



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 10:36 am BST

PDB ID : 5JQV
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 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

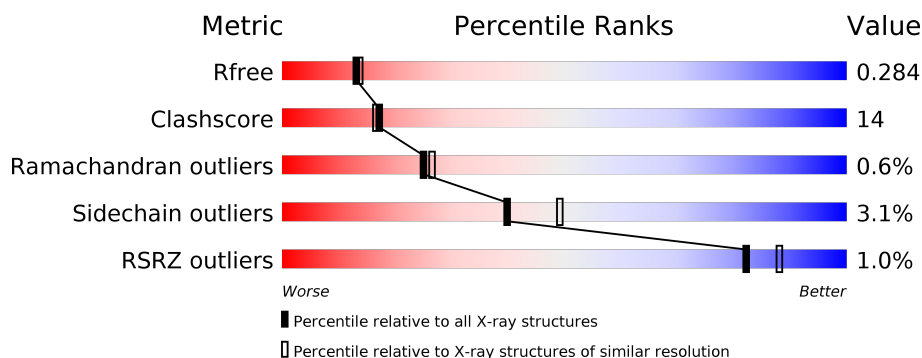
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 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>65%</div> <div>31%</div> <div>••</div> </div> </div>
1	B	471	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>••</div> </div> </div>
1	C	471	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>••</div> </div> </div>
1	D	471	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>•</div> </div> </div>
1	E	471	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>•</div> </div> </div>
1	F	471	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	471	<div><div></div><div>70%</div><div>24%</div><div></div><div></div></div>
1	H	471	% <div><div></div><div>66%</div><div>28%</div><div></div><div></div></div>

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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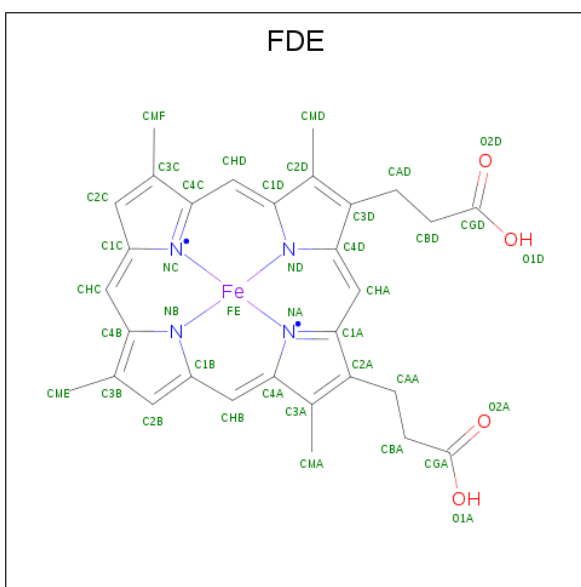
Chain	Residue	Modelled	Actual	Comment	Reference
B	272	TRP	LEU	engineered mutation	UNP P14779
B	322	ILE	LEU	engineered mutation	UNP P14779
B	406	SER	ALA	engineered mutation	UNP P14779
B	464	LEU	-	expression tag	UNP P14779
B	465	GLU	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	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 (three-letter code: FDE) (formula: C₃₀H₂₈FeN₄O₄).



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.

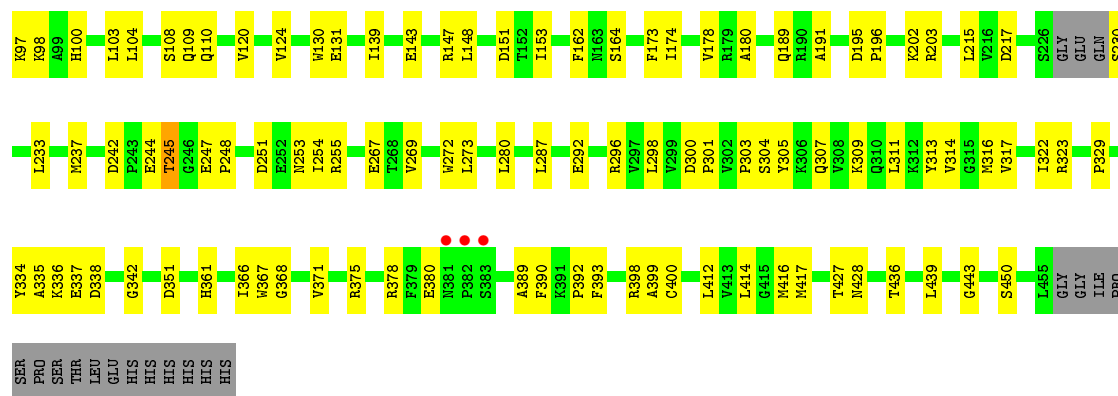
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		
3	B	154	Total	O	0	0
			154	154		
3	C	132	Total	O	0	0
			132	132		
3	D	89	Total	O	0	0
			89	89		

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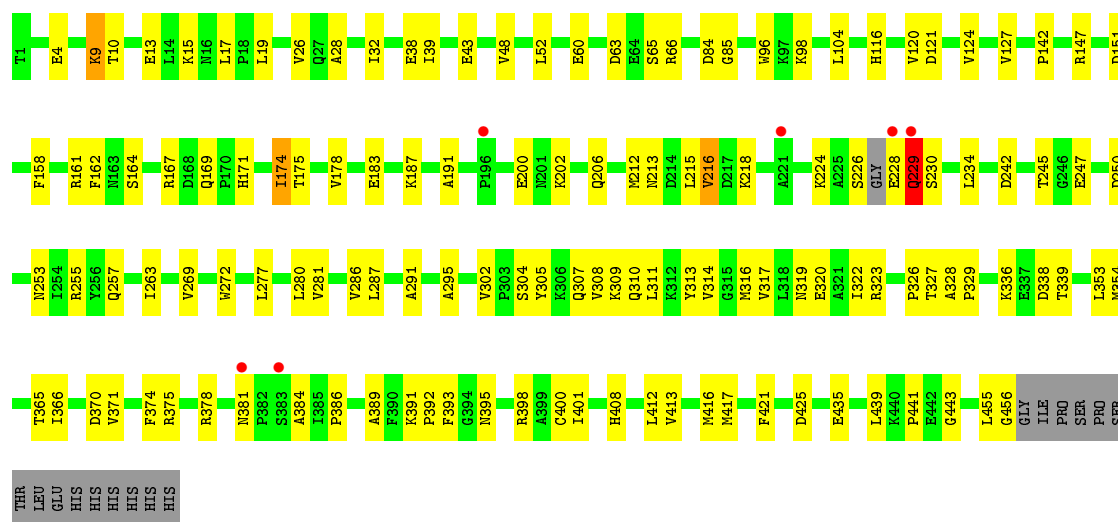
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	164	Total 164	O 164	0	0
3	F	130	Total 130	O 130	0	0
3	G	156	Total 156	O 156	0	0
3	H	179	Total 179	O 179	0	0

THER
I2
M5
K9
G12
E13
L14
L17
P18
L19
Q27
E38
I39
F40
K41
F42
E43
G46
R47
V48
T49
R50
Y51
L52
S53
S54
S55
R56
L57
L58
K59
E60
K69
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K76
F77
V78
R79
D80
F81
D84
F87
T88
S89
W90
E93
W96



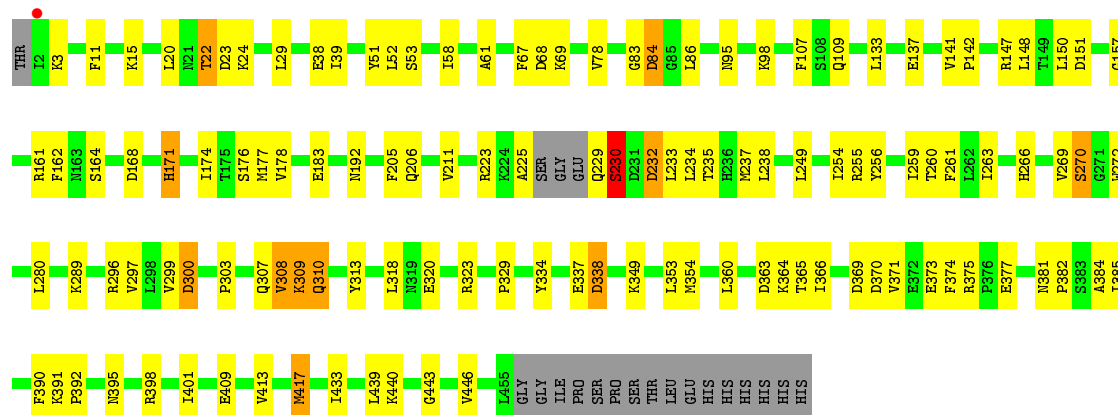
• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain F: 69% 27%

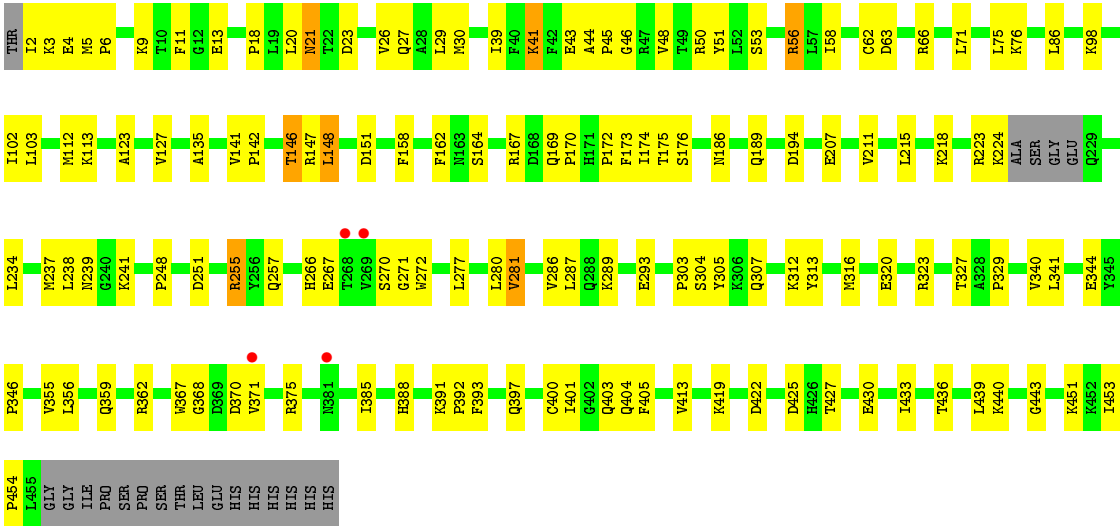


• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain G: 70% 24%



• 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	106.71Å 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) 100.0 (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 0.214 , 0.284	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 , 47.3	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	0.90	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	0.46	0/3665	0.66	3/4969 (0.1%)
1	B	0.46	0/3683	0.67	0/4990
1	C	0.45	0/3637	0.65	1/4935 (0.0%)
1	D	0.42	0/3579	0.62	0/4868
1	E	0.49	0/3678	0.67	0/4986
1	F	0.47	0/3651	0.66	1/4957 (0.0%)
1	G	0.46	0/3681	0.67	0/4992
1	H	0.45	0/3664	0.65	0/4963
All	All	0.46	0/29238	0.66	5/39660 (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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	310	GLN	CA-CB-CG	-7.88	96.06	113.40
1	A	168	ASP	C-N-CA	6.33	137.53	121.70
1	A	4	GLU	C-N-CA	-5.92	106.91	121.70
1	A	52	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	234	LEU	CA-CB-CG	5.16	127.16	115.30

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	119	0
1	B	3597	0	3507	103	0
1	C	3551	0	3453	94	0
1	D	3493	0	3302	84	0
1	E	3589	0	3498	92	0
1	F	3565	0	3440	94	0
1	G	3585	0	3465	92	0
1	H	3578	0	3503	109	0
2	A	39	0	26	1	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	5	0
3	A	159	0	0	36	0
3	B	154	0	0	19	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	18	0
3	H	179	0	0	28	0
All	All	30012	0	27861	786	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 786 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: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
1:A:168:ASP:CG	1:A:169:GLN:H	1.77	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/471 (95%)	433 (96%)	14 (3%)	2 (0%)	34	38
1	B	449/471 (95%)	434 (97%)	14 (3%)	1 (0%)	47	55
1	C	448/471 (95%)	433 (97%)	12 (3%)	3 (1%)	22	22
1	D	450/471 (96%)	432 (96%)	16 (4%)	2 (0%)	34	38
1	E	448/471 (95%)	433 (97%)	13 (3%)	2 (0%)	34	38
1	F	451/471 (96%)	432 (96%)	15 (3%)	4 (1%)	17	17
1	G	450/471 (96%)	435 (97%)	10 (2%)	5 (1%)	14	13
1	H	446/471 (95%)	433 (97%)	10 (2%)	3 (1%)	22	22
All	All	3591/3768 (95%)	3465 (96%)	104 (3%)	22 (1%)	25	26

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%)	360 (96%)	13 (4%)	36	45
1	B	378/414 (91%)	366 (97%)	12 (3%)	39	47
1	C	369/414 (89%)	353 (96%)	16 (4%)	29	36
1	D	345/414 (83%)	340 (99%)	5 (1%)	67	78
1	E	379/414 (92%)	373 (98%)	6 (2%)	62	74
1	F	367/414 (89%)	353 (96%)	14 (4%)	33	41
1	G	373/414 (90%)	356 (95%)	17 (5%)	27	33
1	H	376/414 (91%)	365 (97%)	11 (3%)	42	52
All	All	2960/3312 (89%)	2866 (97%)	94 (3%)	40	47

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	VAL
1	F	9	LYS
1	H	146	THR
1	D	192	ASN
1	E	245	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	388	HIS
1	G	310	GLN
1	E	404	GLN
1	B	116	HIS
1	E	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	B	501	1	32,46,46	6.52	19 (59%)	20,76,76	3.28	11 (55%)
2	FDE	H	501	1	32,46,46	6.52	18 (56%)	20,76,76	3.14	9 (45%)
2	FDE	F	501	1	32,46,46	6.41	16 (50%)	20,76,76	3.25	10 (50%)
2	FDE	C	501	1,3	32,46,46	6.39	16 (50%)	20,76,76	3.51	13 (65%)
2	FDE	A	501	1,3	32,46,46	6.68	18 (56%)	20,76,76	3.51	11 (55%)
2	FDE	G	501	1	32,46,46	6.33	18 (56%)	20,76,76	3.38	10 (50%)
2	FDE	E	501	1,3	32,46,46	6.33	16 (50%)	20,76,76	3.31	9 (45%)
2	FDE	D	501	1	32,46,46	6.32	18 (56%)	20,76,76	3.63	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	B	501	1	-	0/6/86/86	-
2	FDE	H	501	1	-	0/6/86/86	-
2	FDE	F	501	1	-	0/6/86/86	-
2	FDE	C	501	1,3	-	0/6/86/86	-
2	FDE	A	501	1,3	-	0/6/86/86	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDE	G	501	1	-	0/6/86/86	-
2	FDE	E	501	1,3	-	1/6/86/86	-
2	FDE	D	501	1	-	0/6/86/86	-

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	FDE	C3A-C2A	19.87	1.50	1.34
2	A	501	FDE	C3A-C2A	19.69	1.49	1.34
2	B	501	FDE	C3A-C2A	18.43	1.48	1.34
2	G	501	FDE	C3A-C2A	18.21	1.48	1.34
2	F	501	FDE	C3A-C2A	18.07	1.48	1.34

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FDE	C2B-C1B-NB	6.81	117.63	108.63
2	A	501	FDE	CHA-C1A-NA	6.70	123.39	110.75
2	H	501	FDE	CHA-C1A-NA	6.53	123.06	110.75
2	G	501	FDE	CHC-C1C-NC	6.44	122.89	110.75
2	D	501	FDE	CHA-C1A-NA	6.32	122.67	110.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

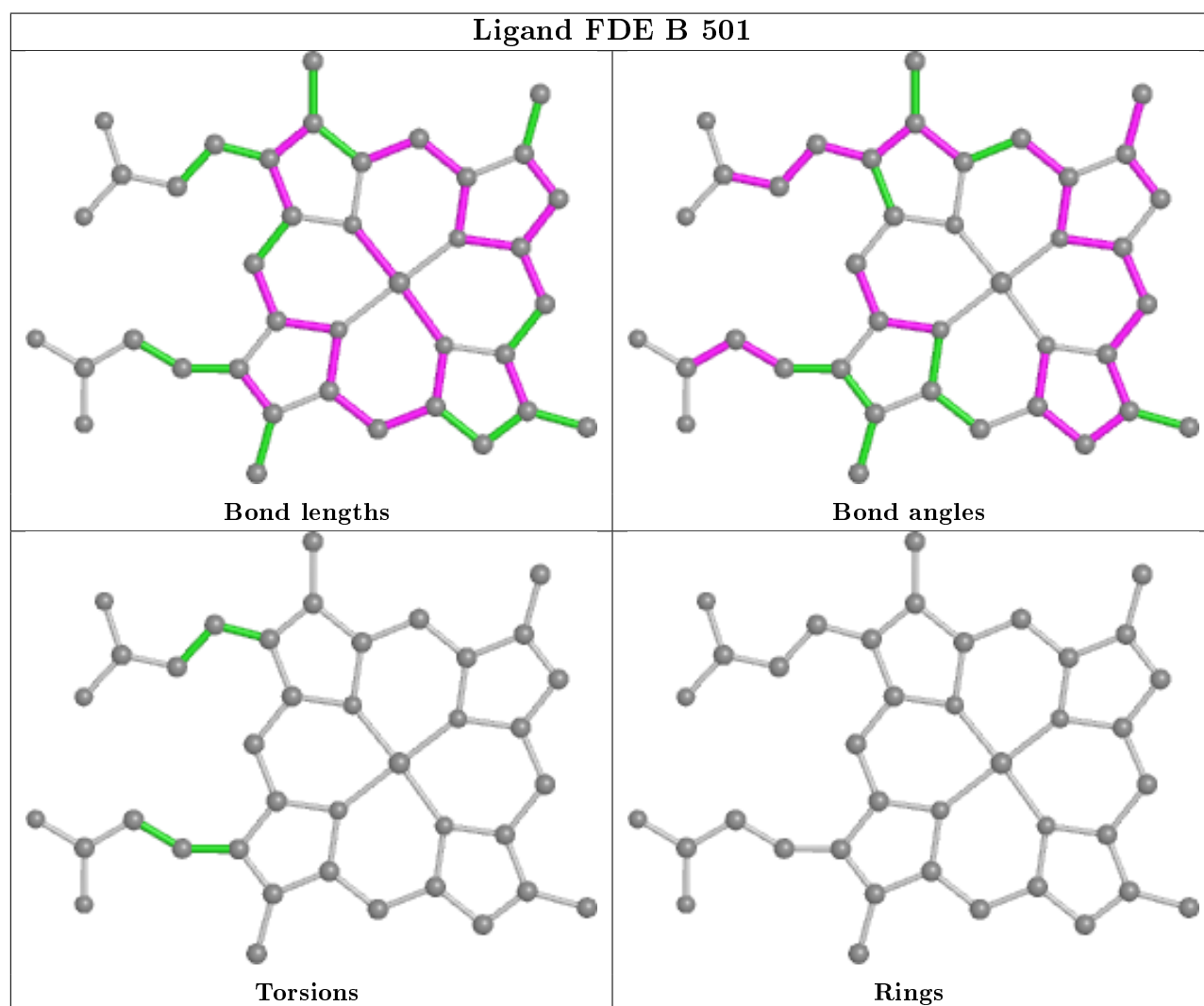
Mol	Chain	Res	Type	Atoms
2	E	501	FDE	C3A-C2A-CAA-CBA

There are no ring outliers.

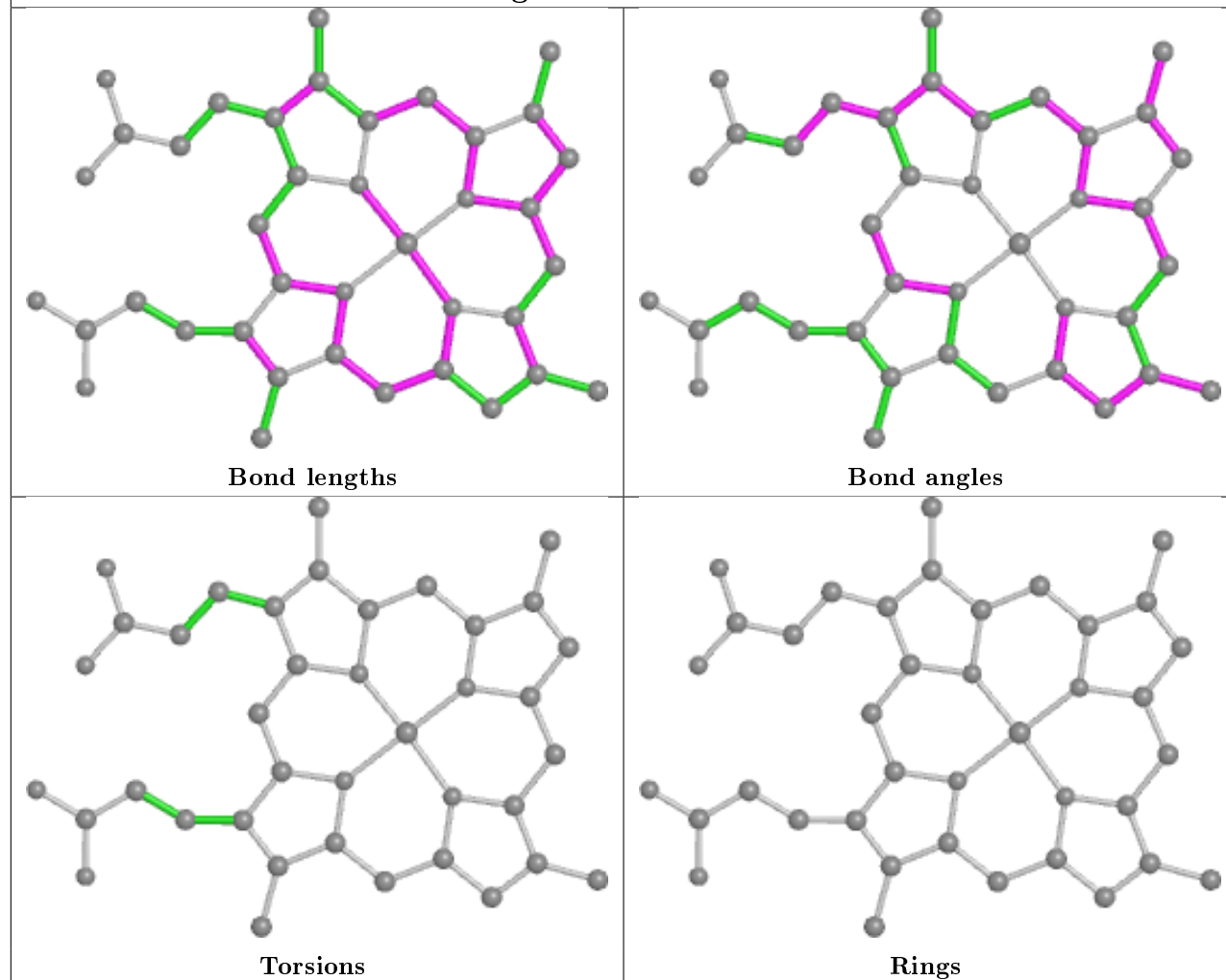
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FDE	2	0
2	H	501	FDE	5	0
2	F	501	FDE	1	0
2	C	501	FDE	1	0
2	A	501	FDE	1	0
2	G	501	FDE	2	0
2	E	501	FDE	1	0
2	D	501	FDE	1	0

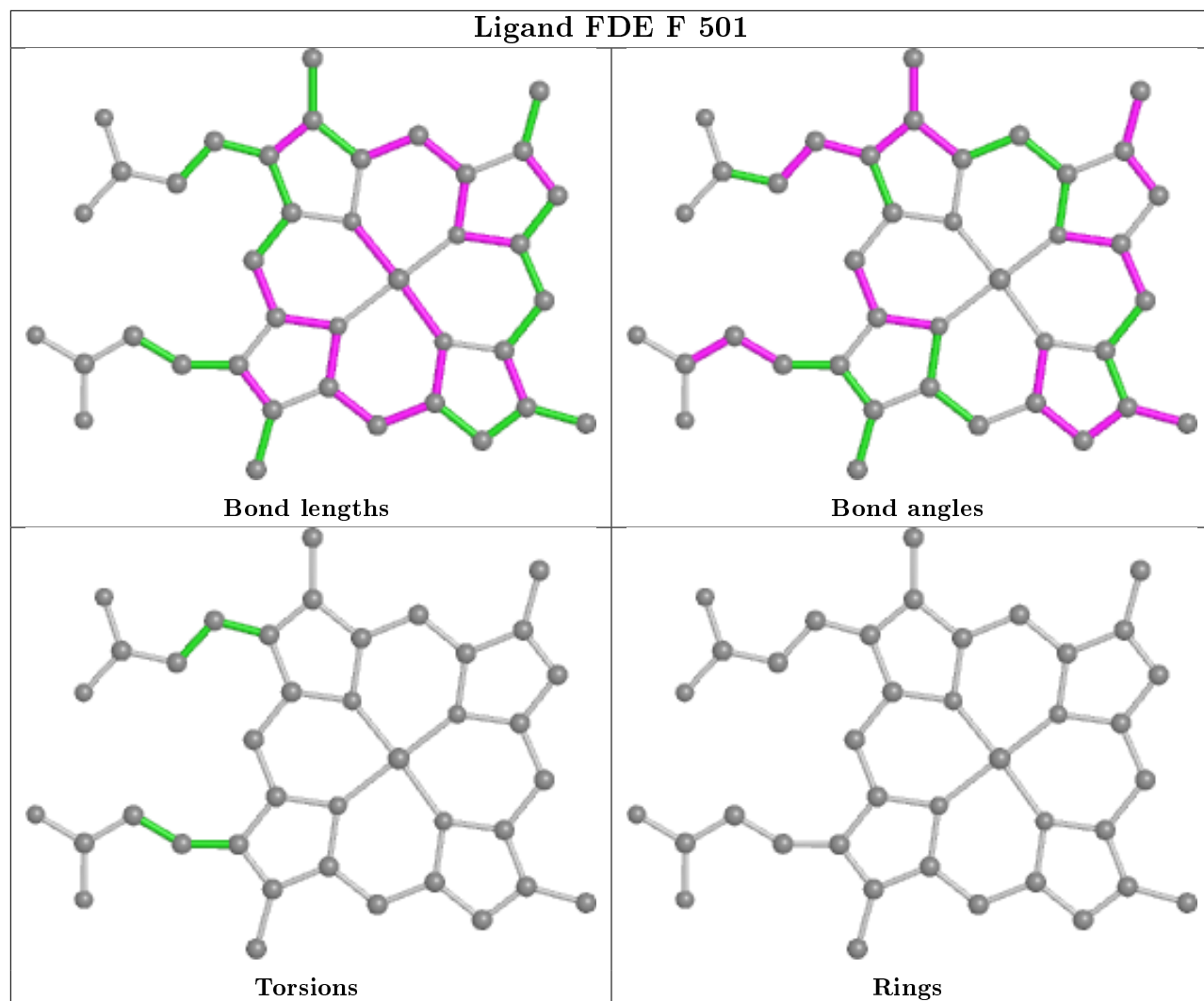
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



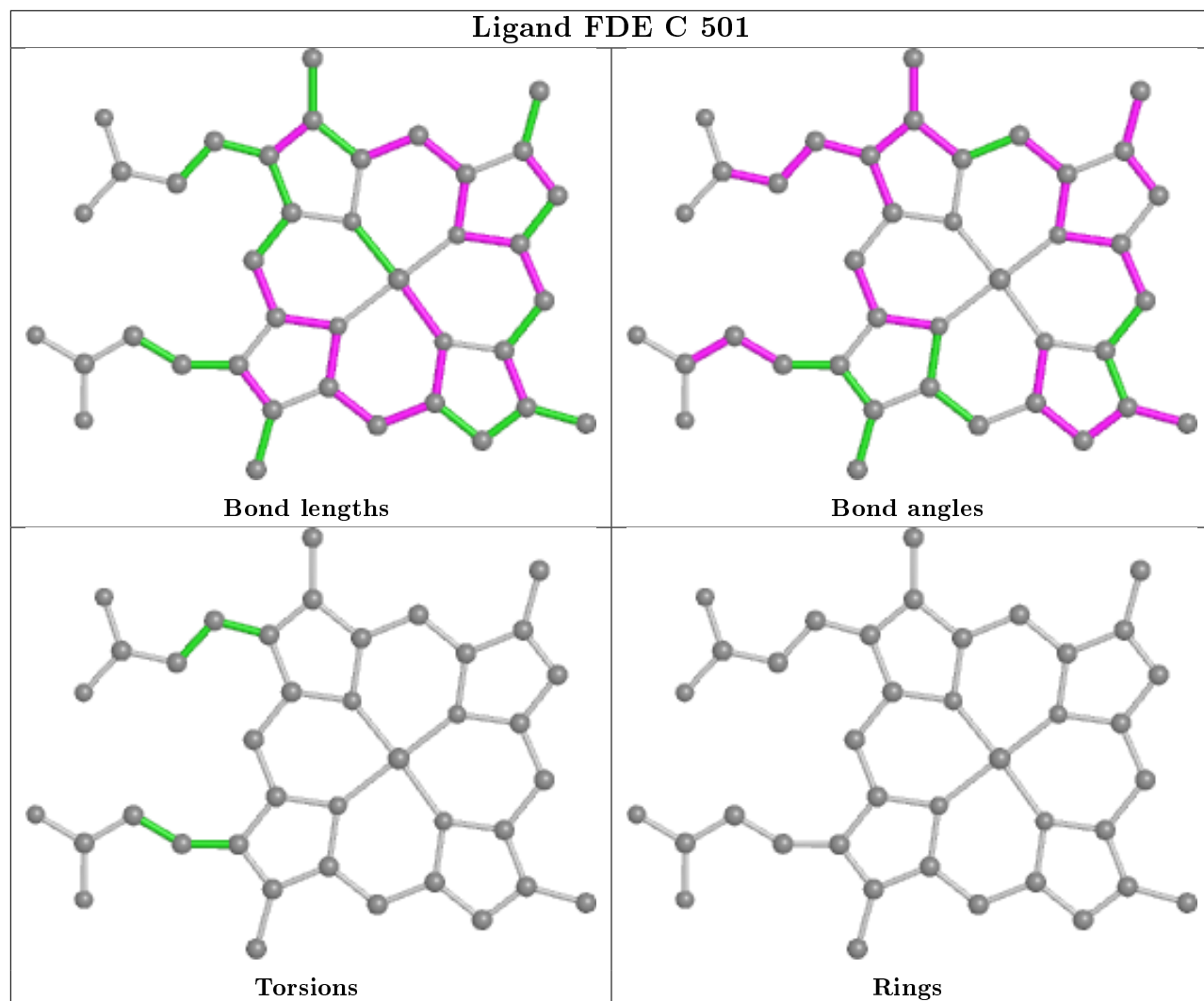
Ligand FDE H 501



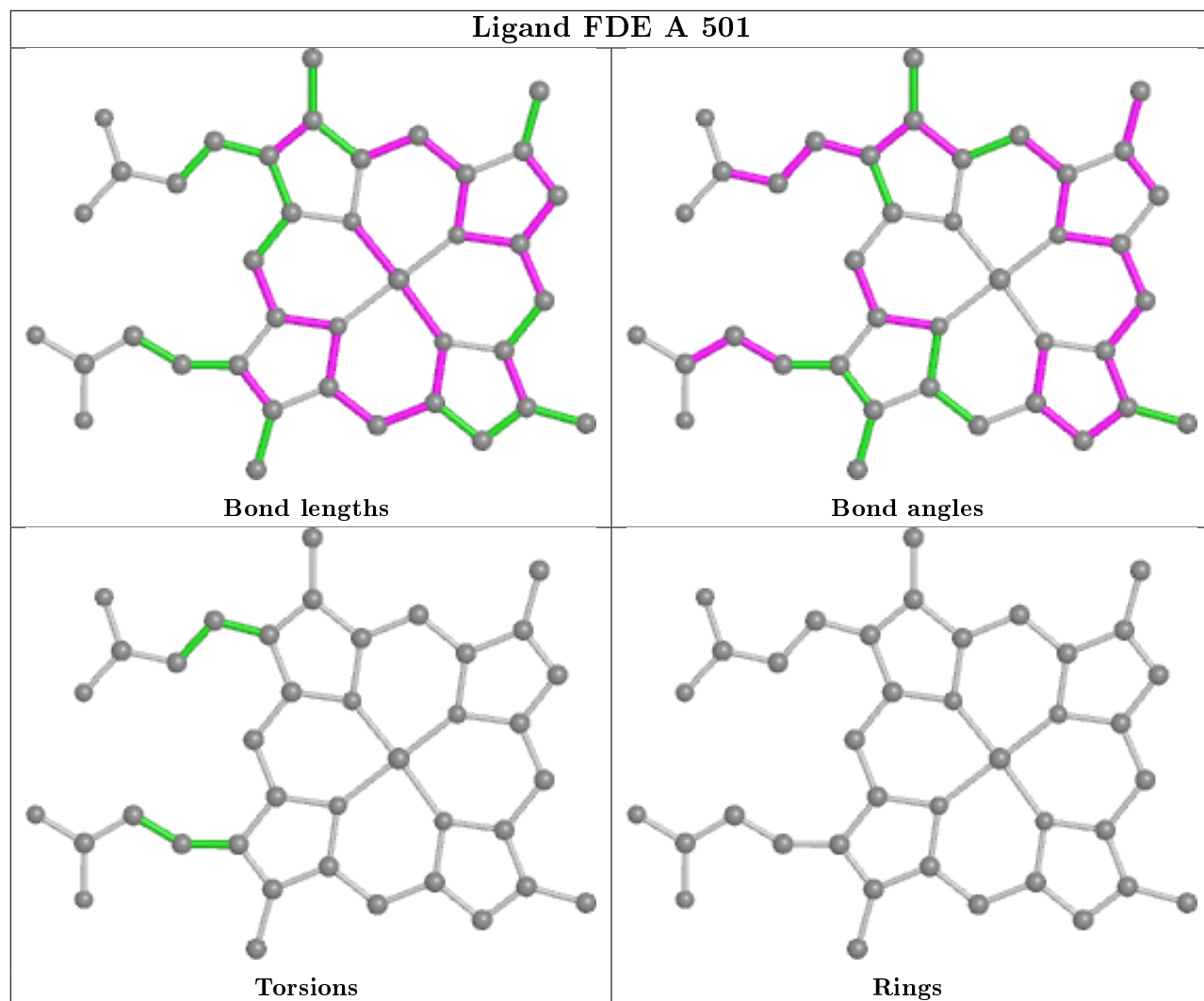
Ligand FDE F 501

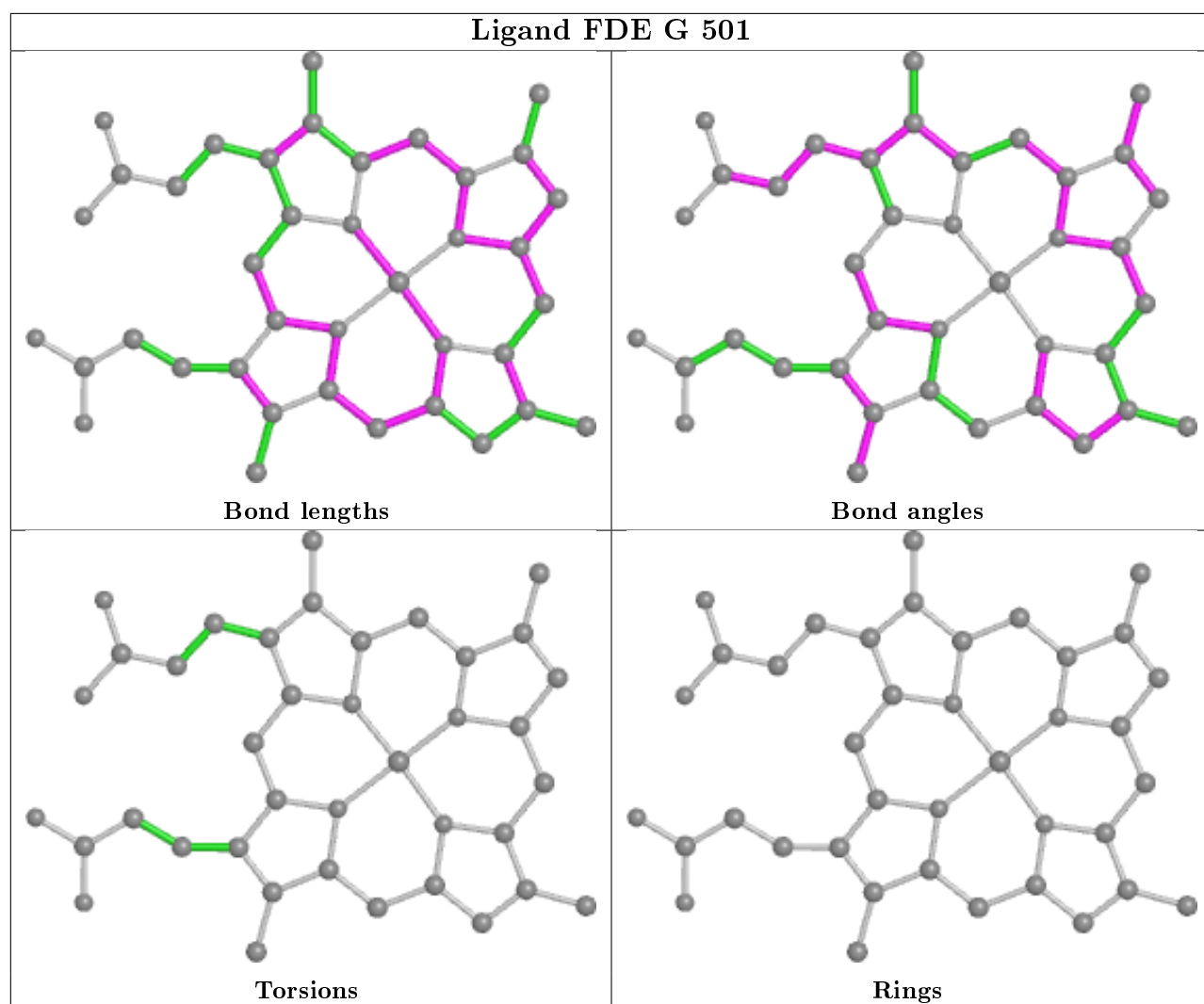


Ligand FDE C 501

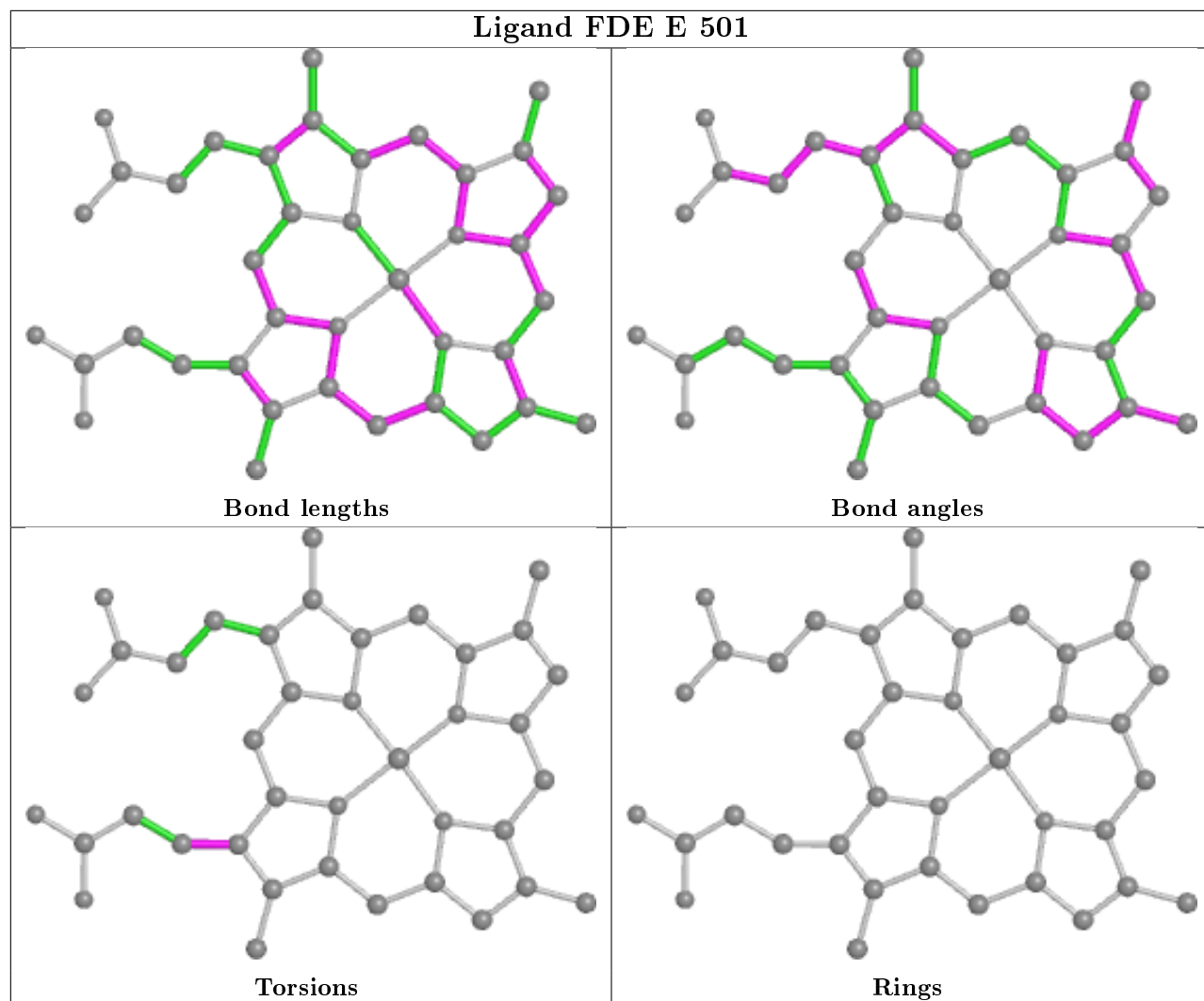


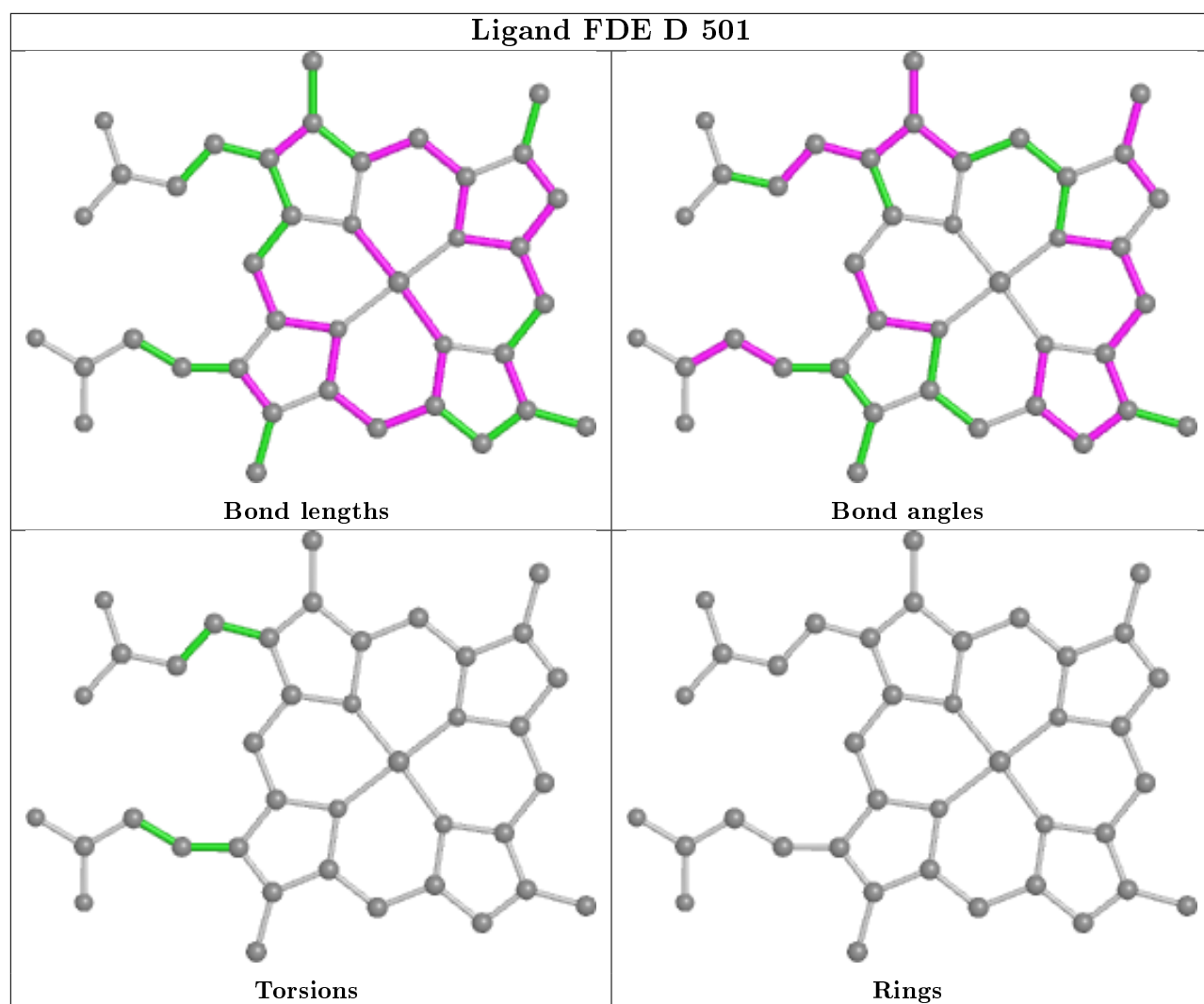
Ligand FDE A 501





Ligand FDE E 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	453/471 (96%)	-0.07	6 (1%) 77 83	10, 22, 39, 56	0
1	B	453/471 (96%)	-0.22	3 (0%) 87 92	7, 18, 36, 52	0
1	C	452/471 (95%)	-0.20	3 (0%) 87 92	10, 22, 37, 52	0
1	D	454/471 (96%)	0.08	11 (2%) 59 68	14, 30, 46, 59	0
1	E	451/471 (95%)	-0.26	3 (0%) 87 92	6, 17, 34, 54	0
1	F	455/471 (96%)	-0.05	6 (1%) 77 83	10, 23, 44, 66	0
1	G	451/471 (95%)	-0.20	1 (0%) 95 97	7, 21, 38, 60	0
1	H	450/471 (95%)	-0.16	4 (0%) 84 89	7, 19, 37, 49	0
All	All	3619/3768 (96%)	-0.14	37 (1%) 82 88	6, 22, 41, 66	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	196	PRO	5.0
1	D	455	LEU	3.6
1	B	225	ALA	3.4
1	F	381	ASN	3.4
1	E	382	PRO	3.3

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 carbohydrates in this entry.

6.4 Ligands

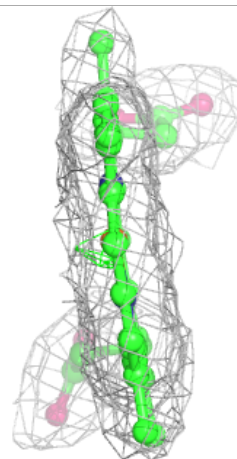
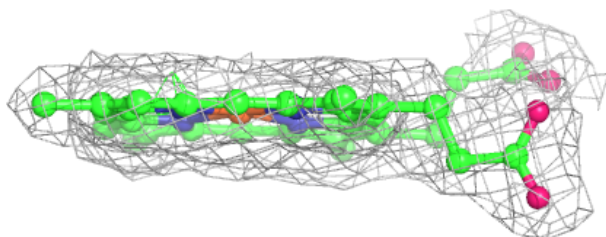
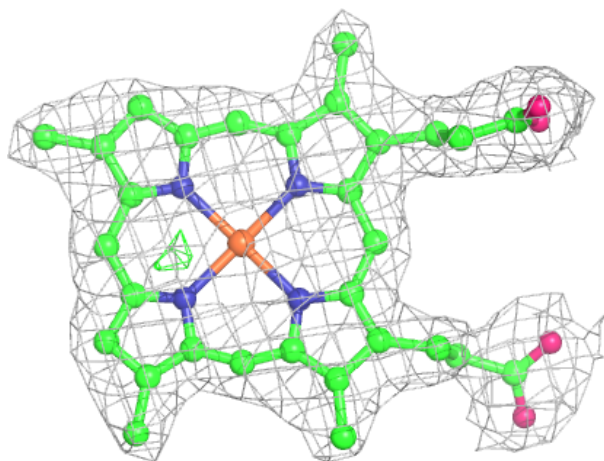
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FDE	B	501	39/39	0.96	0.19	6,9,16,17	0
2	FDE	A	501	39/39	0.96	0.19	8,15,20,26	0
2	FDE	D	501	39/39	0.96	0.19	14,21,29,33	0
2	FDE	C	501	39/39	0.97	0.15	4,10,15,17	0
2	FDE	H	501	39/39	0.97	0.18	6,10,14,19	0
2	FDE	G	501	39/39	0.97	0.17	7,15,21,21	0
2	FDE	E	501	39/39	0.97	0.16	7,10,14,19	0
2	FDE	F	501	39/39	0.97	0.14	7,13,20,23	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.

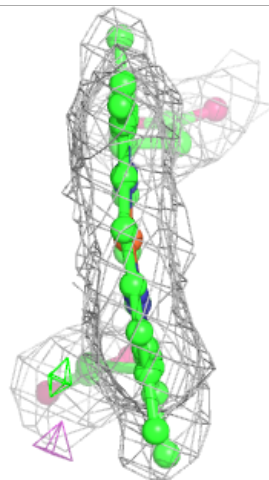
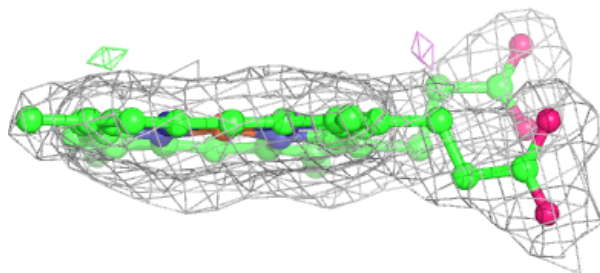
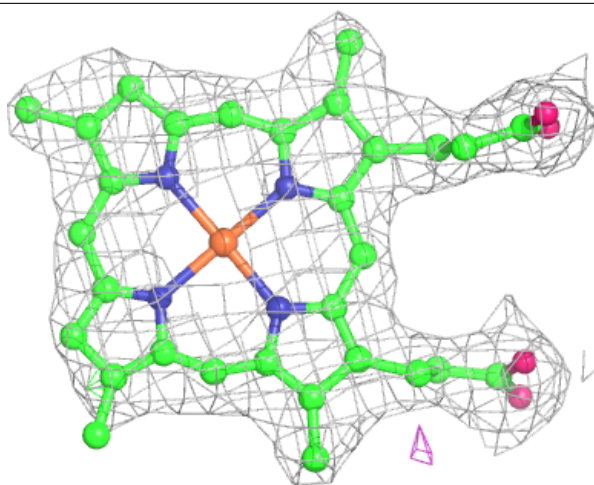
Electron density around FDE B 501:

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



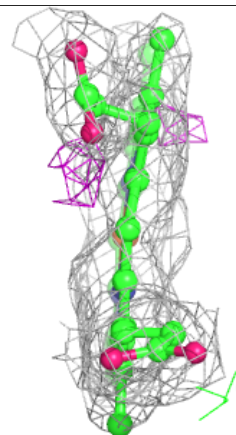
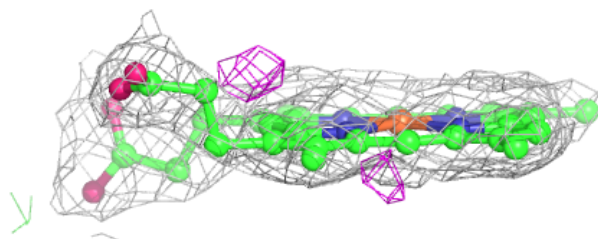
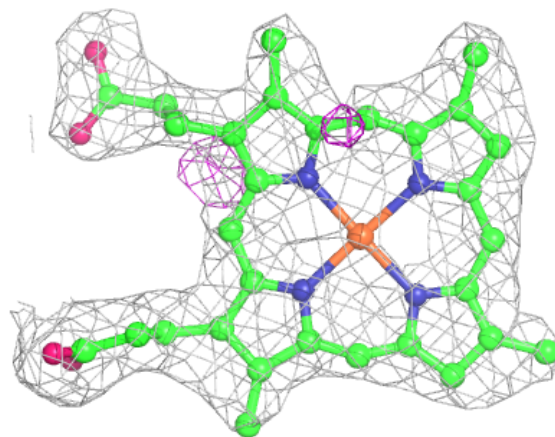
Electron density around FDE A 501:

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



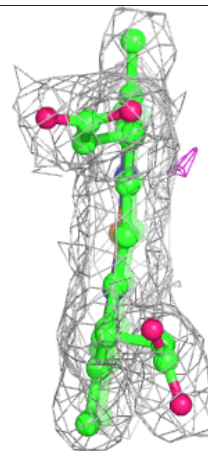
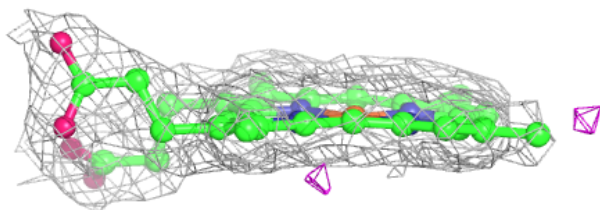
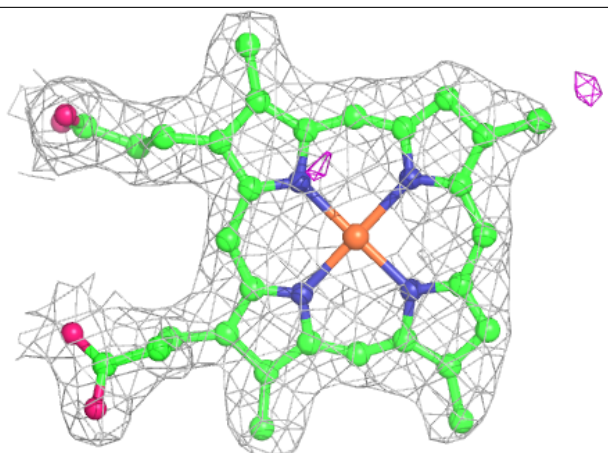
Electron density around FDE D 501:

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



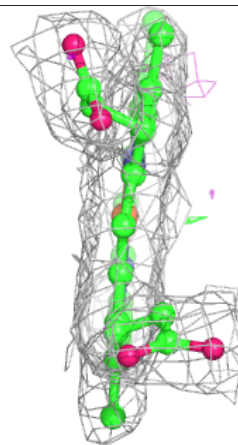
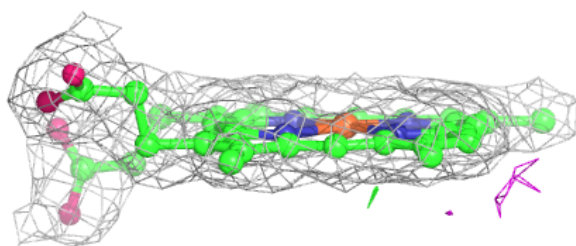
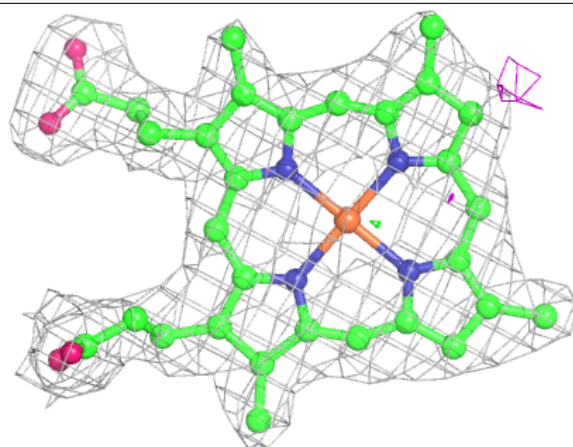
Electron density around FDE C 501:

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



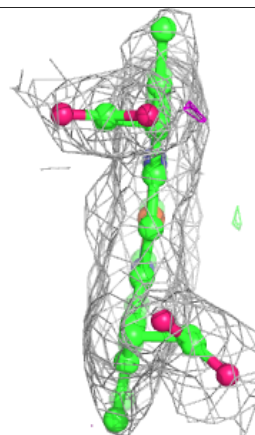
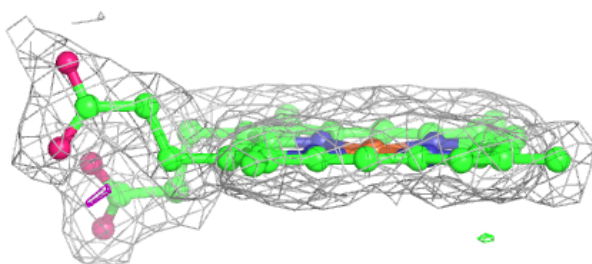
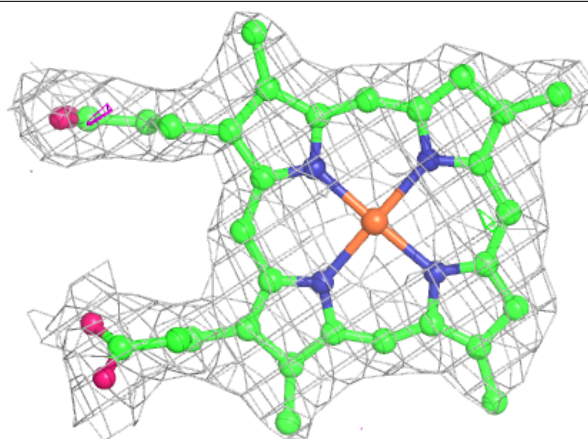
Electron density around FDE H 501:

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



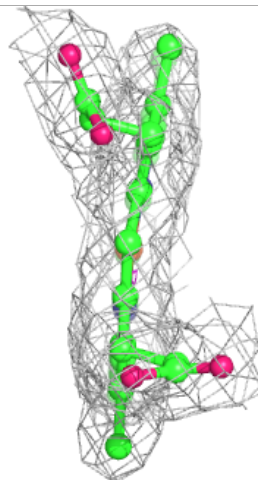
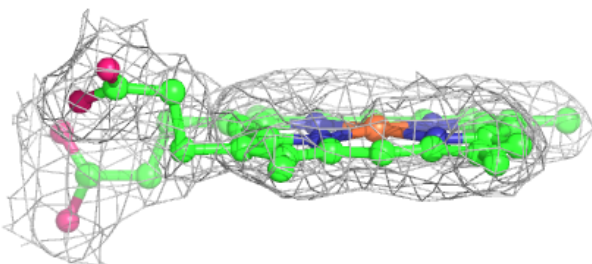
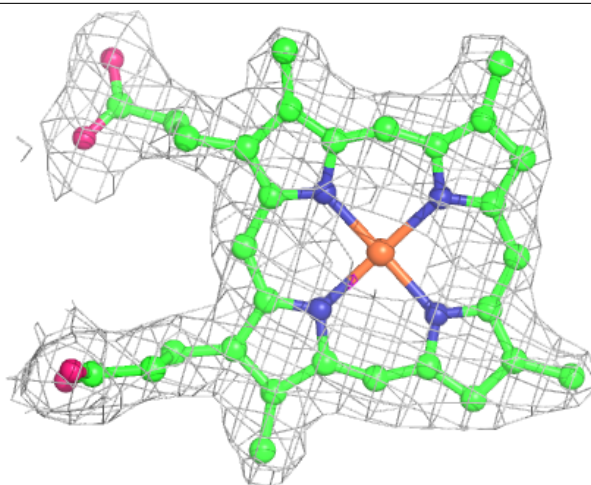
Electron density around FDE G 501:

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



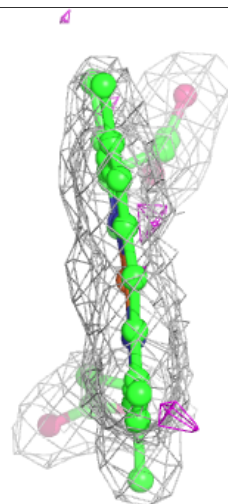
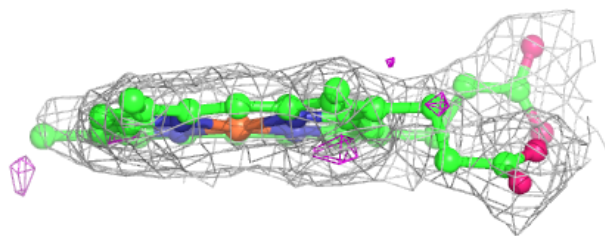
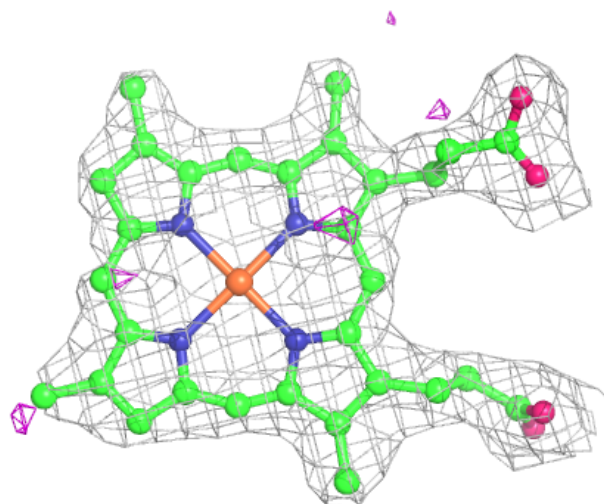
Electron density around FDE E 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.