WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 06:47 PM EDT

|		
PDB ID	:	3T3S
Title	:	Human Cytochrome P450 2A13 in complex with Pilocarpine
Authors	:	DeVore, N.M.; Scott, E.E.
Deposited on	:	2011-07-25
Resolution	:	3.00 Å(reported)

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 3.00 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.

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
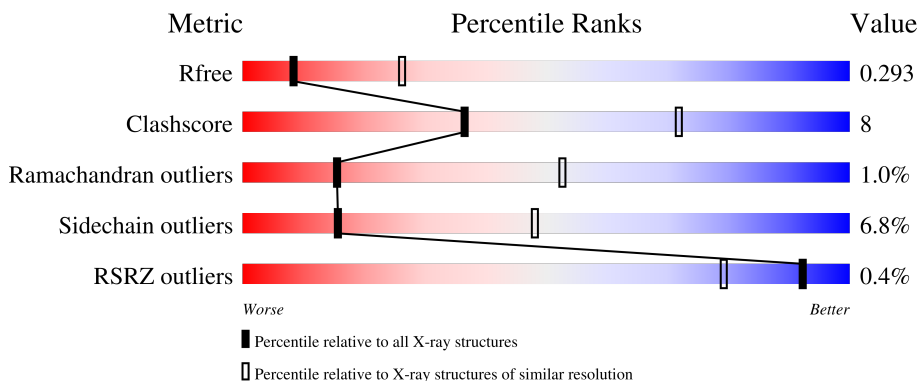
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	476	76%　　19%　・・
1	B	476	72%　　23%　・・
1	C	476	79%　　17%　・・
1	D	476	81%　　15%　・・
1	E	476	78%　　18%　・・

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Mol	Chain	Length	Quality of chain
1	F	476	75% ... 21% ...
1	G	476	74% ... 20% ...
1	H	476	2% 73% ... 23% ...

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
3	9PL	C	1	-	-	X	-
3	9PL	E	1	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 30483 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total 3759	C 2419	N 650	O 672	S 18	0	0	0
1	B	464	Total 3763	C 2421	N 650	O 674	S 18	0	0	0
1	C	464	Total 3755	C 2416	N 649	O 672	S 18	0	0	0
1	D	464	Total 3763	C 2421	N 650	O 674	S 18	0	0	0
1	E	464	Total 3755	C 2416	N 649	O 672	S 18	0	0	0
1	F	464	Total 3747	C 2407	N 650	O 672	S 18	0	0	0
1	G	464	Total 3743	C 2407	N 646	O 672	S 18	0	0	0
1	H	464	Total 3732	C 2396	N 648	O 670	S 18	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP Q16696
A	24	ALA	-	expression tag	UNP Q16696
A	25	LYS	-	expression tag	UNP Q16696
A	26	LYS	-	expression tag	UNP Q16696
A	27	THR	-	expression tag	UNP Q16696
A	28	SER	-	expression tag	UNP Q16696
A	29	SER	-	expression tag	UNP Q16696
A	30	LYS	-	expression tag	UNP Q16696
A	495	HIS	-	expression tag	UNP Q16696
A	496	HIS	-	expression tag	UNP Q16696
A	497	HIS	-	expression tag	UNP Q16696
A	498	HIS	-	expression tag	UNP Q16696
B	23	MET	-	expression tag	UNP Q16696

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W O R L D W I D E
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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	-	expression tag	UNP Q16696
B	25	LYS	-	expression tag	UNP Q16696
B	26	LYS	-	expression tag	UNP Q16696
B	27	THR	-	expression tag	UNP Q16696
B	28	SER	-	expression tag	UNP Q16696
B	29	SER	-	expression tag	UNP Q16696
B	30	LYS	-	expression tag	UNP Q16696
B	495	HIS	-	expression tag	UNP Q16696
B	496	HIS	-	expression tag	UNP Q16696
B	497	HIS	-	expression tag	UNP Q16696
B	498	HIS	-	expression tag	UNP Q16696
C	23	MET	-	expression tag	UNP Q16696
C	24	ALA	-	expression tag	UNP Q16696
C	25	LYS	-	expression tag	UNP Q16696
C	26	LYS	-	expression tag	UNP Q16696
C	27	THR	-	expression tag	UNP Q16696
C	28	SER	-	expression tag	UNP Q16696
C	29	SER	-	expression tag	UNP Q16696
C	30	LYS	-	expression tag	UNP Q16696
C	495	HIS	-	expression tag	UNP Q16696
C	496	HIS	-	expression tag	UNP Q16696
C	497	HIS	-	expression tag	UNP Q16696
C	498	HIS	-	expression tag	UNP Q16696
D	23	MET	-	expression tag	UNP Q16696
D	24	ALA	-	expression tag	UNP Q16696
D	25	LYS	-	expression tag	UNP Q16696
D	26	LYS	-	expression tag	UNP Q16696
D	27	THR	-	expression tag	UNP Q16696
D	28	SER	-	expression tag	UNP Q16696
D	29	SER	-	expression tag	UNP Q16696
D	30	LYS	-	expression tag	UNP Q16696
D	495	HIS	-	expression tag	UNP Q16696
D	496	HIS	-	expression tag	UNP Q16696
D	497	HIS	-	expression tag	UNP Q16696
D	498	HIS	-	expression tag	UNP Q16696
E	23	MET	-	expression tag	UNP Q16696
E	24	ALA	-	expression tag	UNP Q16696
E	25	LYS	-	expression tag	UNP Q16696
E	26	LYS	-	expression tag	UNP Q16696
E	27	THR	-	expression tag	UNP Q16696
E	28	SER	-	expression tag	UNP Q16696
E	29	SER	-	expression tag	UNP Q16696

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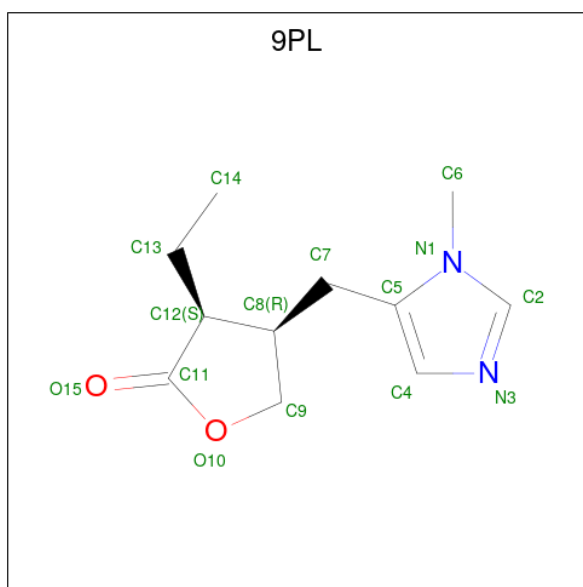| Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	expression tag	UNP Q16696
E	495	HIS	-	expression tag	UNP Q16696
E	496	HIS	-	expression tag	UNP Q16696
E	497	HIS	-	expression tag	UNP Q16696
E	498	HIS	-	expression tag	UNP Q16696
F	23	MET	-	expression tag	UNP Q16696
F	24	ALA	-	expression tag	UNP Q16696
F	25	LYS	-	expression tag	UNP Q16696
F	26	LYS	-	expression tag	UNP Q16696
F	27	THR	-	expression tag	UNP Q16696
F	28	SER	-	expression tag	UNP Q16696
F	29	SER	-	expression tag	UNP Q16696
F	30	LYS	-	expression tag	UNP Q16696
F	495	HIS	-	expression tag	UNP Q16696
F	496	HIS	-	expression tag	UNP Q16696
F	497	HIS	-	expression tag	UNP Q16696
F	498	HIS	-	expression tag	UNP Q16696
G	23	MET	-	expression tag	UNP Q16696
G	24	ALA	-	expression tag	UNP Q16696
G	25	LYS	-	expression tag	UNP Q16696
G	26	LYS	-	expression tag	UNP Q16696
G	27	THR	-	expression tag	UNP Q16696
G	28	SER	-	expression tag	UNP Q16696
G	29	SER	-	expression tag	UNP Q16696
G	30	LYS	-	expression tag	UNP Q16696
G	495	HIS	-	expression tag	UNP Q16696
G	496	HIS	-	expression tag	UNP Q16696
G	497	HIS	-	expression tag	UNP Q16696
G	498	HIS	-	expression tag	UNP Q16696
H	23	MET	-	expression tag	UNP Q16696
H	24	ALA	-	expression tag	UNP Q16696
H	25	LYS	-	expression tag	UNP Q16696
H	26	LYS	-	expression tag	UNP Q16696
H	27	THR	-	expression tag	UNP Q16696
H	28	SER	-	expression tag	UNP Q16696
H	29	SER	-	expression tag	UNP Q16696
H	30	LYS	-	expression tag	UNP Q16696
H	495	HIS	-	expression tag	UNP Q16696
H	496	HIS	-	expression tag	UNP Q16696
H	497	HIS	-	expression tag	UNP Q16696
H	498	HIS	-	expression tag	UNP Q16696

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).

HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (3S,4R)-3-ethyl-4-[(1-methyl-1H-imidazol-5-yl)methyl]dihydrofuran-2(3H)-one (three-letter code: 9PL) (formula: $C_{11}H_{16}N_2O_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		
3	E	1	Total	C	N	O	0	0
			15	11	2	2		
3	F	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		
4	C	4	Total	O	0	0
			4	4		
4	D	5	Total	O	0	0
			5	5		
4	E	8	Total	O	0	0
			8	8		
4	G	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total 4	O 4	0	0

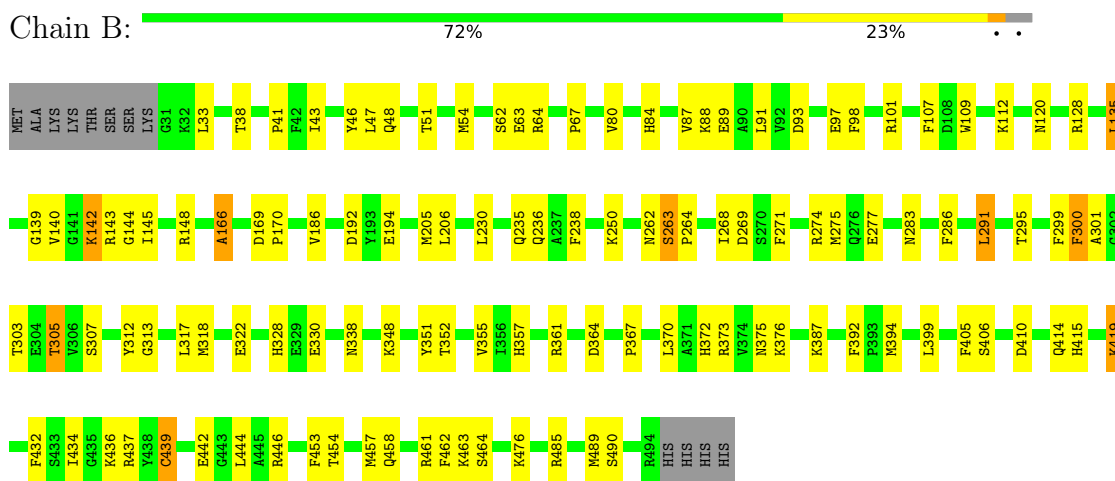# 3 Residue-property plots ⓘ

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.
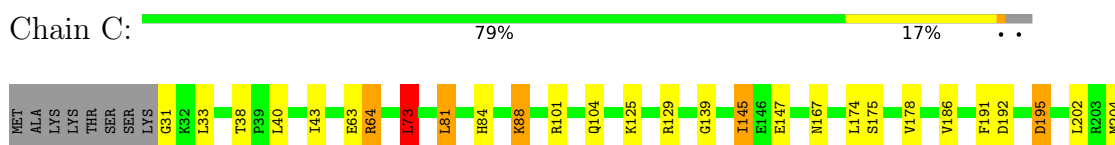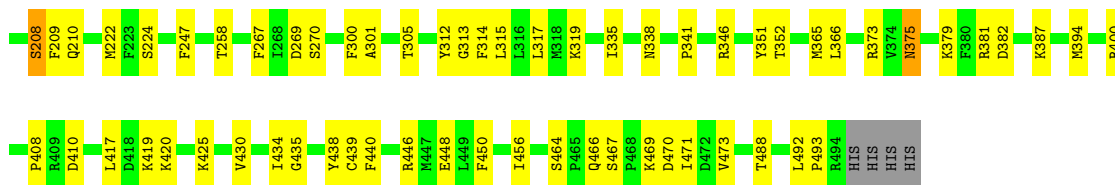
- Molecule 1: Cytochrome P450 2A13

Chain A:
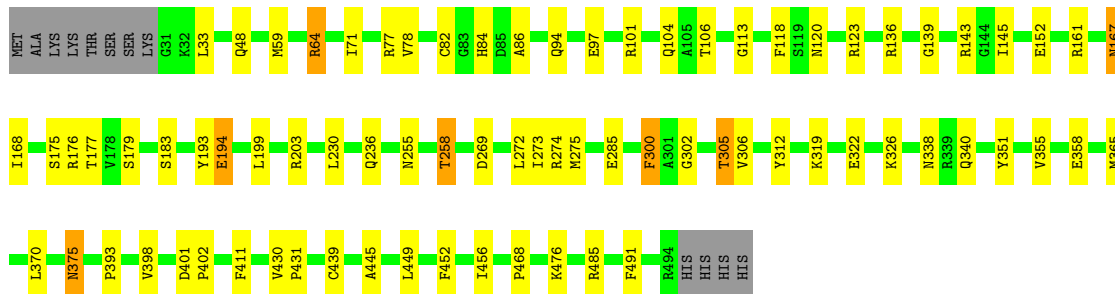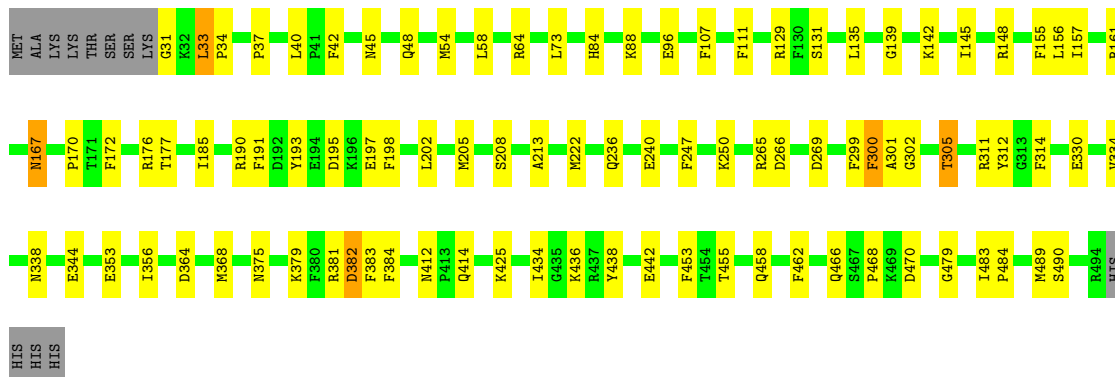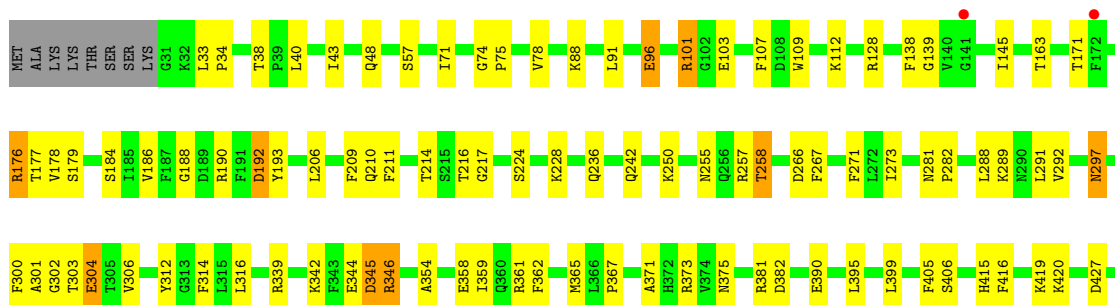

- Molecule 1: Cytochrome P450 2A13

Chain B:

- Molecule 1: Cytochrome P450 2A13

Chain C:

S208 F209 Q210 M222 F223 S224 F247 T258 F267 I268 D269 S270 F300 A301 T305 Y312 G313 F314 L315 L316 L317 M318 K319 I335 N338 P341 R346 Y351 T352 M365 L366 R373 V374 N375 K379 F380 R381 D382 K387 M394 R400

P408 R409 D410 L417 D418 K419 K420 K425 V430 I434 G435 Y438 C439 F440 R446 M447 E448 L449 F450 I456 S464 P465 Q466 S467 P468 K469 D470 I471 D472 V473 T488 L492 P493 R494 HIS HIS HIS HIS

• Molecule 1: Cytochrome P450 2A13

Chain D:　　　　　81%　　　　　15%

MET ALA LYS LYS THR SER SER LYS G31 K32 L33 Q48 M59 R64 I71 R77 V78 C82 G83 H84 D85 A86 Q94 E97 R101 Q104 A105 T106 G113 F118 S119 N120 R123 R136 G139 R143 G144 I145 E152 R161 N167

I168 S175 R176 T177 V178 S179 S183 Y193 E194 L199 R203 L230 Q236 N255 T258 D269 L272 I273 R274 M275 E285 F300 A301 G302 T305 V306 Y312 K319 E322 K326 N338 R339 Q340 Y351 V355 E358 M365

L370 N375 P393 V398 D401 P402 F411 V430 P431 C439 A445 L449 F452 I456 P468 K476 R485 F491 R494 HIS HIS HIS HIS

• Molecule 1: Cytochrome P450 2A13

Chain E:　　　　　78%　　　　　18%

MET ALA LYS LYS THR SER SER LYS G31 K32 L33 P34 P37 L40 P41 F42 N45 Q48 M54 L58 R64 L73 H84 K88 E96 F107 F111 R129 F130 S131 L135 G139 K142 I145 R148 F155 L156 I157 R161

N167 P170 T171 F172 R176 T177 I185 R190 F191 D192 Y193 E194 D195 K196 E197 F198 L202 M205 S208 A213 M222 Q236 E240 F247 K250 R265 D266 D269 F299 F300 A301 G302 T305 R311 Y312 G313 F314 E330 V334

N338 E344 E353 I356 D364 M368 N375 K379 F380 R381 D382 F383 F384 N412 P413 Q414 K425 I434 G435 K436 R437 Y438 E442 F453 T454 T455 Q458 F462 Q466 S467 P468 K469 D470 G479 I483 P484 M489 S490 R494 HIS

HIS HIS HIS

• Molecule 1: Cytochrome P450 2A13

Chain F:　　　　　75%　　　　　21%

MET ALA LYS LYS THR SER SER LYS G31 K32 L33 P34 T38 P39 L40 I43 Q48 S57 I71 G74 P75 V78 K88 L91 E96 R101 G102 E103 F107 D108 W109 K112 R128 F138 G139 V140 G141 I145 T163 T171 F172

R176 T177 V178 S179 S184 I185 V186 F187 G188 D189 R190 F191 D192 Y193 L206 F209 Q210 F211 T214 S215 T216 G217 S224 K228 Q236 Q242 K250 N255 Q256 R257 T258 D266 F267 F271 L272 I273 N281 P282 L288 K289 N290 L291 V292 M297

F300 A301 G302 T303 E304 T305 V306 Y312 G313 F314 L315 L316 R339 K342 F343 E344 D345 R346 A354 E358 I359 Q360 R361 F362 M365 L366 P367 A371 H372 R373 V374 N375 R381 D382 E390 L395 L399 F405 S406 H415 F416 K419 K420 D427

C439 R446 M447 E448 L451 F452 F453 T454 T455 I456 F460 D470 F491 R494 HIS HIS HIS HIS

• Molecule 1: Cytochrome P450 2A13

Chain G:
74%   20%

MET ALA LYS THR SER SER LYS G31 K32 L33 T38 P41 Q48 M54 Y55 N56 K60 R76 H84 K88 L91 V92 E96 S99 G100 R101 F118 K125 R129 R136 G139 V140 G141 I145 R148 E151 F155 L156

L160 T163 T171 F172 F173 R176 T177 V178 I182 F187 G188 D189 R190 F191 D192 D195 F198 R203 S215 T216 G217 Q218 K239 L244 F247 K251 Q256 D266 F267 I268 D269 I273 T284 E285 F286 L296 F300 A301 G302 T305

V306 T309 K319 G336 K337 N338 R339 K342 R346 P350 R361 M365 L366 L370 V374 N375 F380 F383 P386 K387 M394 L395 V398 L399 R409 Q422 D427 A428 F432 S433 I434 G435 K436 R437 Y438 C439 E442 E448

F452 R461 F462 K463 Q466 S467 P468 K469 D470 I471 K476 R485 N486 Y487 T488 M489 S490 F491 L492 P493 R494 HIS HIS HIS HIS

• Molecule 1: Cytochrome P450 2A13

Chain H:
2%
73%   23%

MET ALA LYS THR SER SER LYS G31 K32 L33 P34 N45 Q48 E52 Y55 M59 S62 F69 L73 V78 L81 D85 K88 E89 A90 L91 V92 D93 Q104 L110 Y114 S131 L135 V140 G141 K142 R148 A153

L156 G165 A166 N167 I168 D169 P170 T171 F172 R176 T177 V178 S179 Y193 K196 E197 F198 L199 S200 L201 L202 R203 Q210 T214 S215 T216 S225 Q236 F247 N255 Q256 L259 D260 P261 D266 F267 I268 F271 L272 Q276 E279 K280 N283

L288 K289 N290 L291 V292 L296 N297 L298 V306 T309 L310 R311 Y312 M318 E322 A325 E329 E330 N338 R339 Q340 D345 R346 A347 K348 Y351 T352 E353 A354 V355 I356 H357 E358 I359 Q360 A371 K376 F380 R381 F392 P393 M394 L399 P408

F411 Q414 L417 D418 K419 V430 P431 F432 G435 K436 R437 Y438 C439 F440 G441 L444 A445 R446 M447 E448 L449 F453 M457 S464 P465 Q466 D470 I471 P475 K476 H477 T482 R485 S490 F491 L492 P493 R494 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.50Å 119.86Å 154.87Å 101.01° 101.72° 93.59°	Depositor
Resolution (Å)	102.88 – 3.00 102.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (102.88-3.00) 98.3 (102.87-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.01Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.213 , 0.303 0.217 , 0.293	Depositor DCC
R_{free} test set	4826 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30483	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: 9PL, HEM

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	0.58	1/3856 (0.0%)	0.66	0/5193
1	B	0.49	0/3860	0.67	2/5198 (0.0%)
1	C	0.50	0/3852	0.64	3/5189 (0.1%)
1	D	0.50	0/3860	0.64	0/5198
1	E	0.46	0/3852	0.60	0/5189
1	F	0.48	0/3843	0.58	0/5176
1	G	0.47	0/3840	0.60	0/5174
1	H	0.47	0/3828	0.59	0/5159
All	All	0.49	1/30791 (0.0%)	0.62	5/41476 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	GLU	CD-OE1	-5.12	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	73	LEU	CA-CB-CG	5.37	127.64	115.30
1	C	81	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	33	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	230	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3759	0	3724	51	0
1	B	3763	0	3728	78	0
1	C	3755	0	3713	56	0
1	D	3763	0	3728	50	0
1	E	3755	0	3713	54	0
1	F	3747	0	3699	56	0
1	G	3743	0	3684	59	0
1	H	3732	0	3664	61	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	10	0
2	D	43	0	30	13	0
2	E	43	0	30	5	0
2	F	43	0	30	6	0
2	G	43	0	30	5	0
2	H	43	0	30	5	0
3	A	15	0	15	3	0
3	B	15	0	16	6	0
3	C	15	0	16	12	0
3	D	15	0	16	4	0
3	E	15	0	16	8	0
3	F	15	0	16	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	4	0	0	1	0
4	D	5	0	0	1	0
4	E	8	0	0	1	0
4	G	1	0	0	1	0
4	H	4	0	0	1	0
All	All	30483	0	29988	479	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 8.

The worst 5 of 479 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:C:305:THR:HG21	3:C:1:9PL:H2	1.37	1.05
1:B:305:THR:HG23	3:B:1:9PL:H6B	1.45	0.97
1:C:305:THR:CG2	3:C:1:9PL:H2	1.97	0.95
1:D:64:ARG:CG	1:D:64:ARG:HH11	1.81	0.93
1:B:166:ALA:O	1:B:490:SER:HB3	1.69	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/476 (97%)	445 (96%)	15 (3%)	2 (0%)	34	72
1	B	462/476 (97%)	423 (92%)	31 (7%)	8 (2%)	9	39
1	C	462/476 (97%)	420 (91%)	39 (8%)	3 (1%)	25	64
1	D	462/476 (97%)	421 (91%)	39 (8%)	2 (0%)	34	72
1	E	462/476 (97%)	429 (93%)	25 (5%)	8 (2%)	9	39
1	F	462/476 (97%)	406 (88%)	49 (11%)	7 (2%)	10	42
1	G	462/476 (97%)	424 (92%)	31 (7%)	7 (2%)	10	42
1	H	462/476 (97%)	396 (86%)	65 (14%)	1 (0%)	47	82
All	All	3696/3808 (97%)	3364 (91%)	294 (8%)	38 (1%)	15	53

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	338	ASN
1	F	304	GLU
1	G	336	GLY
1	G	337	LYS
1	G	375	ASN

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	407/419 (97%)	380 (93%)	27 (7%)	16	49
1	B	408/419 (97%)	387 (95%)	21 (5%)	24	60
1	C	406/419 (97%)	377 (93%)	29 (7%)	14	46
1	D	408/419 (97%)	386 (95%)	22 (5%)	22	57
1	E	406/419 (97%)	384 (95%)	22 (5%)	22	57
1	F	404/419 (96%)	370 (92%)	34 (8%)	11	38
1	G	403/419 (96%)	369 (92%)	34 (8%)	11	38
1	H	400/419 (96%)	368 (92%)	32 (8%)	12	40
All	All	3242/3352 (97%)	3021 (93%)	221 (7%)	16	48

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	425	LYS
1	F	312	TYR
1	H	470	ASP
1	H	225	SER
1	E	458	GLN

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	94	GLN
1	H	458	GLN
1	G	422	GLN
1	H	120	ASN
1	D	72	HIS

5.3.3 RNA (i)

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 ⓘ

14 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	HEM	B	500	1,3	41,50,50	1.99	5 (12%)	45,82,82	2.01	15 (33%)
2	HEM	C	500	1,3	41,50,50	1.95	7 (17%)	45,82,82	1.78	9 (20%)
2	HEM	G	500	1	41,50,50	2.33	13 (31%)	45,82,82	1.99	16 (35%)
3	9PL	C	1	2	13,16,16	1.46	1 (7%)	16,22,22	2.56	7 (43%)
3	9PL	F	1	2	13,16,16	1.42	1 (7%)	16,22,22	2.29	5 (31%)
2	HEM	A	500	1,3	41,50,50	1.99	7 (17%)	45,82,82	1.97	13 (28%)
2	HEM	D	500	1,3	41,50,50	1.98	7 (17%)	45,82,82	1.59	6 (13%)
3	9PL	E	1	2	13,16,16	1.44	1 (7%)	16,22,22	2.57	7 (43%)
2	HEM	E	500	1,3	41,50,50	2.30	8 (19%)	45,82,82	1.66	7 (15%)
2	HEM	H	500	1	41,50,50	2.26	10 (24%)	45,82,82	1.65	8 (17%)
3	9PL	B	1	2	13,16,16	1.69	2 (15%)	16,22,22	2.56	6 (37%)
3	9PL	D	1	2	13,16,16	1.44	1 (7%)	16,22,22	2.72	8 (50%)
2	HEM	F	500	1,3	41,50,50	2.13	8 (19%)	45,82,82	1.98	11 (24%)
3	9PL	A	1	2	13,16,16	1.58	2 (15%)	16,22,22	3.20	7 (43%)

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	HEM	B	500	1,3	-	5/12/54/54	-
2	HEM	C	500	1,3	-	2/12/54/54	-
2	HEM	G	500	1	-	4/12/54/54	-
3	9PL	C	1	2	-	4/6/19/19	0/2/2/2
3	9PL	F	1	2	-	1/6/19/19	0/2/2/2
2	HEM	A	500	1,3	-	3/12/54/54	-
2	HEM	D	500	1,3	-	3/12/54/54	-
3	9PL	E	1	2	-	4/6/19/19	0/2/2/2
2	HEM	E	500	1,3	-	4/12/54/54	-
2	HEM	H	500	1	-	7/12/54/54	-
3	9PL	B	1	2	-	3/6/19/19	0/2/2/2
3	9PL	D	1	2	-	4/6/19/19	0/2/2/2
2	HEM	F	500	1,3	-	6/12/54/54	-
3	9PL	A	1	2	-	3/6/19/19	0/2/2/2

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	C3D-C2D	8.44	1.54	1.36
2	F	500	HEM	C3D-C2D	8.19	1.54	1.36
2	E	500	HEM	C3D-C2D	8.13	1.54	1.36
2	A	500	HEM	C3D-C2D	7.76	1.53	1.36
2	B	500	HEM	C3D-C2D	7.61	1.52	1.36

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	9PL	C9-C8-C12	7.41	113.06	101.44
3	E	1	9PL	C9-C8-C12	6.55	111.71	101.44
3	C	1	9PL	C9-C8-C12	6.53	111.68	101.44
3	A	1	9PL	C5-C7-C8	-6.24	100.26	114.25
3	F	1	9PL	C9-C8-C12	6.24	111.22	101.44

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C1A-C2A-CAA-CBA
2	D	500	HEM	C3A-C2A-CAA-CBA

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	500	HEM	C1A-C2A-CAA-CBA
2	F	500	HEM	C3A-C2A-CAA-CBA
2	G	500	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

14 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	3	0
2	C	500	HEM	10	0
2	G	500	HEM	5	0
3	C	1	9PL	12	0
3	F	1	9PL	2	0
2	A	500	HEM	3	0
2	D	500	HEM	13	0
3	E	1	9PL	8	0
2	E	500	HEM	5	0
2	H	500	HEM	5	0
3	B	1	9PL	6	0
3	D	1	9PL	4	0
2	F	500	HEM	6	0
3	A	1	9PL	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 HEM B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM G 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM H 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM F 500

Bond lengths

Bond angles

Torsions

Rings

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, 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(Å²)	Q<0.9
1	A	464/476 (97%)	-0.36	0	100	100	23, 38, 54, 60	0
1	B	464/476 (97%)	-0.29	0	100	100	24, 44, 64, 66	0
1	C	464/476 (97%)	-0.33	0	100	100	26, 45, 71, 76	0
1	D	464/476 (97%)	-0.34	0	100	100	22, 42, 62, 69	0
1	E	464/476 (97%)	-0.25	0	100	100	32, 60, 76, 82	0
1	F	464/476 (97%)	-0.16	2 (0%)	92	79	29, 67, 85, 93	0
1	G	464/476 (97%)	-0.14	2 (0%)	92	79	35, 66, 94, 98	0
1	H	464/476 (97%)	0.14	11 (2%)	59	30	40, 84, 101, 104	0
All	All	3712/3808 (97%)	-0.22	15 (0%)	92	79	22, 54, 91, 104	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	329	GLU	3.4
1	F	172	PHE	3.2
1	H	356	ILE	2.8
1	H	414	GLN	2.5
1	H	355	VAL	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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
3	9PL	C	1	15/15	0.91	0.42	74,75,76,76	0
2	HEM	H	500	43/43	0.95	0.29	80,82,85,85	0
3	9PL	B	1	15/15	0.96	0.36	75,77,79,80	0
3	9PL	E	1	15/15	0.96	0.31	74,75,76,76	0
3	9PL	F	1	15/15	0.96	0.35	74,75,75,76	0
2	HEM	E	500	43/43	0.97	0.24	53,59,61,62	0
2	HEM	G	500	43/43	0.97	0.28	54,58,60,63	0
2	HEM	C	500	43/43	0.97	0.26	34,41,43,46	0
3	9PL	A	1	15/15	0.97	0.39	60,64,70,71	0
2	HEM	F	500	43/43	0.98	0.24	56,62,64,64	0
2	HEM	A	500	43/43	0.98	0.26	28,34,38,40	0
3	9PL	D	1	15/15	0.98	0.28	63,66,71,71	0
2	HEM	D	500	43/43	0.98	0.26	28,38,42,44	0
2	HEM	B	500	43/43	0.98	0.27	29,34,38,40	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.
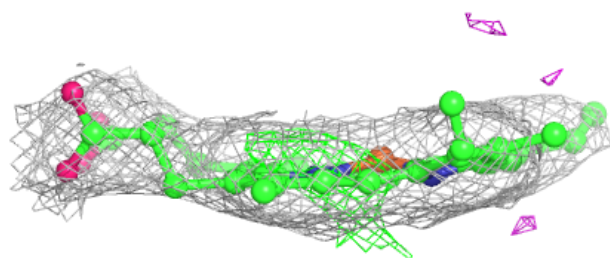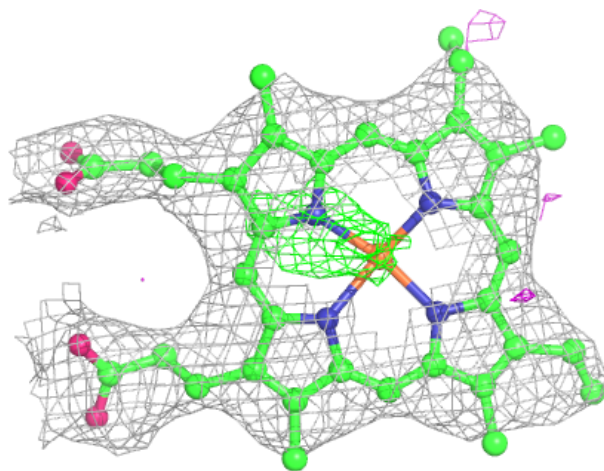
Electron density around HEM H 500:

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

Electron density around HEM E 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
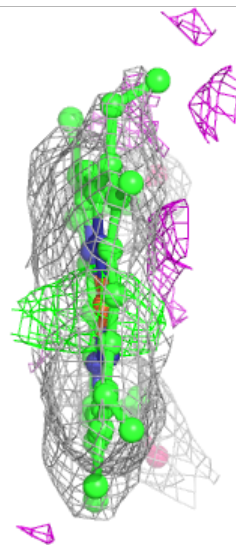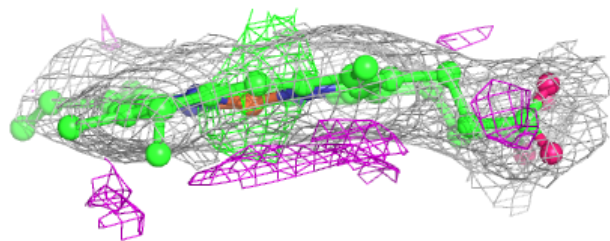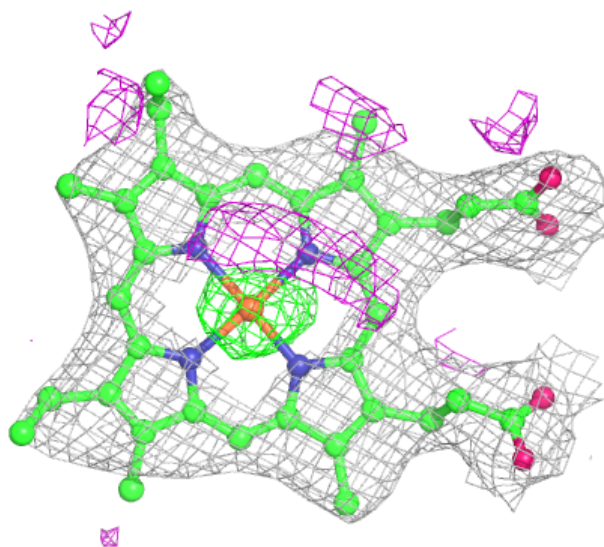mF_o-DF_c (at 3 rmsd) in purple (negative)
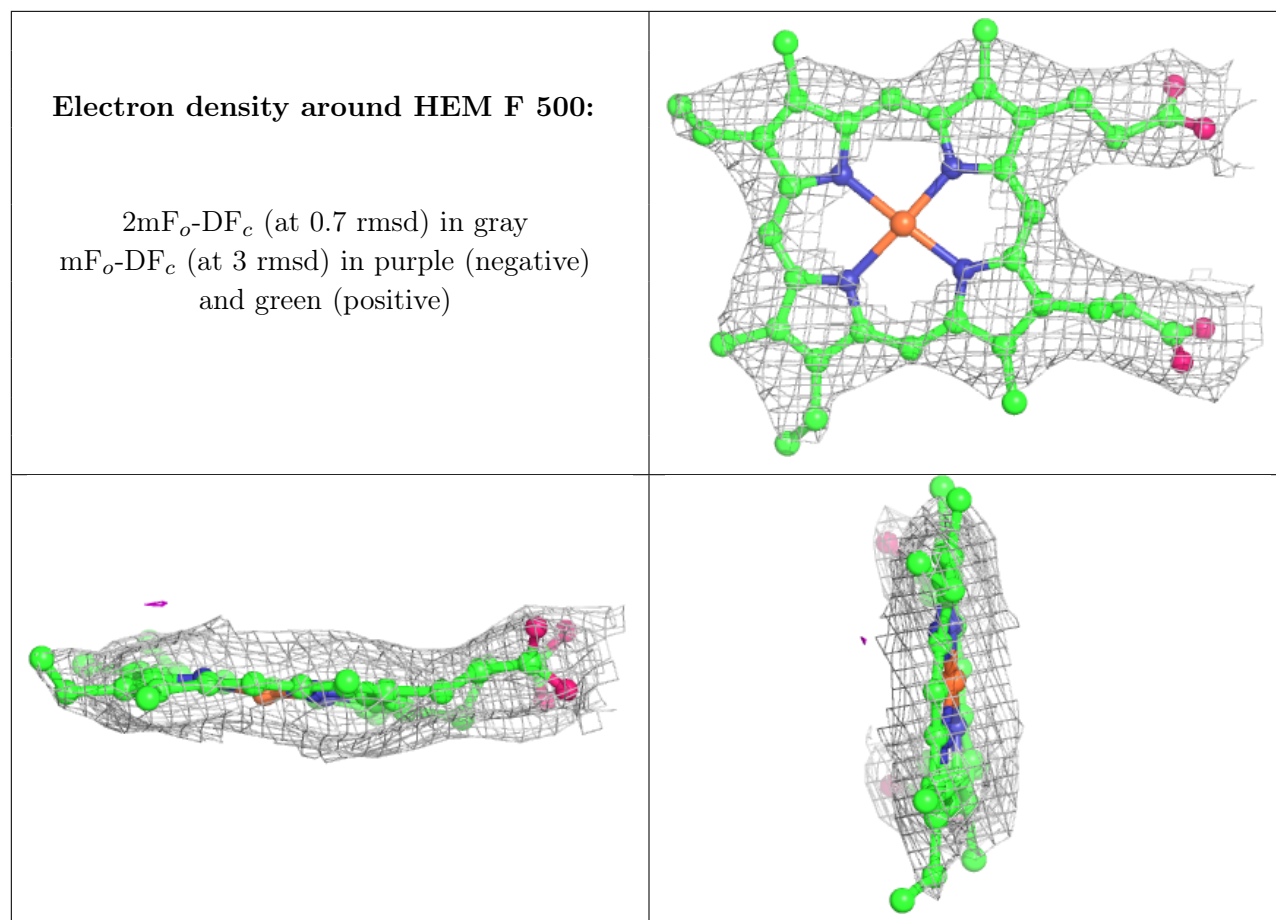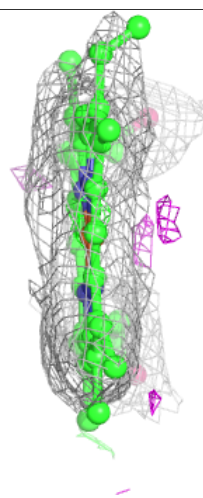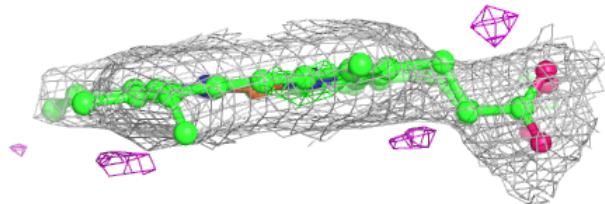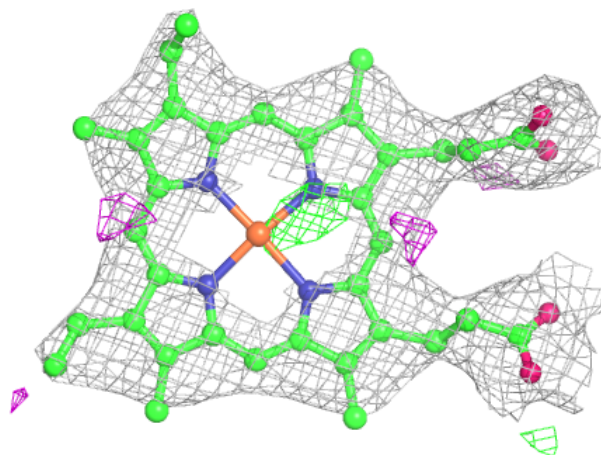and green (positive)
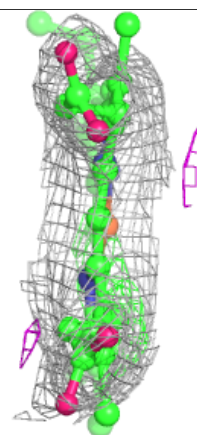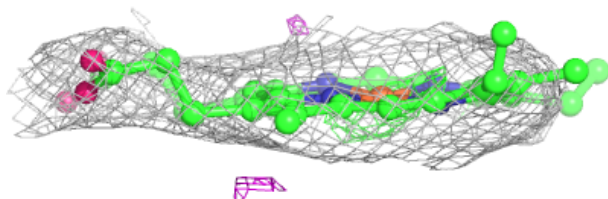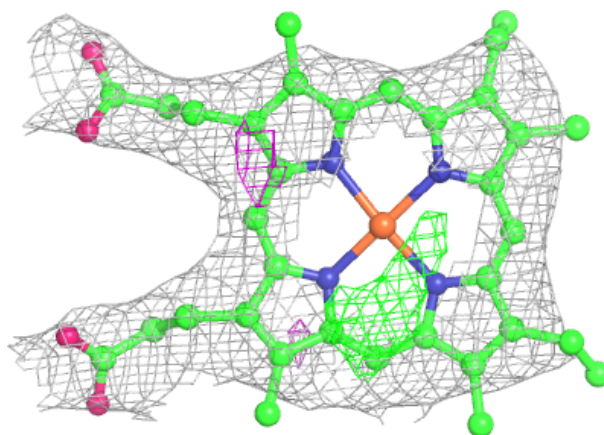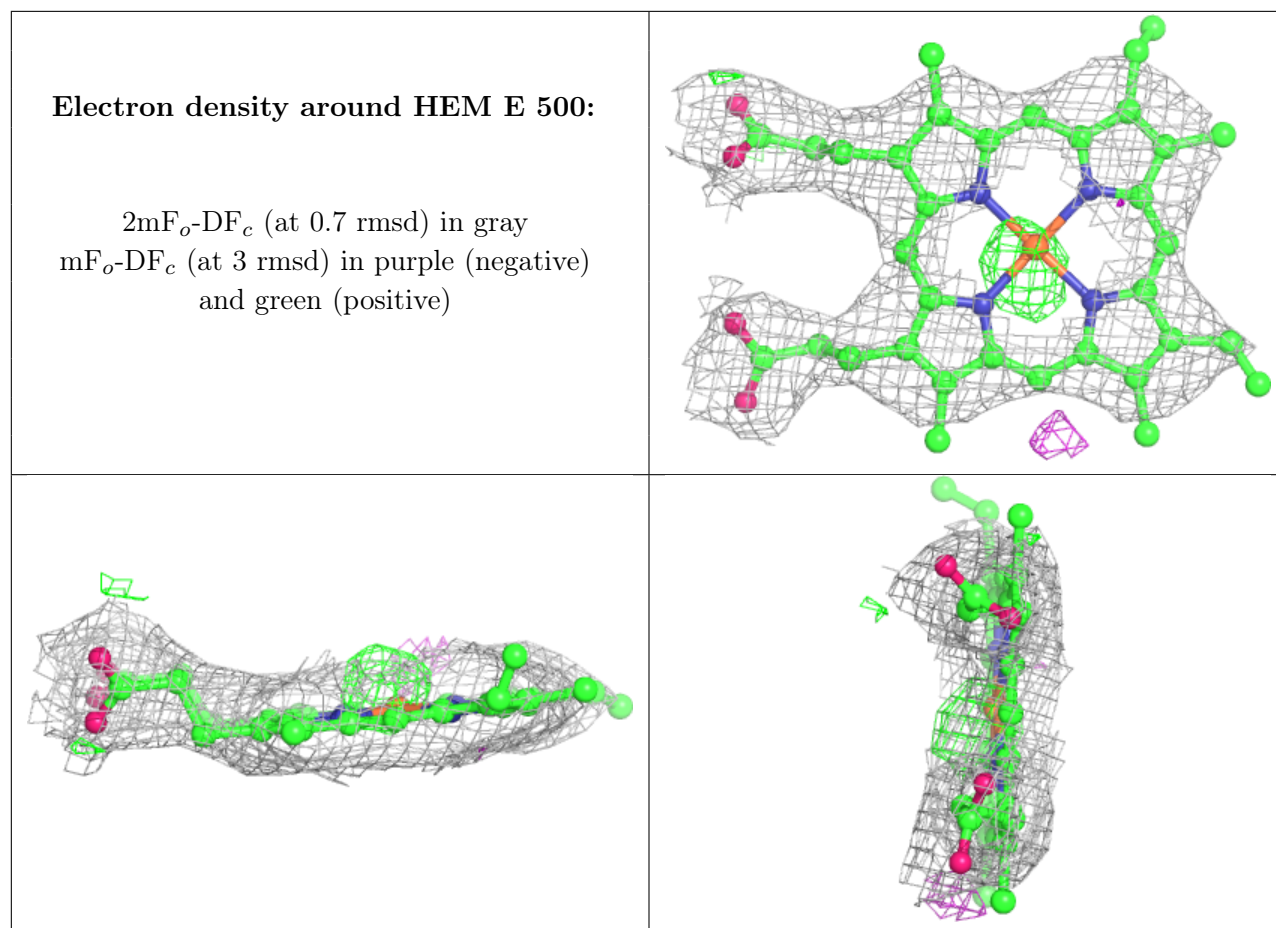
Electron density around HEM G 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
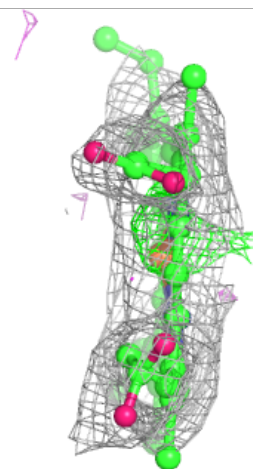
Electron density around HEM C 500:

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

Electron density around HEM F 500:

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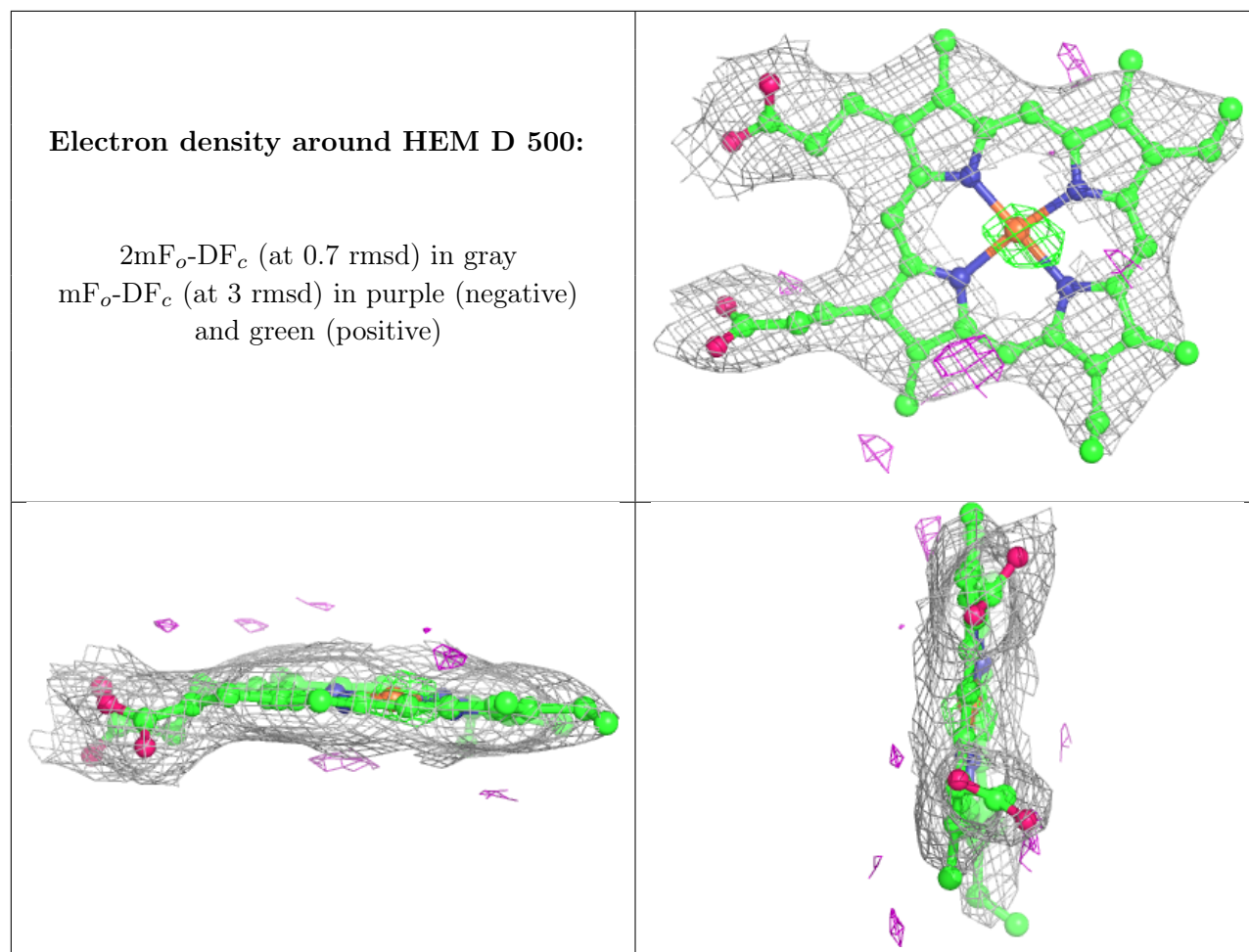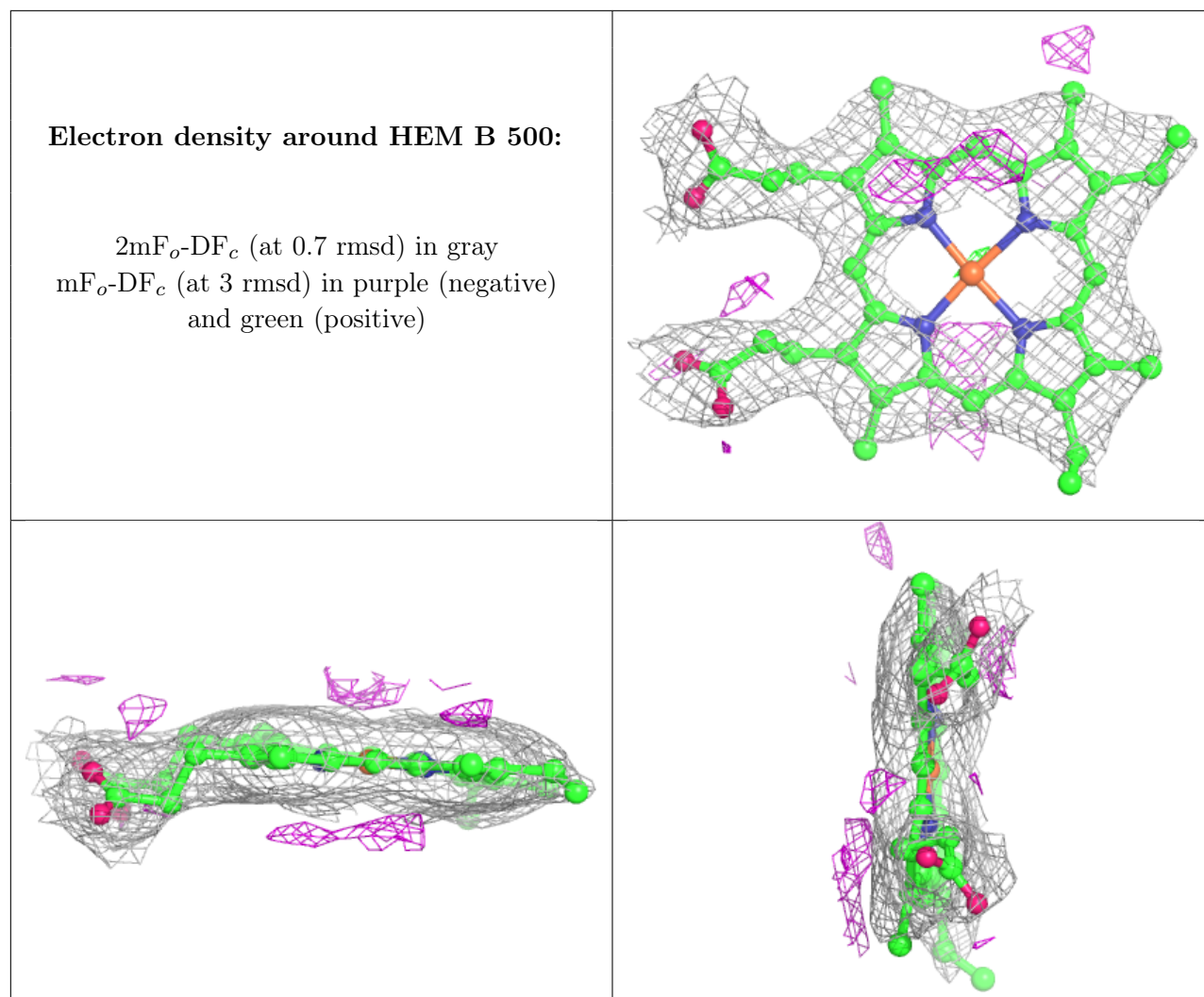mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM A 500:

$2mF_o$-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 500:

$2mF_o$-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 500:

$2mF_o$-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.