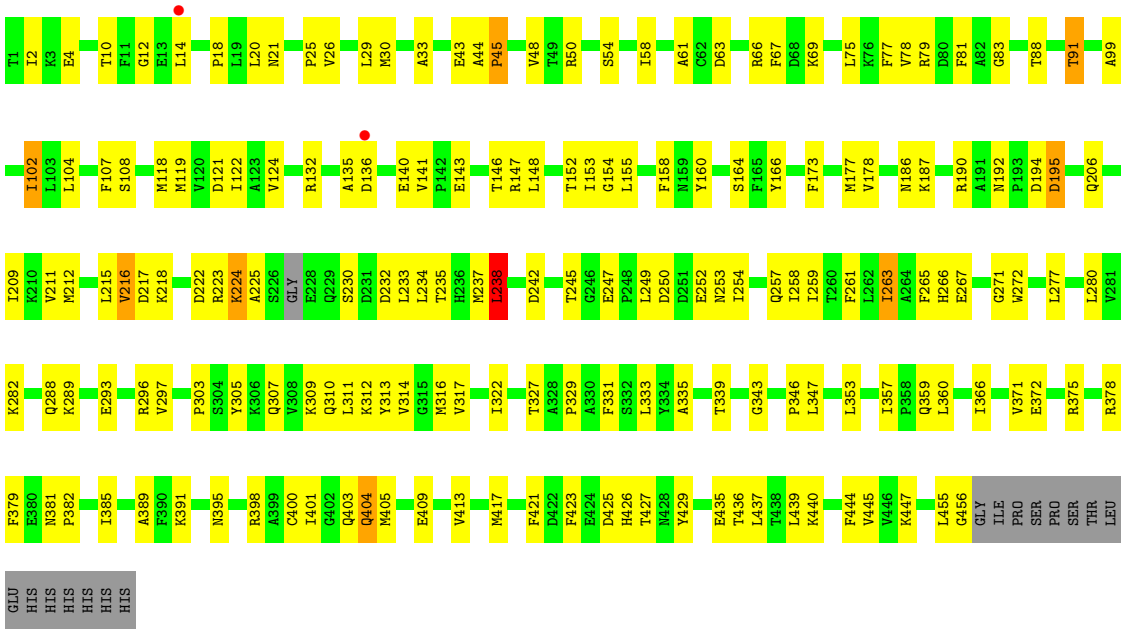
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain E:



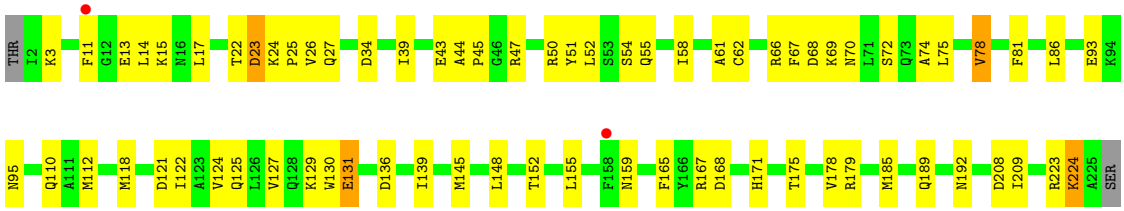
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain F:



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain G:



GLY GLU Q229 D232 L233 L234 T235 H236 M237 L238 N239 D242 T245 D250 I254 A264 F265 H266 E267 T268 W272 L273 S274 F275 Y278 F279 L280 L287 Q288 K289 E293 S304 Y305 K306 Q307 V308 K309 Q310 L311 K312 Y313 Y314 V317 L318 N319 E320 A321 I322

R323 P326 T327 A328 S332 L333 D338 E344 Y345 K349 L353 M354 V355 P358 Q359 L360 T365 I366 W367 G368 D369 D370 V371 F374 R375 P376 E377 R378 F379 E380 N381 P382 S383 A384 H388 A389 F390 K391 P392 F393 G394 N395 R398 A399 C400 Q404 M405 S406

L407 T411 L412 V413 L414 M417 L418 K419 H420 F421 D422 F423 H426 Y429 E430 L431 D432 I433 K434 E435 T436 L437 T438 L439 K440 P441 F444 V445 V446 K447 K451 L455 GLY GLY ILE PRO SER PRO SER THR LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain H:

THR I2 K3 E4 F11 K15 N16 L17 P18 L19 L20 N21 T22 D23 K24 P25 V26 Q27 A28 L29 M30 K31 E38 I39 E43 A44 R47 R50 Y51 L52 S53 S54 G55 R56 L57 I58 K59 E60 A61 C62 D63 E64 S65 R66 F67 D68 K69 N70 L71 K76 D80 F81

L86 K97 K98 I102 S106 M119 V120 V124 Q125 L126 V127 Q128 K129 W130 E131 N134 A135 D136 E137 H138 P142 E143 D144 R147 L148 T152 I153 F162 N163 S164 R167 D168 Q169 P170 H171 I174 M177 V178 L181 D182 E183 Q189 R190 A191

N192 P196 D199 D208 I209 M212 N213 V216 R223 K224 ALA SER GLY GLU Q229 S230 L233 L234 T235 H236 D242 P243 E244 T245 G246 E247 P248 L249 I254 R255 Y256 Q257 I258 I259 L262 I263 A264 F265 H266 G271 W272 V286 E293 K309 K312

Y313 V314 G315 M316 V317 L318 N319 E320 A321 I322 W325 F331 G342 G343 E344 L353 M354 V355 L360 K364 T365 I366 V371 E372 E373 F374 R375 R378 F379 E380 N381 P382 I385 P386 Q387 H388 A389 F390 K391 Q397 C400 E409 V413 L414 M417 L418

K419 H420 F421 D422 F423 H426 K434 E435 T436 L437 K440 P441 K447 P454 L455 GLY GLY ILE PRO SER PRO SER THR LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.06Å 166.30Å 229.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.85 – 2.16 28.85 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.85-2.16) 98.8 (28.85-2.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.16Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.258 , 0.334 0.260 , 0.332	Depositor DCC
R_{free} test set	2000 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 24.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	29916	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FDE

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	0.48	0/3640	0.70	2/4939 (0.0%)
1	B	0.52	0/3665	0.72	2/4972 (0.0%)
1	C	0.49	0/3637	0.73	4/4936 (0.1%)
1	D	0.46	0/3571	0.69	0/4855
1	E	0.49	0/3668	0.70	0/4974
1	F	0.49	0/3629	0.70	0/4930
1	G	0.48	0/3638	0.70	2/4939 (0.0%)
1	H	0.49	0/3657	0.70	0/4955
All	All	0.49	0/29105	0.70	10/39500 (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
1	D	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	ASP	CA-C-N	9.40	138.80	120.94
1	C	168	ASP	C-N-CA	9.40	138.80	120.94
1	A	436	THR	CA-C-N	-6.46	107.87	121.64
1	A	436	THR	C-N-CA	-6.46	107.87	121.64
1	C	436	THR	CA-C-N	-6.17	110.16	121.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	ILE	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	3554	0	3443	125	0
1	B	3578	0	3463	125	0
1	C	3552	0	3444	114	0
1	D	3485	0	3286	132	0
1	E	3579	0	3482	95	0
1	F	3543	0	3387	140	0
1	G	3546	0	3392	145	0
1	H	3571	0	3480	121	0
2	A	39	0	25	1	0
2	B	39	0	25	2	0
2	C	39	0	25	1	0
2	D	39	0	25	2	0
2	E	39	0	25	2	0
2	F	39	0	25	1	0
2	G	39	0	25	3	0
2	H	39	0	25	2	0
3	A	149	0	0	27	0
3	B	189	0	0	21	0
3	C	165	0	0	18	1
3	D	112	0	0	10	0
3	E	155	0	0	10	2
3	F	117	0	0	12	0
3	G	138	0	0	21	0
3	H	171	0	0	23	1
All	All	29916	0	27577	984	2

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 17.

The worst 5 of 984 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)
1:G:272:TRP:CD1	1:G:322:ILE:CD1	2.39	1.05
1:G:272:TRP:NE1	1:G:322:ILE:HD13	1.75	1.02
1:A:68:ASP:HB2	1:A:336:LYS:NZ	1.75	1.01
1:G:272:TRP:CD1	1:G:322:ILE:HD13	1.99	0.96
1:H:106:SER:HG	1:H:236:HIS:HD1	1.10	0.96

All (2) 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)
3:E:715:HOH:O	3:H:734:HOH:O[2_455]	2.02	0.18
3:C:741:HOH:O	3:E:719:HOH:O[2_354]	2.13	0.07

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	448/471 (95%)	429 (96%)	18 (4%)	1 (0%)	43	44
1	B	451/471 (96%)	437 (97%)	13 (3%)	1 (0%)	43	44
1	C	449/471 (95%)	426 (95%)	21 (5%)	2 (0%)	30	26
1	D	450/471 (96%)	427 (95%)	18 (4%)	5 (1%)	11	7
1	E	448/471 (95%)	426 (95%)	19 (4%)	3 (1%)	18	13
1	F	451/471 (96%)	427 (95%)	19 (4%)	5 (1%)	11	7
1	G	449/471 (95%)	431 (96%)	17 (4%)	1 (0%)	43	44
1	H	446/471 (95%)	428 (96%)	18 (4%)	0	100	100
All	All	3592/3768 (95%)	3431 (96%)	143 (4%)	18 (0%)	24	20

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	247	GLU
1	E	225	ALA
1	E	311	LEU
1	F	224	LYS
1	D	245	THR

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	367/415 (88%)	345 (94%)	22 (6%)	17	13
1	B	374/415 (90%)	363 (97%)	11 (3%)	37	39
1	C	368/415 (89%)	351 (95%)	17 (5%)	24	22
1	D	343/415 (83%)	332 (97%)	11 (3%)	34	36
1	E	375/415 (90%)	353 (94%)	22 (6%)	18	13
1	F	360/415 (87%)	343 (95%)	17 (5%)	23	21
1	G	364/415 (88%)	345 (95%)	19 (5%)	21	17
1	H	375/415 (90%)	357 (95%)	18 (5%)	23	20
All	All	2926/3320 (88%)	2789 (95%)	137 (5%)	23	21

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	383	SER
1	H	4	GLU
1	H	216	VAL
1	C	437	LEU
1	C	434	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	55	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	171	HIS
1	G	163	ASN
1	G	397	GLN
1	D	266	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FDE	H	501	1	46,46,46	2.87	25 (54%)	60,76,76	4.17	34 (56%)
2	FDE	F	501	1	46,46,46	2.80	24 (52%)	60,76,76	4.23	35 (58%)
2	FDE	A	501	1,3	46,46,46	2.80	26 (56%)	60,76,76	4.08	33 (55%)
2	FDE	G	501	1	46,46,46	2.71	27 (58%)	60,76,76	4.21	32 (53%)
2	FDE	D	501	1	46,46,46	2.88	24 (52%)	60,76,76	4.14	34 (56%)
2	FDE	B	501	1	46,46,46	2.91	25 (54%)	60,76,76	4.21	31 (51%)
2	FDE	C	501	1	46,46,46	2.81	24 (52%)	60,76,76	4.52	36 (60%)
2	FDE	E	501	1,3	46,46,46	2.84	25 (54%)	60,76,76	4.19	34 (56%)

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
2	FDE	H	501	1	1/1/3/7	3/10/50/50	-
2	FDE	F	501	1	1/1/3/7	2/10/50/50	-
2	FDE	A	501	1,3	1/1/3/7	2/10/50/50	-
2	FDE	G	501	1	1/1/3/7	3/10/50/50	-
2	FDE	D	501	1	1/1/3/7	2/10/50/50	-
2	FDE	B	501	1	1/1/3/7	4/10/50/50	-
2	FDE	C	501	1	1/1/3/7	3/10/50/50	-
2	FDE	E	501	1,3	1/1/3/7	3/10/50/50	-

The worst 5 of 200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FDE	C1B-NB	-6.74	1.30	1.39
2	E	501	FDE	C1B-NB	-6.34	1.31	1.39
2	H	501	FDE	C1B-NB	-6.06	1.31	1.39
2	G	501	FDE	C2A-C3A	5.90	1.49	1.36
2	D	501	FDE	C3D-C2D	5.82	1.49	1.36

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FDE	C1D-CHD-C4C	12.90	153.44	126.02
2	H	501	FDE	CHD-C1D-ND	-12.20	111.17	124.45
2	C	501	FDE	CHD-C4C-NC	-12.14	111.36	124.42
2	B	501	FDE	CHD-C1D-ND	-11.81	111.59	124.45
2	C	501	FDE	CHD-C1D-ND	-11.57	111.85	124.45

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	FDE	ND
2	B	501	FDE	ND
2	C	501	FDE	ND
2	D	501	FDE	ND
2	E	501	FDE	ND

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	FDE	CAD-CBD-CGD-O1D
2	A	501	FDE	CAD-CBD-CGD-O1D
2	B	501	FDE	CAD-CBD-CGD-O2D
2	B	501	FDE	CAD-CBD-CGD-O1D
2	D	501	FDE	CAA-CBA-CGA-O2A

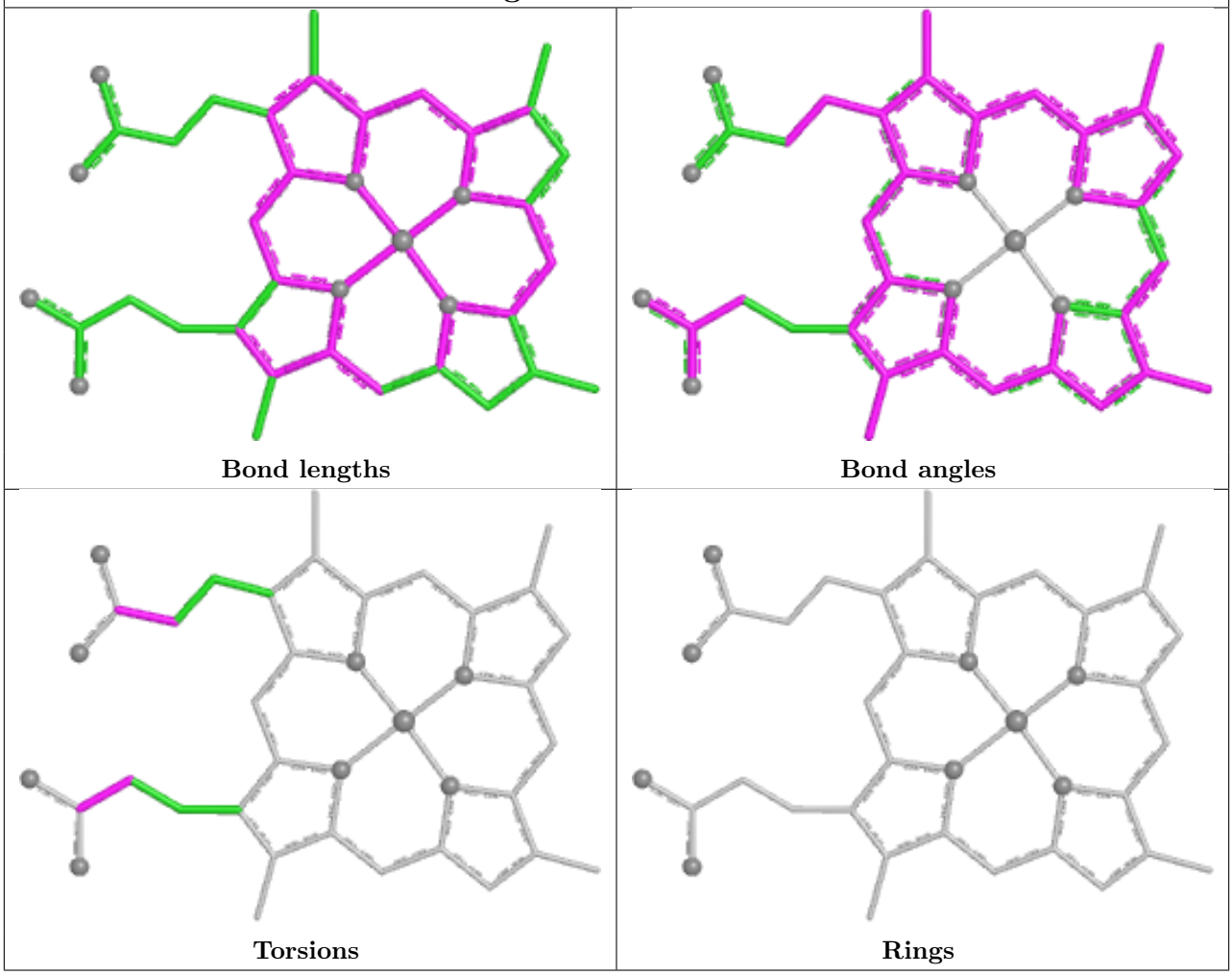
There are no ring outliers.

8 monomers are involved in 14 short contacts:

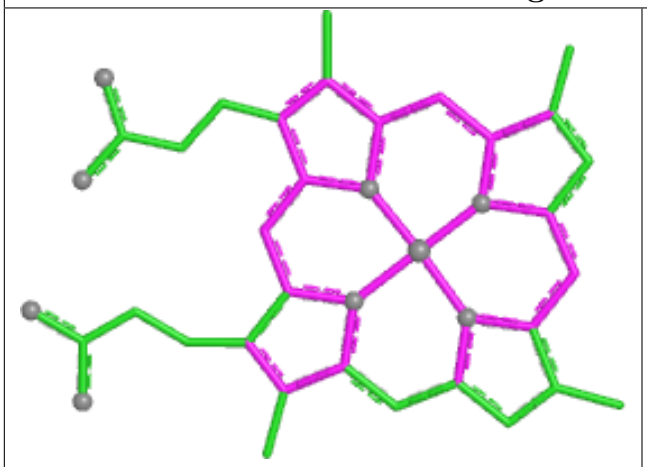
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	FDE	2	0
2	F	501	FDE	1	0
2	A	501	FDE	1	0
2	G	501	FDE	3	0
2	D	501	FDE	2	0
2	B	501	FDE	2	0
2	C	501	FDE	1	0
2	E	501	FDE	2	0

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

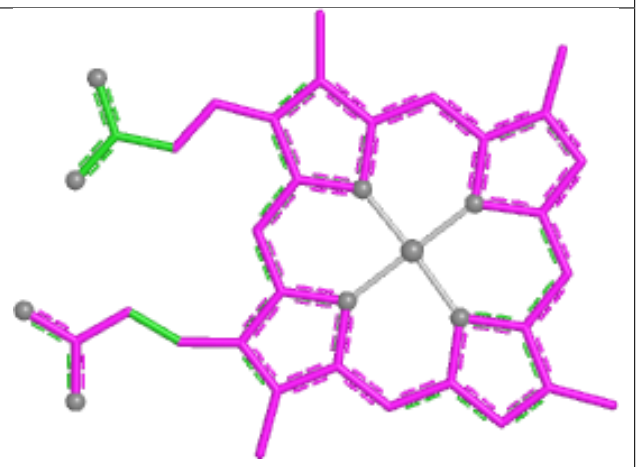
Ligand FDE H 501



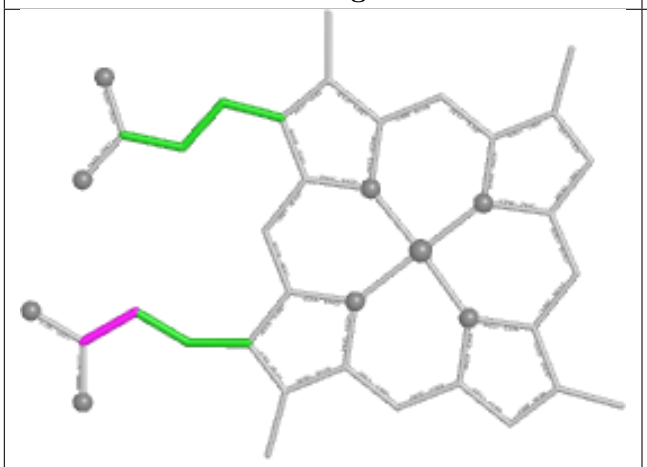
Ligand FDE F 501



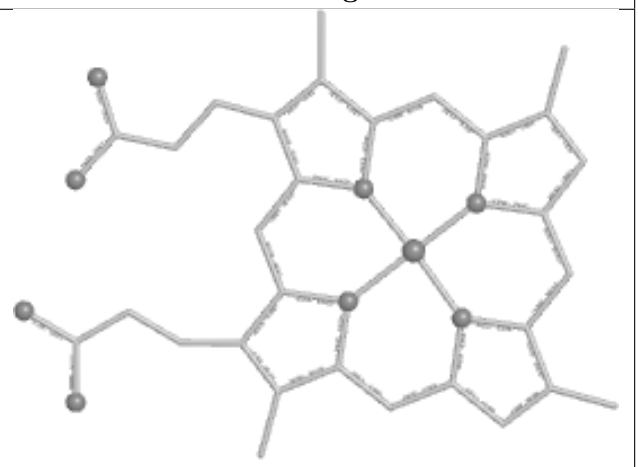
Bond lengths



Bond angles

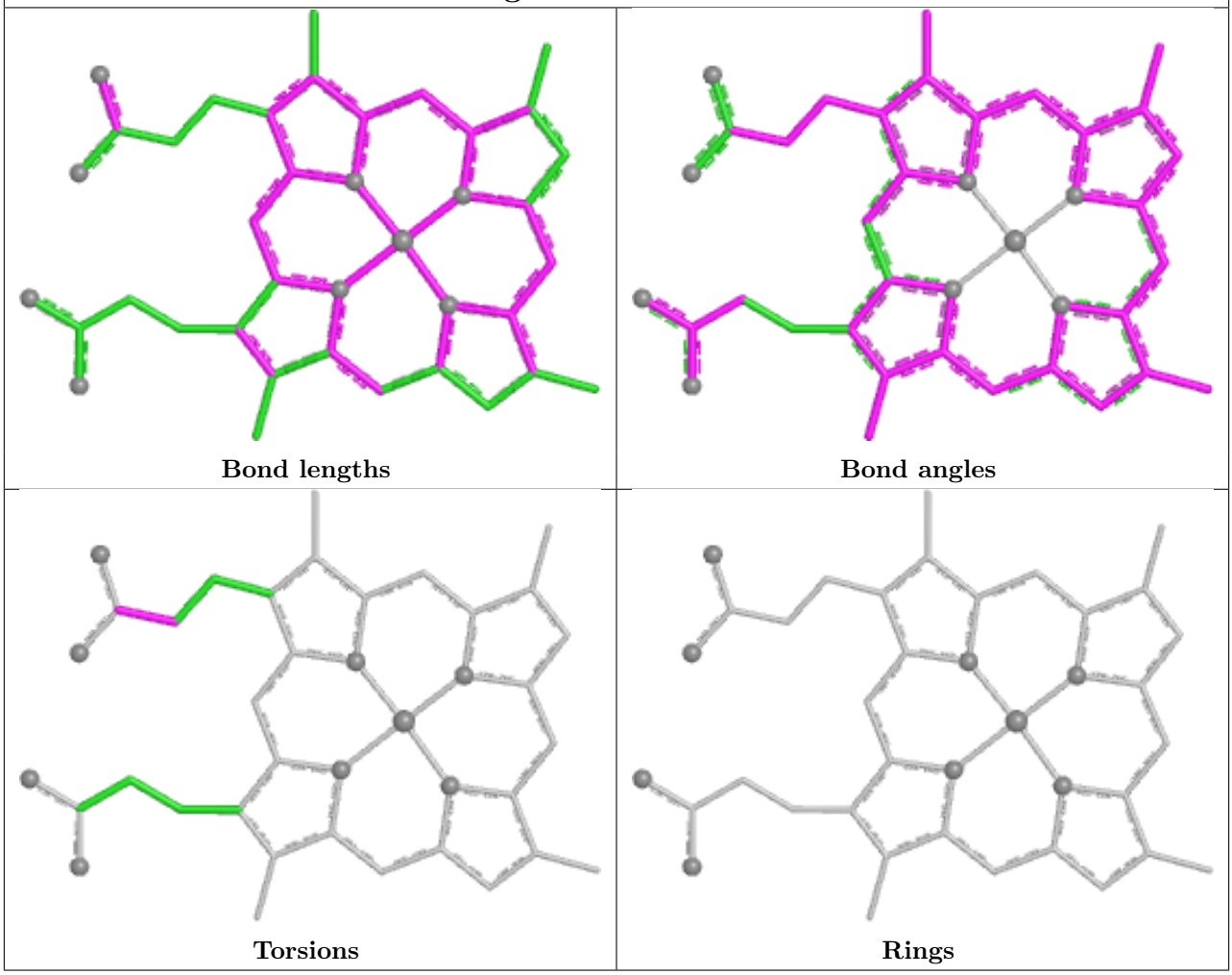


Torsions

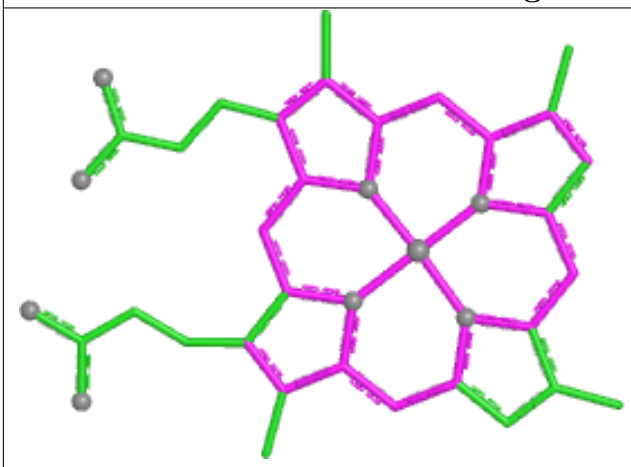


Rings

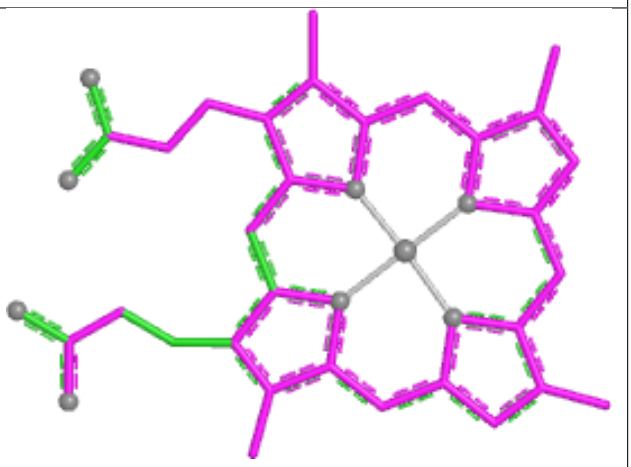
Ligand FDE A 501



Ligand FDE G 501



Bond lengths



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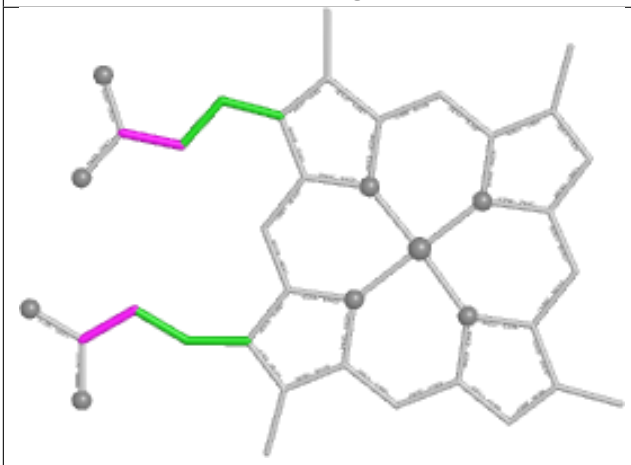
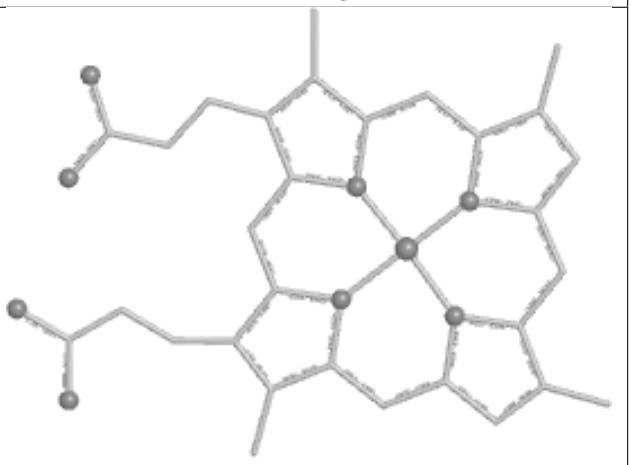
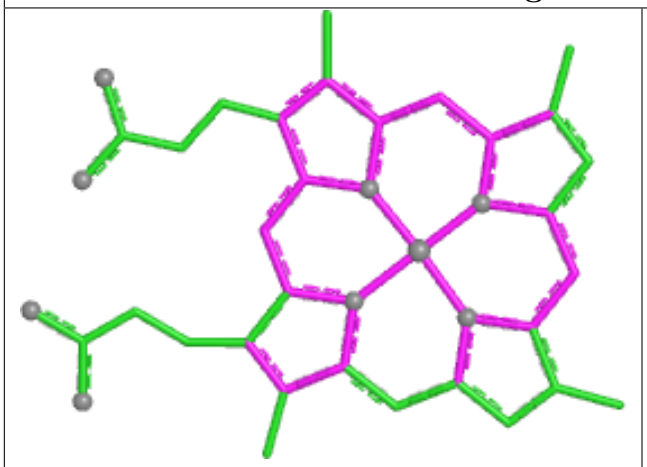


Torsions

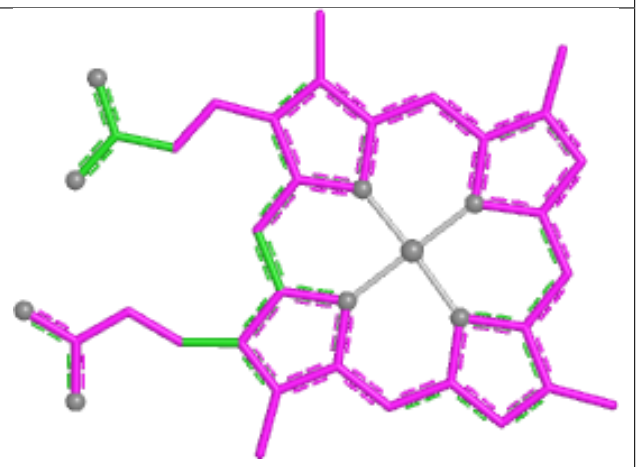


Rings

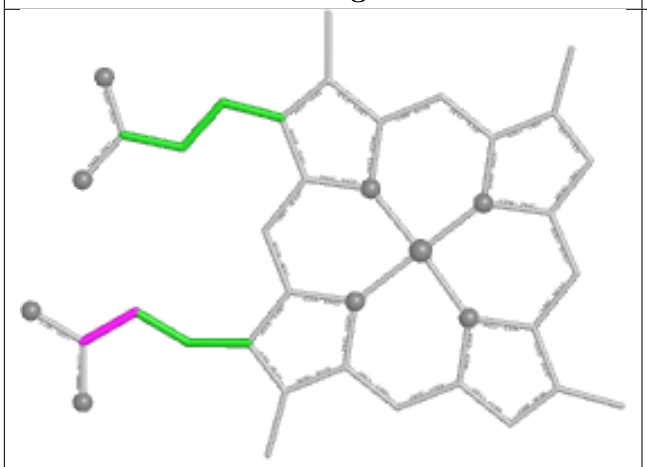
Ligand FDE D 501



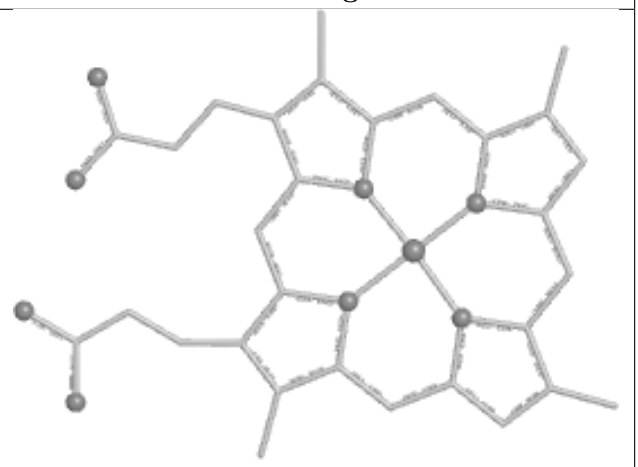
Bond lengths



Bond angles

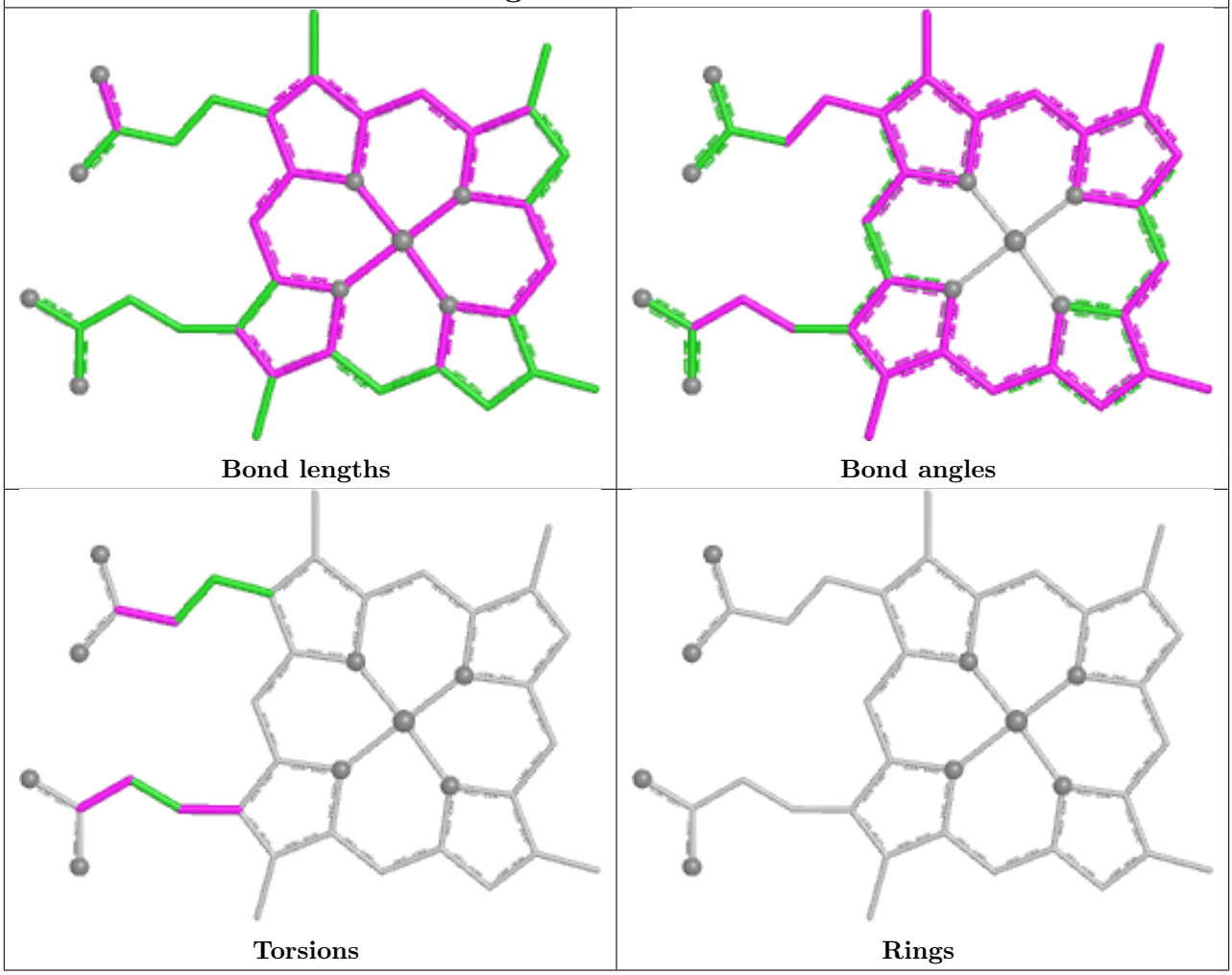


Torsions



Rings

Ligand FDE B 501



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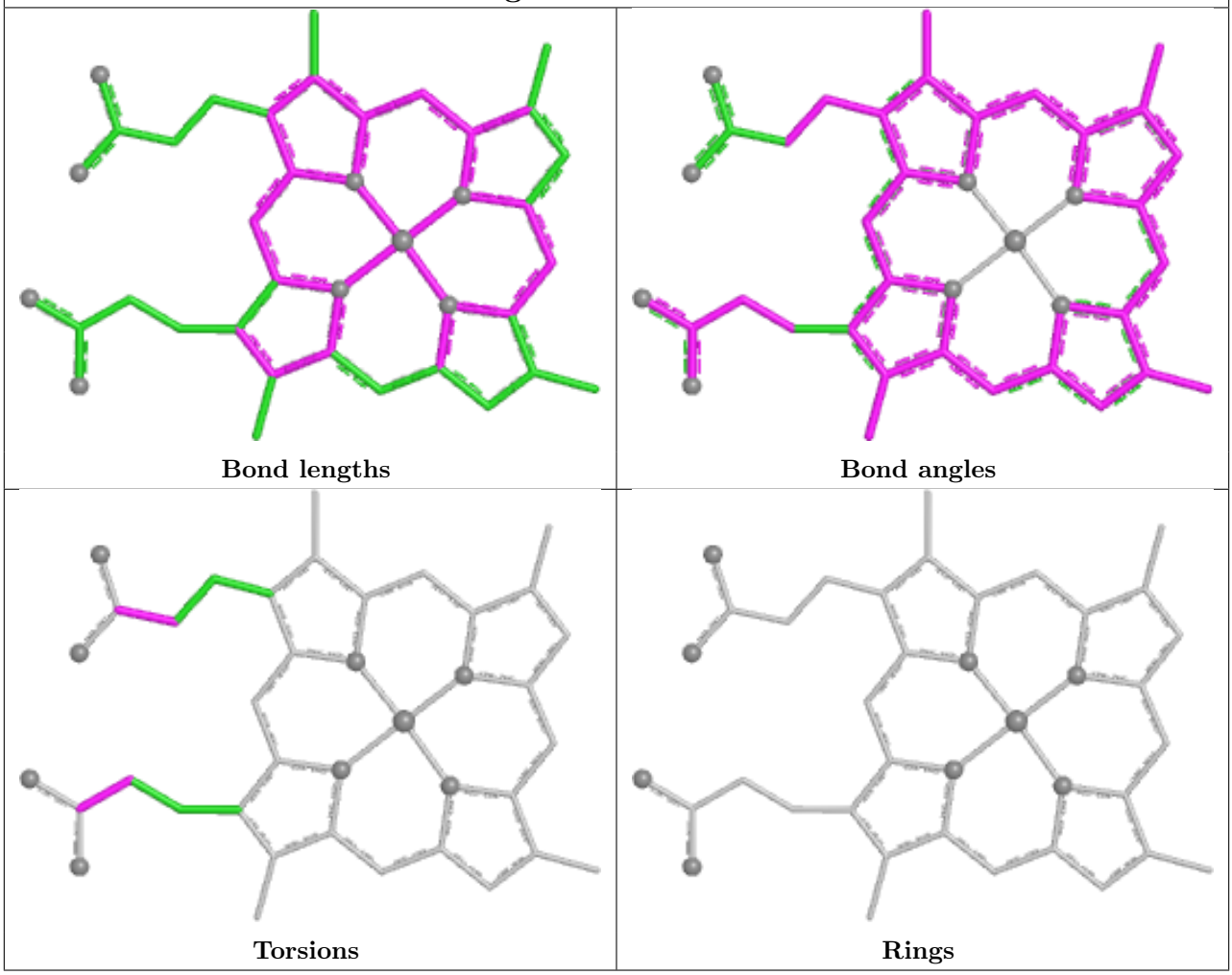
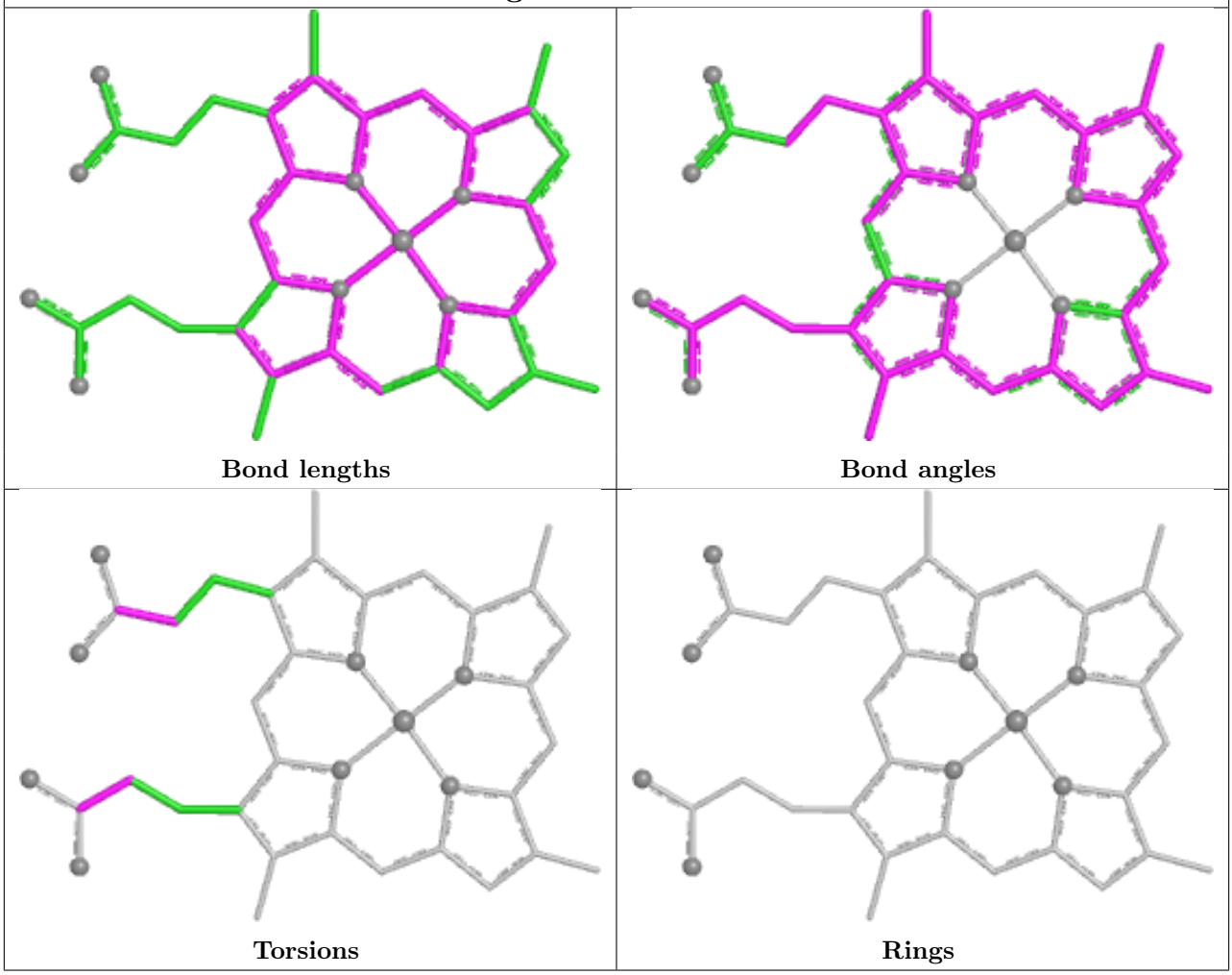


Ligand FDE E 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	452/471 (95%)	-0.20	2 (0%)	88	90	4, 15, 28, 35	0
1	B	453/471 (96%)	-0.33	1 (0%)	91	92	2, 10, 25, 36	0
1	C	453/471 (96%)	-0.29	0	100	100	2, 11, 25, 37	0
1	D	454/471 (96%)	0.02	1 (0%)	91	92	10, 21, 33, 42	0
1	E	451/471 (95%)	-0.24	0	100	100	4, 12, 26, 37	1 (0%)
1	F	455/471 (96%)	-0.06	2 (0%)	88	90	7, 19, 32, 38	0
1	G	451/471 (95%)	-0.12	3 (0%)	84	85	4, 16, 30, 42	2 (0%)
1	H	450/471 (95%)	-0.20	1 (0%)	91	92	3, 13, 26, 36	0
All	All	3619/3768 (96%)	-0.18	10 (0%)	90	91	2, 15, 29, 42	3 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	4.1
1	G	379	PHE	3.3
1	F	136	ASP	2.7
1	D	173	PHE	2.6
1	H	385	ILE	2.5

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

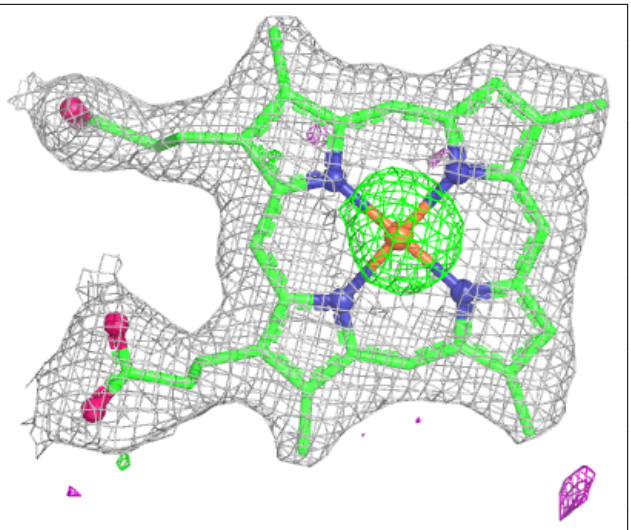
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

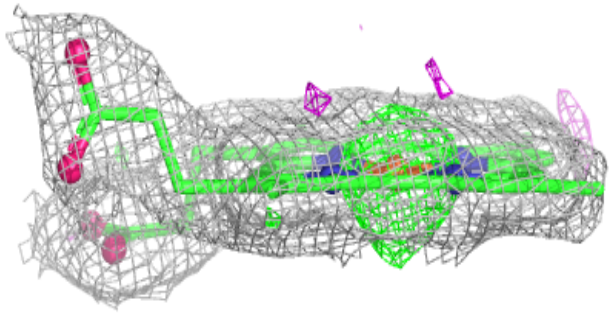
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FDE	A	501	39/39	0.89	0.09	5,10,16,127	0
2	FDE	C	501	39/39	0.97	0.07	2,2,7,10	0
2	FDE	F	501	39/39	0.97	0.07	4,8,18,25	0
2	FDE	G	501	39/39	0.97	0.07	3,6,11,16	0
2	FDE	H	501	39/39	0.97	0.07	2,2,7,7	0
2	FDE	B	501	39/39	0.98	0.06	2,3,11,16	0
2	FDE	D	501	39/39	0.98	0.06	5,10,15,17	0
2	FDE	E	501	39/39	0.98	0.07	2,4,18,24	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 FDE A 501:

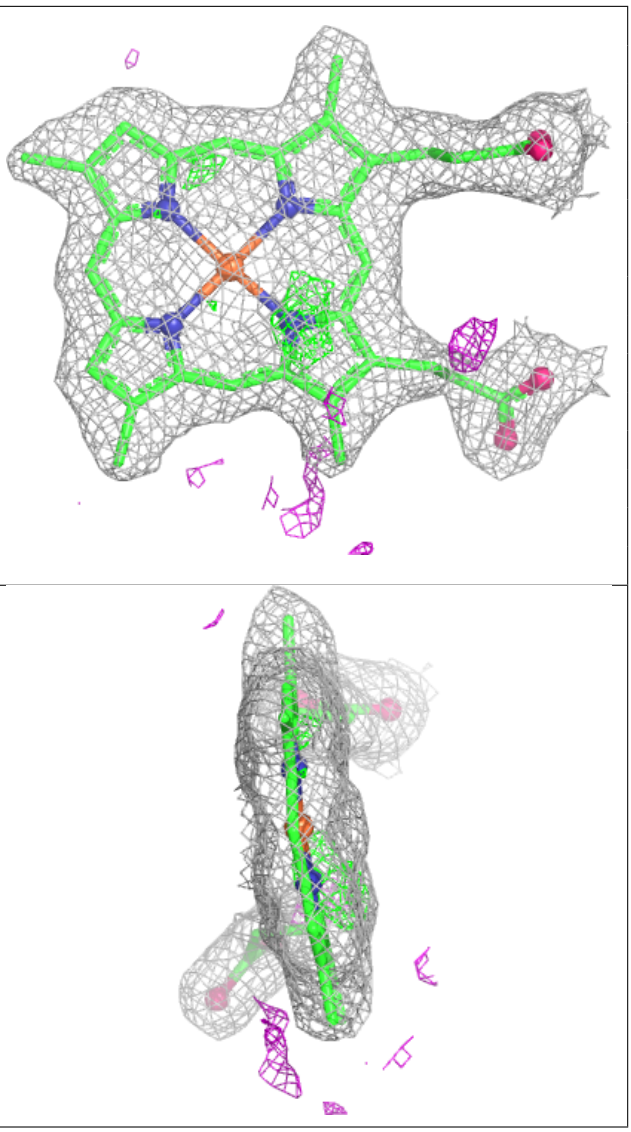
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





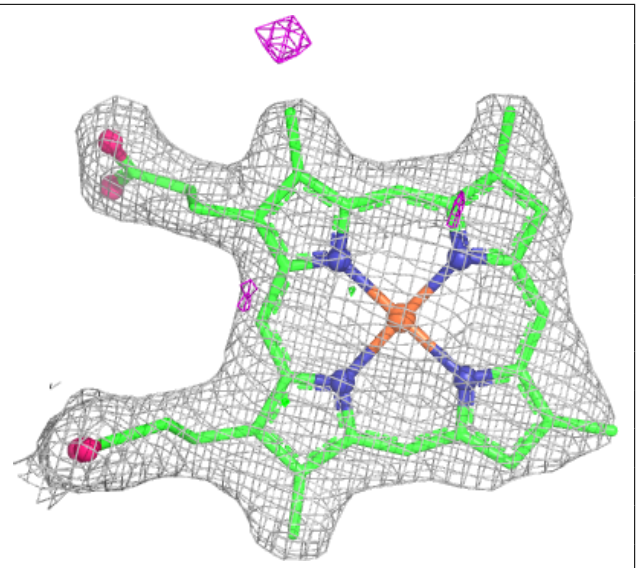
Electron density around FDE C 501:

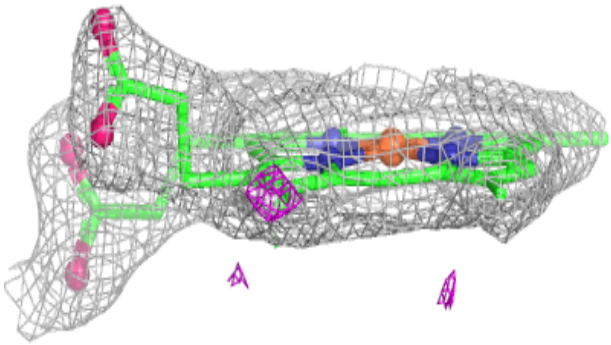
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

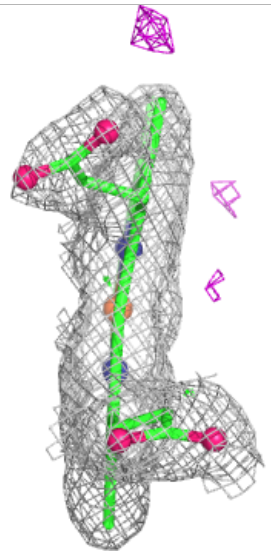


Electron density around FDE F 501:

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

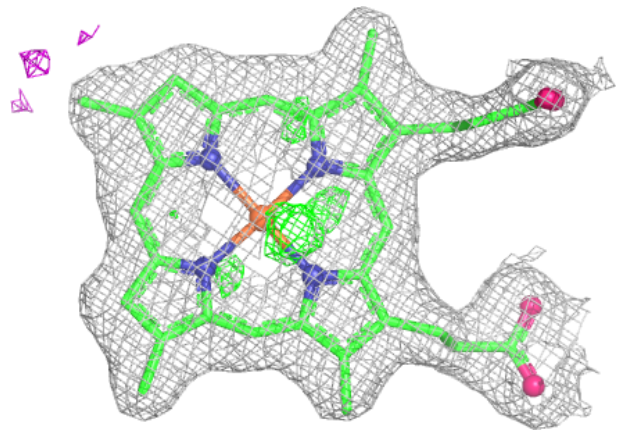


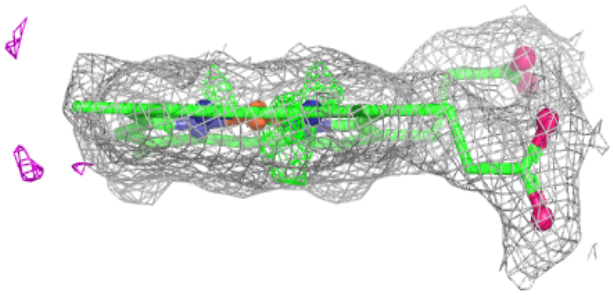


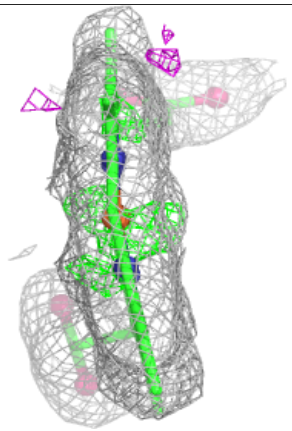


Electron density around FDE G 501:

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

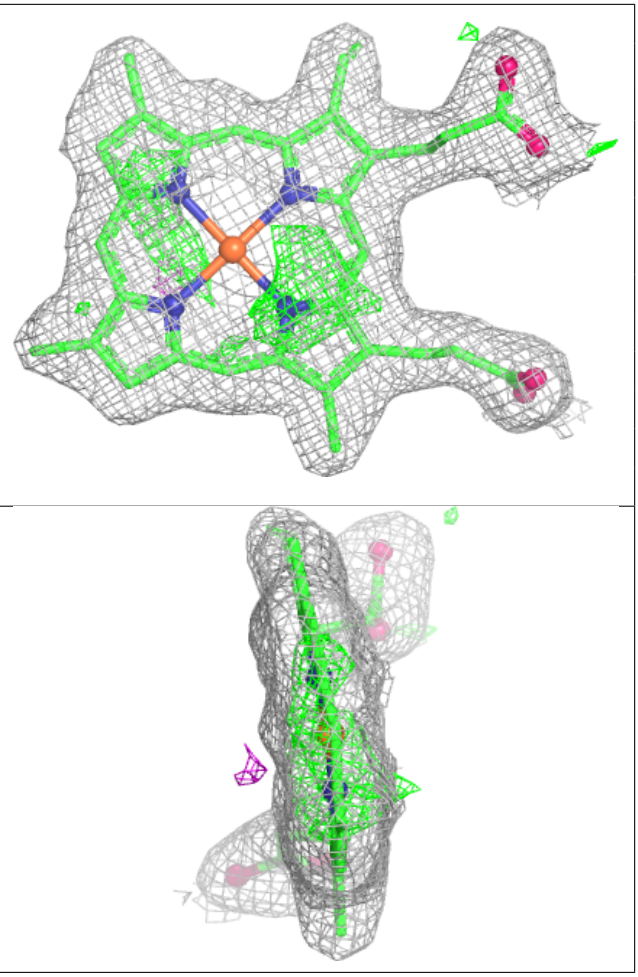






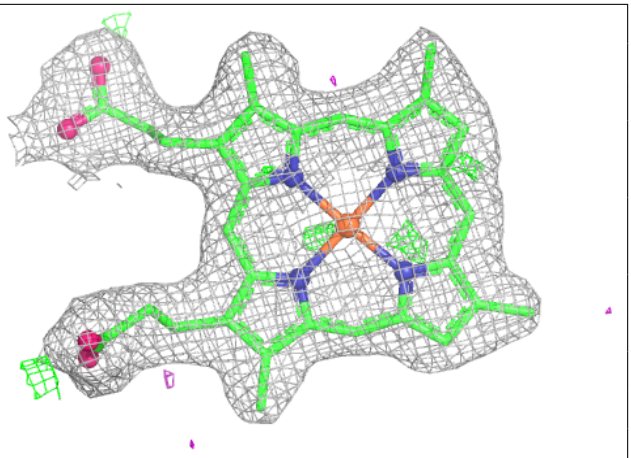
Electron density around FDE H 501:

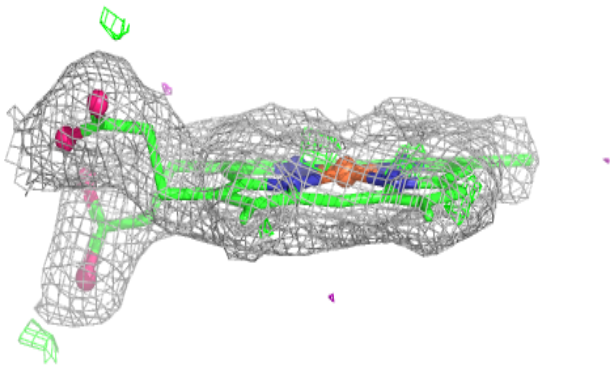
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

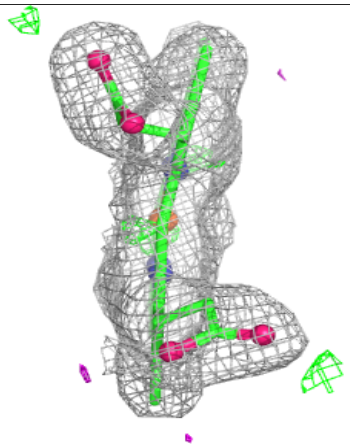


Electron density around FDE B 501:

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

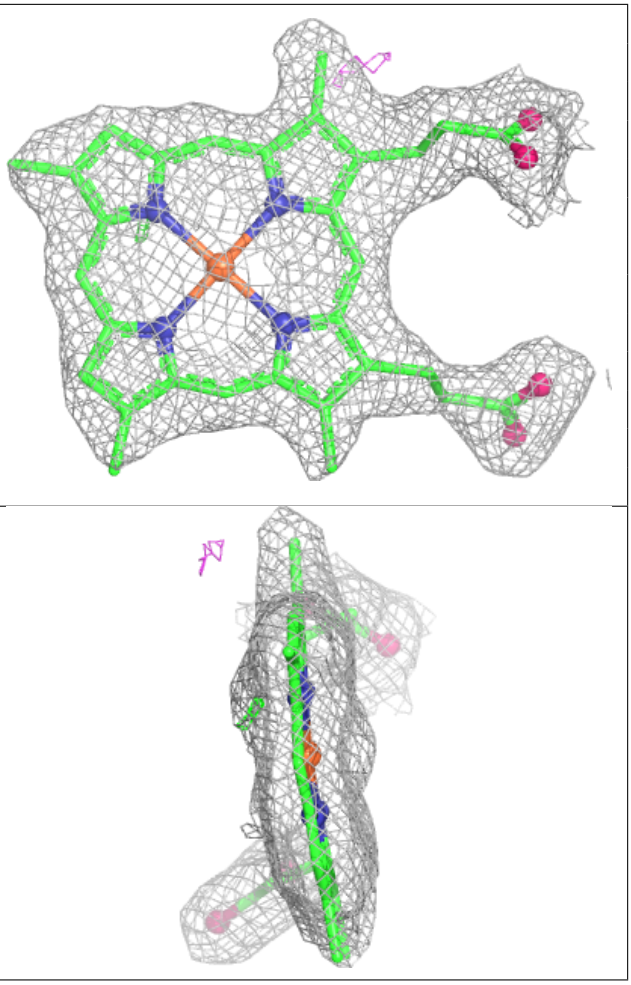


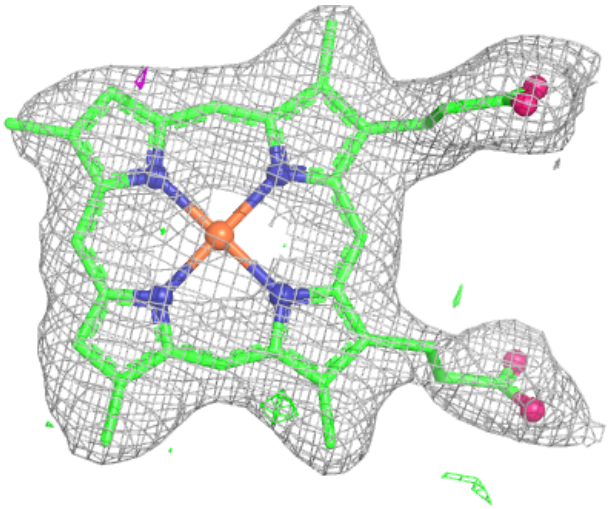
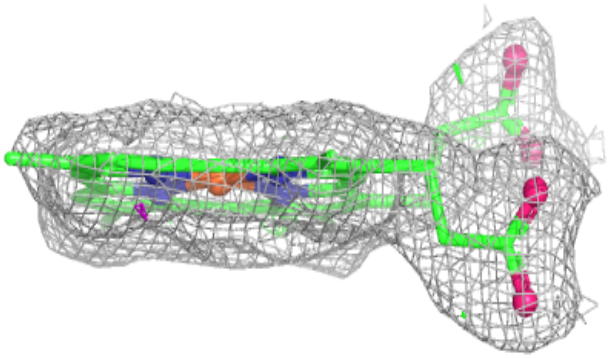
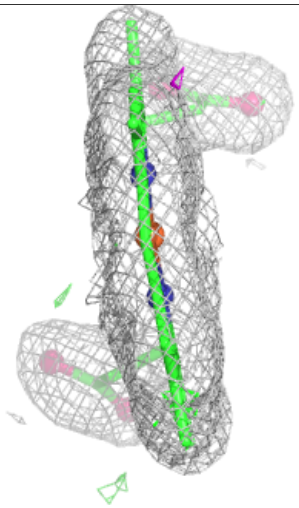




Electron density around FDE D 501:

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



Electron density around FDE E 501: 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.