



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 PM UTC

PDB ID : 3OZW / pdb_00003ozw
Title : The Crystal Structure of flavohemoglobin from *R. eutrophus* in complex with ketoconazole
Authors : El Hammi, E.; Warkentin, E.; Demmer, U.; Ermler, U.; Baciou, L.
Deposited on : 2010-09-27
Resolution : 2.30 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

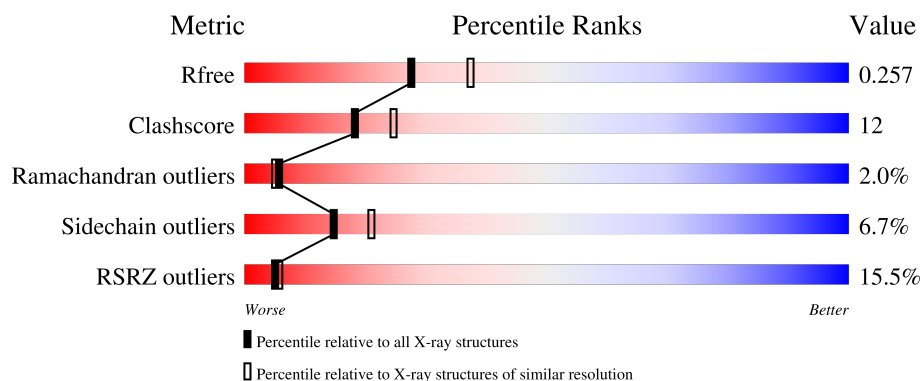
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



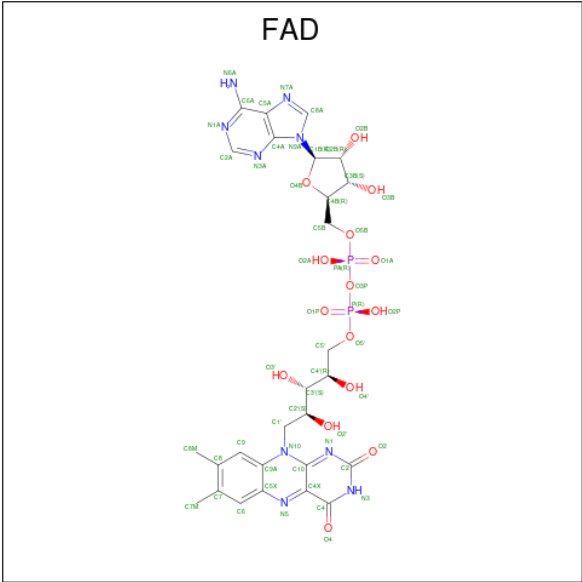
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	11% 79% 17% .
1	B	403	20% 79% 16% ..

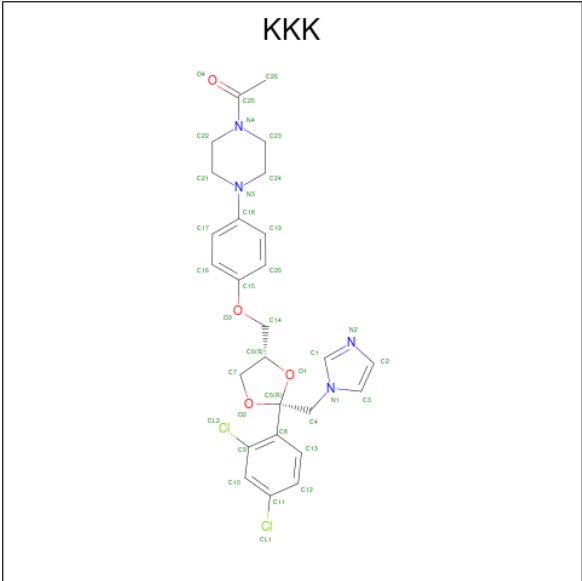
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	KKK	A	413	X	-	-	-
4	KKK	B	413	X	-	-	-



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

- Molecule 4 is 1-acetyl-4-(4-{[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy}phenyl)piperazine (CCD ID: KKK) (formula: C₂₆H₂₈Cl₂N₄O₄).



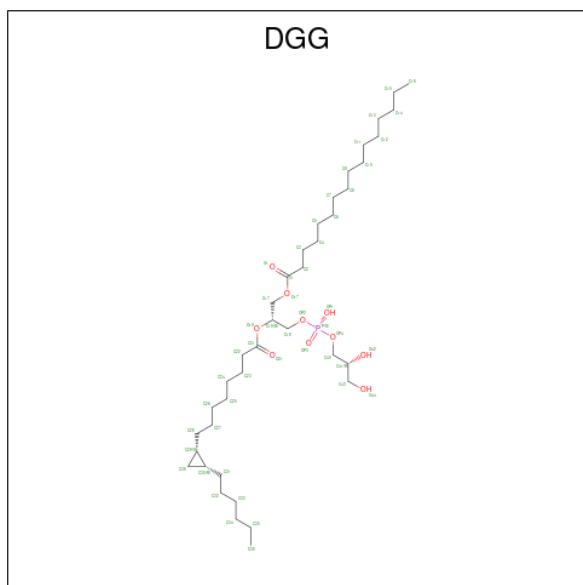
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			36	26	2	4	4		

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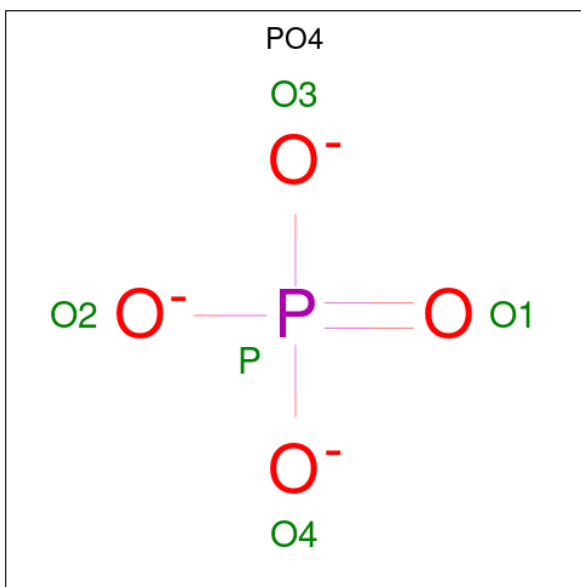
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	
			36	26	2	4	4	
							0	0

- Molecule 5 is 1-[GLYCEROLYLPHOSPHONYL]-2-[8-(2-HEXYL-CYCLOPROPYL)-OCTANAL-1-YL]-3-[HEXADECANAL-1-YL]-GLYCEROL (CCD ID: DGG) (formula: $C_{39}H_{75}O_{10}P$).



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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

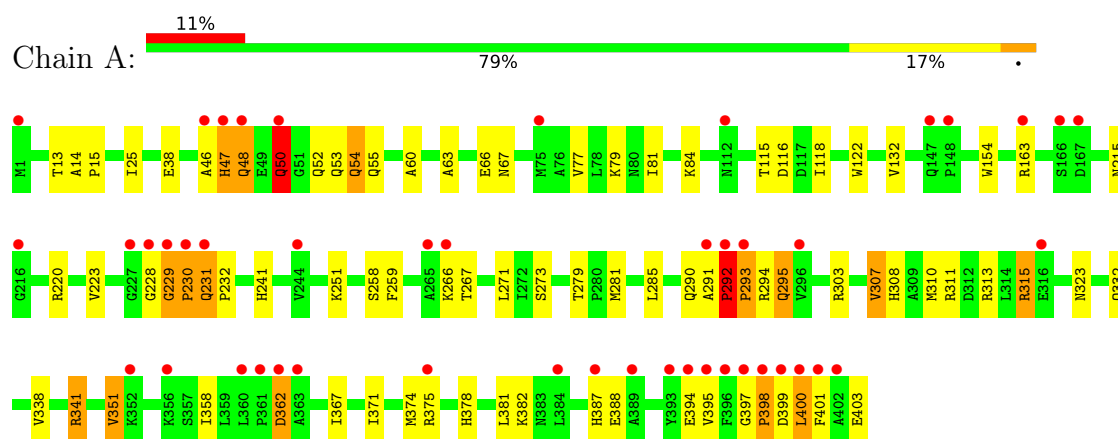
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total	O	0	0
			94	94		
7	B	87	Total	O	0	0
			87	87		

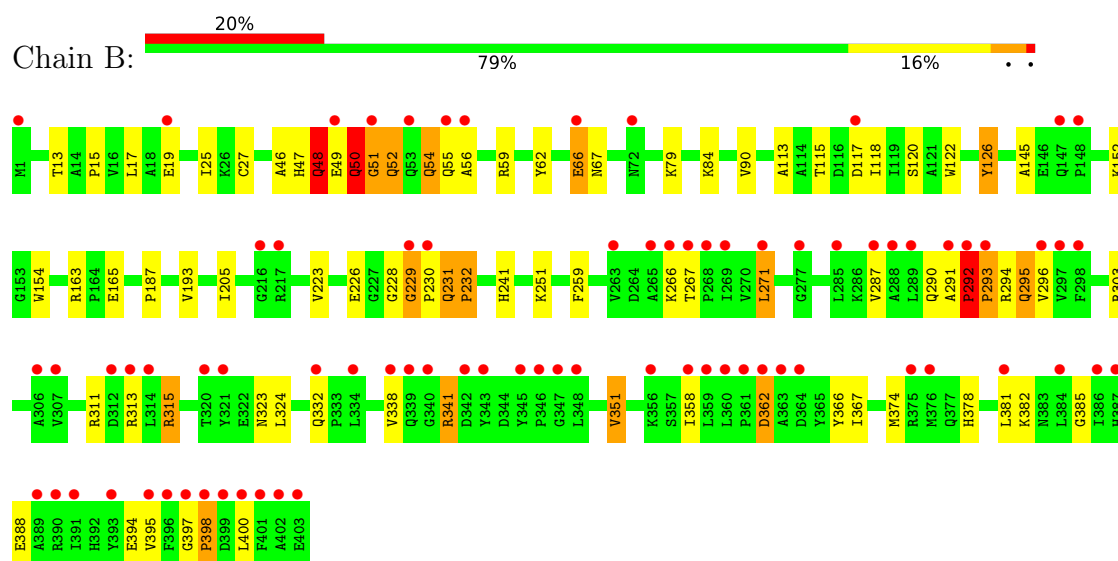
3 Residue-property plots [i](#)

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: 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	87.12Å 87.12Å 292.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.30) 92.7 (30.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.205 , 0.241 0.227 , 0.257	Depositor DCC
R_{free} test set	2573 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6795	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: DGG, HEM, PO4, FAD, KKK

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	0.90	0/3233	1.01	7/4393 (0.2%)
1	B	0.94	2/3253 (0.1%)	1.02	5/4419 (0.1%)
All	All	0.92	2/6486 (0.0%)	1.02	12/8812 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	VAL	CA-CB	5.42	1.59	1.54
1	B	126	TYR	CD1-CE1	5.13	1.54	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	PRO	CA-C-N	7.83	129.63	119.84
1	A	292	PRO	C-N-CA	7.83	129.63	119.84
1	B	292	PRO	CA-C-N	7.82	129.61	119.84
1	B	292	PRO	C-N-CA	7.82	129.61	119.84
1	A	50	GLN	N-CA-C	6.55	119.82	108.76
1	A	279	THR	CA-C-N	-6.44	112.37	119.19
1	A	279	THR	C-N-CA	-6.44	112.37	119.19
1	A	307	VAL	CB-CA-C	6.43	117.89	110.88
1	A	132	VAL	N-CA-C	-6.07	104.82	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	PRO	CA-C-N	-5.99	113.61	119.78
1	B	232	PRO	C-N-CA	-5.99	113.61	119.78
1	B	165	GLU	N-CA-C	-5.56	106.86	113.97

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 ⓘ

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	83	0
1	B	3170	0	3131	69	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	53	0	31	4	0
3	B	53	0	31	1	0
4	A	36	0	28	6	0
4	B	36	0	28	13	0
5	A	19	0	30	11	0
6	A	5	0	0	0	0
7	A	94	0	0	18	0
7	B	87	0	0	10	0
All	All	6795	0	6451	158	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 12.

All (158) 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:117:ASP:HB2	7:B:473:HOH:O	1.17	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:HB2	7:A:496:HOH:O	1.32	1.24
1:B:27:CYS:SG	7:B:491:HOH:O	2.05	1.14
1:B:49:GLU:O	1:B:50:GLN:HB2	1.42	1.10
1:A:341:ARG:HG2	1:A:341:ARG:HH21	1.14	1.03
1:B:341:ARG:HG2	1:B:341:ARG:HH21	1.19	1.02
1:B:27:CYS:CB	7:B:491:HOH:O	2.08	1.02
1:A:291:ALA:HA	1:A:292:PRO:C	1.86	1.01
1:B:54:GLN:HE21	1:B:55:GLN:HE21	1.09	1.00
1:B:27:CYS:HB2	7:B:491:HOH:O	1.62	0.99
1:B:48:GLN:HG3	7:B:440:HOH:O	1.65	0.95
1:B:291:ALA:HA	1:B:292:PRO:C	1.91	0.95
1:A:230:PRO:HG3	1:B:59:ARG:HG2	1.45	0.95
1:A:54:GLN:HE21	1:A:55:GLN:HE21	0.94	0.89
1:A:54:GLN:NE2	1:A:55:GLN:HE21	1.71	0.88
1:A:54:GLN:HE21	1:A:55:GLN:NE2	1.73	0.85
1:A:77:VAL:HG21	5:A:416:DGG:H251	1.60	0.83
1:A:232:PRO:HG2	3:A:405:FAD:C5A	2.07	0.83
1:B:341:ARG:HG2	1:B:341:ARG:NH2	1.95	0.81
1:A:341:ARG:HG2	1:A:341:ARG:NH2	1.89	0.80
1:A:394:GLU:HA	7:A:408:HOH:O	1.82	0.78
1:A:399:ASP:HB3	7:A:415:HOH:O	1.85	0.76
1:A:303:ARG:HG3	1:A:332:GLN:HB2	1.67	0.75
1:A:13:THR:HG21	1:A:118:ILE:HG12	1.70	0.73
1:B:54:GLN:HE21	1:B:55:GLN:NE2	1.86	0.73
1:B:47:HIS:ND1	4:B:413:KKK:H19	2.04	0.72
1:A:230:PRO:CG	1:B:59:ARG:HG2	2.20	0.71
1:B:47:HIS:CE1	4:B:413:KKK:H21A	2.24	0.71
1:A:46:ALA:C	1:A:48:GLN:H	1.98	0.71
1:A:351:VAL:HG22	1:A:358:ILE:HD13	1.73	0.71
1:B:367:ILE:HG22	1:B:374:MET:HG2	1.71	0.70
1:A:60:ALA:HB1	5:A:416:DGG:H391	1.74	0.70
1:B:51:GLY:HA3	1:B:52:GLN:HB2	1.74	0.69
1:A:54:GLN:NE2	1:A:55:GLN:NE2	2.37	0.69
1:A:400:LEU:HD23	7:A:415:HOH:O	1.93	0.68
3:A:405:FAD:H2A	1:B:62:TYR:HE1	1.57	0.68
1:A:67:ASN:OD1	5:A:416:DGG:H232	1.93	0.68
1:A:367:ILE:HG22	1:A:374:MET:HG2	1.76	0.66
1:B:54:GLN:NE2	1:B:55:GLN:HE21	1.90	0.62
1:A:55:GLN:NE2	1:B:113:ALA:HB1	2.14	0.61
1:B:230:PRO:HD2	1:B:231:GLN:HE21	1.65	0.61
1:B:228:GLY:O	1:B:229:GLY:C	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:O	1:A:295:GLN:HB2	2.00	0.61
1:A:400:LEU:CD2	7:A:415:HOH:O	2.47	0.61
3:A:405:FAD:H2A	1:B:62:TYR:CE1	2.35	0.61
1:B:51:GLY:CA	1:B:52:GLN:HB2	2.30	0.60
1:A:259:PHE:CG	1:A:394:GLU:HB2	2.37	0.60
1:A:232:PRO:HG2	3:A:405:FAD:N7A	2.14	0.60
1:B:294:ARG:O	1:B:295:GLN:HB2	2.00	0.60
1:A:398:PRO:HG2	7:A:440:HOH:O	2.02	0.59
1:A:259:PHE:CD2	1:A:394:GLU:HB2	2.36	0.59
1:B:66:GLU:HB3	7:B:484:HOH:O	2.01	0.59
1:B:259:PHE:CD2	1:B:394:GLU:HB2	2.38	0.59
1:A:122:TRP:HZ3	5:A:416:DGG:H332	1.67	0.59
1:A:230:PRO:HD2	1:A:231:GLN:HE21	1.66	0.59
1:A:228:GLY:O	1:A:229:GLY:C	2.46	0.59
1:A:394:GLU:CA	7:A:408:HOH:O	2.48	0.59
1:A:399:ASP:OD1	7:A:408:HOH:O	2.17	0.58
1:A:63:ALA:HB1	5:A:416:DGG:H242	1.86	0.57
1:B:13:THR:HG21	1:B:118:ILE:HG12	1.86	0.57
1:A:163:ARG:NH1	1:A:313:ARG:HH22	2.02	0.57
1:A:46:ALA:C	1:A:48:GLN:N	2.62	0.57
1:B:56:ALA:CB	4:B:413:KKK:H16	2.33	0.57
1:A:77:VAL:CG2	5:A:416:DGG:H251	2.33	0.56
1:A:220:ARG:NH2	1:A:310:MET:CE	2.69	0.56
1:A:294:ARG:O	1:A:295:GLN:CB	2.54	0.56
4:A:413:KKK:CL1	5:A:416:DGG:H322	2.42	0.56
1:B:49:GLU:O	1:B:50:GLN:CB	2.31	0.56
1:A:220:ARG:HH22	1:A:310:MET:CE	2.19	0.55
1:B:351:VAL:HG22	1:B:358:ILE:HD13	1.89	0.55
1:A:77:VAL:HG11	5:A:416:DGG:H231	1.88	0.55
1:A:291:ALA:HA	1:A:293:PRO:N	2.20	0.55
4:A:413:KKK:CL1	5:A:416:DGG:H352	2.44	0.55
1:B:259:PHE:CG	1:B:394:GLU:HB2	2.42	0.55
1:A:220:ARG:NH2	1:A:310:MET:HE1	2.23	0.54
1:B:223:VAL:O	1:B:241:HIS:HE1	1.90	0.54
1:B:46:ALA:O	1:B:49:GLU:HG2	2.08	0.53
1:A:52:GLN:HE22	1:B:19[A]:GLU:HG3	1.74	0.53
1:A:267:THR:OG1	1:A:362:ASP:O	2.26	0.53
1:B:67:ASN:ND2	7:B:484:HOH:O	2.41	0.53
1:B:126:TYR:CE1	2:B:404:HEM:HAB	2.44	0.53
1:B:47:HIS:CE1	4:B:413:KKK:C21	2.91	0.52
1:B:294:ARG:O	1:B:295:GLN:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HD2	1:A:315:ARG:HD3	1.92	0.51
1:B:291:ALA:HA	1:B:293:PRO:N	2.25	0.51
1:B:395:VAL:HG12	1:B:397:GLY:H	1.75	0.51
1:B:303:ARG:HG3	1:B:332:GLN:HB2	1.93	0.51
1:A:308:HIS:CE1	1:A:311:ARG:HG2	2.46	0.51
1:B:47:HIS:C	1:B:49:GLU:H	2.18	0.50
1:A:50:GLN:HG3	1:B:15:PRO:HG2	1.94	0.50
1:A:122:TRP:CZ3	5:A:416:DGG:H332	2.46	0.49
1:A:398:PRO:HB3	7:A:485:HOH:O	2.11	0.49
1:B:385:GLY:HA2	7:B:488:HOH:O	2.12	0.49
1:B:232:PRO:HG2	3:B:405:FAD:C5A	2.43	0.49
1:B:398:PRO:HG3	4:B:413:KKK:H21	1.93	0.49
1:A:351:VAL:HB	7:A:459:HOH:O	2.12	0.49
1:A:53:GLN:HG2	4:A:413:KKK:C20	2.43	0.49
1:B:311:ARG:HD2	1:B:315:ARG:HD3	1.95	0.49
1:B:351:VAL:HG13	1:B:358:ILE:HD11	1.95	0.49
1:B:398:PRO:CG	4:B:413:KKK:H21	2.42	0.49
1:B:115:THR:OG1	1:B:118:ILE:HD12	2.13	0.48
1:A:341:ARG:HH21	1:A:341:ARG:CG	2.03	0.48
2:A:404:HEM:HMB2	2:A:404:HEM:HBB2	1.96	0.48
1:B:398:PRO:CD	4:B:413:KKK:H21	2.43	0.48
4:A:413:KKK:C6	4:A:413:KKK:H13	2.44	0.48
1:A:378:HIS:CD2	1:A:382:LYS:HD2	2.48	0.47
2:A:404:HEM:HBC2	2:A:404:HEM:HHH	1.96	0.47
1:B:145:ALA:HB2	1:B:152:LYS:HG3	1.96	0.47
1:A:223:VAL:O	1:A:241:HIS:HE1	1.97	0.47
1:A:395:VAL:HG12	1:A:397:GLY:H	1.79	0.47
4:A:413:KKK:C6	4:A:413:KKK:C13	2.91	0.47
1:B:193:VAL:O	1:B:205:ILE:HA	2.14	0.47
1:A:273:SER:HB3	1:A:281:MET:HG3	1.97	0.47
1:B:267:THR:OG1	1:B:362:ASP:O	2.32	0.47
1:A:401:PHE:HD2	7:A:440:HOH:O	1.97	0.47
2:A:404:HEM:HBB2	2:A:404:HEM:CMB	2.45	0.47
1:A:115:THR:OG1	1:A:118:ILE:HD12	2.14	0.47
1:A:231:GLN:HE21	1:A:231:GLN:H	1.60	0.47
1:A:77:VAL:HG21	5:A:416:DGG:C25	2.41	0.46
1:A:400:LEU:HD22	1:A:403:GLU:OE2	2.14	0.46
4:A:413:KKK:C3	4:A:413:KKK:C8	2.93	0.46
1:A:395:VAL:N	7:A:408:HOH:O	2.48	0.46
2:A:404:HEM:HHH	2:A:404:HEM:CBC	2.45	0.46
1:B:154:TRP:HB3	1:B:251:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:NZ	7:A:462:HOH:O	2.49	0.46
2:B:404:HEM:HBD2	4:B:413:KKK:H20	1.98	0.46
1:A:231:GLN:H	1:A:231:GLN:NE2	2.14	0.46
1:A:220:ARG:HH22	1:A:310:MET:HE1	1.79	0.45
1:A:38:GLU:HB2	7:A:486:HOH:O	2.17	0.45
1:A:48:GLN:HE21	1:A:48:GLN:C	2.25	0.45
1:A:375:ARG:HG2	7:B:406:HOH:O	2.17	0.45
1:A:14:ALA:N	1:A:15:PRO:CD	2.80	0.44
1:B:49:GLU:OE2	7:B:451:HOH:O	2.21	0.44
1:A:292:PRO:HA	1:A:293:PRO:HD2	1.75	0.44
1:A:398:PRO:CB	7:A:485:HOH:O	2.66	0.44
4:B:413:KKK:H24A	4:B:413:KKK:H17	1.74	0.44
1:A:154:TRP:HB3	1:A:251:LYS:HB3	2.00	0.43
1:A:308:HIS:ND1	1:A:311:ARG:HG2	2.33	0.43
1:B:378:HIS:CD2	1:B:382:LYS:HD2	2.53	0.43
1:A:230:PRO:HG3	1:B:59:ARG:CG	2.33	0.43
1:A:81:ILE:HD13	2:A:404:HEM:HMA1	2.00	0.43
1:B:163:ARG:NH1	1:B:313:ARG:HH22	2.17	0.42
1:A:387:HIS:HB3	7:A:439:HOH:O	2.19	0.42
1:B:17:LEU:HD22	1:B:122:TRP:CE2	2.55	0.42
1:B:56:ALA:HB3	4:B:413:KKK:H16	1.99	0.42
1:B:187:PRO:HG3	1:B:287:VAL:HG21	2.02	0.42
1:A:371:ILE:HG21	1:A:401:PHE:HD1	1.85	0.41
1:A:399:ASP:N	7:A:468:HOH:O	2.52	0.41
1:B:398:PRO:HD3	4:B:413:KKK:C22	2.50	0.41
1:A:293:PRO:HB2	1:A:294:ARG:HA	2.02	0.41
1:B:271:LEU:HD12	1:B:366:TYR:HB2	2.03	0.41
1:B:292:PRO:HA	1:B:293:PRO:HD2	1.77	0.41
1:A:395:VAL:HG23	7:A:408:HOH:O	2.20	0.41
1:B:296:VAL:O	1:B:324:LEU:HA	2.21	0.40
2:B:404:HEM:C4D	4:B:413:KKK:H1	2.56	0.40
1:B:47:HIS:C	1:B:49:GLU:N	2.79	0.40
1:B:398:PRO:HD3	4:B:413:KKK:N4	2.36	0.40
1:A:215:ASN:OD1	1:A:215:ASN:C	2.64	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	7
1	B	403/403 (100%)	382 (95%)	12 (3%)	9 (2%)	5	4
All	All	804/806 (100%)	761 (95%)	27 (3%)	16 (2%)	6	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	292	PRO
1	A	293	PRO
1	A	295	GLN
1	B	48	GLN
1	B	50	GLN
1	B	292	PRO
1	B	293	PRO
1	B	295	GLN
1	A	229	GLY
1	B	51	GLY
1	B	52	GLN
1	B	229	GLY
1	A	398	PRO
1	B	398	PRO
1	A	230	PRO

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	334/334 (100%)	310 (93%)	24 (7%)	13	18
1	B	336/334 (101%)	315 (94%)	21 (6%)	16	23
All	All	670/668 (100%)	625 (93%)	45 (7%)	15	21

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	47	HIS
1	A	48	GLN
1	A	50	GLN
1	A	54	GLN
1	A	66	GLU
1	A	79	LYS
1	A	84	LYS
1	A	231	GLN
1	A	258	SER
1	A	266	LYS
1	A	271	LEU
1	A	285	LEU
1	A	290	GLN
1	A	307	VAL
1	A	315	ARG
1	A	323	ASN
1	A	338	VAL
1	A	341	ARG
1	A	351	VAL
1	A	362	ASP
1	A	381	LEU
1	A	388	GLU
1	A	400	LEU
1	B	25	ILE
1	B	48	GLN
1	B	50	GLN
1	B	54	GLN
1	B	66	GLU
1	B	79	LYS
1	B	84	LYS
1	B	120	SER
1	B	231	GLN
1	B	266	LYS
1	B	271	LEU

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	315	ARG
1	B	323	ASN
1	B	338	VAL
1	B	341	ARG
1	B	351	VAL
1	B	362	ASP
1	B	381	LEU
1	B	388	GLU
1	B	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	GLN
1	A	50	GLN
1	A	54	GLN
1	A	128	ASN
1	A	184	ASN
1	A	231	GLN
1	A	241	HIS
1	A	243	HIS
1	A	339	GLN
1	A	377	GLN
1	A	378	HIS
1	B	4	GLN
1	B	50	GLN
1	B	53	GLN
1	B	55	GLN
1	B	67	ASN
1	B	80	ASN
1	B	231	GLN
1	B	241	HIS
1	B	243	HIS
1	B	339	GLN
1	B	378	HIS

5.3.3 RNA ⓘ

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	404	1,4	50,50,50	2.31	13 (26%)	67,82,82	1.83	12 (17%)
3	FAD	A	405	-	58,58,58	1.38	8 (13%)	85,89,89	1.63	18 (21%)
3	FAD	B	405	-	58,58,58	1.21	7 (12%)	85,89,89	1.60	18 (21%)
4	KKK	A	413	2	40,40,40	1.14	4 (10%)	57,57,57	2.06	14 (24%)
4	KKK	B	413	2	40,40,40	1.45	5 (12%)	57,57,57	2.64	16 (28%)
6	PO4	A	406	-	4,4,4	0.60	0	6,6,6	0.66	0
5	DGG	A	416	-	19,19,50	5.12	2 (10%)	20,22,59	5.61	6 (30%)
2	HEM	A	404	1,4	50,50,50	1.90	9 (18%)	67,82,82	1.43	10 (14%)

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	HEM	B	404	1,4	-	8/14/54/54	-
3	FAD	A	405	-	-	2/34/50/50	0/6/6/6
3	FAD	B	405	-	-	3/34/50/50	0/6/6/6
4	KKK	A	413	2	2/2/5/5	7/24/45/45	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KKK	B	413	2	2/2/5/5	9/24/45/45	0/5/5/5
5	DGG	A	416	-	-	7/16/21/59	0/1/1/1
2	HEM	A	404	1,4	-	5/14/54/54	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	416	DGG	C30-C29	21.78	2.16	1.51
2	B	404	HEM	FE-NB	8.11	2.19	1.94
2	A	404	HEM	C3D-C2D	7.35	1.52	1.36
2	B	404	HEM	C3D-C2D	7.08	1.52	1.36
2	B	404	HEM	FE-ND	6.90	2.16	1.94
3	A	405	FAD	C4X-N5	4.79	1.41	1.30
5	A	416	DGG	O19-C21	4.58	1.46	1.30
4	B	413	KKK	C4-C5	4.55	1.58	1.52
2	A	404	HEM	FE-NA	4.29	2.09	1.95
4	B	413	KKK	C9-CL2	3.94	1.82	1.73
2	A	404	HEM	FE-NC	3.94	2.08	1.95
3	B	405	FAD	C4X-N5	3.87	1.39	1.30
2	B	404	HEM	C1B-NB	-3.46	1.34	1.40
2	A	404	HEM	CMB-C2B	3.43	1.57	1.50
2	B	404	HEM	CAC-C3C	3.40	1.56	1.47
3	A	405	FAD	C10-N1	3.39	1.40	1.33
2	A	404	HEM	C4C-NC	-3.12	1.33	1.39
4	B	413	KKK	C5-C8	-2.98	1.50	1.53
3	A	405	FAD	C1'-C2'	2.96	1.56	1.52
4	A	413	KKK	C5-C8	-2.96	1.50	1.53
4	A	413	KKK	C4-C5	2.94	1.56	1.52
2	B	404	HEM	CMA-C3A	2.88	1.56	1.50
3	A	405	FAD	C2A-N3A	2.88	1.39	1.33
3	A	405	FAD	C2A-N1A	2.84	1.39	1.33
2	A	404	HEM	C2A-C3A	-2.82	1.31	1.38
3	B	405	FAD	C2A-N1A	2.79	1.38	1.33
4	B	413	KKK	C25-N4	2.72	1.43	1.35
2	B	404	HEM	CAB-C3B	2.64	1.54	1.47
3	B	405	FAD	C8A-N7A	2.52	1.36	1.31
2	B	404	HEM	CMC-C2C	2.50	1.55	1.50
2	A	404	HEM	CAB-C3B	2.49	1.54	1.47
2	B	404	HEM	C3C-C2C	-2.48	1.32	1.37
3	B	405	FAD	C2A-N3A	2.35	1.38	1.33
4	A	413	KKK	C25-N4	2.34	1.42	1.35
2	B	404	HEM	CMB-C2B	2.34	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	413	KKK	C11-CL1	2.32	1.79	1.74
2	A	404	HEM	CAC-C3C	2.28	1.53	1.47
3	A	405	FAD	C8A-N7A	2.19	1.35	1.31
2	A	404	HEM	CMC-C2C	2.19	1.55	1.50
3	A	405	FAD	PA-O3P	2.14	1.61	1.59
2	B	404	HEM	C2A-C3A	-2.14	1.33	1.38
3	B	405	FAD	C1'-C2'	2.11	1.55	1.52
2	B	404	HEM	CAA-C2A	2.11	1.56	1.51
4	A	413	KKK	C4-N1	2.09	1.50	1.46
3	B	405	FAD	C5A-N7A	-2.08	1.35	1.39
2	B	404	HEM	C4D-ND	-2.07	1.36	1.40
3	A	405	FAD	C4X-C10	-2.04	1.38	1.44
3	B	405	FAD	C1'-N10	2.02	1.52	1.47

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	416	DGG	C30-C39-C29	16.86	90.38	60.89
4	B	413	KKK	C13-C8-C5	-11.51	111.58	119.18
5	A	416	DGG	C39-C30-C29	-10.90	44.76	59.53
5	A	416	DGG	C39-C29-C30	-10.83	44.86	59.53
5	A	416	DGG	C39-C29-C28	-8.53	105.21	120.62
2	B	404	HEM	C4D-ND-C1D	6.84	113.31	105.21
3	A	405	FAD	N3A-C2A-N1A	-5.79	119.81	128.58
4	A	413	KKK	C5-C4-N1	-5.70	107.80	112.76
4	B	413	KKK	C4-C5-C8	5.68	117.57	109.59
3	B	405	FAD	N3A-C2A-N1A	-5.30	120.56	128.58
4	A	413	KKK	C23-N4-C25	-5.15	109.10	122.96
4	B	413	KKK	C10-C9-C8	-5.10	116.88	121.97
4	A	413	KKK	C13-C8-C5	-5.04	115.85	119.18
4	B	413	KKK	C13-C8-C9	5.04	121.87	116.51
4	B	413	KKK	O1-C5-C8	-4.80	97.33	111.00
3	B	405	FAD	C4X-C10-N10	4.66	123.15	116.48
3	A	405	FAD	C5A-C4A-N3A	-4.58	120.41	126.72
4	A	413	KKK	C24-N3-C18	-4.54	105.74	118.11
4	A	413	KKK	C22-N4-C25	-4.50	110.87	122.96
4	B	413	KKK	O1-C5-C4	4.46	114.90	109.00
4	B	413	KKK	C22-N4-C25	-4.43	111.05	122.96
2	B	404	HEM	CHC-C1C-NC	4.35	129.19	124.45
5	A	416	DGG	C39-C30-C31	-4.28	112.89	120.62
2	B	404	HEM	CBA-CAA-C2A	-4.27	100.72	112.53
4	B	413	KKK	C8-C9-CL2	4.24	126.82	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	413	KKK	C19-C18-N3	-4.23	115.51	121.39
4	B	413	KKK	C5-C8-C9	3.95	126.52	123.72
3	B	405	FAD	C5A-C4A-N3A	-3.88	121.37	126.72
2	B	404	HEM	CBD-CAD-C3D	-3.77	102.10	112.53
3	A	405	FAD	N9A-C8A-N7A	-3.61	108.81	113.94
3	A	405	FAD	C2A-N3A-C4A	3.51	120.39	111.83
2	B	404	HEM	CMB-C2B-C1B	-3.49	119.58	125.03
4	B	413	KKK	C21-N3-C18	-3.46	108.67	118.11
4	B	413	KKK	C23-N4-C25	-3.30	114.09	122.96
2	B	404	HEM	CHC-C4B-NB	-3.27	120.90	124.42
2	A	404	HEM	CHA-C4D-ND	3.26	128.40	124.37
3	A	405	FAD	C4-N3-C2	-3.19	119.97	125.64
4	A	413	KKK	O4-C25-N4	-3.17	117.24	120.98
4	A	413	KKK	O2-C5-C8	3.16	116.79	111.37
2	B	404	HEM	C1B-NB-C4B	3.16	108.94	105.21
3	A	405	FAD	N3A-C4A-N9A	3.10	132.44	127.17
3	A	405	FAD	C5A-N7A-C8A	3.07	108.27	103.45
2	A	404	HEM	CBA-CAA-C2A	-3.05	104.10	112.53
2	B	404	HEM	O1D-CGD-CBD	-3.05	113.43	123.09
4	A	413	KKK	C13-C8-C9	3.03	119.74	116.51
4	A	413	KKK	C14-O3-C15	3.01	124.47	117.85
3	A	405	FAD	C4X-C4-N3	2.99	120.86	113.25
4	B	413	KKK	C23-N4-C22	-2.92	106.73	112.68
2	B	404	HEM	CAD-CBD-CGD	-2.90	105.97	113.67
2	A	404	HEM	C4B-C3B-C2B	2.86	109.91	107.28
4	A	413	KKK	O3-C14-C6	-2.85	101.22	107.79
3	B	405	FAD	N9A-C8A-N7A	-2.81	109.95	113.94
3	B	405	FAD	C2A-N3A-C4A	2.79	118.64	111.83
2	A	404	HEM	C3B-C2B-C1B	-2.63	104.44	106.41
3	A	405	FAD	C4X-C10-N10	2.62	120.23	116.48
3	B	405	FAD	C5A-N7A-C8A	2.57	107.49	103.45
3	B	405	FAD	C10-C4X-N5	-2.56	119.59	124.81
4	B	413	KKK	O3-C14-C6	2.54	113.64	107.79
2	B	404	HEM	CHC-C4B-C3B	2.52	130.10	125.07
2	A	404	HEM	CHA-C4D-C3D	-2.52	120.59	125.23
2	B	404	HEM	C1D-C2D-C3D	-2.49	104.36	106.98
3	B	405	FAD	C4'-C3'-C2'	-2.46	109.47	113.57
3	A	405	FAD	C5'-C4'-C3'	-2.44	107.62	112.22
3	B	405	FAD	C4-N3-C2	-2.43	121.33	125.64
4	A	413	KKK	C21-N3-C18	-2.42	111.52	118.11
3	A	405	FAD	C5X-C9A-N10	2.36	120.10	117.97
2	A	404	HEM	CBD-CAD-C3D	-2.33	106.09	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	HEM	O2D-CGD-CBD	2.32	121.32	114.00
2	A	404	HEM	C1D-C2D-C3D	-2.28	104.58	106.98
3	B	405	FAD	O2-C2-N1	-2.28	118.01	121.80
4	B	413	KKK	C4-N1-C3	-2.28	122.80	127.02
2	A	404	HEM	C4D-ND-C1D	2.27	107.89	105.21
3	A	405	FAD	C1'-C2'-C3'	2.22	115.68	109.66
3	B	405	FAD	C4A-C5A-N7A	-2.21	108.05	110.58
3	B	405	FAD	O2-C2-N3	2.18	122.76	118.58
3	A	405	FAD	C10-C4X-N5	-2.15	120.41	124.81
3	B	405	FAD	C10-N1-C2	2.15	121.50	116.85
4	B	413	KKK	C24-N3-C18	-2.10	112.38	118.11
3	B	405	FAD	O2A-PA-O3P	2.10	112.94	107.27
4	B	413	KKK	C9-C10-C11	2.09	121.09	118.72
4	A	413	KKK	O2-C5-C4	2.09	114.14	109.37
4	A	413	KKK	O1-C5-C8	-2.08	105.06	111.00
3	A	405	FAD	O4-C4-C4X	-2.08	121.05	126.53
3	A	405	FAD	C9A-C5X-N5	-2.08	120.25	122.45
3	B	405	FAD	C5A-C4A-N9A	2.06	108.06	105.81
3	A	405	FAD	C6-C5X-C9A	2.06	121.88	119.05
2	A	404	HEM	O1D-CGD-CBD	-2.06	116.57	123.09
5	A	416	DGG	O19-C21-C22	2.05	120.47	114.00
2	A	404	HEM	C2B-C1B-NB	2.05	112.19	109.84
3	B	405	FAD	C4X-C4-N3	2.04	118.45	113.25
3	A	405	FAD	C4X-C10-N1	-2.03	119.61	124.59
3	B	405	FAD	C1'-C2'-C3'	2.02	115.14	109.66
3	A	405	FAD	C6A-C5A-C4A	2.02	119.93	117.18
3	B	405	FAD	C6A-C5A-C4A	2.00	119.91	117.18

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	413	KKK	C6
4	A	413	KKK	C5
4	B	413	KKK	C6
4	B	413	KKK	C5

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	HEM	C3D-CAD-CBD-CGD
4	A	413	KKK	N1-C4-C5-O2
4	A	413	KKK	N1-C4-C5-C8

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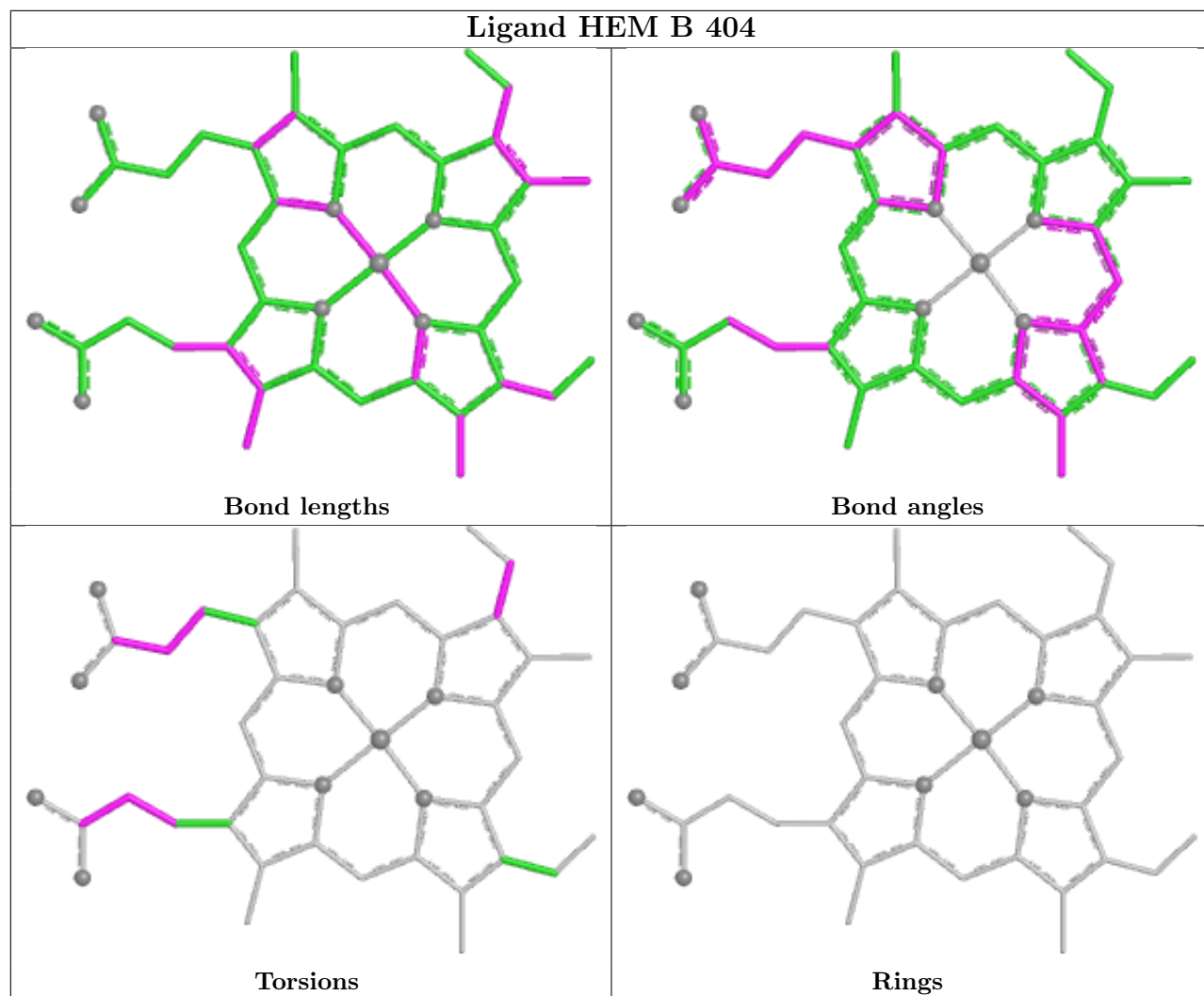
Mol	Chain	Res	Type	Atoms
4	A	413	KKK	O4-C25-N4-C23
4	A	413	KKK	C26-C25-N4-C23
4	B	413	KKK	N1-C4-C5-O2
4	B	413	KKK	N1-C4-C5-C8
4	B	413	KKK	O4-C25-N4-C22
4	B	413	KKK	C26-C25-N4-C22
4	B	413	KKK	O4-C25-N4-C23
4	B	413	KKK	C26-C25-N4-C23
2	B	404	HEM	C3D-CAD-CBD-CGD
4	B	413	KKK	C17-C18-N3-C21
4	B	413	KKK	C19-C18-N3-C21
5	A	416	DGG	C23-C24-C25-C26
4	B	413	KKK	C6-C14-O3-C15
2	B	404	HEM	C2C-C3C-CAC-CBC
5	A	416	DGG	C22-C23-C24-C25
2	B	404	HEM	C4C-C3C-CAC-CBC
5	A	416	DGG	C33-C34-C35-C36
5	A	416	DGG	C30-C31-C32-C33
5	A	416	DGG	C39-C30-C31-C32
3	B	405	FAD	O2'-C2'-C3'-O3'
4	A	413	KKK	C16-C15-O3-C14
5	A	416	DGG	O21-C21-C22-C23
5	A	416	DGG	O19-C21-C22-C23
4	A	413	KKK	C20-C15-O3-C14
2	A	404	HEM	CAD-CBD-CGD-O2D
2	A	404	HEM	CAA-CBA-CGA-O1A
2	B	404	HEM	CAA-CBA-CGA-O2A
2	B	404	HEM	CAD-CBD-CGD-O2D
2	B	404	HEM	C2A-CAA-CBA-CGA
2	A	404	HEM	CAA-CBA-CGA-O2A
2	B	404	HEM	CAA-CBA-CGA-O1A
4	A	413	KKK	O2-C5-C8-C9
2	B	404	HEM	CAD-CBD-CGD-O1D
3	B	405	FAD	O2'-C2'-C3'-C4'
2	A	404	HEM	CAD-CBD-CGD-O1D
3	A	405	FAD	PA-O3P-P-O2P
3	A	405	FAD	C2B-C1B-N9A-C8A
3	B	405	FAD	PA-O3P-P-O2P

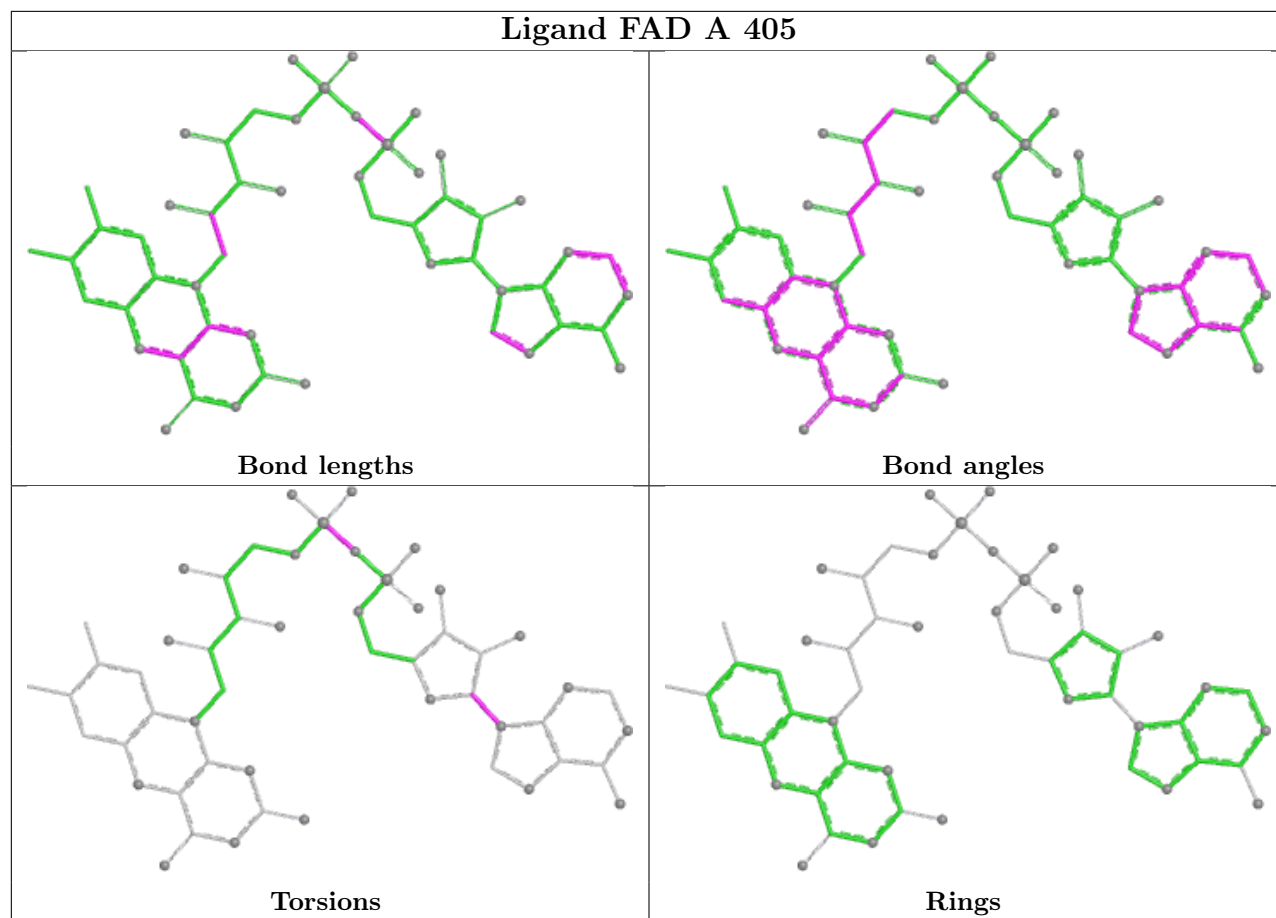
There are no ring outliers.

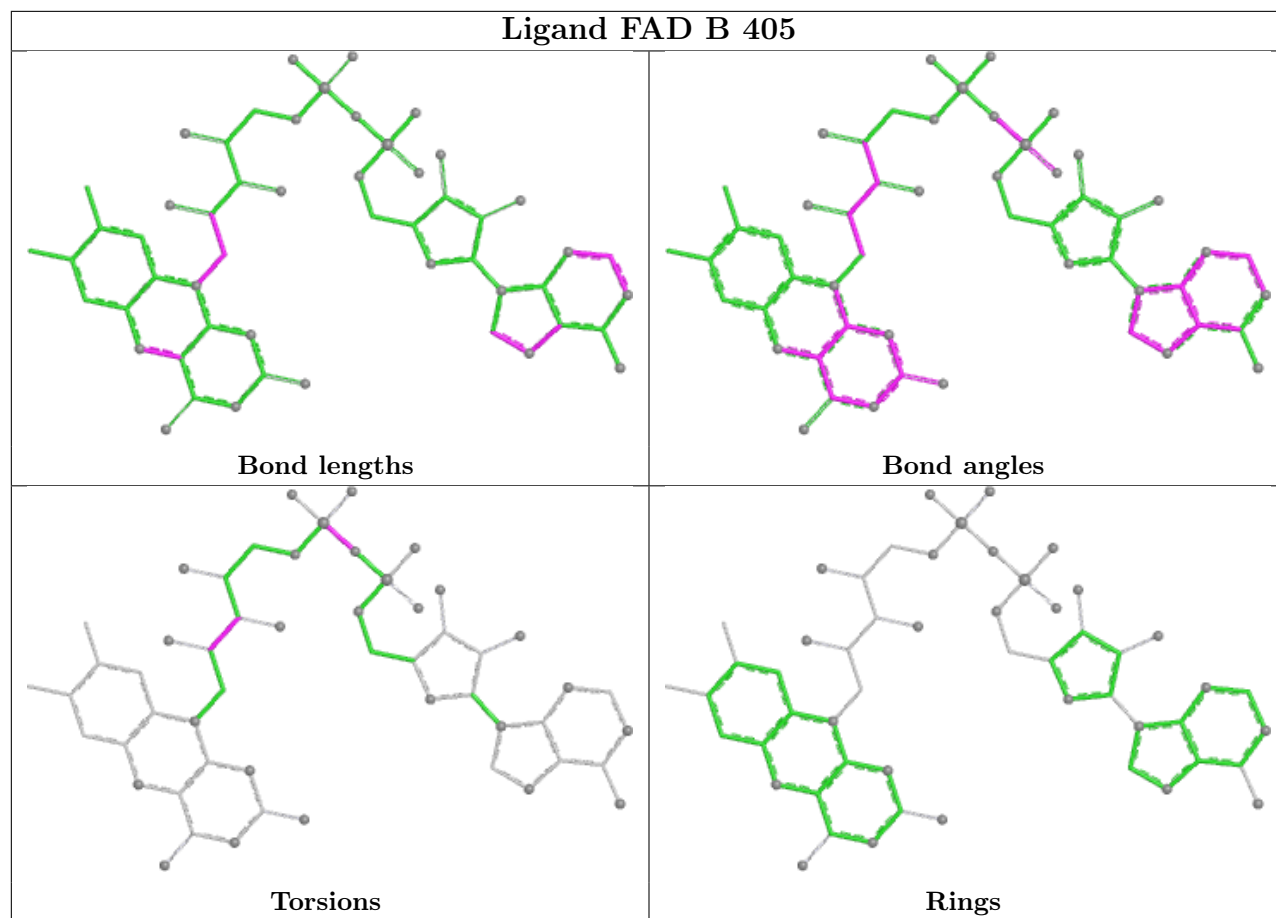
7 monomers are involved in 39 short contacts:

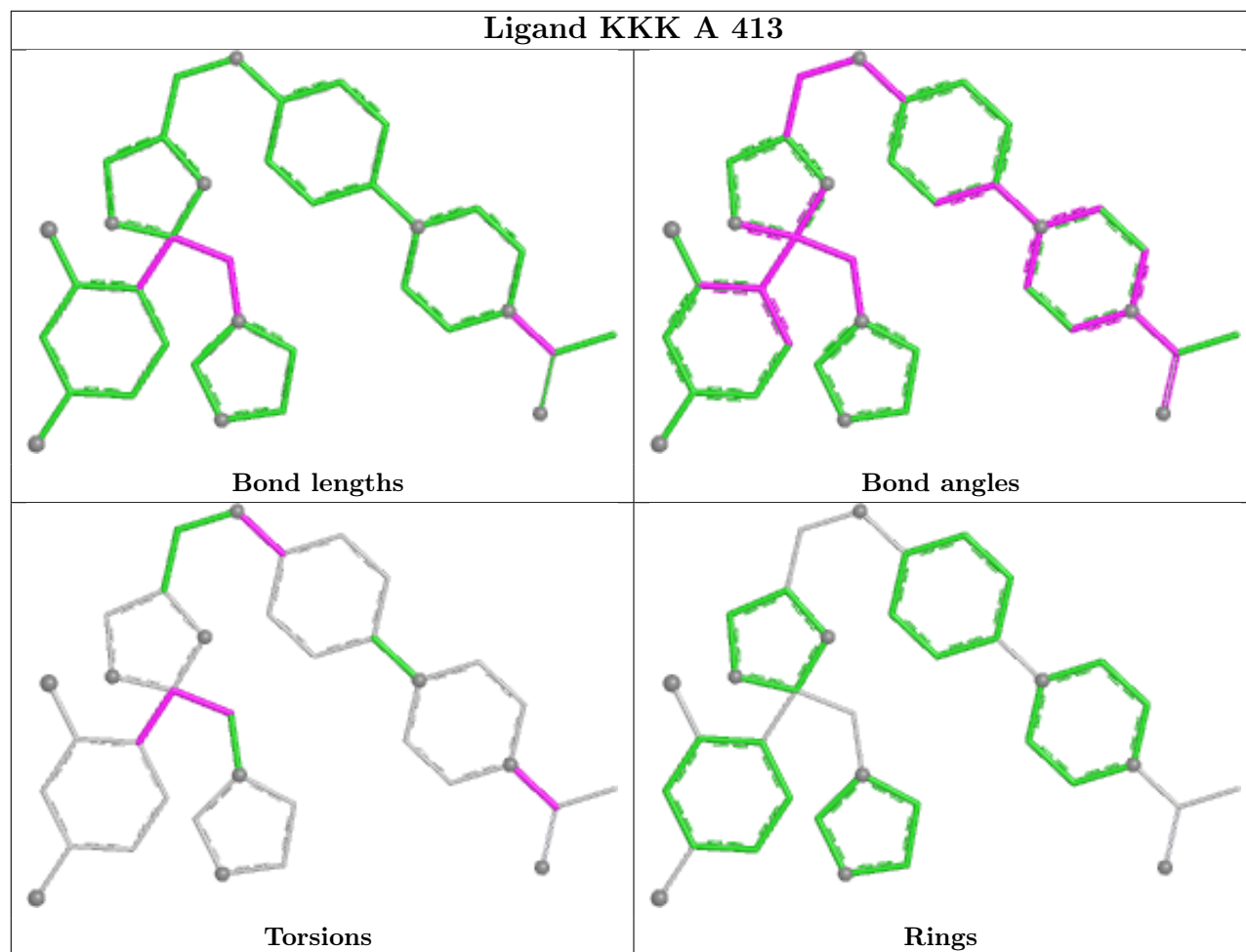
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	HEM	3	0
3	A	405	FAD	4	0
3	B	405	FAD	1	0
4	A	413	KKK	6	0
4	B	413	KKK	13	0
5	A	416	DGG	11	0
2	A	404	HEM	5	0

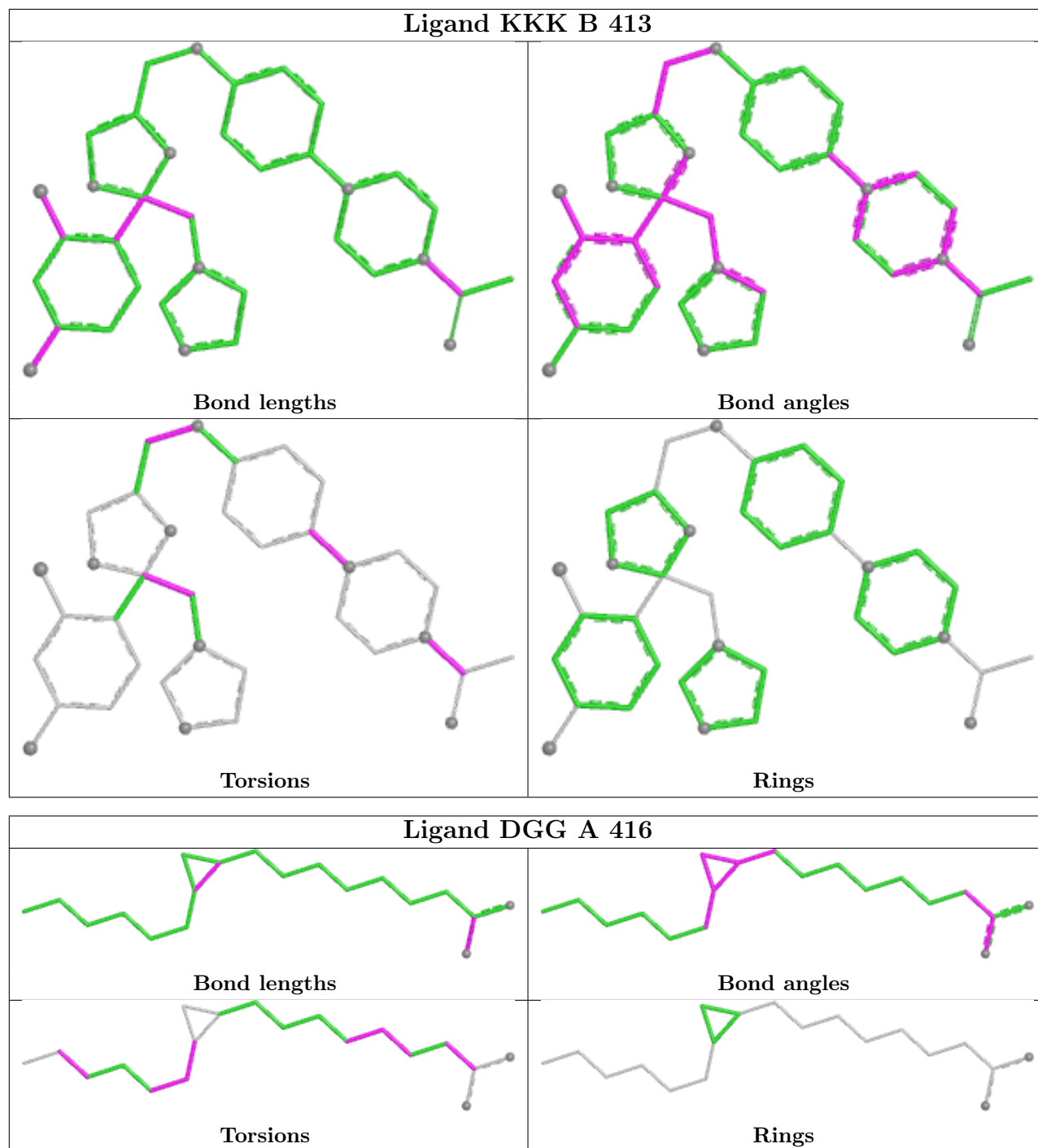
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

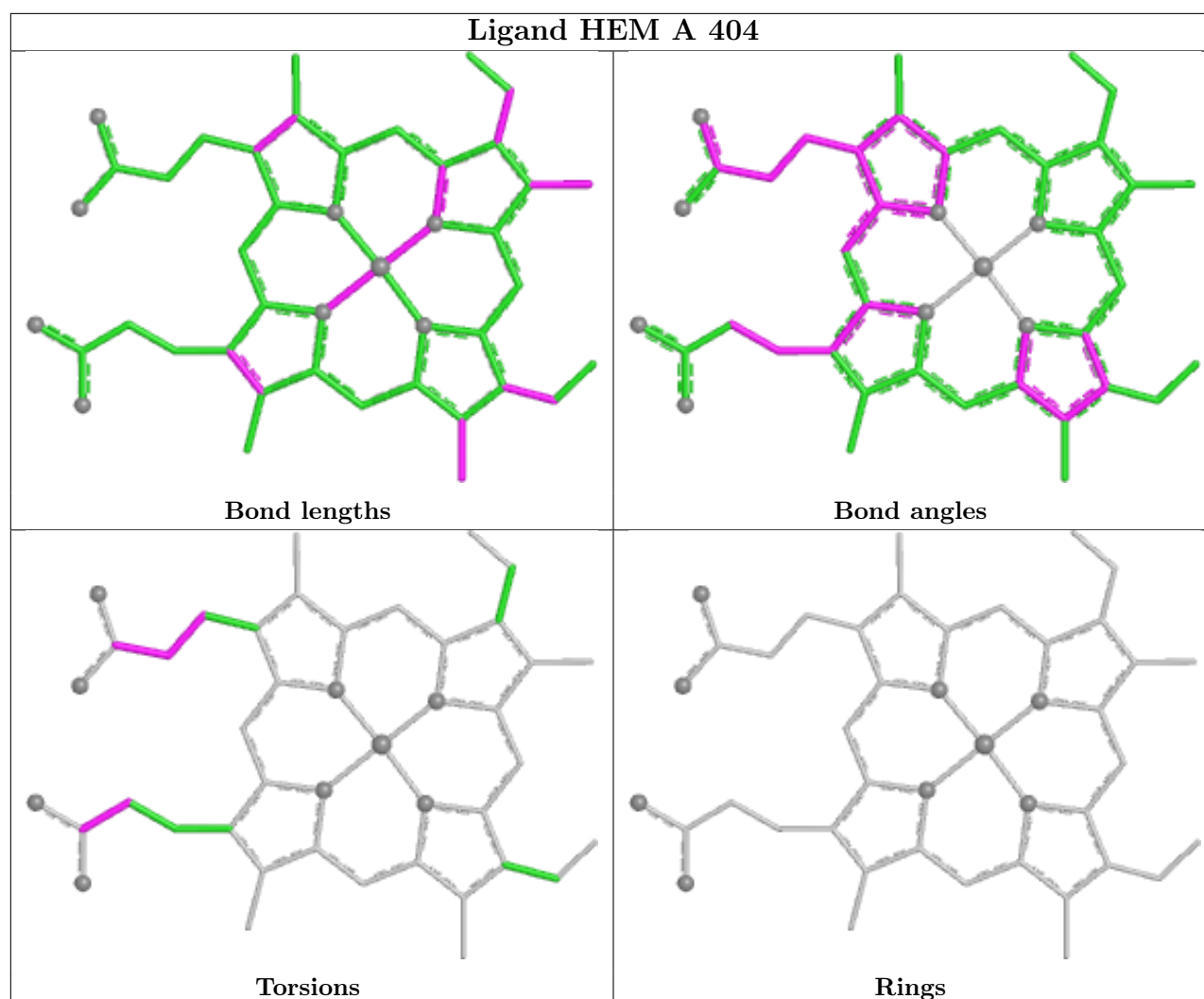












5.7 Other polymers [i](#)

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%)	0.82	46 (11%)	10 11	29, 54, 105, 198	0
1	B	403/403 (100%)	0.97	79 (19%)	3 3	26, 57, 126, 174	2 (0%)
All	All	806/806 (100%)	0.89	125 (15%)	5 6	26, 55, 117, 198	2 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	PHE	9.9
1	A	400	LEU	7.8
1	A	395	VAL	7.7
1	A	402	ALA	7.6
1	A	396	PHE	7.6
1	A	397	GLY	6.3
1	B	393	TYR	6.3
1	B	292	PRO	5.8
1	B	306	ALA	5.6
1	B	401	PHE	5.4
1	B	288	ALA	5.2
1	B	293	PRO	5.1
1	B	400	LEU	5.0
1	A	47	HIS	5.0
1	B	381	LEU	4.7
1	B	51	GLY	4.5
1	B	399	ASP	4.5
1	B	297	VAL	4.3
1	A	398	PRO	4.2
1	B	402	ALA	4.2
1	B	397	GLY	4.1
1	A	293	PRO	4.0
1	A	291	ALA	3.9
1	B	359	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	3.8
1	A	167	ASP	3.8
1	A	230	PRO	3.8
1	B	289	LEU	3.8
1	B	53	GLN	3.7
1	A	292	PRO	3.6
1	B	396	PHE	3.6
1	B	291	ALA	3.5
1	B	1	MET	3.5
1	B	403	GLU	3.5
1	A	361	PRO	3.5
1	B	356	LYS	3.5
1	A	163	ARG	3.4
1	B	363	ALA	3.4
1	B	269	ILE	3.4
1	B	343	TYR	3.4
1	B	307	VAL	3.4
1	A	266	LYS	3.3
1	B	340	GLY	3.2
1	B	268	PRO	3.2
1	B	395	VAL	3.2
1	B	398	PRO	3.2
1	A	362	ASP	3.1
1	B	391	ILE	3.1
1	B	314	LEU	3.1
1	B	321	TYR	3.1
1	B	263	VAL	3.1
1	B	347	GLY	3.1
1	A	399	ASP	3.0
1	B	229	GLY	3.0
1	B	148	PRO	2.9
1	B	334	LEU	2.9
1	B	320	THR	2.9
1	B	348	LEU	2.8
1	B	361	PRO	2.8
1	B	339	GLN	2.8
1	B	387	HIS	2.8
1	B	66	GLU	2.7
1	B	345	TYR	2.7
1	A	387	HIS	2.7
1	A	375	ARG	2.7
1	B	19[A]	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	346	PRO	2.6
1	B	56	ALA	2.6
1	B	230	PRO	2.6
1	A	229	GLY	2.6
1	A	296	VAL	2.6
1	B	296	VAL	2.6
1	A	363	ALA	2.5
1	B	267	THR	2.5
1	B	217[A]	ARG	2.5
1	B	390	ARG	2.5
1	A	231	GLN	2.5
1	B	287	VAL	2.5
1	B	338	VAL	2.5
1	B	386	ILE	2.5
1	A	228	GLY	2.5
1	B	375	ARG	2.4
1	B	298	PHE	2.4
1	B	384	LEU	2.4
1	B	117	ASP	2.4
1	B	265	ALA	2.4
1	A	166	SER	2.4
1	B	360	LEU	2.4
1	B	312	ASP	2.3
1	A	1	MET	2.3
1	B	147	GLN	2.3
1	B	277	GLY	2.3
1	B	376	MET	2.3
1	A	356	LYS	2.3
1	B	342	ASP	2.3
1	A	389	ALA	2.3
1	A	316	GLU	2.3
1	A	384	LEU	2.2
1	B	313	ARG	2.2
1	A	352	LYS	2.2
1	B	362	ASP	2.2
1	A	216	GLY	2.2
1	B	72	ASN	2.2
1	A	227	GLY	2.2
1	B	285	LEU	2.1
1	B	271	LEU	2.1
1	A	75	MET	2.1
1	A	393	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLN	2.1
1	A	265	ALA	2.1
1	B	389	ALA	2.1
1	A	50	GLN	2.1
1	A	112	ASN	2.1
1	B	332	GLN	2.1
1	B	216	GLY	2.1
1	B	49	GLU	2.0
1	A	48	GLN	2.0
1	A	147	GLN	2.0
1	B	364	ASP	2.0
1	A	244	VAL	2.0
1	A	46	ALA	2.0
1	A	360	LEU	2.0
1	A	148	PRO	2.0
1	B	358	ILE	2.0
1	B	266	LYS	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	KKK	A	413	36/36	0.86	0.18	36,62,124,132	0
4	KKK	B	413	36/36	0.86	0.23	32,108,265,275	0
5	DGG	A	416	19/50	0.92	0.12	44,55,96,100	0
6	PO4	A	406	5/5	0.93	0.09	46,65,72,75	0
3	FAD	A	405	53/53	0.97	0.07	22,36,82,90	0
3	FAD	B	405	53/53	0.97	0.06	26,33,60,64	0

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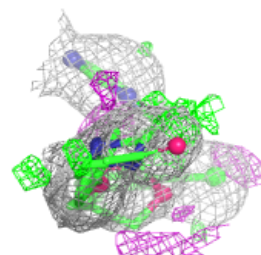
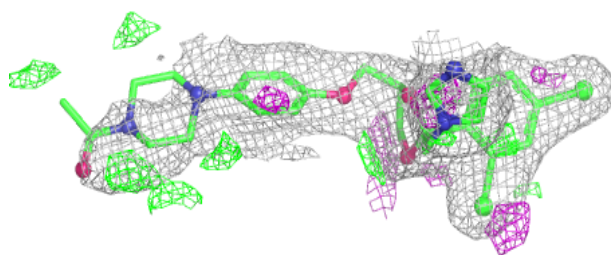
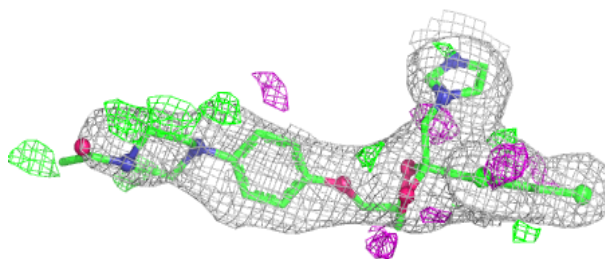
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	404	43/43	0.98	0.07	22,29,62,69	0
2	HEM	B	404	43/43	0.98	0.06	22,29,48,76	0

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.

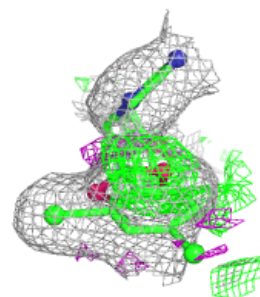
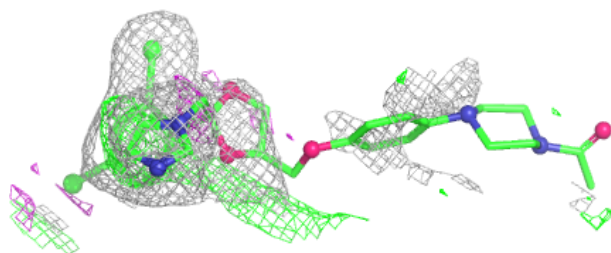
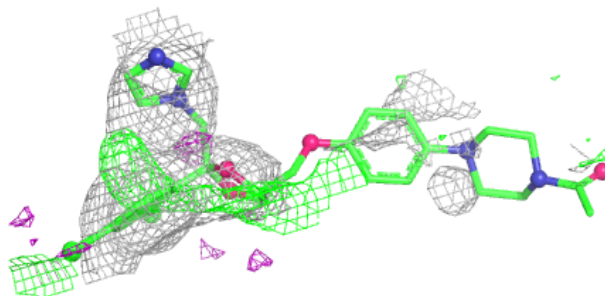
Electron density around KKK A 413:

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

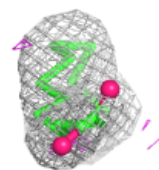
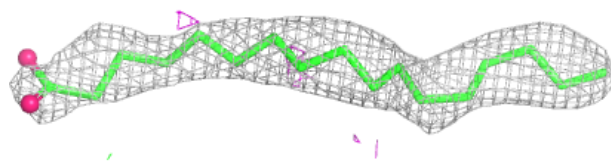
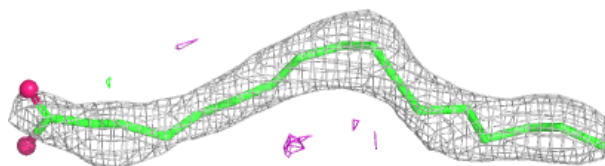


Electron density around KKK B 413:

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

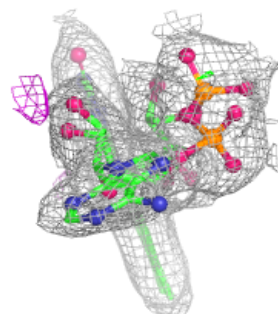
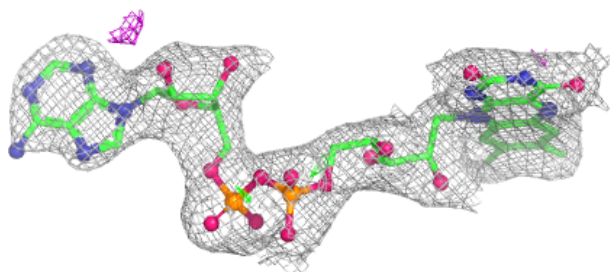
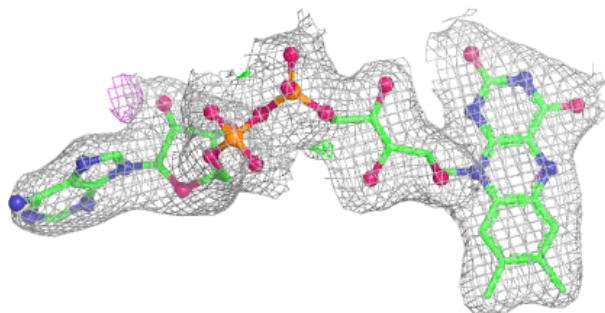
**Electron density around DGG A 416:**

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

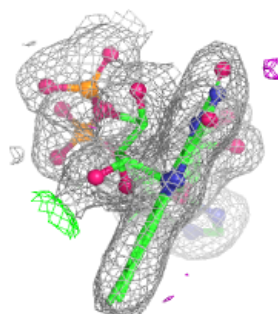
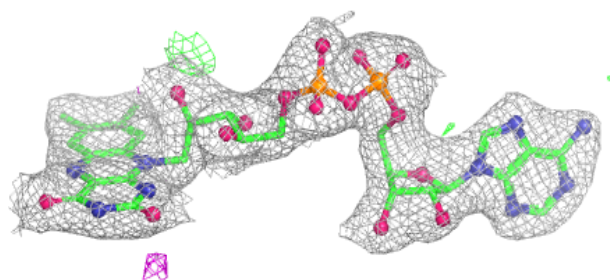
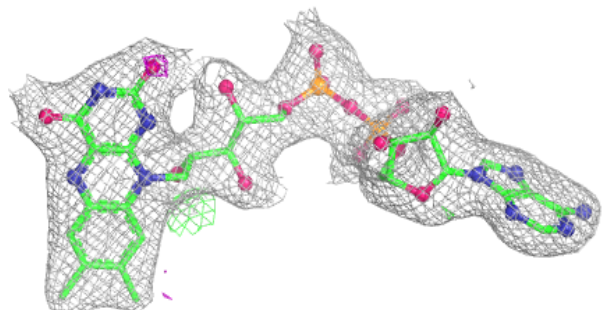


Electron density around FAD A 405:

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

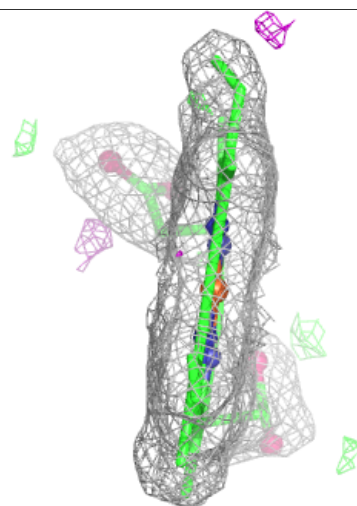
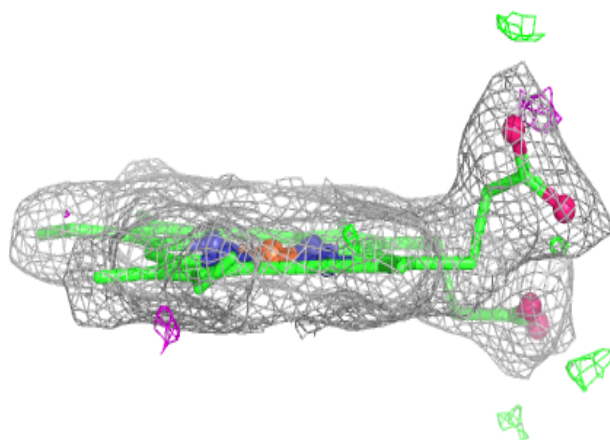
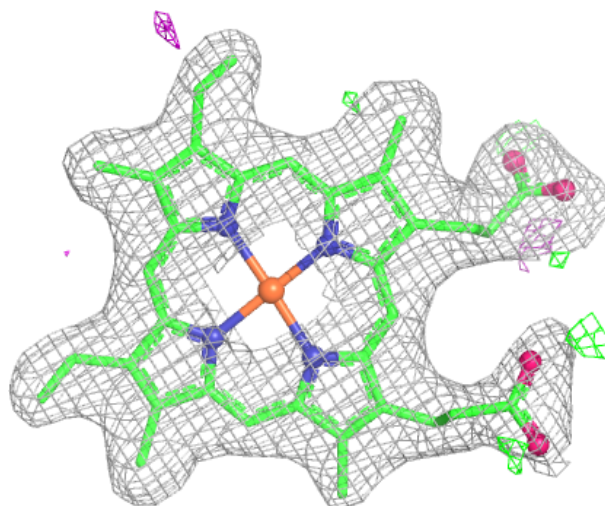
**Electron density around FAD B 405:**

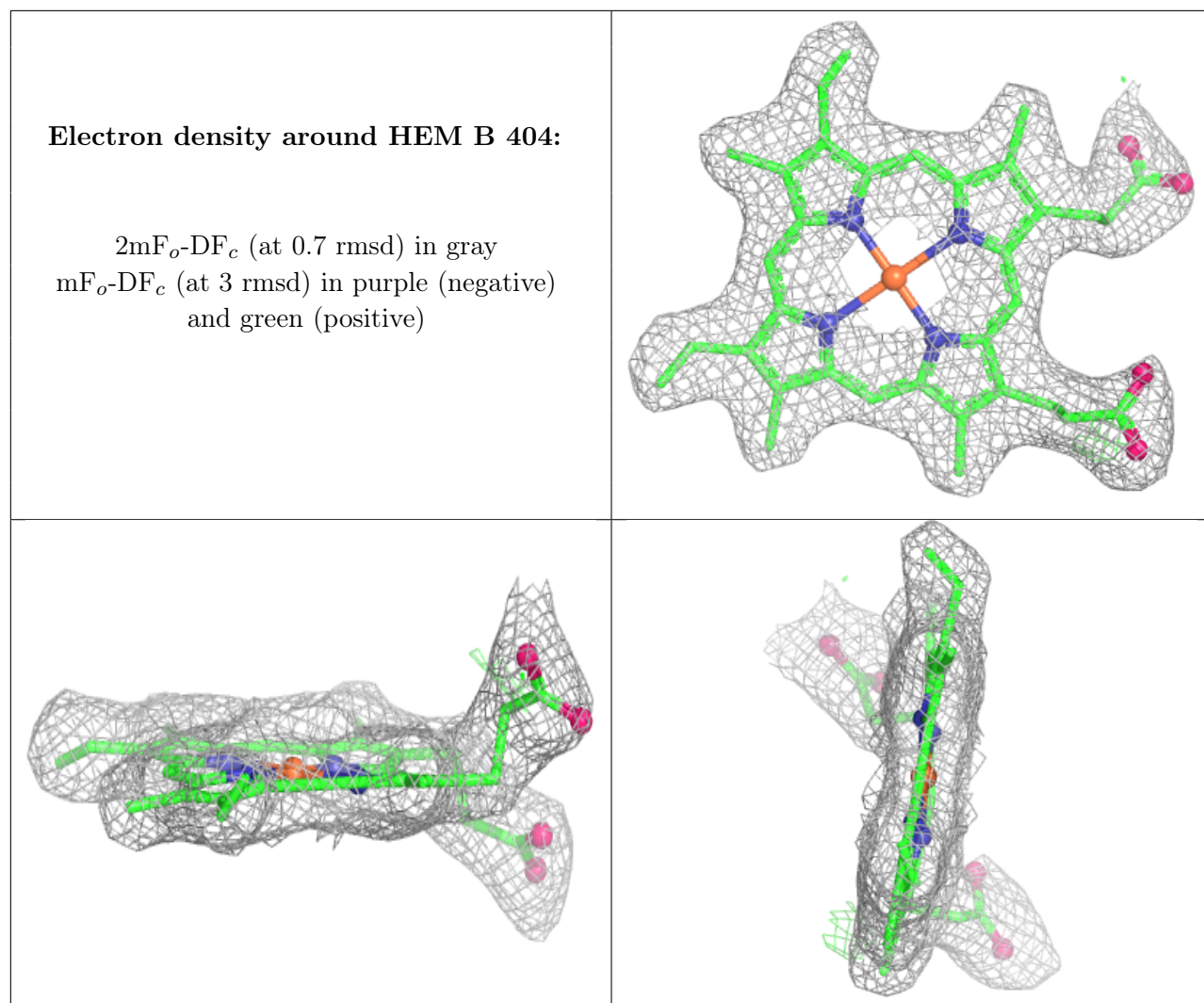
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.