



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 3OZV / pdb_00003ozv
Title : The Crystal Structure of flavohemoglobin from *R. eutrophus* in complex with econazole
Authors : El Hammi, E.; Warkentin, E.; Demmer, U.; Ermler, U.; Baciou, L.
Deposited on : 2010-09-27
Resolution : 2.40 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

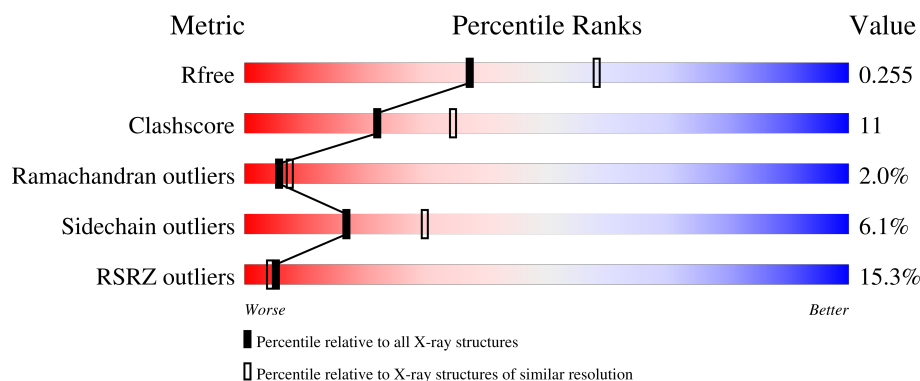
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	403	
1	B	403	

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
5	ECN	A	411	X	-	X	-
5	ECN	B	411	X	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6722 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 Flavohemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	403	Total	C	N	O	S	0	1	0
			3162	2015	543	590	14			
1	A	403	Total	C	N	O	S	0	0	0
			3156	2011	543	588	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



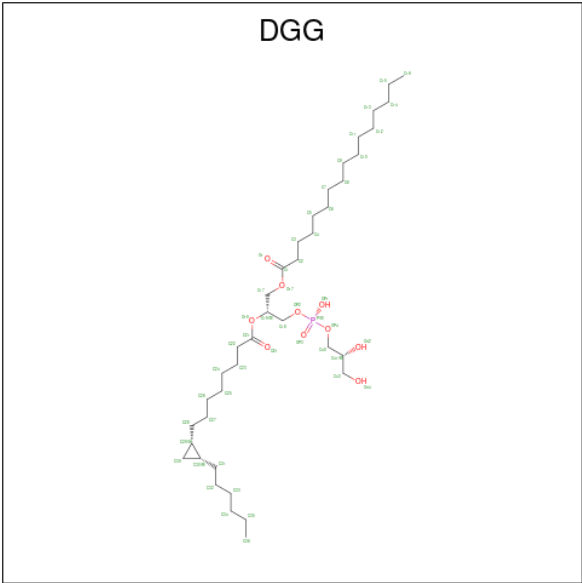
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1-[GLYCEROLYLPHOSPHONYL]-2-[8-(2-HEXYL-CYCLOPROPYL)-OCTANAL-1-YL]-3-[HEXADECANAL-1-YL]-GLYCEROL (CCD ID: DGG) (formula: C₃₉H₇₅O₁₀P).



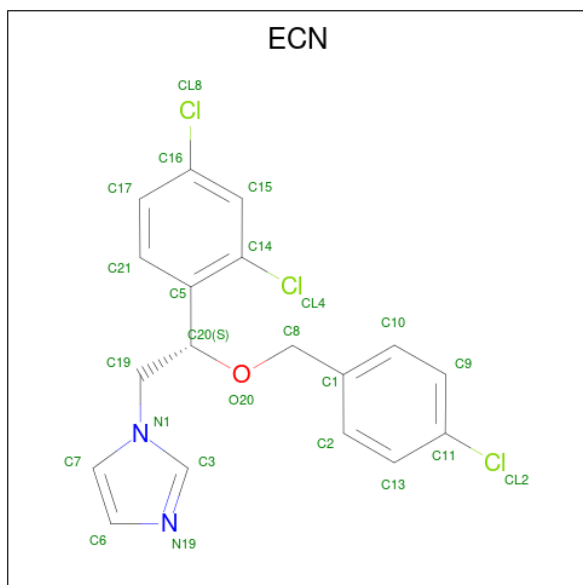
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			19	17	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	17	2		

- Molecule 5 is 1-[(2S)-2-[(4-CHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (CCD ID: ECN) (formula: C₁₈H₁₅Cl₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		
5	A	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

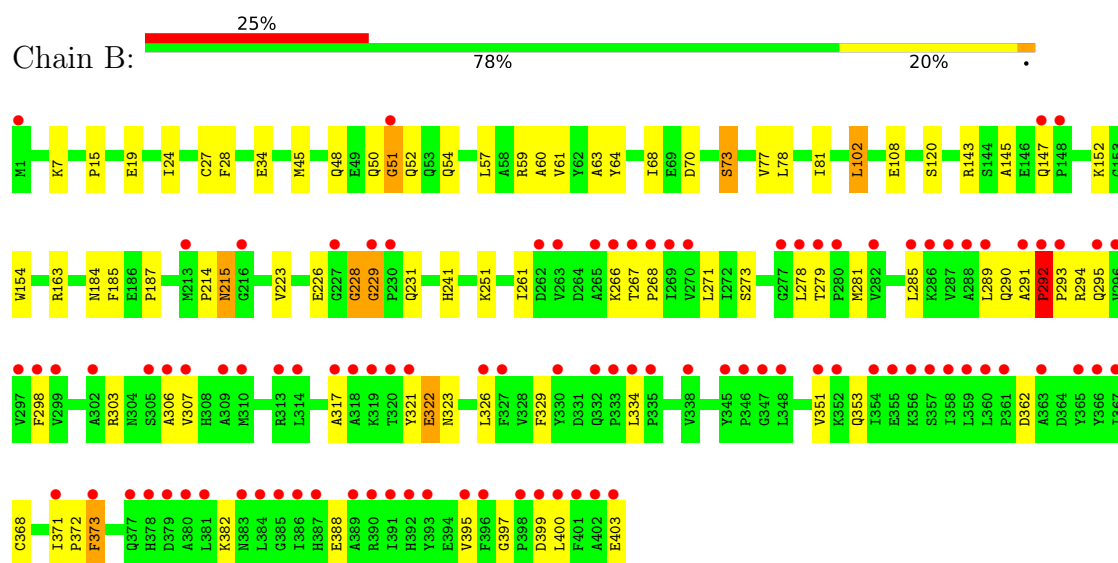
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	58	Total	O	0	0
			58	58		
7	A	63	Total	O	0	0
			63	63		

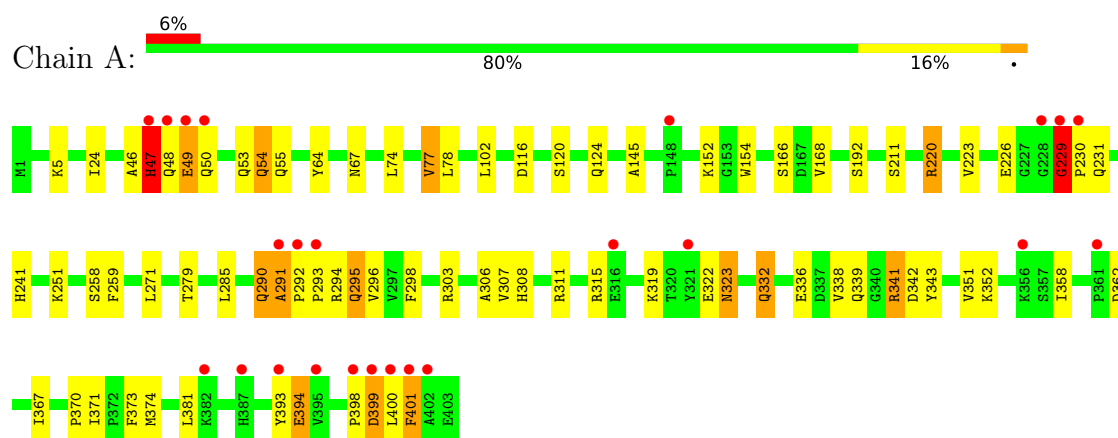
3 Residue-property plots

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: Flavohemoglobin



• Molecule 1: Flavohemoglobin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.22Å 87.22Å 291.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.40) 99.0 (30.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.210 , 0.248 0.227 , 0.255	Depositor DCC
R_{free} test set	2269 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6722	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, DGG, HEM, ECN, PO4

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	0.79	0/3233	1.03	8/4393 (0.2%)
1	B	0.82	0/3242	1.02	7/4405 (0.2%)
All	All	0.81	0/6475	1.02	15/8798 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	229	GLY	CA-C-N	8.69	130.70	119.84
1	A	229	GLY	C-N-CA	8.69	130.70	119.84
1	B	292	PRO	CA-C-N	6.84	128.40	119.84
1	B	292	PRO	C-N-CA	6.84	128.40	119.84
1	A	371	ILE	CA-C-N	-6.08	112.60	119.28
1	A	371	ILE	C-N-CA	-6.08	112.60	119.28
1	A	332	GLN	CA-C-N	5.84	125.78	119.76
1	A	332	GLN	C-N-CA	5.84	125.78	119.76
1	A	279	THR	CA-C-N	-5.83	113.75	119.64
1	A	279	THR	C-N-CA	-5.83	113.75	119.64
1	B	61	VAL	N-CA-CB	5.75	118.35	110.54
1	B	228	GLY	N-CA-C	-5.49	100.17	113.18
1	B	215	ASN	N-CA-C	5.14	121.76	110.80
1	B	279	THR	CA-C-N	-5.05	114.54	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	THR	C-N-CA	-5.05	114.54	119.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	226	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3156	0	3112	61	0
1	B	3162	0	3118	55	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	53	0	31	4	0
3	B	53	0	31	0	0
4	A	19	0	31	6	0
4	B	19	0	31	6	0
5	A	24	0	15	15	0
5	B	24	0	15	18	0
6	A	5	0	0	0	0
7	A	63	0	0	0	0
7	B	58	0	0	1	0
All	All	6722	0	6444	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (139) 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:24:ILE:HG22	5:B:411:ECN:CL2	1.41	1.57
5:A:411:ECN:H10	5:A:411:ECN:C20	1.70	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:CG2	5:B:411:ECN:CL2	2.26	1.19
5:A:411:ECN:H20	5:A:411:ECN:C10	1.53	1.16
5:B:411:ECN:H20	5:B:411:ECN:C10	1.38	1.15
1:A:399:ASP:HA	1:A:400:LEU:HB2	1.28	1.13
1:A:24:ILE:HG21	5:A:411:ECN:CL2	1.85	1.13
5:B:411:ECN:C10	5:B:411:ECN:C20	2.27	1.12
4:A:406:DGG:H352	5:A:411:ECN:H2	1.30	1.11
1:B:77:VAL:HG11	4:B:406:DGG:H241	1.21	1.11
5:B:411:ECN:C20	5:B:411:ECN:H10	1.81	1.10
5:B:411:ECN:H20	5:B:411:ECN:H10	1.18	1.08
1:A:341:ARG:HG2	1:A:341:ARG:HH21	1.21	1.01
1:A:220:ARG:HG2	1:A:220:ARG:HH21	1.32	0.94
1:B:102:LEU:HD13	5:B:411:ECN:C9	2.04	0.87
4:B:406:DGG:H341	5:B:411:ECN:H8C2	1.56	0.85
1:B:371:ILE:HD11	1:B:395:VAL:HG13	1.58	0.84
1:B:63:ALA:HB1	4:B:406:DGG:H242	1.60	0.83
5:B:411:ECN:H10	5:B:411:ECN:C19	2.09	0.82
1:A:54:GLN:HE21	1:A:55:GLN:NE2	1.78	0.81
4:A:406:DGG:H352	5:A:411:ECN:C2	2.09	0.81
1:A:398:PRO:O	1:A:399:ASP:HB2	1.82	0.80
1:A:48:GLN:N	1:A:49:GLU:HA	1.95	0.79
1:B:77:VAL:CG1	4:B:406:DGG:H241	2.09	0.78
1:B:371:ILE:HD11	1:B:395:VAL:CG1	2.12	0.78
5:A:411:ECN:H10	5:A:411:ECN:H20	0.79	0.76
1:A:399:ASP:CA	1:A:400:LEU:HB2	2.12	0.75
5:A:411:ECN:C20	5:A:411:ECN:C10	2.41	0.74
5:A:411:ECN:H10	5:A:411:ECN:CL4	2.26	0.72
1:B:59:ARG:HG3	1:B:59:ARG:HH21	1.55	0.71
1:B:102:LEU:HD13	5:B:411:ECN:C11	2.21	0.70
1:A:211:SER:OG	1:A:220:ARG:NH2	2.26	0.69
1:B:57:LEU:HD11	5:B:411:ECN:H2	1.75	0.68
1:A:374:MET:CE	1:A:393:TYR:HB2	2.24	0.67
1:A:399:ASP:HB3	1:A:401:PHE:N	2.10	0.67
1:A:102:LEU:HD11	5:A:411:ECN:C9	2.25	0.66
1:A:54:GLN:NE2	1:A:55:GLN:NE2	2.43	0.66
4:A:406:DGG:C35	5:A:411:ECN:H2	2.18	0.65
1:A:341:ARG:NH2	1:A:342:ASP:OD1	2.29	0.65
1:B:295:GLN:HB2	1:B:323:ASN:O	1.96	0.64
1:A:220:ARG:HG2	1:A:220:ARG:NH2	2.06	0.64
1:A:303:ARG:HB3	1:A:307:VAL:HG11	1.79	0.64
1:A:341:ARG:HG2	1:A:341:ARG:NH2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:CG2	5:A:411:ECN:CL2	2.75	0.63
1:B:281:MET:HE2	1:B:368:CYS:HB3	1.81	0.62
1:A:47:HIS:CD2	1:A:53:GLN:OE1	2.51	0.62
1:A:226:GLU:HG2	3:A:405:FAD:O3B	2.00	0.62
1:A:399:ASP:HA	1:A:400:LEU:CB	2.16	0.62
1:B:63:ALA:HB1	4:B:406:DGG:C24	2.29	0.62
1:B:77:VAL:HG21	4:B:406:DGG:H261	1.81	0.61
1:A:54:GLN:HE21	1:A:55:GLN:HE21	1.46	0.61
1:B:102:LEU:HD22	5:B:411:ECN:C10	2.30	0.60
1:A:67:ASN:ND2	4:A:406:DGG:H232	2.16	0.60
1:A:398:PRO:O	1:A:399:ASP:CB	2.50	0.60
1:B:59:ARG:HD3	1:B:400:LEU:O	2.03	0.59
1:A:168:VAL:CG2	1:A:307:VAL:HG23	2.32	0.58
1:A:120:SER:O	1:A:124:GLN:HG3	2.04	0.58
2:A:404:HEM:HMB2	2:A:404:HEM:HBB2	1.85	0.58
1:B:329:PHE:HE1	1:B:353:GLN:HE22	1.52	0.58
1:A:48:GLN:N	1:A:49:GLU:CA	2.66	0.57
1:B:45:MET:O	1:B:48:GLN:HB2	2.04	0.57
1:A:211:SER:OG	1:A:220:ARG:HG2	2.05	0.57
1:B:223:VAL:O	1:B:241:HIS:HE1	1.86	0.57
1:B:27:CYS:SG	1:B:108:GLU:OE2	2.63	0.56
1:B:64:TYR:CZ	1:B:68:ILE:HD12	2.40	0.56
2:A:404:HEM:NB	5:A:411:ECN:H3	2.21	0.56
1:A:168:VAL:HG22	1:A:307:VAL:HG23	1.88	0.55
1:B:291:ALA:HA	1:B:292:PRO:C	2.31	0.55
1:B:102:LEU:HD22	5:B:411:ECN:H10	1.89	0.55
2:B:404:HEM:HBB2	2:B:404:HEM:HMB2	1.89	0.55
1:B:372:PRO:O	1:B:373:PHE:HB2	2.06	0.55
1:A:293:PRO:N	1:A:294:ARG:HA	2.22	0.55
1:A:229:GLY:O	1:A:231:GLN:N	2.41	0.53
1:B:143:ARG:O	1:B:147:GLN:HG3	2.07	0.53
1:A:154:TRP:HB3	1:A:251:LYS:HB3	1.91	0.53
1:B:397:GLY:O	1:B:399:ASP:OD1	2.27	0.53
1:A:303:ARG:HB3	1:A:307:VAL:CG1	2.39	0.52
1:A:290:GLN:O	1:A:291:ALA:HB3	2.10	0.51
1:B:102:LEU:HD13	5:B:411:ECN:C10	2.41	0.51
1:B:15:PRO:HG3	3:A:405:FAD:C2A	2.41	0.51
1:B:185:PHE:CE2	1:B:214:PRO:HA	2.46	0.51
1:A:285:LEU:HD12	1:A:296:VAL:HG11	1.91	0.51
1:B:228:GLY:O	1:B:229:GLY:C	2.54	0.50
1:B:371:ILE:CD1	1:B:395:VAL:HG13	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:404:HEM:HBB2	2:A:404:HEM:CMB	2.42	0.50
1:A:351:VAL:HG22	1:A:358:ILE:HG12	1.92	0.50
1:A:367:ILE:HG22	1:A:374:MET:HG2	1.93	0.50
1:B:28:PHE:HB2	5:B:411:ECN:CL2	2.49	0.49
1:A:285:LEU:HD13	1:A:298:PHE:CD1	2.48	0.49
1:B:382:LYS:HE3	1:B:388:GLU:OE1	2.13	0.49
1:A:77:VAL:CG2	4:A:406:DGG:H271	2.44	0.48
1:A:46:ALA:C	1:A:48:GLN:H	2.22	0.47
1:B:371:ILE:HD11	1:B:395:VAL:HG11	1.95	0.47
1:B:145:ALA:HB2	1:B:152:LYS:HG3	1.96	0.47
2:B:404:HEM:HHD	2:B:404:HEM:HBC2	1.96	0.47
2:B:404:HEM:HBB2	2:B:404:HEM:CMB	2.45	0.47
5:B:411:ECN:C9	5:B:411:ECN:CL4	3.00	0.47
1:A:339:GLN:HB3	1:A:343:TYR:CZ	2.50	0.47
2:A:404:HEM:C4B	5:A:411:ECN:H3	2.50	0.47
1:B:154:TRP:HB3	1:B:251:LYS:HB3	1.97	0.46
1:A:374:MET:HE3	1:A:393:TYR:HB2	1.97	0.46
1:B:321:TYR:O	1:B:322:GLU:CB	2.64	0.46
1:A:370:PRO:O	1:A:373:PHE:HB3	2.16	0.46
1:B:329:PHE:HE1	1:B:353:GLN:NE2	2.13	0.46
1:B:7:LYS:HG2	1:B:68:ILE:HG12	1.97	0.46
2:B:404:HEM:NB	5:B:411:ECN:H3	2.30	0.46
1:B:268:PRO:HA	1:B:294:ARG:HG3	1.98	0.45
1:B:50:GLN:O	1:B:51:GLY:C	2.60	0.45
1:B:60:ALA:HB2	1:B:400:LEU:HD13	1.99	0.45
1:A:24:ILE:HD13	5:A:411:ECN:CL2	2.54	0.45
1:B:298:PHE:HB3	1:B:326:LEU:HD12	1.99	0.44
1:A:64:TYR:HB2	4:A:406:DGG:H281	2.00	0.44
1:A:294:ARG:O	1:A:295:GLN:HB2	2.18	0.44
1:B:70:ASP:CG	1:B:73:SER:HB2	2.43	0.43
1:A:102:LEU:HD11	5:A:411:ECN:C11	2.48	0.43
1:B:59:ARG:HG3	1:B:59:ARG:NH2	2.28	0.43
1:A:145:ALA:HB2	1:A:152:LYS:HG3	2.00	0.43
1:B:303:ARG:HB3	1:B:307:VAL:HG21	1.99	0.43
1:A:47:HIS:HD2	1:A:53:GLN:OE1	1.98	0.43
1:A:223:VAL:O	1:A:241:HIS:HE1	2.01	0.43
1:B:317:ALA:O	1:B:321:TYR:HD2	2.02	0.42
1:A:166:SER:HB2	1:A:306:ALA:O	2.19	0.42
1:A:399:ASP:HB3	1:A:400:LEU:C	2.43	0.42
1:B:273:SER:HB3	1:B:281:MET:HG3	2.02	0.42
1:A:168:VAL:HG21	1:A:307:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HD23	1:B:81:ILE:HD12	2.01	0.42
1:B:163:ARG:HE	1:B:163:ARG:HB3	1.72	0.42
1:B:403:GLU:C	7:B:453:HOH:O	2.64	0.41
1:A:292:PRO:HA	1:A:293:PRO:HA	1.73	0.41
1:A:308:HIS:CE1	1:A:311:ARG:HG3	2.55	0.41
1:B:57:LEU:HD11	5:B:411:ECN:C2	2.46	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.93	0.41
1:A:259:PHE:CG	1:A:394:GLU:HB2	2.55	0.41
1:A:323:ASN:ND2	1:A:323:ASN:H	2.18	0.41
1:B:187:PRO:HG2	1:B:261:ILE:HD11	2.02	0.40
1:B:306:ALA:HB2	1:B:334:LEU:HD11	2.03	0.40
1:A:48:GLN:H	1:A:49:GLU:HA	1.83	0.40
1:A:48:GLN:HG2	3:A:405:FAD:C4A	2.51	0.40
1:A:226:GLU:CG	3:A:405:FAD:O3B	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/403 (100%)	379 (94%)	15 (4%)	7 (2%)	7	10
1	B	402/403 (100%)	382 (95%)	11 (3%)	9 (2%)	5	6
All	All	803/806 (100%)	761 (95%)	26 (3%)	16 (2%)	6	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	PRO
1	B	373	PHE
1	A	47	HIS
1	A	230	PRO

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Mol	Chain	Res	Type
1	B	51	GLY
1	B	52	GLN
1	B	215	ASN
1	B	229	GLY
1	A	295	GLN
1	A	399	ASP
1	B	184	ASN
1	B	322	GLU
1	A	50	GLN
1	A	291	ALA
1	A	229	GLY
1	B	292	PRO

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	334/334 (100%)	309 (92%)	25 (8%)	12	21
1	B	335/334 (100%)	318 (95%)	17 (5%)	21	37
All	All	669/668 (100%)	627 (94%)	42 (6%)	17	29

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19[A]	GLU
1	B	19[B]	GLU
1	B	34	GLU
1	B	54	GLN
1	B	73	SER
1	B	102	LEU
1	B	120	SER
1	B	231	GLN
1	B	266	LYS
1	B	267	THR
1	B	271	LEU

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Mol	Chain	Res	Type
1	B	278	LEU
1	B	285	LEU
1	B	289	LEU
1	B	290	GLN
1	B	351	VAL
1	B	362	ASP
1	A	5	LYS
1	A	47	HIS
1	A	49	GLU
1	A	54	GLN
1	A	74	LEU
1	A	77	VAL
1	A	116	ASP
1	A	192	SER
1	A	220	ARG
1	A	258	SER
1	A	271	LEU
1	A	290	GLN
1	A	315	ARG
1	A	319	LYS
1	A	322	GLU
1	A	323	ASN
1	A	332	GLN
1	A	336	GLU
1	A	338	VAL
1	A	341	ARG
1	A	352	LYS
1	A	362	ASP
1	A	381	LEU
1	A	394	GLU
1	A	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	20	HIS
1	B	50	GLN
1	B	53	GLN
1	B	55	GLN
1	B	67	ASN
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	241	HIS
1	B	249	GLN
1	B	332	GLN
1	B	339	GLN
1	B	353	GLN
1	B	377	GLN
1	B	392	HIS
1	A	4	GLN
1	A	47	HIS
1	A	55	GLN
1	A	128	ASN
1	A	241	HIS
1	A	290	GLN
1	A	323	ASN
1	A	339	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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
3	FAD	A	405	-	58,58,58	1.25	5 (8%)	85,89,89	1.67	17 (20%)
4	DGG	A	406	-	19,19,50	1.19	1 (5%)	20,22,59	2.54	3 (15%)
5	ECN	B	411	2	26,26,26	1.33	3 (11%)	35,35,35	2.47	9 (25%)
2	HEM	A	404	1,5	50,50,50	1.69	6 (12%)	67,82,82	1.39	13 (19%)
5	ECN	A	411	2	26,26,26	1.55	5 (19%)	35,35,35	2.87	11 (31%)
3	FAD	B	405	-	58,58,58	1.13	6 (10%)	85,89,89	1.60	16 (18%)
6	PO4	A	407	-	4,4,4	0.83	0	6,6,6	0.58	0
2	HEM	B	404	1,5	50,50,50	2.03	11 (22%)	67,82,82	1.47	10 (14%)
4	DGG	B	406	-	19,19,50	1.22	1 (5%)	20,22,59	2.70	4 (20%)

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
3	FAD	A	405	-	-	2/34/50/50	0/6/6/6
4	DGG	A	406	-	-	10/16/21/59	0/1/1/1
5	ECN	B	411	2	1/1/1/1	4/13/13/13	0/3/3/3
2	HEM	A	404	1,5	-	3/14/54/54	-
5	ECN	A	411	2	1/1/1/1	4/13/13/13	0/3/3/3
3	FAD	B	405	-	-	1/34/50/50	0/6/6/6
2	HEM	B	404	1,5	-	1/14/54/54	-
4	DGG	B	406	-	-	11/16/21/59	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	HEM	C3D-C2D	7.15	1.52	1.36
2	A	404	HEM	C3D-C2D	7.13	1.52	1.36
2	B	404	HEM	FE-ND	6.71	2.15	1.94
2	B	404	HEM	FE-NB	4.97	2.10	1.94
4	A	406	DGG	O19-C21	4.76	1.46	1.30
3	A	405	FAD	C4X-N5	4.71	1.40	1.30
4	B	406	DGG	O19-C21	4.58	1.46	1.30
5	A	411	ECN	C14-CL4	3.91	1.82	1.73
3	B	405	FAD	C4X-N5	3.85	1.39	1.30
5	B	411	ECN	C14-CL4	3.45	1.81	1.73
5	A	411	ECN	C16-CL8	3.34	1.82	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	HEM	CAB-C3B	3.31	1.56	1.47
5	B	411	ECN	C19-C20	3.30	1.57	1.52
2	A	404	HEM	FE-NC	3.26	2.05	1.95
3	A	405	FAD	C2A-N3A	3.16	1.39	1.33
2	B	404	HEM	CAC-C3C	3.03	1.55	1.47
3	A	405	FAD	C2A-N1A	2.89	1.39	1.33
2	B	404	HEM	CAB-C3B	2.85	1.55	1.47
2	B	404	HEM	C1B-NB	-2.79	1.35	1.40
3	A	405	FAD	C10-N1	2.77	1.38	1.33
2	A	404	HEM	FE-NA	2.70	2.04	1.95
5	A	411	ECN	C15-C16	2.70	1.42	1.38
2	A	404	HEM	CAC-C3C	2.65	1.54	1.47
3	B	405	FAD	C2A-N1A	2.64	1.38	1.33
5	A	411	ECN	C19-C20	2.64	1.56	1.52
3	B	405	FAD	C1'-N10	2.61	1.54	1.47
5	A	411	ECN	C15-C14	2.57	1.42	1.38
2	A	404	HEM	C4C-NC	-2.52	1.34	1.39
3	B	405	FAD	C8A-N7A	2.52	1.36	1.31
3	B	405	FAD	C10-N1	2.51	1.38	1.33
2	B	404	HEM	CMB-C2B	2.47	1.55	1.50
2	B	404	HEM	CMA-C3A	2.36	1.55	1.50
2	B	404	HEM	FE-NA	2.30	2.02	1.95
5	B	411	ECN	C5-C20	-2.25	1.46	1.52
3	A	405	FAD	C8A-N7A	2.12	1.35	1.31
3	B	405	FAD	C2A-N3A	2.10	1.37	1.33
2	B	404	HEM	C3C-C2C	-2.03	1.33	1.37
2	B	404	HEM	C2A-C3A	-2.00	1.33	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	411	ECN	O20-C20-C5	-8.86	101.35	112.05
4	B	406	DGG	C39-C30-C31	-8.77	104.77	120.62
5	B	411	ECN	O20-C20-C19	7.78	118.72	106.24
4	A	406	DGG	C39-C29-C28	-7.67	106.77	120.62
4	A	406	DGG	C39-C30-C31	-7.48	107.11	120.62
4	B	406	DGG	C39-C29-C28	-7.34	107.36	120.62
5	B	411	ECN	C21-C5-C14	6.19	123.02	116.82
3	B	405	FAD	N3A-C2A-N1A	-6.13	119.30	128.58
5	A	411	ECN	C5-C14-CL4	-5.59	114.70	120.41
3	A	405	FAD	N3A-C2A-N1A	-5.47	120.30	128.58
5	A	411	ECN	C15-C14-CL4	5.18	126.93	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	HEM	C4D-ND-C1D	5.15	111.31	105.21
5	A	411	ECN	C21-C5-C14	5.14	121.97	116.82
5	A	411	ECN	C15-C16-CL8	5.06	125.51	119.17
3	A	405	FAD	C5A-C4A-N3A	-4.94	119.91	126.72
5	B	411	ECN	C14-C5-C20	-4.73	117.84	122.15
3	A	405	FAD	C4'-C3'-C2'	-4.62	105.89	113.57
5	A	411	ECN	O20-C20-C19	4.62	113.65	106.24
5	B	411	ECN	O20-C20-C5	-4.42	106.72	112.05
2	B	404	HEM	CHC-C1C-NC	4.15	128.97	124.45
2	B	404	HEM	CBA-CAA-C2A	-4.00	101.48	112.53
5	B	411	ECN	C15-C14-C5	-3.88	118.28	122.46
5	A	411	ECN	C15-C14-C5	-3.79	118.37	122.46
5	A	411	ECN	C14-C5-C20	-3.57	118.89	122.15
3	B	405	FAD	C4X-C10-N10	3.56	121.58	116.48
3	A	405	FAD	C2A-N3A-C4A	3.55	120.49	111.83
3	B	405	FAD	C5A-C4A-N3A	-3.53	121.86	126.72
3	A	405	FAD	N3A-C4A-N9A	3.52	133.16	127.17
2	A	404	HEM	CBA-CAA-C2A	-3.46	102.97	112.53
3	A	405	FAD	C4X-C10-N10	3.42	121.38	116.48
3	B	405	FAD	C2A-N3A-C4A	3.21	119.67	111.83
3	B	405	FAD	N9A-C8A-N7A	-3.13	109.50	113.94
2	A	404	HEM	CHA-C4D-ND	3.11	128.22	124.37
3	A	405	FAD	N9A-C8A-N7A	-3.09	109.56	113.94
5	B	411	ECN	C13-C11-CL2	3.04	123.84	119.36
2	A	404	HEM	CHD-C4C-NC	-3.02	121.16	124.45
3	A	405	FAD	C4X-C4-N3	3.00	120.88	113.25
3	A	405	FAD	C4-N3-C2	-2.97	120.36	125.64
3	B	405	FAD	C5X-C9A-N10	2.85	120.54	117.97
3	A	405	FAD	C5A-N7A-C8A	2.84	107.92	103.45
2	A	404	HEM	C4D-ND-C1D	2.83	108.56	105.21
3	B	405	FAD	C1'-C2'-C3'	2.83	117.33	109.66
5	A	411	ECN	O20-C8-C1	2.80	116.32	109.91
5	B	411	ECN	C9-C11-CL2	-2.79	115.24	119.36
5	B	411	ECN	C19-N1-C3	-2.79	123.04	126.96
3	A	405	FAD	C4-C4X-N5	2.76	122.02	118.21
5	A	411	ECN	C17-C16-CL8	-2.66	115.43	119.36
3	B	405	FAD	C4-N3-C2	-2.65	120.93	125.64
3	B	405	FAD	C5A-N7A-C8A	2.62	107.57	103.45
2	B	404	HEM	CAD-C3D-C4D	2.59	129.21	124.70
3	A	405	FAD	C1'-C2'-C3'	2.54	116.55	109.66
3	A	405	FAD	C10-C4X-N5	-2.52	119.66	124.81
2	B	404	HEM	C3C-C2C-C1C	2.47	109.38	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	HEM	CHA-C4D-C3D	-2.47	120.68	125.23
2	B	404	HEM	O2D-CGD-CBD	2.43	121.69	114.00
3	B	405	FAD	C10-C4X-N5	-2.43	119.85	124.81
5	B	411	ECN	C7-N1-C3	2.37	109.67	106.71
3	B	405	FAD	C4A-C5A-N7A	-2.37	107.88	110.58
2	A	404	HEM	CHC-C4B-NB	2.35	126.95	124.42
3	B	405	FAD	C4X-C4-N3	2.34	119.22	113.25
2	A	404	HEM	CMD-C2D-C1D	2.33	128.68	125.03
4	B	406	DGG	O19-C21-C22	2.29	121.25	114.00
2	A	404	HEM	CAD-CBD-CGD	-2.29	107.58	113.67
3	A	405	FAD	C10-N1-C2	2.26	121.74	116.85
2	B	404	HEM	C4D-C3D-C2D	-2.21	103.68	106.89
2	B	404	HEM	CMB-C2B-C1B	-2.18	121.62	125.03
2	B	404	HEM	CHC-C4B-NB	-2.18	122.08	124.42
2	A	404	HEM	C4D-C3D-C2D	-2.17	103.73	106.89
4	A	406	DGG	O19-C21-C22	2.15	120.80	114.00
3	B	405	FAD	C4'-C3'-C2'	-2.15	109.99	113.57
3	B	405	FAD	O4-C4-C4X	-2.15	120.86	126.53
3	B	405	FAD	C9A-C5X-N5	-2.15	120.18	122.45
2	A	404	HEM	CHC-C1C-NC	2.13	126.77	124.45
3	A	405	FAD	C9A-C5X-N5	-2.12	120.21	122.45
2	A	404	HEM	CAD-C3D-C4D	2.12	128.39	124.70
3	B	405	FAD	C2A-N1A-C6A	2.11	122.19	118.73
2	A	404	HEM	C4A-CHB-C1B	-2.10	121.31	126.25
5	A	411	ECN	C8-C1-C2	-2.09	115.83	120.64
3	A	405	FAD	C5A-C6A-N6A	-2.08	118.15	123.29
4	B	406	DGG	O19-C21-O21	-2.02	118.14	123.33
3	A	405	FAD	C6A-C5A-C4A	2.02	119.93	117.18
2	A	404	HEM	CHD-C4C-C3C	2.01	128.59	125.21
2	B	404	HEM	CAC-C3C-C4C	2.00	129.60	124.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	411	ECN	C20
5	A	411	ECN	C20

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	DGG	C29-C30-C31-C32
5	B	411	ECN	N1-C19-C20-O20

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Mol	Chain	Res	Type	Atoms
5	B	411	ECN	N1-C19-C20-C5
5	B	411	ECN	C1-C8-O20-C20
5	A	411	ECN	N1-C19-C20-C5
5	A	411	ECN	C19-C20-O20-C8
5	A	411	ECN	C5-C20-O20-C8
5	A	411	ECN	C1-C8-O20-C20
2	A	404	HEM	C3D-CAD-CBD-CGD
4	B	406	DGG	C30-C31-C32-C33
4	A	406	DGG	C30-C31-C32-C33
4	B	406	DGG	C32-C33-C34-C35
4	A	406	DGG	C32-C33-C34-C35
4	B	406	DGG	C31-C32-C33-C34
4	A	406	DGG	C31-C32-C33-C34
4	A	406	DGG	C22-C23-C24-C25
4	B	406	DGG	C26-C27-C28-C29
5	B	411	ECN	C19-C20-O20-C8
4	B	406	DGG	C22-C23-C24-C25
4	A	406	DGG	C23-C24-C25-C26
2	B	404	HEM	C3D-CAD-CBD-CGD
4	B	406	DGG	C33-C34-C35-C36
4	B	406	DGG	C25-C26-C27-C28
4	A	406	DGG	C27-C28-C29-C39
4	A	406	DGG	C39-C30-C31-C32
2	A	404	HEM	CAD-CBD-CGD-O1D
4	A	406	DGG	O21-C21-C22-C23
2	A	404	HEM	CAD-CBD-CGD-O2D
4	A	406	DGG	O19-C21-C22-C23
4	B	406	DGG	C29-C30-C31-C32
4	B	406	DGG	O21-C21-C22-C23
3	A	405	FAD	O2'-C2'-C3'-O3'
4	B	406	DGG	C23-C24-C25-C26
4	B	406	DGG	O19-C21-C22-C23
3	B	405	FAD	PA-O3P-P-O2P
3	A	405	FAD	PA-O3P-P-O2P

There are no ring outliers.

7 monomers are involved in 50 short contacts:

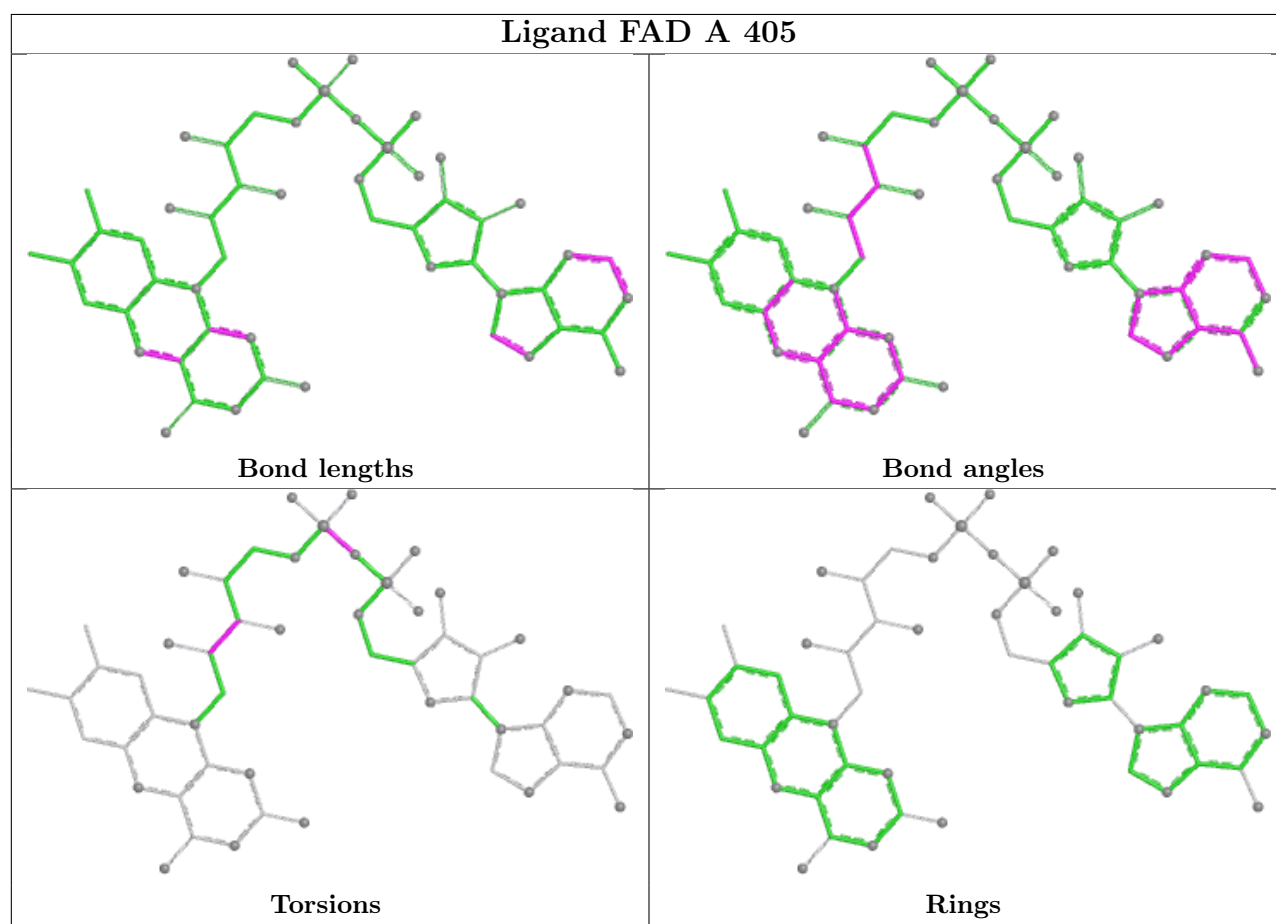
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	FAD	4	0
4	A	406	DGG	6	0
5	B	411	ECN	18	0

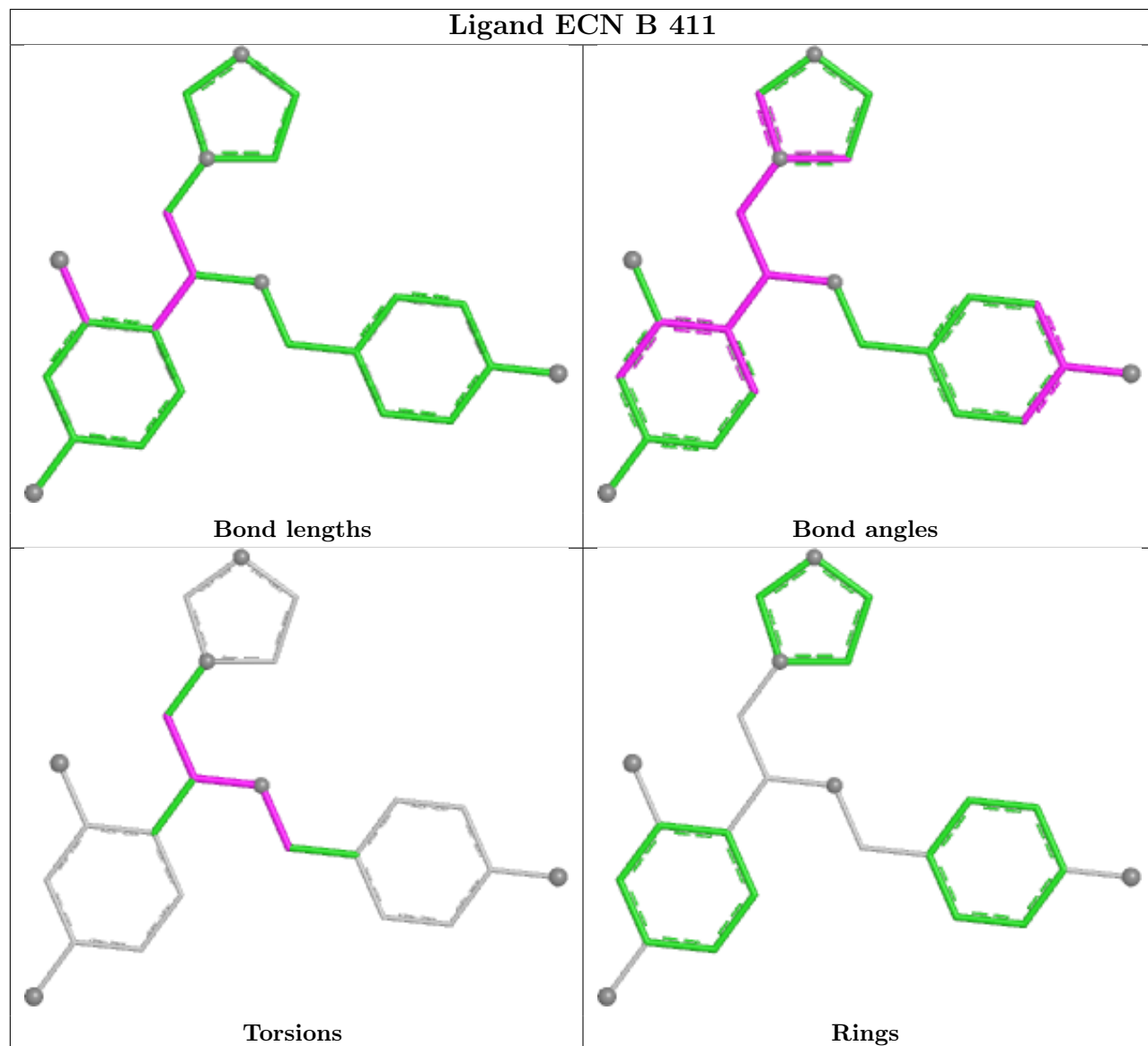
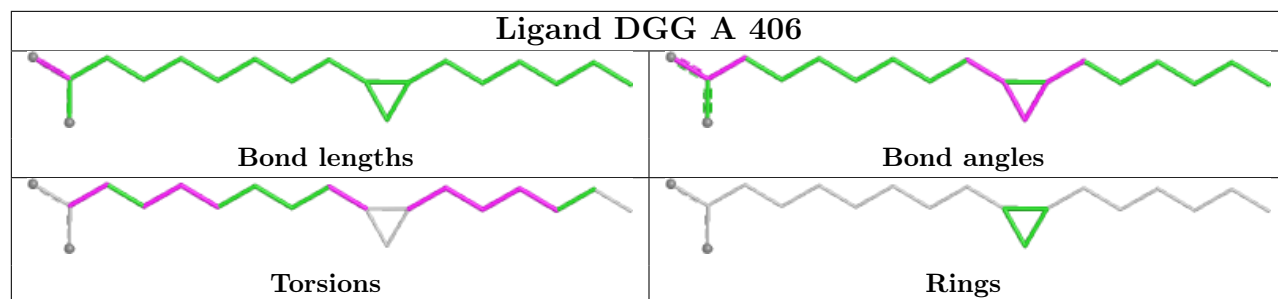
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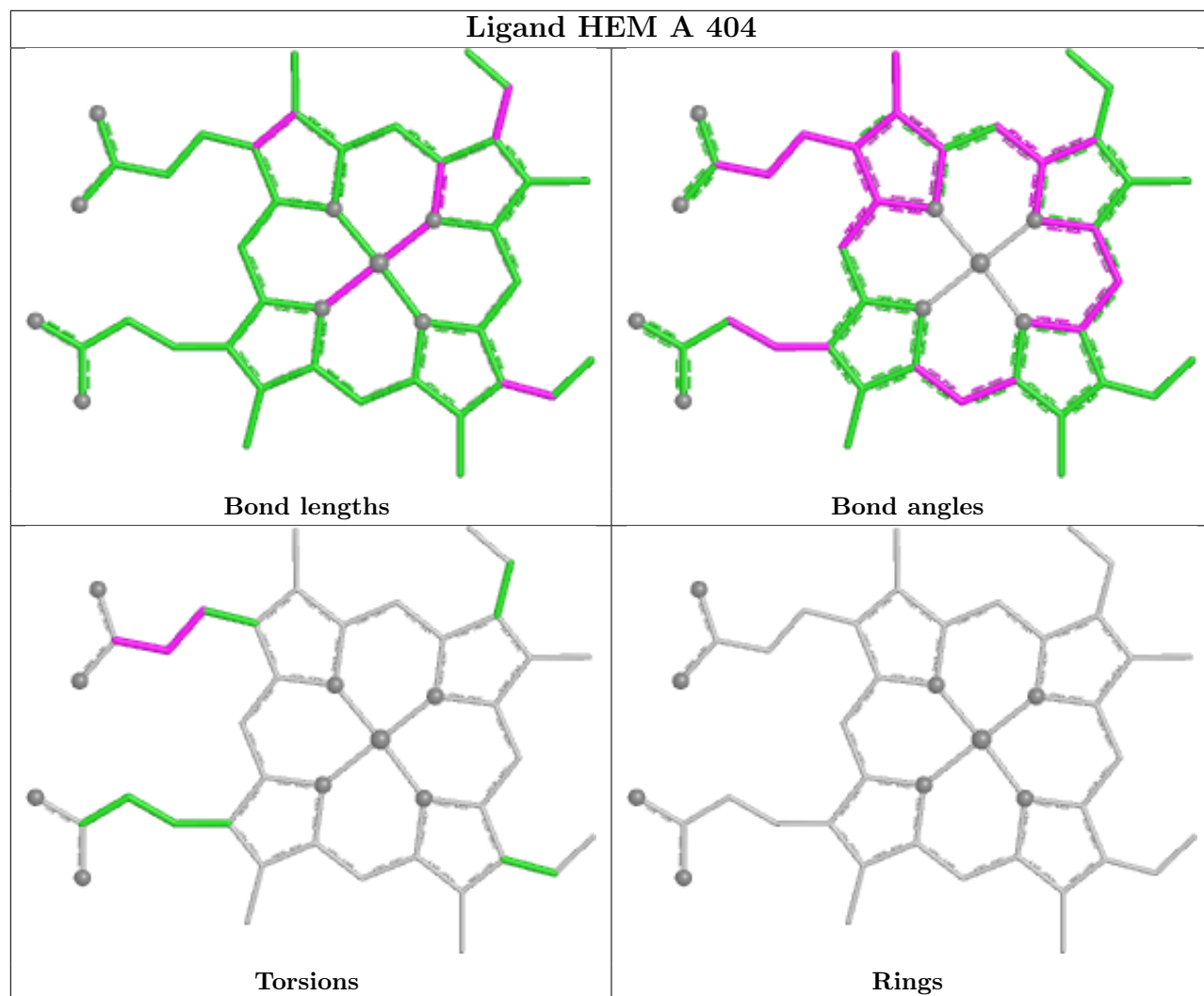
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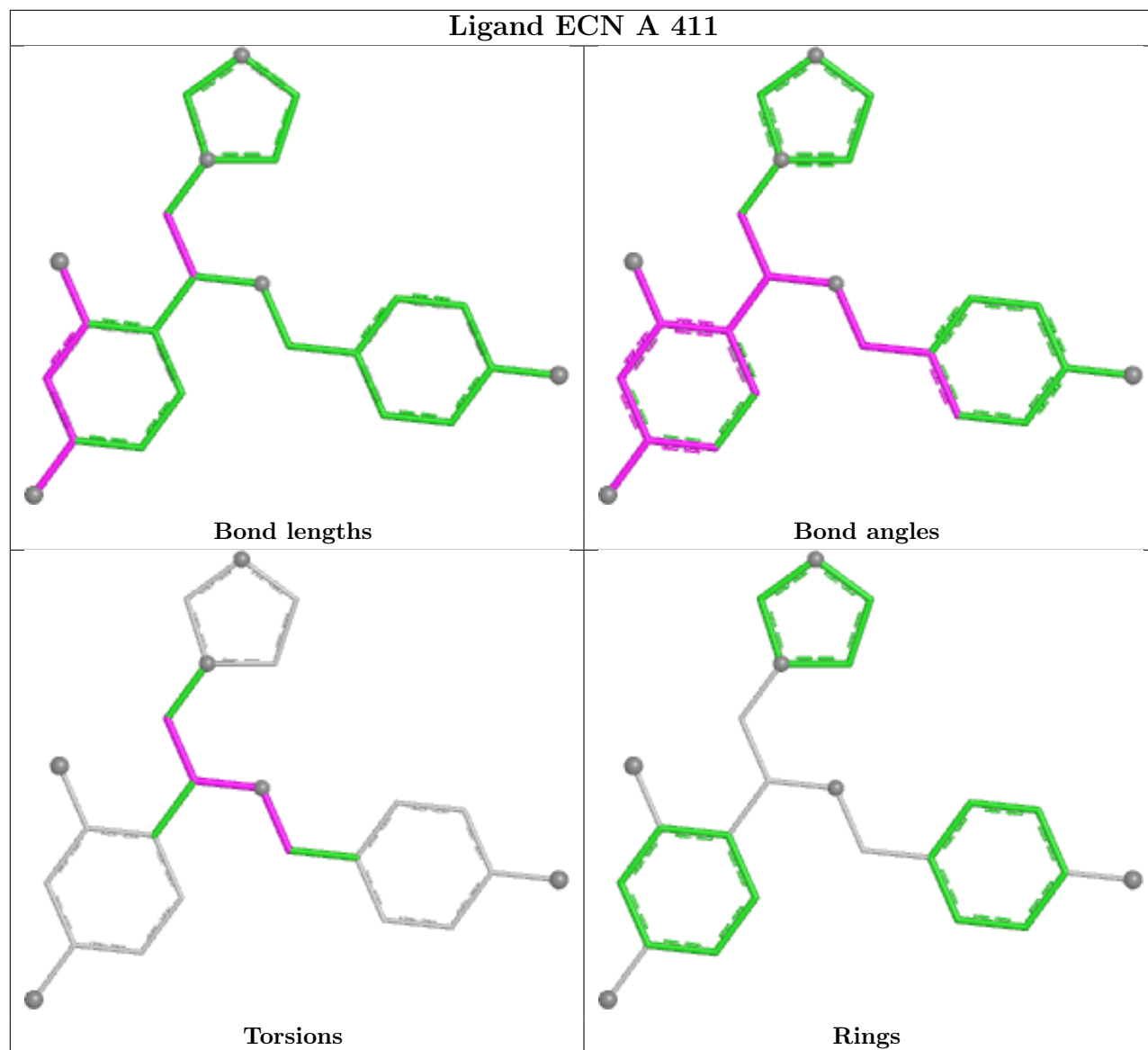
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	HEM	4	0
5	A	411	ECN	15	0
2	B	404	HEM	4	0
4	B	406	DGG	6	0

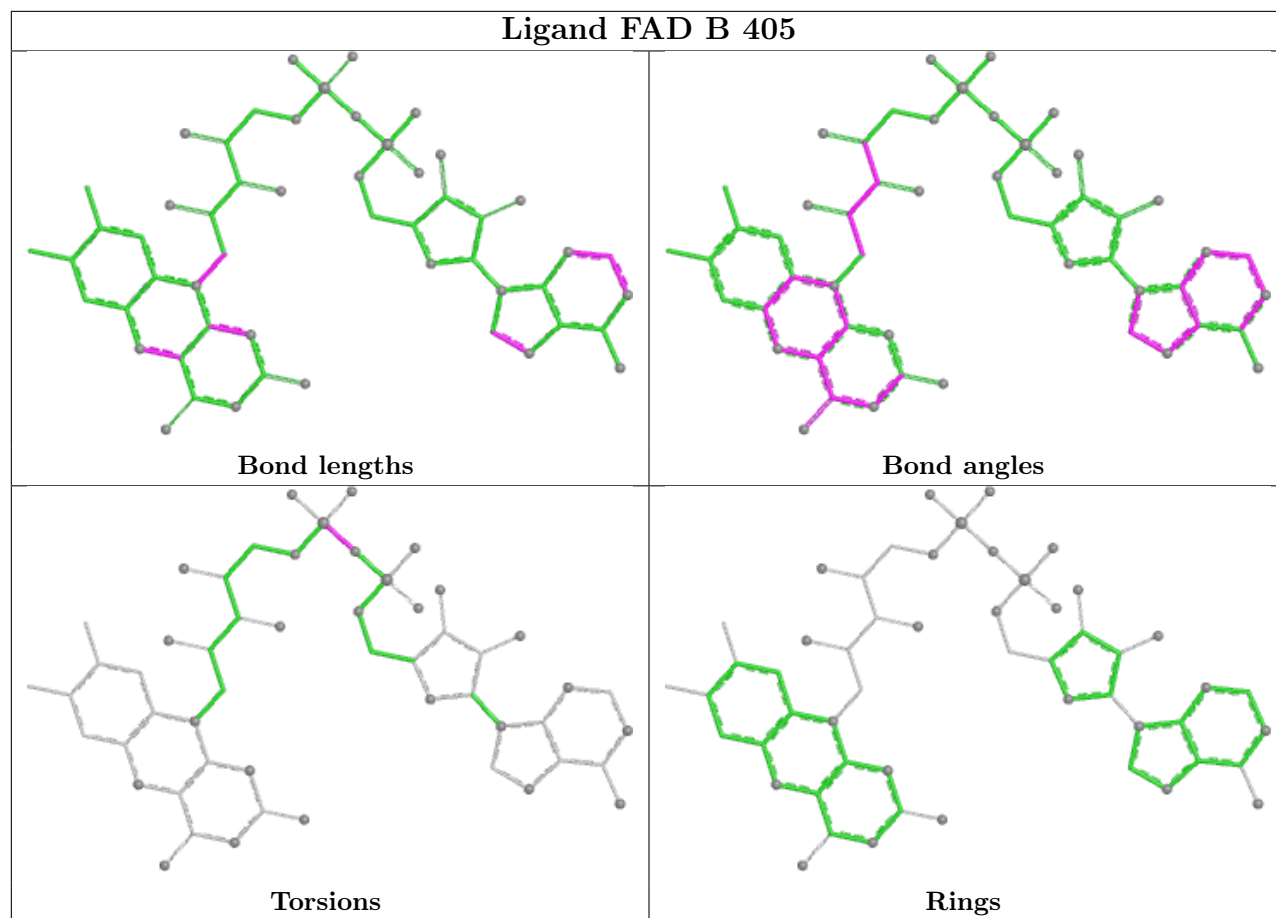
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

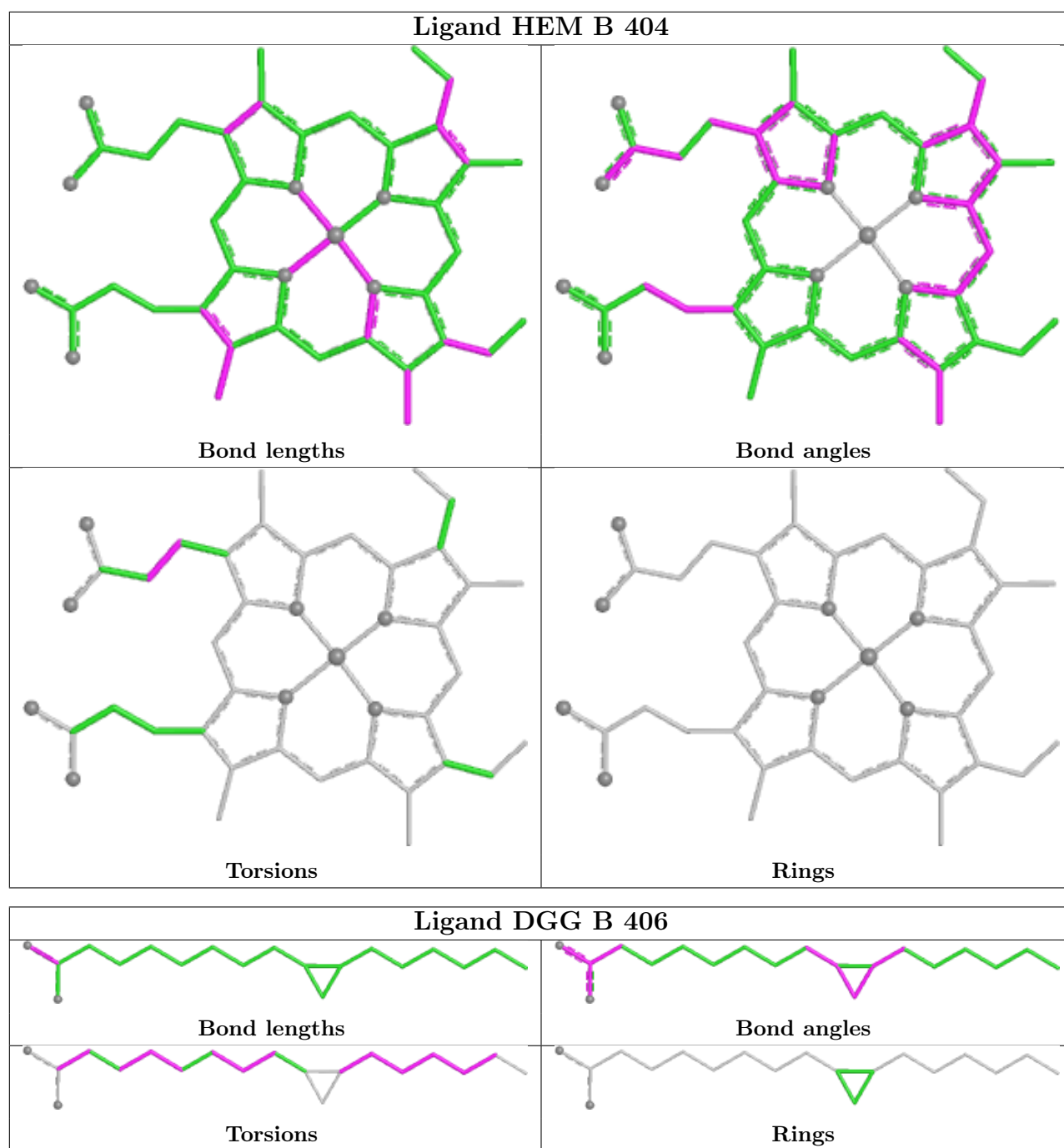












5.7 Other polymers [i](#)

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	403/403 (100%)	0.48	24 (5%) 27 24	28, 55, 102, 170	0
1	B	403/403 (100%)	0.95	99 (24%) 2 1	27, 62, 145, 185	1 (0%)
All	All	806/806 (100%)	0.72	123 (15%) 5 4	27, 57, 134, 185	1 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	ALA	7.1
1	B	381	LEU	6.6
1	A	402	ALA	6.2
1	B	400	LEU	6.0
1	B	292	PRO	5.6
1	A	48	GLN	4.8
1	B	277	GLY	4.8
1	B	306	ALA	4.7
1	B	307	VAL	4.7
1	B	334	LEU	4.6
1	A	400	LEU	4.3
1	B	386	ILE	4.3
1	B	403	GLU	4.3
1	B	399	ASP	4.2
1	B	289	LEU	4.1
1	B	269	ILE	4.1
1	B	356	LYS	4.1
1	B	385	GLY	4.0
1	B	287	VAL	4.0
1	B	288	ALA	3.9
1	B	396	PHE	3.9
1	B	297	VAL	3.8
1	B	359	LEU	3.8
1	A	292	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	47	HIS	3.7
1	A	230	PRO	3.7
1	A	401	PHE	3.7
1	B	266	LYS	3.7
1	B	346	PRO	3.6
1	B	299	VAL	3.6
1	A	395	VAL	3.6
1	B	393	TYR	3.5
1	B	348	LEU	3.4
1	B	320	THR	3.3
1	B	363	ALA	3.3
1	B	282	VAL	3.2
1	B	216	GLY	3.1
1	B	367	ILE	3.1
1	B	148	PRO	3.1
1	B	387	HIS	3.1
1	B	360	LEU	3.1
1	A	399	ASP	3.1
1	B	380	ALA	3.0
1	A	293	PRO	3.0
1	B	298	PHE	3.0
1	B	338	VAL	3.0
1	B	361	PRO	3.0
1	B	319	LYS	3.0
1	A	148	PRO	2.9
1	B	335	PRO	2.9
1	B	296	VAL	2.9
1	A	50	GLN	2.9
1	B	305	SER	2.9
1	B	398	PRO	2.8
1	B	345	TYR	2.8
1	B	354	ILE	2.8
1	B	286	LYS	2.8
1	B	377	GLN	2.8
1	B	395	VAL	2.7
1	B	279	THR	2.7
1	B	263	VAL	2.7
1	B	321	TYR	2.7
1	B	358	ILE	2.6
1	B	293	PRO	2.6
1	B	333	PRO	2.6
1	B	317	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	2.5
1	B	309	ALA	2.5
1	B	357	SER	2.5
1	A	361	PRO	2.5
1	B	51	GLY	2.5
1	B	401	PHE	2.5
1	B	280	PRO	2.5
1	B	378	HIS	2.5
1	B	1	MET	2.5
1	B	278	LEU	2.4
1	A	393	TYR	2.4
1	B	327	PHE	2.4
1	B	389	ALA	2.4
1	A	382	LYS	2.4
1	B	314	LEU	2.4
1	B	302	ALA	2.4
1	B	391	ILE	2.4
1	B	262	ASP	2.4
1	B	392	HIS	2.4
1	A	356	LYS	2.4
1	B	384	LEU	2.3
1	B	265	ALA	2.3
1	B	267	THR	2.3
1	A	229	GLY	2.3
1	B	268	PRO	2.3
1	B	326	LEU	2.3
1	B	371	ILE	2.3
1	B	352	LYS	2.3
1	A	321	TYR	2.3
1	B	229	GLY	2.3
1	B	295	GLN	2.3
1	A	228	GLY	2.2
1	B	285	LEU	2.2
1	A	398	PRO	2.2
1	B	318	ALA	2.2
1	B	332	GLN	2.2
1	A	49	GLU	2.2
1	B	313	ARG	2.2
1	A	387	HIS	2.2
1	B	213	MET	2.2
1	B	379	ASP	2.2
1	B	373	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	365	TYR	2.1
1	B	366	TYR	2.1
1	A	316	GLU	2.1
1	B	270	VAL	2.1
1	B	383	ASN	2.1
1	B	310	MET	2.1
1	B	147	GLN	2.1
1	B	291	ALA	2.1
1	A	291	ALA	2.1
1	B	390	ARG	2.1
1	B	355	GLU	2.1
1	B	330	TYR	2.1
1	B	351	VAL	2.1
1	B	227	GLY	2.1
1	B	230	PRO	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.

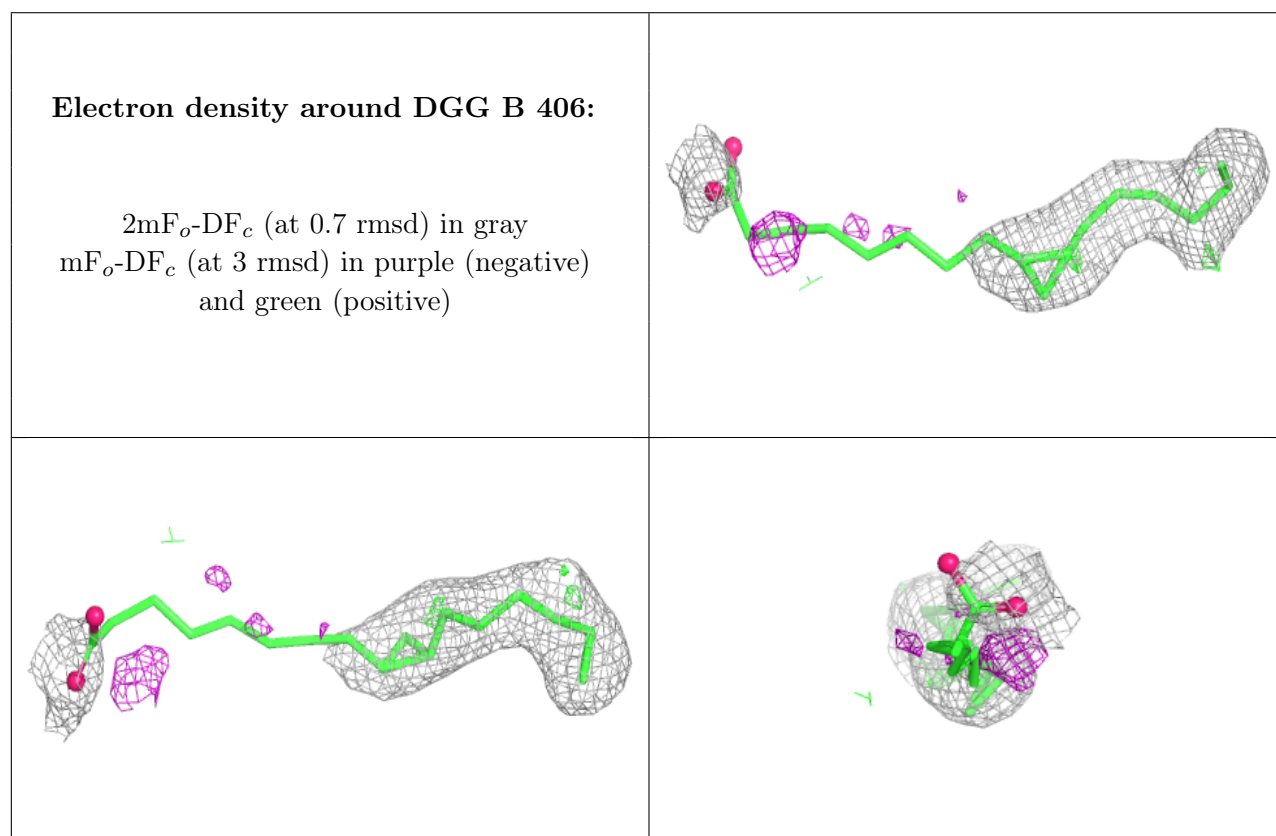
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DGG	B	406	19/50	0.87	0.24	28,71,191,193	0
4	DGG	A	406	19/50	0.88	0.14	45,58,95,97	0
5	ECN	A	411	24/24	0.88	0.16	29,73,99,139	0
6	PO4	A	407	5/5	0.92	0.11	58,70,73,88	0
5	ECN	B	411	24/24	0.95	0.16	31,53,239,322	0
3	FAD	A	405	53/53	0.97	0.07	23,33,80,88	0
3	FAD	B	405	53/53	0.97	0.07	24,35,55,63	0
2	HEM	A	404	43/43	0.98	0.07	21,29,66,82	0

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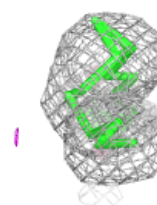
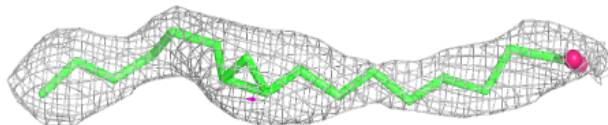
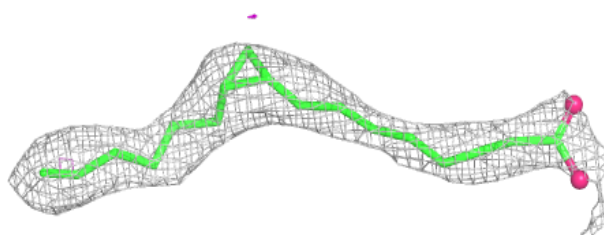
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	404	43/43	0.98	0.07	19,32,56,80	0

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.

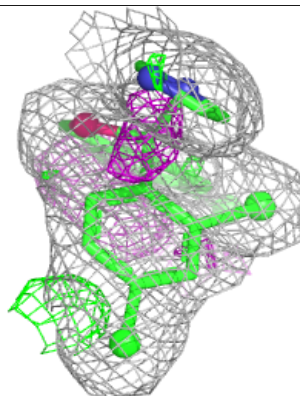
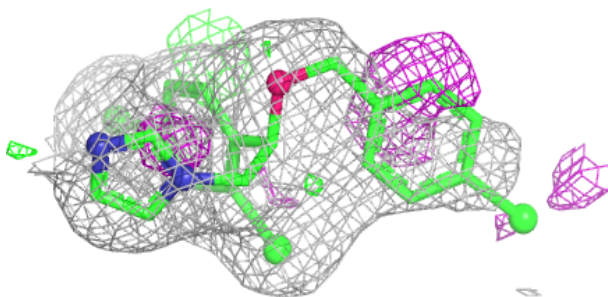
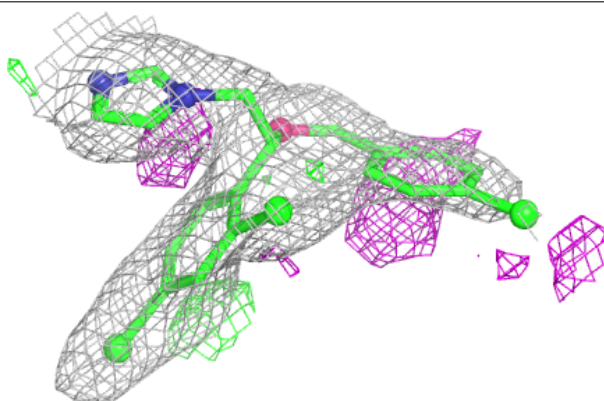


Electron density around DGG A 406:

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

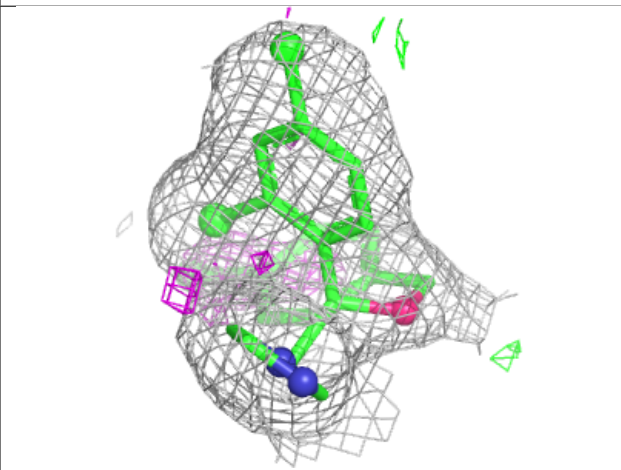
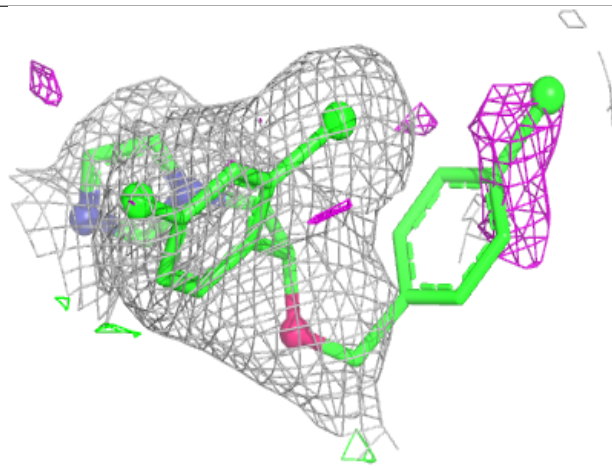
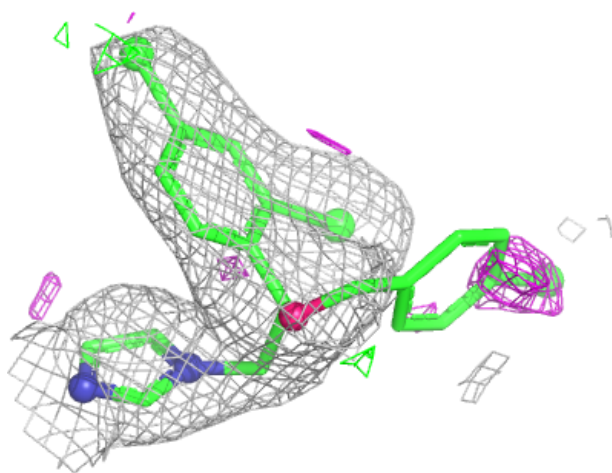
**Electron density around ECN A 411:**

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



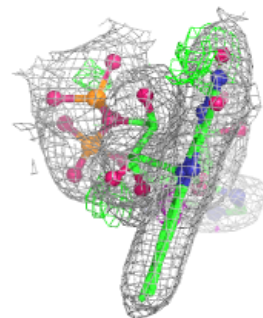
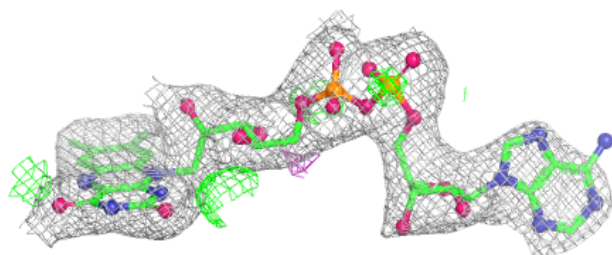
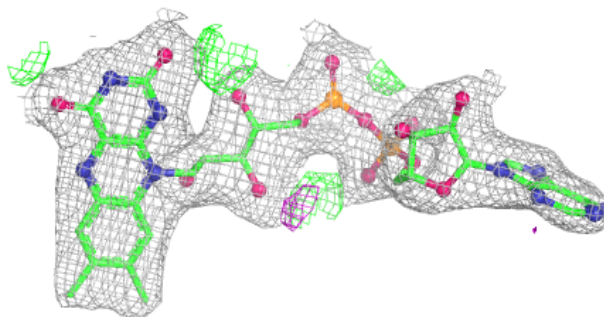
Electron density around ECN B 411:

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

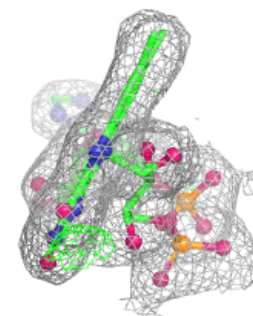
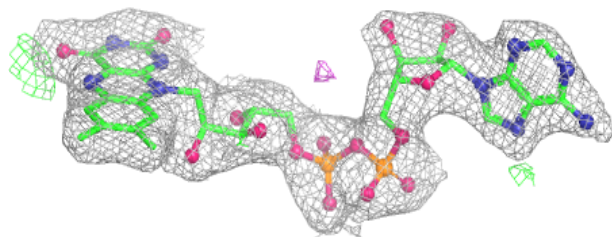
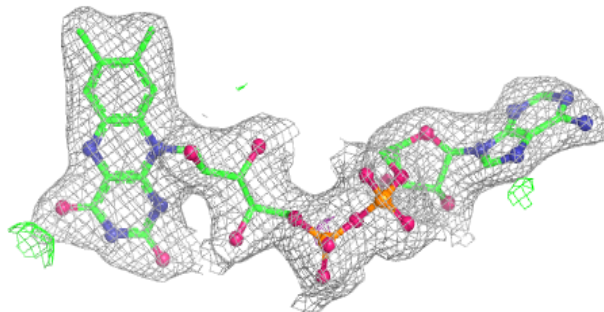


Electron density around FAD A 405:

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

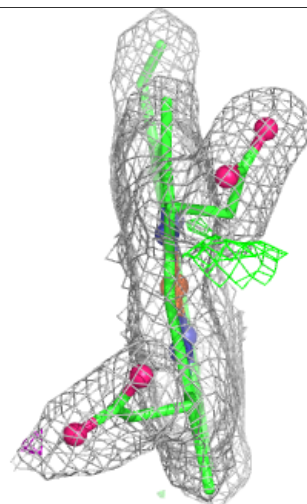
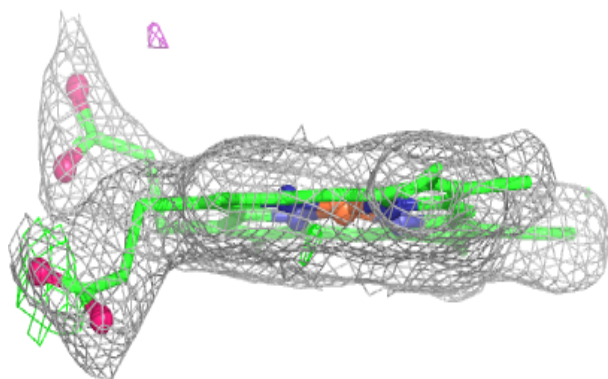
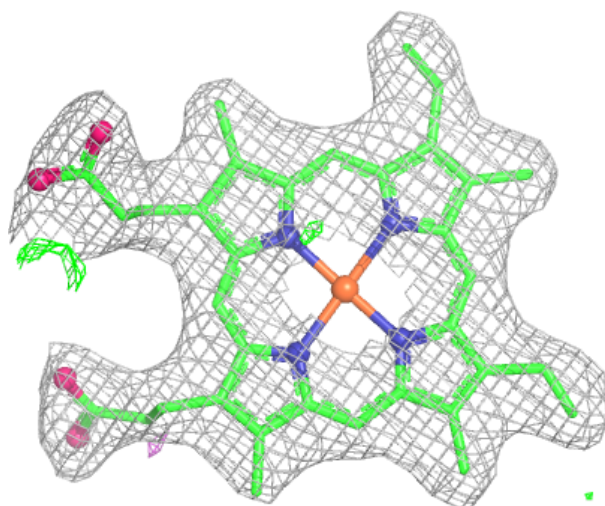
**Electron density around FAD B 405:**

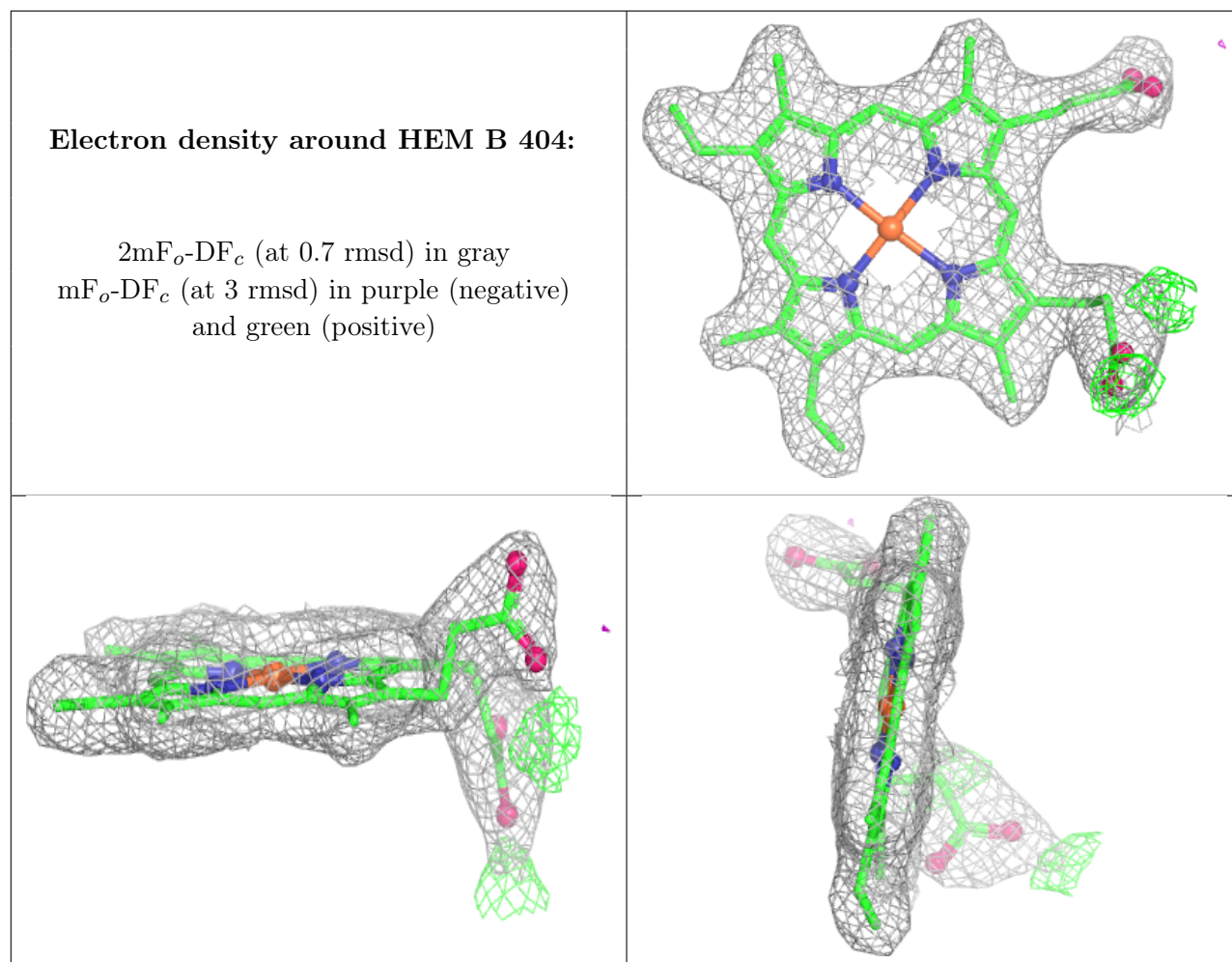
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 404:

$2mF_o-DF_c$ (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.