



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:20 AM UTC

PDB ID : 1CQX / pdb_00001cqx
Title : Crystal structure of the flavohemoglobin from *Alcaligenes eutrophus* at 1.75 Å resolution
Authors : Ermler, U.; Siddiqui, R.A.; Cramm, R.; Friedrich, B.
Deposited on : 1999-08-12
Resolution : 1.75 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

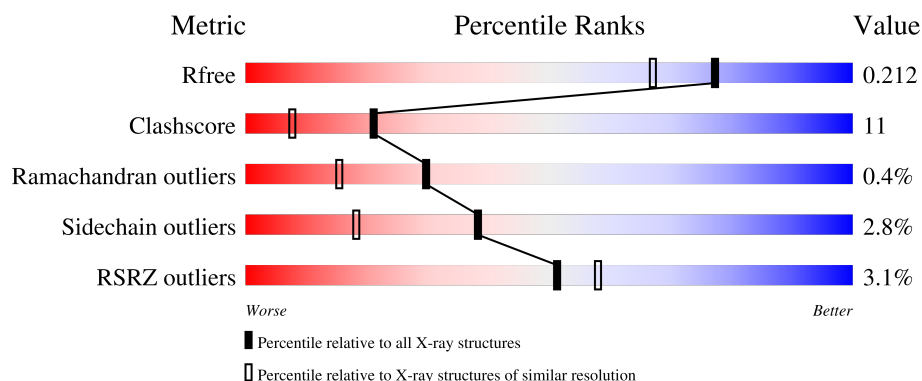
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	3% 77% 22%
1	B	403	3% 83% 15% .

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	DGG	B	406	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7180 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.

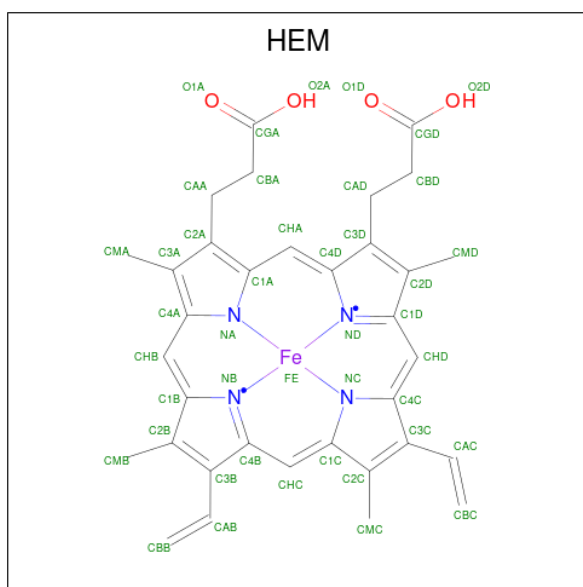
- Molecule 1 is a protein called FLAVOHEMOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3158	2012	543	589	14			
1	B	403	Total	C	N	O	S	0	0	0
			3158	2012	543	589	14			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

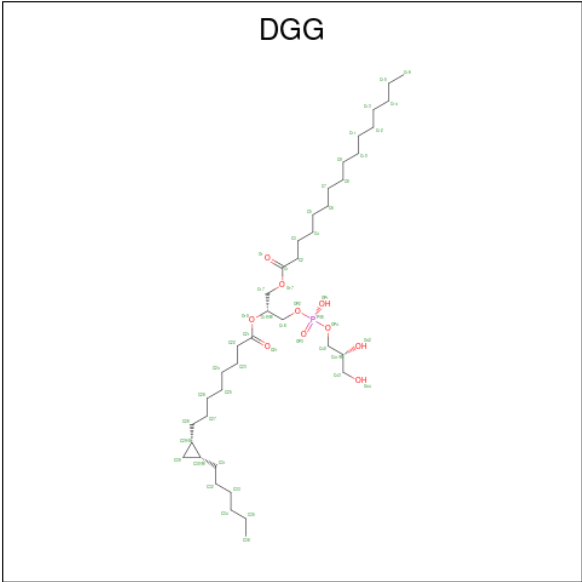
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			45	36	8	1		
5	B	1	Total	C	O	P	0	0
			45	36	8	1		

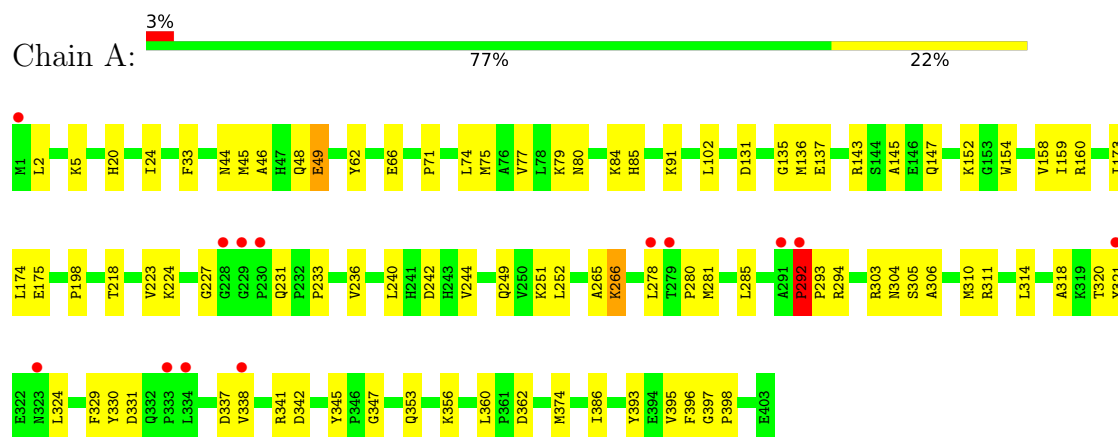
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	267	Total	O	0	0
			267	267		
6	B	314	Total	O	0	0
			314	314		

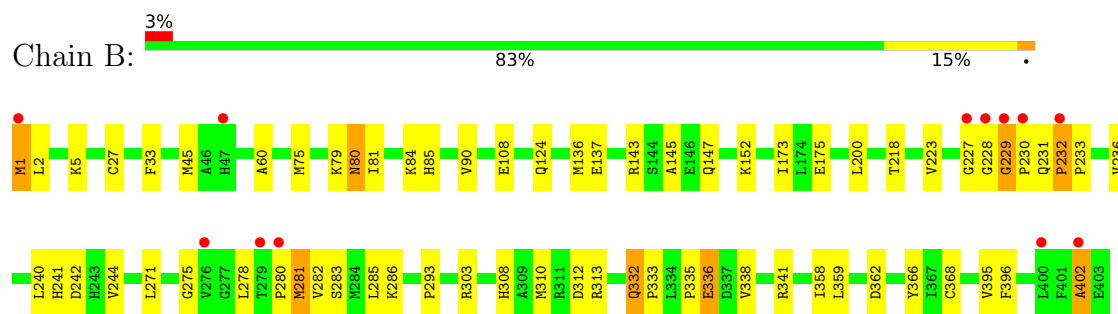
3 Residue-property plots

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: FLAVOHEMOPROTEIN



• Molecule 1: FLAVOHEMOPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.20Å 85.80Å 103.90Å 90.00° 81.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.75 10.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	89.7 (10.00-1.75) 84.4 (10.00-1.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.76Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.215 (Not available) , 0.212	Depositor DCC
R_{free} test set	4066 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.7	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	0.96	EDS
Total number of atoms	7180	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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, FAD, NA

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	0.41	0/3235	0.97	11/4395 (0.3%)
1	B	0.42	0/3235	0.93	7/4395 (0.2%)
All	All	0.41	0/6470	0.95	18/8790 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	PRO	CA-C-N	-9.38	107.59	120.25
1	A	292	PRO	C-N-CA	-9.38	107.59	120.25
1	A	397	GLY	CA-C-N	9.15	129.93	120.04
1	A	397	GLY	C-N-CA	9.15	129.93	120.04
1	A	236	VAL	N-CA-C	8.13	118.93	110.72
1	B	236	VAL	N-CA-C	7.35	118.14	110.72
1	A	242	ASP	N-CA-C	5.90	120.55	113.23
1	B	395	VAL	N-CA-C	-5.87	101.96	109.30
1	A	395	VAL	N-CA-C	-5.86	101.98	109.30
1	B	402	ALA	N-CA-C	5.85	117.35	110.97
1	B	229	GLY	N-CA-C	-5.71	100.69	112.34
1	A	223	VAL	N-CA-C	5.66	116.00	107.80
1	B	242	ASP	N-CA-C	5.62	120.25	113.17
1	A	2	LEU	N-CA-C	5.34	118.25	109.76
1	B	332	GLN	CA-C-N	5.31	125.30	119.89
1	B	332	GLN	C-N-CA	5.31	125.30	119.89
1	A	281	MET	N-CA-C	5.14	117.62	111.71
1	A	294	ARG	N-CA-C	-5.09	101.46	109.50

There are no chirality outliers.

There are no planarity outliers.

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	3158	0	3114	73	0
1	B	3158	0	3114	68	0
2	A	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
5	A	45	0	67	5	0
5	B	45	0	67	4	0
6	A	267	0	0	7	0
6	B	314	0	0	4	0
All	All	7180	0	6484	144	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 (144) 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:175:GLU:HG2	1:B:218:THR:HG22	1.27	1.13
1:A:175:GLU:HG2	1:A:218:THR:HG22	1.48	0.95
1:A:292:PRO:HB2	1:A:293:PRO:CD	1.99	0.93
1:B:227:GLY:HA3	1:B:233:PRO:HA	1.53	0.91
1:A:292:PRO:HB2	1:A:293:PRO:HD2	1.54	0.88
1:B:45:MET:HE2	1:B:45:MET:HA	1.55	0.86
1:A:131:ASP:O	1:B:1:MET:HG3	1.80	0.81
1:A:44:ASN:ND2	1:A:46:ALA:H	1.80	0.80
1:A:266:LYS:N	1:A:266:LYS:HD3	1.98	0.79
1:A:45:MET:HA	1:A:45:MET:HE2	1.64	0.79
1:A:174:LEU:HD13	1:A:252:LEU:HD11	1.69	0.75
1:A:310:MET:HE3	1:A:310:MET:HA	1.69	0.74
1:B:79:LYS:HA	1:B:136:MET:HE1	1.70	0.72
1:B:145:ALA:CB	1:B:152:LYS:HE3	2.20	0.71
1:A:80:ASN:HB2	6:A:594:HOH:O	1.91	0.69
1:B:145:ALA:HB2	1:B:152:LYS:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ALA:HB2	1:B:152:LYS:HG3	1.79	0.65
1:A:356:LYS:HD3	1:A:356:LYS:H	1.61	0.65
1:B:240:LEU:HD23	1:B:244:VAL:HG21	1.77	0.64
5:A:406:DGG:H351	5:A:406:DGG:HC81	1.80	0.64
1:A:44:ASN:HD22	1:A:45:MET:N	1.97	0.63
1:B:175:GLU:CG	1:B:218:THR:HG22	2.16	0.63
1:A:338:VAL:O	1:A:341:ARG:HG2	1.99	0.63
1:A:71:PRO:O	1:A:75:MET:HG2	2.00	0.62
1:A:224:LYS:HD3	1:A:398:PRO:O	2.00	0.62
1:A:44:ASN:HD22	1:A:44:ASN:C	2.06	0.62
5:A:406:DGG:H131	5:A:406:DGG:HC91	1.81	0.62
1:B:81:ILE:HD11	5:B:406:DGG:HC42	1.82	0.61
1:A:265:ALA:C	1:A:266:LYS:HD3	2.26	0.60
1:A:321:TYR:HD2	1:A:324:LEU:HB2	1.66	0.60
1:B:1:MET:C	1:B:1:MET:HE2	2.25	0.60
1:A:175:GLU:CG	1:A:218:THR:HG22	2.27	0.60
1:A:338:VAL:HB	1:A:341:ARG:HE	1.66	0.59
1:B:1:MET:SD	6:B:1546:HOH:O	2.57	0.58
1:A:280:PRO:HD2	1:A:396:PHE:CE2	2.40	0.57
1:B:60:ALA:HB3	5:B:406:DGG:H361	1.85	0.57
1:A:337:ASP:HA	1:A:342:ASP:OD1	2.05	0.57
1:A:311:ARG:HD2	1:A:311:ARG:C	2.29	0.56
1:B:278:LEU:HD23	1:B:310:MET:HE3	1.86	0.56
6:A:698:HOH:O	1:B:1:MET:HB2	2.04	0.56
1:B:80:ASN:HB2	6:B:1688:HOH:O	2.06	0.56
1:A:280:PRO:HD2	1:A:396:PHE:CZ	2.41	0.56
1:A:49:GLU:O	1:A:49:GLU:HG3	2.04	0.55
1:A:198:PRO:HD2	6:A:660:HOH:O	2.06	0.55
1:A:310:MET:HE2	1:A:314:LEU:HG	1.89	0.55
1:A:329:PHE:HA	1:A:345:TYR:O	2.07	0.55
1:A:304:ASN:HA	1:A:330:TYR:CD2	2.41	0.55
1:A:227:GLY:HA3	1:A:233:PRO:HA	1.89	0.54
1:A:159:ILE:HD13	1:A:174:LEU:HD23	1.89	0.54
1:B:60:ALA:CB	5:B:406:DGG:H361	2.37	0.54
1:B:271:LEU:HD23	1:B:366:TYR:HB2	1.89	0.54
1:A:154:TRP:HB3	1:A:251:LYS:HB3	1.89	0.53
1:A:173:ILE:HD12	1:A:173:ILE:N	2.23	0.53
1:A:79:LYS:HA	1:A:136:MET:HE1	1.91	0.53
1:A:44:ASN:HD22	1:A:46:ALA:H	1.54	0.53
6:A:562:HOH:O	1:B:5:LYS:HG3	2.08	0.53
1:B:275:GLY:O	1:B:402:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	1:B:2:LEU:HA	1.90	0.53
1:A:338:VAL:HB	1:A:341:ARG:NE	2.24	0.52
1:B:33:PHE:CE1	1:B:45:MET:HE1	2.44	0.52
1:B:79:LYS:HA	1:B:136:MET:CE	2.38	0.52
1:B:358:ILE:C	1:B:358:ILE:HD12	2.35	0.52
1:A:62:TYR:O	1:A:66:GLU:HG3	2.10	0.52
1:B:1:MET:HE1	1:B:124:GLN:OE1	2.10	0.52
1:B:335:PRO:HD2	1:B:336:GLU:OE2	2.10	0.52
1:B:90:VAL:HG13	3:B:404:HEM:HAC	1.92	0.51
1:A:303:ARG:HA	1:A:331:ASP:OD2	2.10	0.51
1:A:331:ASP:HA	1:A:347:GLY:CA	2.41	0.51
1:A:386:ILE:HD11	6:A:753:HOH:O	2.11	0.51
1:A:102:LEU:HD22	5:A:406:DGG:H321	1.92	0.50
1:B:281:MET:HE2	1:B:368:CYS:SG	2.51	0.50
1:A:305:SER:O	1:A:306:ALA:C	2.53	0.50
4:A:405:FAD:H8A	6:A:518:HOH:O	2.11	0.50
1:A:231:GLN:NE2	1:A:231:GLN:HA	2.26	0.49
1:B:1:MET:HE2	1:B:2:LEU:HD12	1.93	0.49
1:B:75:MET:O	1:B:79:LYS:HG3	2.13	0.49
1:A:159:ILE:HD13	1:A:174:LEU:CD2	2.42	0.49
1:A:353:GLN:O	1:A:356:LYS:NZ	2.46	0.49
1:A:85:HIS:ND1	1:A:137:GLU:OE2	2.44	0.48
1:B:175:GLU:HG2	1:B:218:THR:CG2	2.19	0.48
1:A:79:LYS:CA	1:A:136:MET:HE1	2.43	0.48
1:A:145:ALA:HB2	1:A:152:LYS:HE3	1.95	0.48
1:B:79:LYS:CA	1:B:136:MET:HE1	2.41	0.48
1:A:131:ASP:O	1:B:1:MET:CG	2.58	0.48
5:A:406:DGG:H311	5:A:406:DGG:H281	1.59	0.48
1:B:336:GLU:H	1:B:336:GLU:CD	2.22	0.48
1:B:45:MET:HA	1:B:45:MET:CE	2.37	0.48
1:A:240:LEU:HD23	1:A:244:VAL:HG21	1.95	0.47
5:A:406:DGG:O21	5:A:406:DGG:C18	2.60	0.47
5:B:406:DGG:H311	5:B:406:DGG:H281	1.55	0.47
1:B:79:LYS:HG2	1:B:136:MET:CE	2.45	0.46
1:B:231:GLN:OE1	1:B:232:PRO:HD2	2.16	0.46
1:B:278:LEU:HD23	1:B:310:MET:CE	2.46	0.46
1:B:85:HIS:ND1	1:B:137:GLU:OE2	2.42	0.46
1:A:158:VAL:HG22	1:A:249:GLN:HG2	1.98	0.45
1:B:27:CYS:SG	1:B:108:GLU:OE1	2.74	0.45
1:B:143:ARG:O	1:B:147:GLN:HG2	2.17	0.45
1:B:173:ILE:N	1:B:173:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:2:LEU:HD12	2.47	0.45
1:A:318:ALA:HA	1:A:324:LEU:HD23	1.99	0.45
1:B:45:MET:HE2	1:B:45:MET:CA	2.38	0.45
1:B:143:ARG:HG2	1:B:143:ARG:NH2	2.31	0.44
1:A:160:ARG:NH1	6:A:735:HOH:O	2.44	0.44
1:A:74:LEU:O	1:A:77:VAL:HG22	2.17	0.44
1:A:331:ASP:HA	1:A:347:GLY:HA2	2.00	0.44
1:A:356:LYS:HD3	1:A:356:LYS:N	2.29	0.44
1:A:356:LYS:H	1:A:356:LYS:CD	2.30	0.43
4:B:405:FAD:H8A	6:B:1545:HOH:O	2.17	0.43
1:A:266:LYS:N	1:A:266:LYS:CD	2.71	0.43
1:A:45:MET:HE2	1:A:45:MET:CA	2.44	0.43
1:A:33:PHE:CE1	1:A:45:MET:HE1	2.54	0.43
1:A:311:ARG:HD2	1:A:311:ARG:O	2.17	0.43
1:B:332:GLN:N	1:B:333:PRO:HD3	2.33	0.43
1:A:143:ARG:CZ	1:A:147:GLN:OE1	2.67	0.43
1:A:231:GLN:HA	1:A:231:GLN:HE21	1.83	0.43
1:B:1:MET:CE	1:B:1:MET:O	2.67	0.43
1:B:280:PRO:HB2	1:B:396:PHE:CZ	2.54	0.43
1:A:374:MET:HB3	1:A:393:TYR:CD2	2.54	0.43
1:B:338:VAL:HG23	1:B:341:ARG:HH11	1.83	0.43
1:A:48:GLN:HG2	1:A:49:GLU:N	2.33	0.42
1:A:145:ALA:CB	1:A:152:LYS:HE3	2.49	0.42
1:A:135:GLY:HA2	1:B:1:MET:HE3	2.02	0.42
1:A:143:ARG:NH1	1:A:147:GLN:OE1	2.52	0.42
1:B:223:VAL:O	1:B:241:HIS:HE1	2.02	0.42
1:A:44:ASN:ND2	1:A:44:ASN:C	2.74	0.41
1:B:313:ARG:HD2	1:B:313:ARG:HA	1.90	0.41
1:B:283:SER:HA	1:B:286:LYS:CE	2.50	0.41
1:B:308:HIS:ND1	1:B:312:ASP:OD2	2.53	0.41
1:A:135:GLY:HA3	1:B:1:MET:HG2	2.01	0.41
1:A:160:ARG:HA	1:A:160:ARG:HD3	1.89	0.41
1:B:1:MET:HE2	1:B:2:LEU:N	2.36	0.41
1:B:79:LYS:HG2	1:B:136:MET:HE3	2.03	0.41
1:A:160:ARG:HE	1:A:175:GLU:HB2	1.85	0.41
1:B:1:MET:HE2	1:B:1:MET:O	2.21	0.41
1:B:358:ILE:HD12	1:B:359:LEU:N	2.36	0.41
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.97	0.41
1:B:143:ARG:HG2	1:B:143:ARG:HH21	1.86	0.40
1:B:228:GLY:O	1:B:229:GLY:C	2.65	0.40
1:B:232:PRO:HA	1:B:233:PRO:HD2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HH21	1:B:303:ARG:HG2	1.85	0.40
1:A:20:HIS:O	1:A:24:ILE:HG13	2.20	0.40
1:B:283:SER:HA	1:B:286:LYS:HE3	2.03	0.40
1:B:293:PRO:HD2	6:B:1669:HOH:O	2.22	0.40
1:B:1:MET:HE2	1:B:2:LEU:CA	2.51	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%)	385 (96%)	15 (4%)	1 (0%)	43	27
1	B	401/403 (100%)	388 (97%)	11 (3%)	2 (0%)	24	11
All	All	802/806 (100%)	773 (96%)	26 (3%)	3 (0%)	30	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	B	230	PRO
1	B	232	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%)	324 (97%)	10 (3%)	36	16
1	B	334/334 (100%)	325 (97%)	9 (3%)	39	19
All	All	668/668 (100%)	649 (97%)	19 (3%)	38	18

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	49	GLU
1	A	84	LYS
1	A	91	LYS
1	A	266	LYS
1	A	278	LEU
1	A	285	LEU
1	A	320	THR
1	A	360	LEU
1	A	362	ASP
1	B	1	MET
1	B	80	ASN
1	B	84	LYS
1	B	200	LEU
1	B	281	MET
1	B	282	VAL
1	B	285	LEU
1	B	336	GLU
1	B	362	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	44	ASN
1	A	47	HIS
1	A	80	ASN
1	A	128	ASN
1	A	184	ASN
1	A	207	GLN
1	A	231	GLN
1	A	241	HIS
1	A	249	GLN
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	323	ASN
1	A	332	GLN
1	A	353	GLN
1	A	377	GLN
1	B	20	HIS
1	B	48	GLN
1	B	52	GLN
1	B	53	GLN
1	B	184	ASN
1	B	241	HIS
1	B	245	ASN
1	B	249	GLN
1	B	339	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DGG	B	406	-	45,45,50	1.19	5 (11%)	49,53,59	1.75	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	A	405	-	58,58,58	1.41	10 (17%)	85,89,89	1.46	10 (11%)
3	HEM	B	404	1	50,50,50	1.46	6 (12%)	67,82,82	1.50	12 (17%)
3	HEM	A	404	1	50,50,50	1.52	7 (14%)	67,82,82	1.42	9 (13%)
4	FAD	B	405	-	58,58,58	1.54	15 (25%)	85,89,89	1.46	9 (10%)
5	DGG	A	406	-	45,45,50	1.23	4 (8%)	49,53,59	1.64	7 (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
5	DGG	B	406	-	1/1/6/7	16/46/51/59	0/1/1/1
4	FAD	A	405	-	-	2/34/50/50	0/6/6/6
3	HEM	B	404	1	-	4/14/54/54	-
4	FAD	B	405	-	-	1/34/50/50	0/6/6/6
5	DGG	A	406	-	-	22/46/51/59	0/1/1/1
3	HEM	A	404	1	-	4/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	DGG	O17-C17	-5.28	1.33	1.45
3	B	404	HEM	CBB-CAB	4.88	1.53	1.30
3	A	404	HEM	CBB-CAB	4.72	1.53	1.30
3	B	404	HEM	CBC-CAC	4.63	1.52	1.30
3	A	404	HEM	CBC-CAC	4.49	1.52	1.30
4	B	405	FAD	C5X-N5	-3.48	1.33	1.39
5	B	406	DGG	P-OP2	-3.41	1.49	1.60
4	A	405	FAD	O5'-C5'	3.34	1.57	1.44
3	A	404	HEM	CAC-C3C	-3.29	1.38	1.47
4	A	405	FAD	C5A-C4A	3.21	1.44	1.39
3	B	404	HEM	C1D-ND	3.03	1.44	1.38
3	A	404	HEM	FE-NC	3.01	2.05	1.95
4	B	405	FAD	C5A-C4A	2.94	1.44	1.39
5	B	406	DGG	C18-C19	-2.91	1.41	1.50
4	B	405	FAD	C9A-C5X	2.84	1.45	1.41
5	A	406	DGG	C18-C19	-2.77	1.42	1.50
5	A	406	DGG	P-OP2	-2.77	1.51	1.60
5	B	406	DGG	O17-C1	2.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	FAD	P-O3P	2.70	1.62	1.59
4	A	405	FAD	C9A-C5X	2.67	1.45	1.41
4	B	405	FAD	P-O2P	-2.62	1.43	1.55
4	B	405	FAD	PA-O5B	-2.58	1.49	1.59
5	B	406	DGG	P-OP1	-2.57	1.45	1.54
4	B	405	FAD	C4A-N3A	2.54	1.39	1.34
3	B	404	HEM	CAC-C3C	-2.50	1.40	1.47
5	A	406	DGG	O19-C19	-2.48	1.40	1.46
4	A	405	FAD	C9-C8	2.47	1.43	1.39
5	B	406	DGG	O19-C19	-2.46	1.40	1.46
4	B	405	FAD	C5A-N7A	2.43	1.43	1.39
3	B	404	HEM	C4D-C3D	2.41	1.49	1.45
4	B	405	FAD	C9-C9A	2.40	1.43	1.39
4	B	405	FAD	P-O1P	-2.39	1.42	1.50
4	A	405	FAD	P-O5'	-2.38	1.50	1.59
4	A	405	FAD	PA-O5B	-2.35	1.50	1.59
4	B	405	FAD	PA-O2A	-2.35	1.44	1.55
4	B	405	FAD	P-O5'	-2.26	1.50	1.59
3	B	404	HEM	CAB-C3B	-2.25	1.41	1.47
3	A	404	HEM	FE-NB	2.23	2.01	1.94
3	A	404	HEM	C1D-ND	2.22	1.43	1.38
3	A	404	HEM	C2A-C3A	-2.21	1.33	1.38
4	A	405	FAD	PA-O3P	2.19	1.61	1.59
4	A	405	FAD	C4A-N9A	2.12	1.42	1.37
4	A	405	FAD	P-O2P	-2.08	1.45	1.55
4	A	405	FAD	P-O1P	-2.08	1.43	1.50
4	B	405	FAD	O5'-C5'	2.04	1.52	1.44
4	B	405	FAD	C4X-N5	2.03	1.35	1.30
4	B	405	FAD	C3B-C4B	2.02	1.58	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	DGG	C39-C30-C31	-7.17	107.66	120.62
5	B	406	DGG	C39-C29-C28	-7.02	107.94	120.62
5	B	406	DGG	C39-C30-C31	-6.99	107.98	120.62
5	A	406	DGG	C39-C29-C28	-4.83	111.90	120.62
4	B	405	FAD	C4A-C5A-N7A	-4.54	105.39	110.58
4	A	405	FAD	C4A-C5A-N7A	-4.38	105.57	110.58
3	A	404	HEM	C3B-C4B-NB	4.29	112.55	109.47
3	B	404	HEM	C2D-C1D-ND	4.18	114.73	109.90
3	A	404	HEM	C4B-C3B-C2B	-4.06	103.55	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	FAD	C4A-N9A-C1B	-3.94	117.42	126.63
4	A	405	FAD	C5A-C4A-N3A	-3.92	121.32	126.72
4	B	405	FAD	C5A-N7A-C8A	3.81	109.44	103.45
4	B	405	FAD	C6A-C5A-N7A	3.74	139.29	132.09
3	B	404	HEM	C4C-NC-C1C	-3.56	100.02	105.82
3	B	404	HEM	C3B-C4B-NB	3.48	111.97	109.47
3	A	404	HEM	C3B-C2B-C1B	3.40	108.96	106.41
4	A	405	FAD	C5A-N7A-C8A	3.15	108.41	103.45
3	B	404	HEM	C4D-ND-C1D	-3.15	101.48	105.21
4	A	405	FAD	C6-C5X-C9A	3.01	123.19	119.05
5	B	406	DGG	O19-C21-C22	2.95	117.86	111.48
4	A	405	FAD	C9A-C5X-N5	-2.91	119.37	122.45
4	A	405	FAD	O4B-C1B-C2B	-2.89	100.43	106.62
5	A	406	DGG	O17-C17-C19	2.85	116.61	108.40
3	B	404	HEM	C1D-C2D-C3D	-2.76	104.08	106.98
4	B	405	FAD	N9A-C8A-N7A	-2.75	110.04	113.94
4	A	405	FAD	O4'-C4'-C5'	-2.73	103.96	109.99
4	B	405	FAD	C6-C5X-C9A	2.72	122.79	119.05
4	A	405	FAD	O2-C2-N1	-2.69	117.34	121.80
4	B	405	FAD	C1B-N9A-C8A	2.65	132.97	127.09
3	B	404	HEM	CBD-CAD-C3D	2.65	119.85	112.53
4	A	405	FAD	C4-N3-C2	-2.64	120.95	125.64
4	B	405	FAD	C4A-N9A-C8A	2.64	108.51	105.74
3	B	404	HEM	C1B-NB-C4B	-2.55	102.18	105.21
5	A	406	DGG	OP2-P-OP3	2.31	112.68	106.44
3	A	404	HEM	C4A-NA-C1A	-2.30	102.06	105.82
5	A	406	DGG	O17-C1-O1	-2.29	117.91	123.63
5	B	406	DGG	O19-C19-C18	2.23	116.36	108.34
5	A	406	DGG	O19-C21-C22	2.23	116.30	111.48
3	A	404	HEM	C4A-C3A-C2A	-2.20	104.30	106.82
3	B	404	HEM	CHC-C1C-NC	-2.17	122.09	124.45
5	B	406	DGG	O17-C17-C19	2.16	114.63	108.40
3	A	404	HEM	C4C-NC-C1C	-2.13	102.35	105.82
3	A	404	HEM	C2C-C1C-NC	2.13	113.58	109.64
3	B	404	HEM	C4A-NA-C1A	-2.12	102.36	105.82
3	B	404	HEM	C2A-C1A-NA	2.12	112.50	110.15
5	B	406	DGG	OP1-P-OP2	2.11	112.17	106.67
4	A	405	FAD	N3A-C4A-N9A	2.10	130.74	127.17
3	A	404	HEM	C4D-ND-C1D	-2.10	102.72	105.21
4	B	405	FAD	C4-N3-C2	-2.10	121.91	125.64
3	A	404	HEM	C3A-C4A-NA	2.04	113.41	110.14
5	B	406	DGG	O17-C1-O1	-2.04	118.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	HEM	C4A-C3A-C2A	2.04	109.15	106.82
5	A	406	DGG	C27-C28-C29	-2.03	108.14	115.11
3	B	404	HEM	O2D-CGD-CBD	2.00	120.33	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	406	DGG	C19

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	HEM	C2C-C3C-CAC-CBC
3	A	404	HEM	C4C-C3C-CAC-CBC
3	B	404	HEM	C2C-C3C-CAC-CBC
3	B	404	HEM	C4C-C3C-CAC-CBC
5	A	406	DGG	C18-OP2-P-OP1
5	A	406	DGG	C18-OP2-P-OP4
5	B	406	DGG	C18-OP2-P-OP1
5	B	406	DGG	C18-OP2-P-OP4
5	A	406	DGG	C3-C4-C5-C6
5	A	406	DGG	C1-C2-C3-C4
5	B	406	DGG	O21-C21-O19-C19
5	A	406	DGG	O1-C1-O17-C17
5	B	406	DGG	C11-C12-C13-C14
5	B	406	DGG	C22-C21-O19-C19
5	B	406	DGG	C31-C32-C33-C34
5	A	406	DGG	O21-C21-O19-C19
5	B	406	DGG	C1-C2-C3-C4
5	A	406	DGG	C18-OP2-P-OP3
5	B	406	DGG	C18-OP2-P-OP3
5	B	406	DGG	C10-C11-C12-C13
5	A	406	DGG	C11-C12-C13-C14
5	B	406	DGG	C9-C10-C11-C12
5	B	406	DGG	C30-C31-C32-C33
5	A	406	DGG	OP2-C18-C19-O19
5	B	406	DGG	C23-C24-C25-C26
4	A	405	FAD	C2B-C1B-N9A-C8A
5	A	406	DGG	OP2-C18-C19-C17
5	A	406	DGG	C9-C10-C11-C12
5	A	406	DGG	C2-C3-C4-C5
5	B	406	DGG	C5-C6-C7-C8

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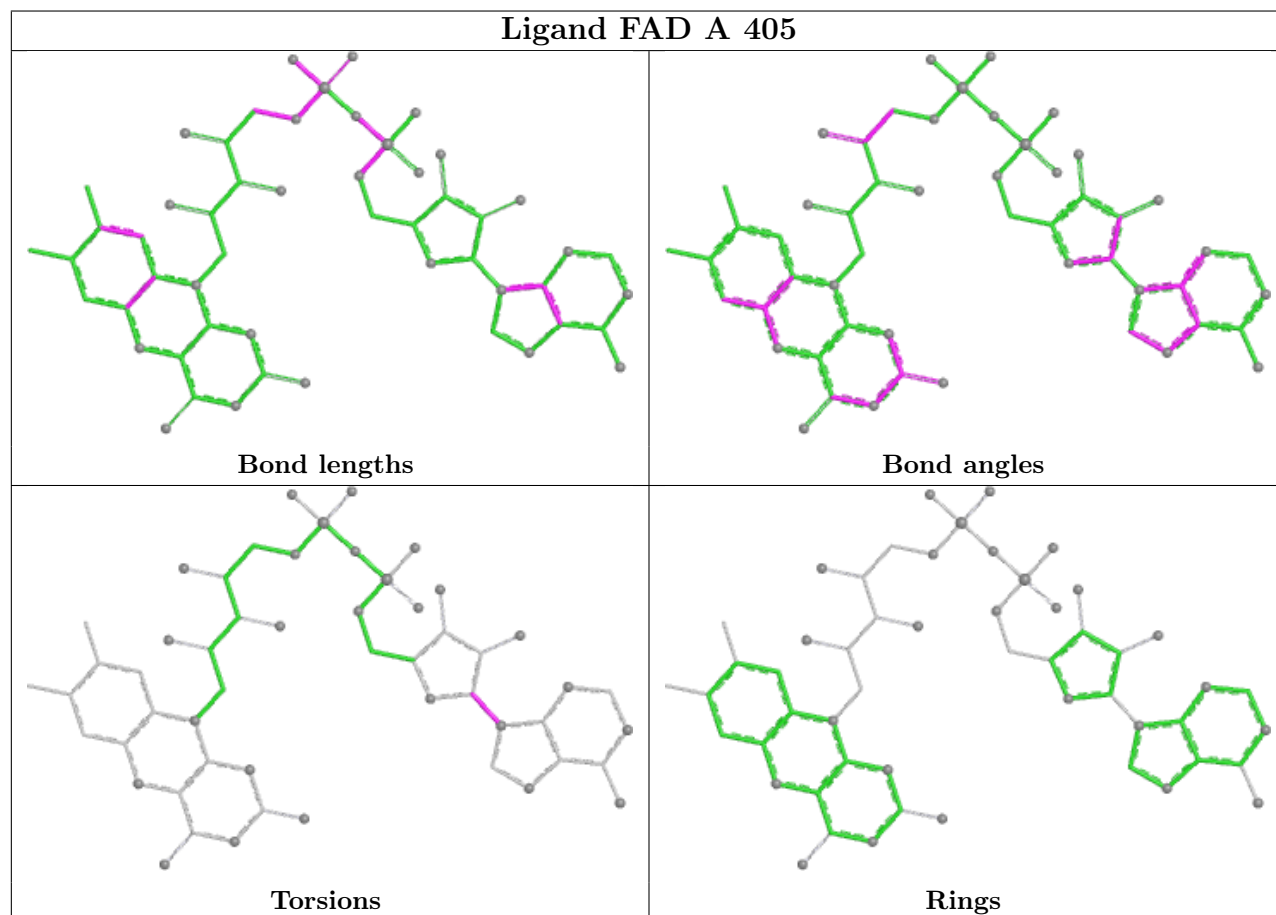
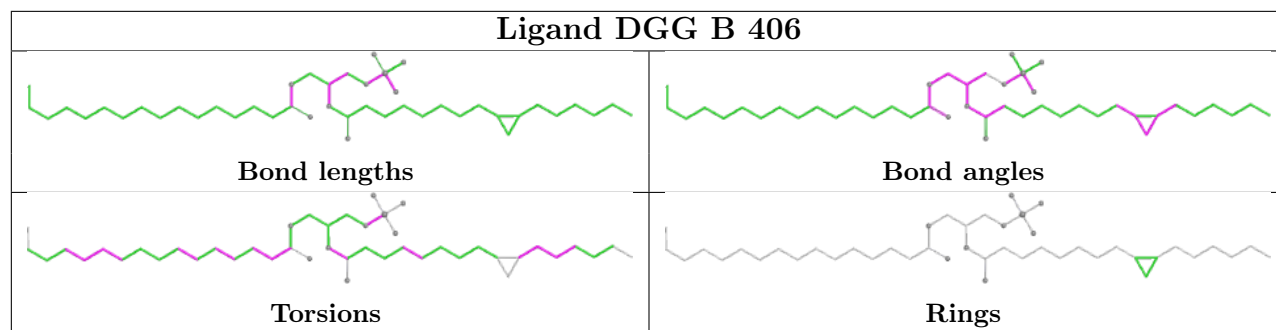
Mol	Chain	Res	Type	Atoms
5	A	406	DGG	C24-C25-C26-C27
5	A	406	DGG	C18-C19-O19-C21
5	A	406	DGG	C10-C11-C12-C13
5	A	406	DGG	C2-C1-O17-C17
5	A	406	DGG	C11-C10-C9-C8
5	A	406	DGG	C4-C5-C6-C7
5	B	406	DGG	C3-C4-C5-C6
3	A	404	HEM	CAD-CBD-CGD-O2D
5	A	406	DGG	C17-C19-O19-C21
3	A	404	HEM	CAD-CBD-CGD-O1D
5	A	406	DGG	O17-C1-C2-C3
3	B	404	HEM	CAD-CBD-CGD-O1D
5	A	406	DGG	C30-C31-C32-C33
5	B	406	DGG	O17-C1-C2-C3
4	A	405	FAD	C2B-C1B-N9A-C4A
3	B	404	HEM	CAD-CBD-CGD-O2D
5	B	406	DGG	C29-C30-C31-C32
4	B	405	FAD	PA-O3P-P-O2P
5	A	406	DGG	C6-C7-C8-C9

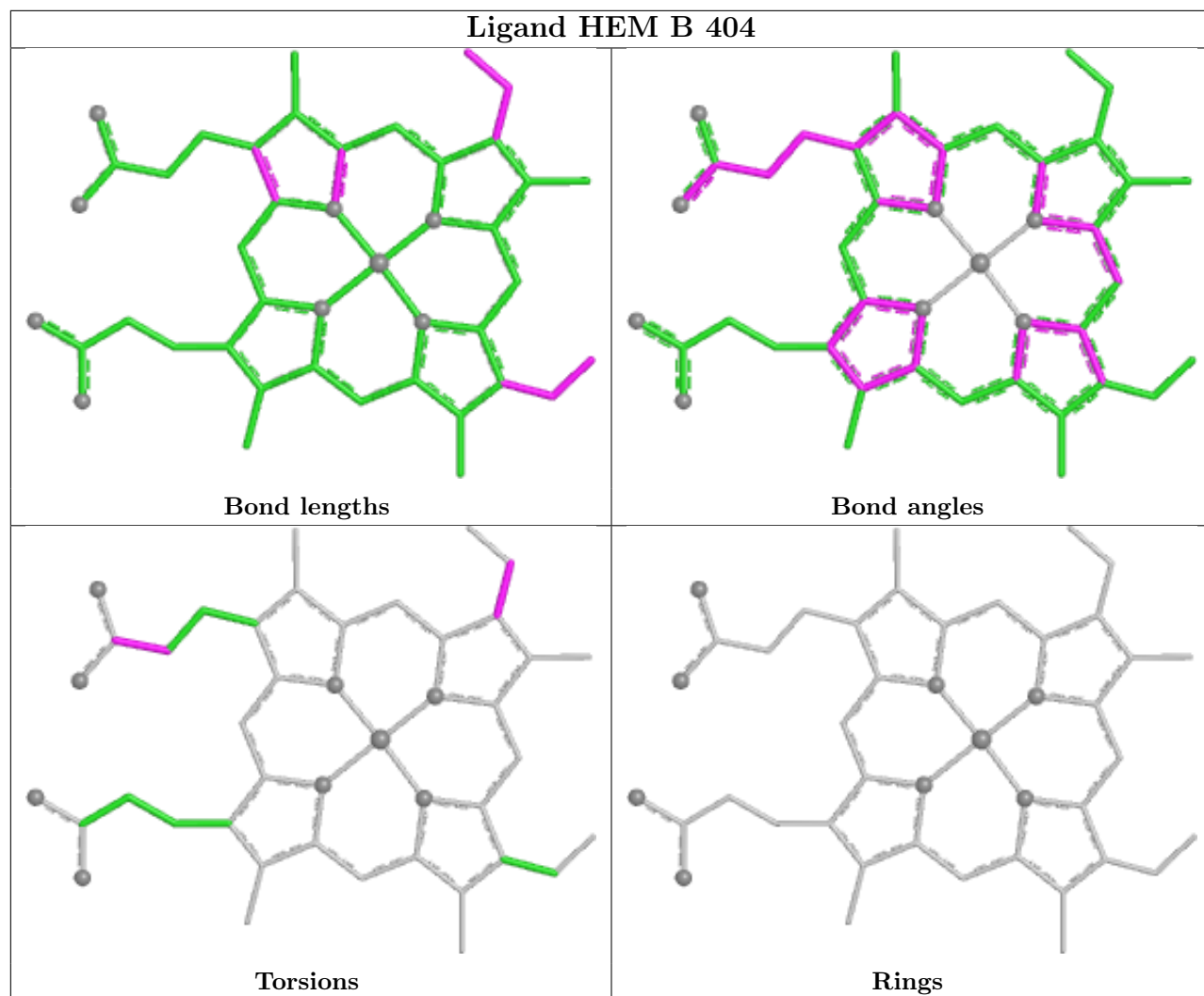
There are no ring outliers.

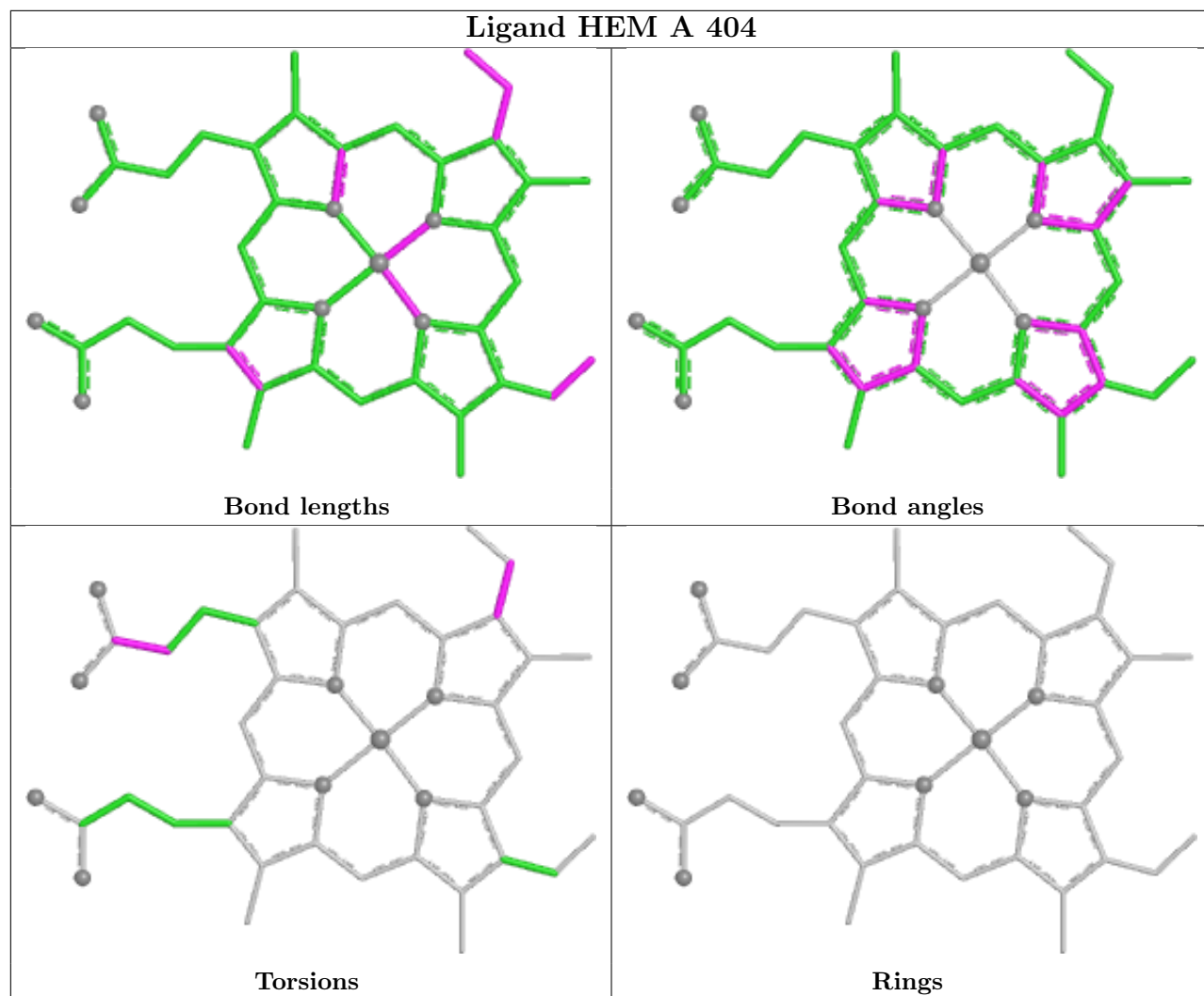
5 monomers are involved in 12 short contacts:

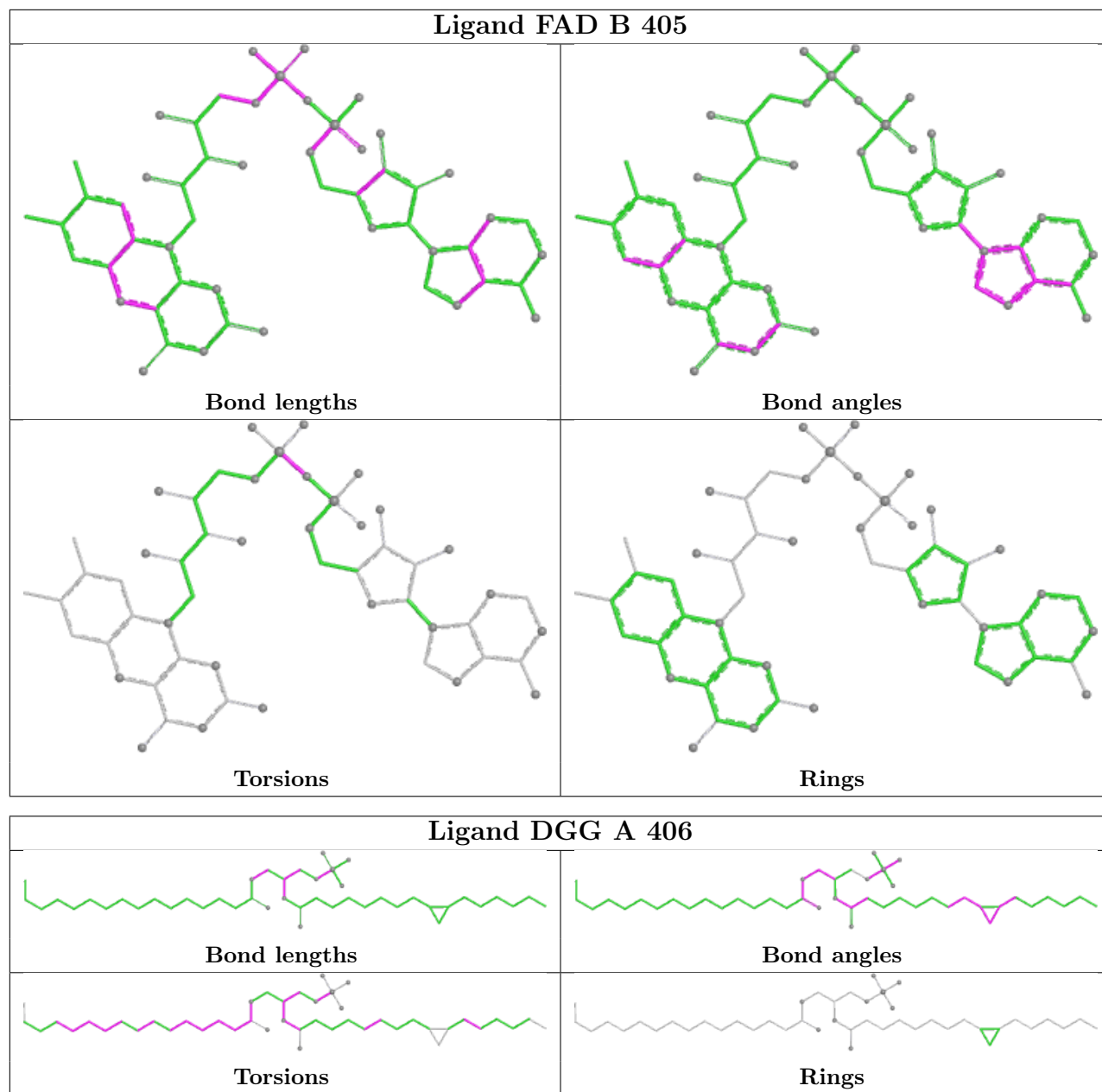
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	DGG	4	0
4	A	405	FAD	1	0
3	B	404	HEM	1	0
4	B	405	FAD	1	0
5	A	406	DGG	5	0

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%)	0.03	13 (3%)	50	57	11, 26, 55, 63	0
1	B	403/403 (100%)	-0.12	12 (2%)	52	59	11, 23, 46, 69	0
All	All	806/806 (100%)	-0.05	25 (3%)	51	58	11, 24, 52, 69	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	PRO	4.0
1	A	321	TYR	3.9
1	A	291	ALA	3.8
1	B	276	VAL	3.4
1	A	230	PRO	3.4
1	A	279	THR	3.2
1	B	229	GLY	3.2
1	A	292	PRO	3.1
1	B	232	PRO	3.1
1	B	228	GLY	3.1
1	B	1	MET	3.0
1	A	323	ASN	2.9
1	A	229	GLY	2.7
1	A	228	GLY	2.7
1	B	279	THR	2.5
1	B	227	GLY	2.4
1	A	338	VAL	2.4
1	B	47	HIS	2.4
1	A	1	MET	2.4
1	B	402	ALA	2.3
1	B	280	PRO	2.3
1	A	278	LEU	2.3
1	A	334	LEU	2.2
1	B	400	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	PRO	2.1

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](#)

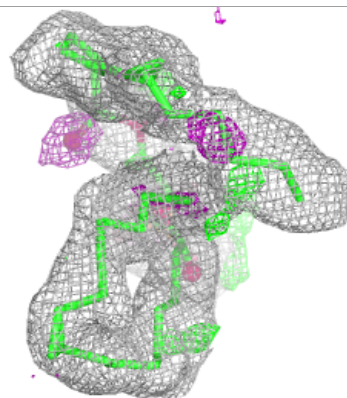
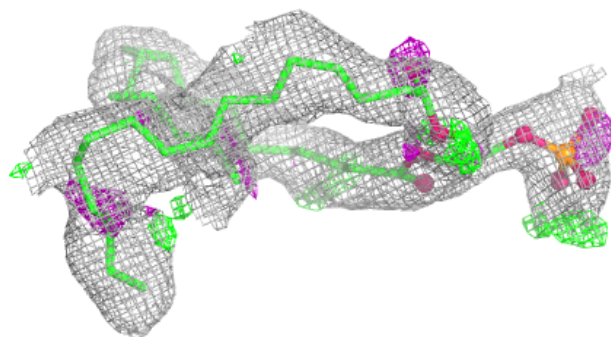
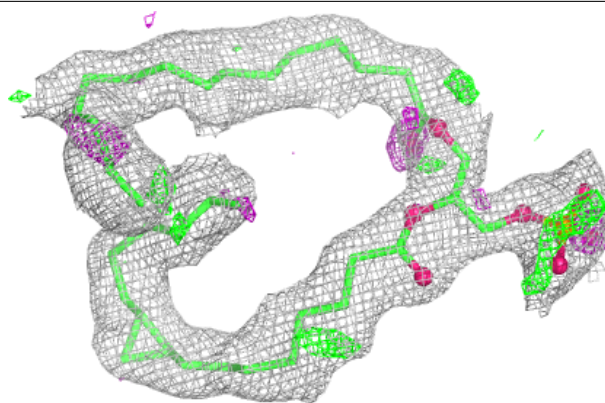
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NA	A	490	1/1	0.78	0.26	41,41,41,41	0
5	DGG	A	406	45/50	0.86	0.08	24,28,37,40	0
5	DGG	B	406	45/50	0.88	0.08	24,28,35,37	0
4	FAD	B	405	53/53	0.98	0.05	10,15,52,52	0
3	HEM	A	404	43/43	0.98	0.05	9,14,33,36	0
4	FAD	A	405	53/53	0.98	0.05	10,15,46,47	0
3	HEM	B	404	43/43	0.99	0.05	9,12,27,33	0

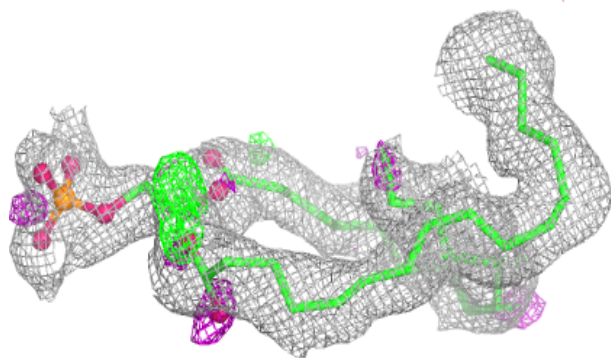
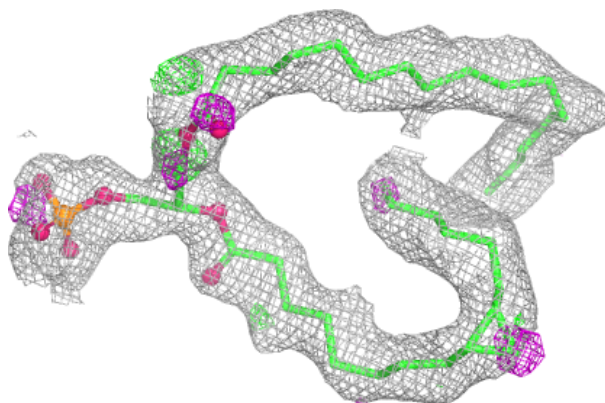
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

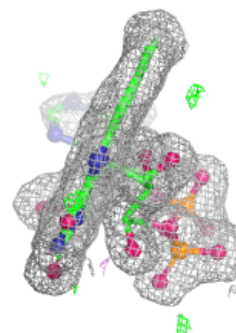
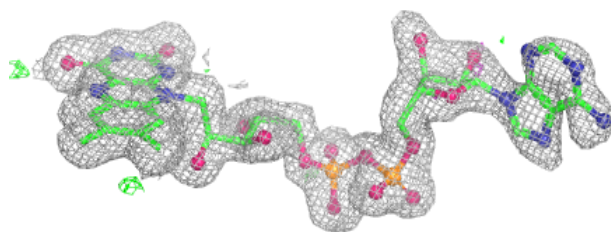
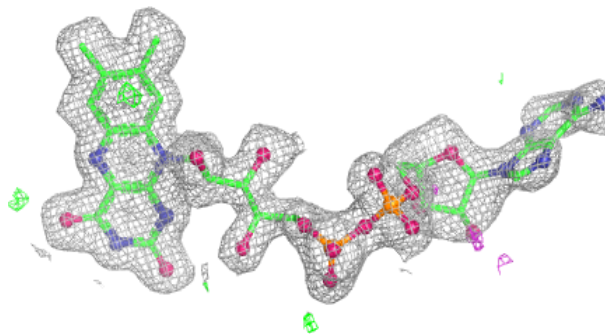
**Electron density around DGG B 406:**

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



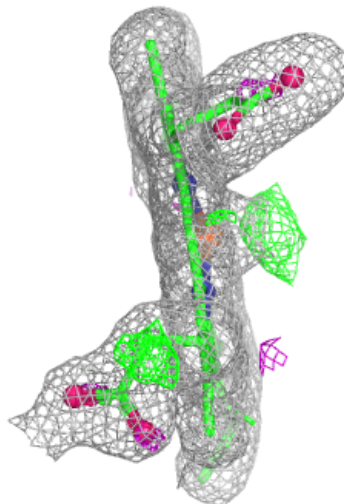
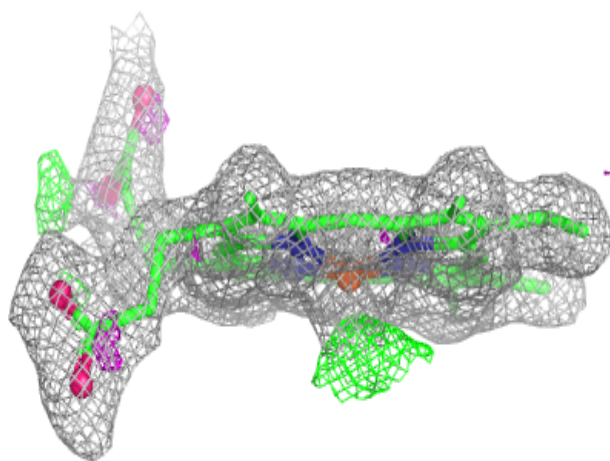
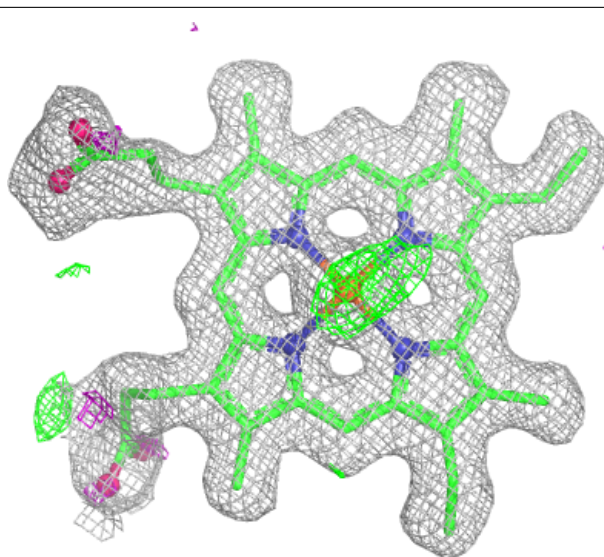
Electron density around FAD B 405:

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



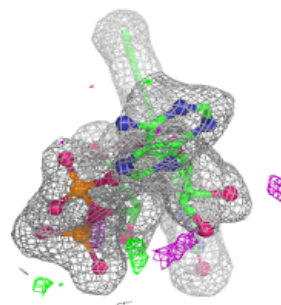
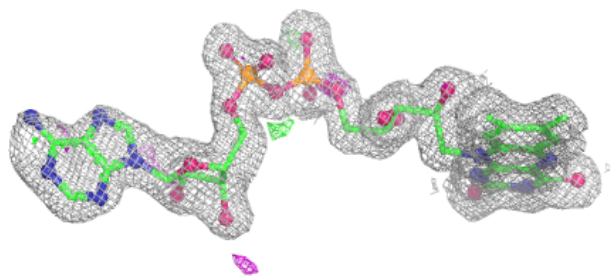
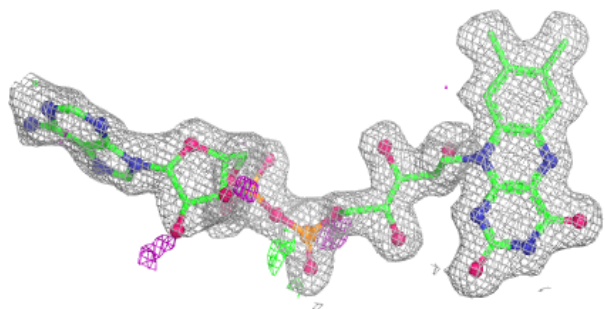
Electron density around HEM A 404:

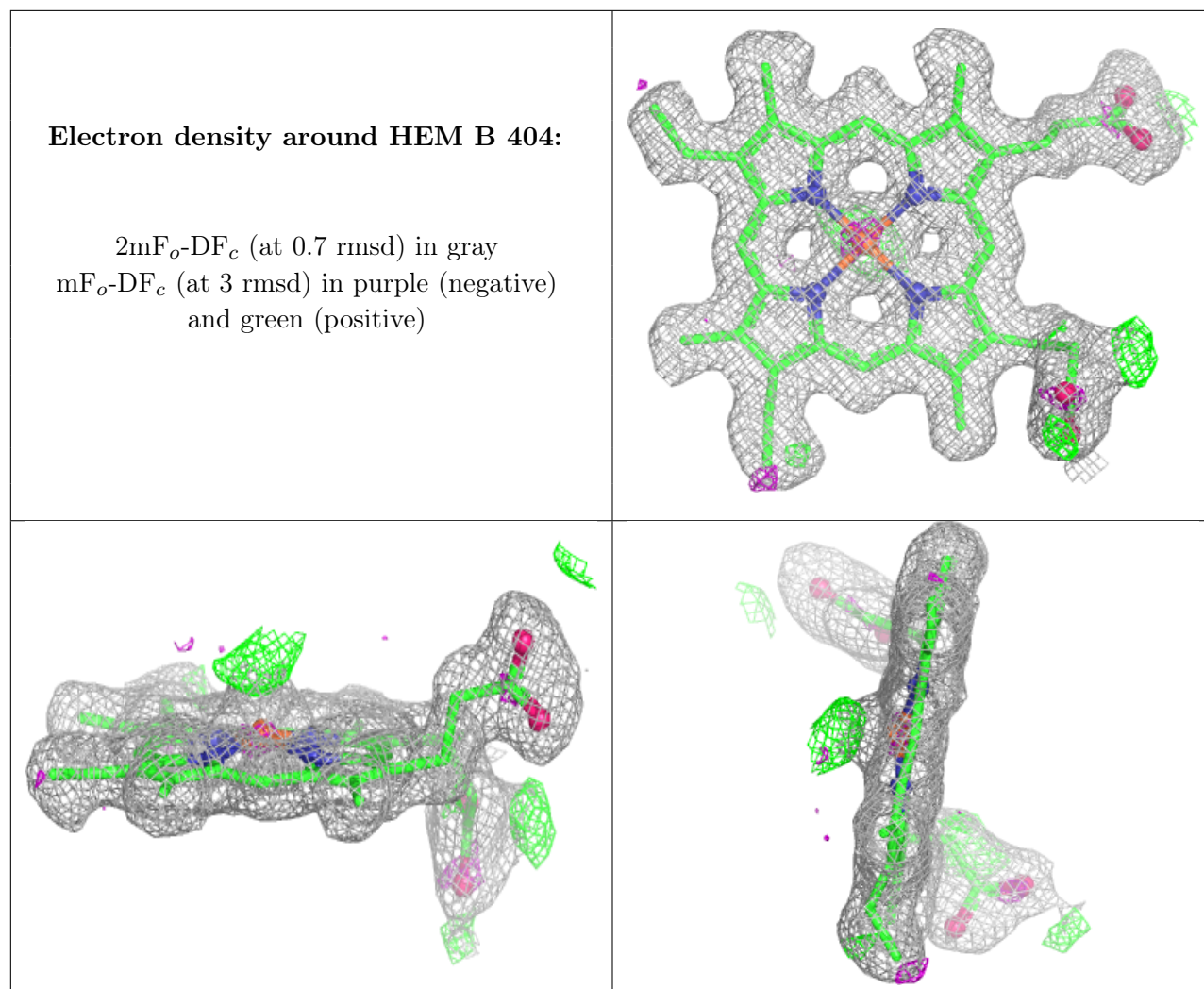
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.