



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 7ZLT / pdb_00007zlt
Title : Crystal structure of CYP125 from Mycobacterium tuberculosis in complex with an inhibitor
Authors : Snee, M.; Kavanagh, M.; Levy, C.
Deposited on : 2022-04-15
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

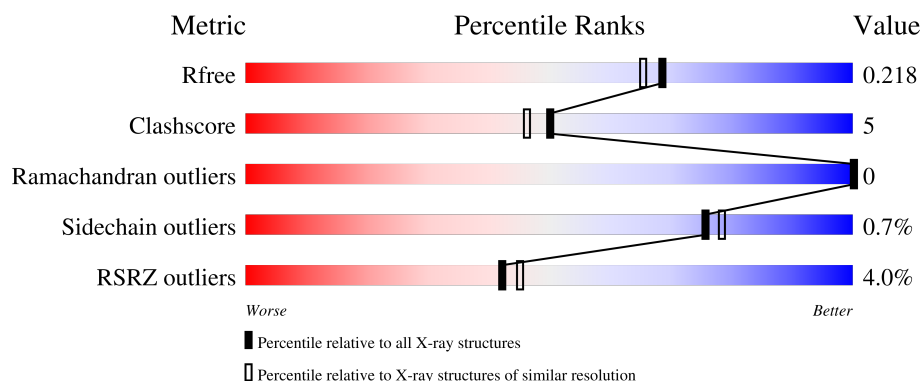
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	418	3% 89% 9% .
1	B	418	6% 86% 11% .
1	C	418	3% 89% 10% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20627 atoms, of which 9806 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.

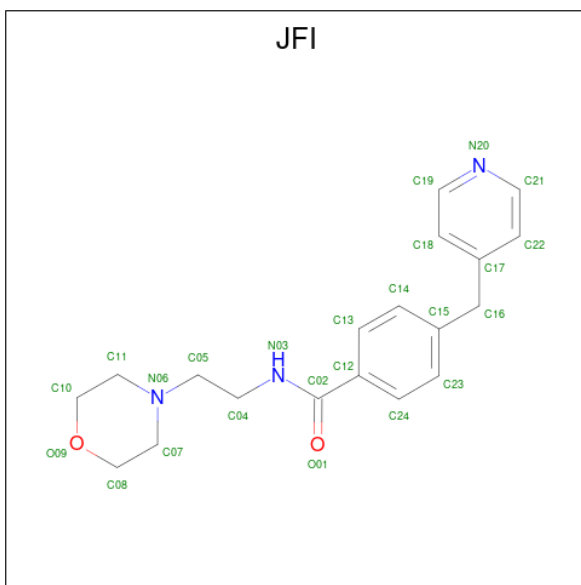
- Molecule 1 is a protein called Steroid C26-monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	H	N	O	S	0	24	0
			6639	2137	3287	573	625	17			
1	B	405	Total	C	H	N	O	S	0	7	0
			6283	2033	3075	560	601	14			
1	C	415	Total	C	H	N	O	S	0	21	0
			6632	2138	3262	585	629	18			

There are 6 discrepancies between the modelled and reference sequences:

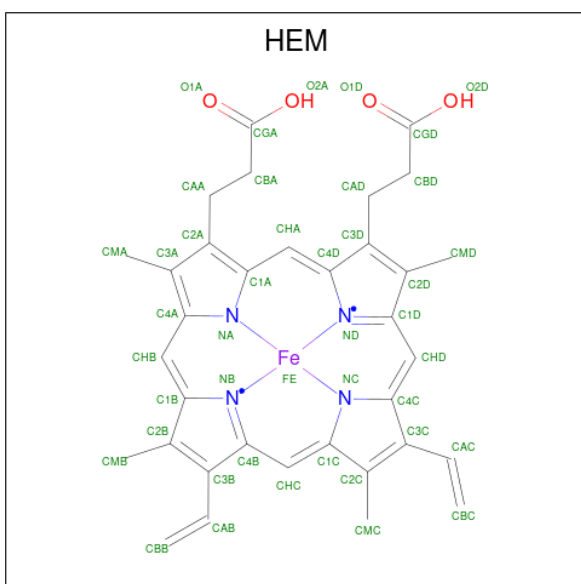
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	-	expression tag	UNP P9WPP1
A	17	GLY	-	expression tag	UNP P9WPP1
B	16	ASN	-	expression tag	UNP P9WPP1
B	17	GLY	-	expression tag	UNP P9WPP1
C	16	ASN	-	expression tag	UNP P9WPP1
C	17	GLY	-	expression tag	UNP P9WPP1

- Molecule 2 is {N}-(2-morpholin-4-ylethyl)-4-(pyridin-4-ylmethyl)benzamide (CCD ID: JFI) (formula: C₁₉H₂₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



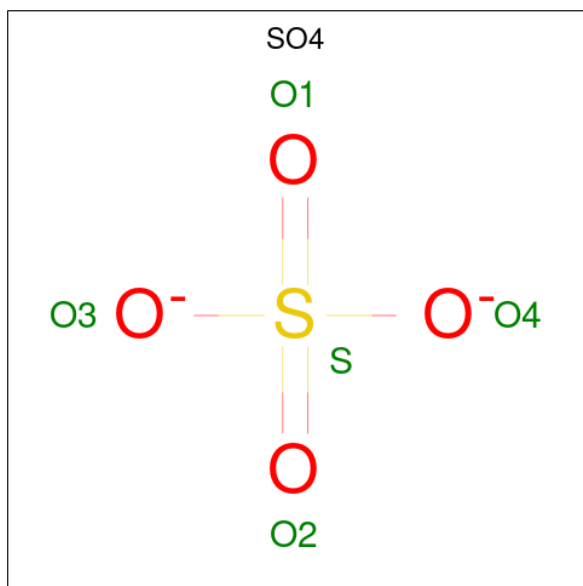
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	1
			94	38	46	6	4		
2	B	1	Total	C	H	N	O	0	0
			47	19	23	3	2		
2	C	1	Total	C	H	N	O	0	0
			47	19	23	3	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

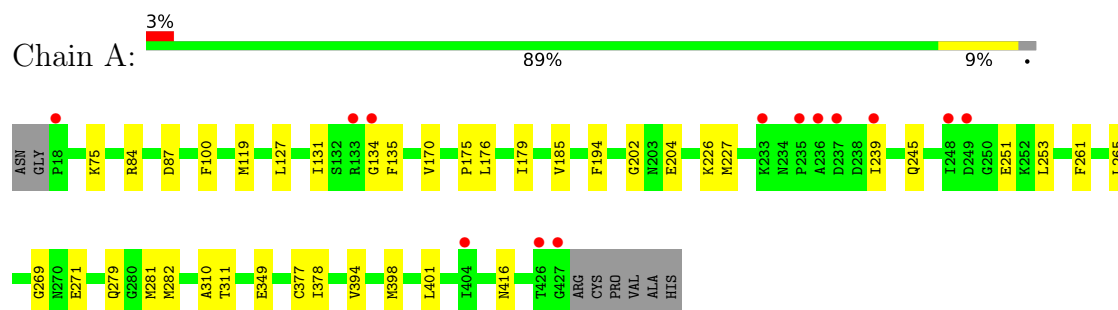
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	283	Total O 283 283	0	0
6	B	161	Total O 161 161	0	0
6	C	151	Total O 151 151	0	0

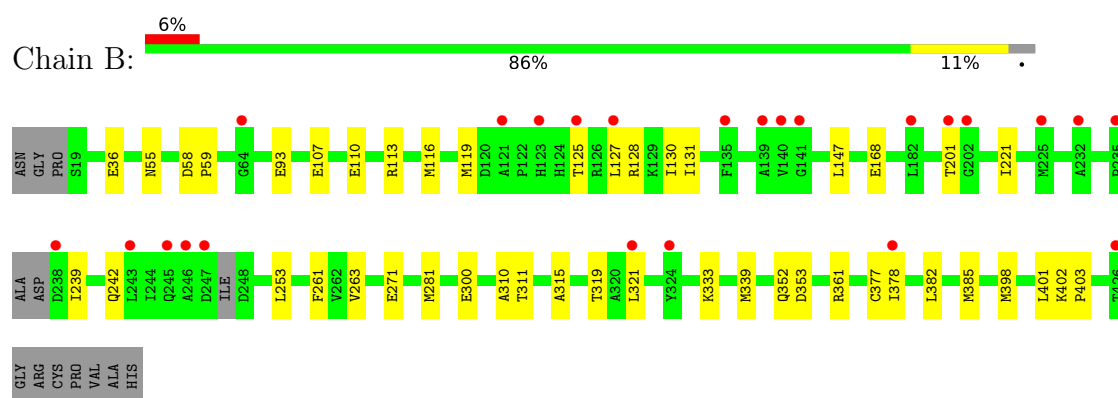
3 Residue-property plots [i](#)

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.

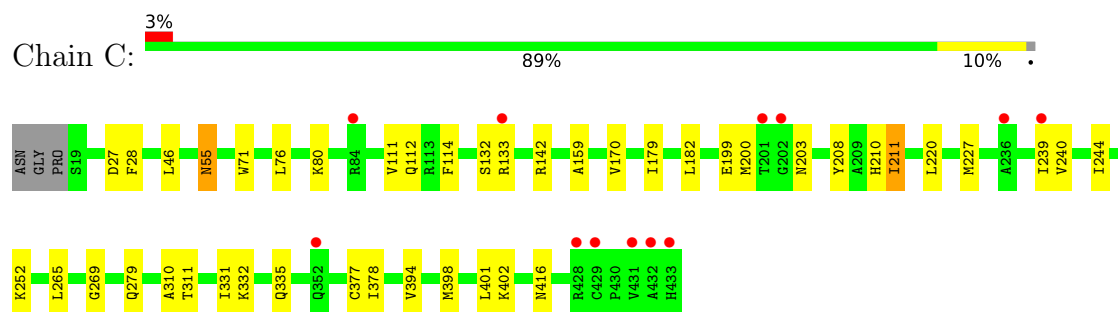
- Molecule 1: Steroid C26-monooxygenase



- Molecule 1: Steroid C26-monooxygenase



- Molecule 1: Steroid C26-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.97Å 68.44Å 144.46Å 90.00° 93.83° 90.00°	Depositor
Resolution (Å)	61.11 – 1.90 61.11 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.11-1.90) 93.0 (61.11-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.184 , 0.220 0.187 , 0.218	Depositor DCC
R_{free} test set	5032 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20627	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: JFI, HEM, SO4, CL

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	0.37	0/3506	0.53	0/4754
1	B	0.27	0/3311	0.41	0/4493
1	C	0.27	0/3512	0.43	0/4765
All	All	0.31	0/10329	0.46	0/14012

There are no bond length outliers.

There are no bond angle outliers.

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	3352	3287	3285	37	0
1	B	3208	3075	3074	34	1
1	C	3370	3262	3249	29	1
2	A	48	46	0	0	0
2	B	24	23	0	0	0
2	C	24	23	0	0	0
3	A	43	30	30	3	0
3	B	43	30	30	4	0
3	C	43	30	30	4	0
4	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	25	0	0	1	0
4	C	30	0	0	0	0
5	A	1	0	0	0	0
6	A	283	0	0	5	1
6	B	161	0	0	2	0
6	C	151	0	0	2	0
All	All	10821	9806	9698	105	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 5.

All (105) 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:119:MET:HE1	1:B:127:LEU:CD1	2.08	0.83
1:A:87[B]:ASP:OD2	6:A:601:HOH:O	2.06	0.73
1:B:119:MET:HE1	1:B:127:LEU:HD12	1.76	0.68
1:C:112:GLN:OE1	6:C:601:HOH:O	2.12	0.68
1:A:179[B]:ILE:HD11	1:A:269:GLY:C	2.19	0.67
3:A:502:HEM:HBC2	3:A:502:HEM:HMC2	1.78	0.65
1:B:36[A]:GLU:OE1	6:B:601:HOH:O	2.15	0.65
1:B:300:GLU:H	1:B:300:GLU:CD	2.05	0.64
1:B:93:GLU:HG2	1:B:319:THR:HG21	1.81	0.63
1:B:119:MET:HE1	1:B:127:LEU:HD13	1.81	0.62
1:A:271:GLU:HG3	6:A:650:HOH:O	2.00	0.61
1:A:175:PRO:O	1:A:179[B]:ILE:HD12	2.00	0.61
1:A:279[A]:GLN:OE1	1:A:416:ASN:ND2	2.35	0.59
1:C:132:SER:HA	1:C:378:ILE:HD11	1.85	0.58
1:A:176[B]:LEU:HD22	1:A:194[B]:PHE:CD1	2.38	0.58
1:A:281[B]:MET:CE	1:A:394:VAL:HG11	2.33	0.58
1:A:179[B]:ILE:HD11	1:A:269:GLY:HA3	1.87	0.57
1:B:131:ILE:HD13	1:B:261:PHE:CD1	2.40	0.56
1:C:239:ILE:HD12	1:C:239:ILE:H	1.69	0.56
3:B:502:HEM:HBC2	3:B:502:HEM:HMC2	1.88	0.56
1:A:185:VAL:HG22	1:A:227[A]:MET:HE1	1.87	0.55
1:A:176[B]:LEU:HD22	1:A:194[B]:PHE:CG	2.41	0.55
1:C:244:ILE:O	1:C:252:LYS:NZ	2.34	0.54
1:C:170:VAL:O	6:C:602:HOH:O	2.19	0.54
1:B:201:THR:HB	1:B:271:GLU:OE1	2.08	0.53
1:B:128:ARG:NH2	1:B:378:ILE:HG22	2.24	0.53
1:B:128:ARG:CZ	1:B:378:ILE:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HD11	1:A:253:LEU:HD11	1.91	0.52
1:B:352:GLN:HA	1:B:352:GLN:OE1	2.09	0.52
1:B:382:LEU:HD23	3:B:502:HEM:HBC2	1.92	0.52
1:B:402:LYS:HE3	1:B:403:PRO:HD2	1.92	0.50
1:A:179[B]:ILE:HD11	1:A:269:GLY:CA	2.41	0.50
1:A:75:LYS:NZ	1:A:349:GLU:HG3	2.27	0.49
1:B:110:GLU:OE1	1:B:113:ARG:NH1	2.45	0.49
1:B:221:ILE:HG13	1:B:263:VAL:HG21	1.95	0.49
1:A:179[B]:ILE:HD11	1:A:269:GLY:O	2.12	0.49
1:B:281:MET:CE	1:B:401:LEU:HD21	2.43	0.49
1:A:281[B]:MET:HE3	1:A:394:VAL:HG11	1.95	0.49
1:A:131:ILE:CD1	1:A:253:LEU:HD11	2.43	0.48
1:C:159:ALA:HB2	1:C:398[B]:MET:HG3	1.96	0.48
1:A:251:GLU:HA	1:A:251:GLU:OE1	2.13	0.48
1:A:131:ILE:HD12	1:A:261:PHE:CD1	2.49	0.47
1:B:127:LEU:O	1:B:131:ILE:HG13	2.14	0.47
1:C:239:ILE:HD12	1:C:239:ILE:N	2.29	0.47
1:C:71:TRP:CD1	1:C:331:ILE:HD12	2.50	0.47
1:A:119:MET:HE1	1:A:127:LEU:HD11	1.97	0.46
1:C:401[A]:LEU:HD23	1:C:402:LYS:N	2.30	0.46
1:A:281[B]:MET:HE1	1:A:394:VAL:HG11	1.98	0.46
1:C:208:TYR:HA	1:C:210:HIS:CE1	2.50	0.46
1:A:310:ALA:O	1:A:311:THR:C	2.59	0.45
1:B:116:MET:HA	1:B:119:MET:HE2	1.98	0.45
1:C:227[B]:MET:HE2	1:C:240:VAL:HG21	1.98	0.45
1:A:377:CYS:HA	3:A:502:HEM:CHA	2.46	0.45
1:C:377:CYS:HA	3:C:502:HEM:CHA	2.46	0.45
3:A:502:HEM:HBC2	3:A:502:HEM:CMC	2.46	0.45
1:B:281:MET:HE1	1:B:401:LEU:HD21	1.99	0.45
1:C:394:VAL:HG13	1:C:398[B]:MET:HE2	1.99	0.45
1:B:239:ILE:HA	1:B:242:GLN:HG3	1.99	0.45
3:C:502:HEM:CMC	3:C:502:HEM:HBC2	2.46	0.45
1:B:361:ARG:NH1	4:B:504:SO4:O2	2.42	0.44
1:A:84:ARG:NH2	6:A:615:HOH:O	2.48	0.44
1:C:182:LEU:O	1:C:239:ILE:HD13	2.18	0.44
3:B:502:HEM:HBC2	3:B:502:HEM:CMC	2.47	0.44
1:C:332:LYS:O	1:C:335:GLN:HB2	2.18	0.44
3:C:502:HEM:HBC2	3:C:502:HEM:HMC1	1.99	0.44
1:A:170:VAL:HG21	1:A:398[B]:MET:HE1	1.99	0.44
1:B:310:ALA:O	1:B:311:THR:C	2.61	0.44
1:B:107:GLU:OE1	1:B:107:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200[A]:MET:HE1	1:C:220:LEU:CD1	2.48	0.44
1:B:321:LEU:O	1:B:333:LYS:NZ	2.47	0.43
1:B:130:ILE:HG21	1:B:253:LEU:CD2	2.49	0.43
1:B:398:MET:O	1:B:401:LEU:HD22	2.18	0.43
1:C:182:LEU:HD23	1:C:265:LEU:HD21	2.00	0.43
1:A:261:PHE:CZ	1:A:265:LEU:HD22	2.53	0.43
1:B:271:GLU:OE2	6:B:602:HOH:O	2.21	0.43
1:A:394:VAL:HG22	1:A:398[B]:MET:HE2	2.00	0.43
1:C:28:PHE:CE2	1:C:46:LEU:HD11	2.53	0.43
1:A:135:PHE:CE1	1:A:378[A]:ILE:HD12	2.54	0.43
1:C:200[A]:MET:HE1	1:C:220:LEU:HD13	2.01	0.43
1:B:107:GLU:H	1:B:107:GLU:CD	2.26	0.43
1:C:199:GLU:O	1:C:211[B]:ILE:CG2	2.67	0.43
1:A:261:PHE:CZ	1:A:265:LEU:CD2	3.02	0.42
1:C:269:GLY:HA2	3:C:502:HEM:HMC3	2.01	0.42
1:A:226:LYS:HE2	1:B:353:ASP:OD2	2.19	0.42
1:A:100:PHE:C	1:A:204:GLU:OE2	2.62	0.42
1:C:279:GLN:HE22	1:C:416:ASN:ND2	2.17	0.42
1:C:200[A]:MET:CE	1:C:220:LEU:CD1	2.97	0.42
1:A:202:GLY:HA2	6:A:660:HOH:O	2.19	0.42
1:B:58:ASP:HB3	1:B:59:PRO:HD2	2.02	0.42
1:C:111:VAL:HG23	1:C:114:PHE:CE2	2.55	0.42
1:C:27:ASP:HA	1:C:55:ASN:HD21	1.85	0.42
1:C:76:LEU:HD21	1:C:80:LYS:HD2	2.01	0.42
1:B:147:LEU:HD12	1:B:385:MET:HE3	2.01	0.41
1:B:377:CYS:HA	3:B:502:HEM:CHA	2.50	0.41
1:C:310:ALA:O	1:C:311:THR:C	2.64	0.41
1:A:279[B]:GLN:NE2	1:A:282:MET:CE	2.84	0.41
1:B:93:GLU:HB3	1:B:319:THR:HB	2.03	0.41
1:A:134:GLY:O	1:A:239:ILE:HG21	2.21	0.41
1:A:204:GLU:HG3	6:A:662:HOH:O	2.21	0.40
1:C:179:ILE:HG23	1:C:265:LEU:HD23	2.04	0.40
1:B:315:ALA:HA	1:B:339:MET:O	2.21	0.40
1:A:131:ILE:HD12	1:A:261:PHE:CE1	2.56	0.40

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)
6:A:827:HOH:O	6:A:827:HOH:O[2_556]	1.73	0.47
1:B:168:GLU:OE1	1:C:142:ARG:HH21[4_555]	1.38	0.22

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	432/418 (103%)	423 (98%)	9 (2%)	0	100	100
1	B	408/418 (98%)	399 (98%)	9 (2%)	0	100	100
1	C	434/418 (104%)	421 (97%)	13 (3%)	0	100	100
All	All	1274/1254 (102%)	1243 (98%)	31 (2%)	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	358/341 (105%)	356 (99%)	2 (1%)	78	81
1	B	332/341 (97%)	330 (99%)	2 (1%)	78	81
1	C	355/341 (104%)	348 (98%)	7 (2%)	48	46
All	All	1045/1023 (102%)	1034 (99%)	11 (1%)	76	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401[A]	LEU
1	A	401[B]	LEU
1	B	55	ASN
1	B	125	THR
1	C	55	ASN

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Mol	Chain	Res	Type
1	C	133[A]	ARG
1	C	133[B]	ARG
1	C	203[A]	ASN
1	C	203[B]	ASN
1	C	211[A]	ILE
1	C	211[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	ASN
1	C	148	GLN
1	C	245	GLN
1	C	330	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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	SO4	C	505	-	4,4,4	0.29	0	6,6,6	0.16	0
2	JFI	A	501[B]	3	26,26,26	2.35	4 (15%)	33,33,33	1.61	6 (18%)
2	JFI	C	501	3	26,26,26	2.24	4 (15%)	33,33,33	1.48	5 (15%)
2	JFI	B	501	3	26,26,26	2.23	4 (15%)	33,33,33	1.28	5 (15%)
4	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.13	0
4	SO4	B	507	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.13	0
3	HEM	C	502	2,1	50,50,50	1.42	7 (14%)	67,82,82	1.10	4 (5%)
4	SO4	B	506	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	C	503	-	4,4,4	0.20	0	6,6,6	0.10	0
4	SO4	B	505	-	4,4,4	0.26	0	6,6,6	0.16	0
2	JFI	A	501[A]	3	26,26,26	2.24	4 (15%)	33,33,33	1.29	3 (9%)
4	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.21	0
3	HEM	A	502	2,1	50,50,50	1.28	5 (10%)	67,82,82	0.93	2 (2%)
4	SO4	C	507	-	4,4,4	0.28	0	6,6,6	0.16	0
4	SO4	A	505	-	4,4,4	0.21	0	6,6,6	0.25	0
4	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.11	0
3	HEM	B	502	2,1	50,50,50	1.36	5 (10%)	67,82,82	1.19	4 (5%)
4	SO4	C	508	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.09	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
2	JFI	A	501[A]	3	-	0/14/22/22	0/3/3/3
2	JFI	B	501	3	-	0/14/22/22	0/3/3/3
3	HEM	B	502	2,1	-	2/14/54/54	-
3	HEM	A	502	2,1	-	2/14/54/54	-
2	JFI	A	501[B]	3	-	1/14/22/22	0/3/3/3
3	HEM	C	502	2,1	-	2/14/54/54	-
2	JFI	C	501	3	-	1/14/22/22	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	JFI	C05-N06	-8.62	1.27	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	JFI	C05-N06	-8.51	1.28	1.47
2	C	501	JFI	C05-N06	-8.28	1.28	1.47
2	A	501[A]	JFI	C05-N06	-7.79	1.29	1.47
2	A	501[B]	JFI	C02-N03	6.19	1.47	1.33
2	A	501[A]	JFI	C02-N03	6.04	1.47	1.33
2	C	501	JFI	C02-N03	5.87	1.46	1.33
2	B	501	JFI	C02-N03	5.33	1.45	1.33
3	B	502	HEM	FE-ND	4.12	2.07	1.94
3	C	502	HEM	FE-ND	3.82	2.06	1.94
2	A	501[B]	JFI	C07-N06	-3.57	1.37	1.46
3	C	502	HEM	FE-NC	3.50	2.06	1.95
3	B	502	HEM	FE-NC	3.35	2.06	1.95
2	A	501[A]	JFI	C07-N06	-3.10	1.38	1.46
2	B	501	JFI	C07-N06	-3.01	1.38	1.46
2	A	501[A]	JFI	C11-N06	-2.99	1.38	1.46
3	B	502	HEM	CAB-C3B	2.98	1.55	1.47
3	A	502	HEM	CAC-C3C	2.95	1.55	1.47
2	C	501	JFI	C07-N06	-2.85	1.39	1.46
3	C	502	HEM	CAB-C3B	2.79	1.54	1.47
3	B	502	HEM	CAC-C3C	2.76	1.54	1.47
2	C	501	JFI	C11-N06	-2.74	1.39	1.46
2	B	501	JFI	C11-N06	-2.74	1.39	1.46
2	A	501[B]	JFI	C11-N06	-2.64	1.39	1.46
3	C	502	HEM	FE-NB	2.53	2.02	1.94
3	C	502	HEM	CAC-C3C	2.48	1.54	1.47
3	A	502	HEM	CAB-C3B	2.20	1.53	1.47
3	C	502	HEM	CMD-C2D	2.20	1.55	1.50
3	A	502	HEM	CMC-C2C	2.15	1.55	1.50
3	B	502	HEM	CMA-C3A	2.14	1.55	1.50
3	A	502	HEM	CAA-C2A	2.08	1.56	1.51
3	C	502	HEM	CMC-C2C	2.04	1.55	1.50
3	A	502	HEM	FE-ND	2.01	2.01	1.94

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	JFI	C10-C11-N06	5.32	118.21	110.12
2	C	501	JFI	C11-N06-C07	3.81	117.04	108.84
2	C	501	JFI	C08-C07-N06	3.78	115.86	110.12
2	C	501	JFI	C10-C11-N06	3.63	115.63	110.12
2	A	501[A]	JFI	C08-C07-N06	3.41	115.30	110.12
2	A	501[A]	JFI	C10-C11-N06	3.23	115.03	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	JFI	C11-N06-C07	2.97	115.23	108.84
3	B	502	HEM	C3B-C2B-C1B	2.93	108.61	106.41
3	C	502	HEM	C1B-NB-C4B	2.81	108.54	105.21
3	C	502	HEM	C4D-ND-C1D	2.58	108.27	105.21
2	A	501[B]	JFI	O09-C10-C11	2.57	117.30	111.77
3	B	502	HEM	C4D-ND-C1D	2.53	108.20	105.21
2	B	501	JFI	C04-N03-C02	-2.48	116.51	122.11
3	B	502	HEM	C1B-NB-C4B	2.46	108.12	105.21
2	B	501	JFI	C11-N06-C07	2.43	114.08	108.84
2	B	501	JFI	C12-C02-N03	2.43	122.17	117.12
2	B	501	JFI	O01-C02-N03	-2.40	117.91	122.59
2	A	501[B]	JFI	C21-N20-C19	2.26	122.03	116.86
2	A	501[A]	JFI	C21-N20-C19	2.24	121.99	116.86
3	B	502	HEM	CHD-C4C-NC	2.24	126.89	124.45
2	C	501	JFI	C21-N20-C19	2.24	121.98	116.86
2	B	501	JFI	C22-C21-N20	-2.20	119.85	123.60
3	C	502	HEM	C3B-C4B-NB	-2.17	107.91	109.47
2	A	501[B]	JFI	C10-O09-C08	2.09	116.65	109.88
3	A	502	HEM	CMA-C3A-C4A	-2.06	122.28	125.42
3	C	502	HEM	C3B-C2B-C1B	2.05	107.95	106.41
3	A	502	HEM	C4D-ND-C1D	2.04	107.62	105.21
2	C	501	JFI	C05-C04-N03	2.01	115.44	111.56
2	A	501[B]	JFI	C22-C21-N20	-2.00	120.19	123.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

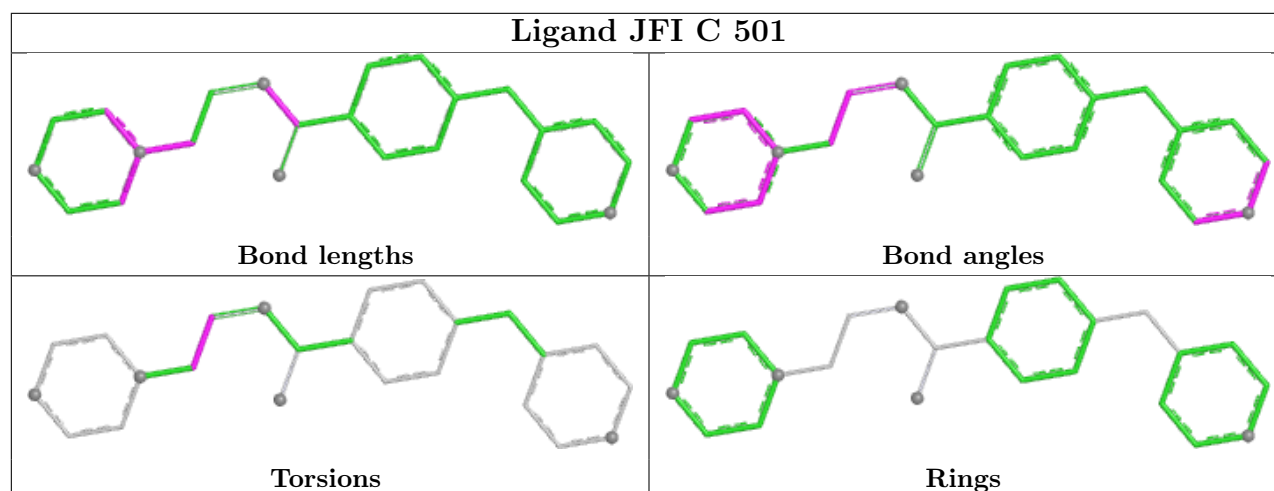
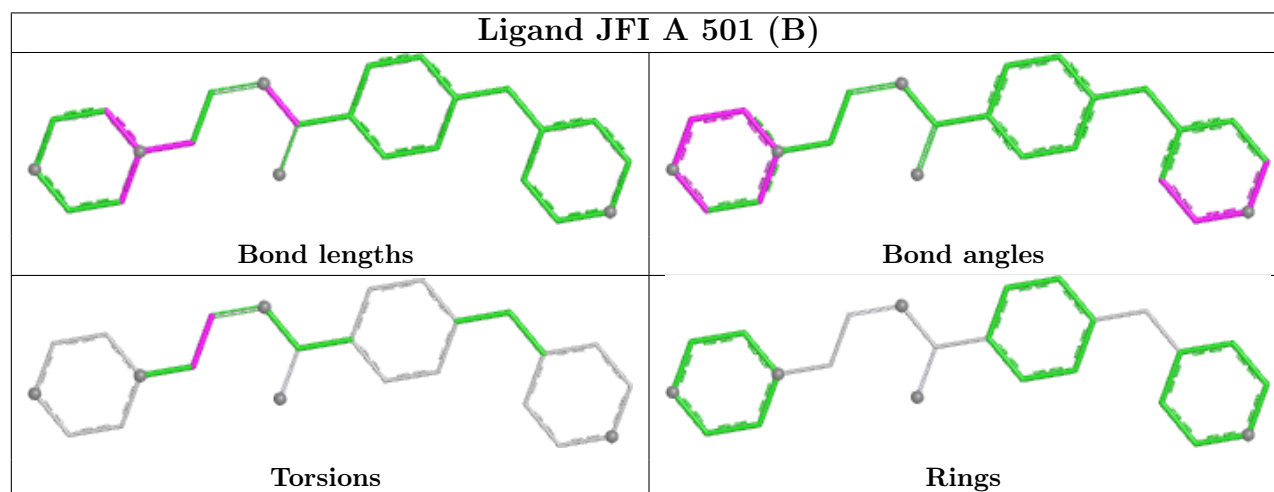
Mol	Chain	Res	Type	Atoms
3	B	502	HEM	C1A-C2A-CAA-CBA
3	A	502	HEM	C1A-C2A-CAA-CBA
2	C	501	JFI	N03-C04-C05-N06
3	A	502	HEM	C3A-C2A-CAA-CBA
3	B	502	HEM	C3A-C2A-CAA-CBA
3	C	502	HEM	C1A-C2A-CAA-CBA
2	A	501[B]	JFI	N03-C04-C05-N06
3	C	502	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

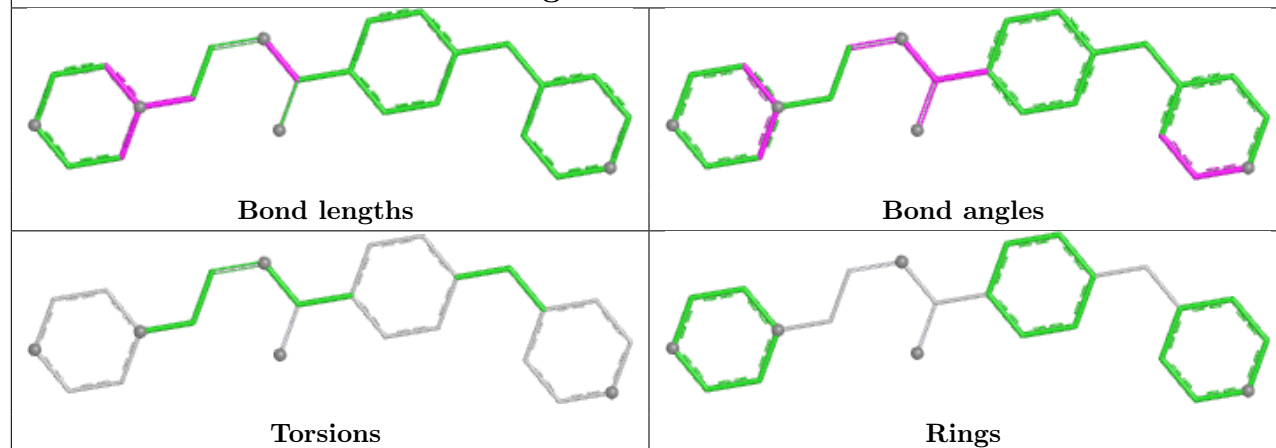
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	HEM	4	0
4	B	504	SO4	1	0
3	A	502	HEM	3	0
3	B	502	HEM	4	0

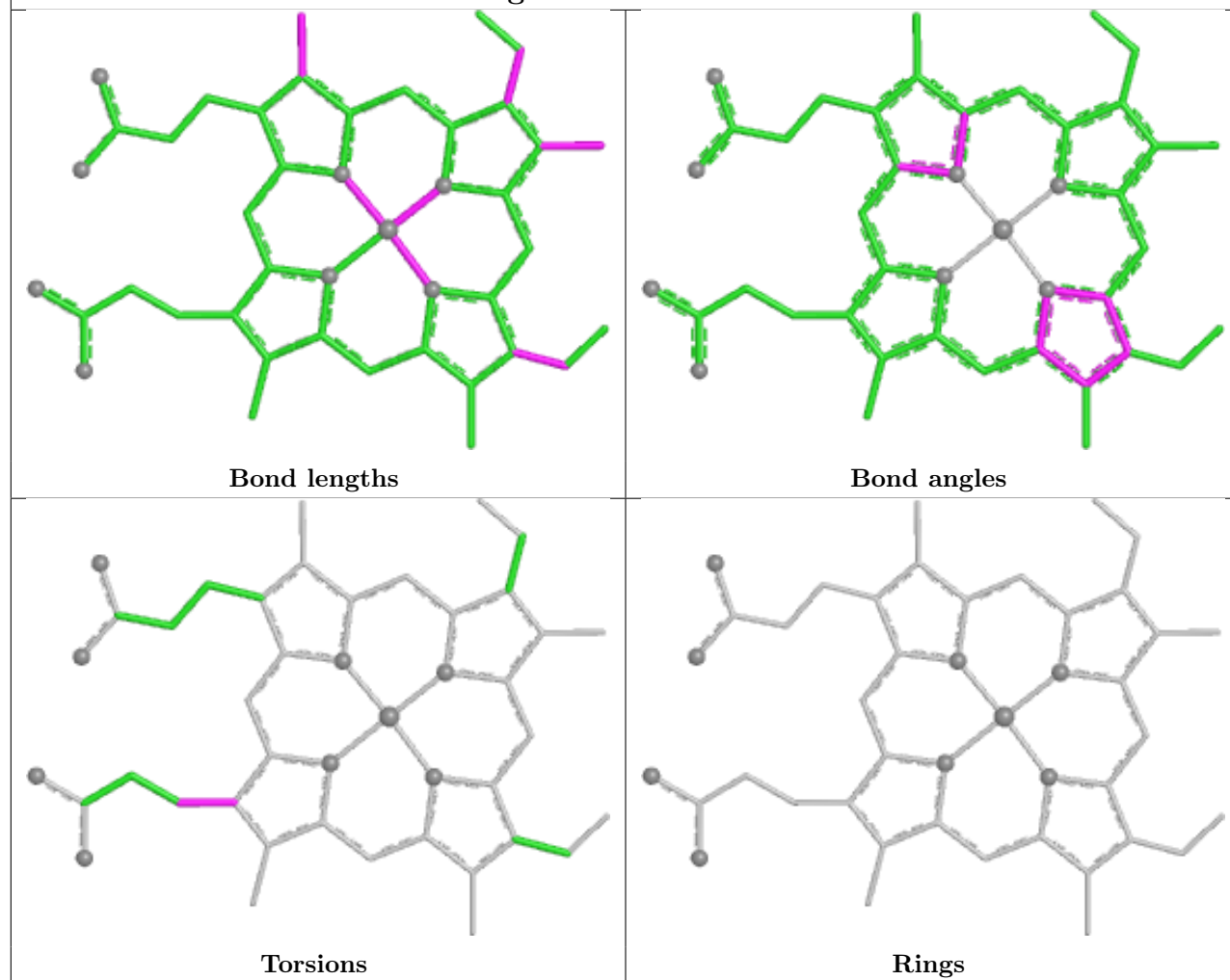
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

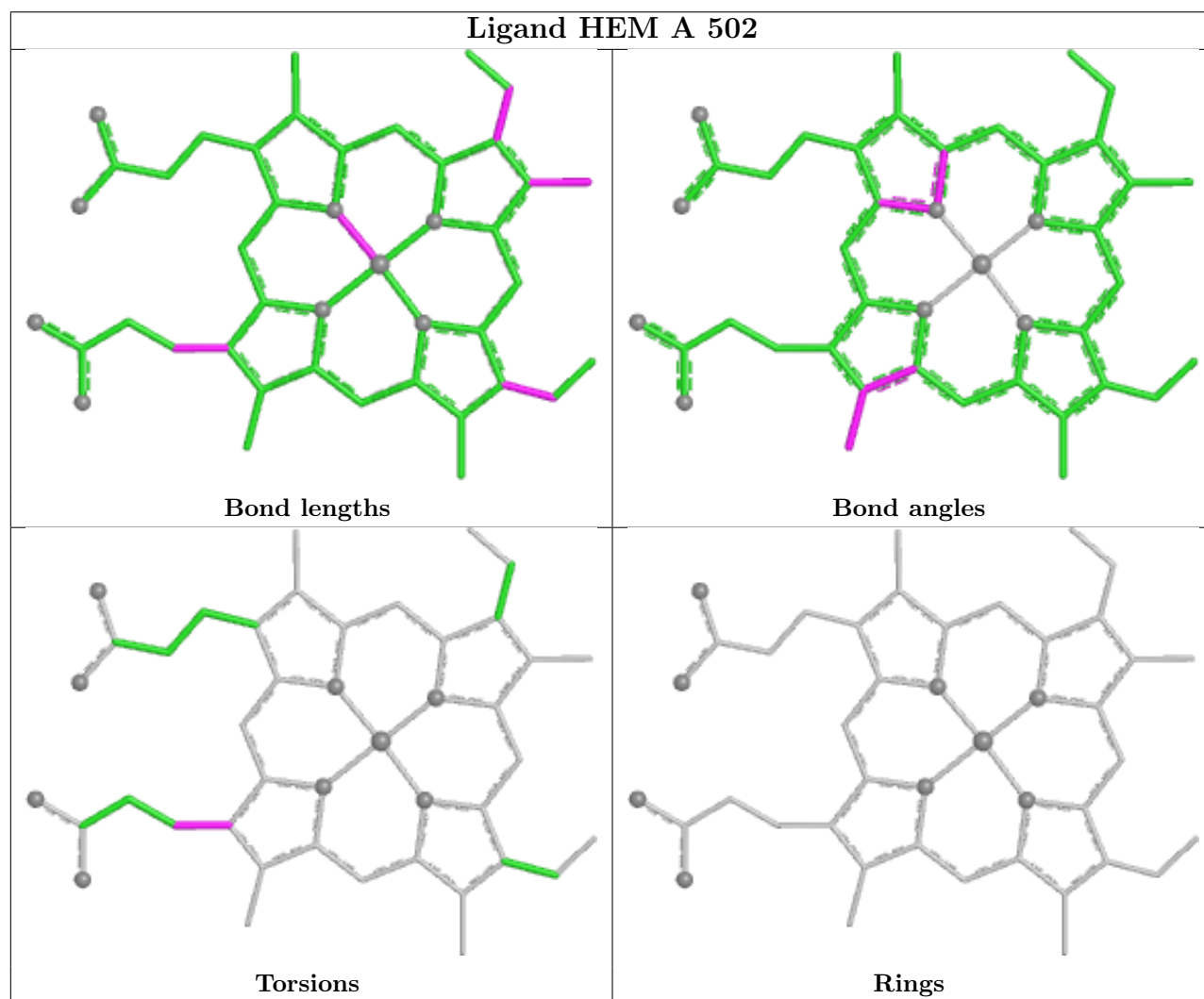
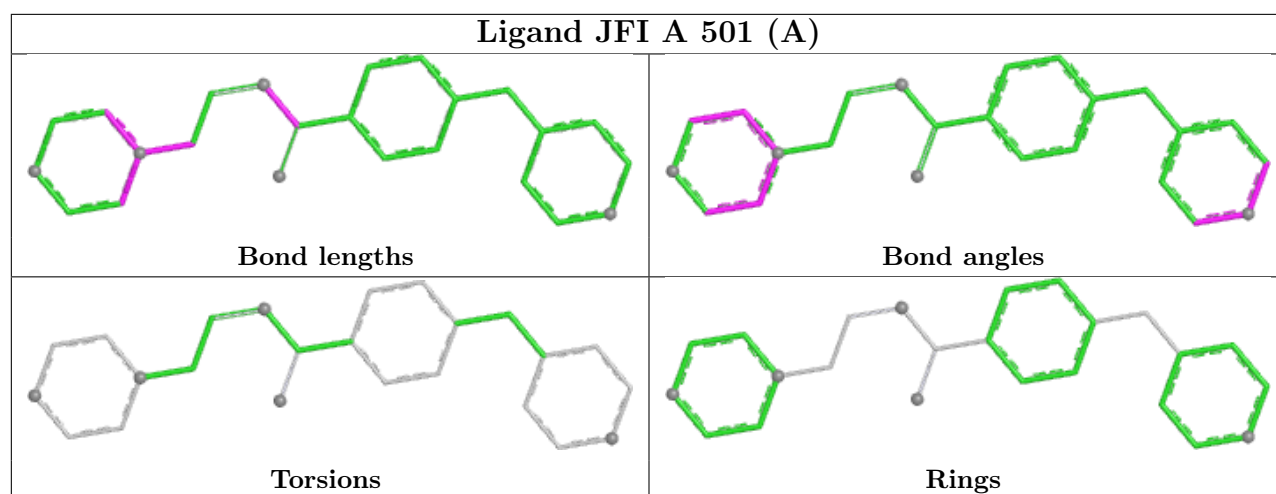


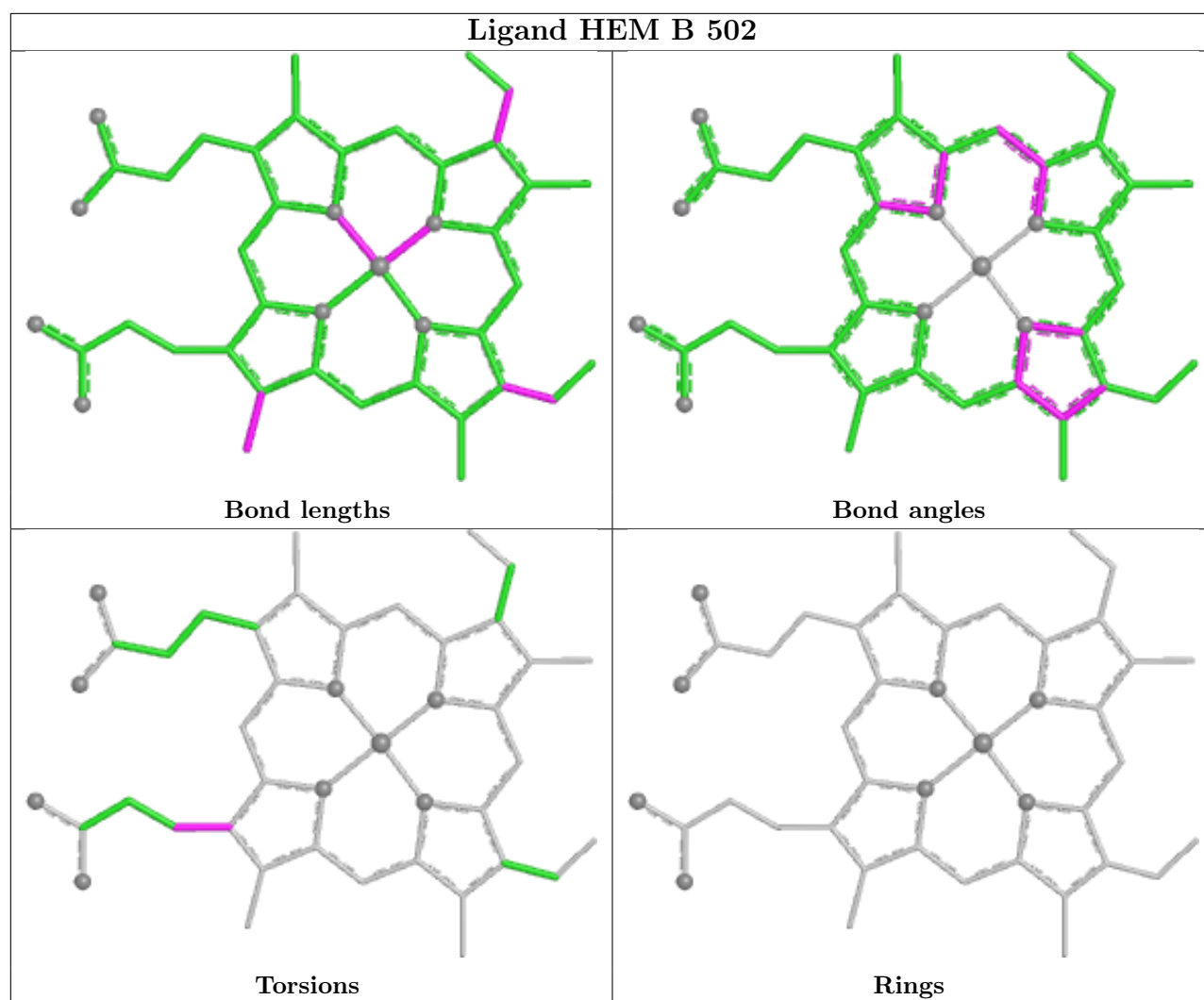
Ligand JFI B 501



Ligand HEM C 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

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	410/418 (98%)	-0.07	13 (3%) 50 54	14, 34, 64, 88	24 (5%)
1	B	405/418 (96%)	0.44	24 (5%) 28 30	19, 50, 81, 97	7 (1%)
1	C	415/418 (99%)	0.28	12 (2%) 53 57	21, 47, 71, 79	19 (4%)
All	All	1230/1254 (98%)	0.21	49 (3%) 42 45	14, 44, 75, 97	50 (4%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	4.0
1	A	427	GLY	3.9
1	C	239	ILE	3.7
1	A	237	ASP	3.6
1	A	236	ALA	3.5
1	C	433	HIS	3.3
1	C	432	ALA	3.2
1	A	248	ILE	3.1
1	C	431	VAL	3.1
1	C	201[A]	THR	3.1
1	B	247	ASP	3.0
1	B	235	PRO	3.0
1	B	121	ALA	2.9
1	A	249	ASP	2.9
1	B	232	ALA	2.6
1	C	202[A]	GLY	2.6
1	C	352[A]	GLN	2.6
1	C	428	ARG	2.6
1	A	233	LYS	2.6
1	A	133	ARG	2.6
1	B	426	THR	2.5
1	B	238	ASP	2.5
1	B	127	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	2.4
1	B	246	ALA	2.4
1	B	245	GLN	2.3
1	C	133[A]	ARG	2.3
1	B	123	HIS	2.3
1	A	18	PRO	2.3
1	B	321	LEU	2.3
1	A	134	GLY	2.3
1	B	225	MET	2.3
1	B	182	LEU	2.2
1	A	404	ILE	2.2
1	C	236	ALA	2.2
1	C	429	CYS	2.2
1	B	135	PHE	2.1
1	B	141	GLY	2.1
1	B	125	THR	2.1
1	B	378	ILE	2.1
1	B	140	VAL	2.1
1	A	235	PRO	2.1
1	B	243	LEU	2.1
1	C	84	ARG	2.1
1	B	324	TYR	2.0
1	B	201	THR	2.0
1	A	239	ILE	2.0
1	A	426	THR	2.0
1	B	64	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

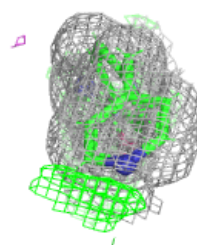
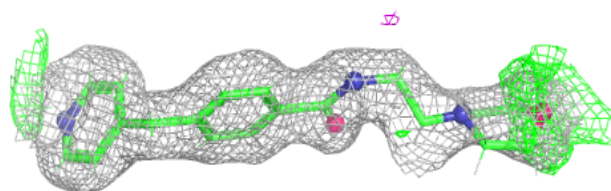
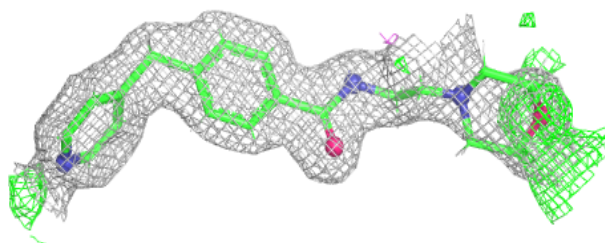
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	504	5/5	0.54	0.11	88,89,92,115	0
4	SO4	B	506	5/5	0.67	0.10	78,78,83,104	5
4	SO4	C	503	5/5	0.78	0.15	52,65,72,75	5
4	SO4	C	505	5/5	0.78	0.11	52,55,68,72	5
4	SO4	B	504	5/5	0.79	0.29	38,47,57,59	5
4	SO4	C	506	5/5	0.79	0.10	58,64,72,83	5
4	SO4	C	507	5/5	0.83	0.14	55,61,67,76	5
4	SO4	C	508	5/5	0.83	0.10	66,67,77,87	0
4	SO4	B	505	5/5	0.84	0.11	40,47,51,55	5
4	SO4	A	504	5/5	0.84	0.09	42,49,62,68	5
2	JFI	A	501[A]	24/24	0.87	0.13	22,31,46,47	47
2	JFI	A	501[B]	24/24	0.87	0.13	21,30,40,51	47
4	SO4	B	507	5/5	0.87	0.08	65,73,82,83	0
4	SO4	A	503	5/5	0.89	0.11	46,48,54,63	5
5	CL	A	506	1/1	0.89	0.14	62,62,62,62	0
4	SO4	B	503	5/5	0.91	0.09	55,62,78,78	5
4	SO4	A	505	5/5	0.91	0.09	54,57,62,76	0
2	JFI	B	501	24/24	0.92	0.10	34,51,71,73	0
2	JFI	C	501	24/24	0.94	0.10	32,45,75,84	0
3	HEM	C	502	43/43	0.98	0.07	30,38,49,58	0
3	HEM	B	502	43/43	0.98	0.08	31,42,57,61	0
3	HEM	A	502	43/43	0.99	0.06	20,24,33,45	0

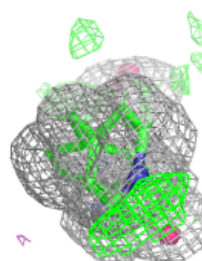
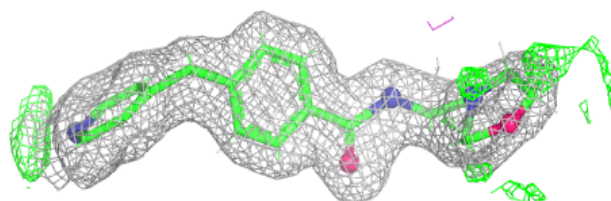
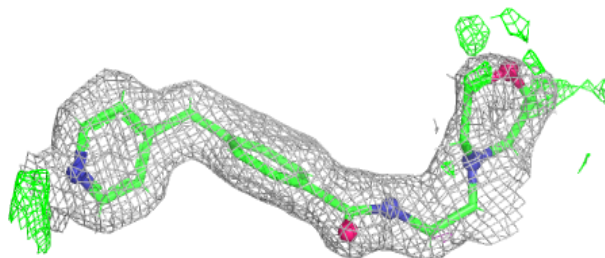
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JFI A 501 (A):

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

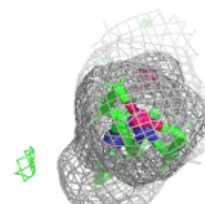
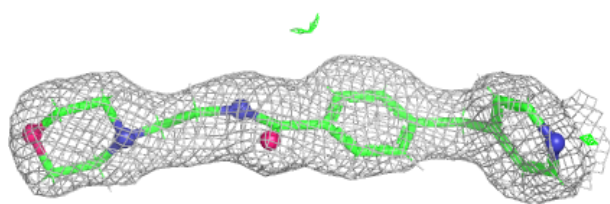
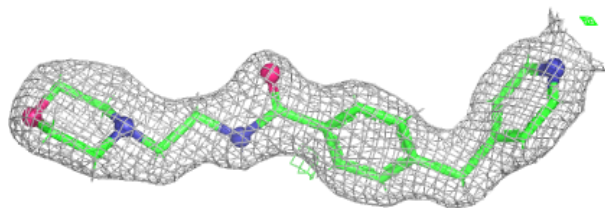
**Electron density around JFI A 501 (B):**

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

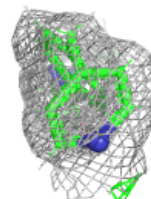
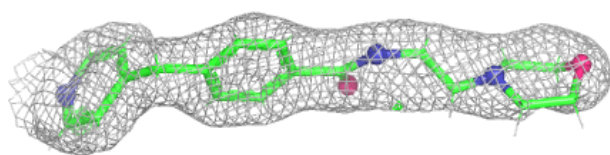
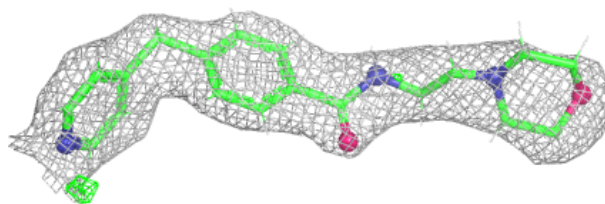


Electron density around JFI B 501:

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

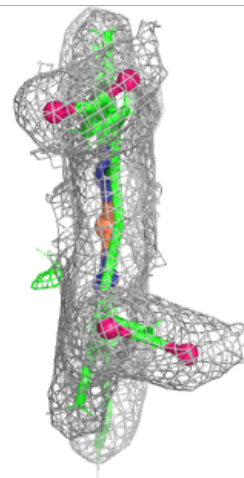
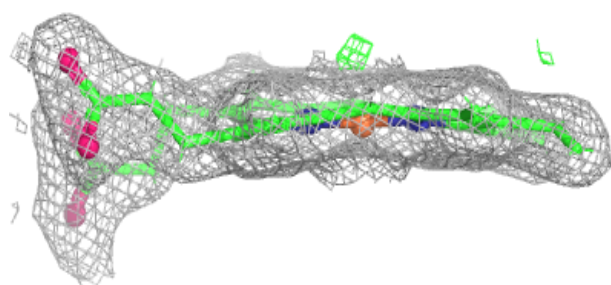
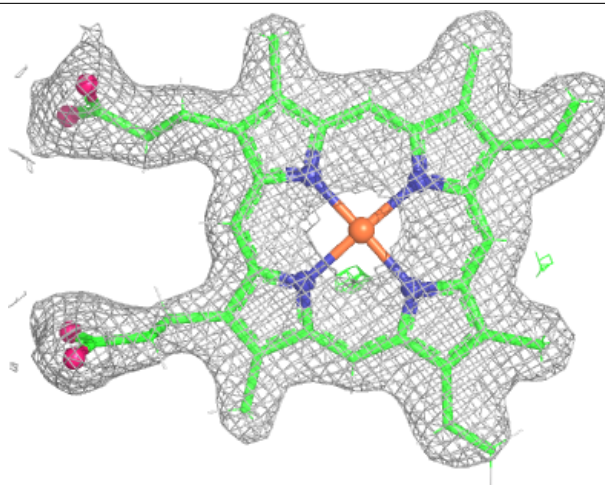
**Electron density around JFI C 501:**

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



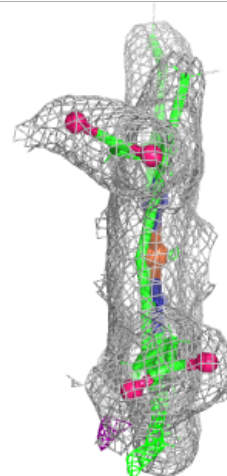
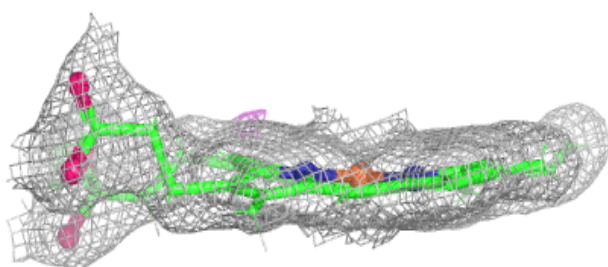
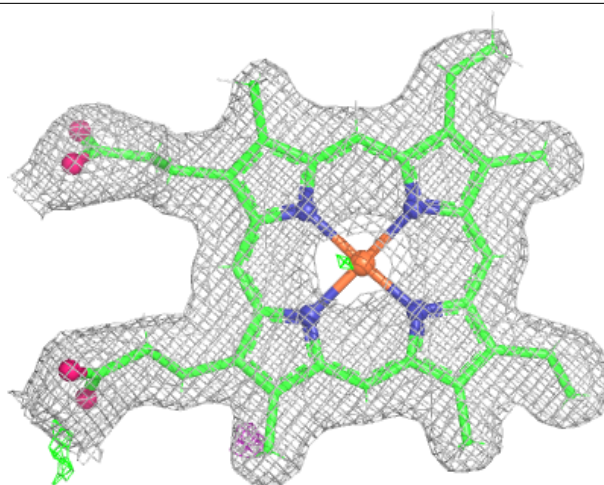
Electron density around HEM C 502:

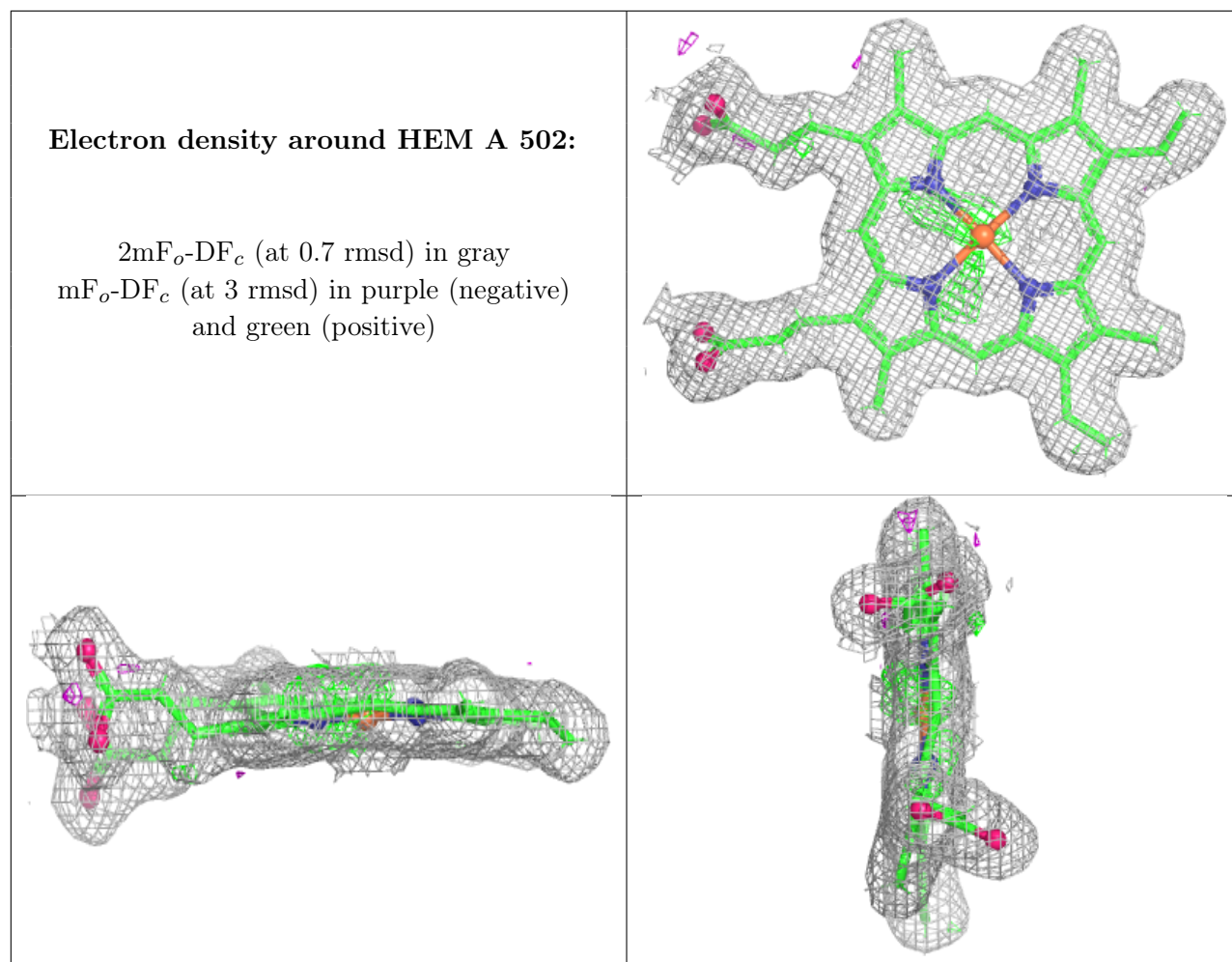
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.