



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:12 am BST

PDB ID : 5JQU
Title : Crystal structure of Cytochrome P450 BM3 heme domain G265F/T269V/L272 W/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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

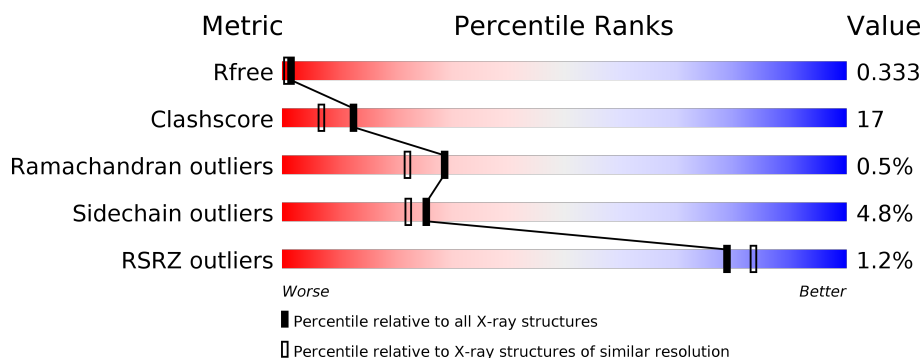
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>• •</div> </div> </div>
1	B	471	<div> <div></div> <div> <div>65%</div> <div>30%</div> <div>• •</div> </div> </div>
1	C	471	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• •</div> </div> </div>
1	D	471	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>• •</div> </div> </div>
1	E	471	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
1	F	471	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	471	<div><div>%</div><div><div></div></div><div>59%34%</div><div></div></div>
1	H	471	<div><div>%</div><div><div></div></div><div>62%32%</div><div></div></div>

2 Entry composition

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

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

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- The ORTEP diagram illustrates the molecular structure of FDE. The central iron atom (Fe) is coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various substituents such as methyl (CMF, CMD, CME, CMA), ethyl (CHD, CHB, CHA), and propyl (CAD, CAA, CBA) groups, and two carboxylic acid groups (O2D, O1D and O2A, O1A). The diagram is labeled with atom names and displacement ellipsoids at the 50% probability level.



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

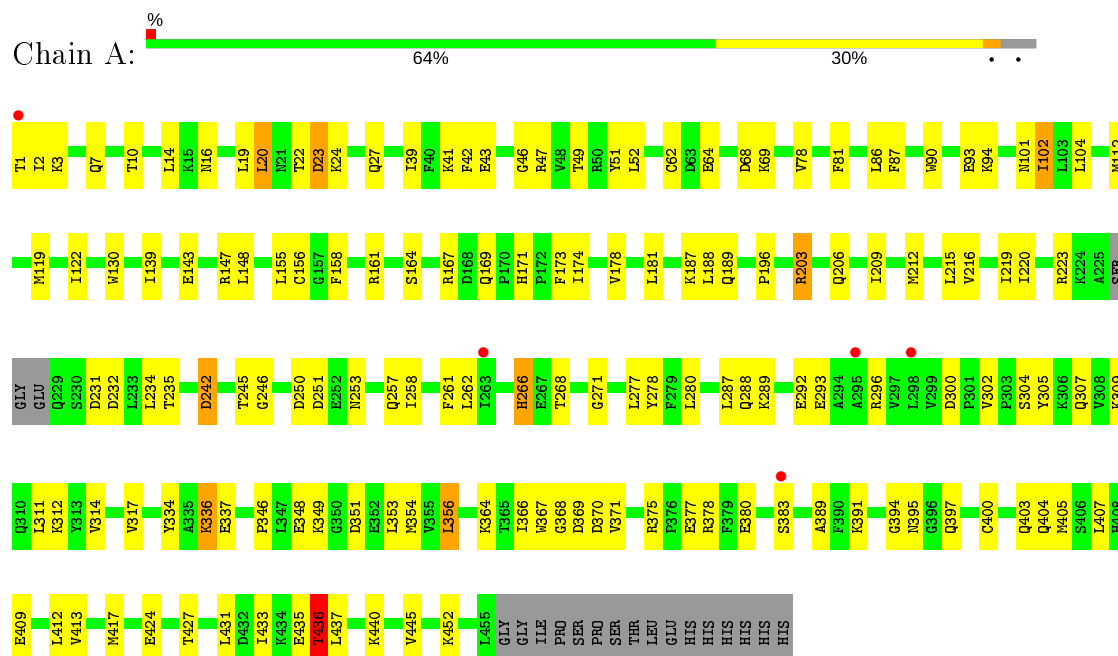
- Molecule 3 is water.

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

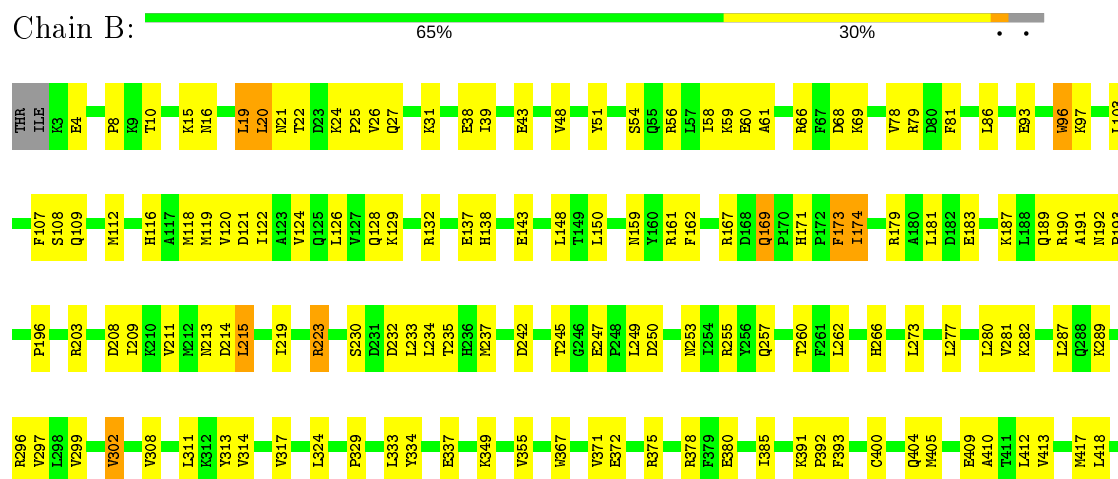
3 Residue-property plots [i](#)

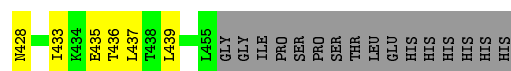
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

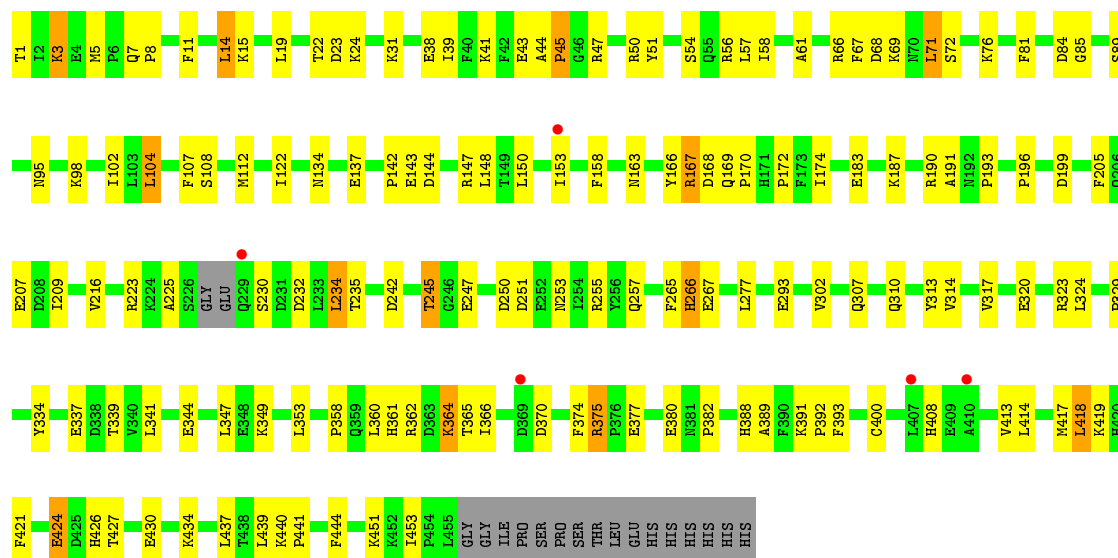


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

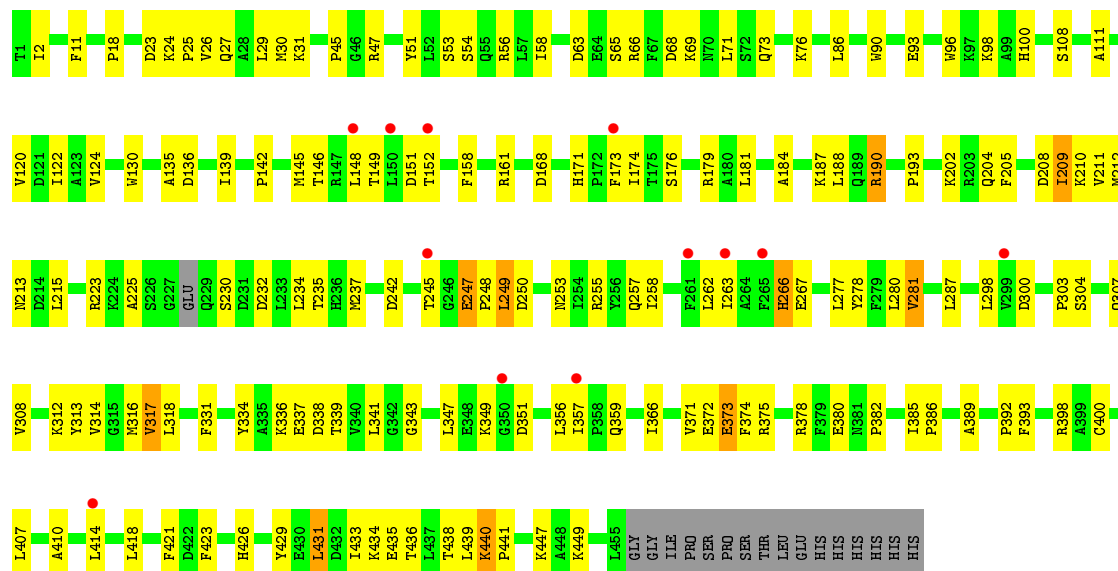




- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

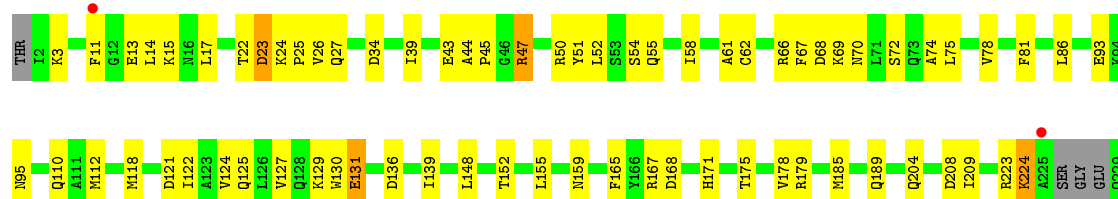


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



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





4 Data and refinement statistics

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) 98.9 (28.85-2.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.16Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.258 , 0.334 0.259 , 0.333	Depositor DCC
R_{free} test set	2000 reflections (0.94%)	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)	0.21 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	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.*

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 [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	0.53	0/3640	0.70	3/4939 (0.1%)
1	B	0.56	0/3665	0.72	1/4972 (0.0%)
1	C	0.53	0/3637	0.72	3/4936 (0.1%)
1	D	0.51	0/3571	0.69	2/4855 (0.0%)
1	E	0.54	1/3668 (0.0%)	0.70	1/4974 (0.0%)
1	F	0.54	2/3629 (0.1%)	0.68	1/4930 (0.0%)
1	G	0.53	0/3638	0.70	1/4939 (0.0%)
1	H	0.51	0/3657	0.70	0/4955
All	All	0.53	3/29105 (0.0%)	0.70	12/39500 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	156	CYS	CB-SG	-6.66	1.71	1.82
1	F	400	CYS	CB-SG	-6.36	1.71	1.82
1	F	156	CYS	CB-SG	-5.72	1.72	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	C	168	ASP	C-N-CA	6.84	138.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	232	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	356	LEU	CA-CB-CG	6.11	129.36	115.30
1	C	71	LEU	CA-CB-CG	5.79	128.62	115.30

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	121	0
1	B	3578	0	3463	114	0
1	C	3552	0	3444	109	0
1	D	3485	0	3286	116	0
1	E	3579	0	3482	90	0
1	F	3543	0	3387	138	0
1	G	3546	0	3392	143	0
1	H	3571	0	3480	121	0
2	A	39	0	25	2	0
2	B	39	0	25	2	0
2	C	39	0	25	2	0
2	D	39	0	25	2	0
2	E	39	0	25	3	0
2	F	39	0	25	1	0
2	G	39	0	25	4	0
2	H	39	0	25	3	0
3	A	149	0	0	27	0
3	B	189	0	0	21	0
3	C	165	0	0	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	171	0	0	23	1
All	All	29916	0	27577	941	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 941 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:G:391:LYS:NZ	3:G:601:HOH:O	1.92	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

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%)	47	46
1	B	451/471 (96%)	437 (97%)	13 (3%)	1 (0%)	47	46
1	C	449/471 (95%)	426 (95%)	21 (5%)	2 (0%)	34	29
1	D	450/471 (96%)	427 (95%)	18 (4%)	5 (1%)	14	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	448/471 (95%)	426 (95%)	19 (4%)	3 (1%)	22	15
1	F	451/471 (96%)	427 (95%)	19 (4%)	5 (1%)	14	8
1	G	449/471 (95%)	431 (96%)	17 (4%)	1 (0%)	47	46
1	H	446/471 (95%)	428 (96%)	18 (4%)	0	100	100
All	All	3592/3768 (95%)	3431 (96%)	143 (4%)	18 (0%)	29	22

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 ⓘ

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%)	348 (95%)	19 (5%)	23	19
1	B	374/415 (90%)	361 (96%)	13 (4%)	36	34
1	C	368/415 (89%)	351 (95%)	17 (5%)	27	23
1	D	343/415 (83%)	330 (96%)	13 (4%)	33	31
1	E	375/415 (90%)	358 (96%)	17 (4%)	27	24
1	F	360/415 (87%)	337 (94%)	23 (6%)	17	12
1	G	364/415 (88%)	344 (94%)	20 (6%)	21	17
1	H	375/415 (90%)	356 (95%)	19 (5%)	24	20
All	All	2926/3320 (88%)	2785 (95%)	141 (5%)	25	22

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	22	THR
1	E	445	VAL
1	H	212	MET
1	E	102	ILE
1	E	266	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	110	GLN
1	E	266	HIS
1	F	387	GLN
1	D	403	GLN
1	F	359	GLN

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 carbohydrates 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	32,46,46	6.93	19 (59%)	20,76,76	3.33	10 (50%)
2	FDE	C	501	1	32,46,46	6.44	18 (56%)	20,76,76	3.43	11 (55%)
2	FDE	E	501	1,3	32,46,46	6.69	16 (50%)	20,76,76	3.57	9 (45%)
2	FDE	A	501	1,3	32,46,46	6.46	16 (50%)	20,76,76	3.80	11 (55%)
2	FDE	G	501	1	32,46,46	6.67	18 (56%)	20,76,76	3.51	10 (50%)
2	FDE	D	501	1	32,46,46	6.51	18 (56%)	20,76,76	3.50	10 (50%)
2	FDE	F	501	1	32,46,46	6.51	18 (56%)	20,76,76	3.79	10 (50%)
2	FDE	B	501	1	32,46,46	6.77	17 (53%)	20,76,76	3.22	10 (50%)

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	-	0/6/86/86	-
2	FDE	C	501	1	-	0/6/86/86	-
2	FDE	E	501	1,3	-	1/6/86/86	-
2	FDE	A	501	1,3	-	0/6/86/86	-
2	FDE	G	501	1	-	0/6/86/86	-
2	FDE	D	501	1	-	2/6/86/86	-
2	FDE	F	501	1	-	0/6/86/86	-
2	FDE	B	501	1	-	1/6/86/86	-

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	FDE	C3A-C2A	19.14	1.49	1.34
2	H	501	FDE	C3A-C2A	18.70	1.49	1.34
2	E	501	FDE	C3A-C2A	18.64	1.49	1.34
2	B	501	FDE	C3A-C2A	18.31	1.48	1.34
2	D	501	FDE	C3A-C2A	18.25	1.48	1.34

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FDE	CBD-CAD-C3D	-9.95	94.14	112.49
2	H	501	FDE	CHA-C1A-NA	7.33	124.58	110.75
2	E	501	FDE	CHA-C1A-NA	7.16	124.25	110.75
2	A	501	FDE	CHC-C1C-NC	7.02	123.99	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	FDE	CHA-C1A-NA	6.77	123.53	110.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	FDE	C3A-C2A-CAA-CBA
2	D	501	FDE	C1A-C2A-CAA-CBA
2	B	501	FDE	C2A-CAA-CBA-CGA
2	D	501	FDE	C3A-C2A-CAA-CBA

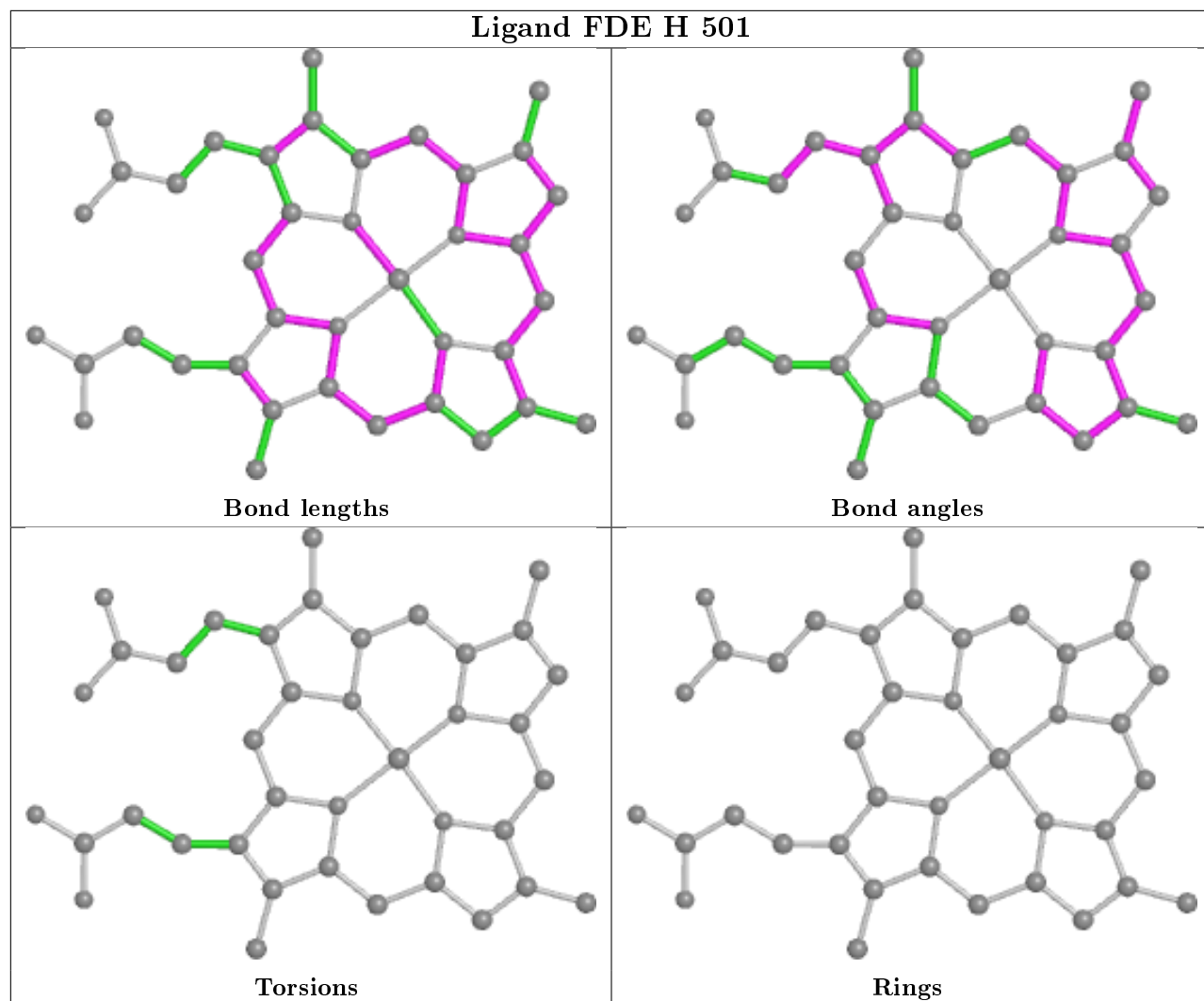
There are no ring outliers.

8 monomers are involved in 19 short contacts:

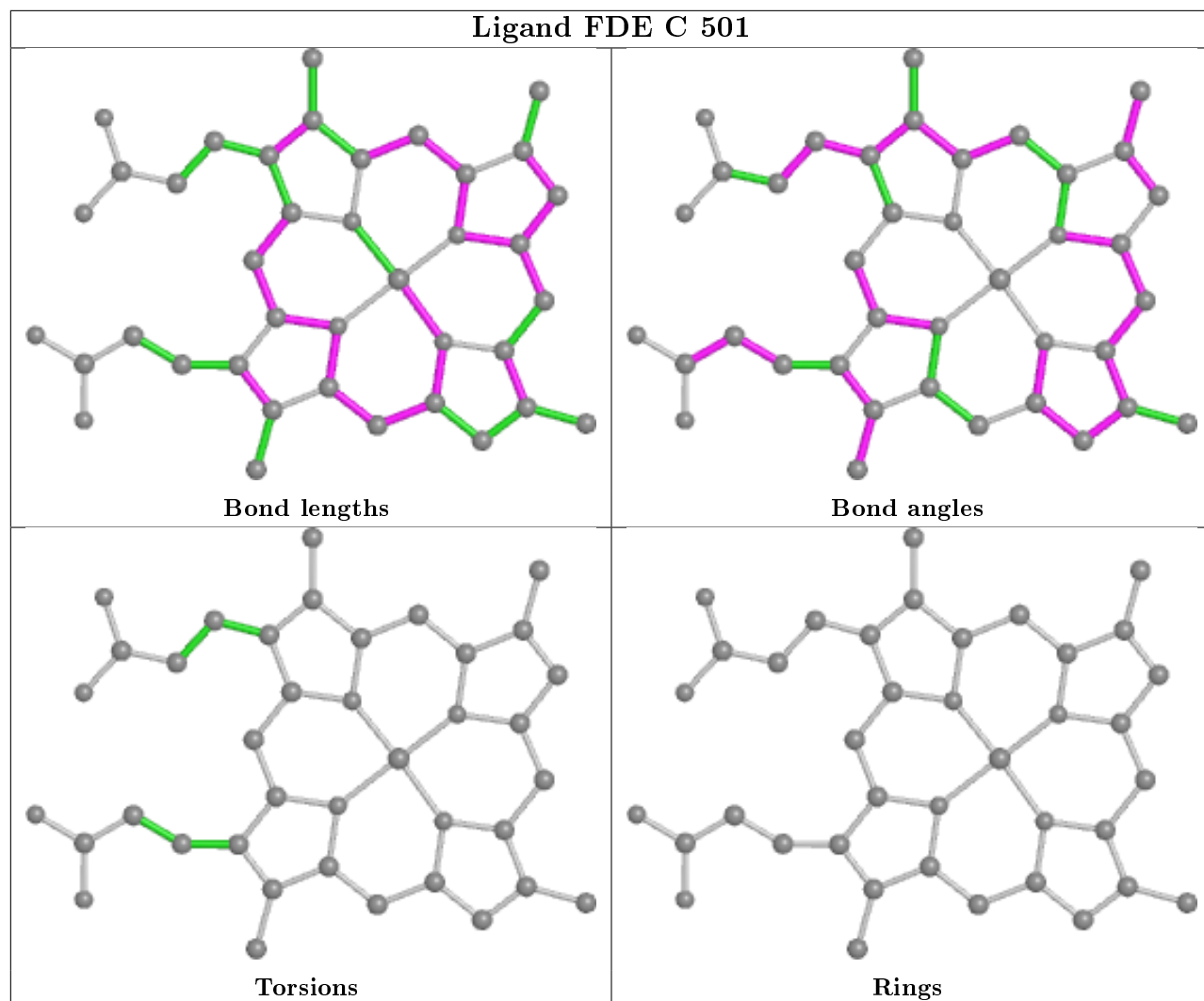
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	FDE	3	0
2	C	501	FDE	2	0
2	E	501	FDE	3	0
2	A	501	FDE	2	0
2	G	501	FDE	4	0
2	D	501	FDE	2	0
2	F	501	FDE	1	0
2	B	501	FDE	2	0

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.

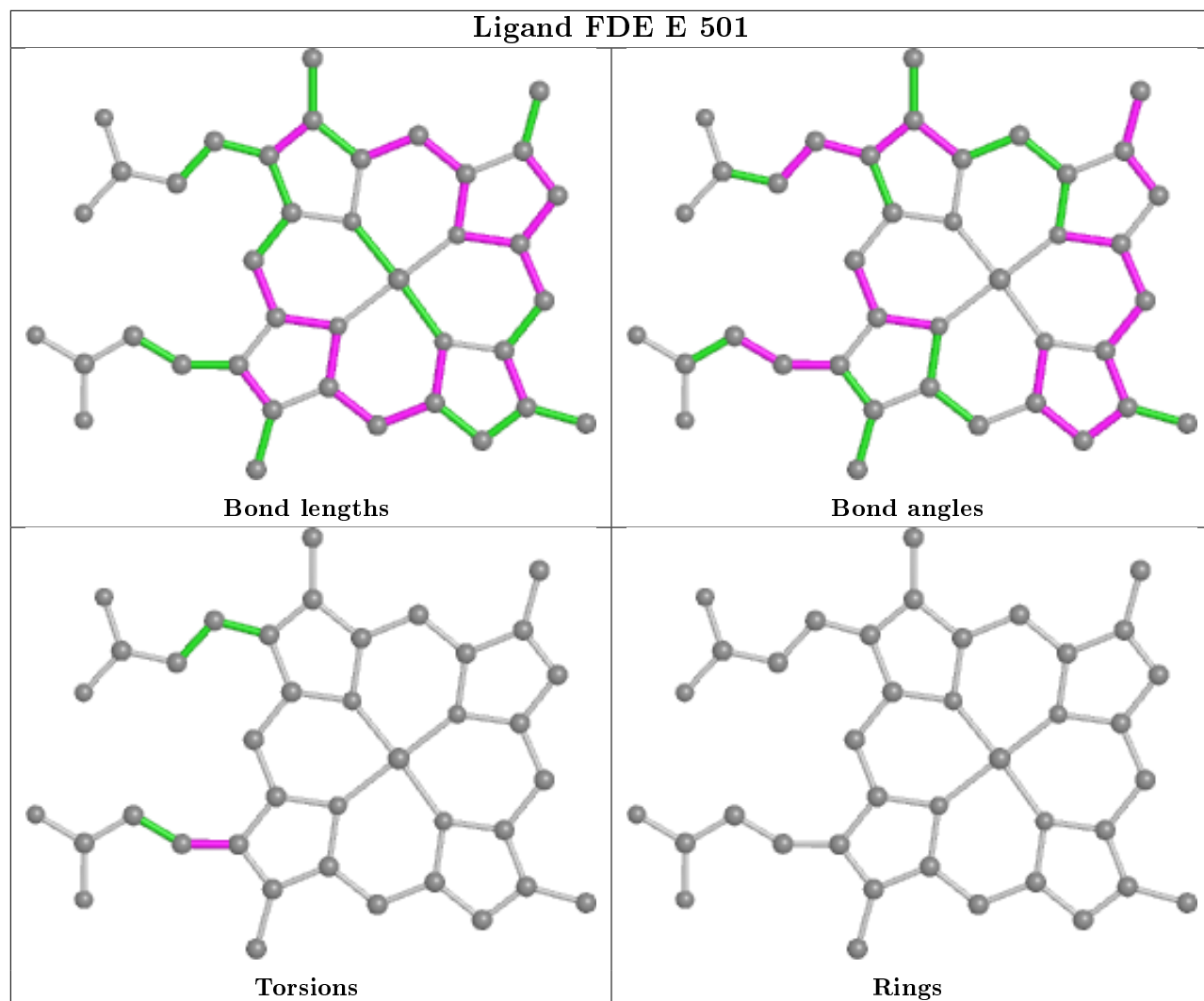
Ligand FDE H 501



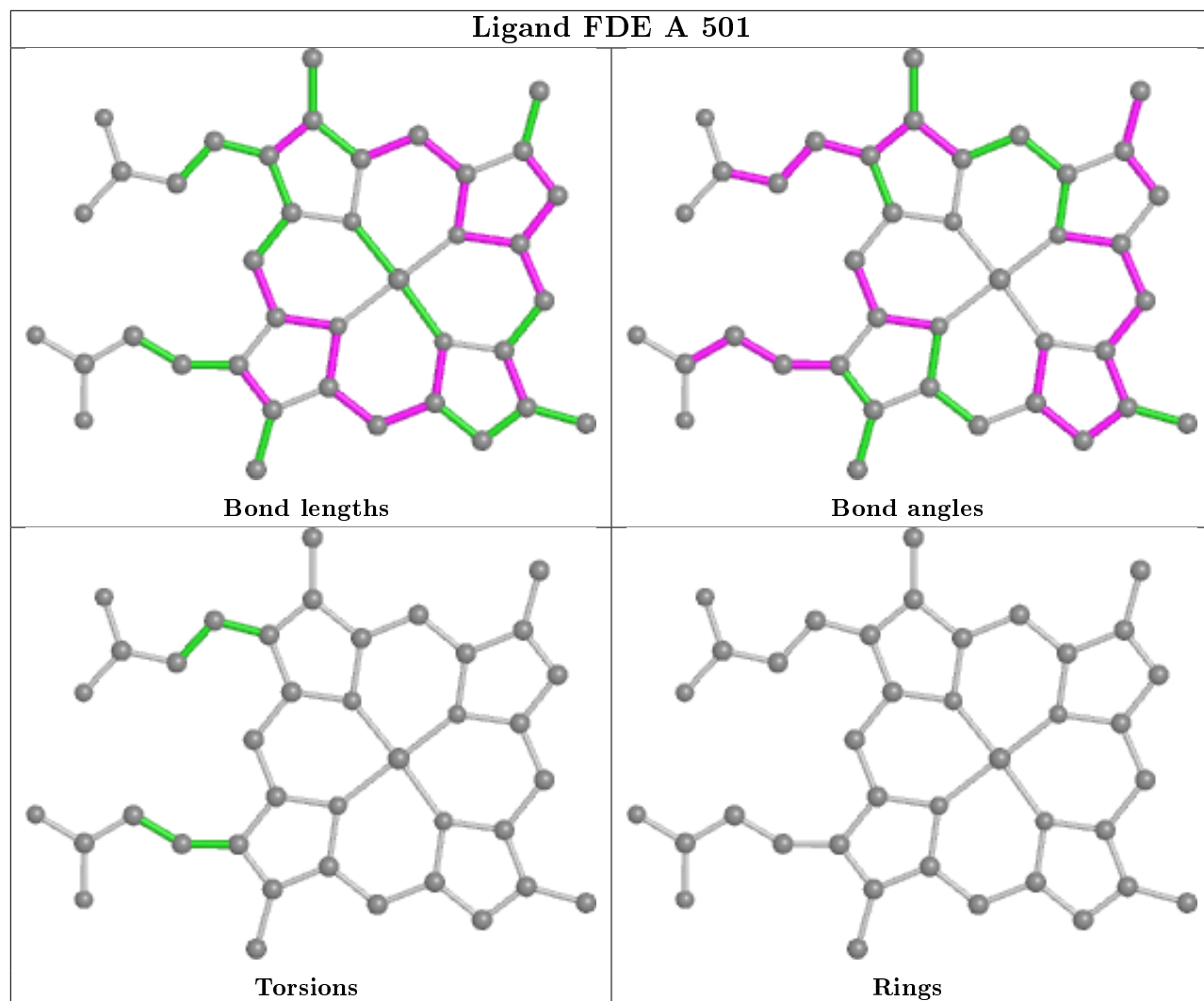
Ligand FDE C 501



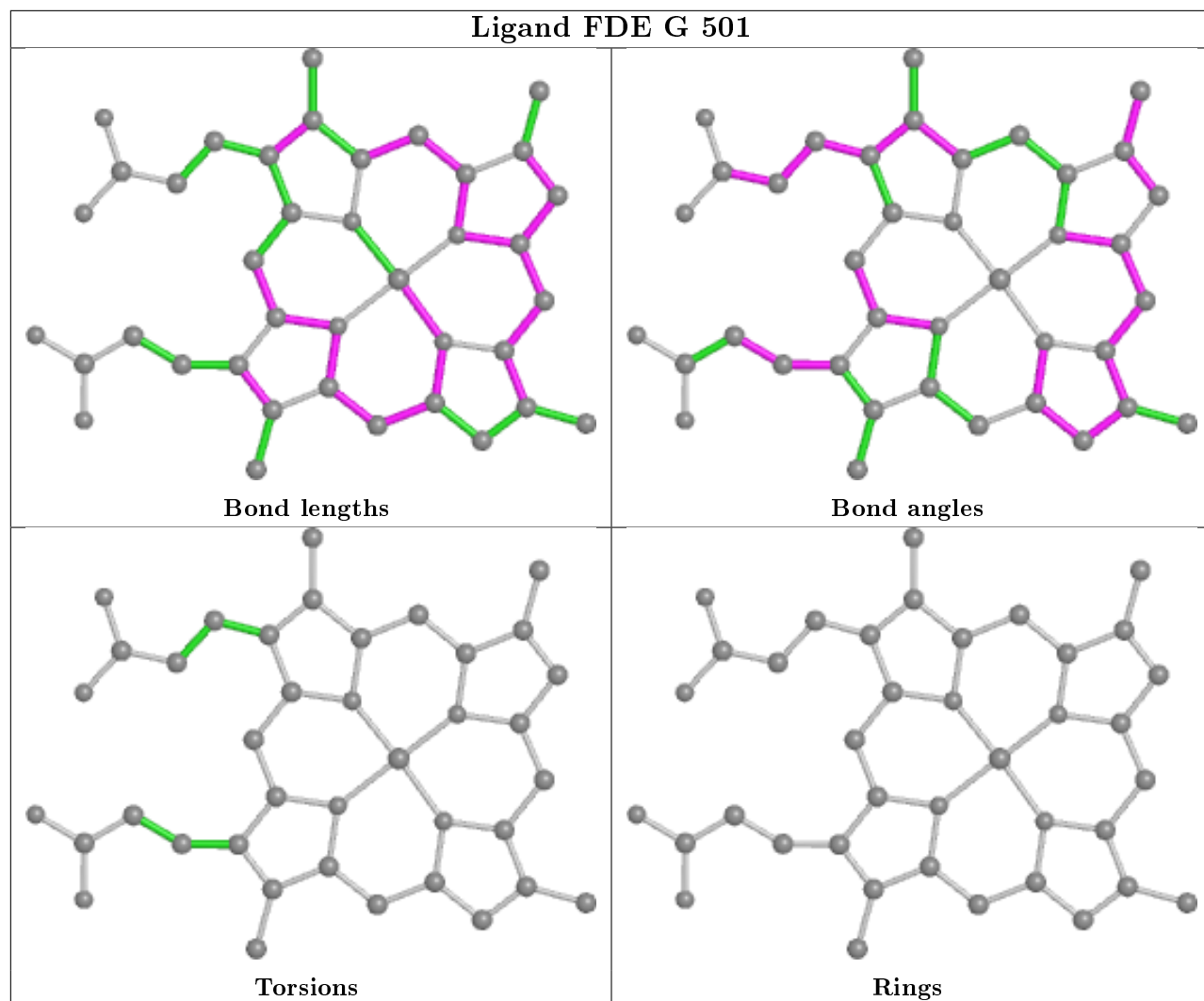
Ligand FDE E 501

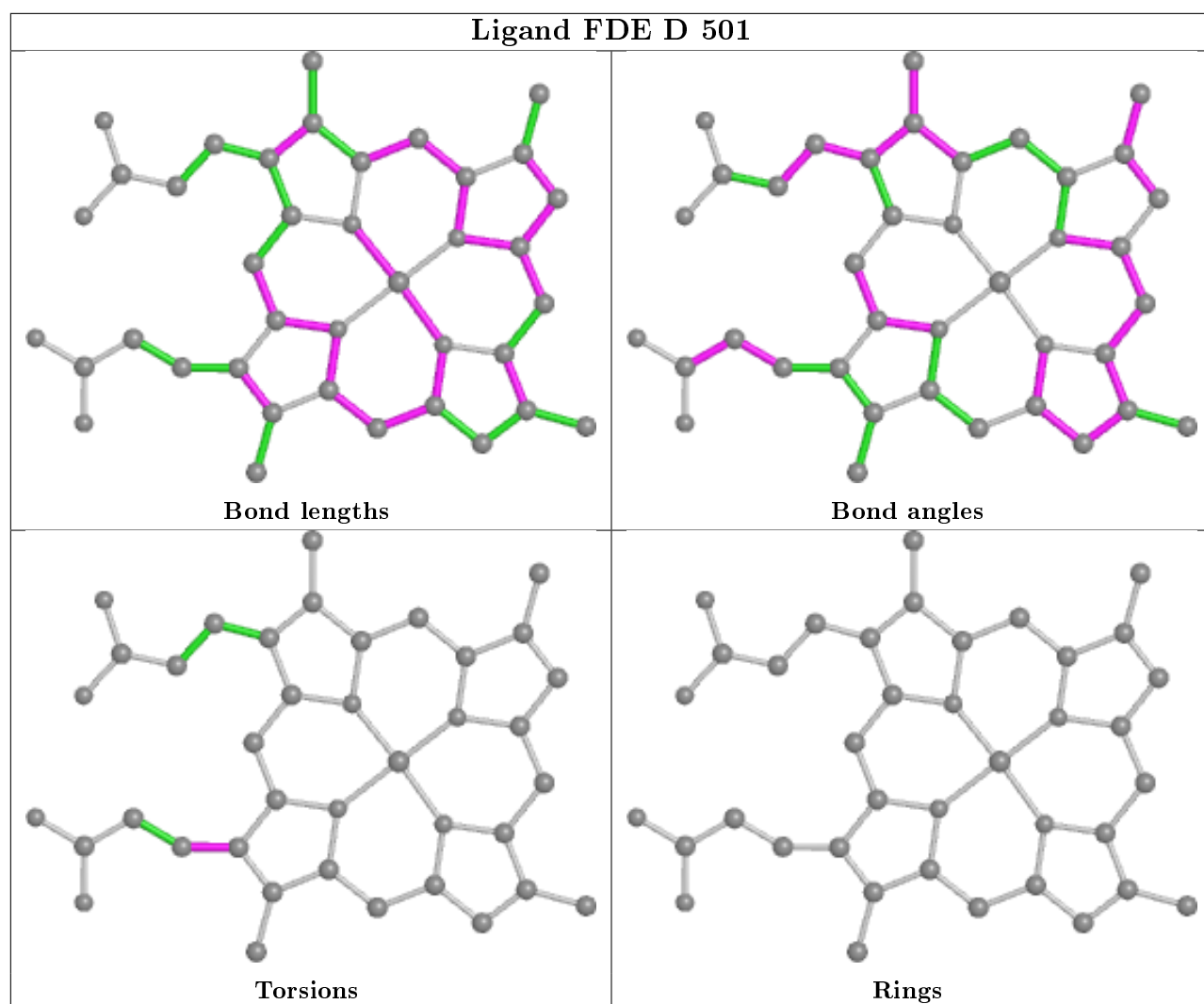


Ligand FDE A 501

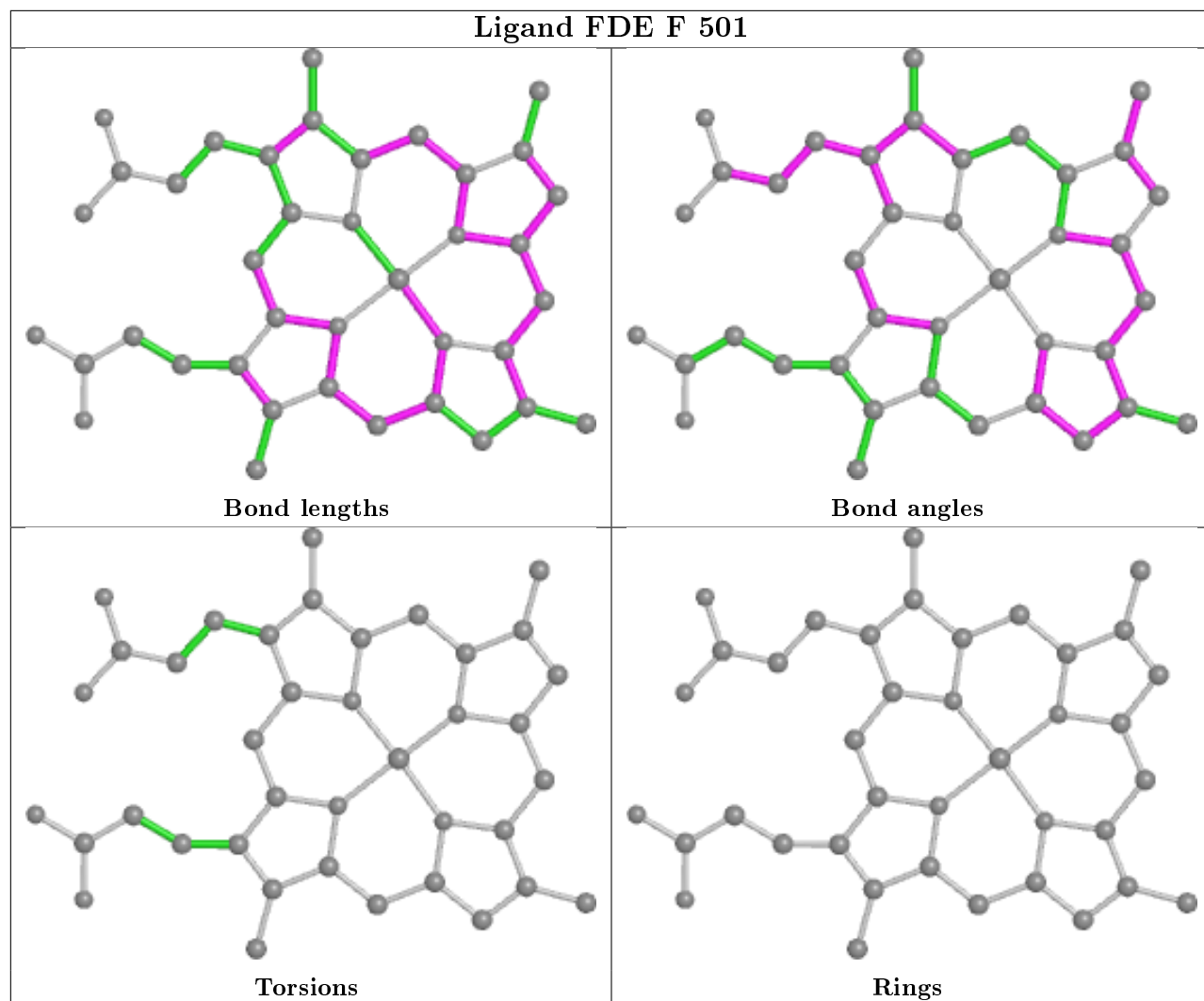


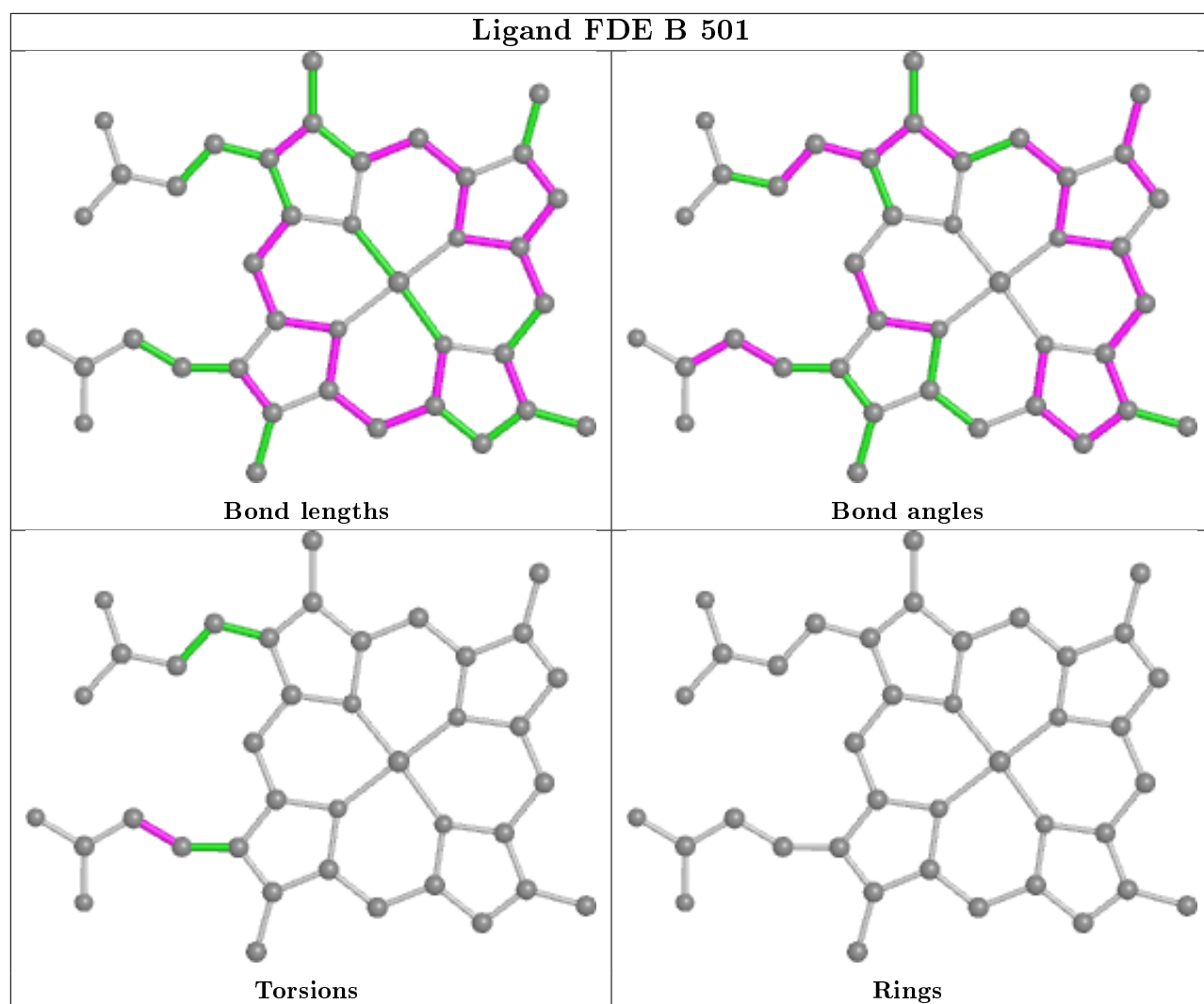
Ligand FDE G 501





Ligand FDE F 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/471 (95%)	0.14	5 (1%) 80 85	4, 15, 28, 35	0
1	B	453/471 (96%)	0.01	0 100 100	2, 10, 25, 36	0
1	C	453/471 (96%)	0.03	5 (1%) 80 85	2, 11, 25, 37	0
1	D	454/471 (96%)	0.30	12 (2%) 56 64	10, 21, 33, 42	0
1	E	451/471 (95%)	0.06	4 (0%) 84 88	4, 12, 26, 37	0
1	F	455/471 (96%)	0.20	8 (1%) 68 75	7, 19, 32, 38	0
1	G	451/471 (95%)	0.10	6 (1%) 77 82	4, 16, 32, 42	0
1	H	450/471 (95%)	0.10	4 (0%) 84 88	3, 13, 26, 36	0
All	All	3619/3768 (96%)	0.12	44 (1%) 79 83	2, 15, 29, 42	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	6.5
1	F	191	ALA	4.6
1	G	379	PHE	3.8
1	D	173	PHE	3.7
1	G	11	PHE	3.7

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 carbohydrates in this entry.

6.4 Ligands

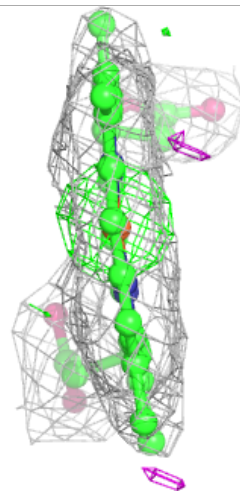
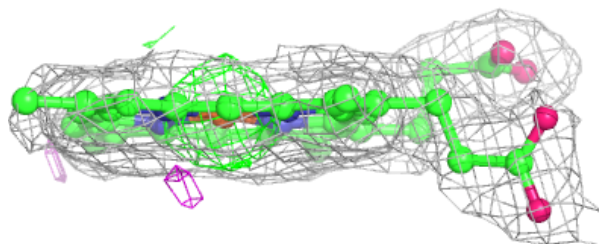
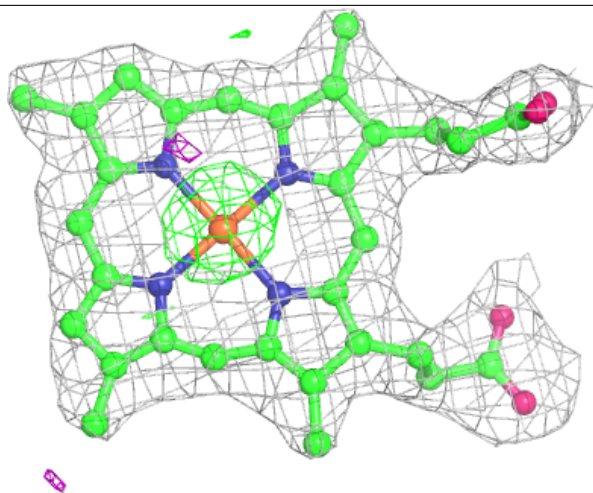
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FDE	A	501	39/39	0.82	0.19	5,10,16,127	0
2	FDE	C	501	39/39	0.93	0.19	2,2,7,10	0
2	FDE	H	501	39/39	0.94	0.18	2,2,7,7	0
2	FDE	G	501	39/39	0.94	0.17	3,6,11,16	0
2	FDE	D	501	39/39	0.94	0.18	5,10,15,17	0
2	FDE	F	501	39/39	0.94	0.15	4,8,18,25	0
2	FDE	E	501	39/39	0.95	0.17	2,4,18,24	0
2	FDE	B	501	39/39	0.95	0.18	2,3,11,16	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.

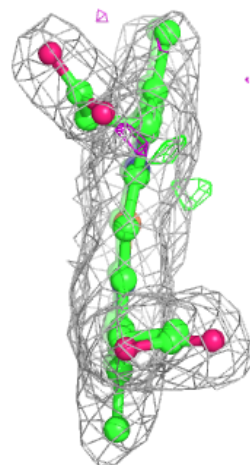
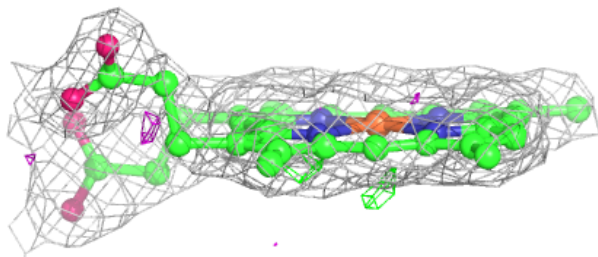
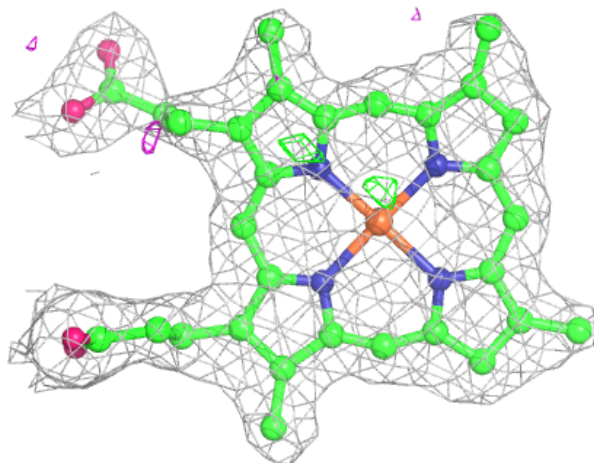
Electron density around FDE A 501:

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



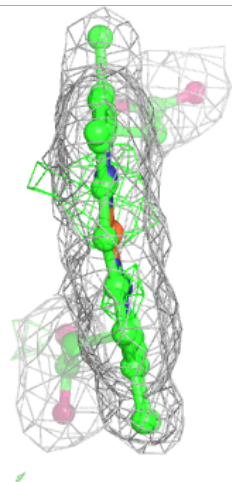
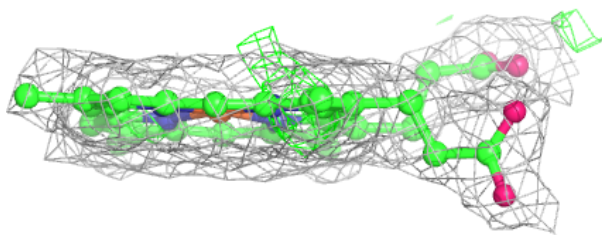
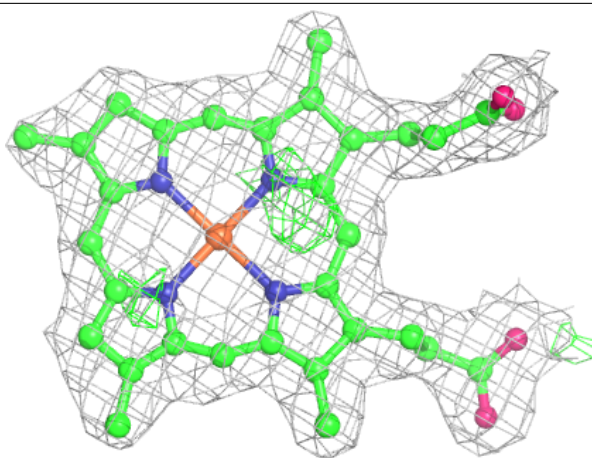
Electron density around FDE C 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



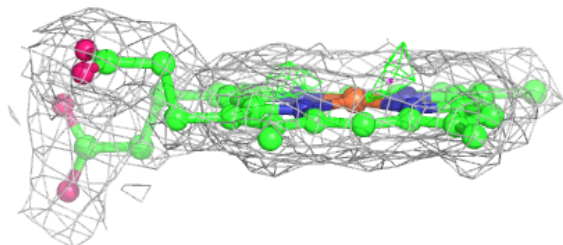
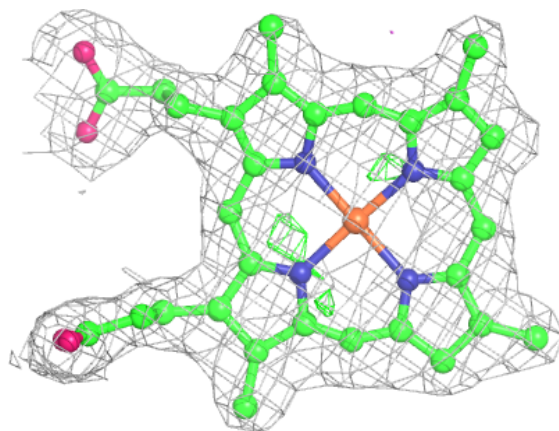
Electron density around FDE H 501:

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



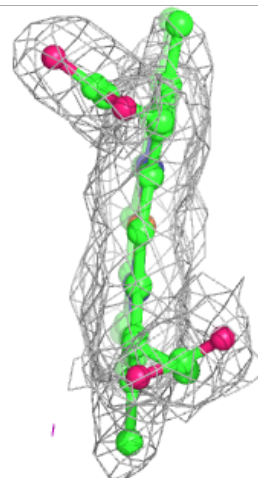
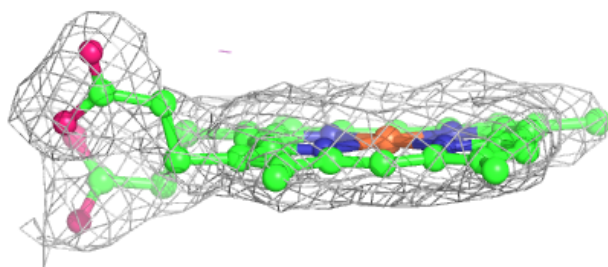
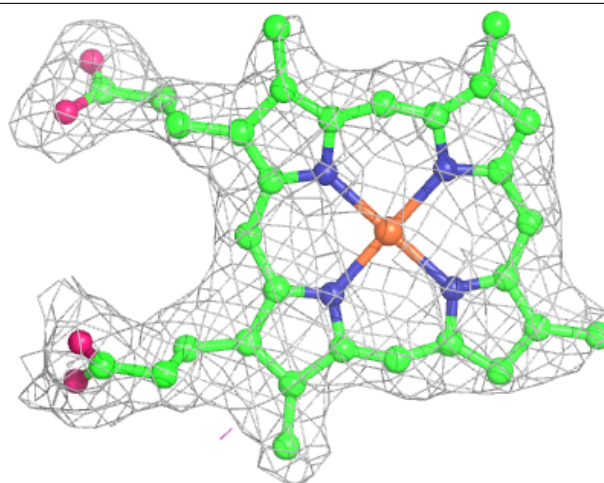
Electron density around FDE G 501:

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



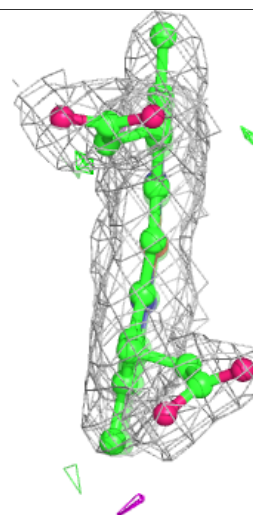
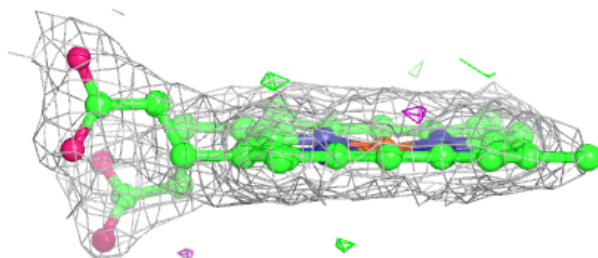
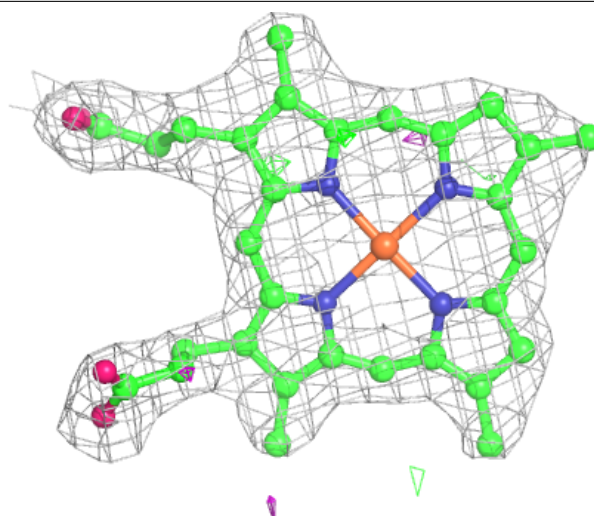
Electron density around FDE D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



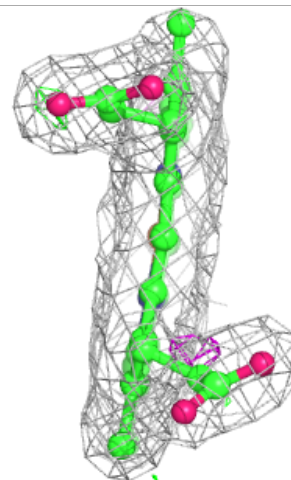
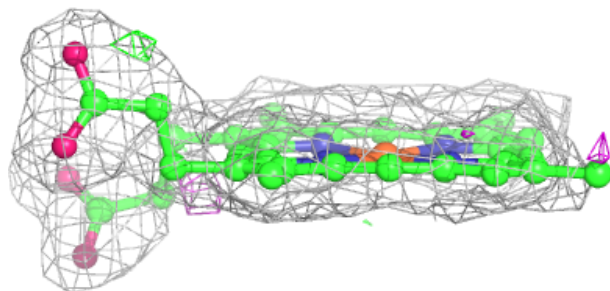
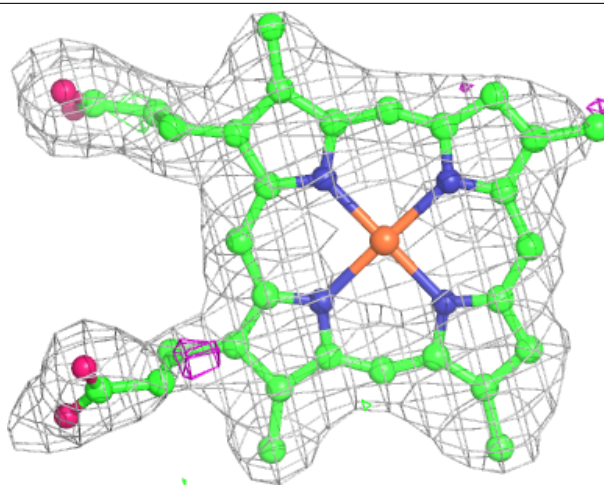
Electron density around FDE F 501:

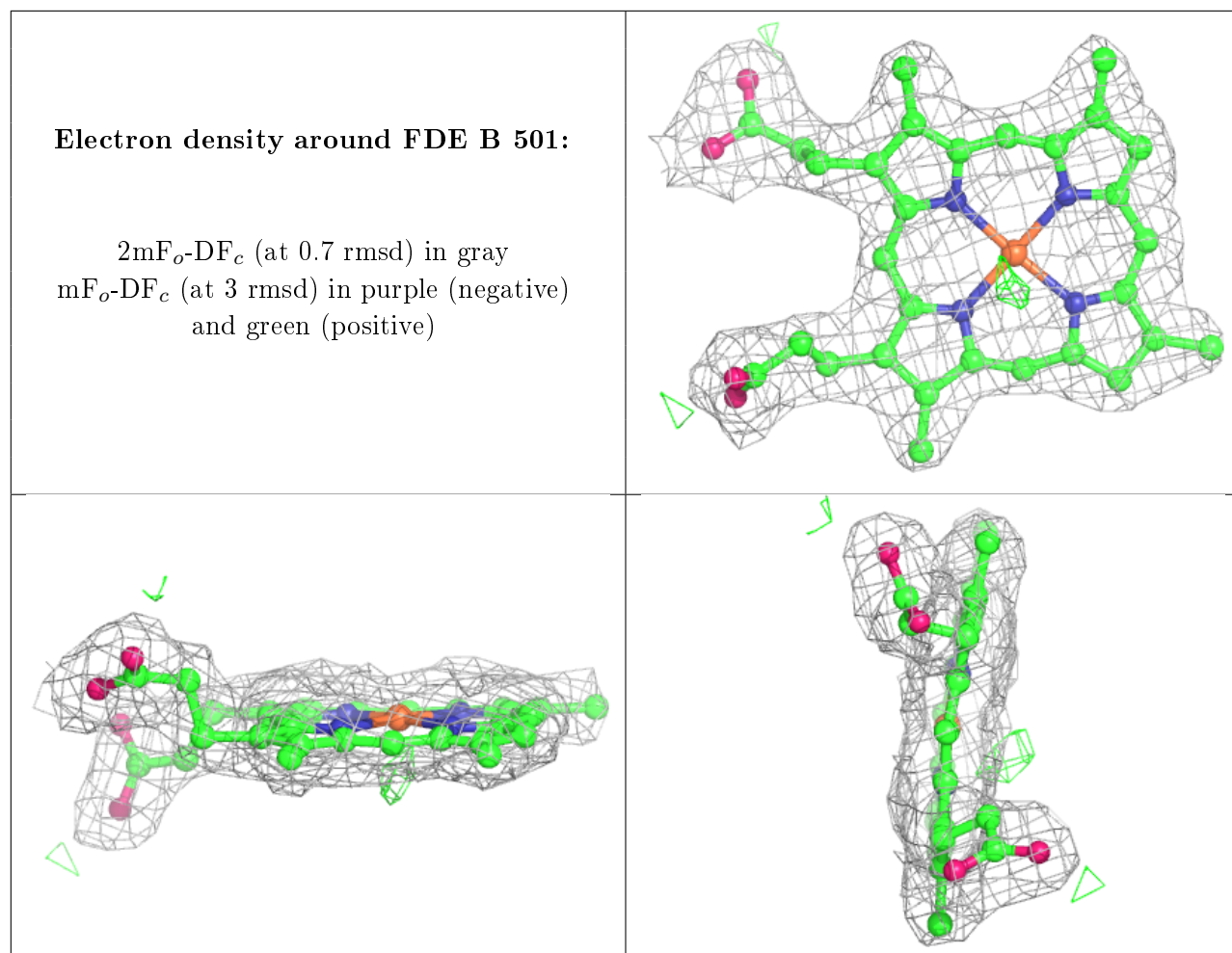
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FDE 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 ⓘ

There are no such residues in this entry.