



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 2, 2026 – 10:18 PM EDT

PDB ID : 5JQV / pdb_00005jqv
Title : Crystal structure of Cytochrome P450 BM3 heme domain T269V/L272W/L322I/A406S (WIVS) 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 : 2.34 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (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

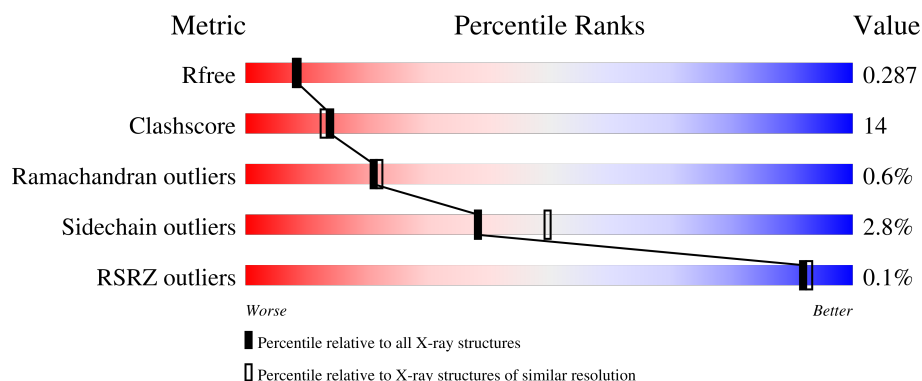
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	 65% 30% . .
1	B	471	 65% 30% . .
1	C	471	 69% 25% . .
1	D	471	 70% 26% .

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Mol	Chain	Length	Quality of chain
1	E	471	
1	F	471	
1	G	471	
1	H	471	

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

There are 3 unique types of molecules in this entry. The entry contains 30012 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
1	A	453	Total	C	N	O	S	0	0	0
			3579	2300	609	653	17			
1	B	453	Total	C	N	O	S	0	0	0
			3597	2307	611	662	17			
1	C	452	Total	C	N	O	S	0	0	0
			3551	2284	602	648	17			
1	D	454	Total	C	N	O	S	0	0	0
			3493	2250	590	636	17			
1	E	451	Total	C	N	O	S	0	1	0
			3589	2302	608	662	17			
1	F	455	Total	C	N	O	S	0	0	0
			3565	2292	602	654	17			
1	G	451	Total	C	N	O	S	0	3	0
			3585	2300	607	661	17			
1	H	450	Total	C	N	O	S	0	0	0
			3578	2300	608	653	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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
A	471	HIS	-	expression tag	UNP P14779
B	269	VAL	THR	engineered mutation	UNP P14779

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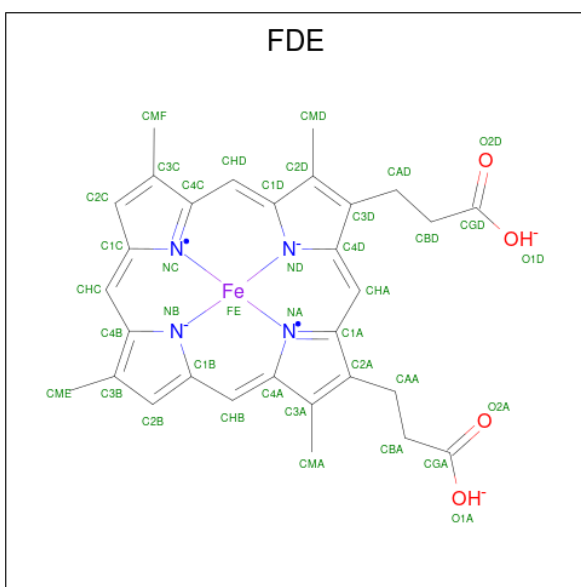
Chain	Residue	Modelled	Actual	Comment	Reference
B	272	TRP	LEU	engineered mutation	UNP P14779
B	322	ILE	LEU	engineered mutation	UNP P14779
B	406	SER	ALA	engineered mutation	UNP P14779
B	464	LEU	-	expression tag	UNP P14779
B	465	GLU	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	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	269	VAL	THR	engineered mutation	UNP P14779
C	272	TRP	LEU	engineered mutation	UNP P14779
C	322	ILE	LEU	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	269	VAL	THR	engineered mutation	UNP P14779
D	272	TRP	LEU	engineered mutation	UNP P14779
D	322	ILE	LEU	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
D	471	HIS	-	expression tag	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	269	VAL	THR	engineered mutation	UNP P14779
F	272	TRP	LEU	engineered mutation	UNP P14779
F	322	ILE	LEU	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	269	VAL	THR	engineered mutation	UNP P14779
G	272	TRP	LEU	engineered mutation	UNP P14779
G	322	ILE	LEU	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
G	471	HIS	-	expression tag	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	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	
2	A	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	B	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	C	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	D	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	E	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	F	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	G	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	H	1	Total 39	C 30	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	159	Total O 159 159	0	0
3	B	154	Total O 154 154	0	0
3	C	132	Total O 132 132	0	0
3	D	89	Total O 89 89	0	0

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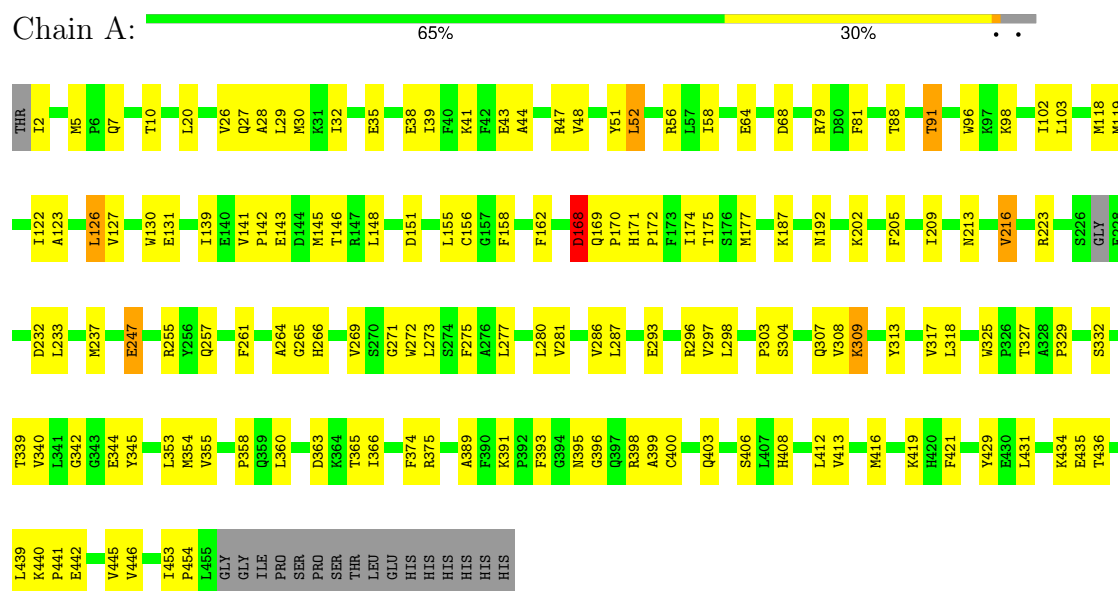
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	164	Total 164	O 164	0	0
3	F	130	Total 130	O 130	0	0
3	G	156	Total 156	O 156	0	0
3	H	179	Total 179	O 179	0	0

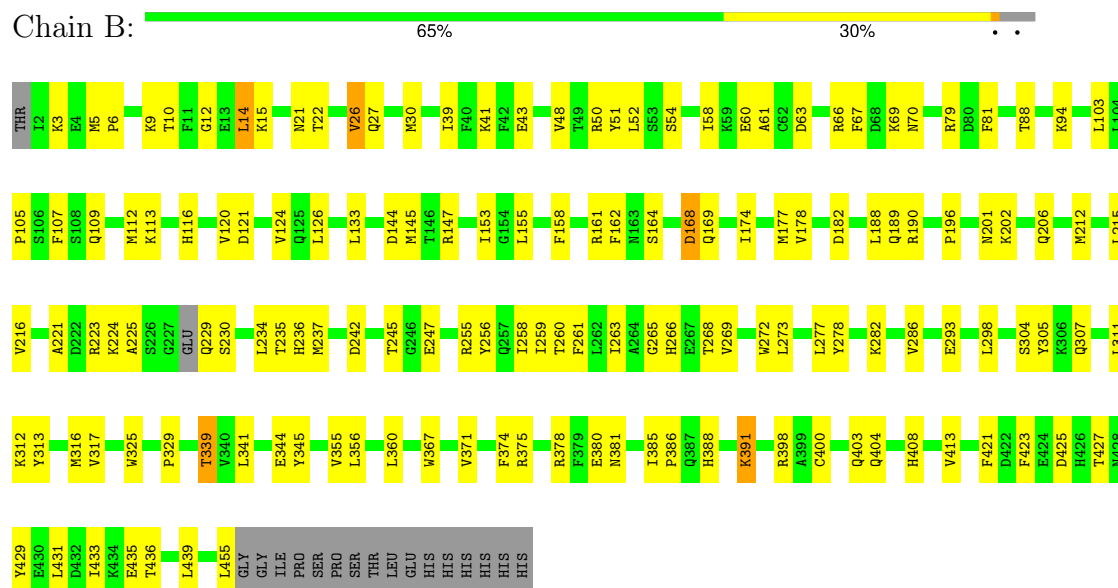
3 Residue-property plots

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.

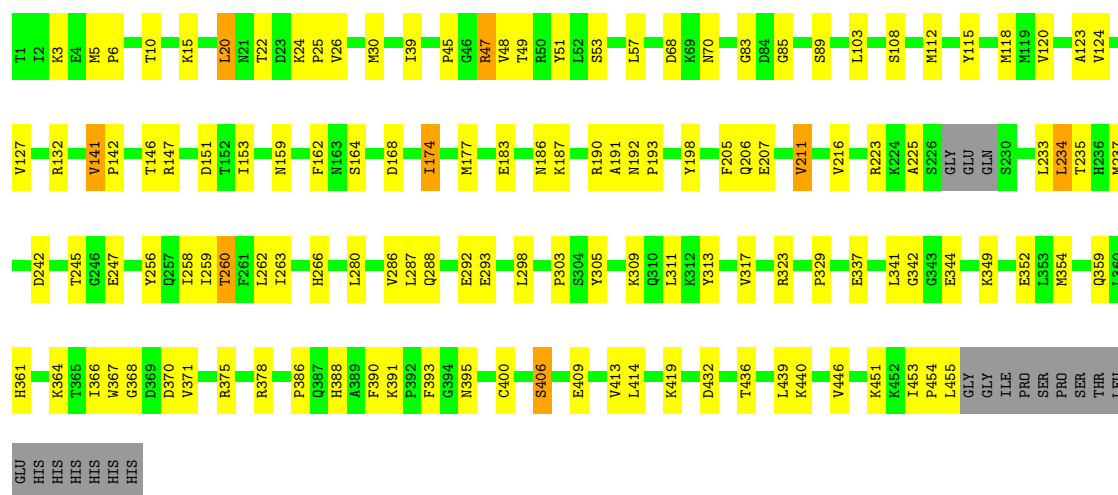
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



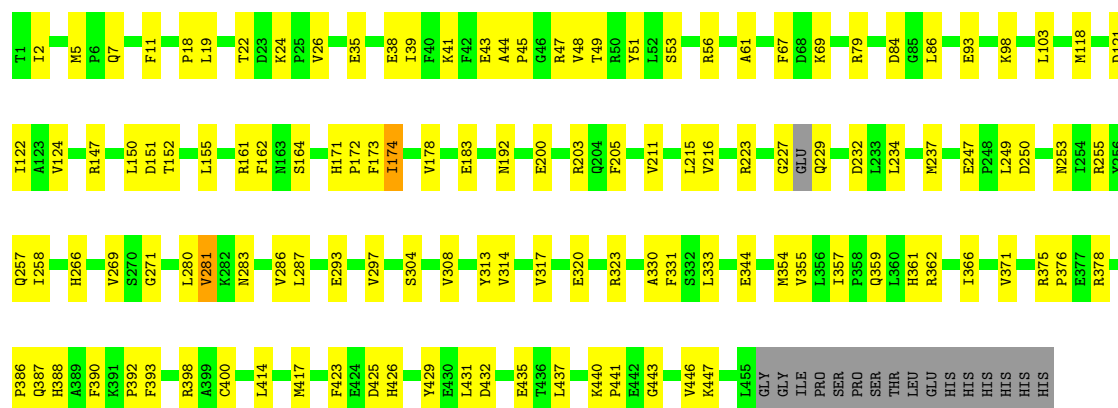
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



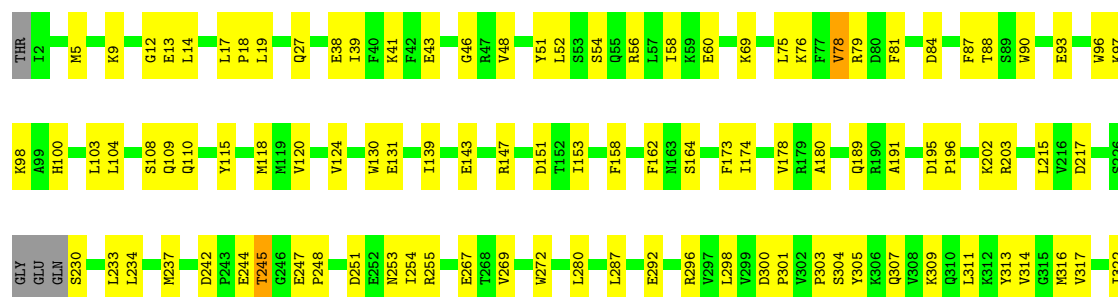
Chain C: 69% 25% . .

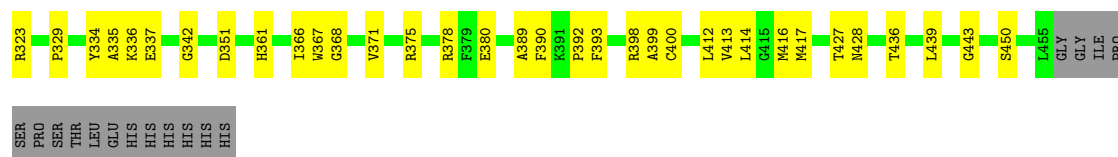


Chain D: 70% 26% .



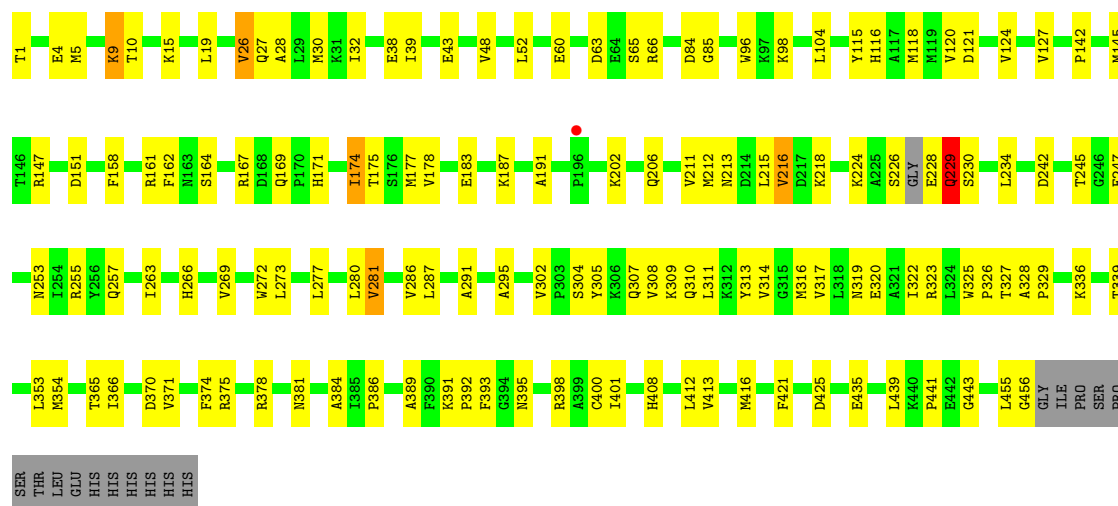
Chain E: 67% 28% .





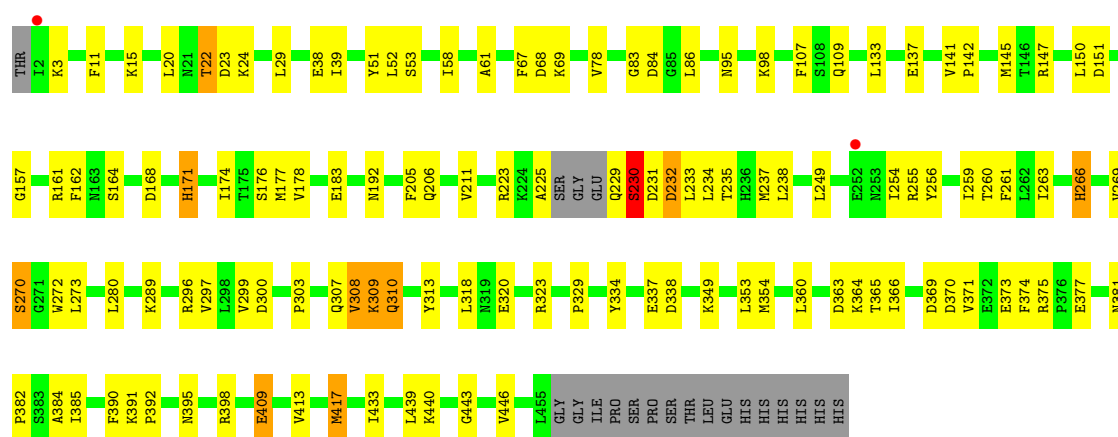
● Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain F: 67% 28% . .



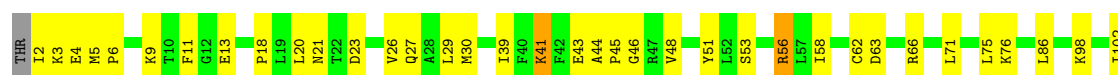
● Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain G: 69% 24% . .



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

Chain H: 67% 27% . .



THR	L103	N239	Q359	
LEU	K113	G240	R362	
GLU	A123	K241	W367	
HIS	V127	P248	G368	
HIS	A135	D251	D369	
HIS	V141	R255	D370	
HIS	P142	Y256	V371	
	T146	Q257	R375	
	R147	H266	I385	
	L148	E267	H388	
	D151	S270	K391	
	F158	G271	P392	
	F162	W272	F393	
	N163	L277	Q397	
	S164	L280	C400	
	R167	V281	Q403	
	D168	V286	V413	
	Q169	L287	V416	
	P170	K289	M416	
	H171	E293	K419	
	P172	P303	D422	
	F173	S304	D425	
	I174	Y305	H426	
	T175	K306	T427	
	S176	Q307	I433	
	N186	Y313	K434	
	Q189	M316	E435	
	E207	E320	T436	
	V211	R323	L439	
	L215	T327	K440	
	K218	A328	G443	
	R223	P329	K451	
	K224	V340	K452	
	ALA	L341	I453	
	SER	E344	P454	
	GLY	Y345	L455	
	GLU	P346	GLY	
	Q229	V355	GLY	
	L234	I357	ILE	
	M237	P358	PRO	
	L238		SER	
			PRO	
			SER	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.71Å 167.41Å 228.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.97 – 2.34 32.97 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.97-2.34) 99.9 (32.97-2.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.284 0.215 , 0.287	Depositor DCC
R_{free} test set	1628 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30012	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/3665	0.66	2/4969 (0.0%)
1	B	0.41	0/3683	0.65	2/4990 (0.0%)
1	C	0.39	0/3637	0.64	0/4935
1	D	0.37	0/3579	0.60	0/4868
1	E	0.43	0/3678	0.66	0/4986
1	F	0.45	0/3651	0.65	1/4957 (0.0%)
1	G	0.41	0/3681	0.64	2/4992 (0.0%)
1	H	0.40	0/3664	0.65	2/4963 (0.0%)
All	All	0.41	0/29238	0.64	9/39660 (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	G	0	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	310	GLN	CA-CB-CG	-9.02	96.06	114.10
1	A	168	ASP	CA-C-N	7.35	137.53	124.01
1	A	168	ASP	C-N-CA	7.35	137.53	124.01
1	G	231	ASP	N-CA-C	5.84	118.96	107.98
1	B	436	THR	CA-C-N	-5.43	112.10	121.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	230	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3579	0	3486	126	0
1	B	3597	0	3507	112	0
1	C	3551	0	3453	93	0
1	D	3493	0	3302	86	0
1	E	3589	0	3498	98	0
1	F	3565	0	3440	98	0
1	G	3585	0	3465	95	0
1	H	3578	0	3503	108	0
2	A	39	0	26	0	0
2	B	39	0	26	2	0
2	C	39	0	26	1	0
2	D	39	0	26	1	0
2	E	39	0	26	1	0
2	F	39	0	25	1	0
2	G	39	0	26	2	0
2	H	39	0	26	4	0
3	A	159	0	0	35	0
3	B	154	0	0	20	0
3	C	132	0	0	18	0
3	D	89	0	0	5	0
3	E	164	0	0	23	0
3	F	130	0	0	12	0
3	G	156	0	0	19	0
3	H	179	0	0	28	0
All	All	30012	0	27861	815	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 14.

The worst 5 of 815 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:A:168:ASP:CG	1:A:169:GLN:H	1.77	0.92
1:F:228:GLU:CB	3:F:707:HOH:O	2.19	0.90
1:A:142:PRO:O	3:A:601:HOH:O	1.89	0.89
1:B:145:MET:SD	3:B:728:HOH:O	2.30	0.88
1:E:27:GLN:NE2	3:E:603:HOH:O	2.07	0.87

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	449/471 (95%)	433 (96%)	14 (3%)	2 (0%)	30	32
1	B	449/471 (95%)	434 (97%)	14 (3%)	1 (0%)	43	50
1	C	448/471 (95%)	433 (97%)	12 (3%)	3 (1%)	18	18
1	D	450/471 (96%)	432 (96%)	16 (4%)	2 (0%)	30	32
1	E	448/471 (95%)	433 (97%)	13 (3%)	2 (0%)	30	32
1	F	451/471 (96%)	432 (96%)	15 (3%)	4 (1%)	14	13
1	G	450/471 (96%)	435 (97%)	10 (2%)	5 (1%)	11	10
1	H	446/471 (95%)	433 (97%)	10 (2%)	3 (1%)	18	18
All	All	3591/3768 (95%)	3465 (96%)	104 (3%)	22 (1%)	21	22

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	E	191	ALA
1	G	310	GLN
1	B	224	LYS
1	C	225	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/414 (90%)	362 (97%)	11 (3%)	37	48
1	B	378/414 (91%)	365 (97%)	13 (3%)	32	42
1	C	369/414 (89%)	354 (96%)	15 (4%)	27	35
1	D	345/414 (83%)	338 (98%)	7 (2%)	48	61
1	E	379/414 (92%)	374 (99%)	5 (1%)	61	73
1	F	367/414 (89%)	354 (96%)	13 (4%)	32	41
1	G	373/414 (90%)	359 (96%)	14 (4%)	29	38
1	H	376/414 (91%)	370 (98%)	6 (2%)	55	67
All	All	2960/3312 (89%)	2876 (97%)	84 (3%)	38	50

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	224	LYS
1	G	192[B]	ASN
1	F	230	SER
1	G	23	ASP
1	G	297	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	388	HIS
1	G	253	ASN
1	F	408	HIS
1	G	186	ASN
1	G	310	GLN

5.3.3 RNA ⓘ

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	A	501	1,3	46,46,46	2.89	25 (54%)	60,76,76	4.04	33 (55%)
2	FDE	E	501	1,3	46,46,46	2.88	24 (52%)	60,76,76	4.03	32 (53%)
2	FDE	G	501	1	46,46,46	2.89	24 (52%)	60,76,76	4.07	35 (58%)
2	FDE	H	501	1	46,46,46	2.88	25 (54%)	60,76,76	3.98	30 (50%)
2	FDE	F	501	1	46,46,46	2.94	26 (56%)	60,76,76	4.09	34 (56%)
2	FDE	C	501	1,3	46,46,46	2.95	24 (52%)	60,76,76	3.98	30 (50%)
2	FDE	D	501	1	46,46,46	2.89	24 (52%)	60,76,76	4.09	32 (53%)
2	FDE	B	501	1	46,46,46	2.86	23 (50%)	60,76,76	4.16	32 (53%)

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	A	501	1,3	1/1/3/7	0/10/50/50	-
2	FDE	E	501	1,3	1/1/3/7	3/10/50/50	-
2	FDE	G	501	1	1/1/3/7	4/10/50/50	-
2	FDE	H	501	1	1/1/3/7	2/10/50/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDE	F	501	1	1/1/3/7	4/10/50/50	-
2	FDE	C	501	1,3	1/1/3/7	2/10/50/50	-
2	FDE	D	501	1	1/1/3/7	4/10/50/50	-
2	FDE	B	501	1	1/1/3/7	3/10/50/50	-

The worst 5 of 195 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	FDE	C2A-C3A	6.17	1.50	1.36
2	A	501	FDE	C2A-C3A	6.10	1.49	1.36
2	C	501	FDE	C3D-C2D	5.88	1.49	1.36
2	B	501	FDE	C1B-NB	-5.79	1.31	1.39
2	B	501	FDE	C3D-C2D	5.77	1.49	1.36

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FDE	CHD-C1D-ND	-11.83	111.58	124.45
2	A	501	FDE	CHD-C1D-ND	-11.56	111.86	124.45
2	B	501	FDE	C1D-CHD-C4C	11.51	150.48	126.02
2	G	501	FDE	CHD-C1D-ND	-11.49	111.95	124.45
2	C	501	FDE	CHD-C1D-ND	-11.47	111.96	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	B	501	FDE	CAD-CBD-CGD-O2D
2	B	501	FDE	CAD-CBD-CGD-O1D
2	D	501	FDE	CAD-CBD-CGD-O2D
2	H	501	FDE	CAD-CBD-CGD-O2D
2	E	501	FDE	CAD-CBD-CGD-O2D

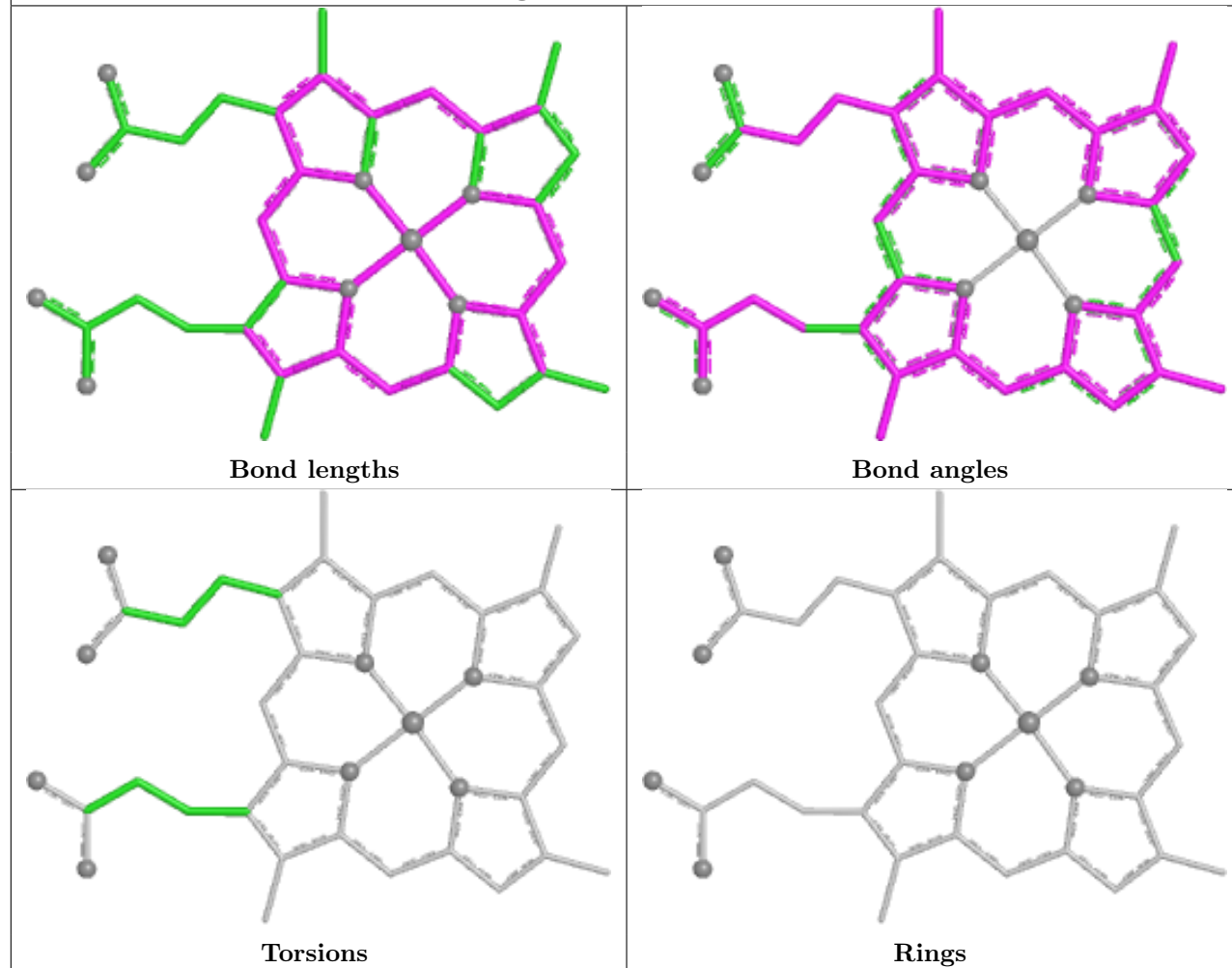
There are no ring outliers.

7 monomers are involved in 12 short contacts:

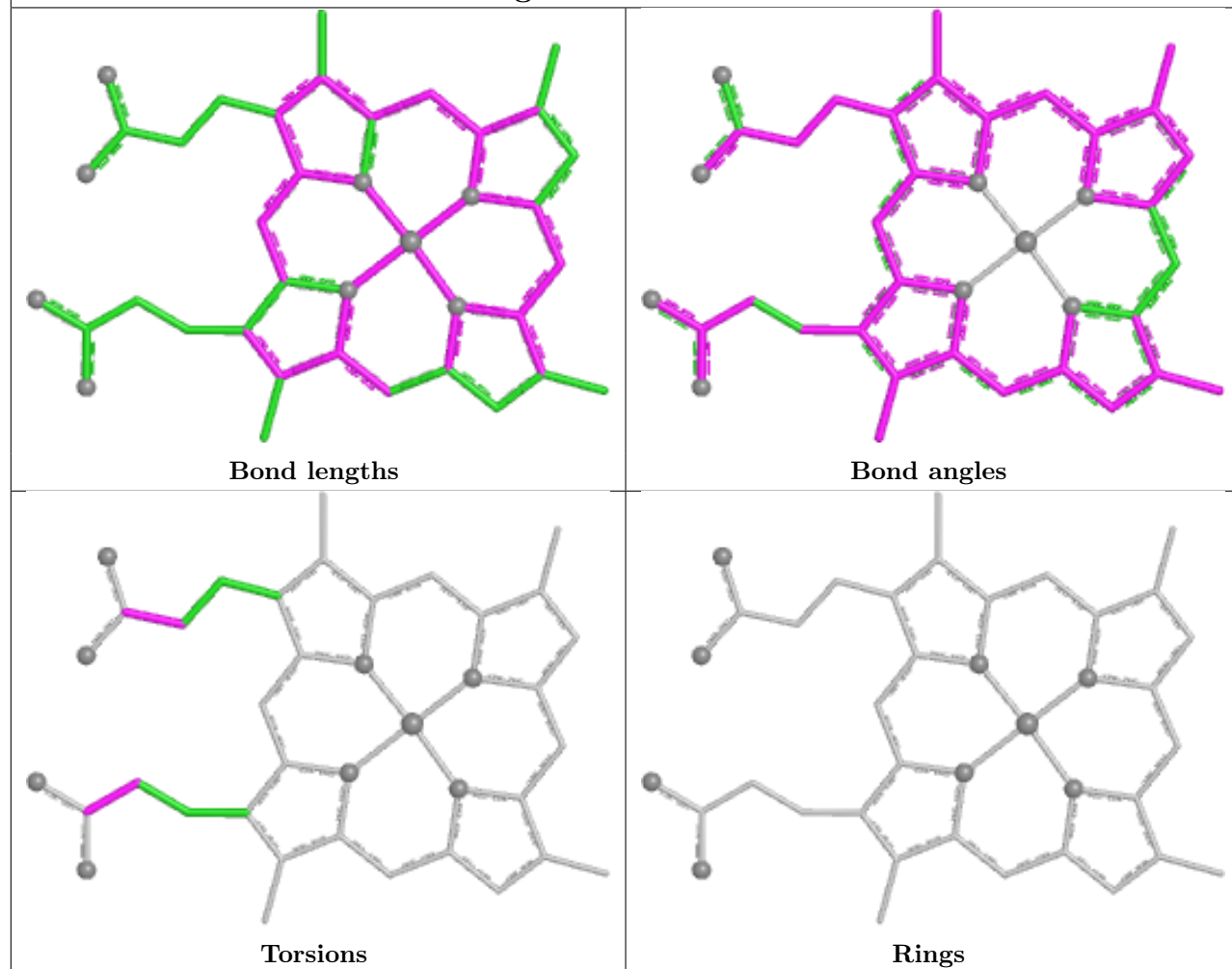
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	FDE	1	0
2	G	501	FDE	2	0
2	H	501	FDE	4	0
2	F	501	FDE	1	0
2	C	501	FDE	1	0
2	D	501	FDE	1	0
2	B	501	FDE	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

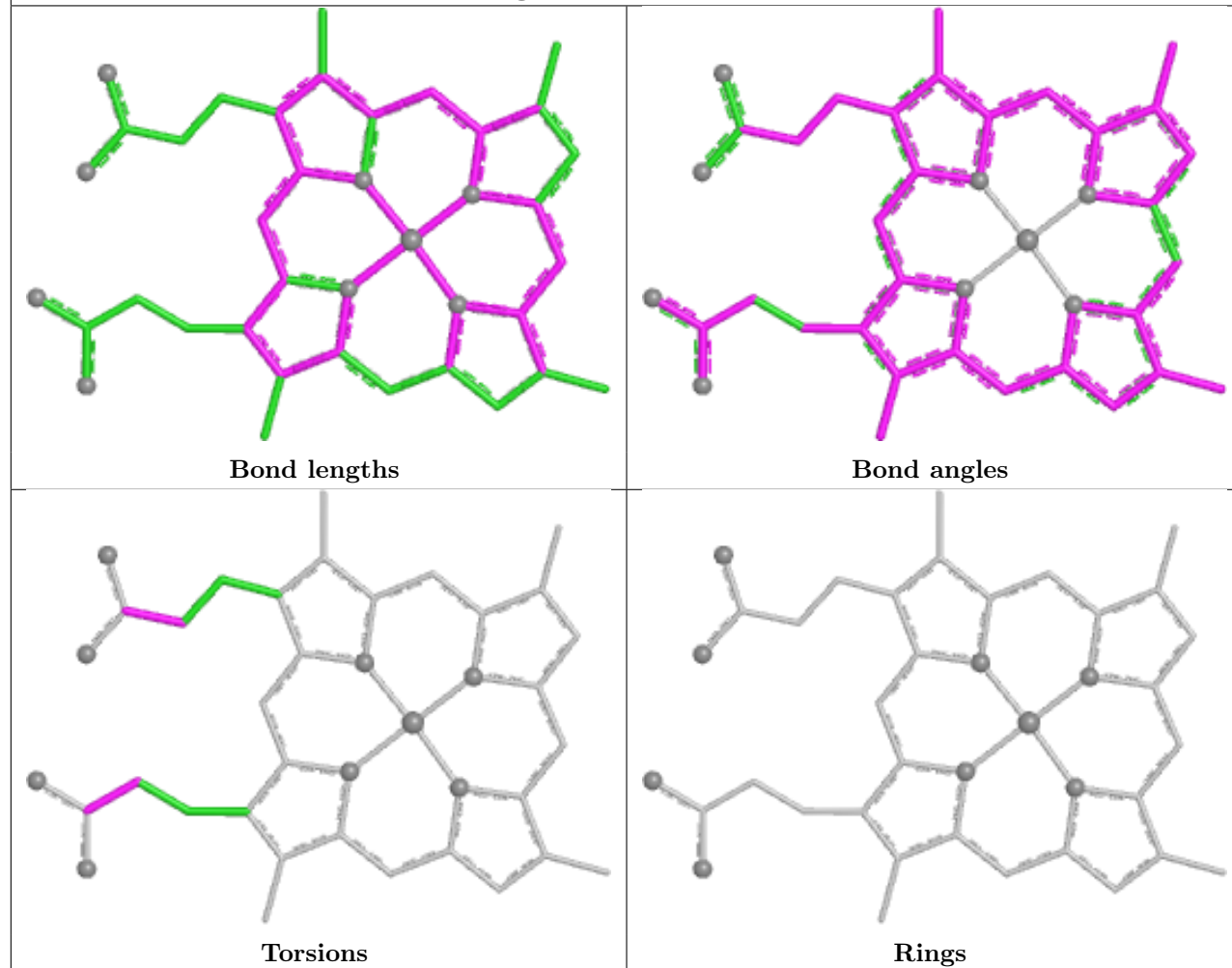
Ligand FDE A 501



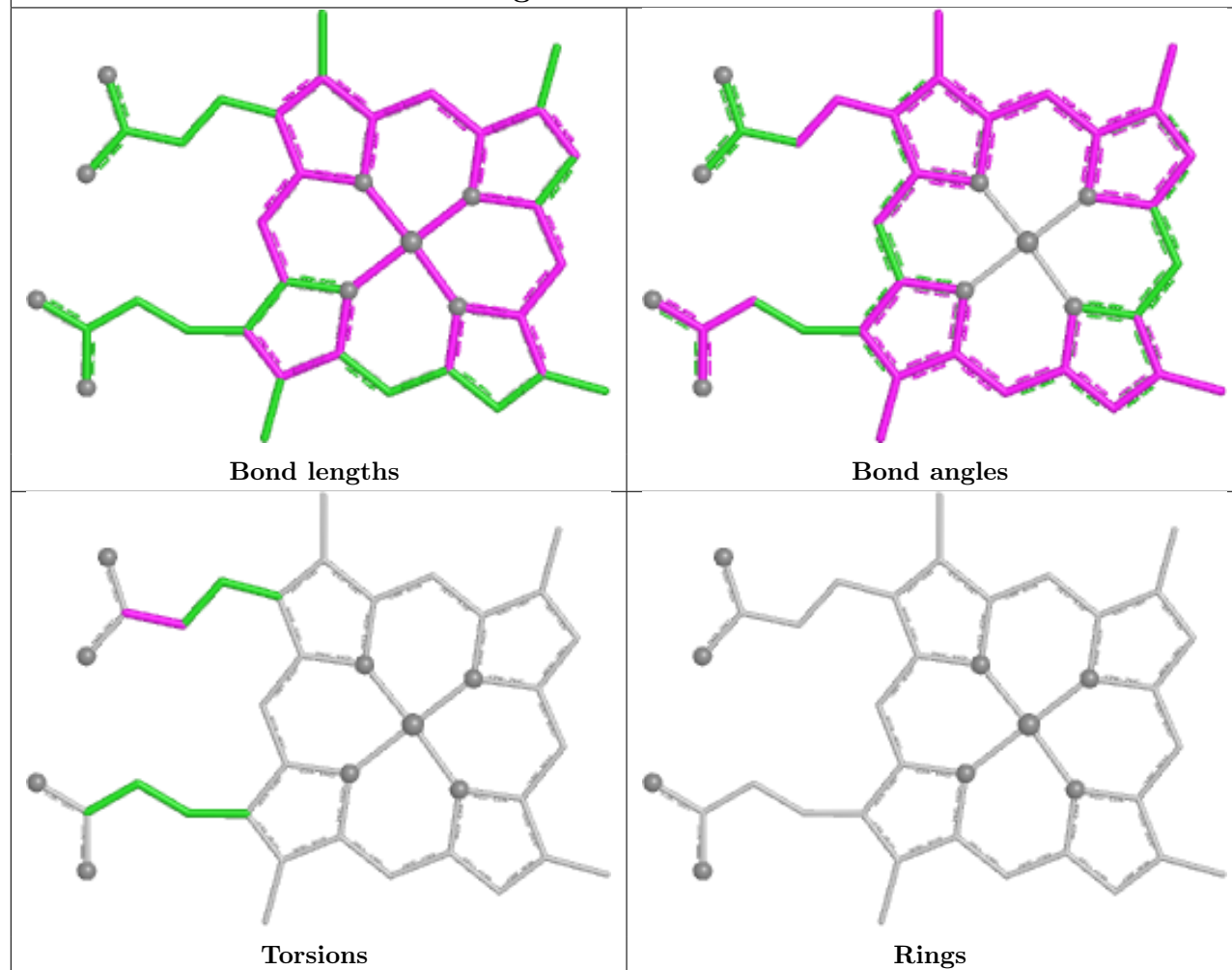
Ligand FDE E 501



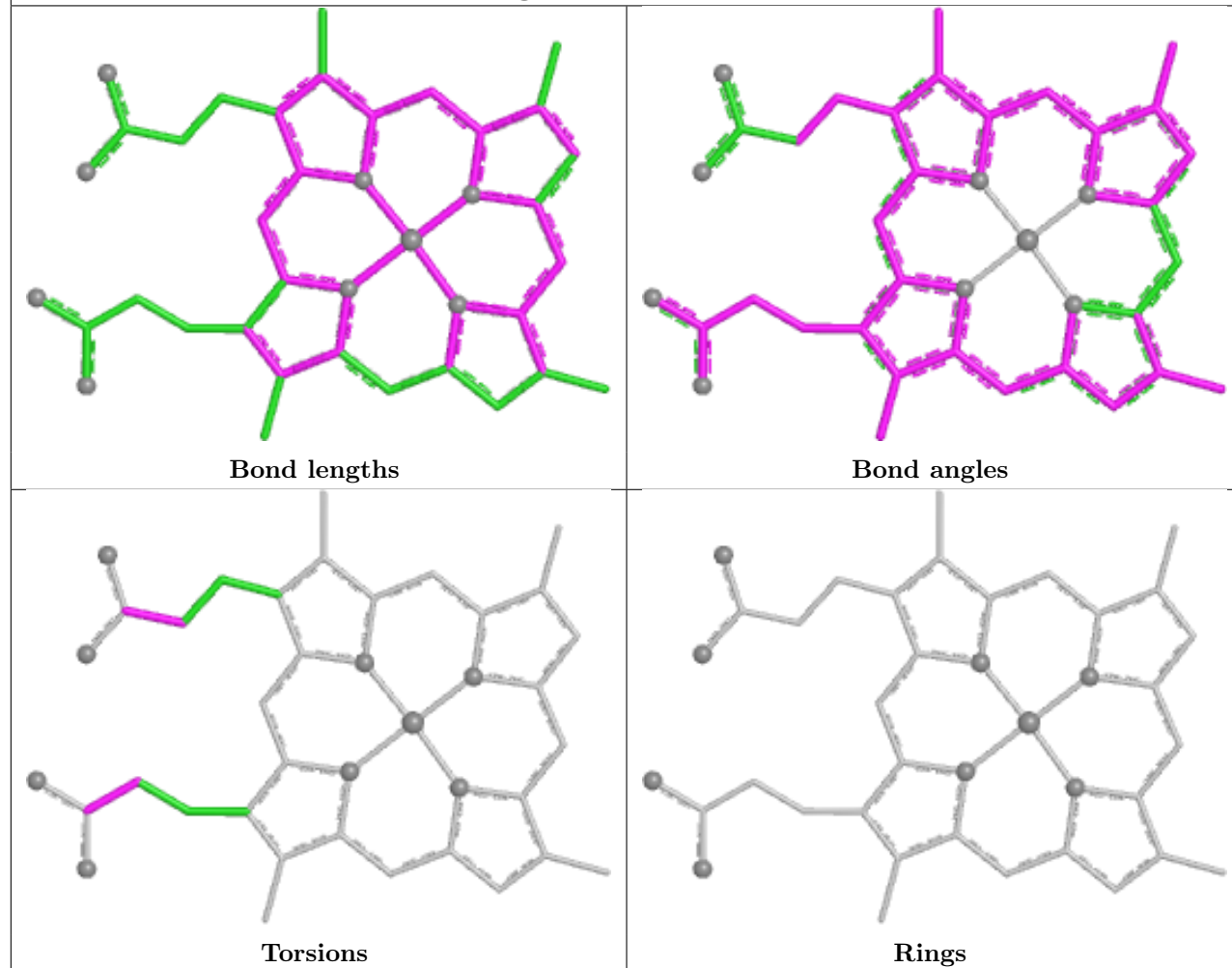
Ligand FDE G 501



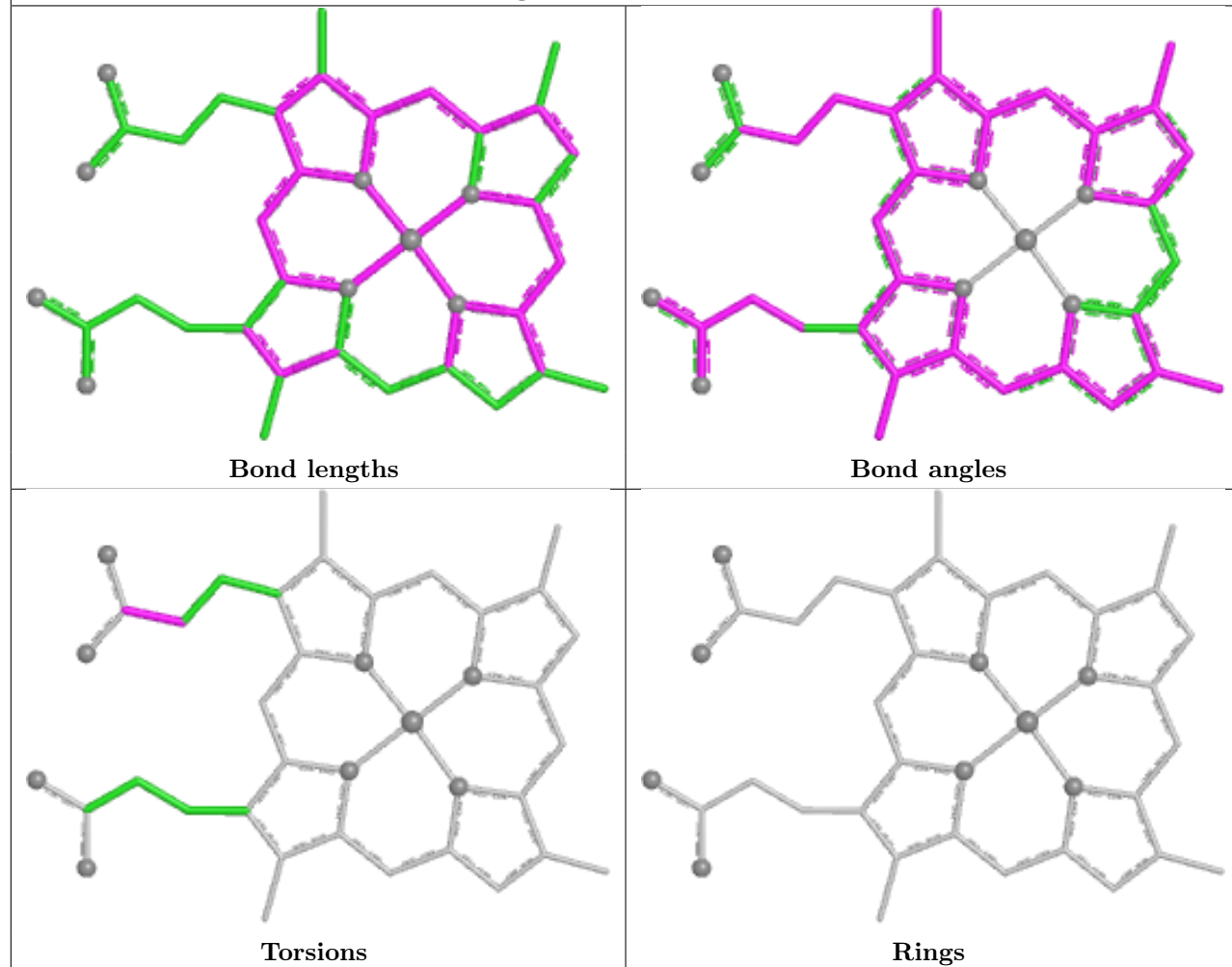
Ligand FDE H 501



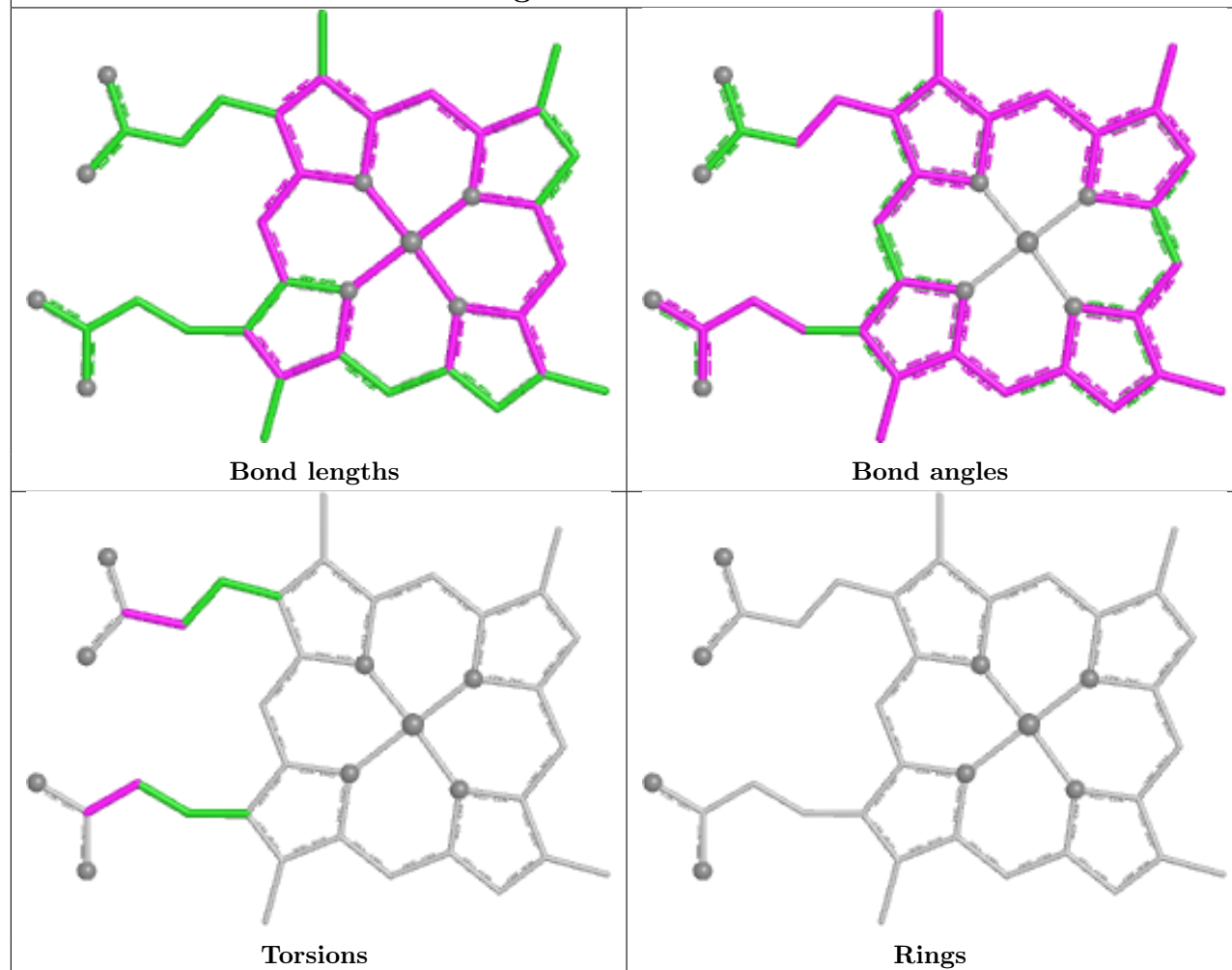
Ligand FDE F 501

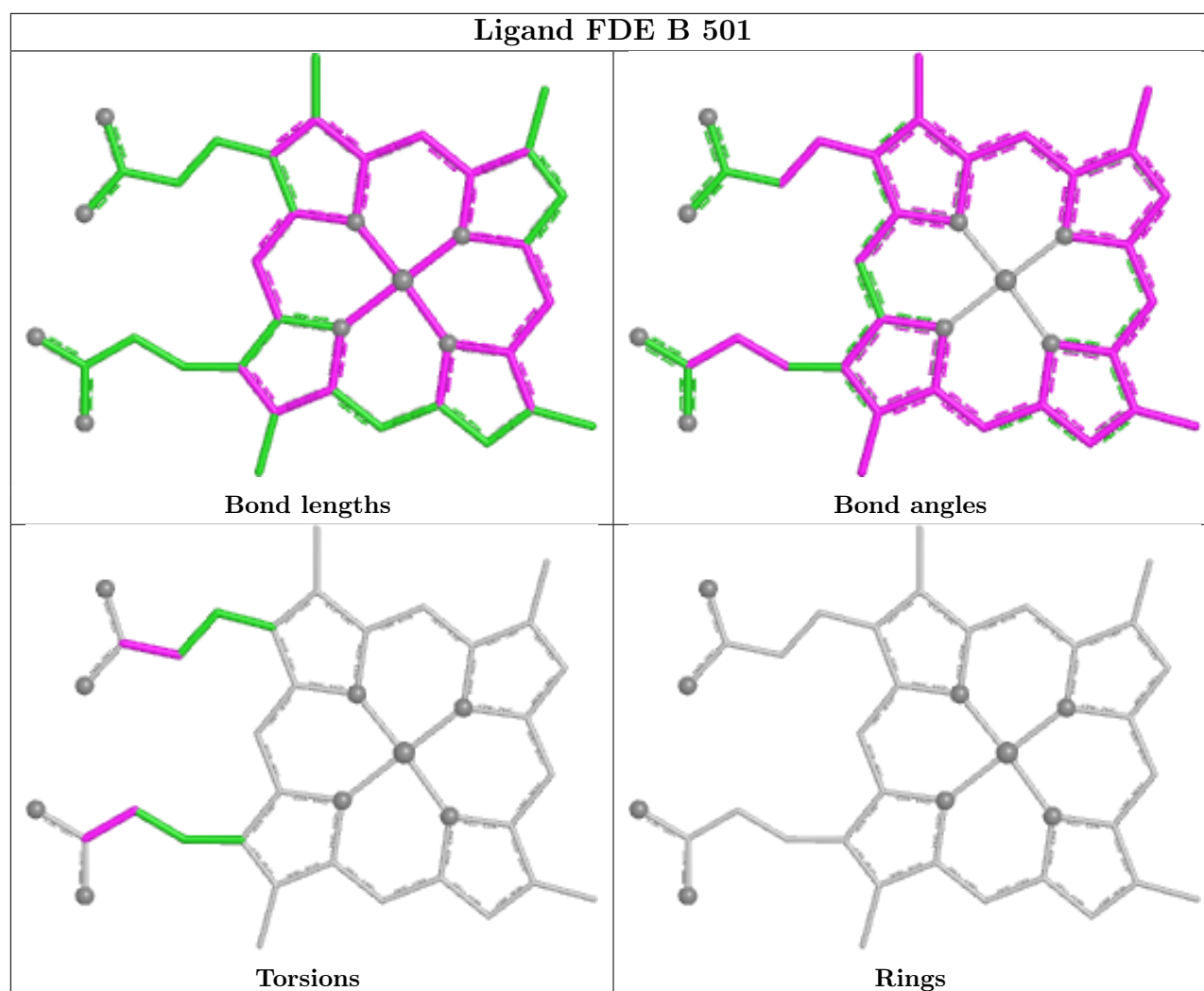


Ligand FDE C 501



Ligand FDE D 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	453/471 (96%)	-0.35	0	100 100	10, 22, 39, 56	0
1	B	453/471 (96%)	-0.49	0	100 100	7, 18, 36, 52	0
1	C	452/471 (95%)	-0.39	0	100 100	10, 22, 37, 52	0
1	D	454/471 (96%)	-0.10	0	100 100	14, 30, 46, 59	0
1	E	451/471 (95%)	-0.46	0	100 100	6, 17, 33, 54	1 (0%)
1	F	455/471 (96%)	-0.26	1 (0%)	91 92	10, 23, 44, 66	0
1	G	451/471 (95%)	-0.37	2 (0%)	88 90	7, 21, 37, 60	3 (0%)
1	H	450/471 (95%)	-0.43	0	100 100	7, 19, 37, 49	0
All	All	3619/3768 (96%)	-0.36	3 (0%)	92 93	6, 22, 40, 66	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	196	PRO	3.7
1	G	252[A]	GLU	3.3
1	G	2	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

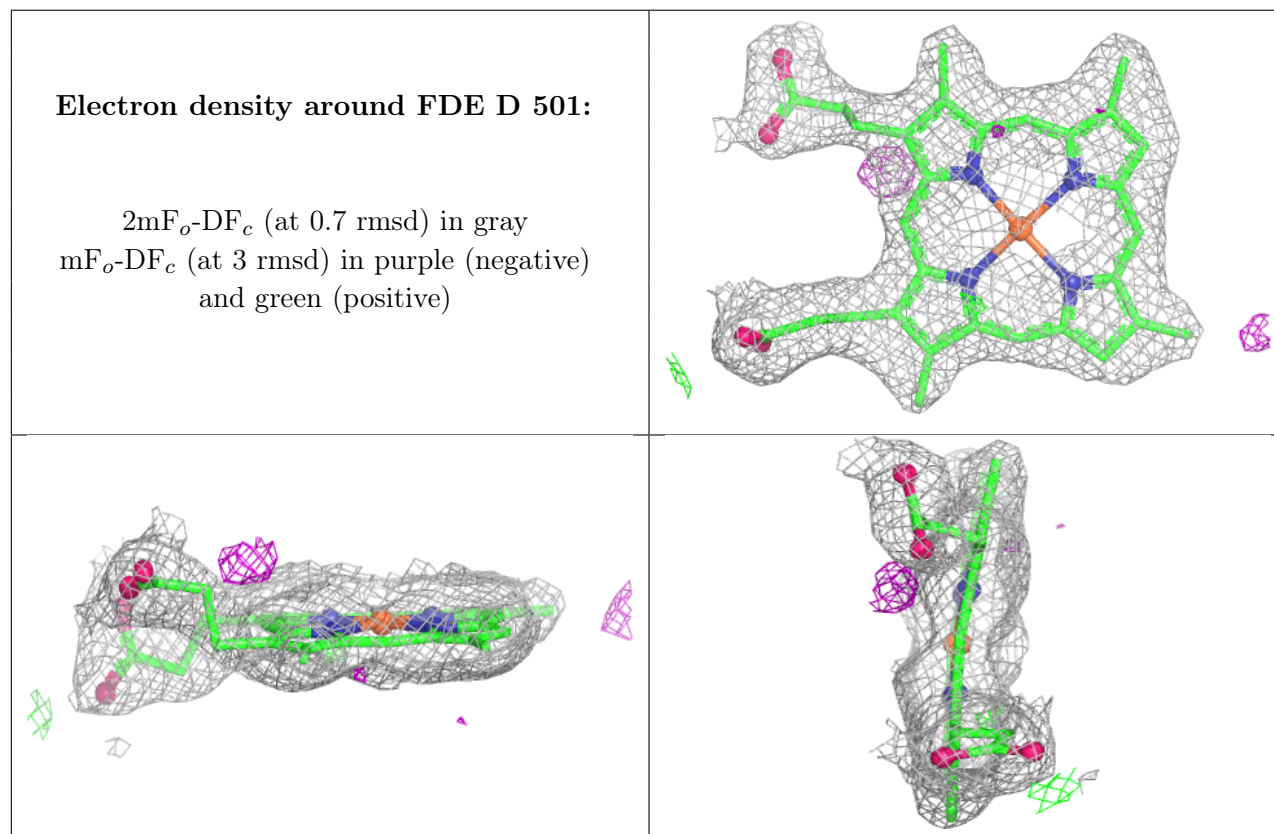
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

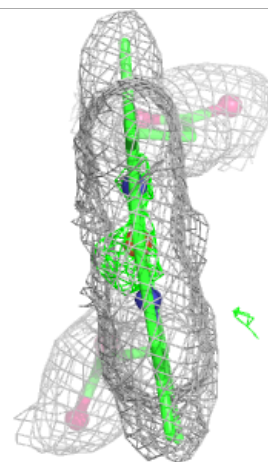
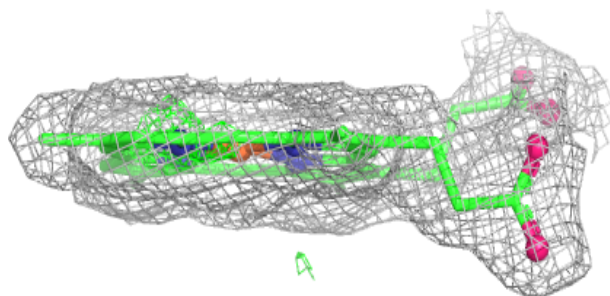
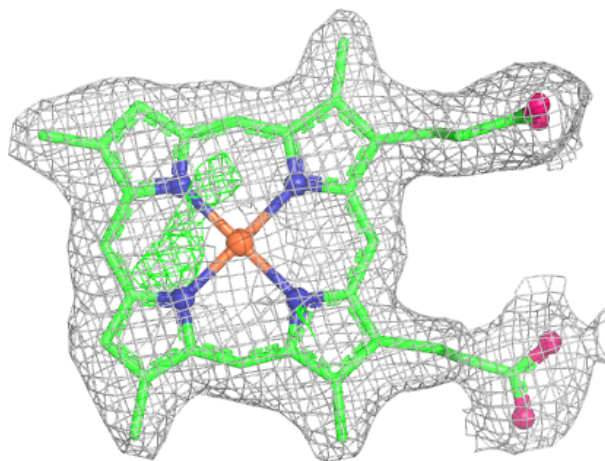
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FDE	D	501	39/39	0.97	0.07	14,21,29,33	0
2	FDE	B	501	39/39	0.98	0.06	6,9,16,17	0
2	FDE	C	501	39/39	0.98	0.06	4,10,15,17	0
2	FDE	A	501	39/39	0.98	0.06	8,15,20,26	0
2	FDE	E	501	39/39	0.98	0.06	7,10,14,19	0
2	FDE	F	501	39/39	0.98	0.05	7,13,20,23	0
2	FDE	G	501	39/39	0.98	0.05	7,15,21,21	0
2	FDE	H	501	39/39	0.99	0.05	6,10,14,19	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.



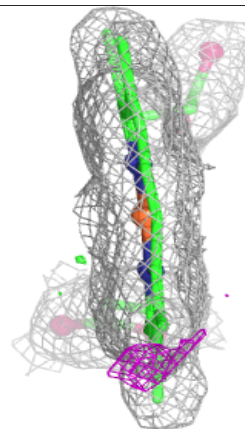
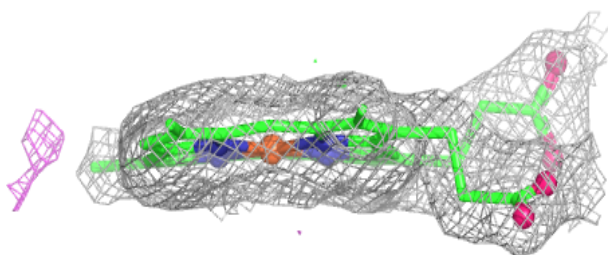
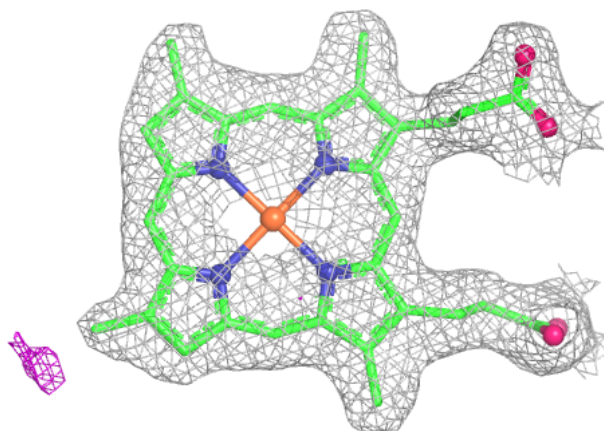
Electron density around FDE B 501:

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



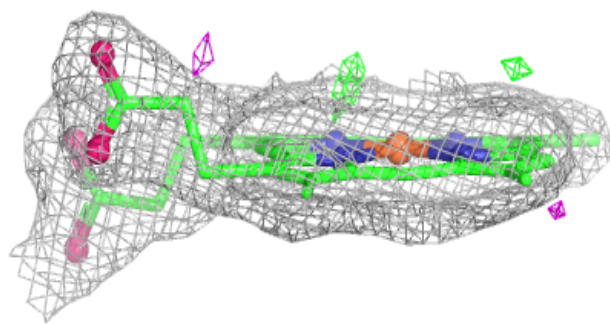
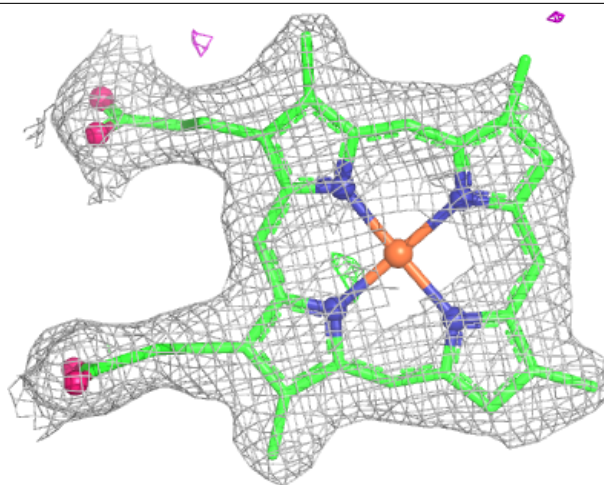
Electron density around FDE C 501:

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



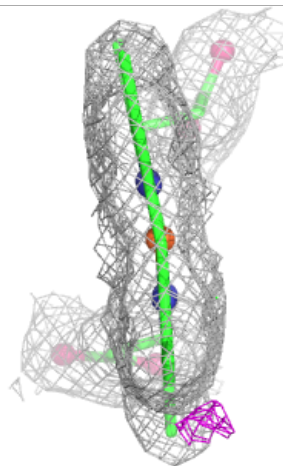
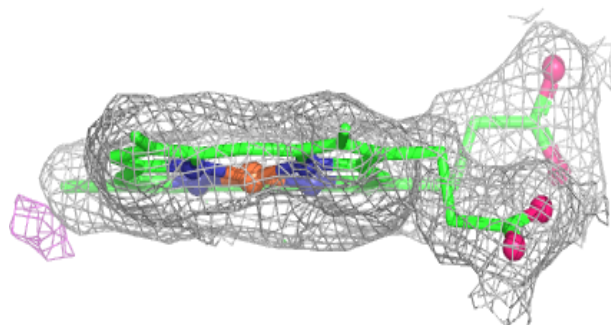
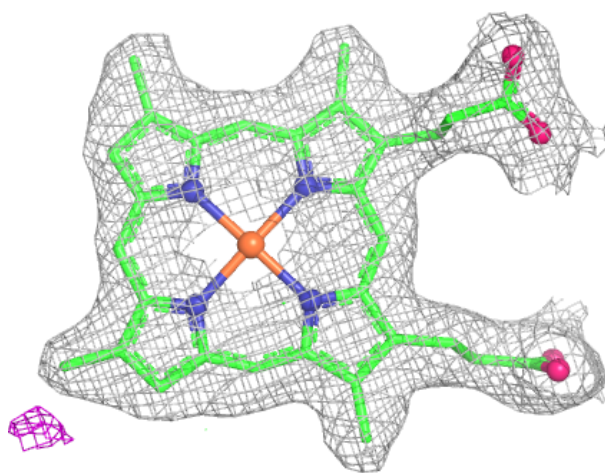
Electron density around FDE A 501:

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



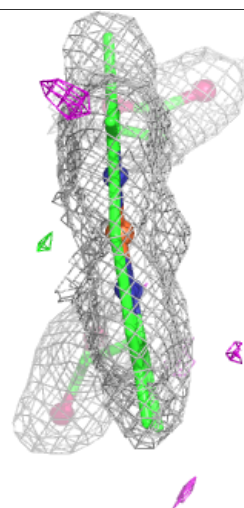
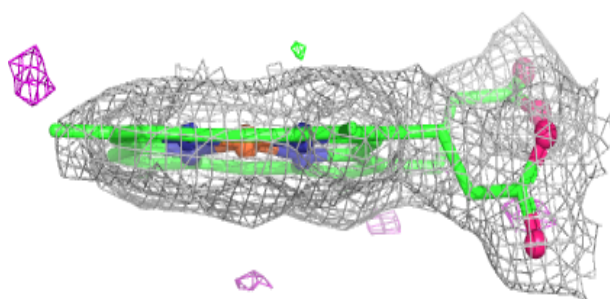
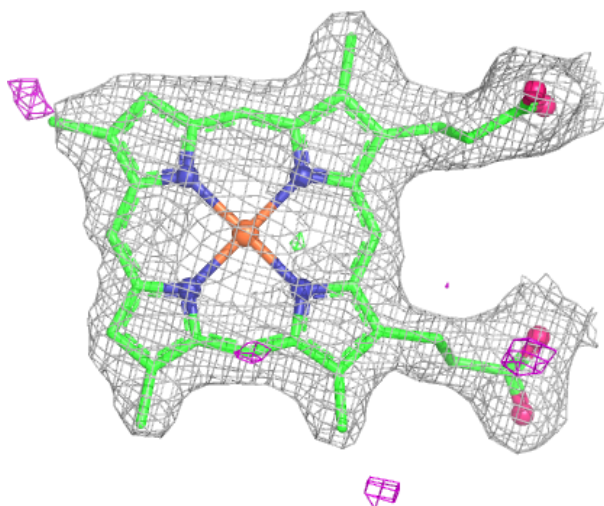
Electron density around FDE E 501:

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



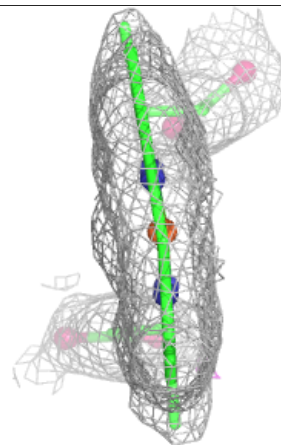
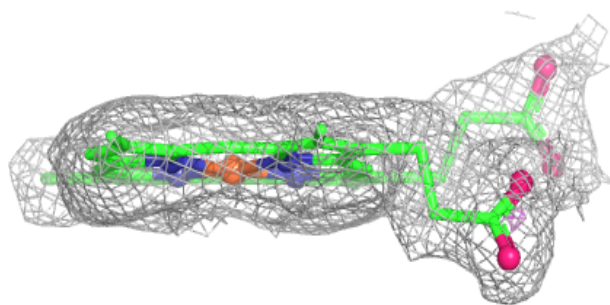
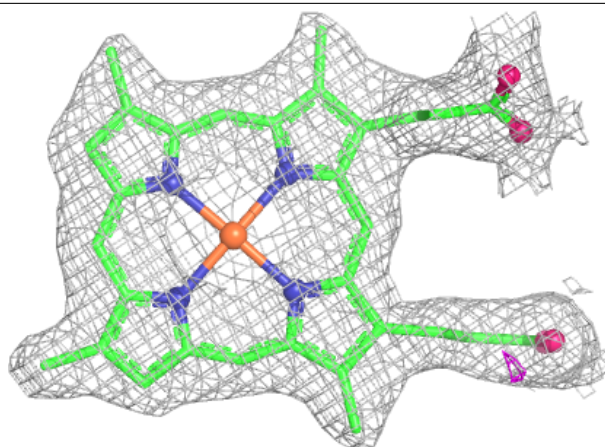
Electron density around FDE F 501:

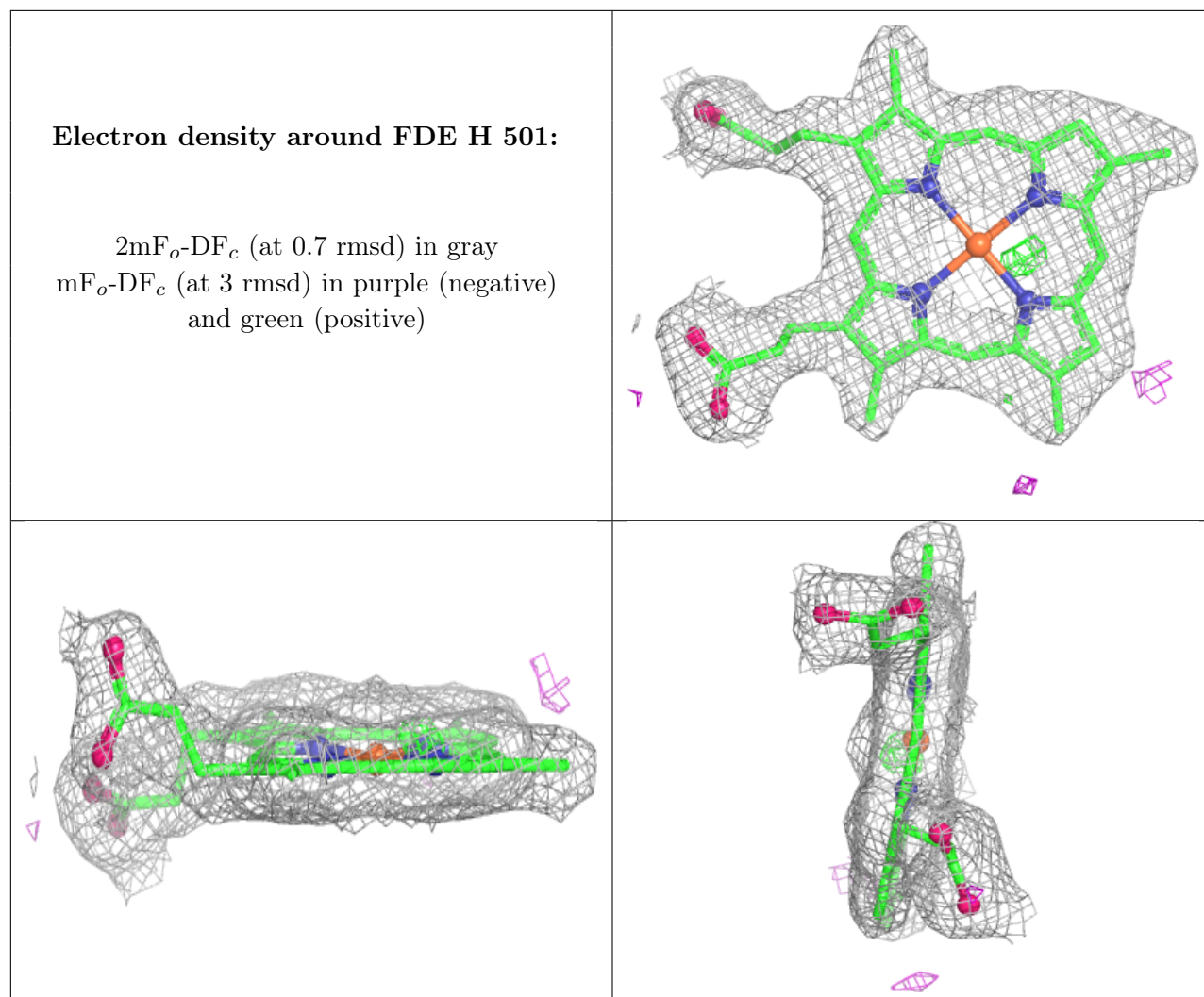
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.