



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:08 PM UTC

PDB ID : 9WMC / pdb\_00009wmc  
Title : Crystal structure of a P450 BM3 heme domain mutant in complex with Alpha-Zearalanol  
Authors : Liu, Z.W.; Huang, J.-W.; Chen, C.-C.; Guo, R.-T.  
Deposited on : 2025-09-03  
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

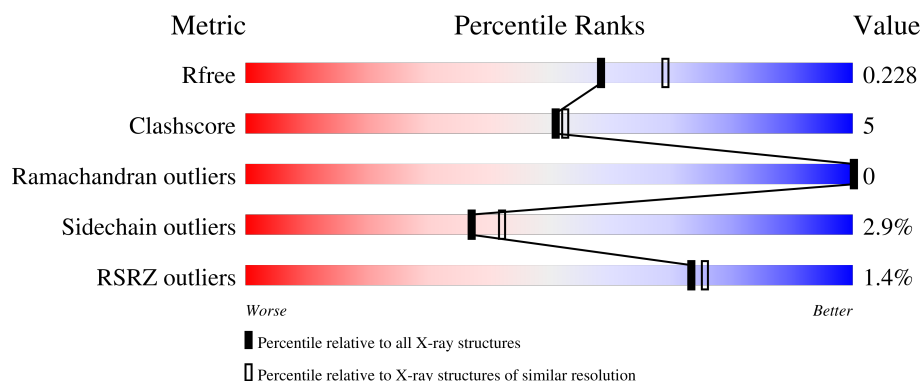
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

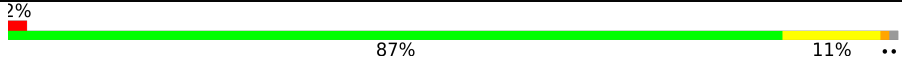

The reported resolution of this entry is 2.09 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	455	
1	B	455	

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
4	PEG	A	504	-	-	X	-
4	PEG	B	503	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8092 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	451	Total	C	N	O	S	0	2	0
			3648	2330	620	683	15			
1	B	451	Total	C	N	O	S	0	2	0
			3648	2330	619	684	15			

There are 28 discrepancies between the modelled and reference sequences:

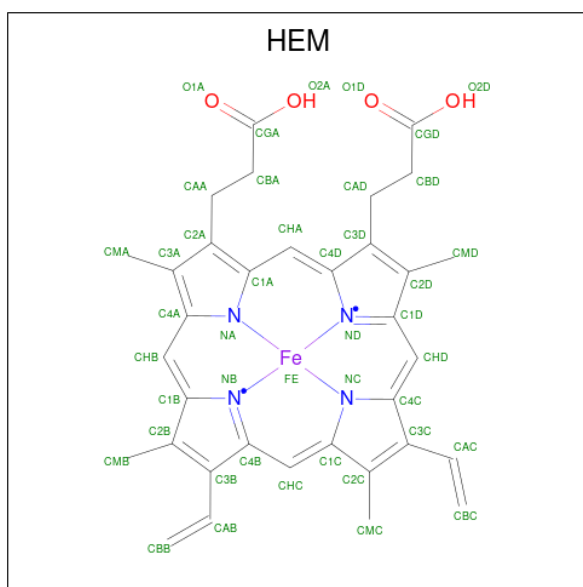
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	conflict	UNP P14779
A	48	TRP	ARG	conflict	UNP P14779
A	73	TRP	SER	conflict	UNP P14779
A	77	ASN	LYS	conflict	UNP P14779
A	79	LEU	VAL	conflict	UNP P14779
A	81	GLU	ASP	conflict	UNP P14779
A	82	ILE	PHE	conflict	UNP P14779
A	83	GLN	ALA	conflict	UNP P14779
A	88	GLY	PHE	conflict	UNP P14779
A	89	LEU	THR	conflict	UNP P14779
A	178	THR	MET	conflict	UNP P14779
A	186	GLN	MET	conflict	UNP P14779
A	206	ILE	PHE	conflict	UNP P14779
A	210	THR	ILE	conflict	UNP P14779
B	2	ALA	THR	conflict	UNP P14779
B	48	TRP	ARG	conflict	UNP P14779
B	73	TRP	SER	conflict	UNP P14779
B	77	ASN	LYS	conflict	UNP P14779
B	79	LEU	VAL	conflict	UNP P14779
B	81	GLU	ASP	conflict	UNP P14779
B	82	ILE	PHE	conflict	UNP P14779
B	83	GLN	ALA	conflict	UNP P14779
B	88	GLY	PHE	conflict	UNP P14779
B	89	LEU	THR	conflict	UNP P14779
B	178	THR	MET	conflict	UNP P14779

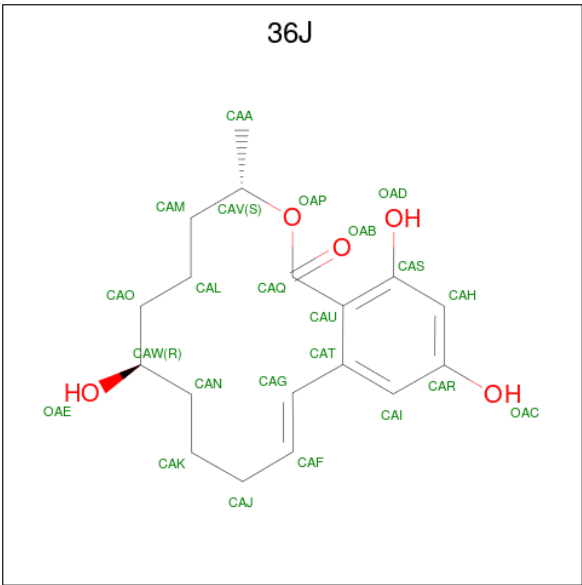
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Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLN	MET	conflict	UNP P14779
B	206	ILE	PHE	conflict	UNP P14779
B	210	THR	ILE	conflict	UNP P14779

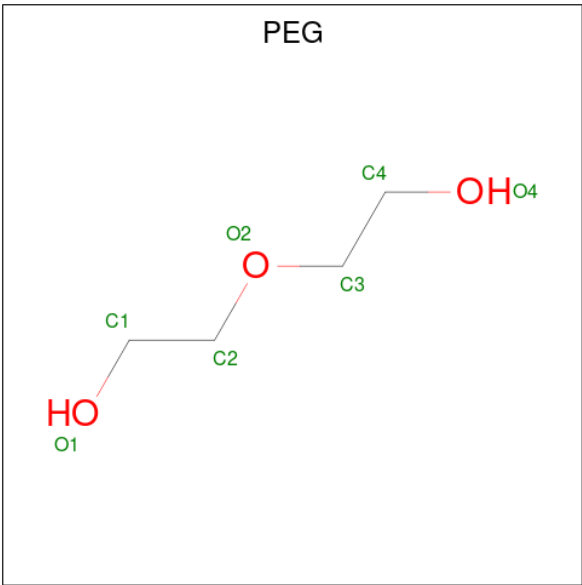
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	18	5		
3	B	1	Total	C	O	0	0
			23	18	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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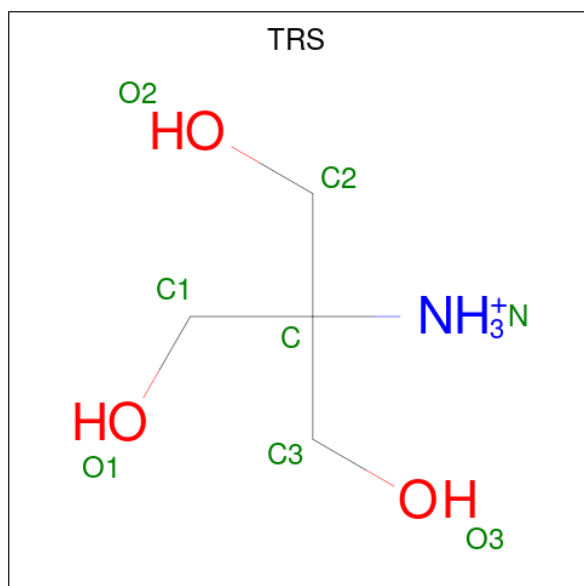
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ni	0	0
			2	2		
5	B	2	Total	Ni	0	0
			2	2		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	319	Total	O	0	0
			319	319		

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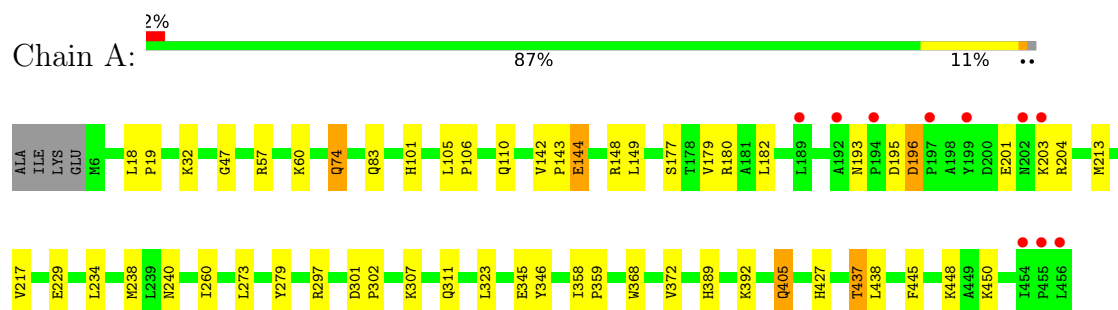
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	305	Total 305	O 305	0	0



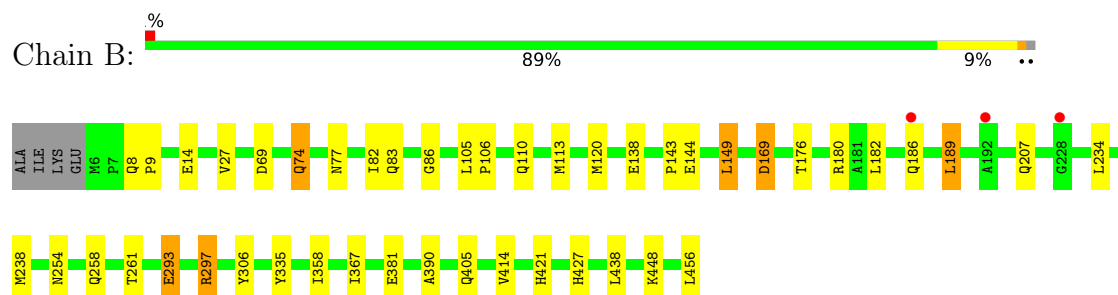
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.54Å 146.83Å 62.68Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	34.95 – 2.09 34.95 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.95-2.09) 99.0 (34.95-2.09)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.178 , 0.220 0.187 , 0.228	Depositor DCC
$R_{free}$ test set	2991 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, NI, TRS, PEG, 36J

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	1.01	0/3741	1.39	3/5065 (0.1%)
1	B	1.03	0/3741	1.37	4/5065 (0.1%)
All	All	1.02	0/7482	1.38	7/10130 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASN	CA-C-N	6.55	126.21	119.92
1	A	240	ASN	C-N-CA	6.55	126.21	119.92
1	B	358	ILE	O-C-N	-5.63	116.81	120.42
1	A	144	GLU	CB-CG-CD	5.54	122.02	112.60
1	B	138	GLU	CA-C-N	5.34	128.45	120.87
1	B	138	GLU	C-N-CA	5.34	128.45	120.87
1	B	169	ASP	N-CA-C	-5.26	106.87	113.28

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3648	0	3611	33	0
1	B	3648	0	3609	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	23	0	22	3	0
3	B	23	0	22	2	0
4	A	21	0	30	6	0
4	B	7	0	10	6	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	B	8	0	12	2	0
7	A	319	0	0	6	1
7	B	305	0	0	5	0
All	All	8092	0	7376	77	1

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 5.

All (77) 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:B:293[B]:GLU:OE1	1:B:297:ARG:NH1	1.99	0.96
1:B:77:ASN:HB2	7:B:601:HOH:O	1.72	0.89
1:A:110:GLN:OE1	1:A:405[B]:GLN:NE2	2.10	0.84
1:A:311:GLN:NE2	7:A:603:HOH:O	2.10	0.83
1:B:83:GLN:NE2	3:B:502:36J:OAC	2.10	0.83
1:A:346:TYR:OH	7:A:602:HOH:O	2.06	0.73
1:A:83:GLN:NE2	3:A:502:36J:OAC	2.22	0.73
4:A:503:PEG:H31	1:B:381:GLU:HB2	1.71	0.72
1:A:389:HIS:HA	1:A:392:LYS:HD3	1.71	0.70
1:B:110:GLN:NE2	1:B:306:TYR:OH	2.24	0.70
1:B:74:GLN:HE21	1:B:74:GLN:H	1.45	0.65
1:B:438:LEU:HA	4:B:503:PEG:H12	1.80	0.64
1:B:77:ASN:ND2	7:B:601:HOH:O	2.15	0.62
1:B:74:GLN:H	1:B:74:GLN:NE2	1.98	0.61
1:B:186:GLN:O	1:B:189:LEU:HB2	2.00	0.60
1:A:311:GLN:HG3	7:A:914:HOH:O	2.01	0.59
1:A:60:LYS:HE2	1:B:293[B]:GLU:OE2	2.04	0.57
1:A:47:GLY:N	7:A:601:HOH:O	1.77	0.57
1:A:148:ARG:HH22	4:A:504:PEG:C4	2.19	0.55
1:A:142:VAL:HB	1:A:143:PRO:HD3	1.88	0.55
1:B:149:LEU:HD21	1:B:414:VAL:HG21	1.89	0.55
1:A:74:GLN:NE2	1:A:74:GLN:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:NE2	4:B:503:PEG:C2	2.71	0.53
1:B:293[B]:GLU:CD	1:B:297:ARG:NH1	2.66	0.51
1:A:101:HIS:CE1	1:A:105:LEU:HD11	2.45	0.51
1:B:186:GLN:HE21	4:B:503:PEG:H21	1.75	0.51
1:A:74:GLN:H	1:A:74:GLN:HE21	1.59	0.51
1:A:279:TYR:HA	1:A:445:PHE:CZ	2.46	0.51
3:A:502:36J:CAQ	3:A:502:36J:CAL	2.89	0.50
1:A:193:ASN:O	1:A:196:ASP:HB2	2.11	0.50
1:B:82:ILE:HG13	1:B:83:GLN:HG3	1.92	0.50
1:B:176:THR:HG22	1:B:180:ARG:NH1	2.27	0.50
1:B:186:GLN:HE21	4:B:503:PEG:C2	2.26	0.49
1:B:293[B]:GLU:CD	1:B:297:ARG:HH11	2.21	0.49
4:A:503:PEG:H41	7:A:697:HOH:O	2.12	0.49
1:B:186:GLN:NE2	4:B:503:PEG:H22	2.28	0.48
1:B:77:ASN:HD21	6:B:504:TRS:H12	1.78	0.48
1:B:367:ILE:HG21	1:B:390:ALA:HB1	1.96	0.48
1:A:57:ARG:NH2	1:A:345:GLU:OE2	2.47	0.47
1:B:182:LEU:HD22	1:B:438:LEU:HD12	1.97	0.46
1:B:254:ASN:O	1:B:258:GLN:HG2	2.15	0.46
1:A:144:GLU:HG2	4:A:504:PEG:O4	2.16	0.46
1:A:217:VAL:CG2	1:A:260:ILE:HD11	2.46	0.46
1:B:74:GLN:NE2	1:B:74:GLN:N	2.64	0.46
1:A:234:LEU:HG	1:A:238:MET:HE3	1.97	0.46
1:B:86:GLY:HA3	1:B:261:THR:OG1	2.16	0.46
1:B:186:GLN:NE2	7:B:612:HOH:O	2.46	0.46
1:B:427:HIS:ND1	1:B:448:LYS:HE2	2.31	0.45
1:A:18:LEU:HB3	1:A:19:PRO:HD3	1.98	0.45
1:A:148:ARG:HH22	4:A:504:PEG:H41	1.82	0.45
1:A:297:ARG:HD2	7:A:888:HOH:O	2.16	0.45
1:A:427:HIS:ND1	1:A:448:LYS:HE2	2.32	0.45
1:A:273:LEU:HD13	1:A:323:LEU:HG	1.99	0.44
1:B:113:MET:HE1	1:B:120:MET:HE1	1.99	0.44
1:A:358:ILE:N	1:A:359:PRO:CD	2.82	0.43
1:B:77:ASN:HD21	6:B:504:TRS:C1	2.30	0.43
1:A:105:LEU:N	1:A:106:PRO:CD	2.82	0.43
1:A:148:ARG:NH2	4:A:504:PEG:H41	2.34	0.43
1:B:8:GLN:HG3	1:B:9:PRO:HD2	2.00	0.43
1:A:427:HIS:CG	1:A:448:LYS:HE2	2.54	0.42
1:B:421:HIS:HE1	7:B:866:HOH:O	2.01	0.42
1:A:182:LEU:HD22	1:A:438:LEU:HD12	2.01	0.42
1:B:110:GLN:OE1	1:B:405:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:CE	1:B:293[B]:GLU:OE2	2.67	0.42
1:B:234:LEU:HG	1:B:238:MET:HE3	2.01	0.42
1:B:143:PRO:HD2	1:B:144:GLU:OE1	2.20	0.41
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.86	0.41
1:A:368:TRP:HB2	1:A:372:VAL:HG12	2.02	0.41
3:A:502:36J:CAQ	3:A:502:36J:H4	2.51	0.41
1:B:27:VAL:HG23	4:B:503:PEG:H11	2.03	0.41
1:A:179:VAL:HG13	1:A:437:THR:HG21	2.03	0.41
1:A:301:ASP:HB3	1:A:302:PRO:HD2	2.03	0.41
1:B:69:ASP:HB3	1:B:335:TYR:CE1	2.56	0.41
1:B:105:LEU:N	1:B:106:PRO:CD	2.83	0.41
1:B:14:GLU:HB2	7:B:892:HOH:O	2.21	0.41
1:B:427:HIS:CG	1:B:448:LYS:HE2	2.56	0.41
3:B:502:36J:OAP	3:B:502:36J:CAG	2.70	0.40

All (1) 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)
7:A:893:HOH:O	7:A:913:HOH:O[1_655]	2.13	0.07

## 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	451/455 (99%)	437 (97%)	14 (3%)	0	100	100
1	B	451/455 (99%)	434 (96%)	17 (4%)	0	100	100
All	All	902/910 (99%)	871 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	397/398 (100%)	380 (96%)	17 (4%)	26	27
1	B	397/398 (100%)	389 (98%)	8 (2%)	48	56
All	All	794/796 (100%)	769 (97%)	25 (3%)	37	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	74	GLN
1	A	149	LEU
1	A	177	SER
1	A	180	ARG
1	A	195	ASP
1	A	196	ASP
1	A	201	GLU
1	A	203	LYS
1	A	204	ARG
1	A	213	MET
1	A	229	GLU
1	A	307	LYS
1	A	405[A]	GLN
1	A	405[B]	GLN
1	A	437	THR
1	A	450	LYS
1	B	74	GLN
1	B	149	LEU
1	B	169	ASP
1	B	189	LEU
1	B	293[A]	GLU
1	B	293[B]	GLU
1	B	297	ARG
1	B	456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	74	GLN
1	A	83	GLN
1	A	190	GLN
1	A	205	GLN
1	A	360	GLN
1	B	74	GLN
1	B	77	ASN
1	B	83	GLN
1	B	96	ASN
1	B	110	GLN
1	B	111	GLN
1	B	139	HIS
1	B	164	ASN
1	B	186	GLN
1	B	207	GLN
1	B	311	GLN
1	B	360	GLN
1	B	388	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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
4	PEG	A	503	-	6,6,6	0.30	0	5,5,5	0.28	0
2	HEM	A	501	1	50,50,50	1.66	9 (18%)	67,82,82	1.49	10 (14%)
2	HEM	B	501	1	50,50,50	1.74	10 (20%)	67,82,82	1.52	9 (13%)
4	PEG	A	504	-	6,6,6	0.58	0	5,5,5	0.45	0
3	36J	B	502	-	24,24,24	0.50	0	32,32,32	0.62	0
4	PEG	A	505	-	6,6,6	0.40	0	5,5,5	0.27	0
6	TRS	B	504	-	7,7,7	0.20	0	9,9,9	0.39	0
3	36J	A	502	-	24,24,24	0.52	0	32,32,32	0.56	0
4	PEG	B	503	-	6,6,6	0.45	0	5,5,5	0.22	0

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
4	PEG	A	503	-	-	4/4/4/4	-
2	HEM	A	501	1	-	0/14/54/54	-
2	HEM	B	501	1	-	1/14/54/54	-
4	PEG	A	504	-	-	2/4/4/4	-
3	36J	B	502	-	-	2/22/22/22	0/2/2/2
4	PEG	A	505	-	-	2/4/4/4	-
6	TRS	B	504	-	-	8/9/9/9	-
3	36J	A	502	-	-	8/22/22/22	1/2/2/2
4	PEG	B	503	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	5.61	2.12	1.94
2	B	501	HEM	C1B-NB	-5.00	1.31	1.40
2	B	501	HEM	FE-NC	4.70	2.10	1.95
2	B	501	HEM	FE-NB	4.11	2.07	1.94
2	A	501	HEM	C4B-NB	-3.55	1.31	1.38
2	A	501	HEM	FE-NC	3.43	2.06	1.95
2	A	501	HEM	FE-NA	3.17	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C4D-ND	-3.14	1.34	1.40
2	B	501	HEM	C4B-NB	-3.03	1.32	1.38
2	A	501	HEM	C4D-ND	-2.84	1.35	1.40
2	B	501	HEM	C4A-NA	-2.70	1.34	1.39
2	A	501	HEM	C3B-C4B	2.47	1.49	1.44
2	A	501	HEM	C1B-NB	-2.42	1.36	1.40
2	A	501	HEM	C1C-C2C	-2.40	1.40	1.45
2	B	501	HEM	C3B-C4B	2.28	1.49	1.44
2	A	501	HEM	CBA-CGA	2.24	1.55	1.50
2	B	501	HEM	C1C-C2C	-2.22	1.40	1.45
2	B	501	HEM	O1A-CGA	2.22	1.29	1.22
2	B	501	HEM	C4C-NC	-2.09	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHC-C4B-NB	4.88	129.68	124.42
2	B	501	HEM	C1B-NB-C4B	3.67	109.55	105.21
2	A	501	HEM	CHD-C4C-NC	3.56	128.33	124.45
2	B	501	HEM	CHD-C1D-ND	3.39	128.07	124.42
2	A	501	HEM	CHA-C4D-ND	3.27	128.41	124.37
2	A	501	HEM	C1B-NB-C4B	3.20	108.99	105.21
2	A	501	HEM	CHD-C1D-ND	3.13	127.79	124.42
2	B	501	HEM	CHD-C1D-C2D	-2.94	120.39	125.03
2	B	501	HEM	O2D-CGD-CBD	2.88	123.11	114.00
2	A	501	HEM	CAD-C3D-C4D	2.79	129.57	124.70
2	A	501	HEM	C4C-NC-C1C	2.77	110.34	105.82
2	A	501	HEM	CHB-C1B-NB	2.71	127.71	124.37
2	A	501	HEM	O2A-CGA-CBA	2.59	122.19	114.00
2	A	501	HEM	CHA-C4D-C3D	-2.59	120.46	125.23
2	A	501	HEM	CHC-C4B-NB	2.50	127.11	124.42
2	B	501	HEM	O2A-CGA-CBA	2.43	121.69	114.00
2	B	501	HEM	C4B-C3B-C2B	-2.40	105.07	107.28
2	B	501	HEM	O2D-CGD-O1D	-2.17	117.75	123.33
2	B	501	HEM	CBD-CAD-C3D	-2.13	106.63	112.53

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	36J	CAL-CAM-CAV-CAA
3	A	502	36J	CAL-CAM-CAV-OAP

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Mol	Chain	Res	Type	Atoms
3	A	502	36J	CAJ-CAF-CAG-CAT
6	B	504	TRS	C3-C-C1-O1
6	B	504	TRS	C1-C-C2-O2
4	B	503	PEG	O1-C1-C2-O2
4	A	503	PEG	O2-C3-C4-O4
4	B	503	PEG	O2-C3-C4-O4
3	A	502	36J	CAK-CAN-CAW-CAO
6	B	504	TRS	C3-C-C2-O2
4	A	504	PEG	O2-C3-C4-O4
4	A	505	PEG	O1-C1-C2-O2
4	A	505	PEG	O2-C3-C4-O4
6	B	504	TRS	N-C-C1-O1
4	A	504	PEG	C1-C2-O2-C3
4	A	503	PEG	O1-C1-C2-O2
4	A	503	PEG	C4-C3-O2-C2
6	B	504	TRS	C2-C-C1-O1
6	B	504	TRS	C1-C-C3-O3
4	A	503	PEG	C1-C2-O2-C3
3	A	502	36J	CAL-CAO-CAW-OAE
6	B	504	TRS	N-C-C2-O2
3	A	502	36J	CAL-CAO-CAW-CAN
3	A	502	36J	CAF-CAJ-CAK-CAN
3	A	502	36J	OAB-CAQ-CAU-CAT
3	B	502	36J	CAF-CAG-CAT-CAI
3	B	502	36J	CAF-CAG-CAT-CAU
6	B	504	TRS	N-C-C3-O3
2	B	501	HEM	CAA-CBA-CGA-O2A

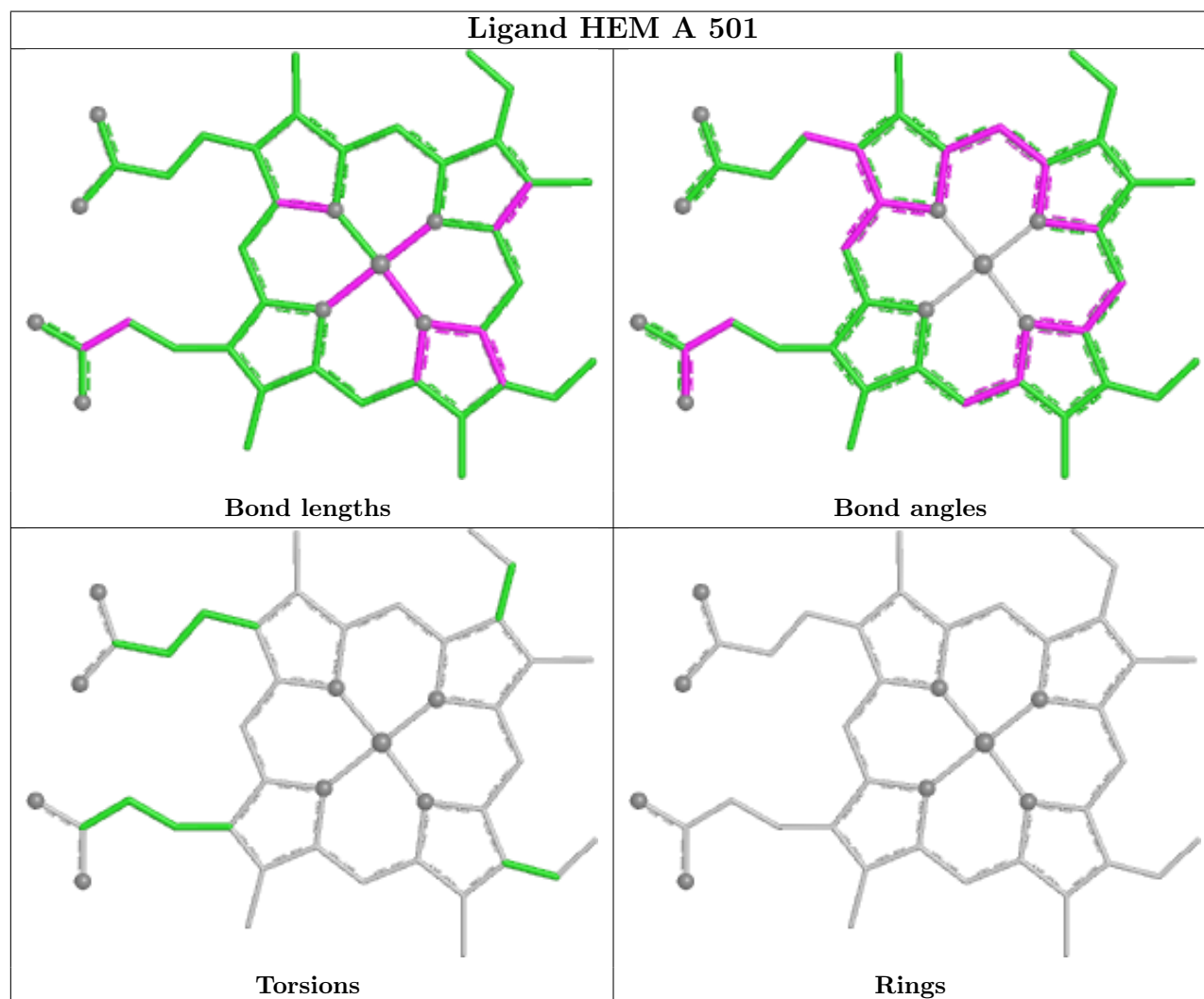
All (1) ring outliers are listed below:

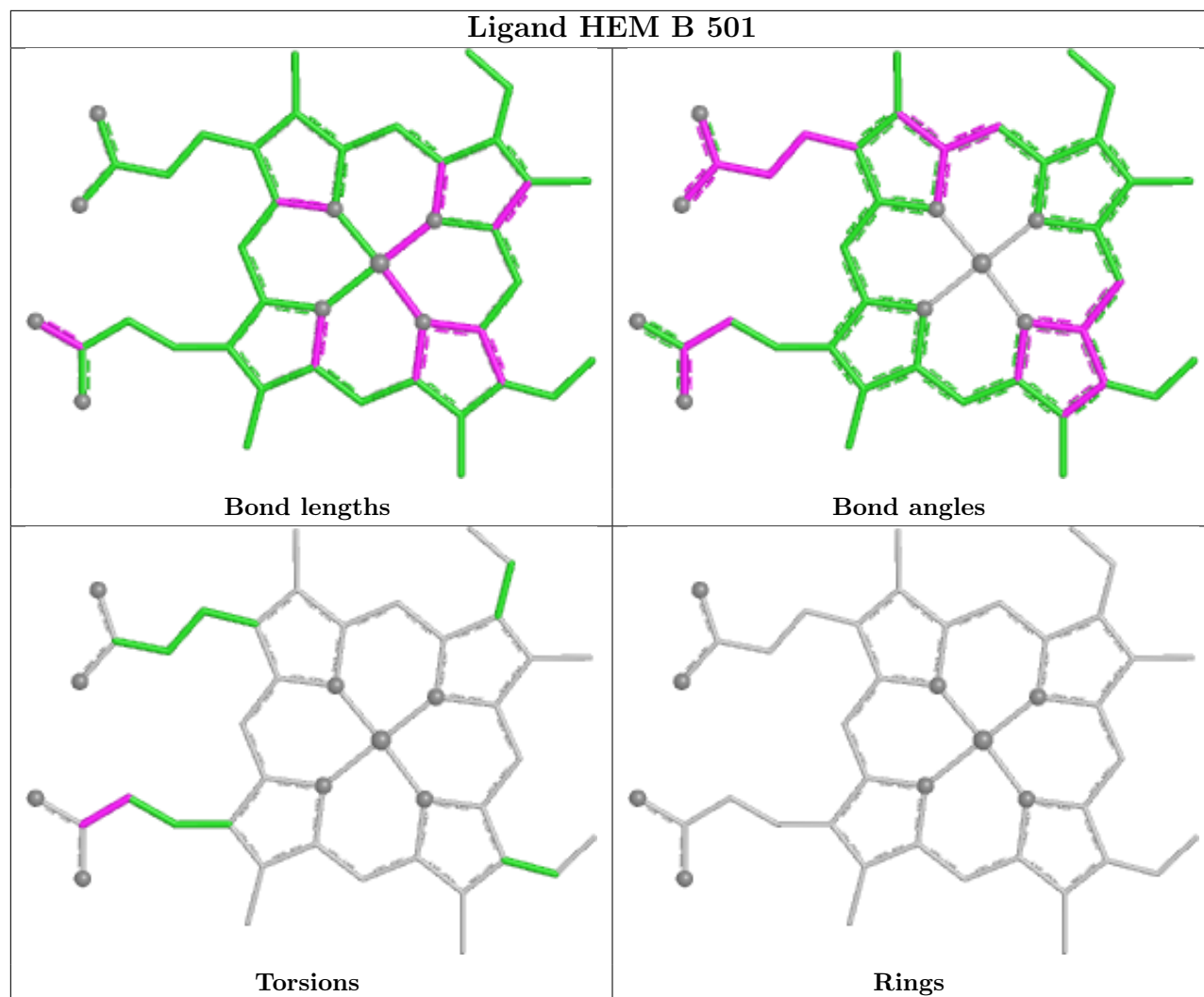
Mol	Chain	Res	Type	Atoms
3	A	502	36J	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C

6 monomers are involved in 19 short contacts:

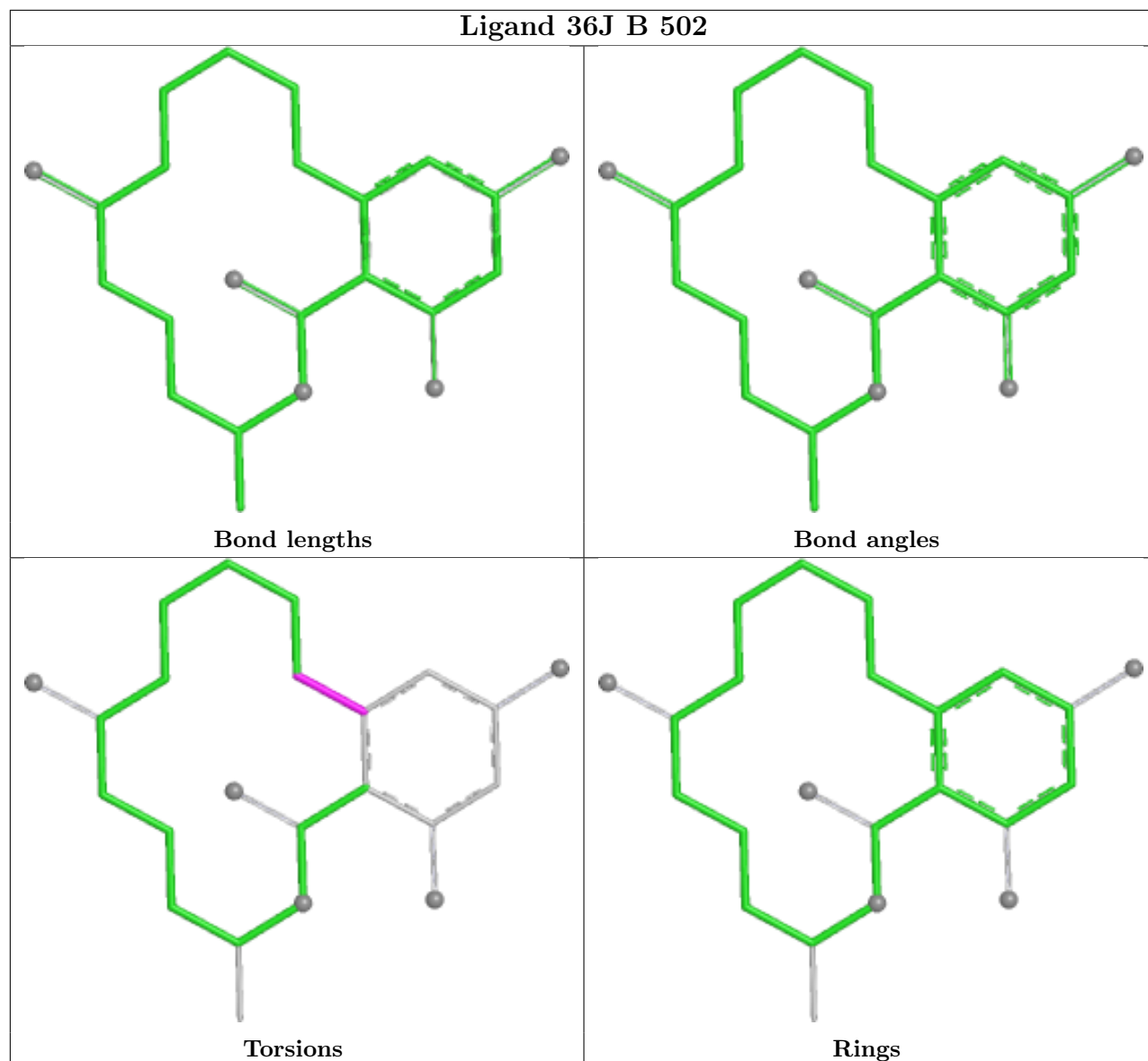
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PEG	2	0
4	A	504	PEG	4	0
3	B	502	36J	2	0
6	B	504	TRS	2	0
3	A	502	36J	3	0
4	B	503	PEG	6	0

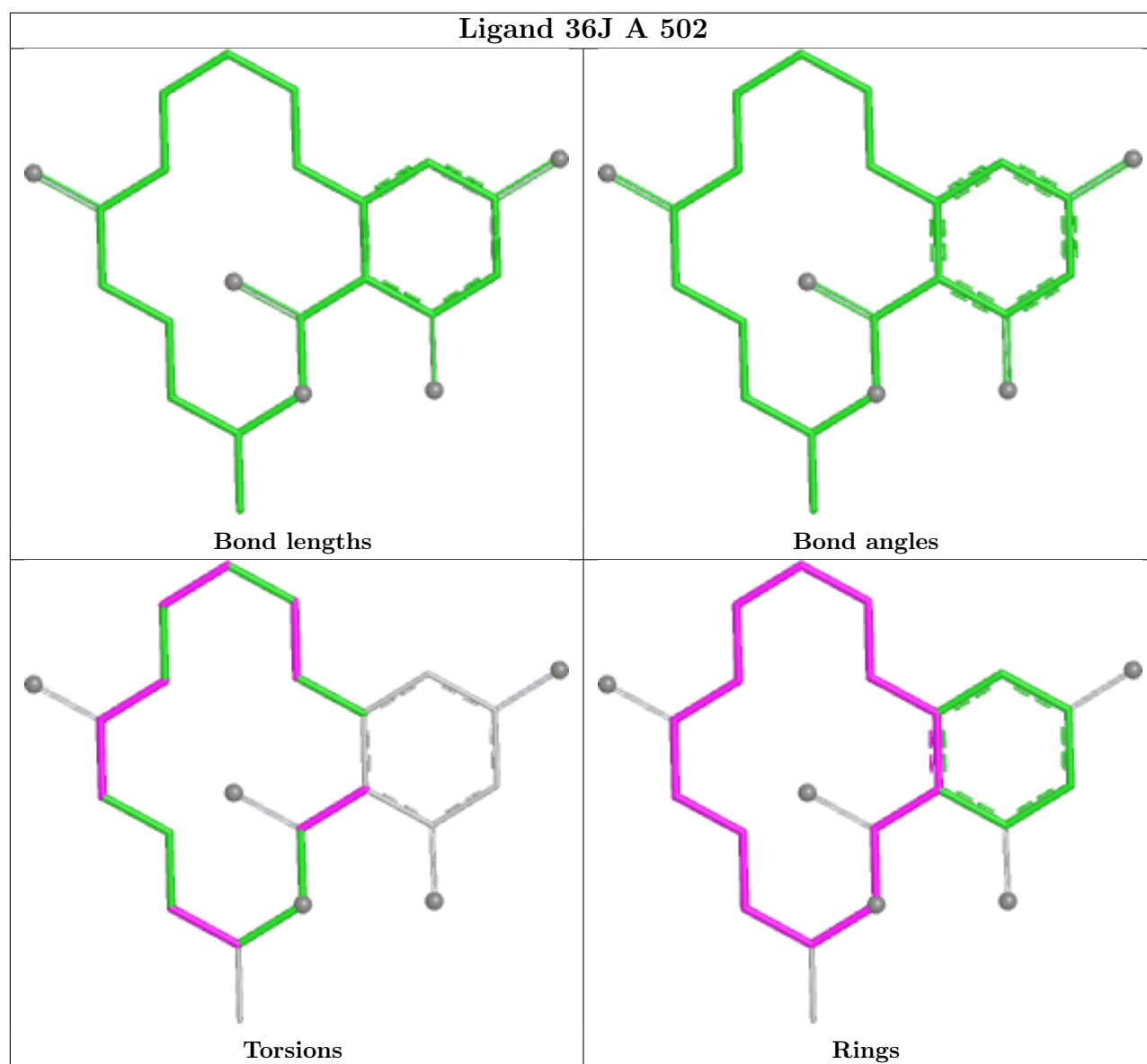
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 36J B 502





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	451/455 (99%)	-0.15	10 (2%) 62 65	15, 29, 65, 83	3 (0%)
1	B	451/455 (99%)	-0.15	3 (0%) 84 86	15, 30, 57, 82	3 (0%)
All	All	902/910 (99%)	-0.15	13 (1%) 73 75	15, 30, 60, 83	6 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	LEU	3.3
1	A	197	PRO	2.7
1	B	228	GLY	2.6
1	A	199	TYR	2.6
1	A	202	ASN	2.5
1	A	454	ILE	2.4
1	A	192	ALA	2.3
1	B	192	ALA	2.3
1	A	203	LYS	2.3
1	A	189	LEU	2.2
1	A	455	PRO	2.1
1	A	194	PRO	2.1
1	B	186	GLN	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

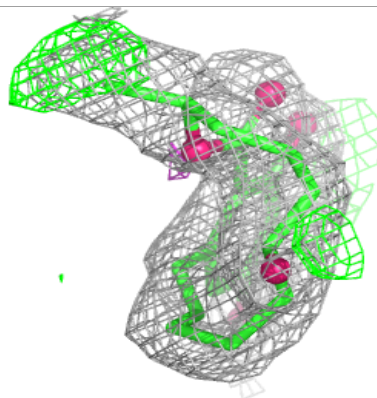
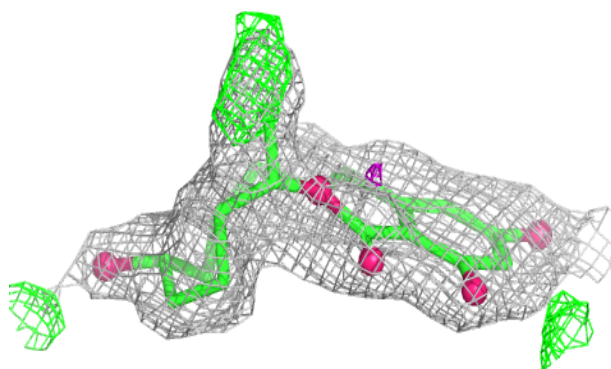
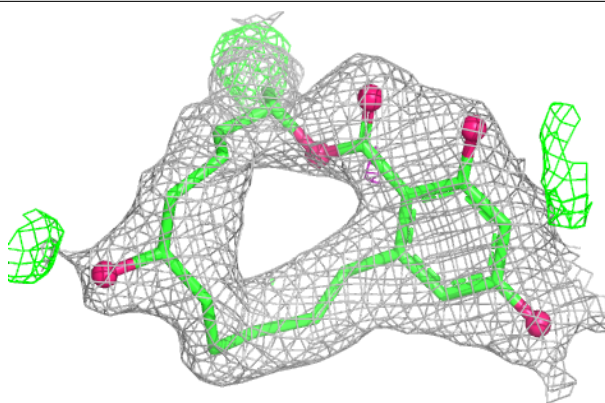
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	TRS	B	504	8/8	0.75	0.19	71,74,78,84	0
4	PEG	A	505	7/7	0.80	0.15	43,53,54,54	0
5	NI	B	506	1/1	0.80	0.10	95,95,95,95	0
4	PEG	A	503	7/7	0.80	0.17	52,55,59,60	0
3	36J	B	502	23/23	0.81	0.14	42,47,57,58	0
4	PEG	A	504	7/7	0.82	0.15	31,48,55,57	0
3	36J	A	502	23/23	0.82	0.16	43,51,59,61	0
4	PEG	B	503	7/7	0.83	0.18	37,54,59,60	0
5	NI	A	507	1/1	0.85	0.12	82,82,82,82	0
5	NI	B	505	1/1	0.92	0.07	72,72,72,72	0
5	NI	A	506	1/1	0.95	0.07	65,65,65,65	0
2	HEM	A	501	43/43	0.98	0.05	18,20,23,24	0
2	HEM	B	501	43/43	0.99	0.05	18,19,22,23	0

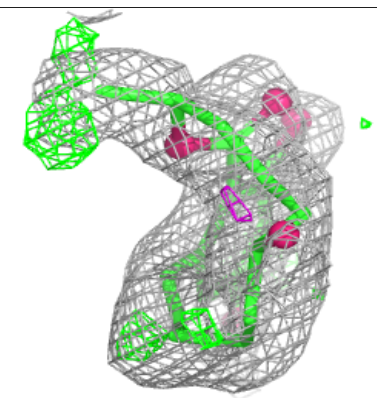
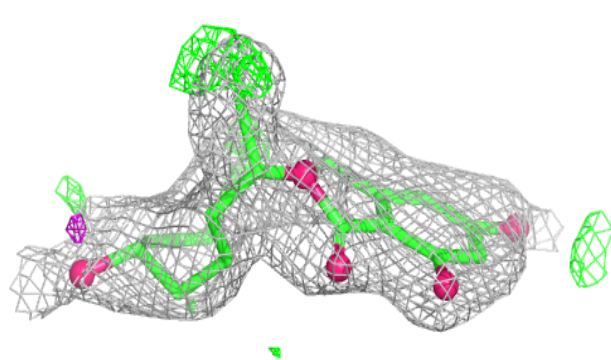
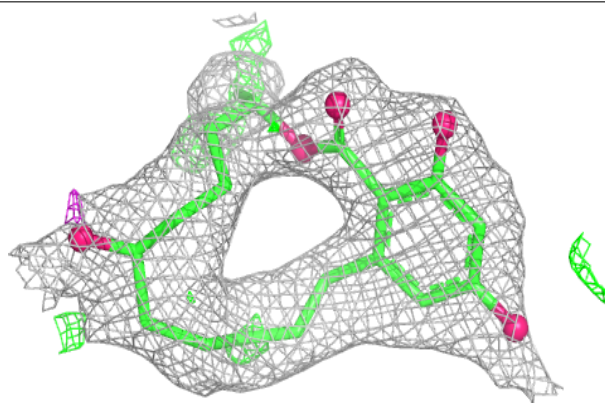
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 36J B 502:**

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

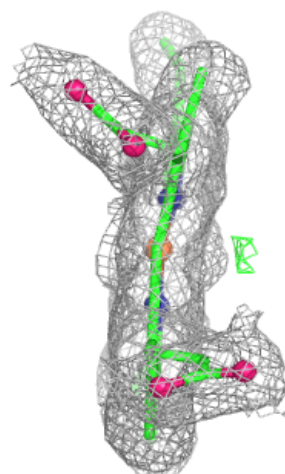
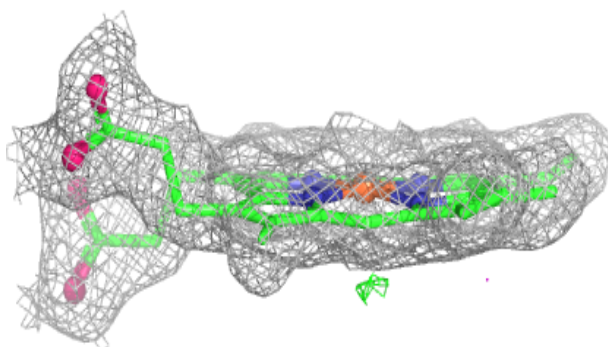
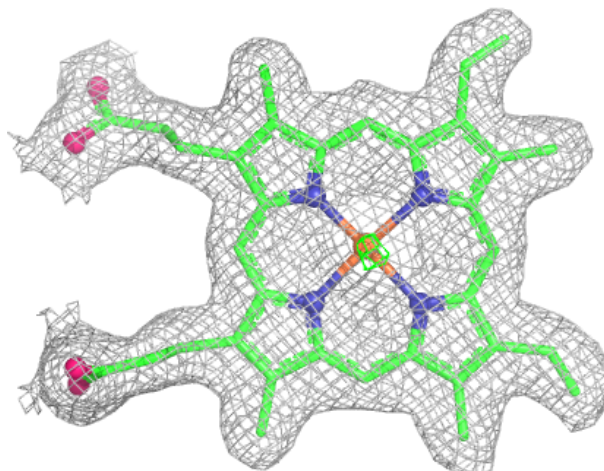
**Electron density around 36J A 502:**

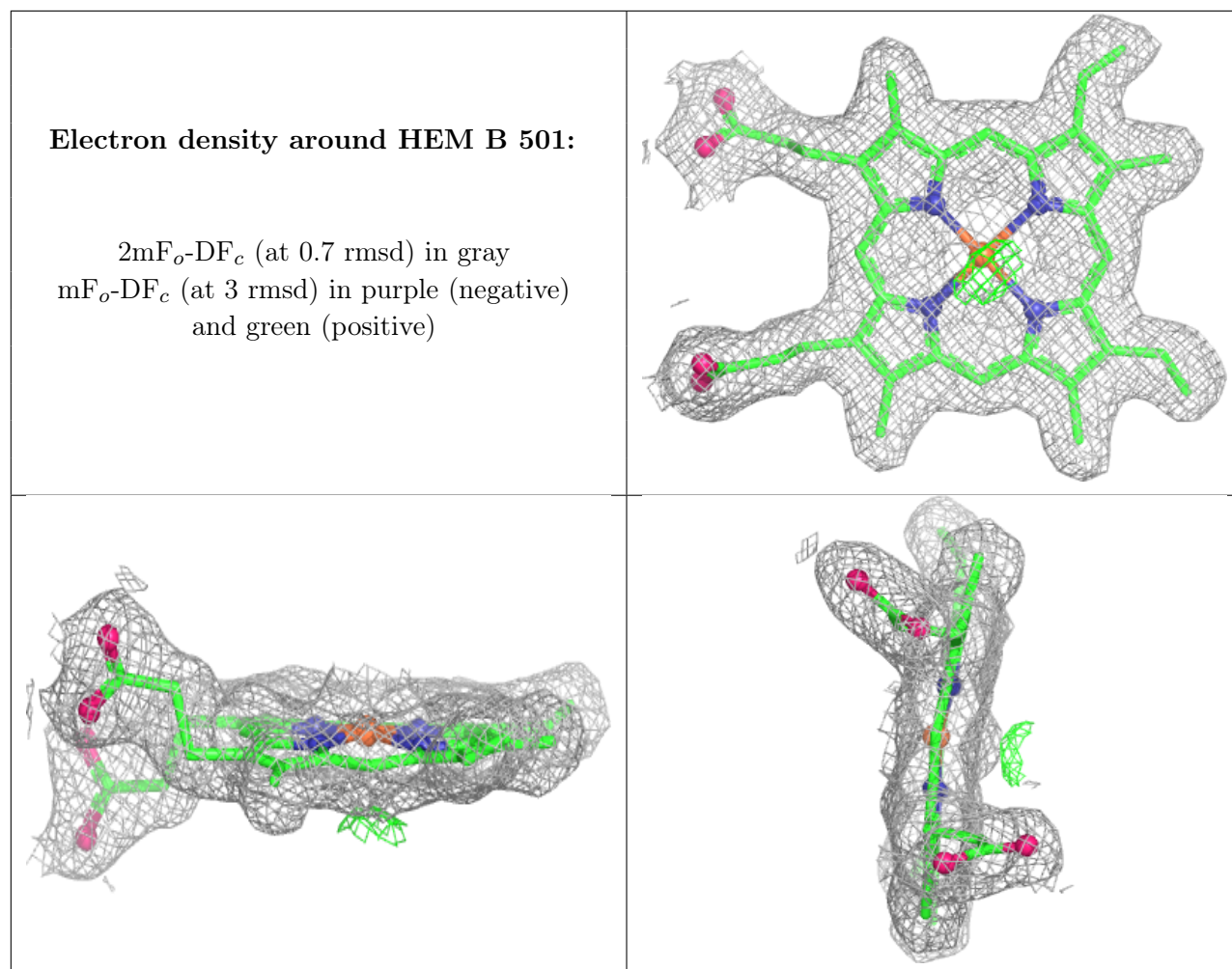
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 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.