



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 PM UTC

PDB ID : 6H1L / pdb_00006h1l
Title : Structure of the BM3 heme domain in complex with tioconazole
Authors : Jeffreys, L.N.; Munro, A.W.M.; Leys, D.
Deposited on : 2018-07-12
Resolution : 1.97 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

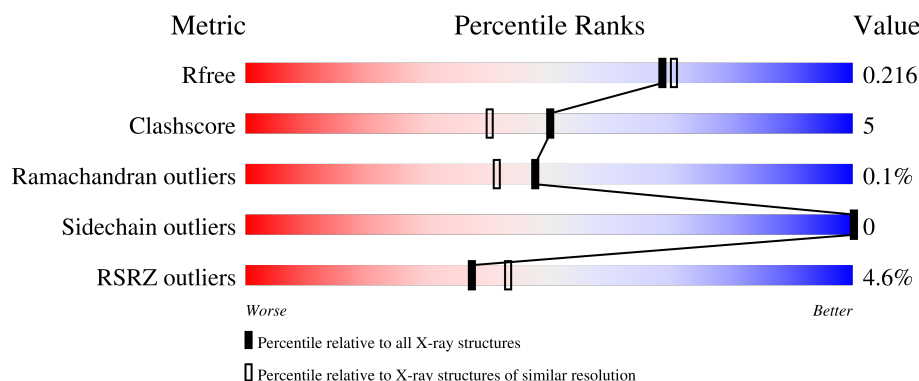
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	457	4% 87% 11%
1	B	457	5% 90% 9%

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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.

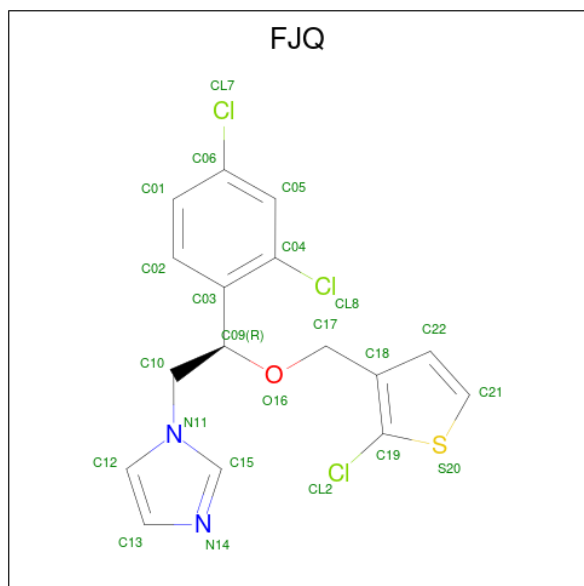
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total 3666	C 2343	N 624	O 682	S 17	0	5	0
1	B	454	Total 3701	C 2364	N 630	O 690	S 17	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

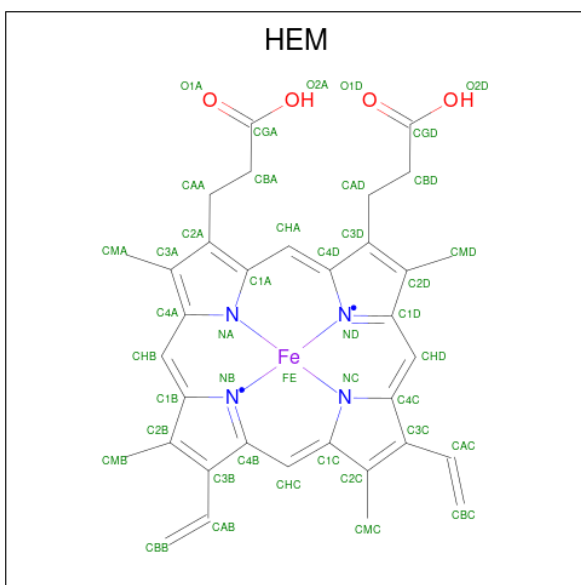
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	conflict	UNP F2Q7T0
A	87	VAL	PHE	conflict	UNP F2Q7T0
B	82	PHE	ALA	conflict	UNP F2Q7T0
B	87	VAL	PHE	conflict	UNP F2Q7T0

- Molecule 2 is Tioconazole (CCD ID: FJQ) (formula: $\text{C}_{16}\text{H}_{13}\text{Cl}_3\text{N}_2\text{OS}$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 16	Cl 3	N 2	O 1	S 1	0	0
2	B	1	Total 23	C 16	Cl 3	N 2	O 1	S 1	0	0

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



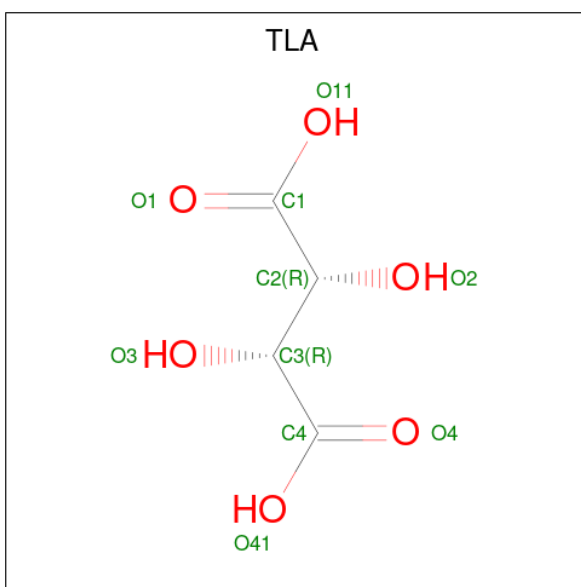
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



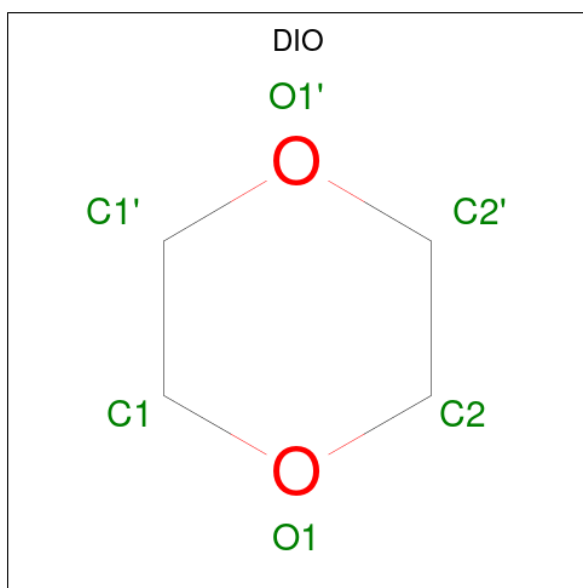
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



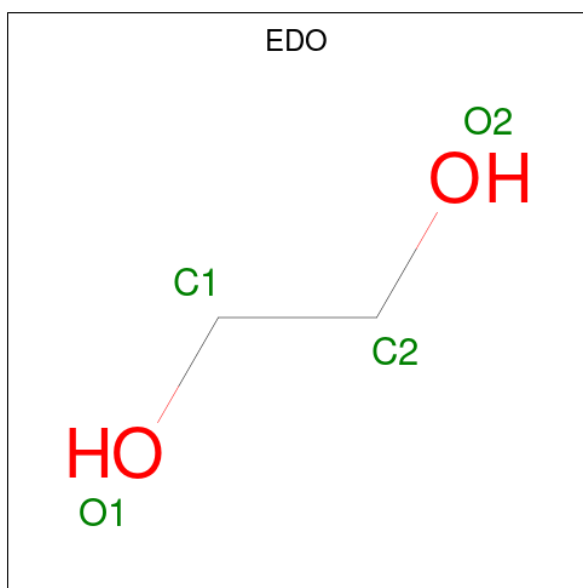
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

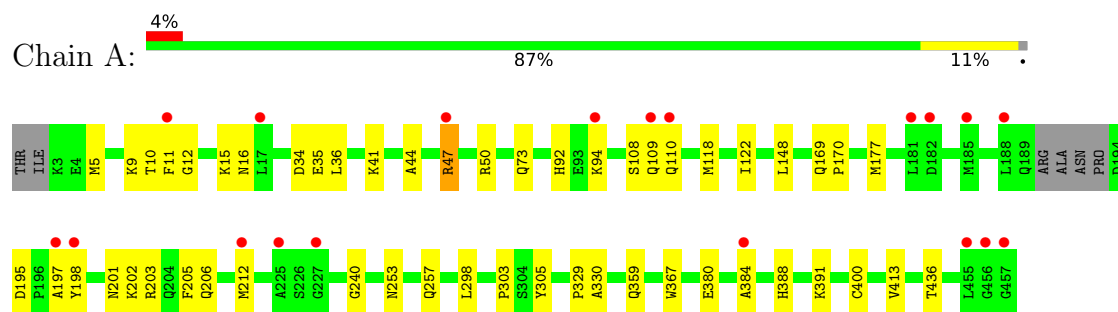
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	234	Total 234	O 234	0	0
9	B	269	Total 269	O 269	0	0

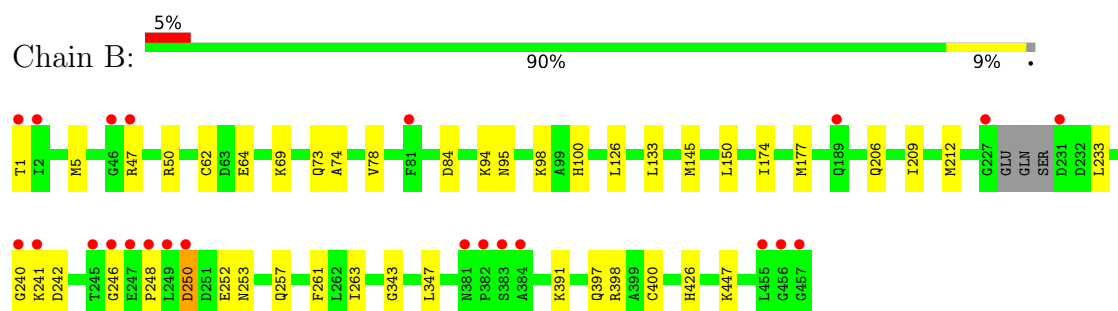
3 Residue-property plots [i](#)

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, α , β , γ	58.98Å 150.85Å 61.00Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	60.69 – 1.97 60.69 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.5 (60.69-1.97) 98.5 (60.69-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.189 , 0.215 0.191 , 0.216	Depositor DCC
R_{free} test set	3634 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: HEM, EDO, FJQ, TLA, PO4, DIO, PEG

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	0.23	0/3758	0.44	1/5075 (0.0%)
1	B	0.20	0/3788	0.39	0/5117
All	All	0.22	0/7546	0.41	1/10192 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH2	-7.04	112.87	119.20

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	3666	0	3647	43	0
1	B	3701	0	3676	32	0
2	A	23	0	0	2	0
2	B	23	0	0	1	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	4	0	0
6	A	6	0	8	2	0
7	A	24	0	36	6	0
7	B	16	0	24	1	0
8	B	7	0	10	2	0
9	A	234	0	0	5	4
9	B	269	0	0	2	2
All	All	8080	0	7465	80	4

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 (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HH22	1:A:73:GLN:CD	1.78	0.91
1:B:1:THR:OG1	1:B:343:GLY:O	1.90	0.90
1:A:240:GLY:HA2	7:A:512:EDO:H21	1.54	0.89
1:B:150:LEU:HD22	1:B:174:ILE:HD11	1.57	0.87
1:B:250:ASP:OD2	1:B:252:GLU:N	2.18	0.77
1:B:206:GLN:OE1	9:B:601:HOH:O	2.07	0.73
1:A:169:GLN:HG3	1:A:170:PRO:HD2	1.71	0.72
1:A:367:TRP:HA	6:A:506:DIO:H11	1.71	0.72
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.75	0.69
1:A:35:GLU:HG2	1:A:36:LEU:HD23	1.76	0.66
1:A:47:ARG:HH22	1:A:73:GLN:NE2	1.93	0.66
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.78	0.63
1:A:329:PRO:HD2	7:A:509:EDO:H12	1.80	0.63
2:A:501:FJQ:CL7	7:A:509:EDO:O2	2.54	0.61
1:A:47:ARG:NH2	1:A:73:GLN:CD	2.54	0.61
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.85	0.58
3:B:502:HEM:HBC2	3:B:502:HEM:HMC2	1.86	0.57
1:B:242:ASP:O	1:B:246:GLY:N	2.39	0.56
1:A:436:THR:O	7:A:508:EDO:H22	2.07	0.55
1:B:240:GLY:O	1:B:248:PRO:HB3	2.07	0.55
1:A:10:THR:HG22	1:A:12[A]:GLY:H	1.71	0.55
1:A:10:THR:HG22	1:A:12[B]:GLY:H	1.71	0.55
1:A:169:GLN:HG3	1:A:170:PRO:CD	2.36	0.54
1:A:391:LYS:NZ	9:A:610:HOH:O	2.40	0.54
1:A:202:LYS:O	1:A:206:GLN:HG2	2.08	0.53
1:A:195:ASP:HB3	1:A:198:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:508:EDO:H21	9:A:673:HOH:O	2.08	0.52
1:B:98:LYS:HG3	1:B:242:ASP:HB2	1.91	0.52
1:A:5:MET:HE3	1:A:50[B]:ARG:HE	1.75	0.51
1:A:5:MET:HG2	1:A:41:LYS:HB2	1.93	0.50
1:A:400:CYS:HB2	3:A:502:HEM:NA	2.28	0.48
1:A:44:ALA:HB3	1:A:47:ARG:HE	1.79	0.48
1:A:253:ASN:O	1:A:257:GLN:HG2	2.13	0.48
1:B:209:ILE:HD12	8:B:508:PEG:H31	1.96	0.47
1:A:201:ASN:C	1:A:203:ARG:H	2.21	0.47
1:B:241:LYS:CG	1:B:246:GLY:HA2	2.44	0.47
1:A:9:LYS:O	1:A:16:ASN:ND2	2.46	0.47
1:B:84:ASP:OD2	1:B:95:ASN:ND2	2.46	0.47
1:B:126:LEU:HD21	1:B:145:MET:HE1	1.97	0.46
1:B:100:HIS:HD2	9:B:609:HOH:O	1.97	0.46
1:B:241:LYS:HG3	1:B:246:GLY:HA2	1.96	0.46
1:A:384:ALA:O	6:A:506:DIO:H22	2.15	0.46
1:B:250:ASP:OD2	1:B:253:ASN:N	2.41	0.46
1:A:73:GLN:HG2	9:A:768:HOH:O	2.14	0.46
1:B:47:ARG:HH21	1:B:73:GLN:HB3	1.81	0.46
1:B:5:MET:HE1	1:B:50[B]:ARG:HD3	1.97	0.45
1:A:195:ASP:OD2	1:A:197:ALA:N	2.48	0.45
1:A:34:ASP:OD1	1:A:359:GLN:NE2	2.47	0.45
1:B:133:LEU:O	7:B:506:EDO:O1	2.34	0.45
1:A:177:MET:HB2	1:A:212:MET:HE3	1.98	0.44
3:A:502:HEM:HBC2	3:A:502:HEM:HMC2	2.00	0.44
1:B:78:VAL:HG11	2:B:501:FJQ:CL2	2.55	0.44
1:A:330:ALA:O	7:A:509:EDO:H22	2.16	0.44
1:B:73:GLN:HG3	1:B:74:ALA:N	2.33	0.44
1:A:11:PHE:HD1	1:A:15:LYS:O	2.01	0.43
1:A:177:MET:HE3	1:A:212:MET:HE1	2.00	0.43
1:A:118:MET:HE1	9:A:613:HOH:O	2.18	0.43
1:A:380:GLU:OE2	9:A:601:HOH:O	2.21	0.43
1:B:69:LYS:HD3	1:B:398:ARG:CZ	2.48	0.43
1:A:109:GLN:OE1	1:A:305:TYR:OH	2.32	0.43
1:B:94:LYS:HE2	1:B:98:LYS:NZ	2.34	0.43
1:B:233:LEU:HD21	1:B:261:PHE:CD2	2.54	0.43
1:B:50[B]:ARG:NH1	1:B:347:LEU:HD23	2.33	0.42
1:B:64:GLU:OE2	1:B:397:GLN:HG2	2.20	0.42
1:B:177:MET:HE3	1:B:263:ILE:HD11	2.02	0.42
1:A:177:MET:HE3	1:A:212:MET:CE	2.50	0.42
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:MET:HE3	1:B:5:MET:HB2	1.75	0.42
1:A:92:HIS:H	1:A:92:HIS:HD1	1.67	0.41
2:A:501:FJQ:C02	2:A:501:FJQ:C17	2.99	0.41
1:B:47:ARG:HH11	1:B:47:ARG:HB2	1.86	0.41
1:B:253:ASN:O	1:B:257:GLN:HG2	2.20	0.41
1:A:94[B]:LYS:HD3	1:A:94[B]:LYS:HA	1.76	0.41
1:A:73:GLN:HE21	1:A:73:GLN:HB3	1.60	0.41
1:B:426:HIS:CD2	1:B:447:LYS:HE3	2.55	0.41
1:A:203:ARG:C	1:A:205:PHE:N	2.78	0.41
1:B:212:MET:HE3	8:B:508:PEG:H21	2.03	0.41
1:B:400:CYS:HB2	3:B:502:HEM:NA	2.36	0.41
1:A:108:SER:C	1:A:110:GLN:H	2.29	0.40
1:A:298:LEU:HD22	1:A:303:PRO:HB3	2.04	0.40

All (4) 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)
9:A:805:HOH:O	9:B:862:HOH:O[1_455]	2.02	0.18
9:A:746:HOH:O	9:B:786:HOH:O[2_646]	2.03	0.17
9:A:790:HOH:O	9:A:823:HOH:O[1_554]	2.03	0.17
9:A:811:HOH:O	9:A:826:HOH:O[1_455]	2.14	0.06

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	452/457 (99%)	431 (95%)	21 (5%)	0	100	100
1	B	456/457 (100%)	441 (97%)	14 (3%)	1 (0%)	43	36
All	All	908/914 (99%)	872 (96%)	35 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	ASP

5.3.2 Protein sidechains [i](#)

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	399/400 (100%)	399 (100%)	0	100	100
1	B	402/400 (100%)	402 (100%)	0	100	100
All	All	801/800 (100%)	801 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	73	GLN
1	A	110	GLN
1	B	110	GLN
1	B	159	ASN
1	B	420	HIS

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](#)

20 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	$\# Z > 2$
7	EDO	A	508	-	3,3,3	0.38	0	2,2,2	0.35	0
7	EDO	A	512	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	A	510	-	3,3,3	0.39	0	2,2,2	0.37	0
7	EDO	A	507	-	3,3,3	0.38	0	2,2,2	0.82	0
4	PO4	A	504	-	4,4,4	0.86	0	6,6,6	0.53	0
7	EDO	B	506	-	3,3,3	0.42	0	2,2,2	0.48	0
7	EDO	A	509	-	3,3,3	0.43	0	2,2,2	0.27	0
2	FJQ	B	501	3	24,25,25	1.37	3 (12%)	28,34,34	1.81	6 (21%)
5	TLA	A	505	-	9,9,9	1.01	0	12,12,12	1.29	2 (16%)
6	DIO	A	506	-	6,6,6	0.68	0	6,6,6	0.46	0
8	PEG	B	508	-	6,6,6	0.50	0	5,5,5	0.27	0
7	EDO	B	505	-	3,3,3	0.48	0	2,2,2	0.34	0
4	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.45	0
7	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.39	0
2	FJQ	A	501	3	24,25,25	1.35	3 (12%)	28,34,34	1.63	6 (21%)
4	PO4	B	503	-	4,4,4	0.90	0	6,6,6	0.51	0
7	EDO	B	507	-	3,3,3	0.50	0	2,2,2	0.20	0
3	HEM	B	502	1,2	50,50,50	1.40	9 (18%)	67,82,82	1.17	5 (7%)
7	EDO	A	511	-	3,3,3	0.42	0	2,2,2	0.45	0
3	HEM	A	502	1,2	50,50,50	1.40	7 (14%)	67,82,82	1.10	2 (2%)

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
5	TLA	A	505	-	-	2/12/12/12	-
2	FJQ	A	501	3	-	1/13/13/13	0/3/3/3
7	EDO	A	508	-	-	1/1/1/1	-
7	EDO	B	506	-	-	1/1/1/1	-
7	EDO	A	512	-	-	1/1/1/1	-
8	PEG	B	508	-	-	1/4/4/4	-
7	EDO	B	507	-	-	0/1/1/1	-
7	EDO	B	505	-	-	1/1/1/1	-
6	DIO	A	506	-	-	-	0/1/1/1
7	EDO	A	510	-	-	0/1/1/1	-
7	EDO	A	509	-	-	1/1/1/1	-
7	EDO	B	504	-	-	0/1/1/1	-
2	FJQ	B	501	3	-	0/13/13/13	0/3/3/3
7	EDO	A	507	-	-	0/1/1/1	-
3	HEM	B	502	1,2	-	2/14/54/54	-
7	EDO	A	511	-	-	0/1/1/1	-
3	HEM	A	502	1,2	-	2/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FJQ	C19-CL2	3.80	1.78	1.71
3	B	502	HEM	FE-NB	3.70	2.06	1.94
3	A	502	HEM	FE-NA	3.67	2.07	1.95
2	A	501	FJQ	C19-CL2	3.55	1.78	1.71
3	B	502	HEM	FE-ND	3.34	2.05	1.94
3	B	502	HEM	CAC-C3C	3.17	1.55	1.47
3	A	502	HEM	CAC-C3C	3.16	1.55	1.47
3	A	502	HEM	FE-NC	3.13	2.05	1.95
3	A	502	HEM	CAB-C3B	3.00	1.55	1.47
3	B	502	HEM	CAB-C3B	2.83	1.54	1.47
3	B	502	HEM	FE-NA	2.76	2.04	1.95
3	A	502	HEM	FE-NB	2.75	2.03	1.94
3	B	502	HEM	FE-NC	2.65	2.03	1.95
3	A	502	HEM	FE-ND	2.59	2.02	1.94
2	A	501	FJQ	C17-C18	2.49	1.53	1.50
2	B	501	FJQ	C17-C18	2.45	1.53	1.50
3	A	502	HEM	CMB-C2B	2.25	1.55	1.50
2	A	501	FJQ	C04-CL8	2.17	1.78	1.73
3	B	502	HEM	CMC-C2C	2.14	1.55	1.50
2	B	501	FJQ	C04-CL8	2.12	1.78	1.73
3	B	502	HEM	CMB-C2B	2.07	1.55	1.50
3	B	502	HEM	C2A-C3A	-2.02	1.33	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FJQ	CL2-C19-S20	5.24	128.40	119.28
2	B	501	FJQ	C22-C21-S20	-4.41	104.96	112.86
2	A	501	FJQ	C22-C21-S20	-4.30	105.16	112.86
2	A	501	FJQ	CL2-C19-S20	3.69	125.70	119.28
3	B	502	HEM	C4D-ND-C1D	3.07	108.84	105.21
2	B	501	FJQ	O16-C17-C18	2.96	111.05	107.75
2	A	501	FJQ	O16-C17-C18	2.82	110.89	107.75
2	B	501	FJQ	C04-C03-C09	-2.71	119.68	122.15
3	B	502	HEM	C1B-NB-C4B	2.67	108.37	105.21
2	A	501	FJQ	C02-C03-C04	2.63	119.45	116.82
3	A	502	HEM	C4D-ND-C1D	2.48	108.15	105.21
5	A	505	TLA	O41-C4-C3	2.48	120.20	113.31
3	B	502	HEM	C3D-C4D-ND	-2.40	107.53	110.17
5	A	505	TLA	O11-C1-C2	2.35	119.85	113.31
2	A	501	FJQ	C04-C03-C09	-2.31	120.04	122.15
3	A	502	HEM	C3D-C4D-ND	-2.18	107.78	110.17
2	B	501	FJQ	C10-C09-C03	-2.06	106.17	110.28
3	B	502	HEM	C2D-C1D-ND	-2.06	107.52	109.90
2	A	501	FJQ	C05-C04-C03	-2.04	120.26	122.46
2	B	501	FJQ	C02-C03-C04	2.03	118.86	116.82
3	B	502	HEM	C2A-C1A-NA	-2.01	107.92	110.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	TLA	O1-C1-C2-O2
5	A	505	TLA	O11-C1-C2-O2
7	A	509	EDO	O1-C1-C2-O2
8	B	508	PEG	C1-C2-O2-C3
2	A	501	FJQ	C03-C09-O16-C17
3	A	502	HEM	CAD-CBD-CGD-O2D
3	B	502	HEM	CAD-CBD-CGD-O2D
7	A	508	EDO	O1-C1-C2-O2
7	B	506	EDO	O1-C1-C2-O2
3	B	502	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O1D
7	B	505	EDO	O1-C1-C2-O2
7	A	512	EDO	O1-C1-C2-O2

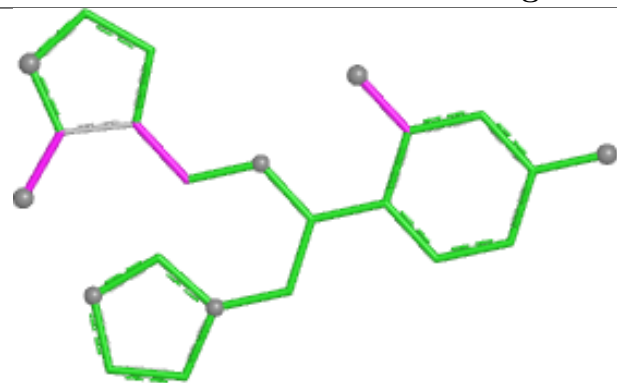
There are no ring outliers.

10 monomers are involved in 17 short contacts:

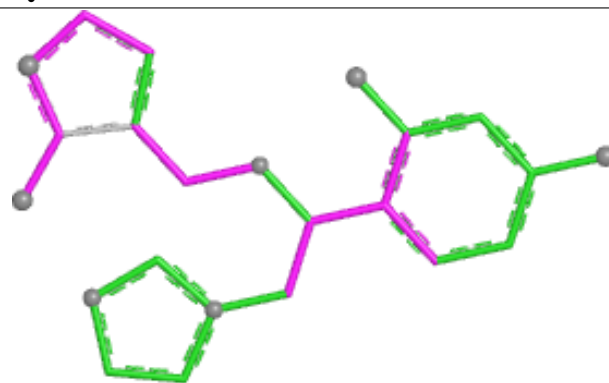
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	EDO	2	0
7	A	512	EDO	1	0
7	B	506	EDO	1	0
7	A	509	EDO	3	0
2	B	501	FJQ	1	0
6	A	506	DIO	2	0
8	B	508	PEG	2	0
2	A	501	FJQ	2	0
3	B	502	HEM	2	0
3	A	502	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

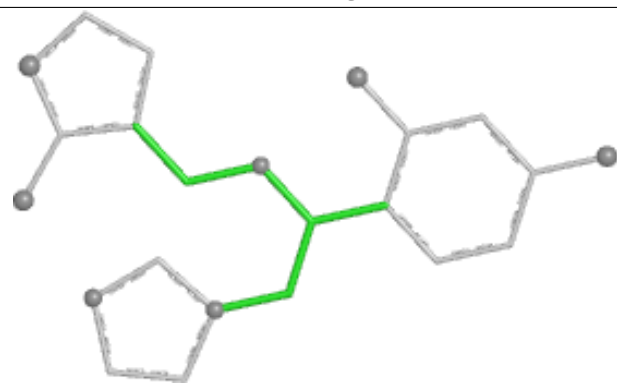
Ligand FJQ B 501



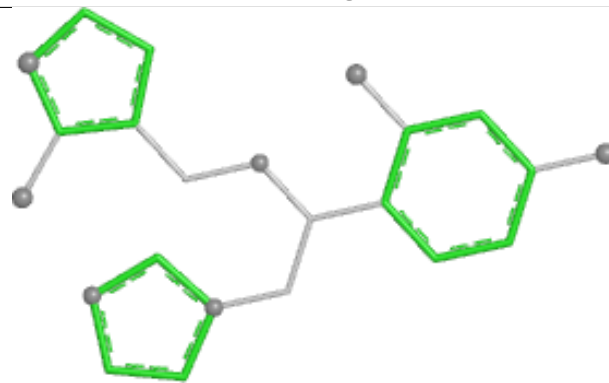
Bond lengths



Bond angles

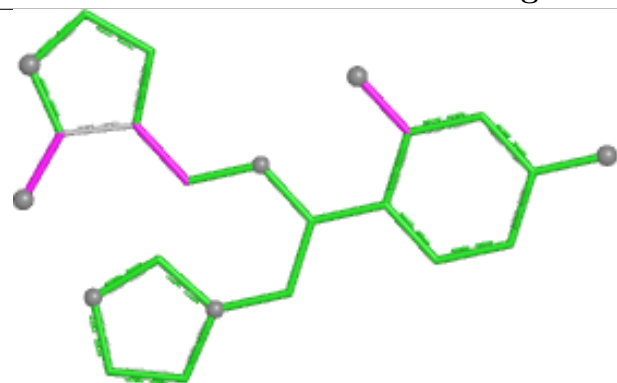


Torsions

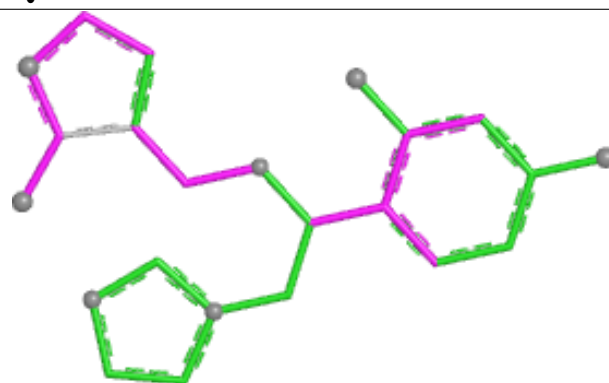


Rings

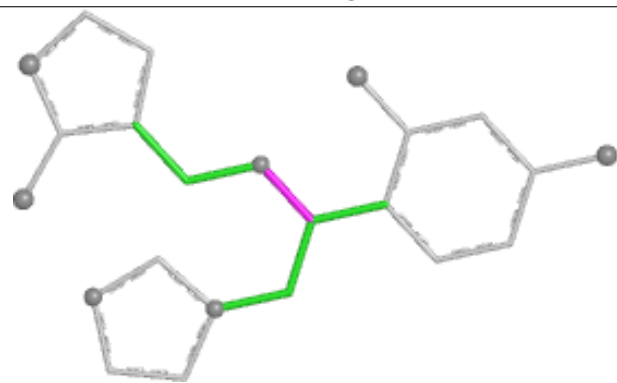
Ligand FJQ A 501



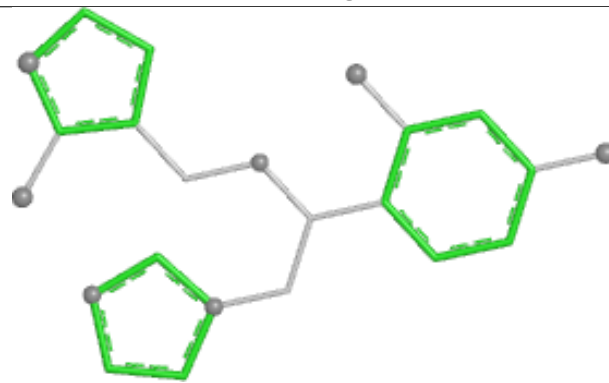
Bond lengths



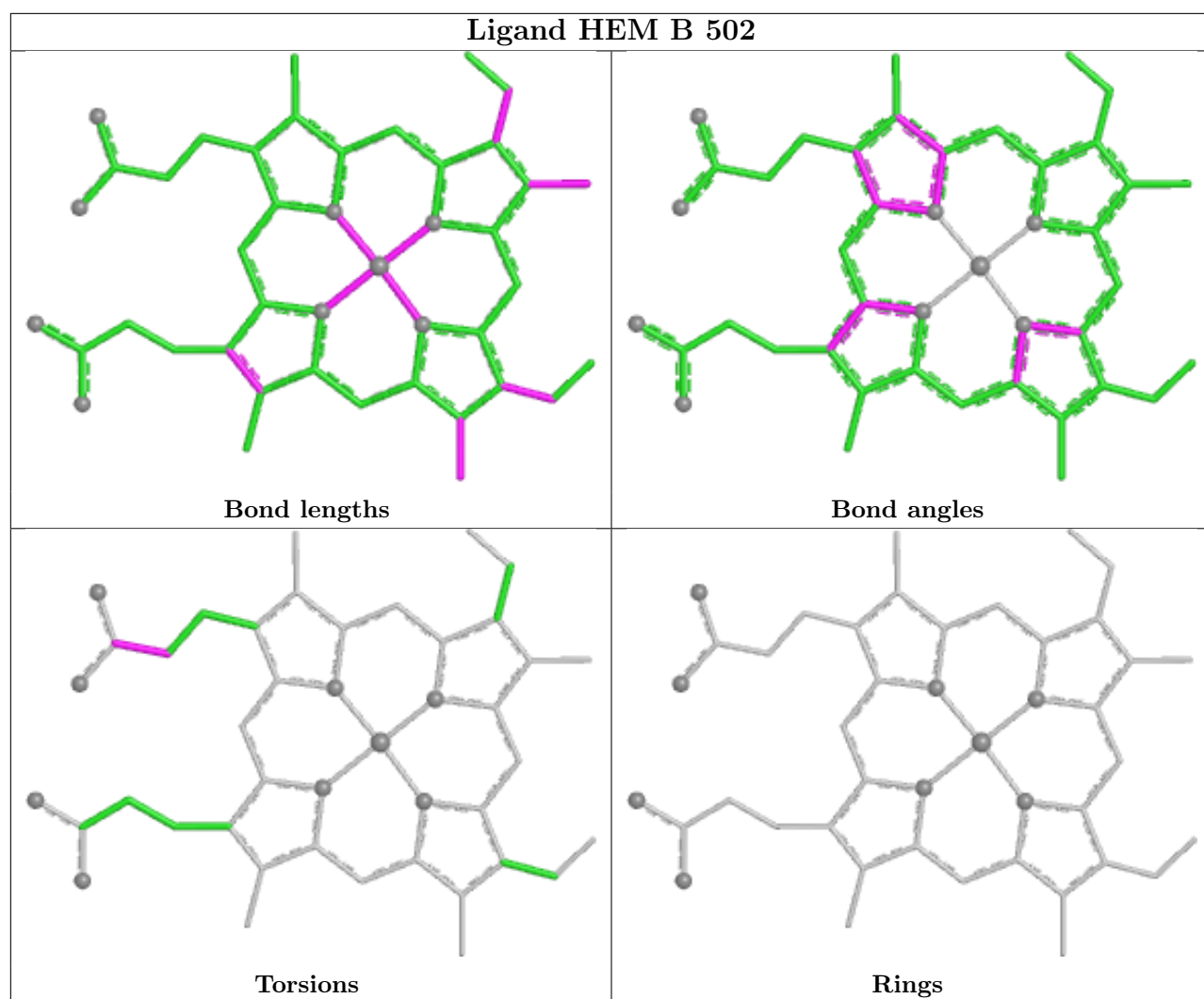
Bond angles

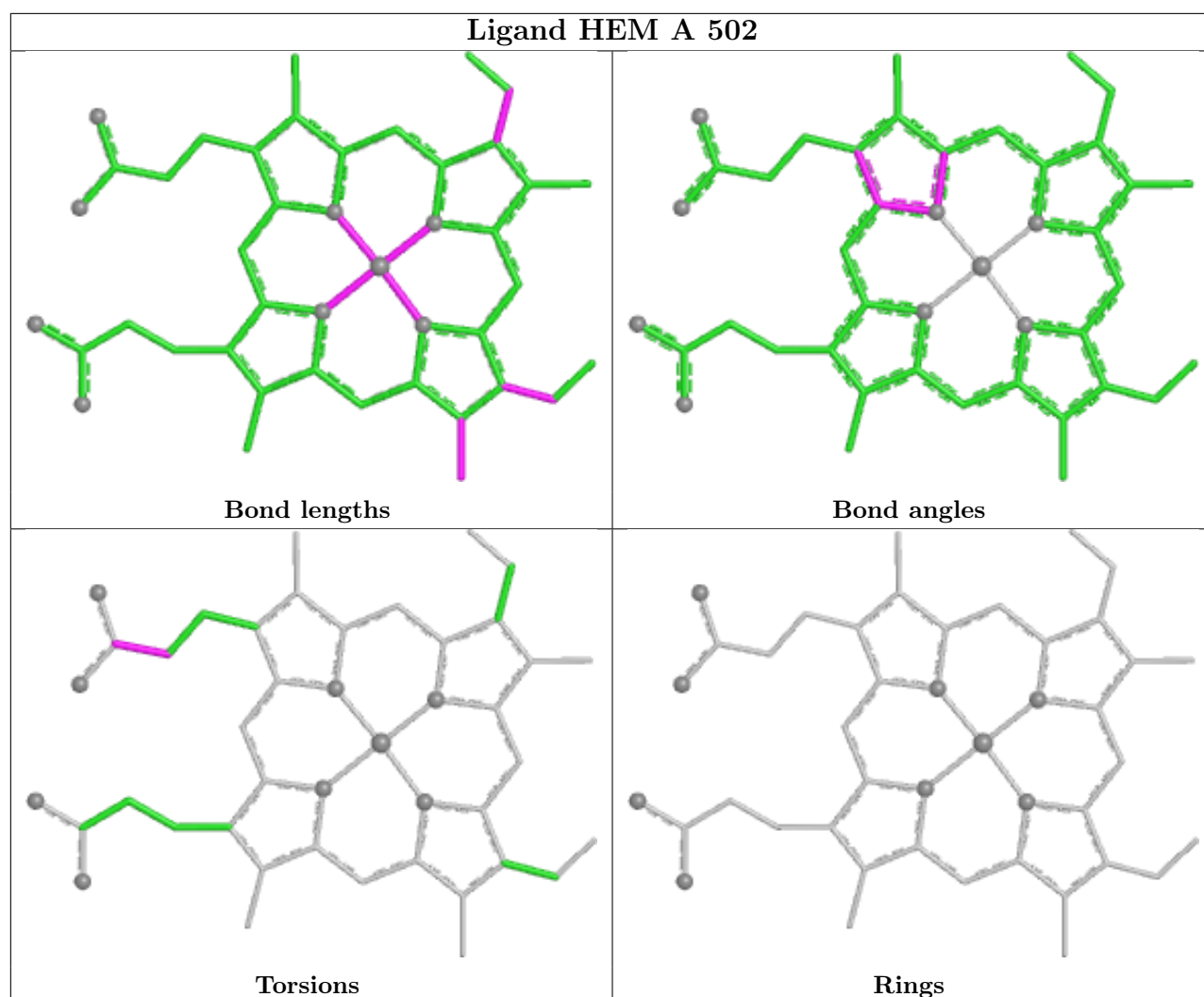


Torsions



Rings





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	451/457 (98%)	0.34	19 (4%)	40 47	19, 39, 71, 103	5 (1%)
1	B	454/457 (99%)	0.26	23 (5%)	33 39	16, 38, 63, 87	6 (1%)
All	All	905/914 (99%)	0.30	42 (4%)	37 43	16, 39, 67, 103	11 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	PRO	5.0
1	B	249	LEU	3.1
1	A	197	ALA	3.1
1	A	17	LEU	3.1
1	B	1	THR	3.0
1	A	188	LEU	3.0
1	B	383	SER	3.0
1	B	227	GLY	3.0
1	B	46	GLY	2.9
1	B	457	GLY	2.9
1	A	198	TYR	2.9
1	A	11	PHE	2.9
1	B	245	THR	2.8
1	A	185	MET	2.7
1	B	240	GLY	2.7
1	A	182	ASP	2.6
1	B	382	PRO	2.6
1	B	246	GLY	2.6
1	B	456	GLY	2.5
1	B	81	PHE	2.5
1	A	47	ARG	2.5
1	B	247	GLU	2.4
1	B	250	ASP	2.4
1	B	241	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	384	ALA	2.4
1	A	455	LEU	2.4
1	A	109	GLN	2.3
1	B	381	ASN	2.3
1	A	212	MET	2.3
1	B	47	ARG	2.3
1	A	181	LEU	2.3
1	B	455	LEU	2.2
1	A	110	GLN	2.2
1	A	94[A]	LYS	2.1
1	A	225	ALA	2.1
1	B	189	GLN	2.1
1	B	384	ALA	2.1
1	B	231	ASP	2.1
1	A	456	GLY	2.1
1	B	2	ILE	2.0
1	A	457	GLY	2.0
1	A	227	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(Å ²)	Q<0.9
4	PO4	A	504	5/5	0.60	0.12	66,68,89,91	0
7	EDO	A	507	4/4	0.76	0.19	55,59,60,61	0
7	EDO	A	508	4/4	0.76	0.25	47,49,52,56	0
8	PEG	B	508	7/7	0.77	0.16	50,56,57,65	0
7	EDO	B	505	4/4	0.78	0.20	47,48,51,53	0

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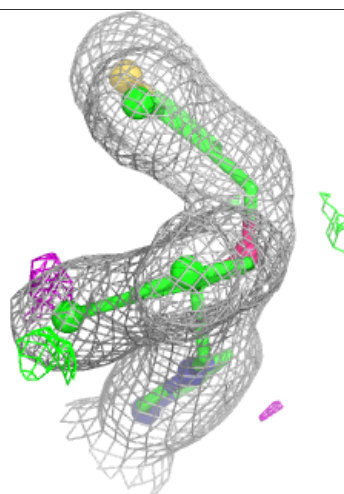
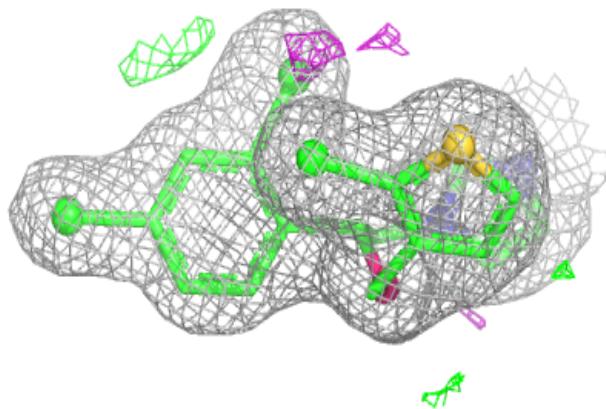
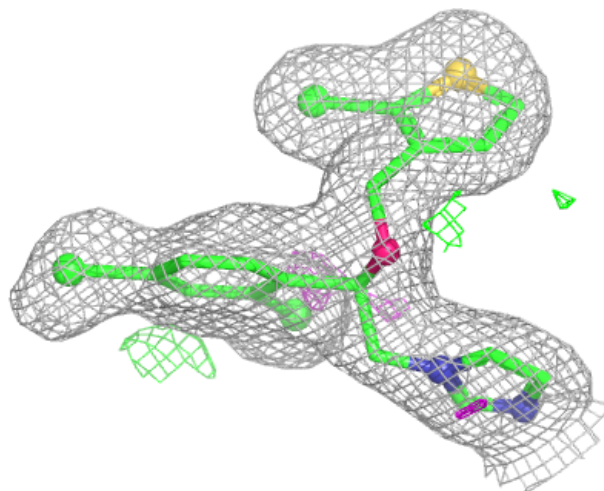
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TLA	A	505	10/10	0.80	0.12	48,62,68,72	0
7	EDO	B	506	4/4	0.80	0.18	39,39,49,52	0
7	EDO	A	509	4/4	0.80	0.20	36,40,48,60	0
7	EDO	A	512	4/4	0.81	0.16	52,53,54,62	0
6	DIO	A	506	6/6	0.81	0.15	52,60,61,65	0
4	PO4	A	503	5/5	0.87	0.10	50,58,65,78	0
7	EDO	A	510	4/4	0.87	0.17	50,51,53,60	0
7	EDO	B	504	4/4	0.88	0.15	51,52,54,60	0
4	PO4	B	503	5/5	0.88	0.10	44,54,60,69	0
7	EDO	A	511	4/4	0.90	0.19	40,48,52,55	0
7	EDO	B	507	4/4	0.91	0.12	34,45,51,54	0
2	FJQ	B	501	23/23	0.95	0.09	32,41,48,66	0
2	FJQ	A	501	23/23	0.96	0.07	22,33,39,54	0
3	HEM	B	502	43/43	0.98	0.06	24,31,39,47	0
3	HEM	A	502	43/43	0.99	0.05	23,27,30,32	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.

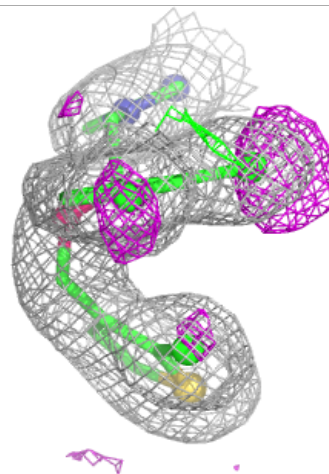
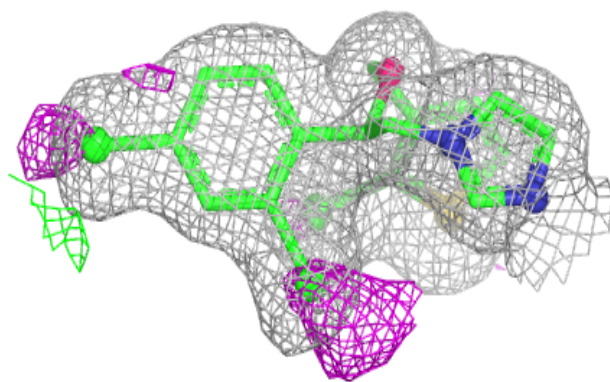
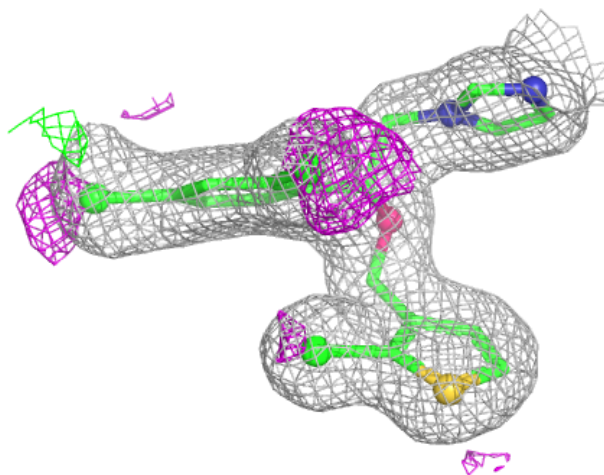
Electron density around FJQ B 501:

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



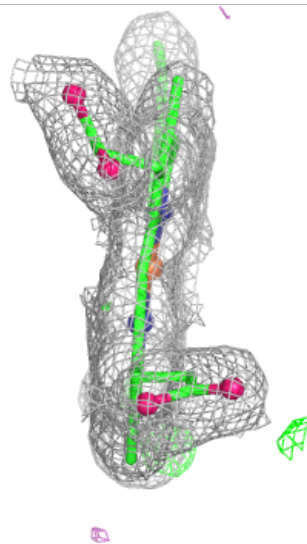
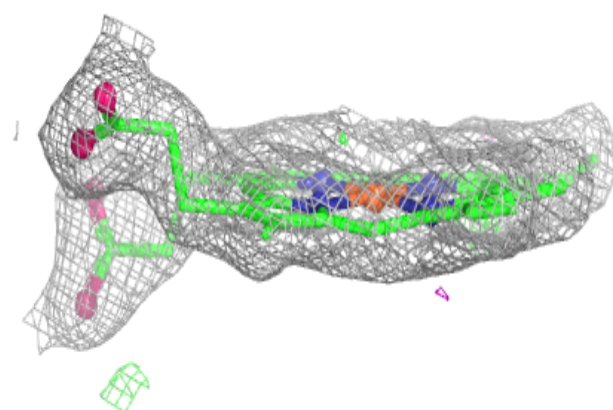
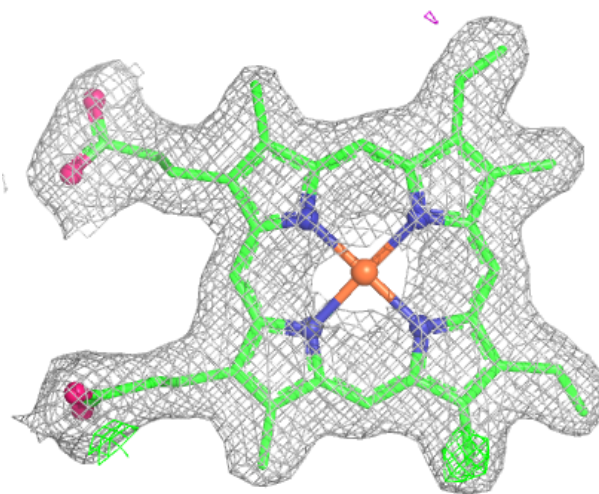
Electron density around FJQ A 501:

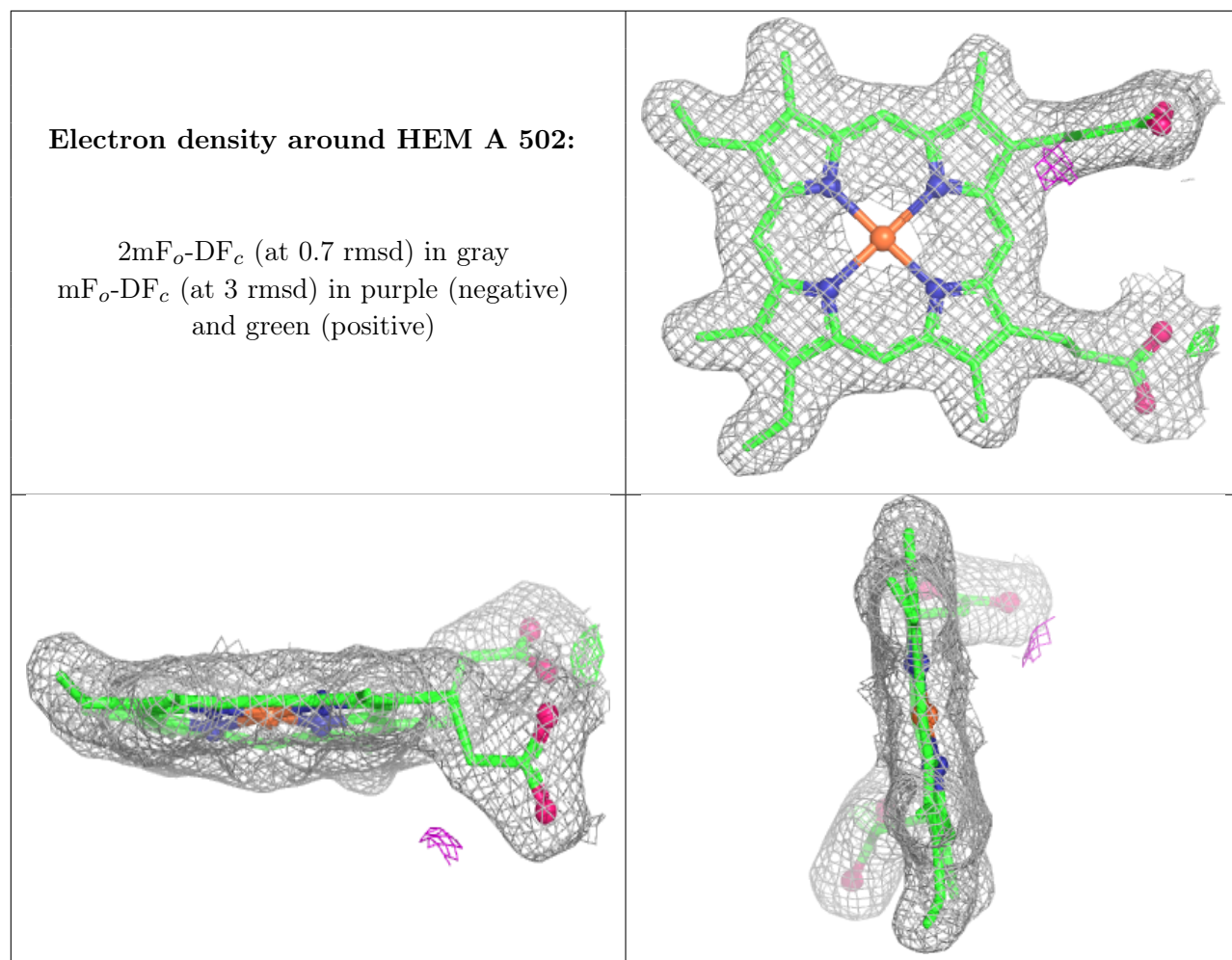
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.