



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:22 pm BST

PDB ID : 6J79
Title : Fusion protein of heme oxygenase-1 and NADPH-cytochrome P450 reductase (13aa)
Authors : Sugishima, M.; Wada, K.
Deposited on : 2019-01-17
Resolution : 3.33 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

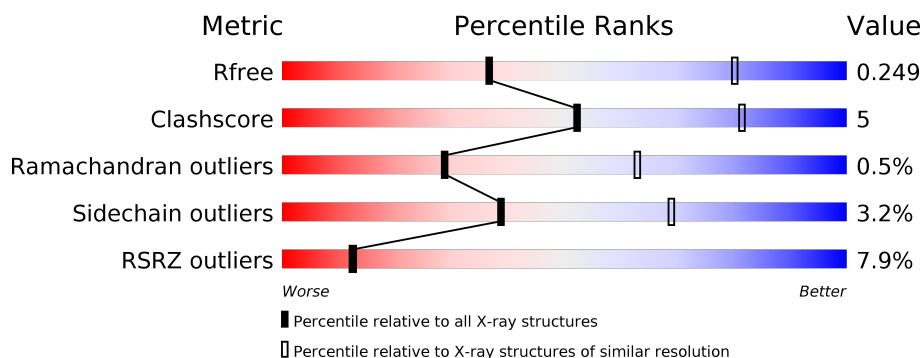
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 on 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	871	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	871	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13345 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 Heme oxygenase 1,NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6558	4168	1128	1233	29			
1	B	813	Total	C	N	O	S	0	0	0
			6517	4144	1121	1224	28			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P06762
A	-18	GLY	-	expression tag	UNP P06762
A	-17	SER	-	expression tag	UNP P06762
A	-16	SER	-	expression tag	UNP P06762
A	-15	HIS	-	expression tag	UNP P06762
A	-14	HIS	-	expression tag	UNP P06762
A	-13	HIS	-	expression tag	UNP P06762
A	-12	HIS	-	expression tag	UNP P06762
A	-11	HIS	-	expression tag	UNP P06762
A	-10	HIS	-	expression tag	UNP P06762
A	-9	SER	-	expression tag	UNP P06762
A	-8	SER	-	expression tag	UNP P06762
A	-7	GLY	-	expression tag	UNP P06762
A	-6	LEU	-	expression tag	UNP P06762
A	-5	VAL	-	expression tag	UNP P06762
A	-4	PRO	-	expression tag	UNP P06762
A	-3	ARG	-	expression tag	UNP P06762
A	-2	GLY	-	expression tag	UNP P06762
A	-1	SER	-	expression tag	UNP P06762
A	0	HIS	-	expression tag	UNP P06762
A	222	PRO	THR	engineered mutation	UNP P06762
A	230	ALA	PRO	engineered mutation	UNP P06762
A	234	MET	-	linker	UNP P06762
A	?	-	THR	deletion	UNP P00388
A	?	-	GLY	deletion	UNP P00388

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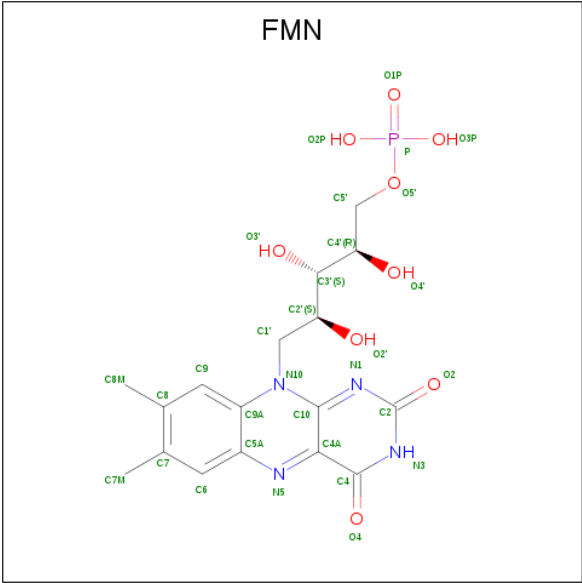
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P00388
A	?	-	GLU	deletion	UNP P00388
B	-19	MET	-	initiating methionine	UNP P06762
B	-18	GLY	-	expression tag	UNP P06762
B	-17	SER	-	expression tag	UNP P06762
B	-16	SER	-	expression tag	UNP P06762
B	-15	HIS	-	expression tag	UNP P06762
B	-14	HIS	-	expression tag	UNP P06762
B	-13	HIS	-	expression tag	UNP P06762
B	-12	HIS	-	expression tag	UNP P06762
B	-11	HIS	-	expression tag	UNP P06762
B	-10	HIS	-	expression tag	UNP P06762
B	-9	SER	-	expression tag	UNP P06762
B	-8	SER	-	expression tag	UNP P06762
B	-7	GLY	-	expression tag	UNP P06762
B	-6	LEU	-	expression tag	UNP P06762
B	-5	VAL	-	expression tag	UNP P06762
B	-4	PRO	-	expression tag	UNP P06762
B	-3	ARG	-	expression tag	UNP P06762
B	-2	GLY	-	expression tag	UNP P06762
B	-1	SER	-	expression tag	UNP P06762
B	0	HIS	-	expression tag	UNP P06762
B	222	PRO	THR	engineered mutation	UNP P06762
B	230	ALA	PRO	engineered mutation	UNP P06762
B	234	MET	-	linker	UNP P06762
B	?	-	THR	deletion	UNP P00388
B	?	-	GLY	deletion	UNP P00388
B	?	-	GLU	deletion	UNP P00388
B	?	-	GLU	deletion	UNP P00388

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by author).



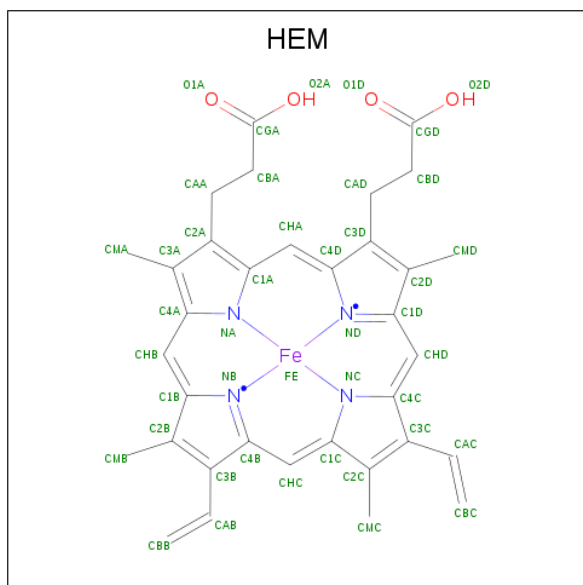
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

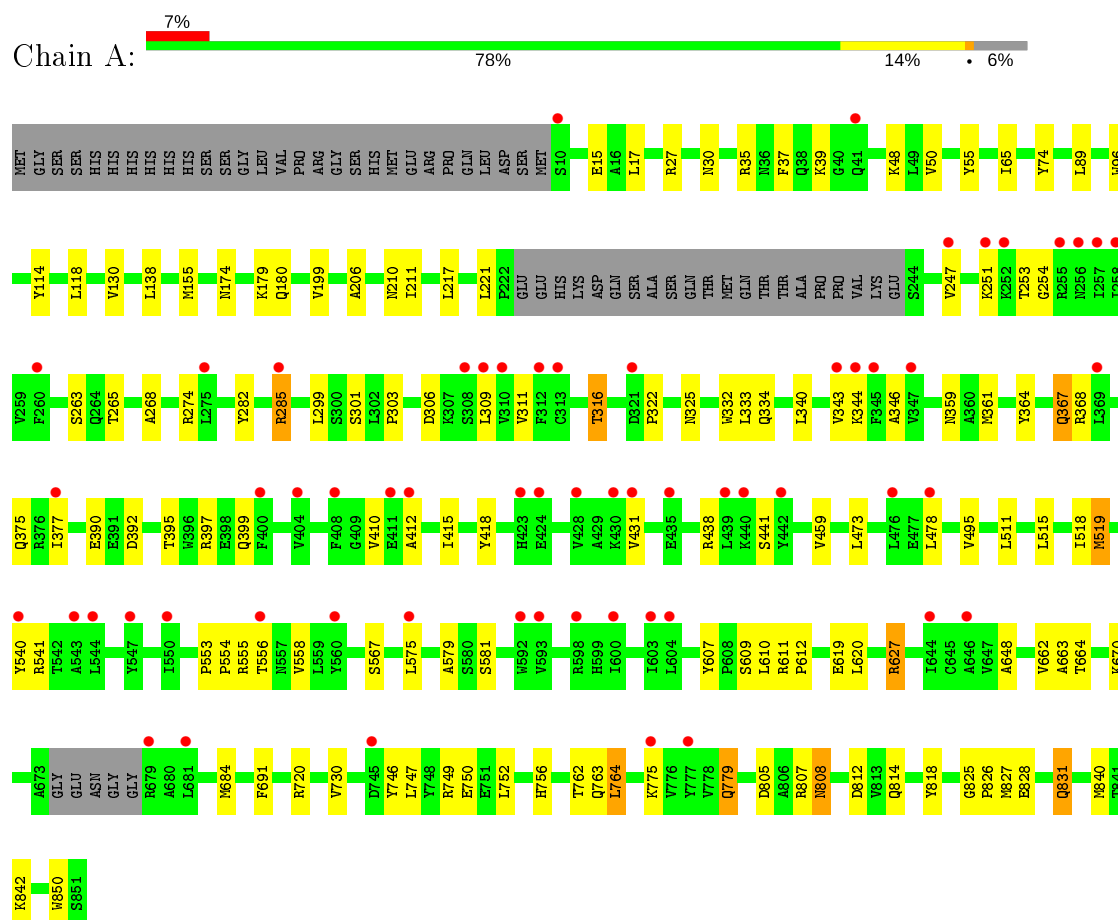
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by author).



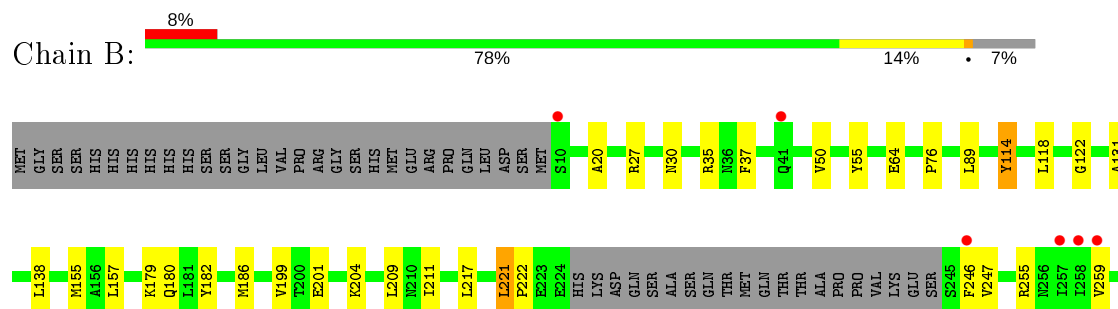
3 Residue-property plots [i](#)

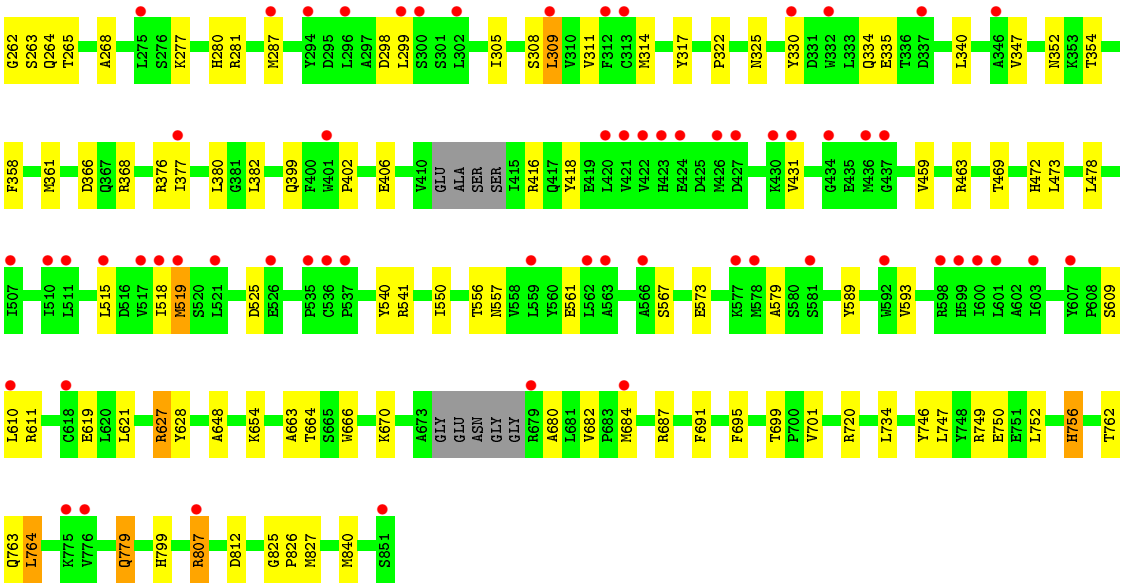
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Heme oxygenase 1,NADPH–cytochrome P450 reductase



- Molecule 1: Heme oxygenase 1,NADPH–cytochrome P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.36Å 159.78Å 189.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 3.33 43.67 – 3.33	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.67-3.33) 99.1 (43.67-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.202 , 0.248 0.202 , 0.249	Depositor DCC
R_{free} test set	1873 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13345	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: FMN, HEM, FAD

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	0.24	0/6719	0.41	0/9098
1	B	0.25	0/6676	0.42	0/9042
All	All	0.25	0/13395	0.41	0/18140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6558	0	6360	72	0
1	B	6517	0	6303	73	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
5	A	6	0	0	0	0
5	B	10	0	0	1	0
All	All	13345	0	12821	143	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 5.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG12	1:A:217:LEU:HD13	1.64	0.79
1:B:50:VAL:HG12	1:B:217:LEU:HD13	1.65	0.79
1:B:352:ASN:ND2	1:B:354:THR:OG1	2.14	0.78
1:A:395:THR:O	1:A:399:GLN:NE2	2.23	0.71
1:B:779:GLN:HG2	1:B:812:ASP:HB3	1.74	0.69
1:A:344:LYS:HB3	1:A:377:ILE:HD11	1.73	0.69
1:B:309:LEU:HD21	1:B:377:ILE:HG13	1.75	0.69
1:A:515:LEU:HB3	1:A:541:ARG:HB2	1.77	0.67
1:B:406:GLU:HG3	1:B:579:ALA:HB3	1.78	0.66
1:A:431:VAL:HG21	1:A:518:ILE:HD13	1.77	0.65
1:A:55:TYR:HA	1:A:89:LEU:HD13	1.78	0.65
1:B:515:LEU:HB3	1:B:541:ARG:HB2	1.79	0.64
1:B:259:VAL:HG13	1:B:311:VAL:HG23	1.80	0.64
1:B:55:TYR:HA	1:B:89:LEU:HD13	1.81	0.63
1:A:478:LEU:HD23	1:A:684:MET:HG2	1.80	0.62
1:B:699:THR:O	1:B:720:ARG:NH2	2.29	0.62
1:B:180:GLN:NE2	1:B:840:MET:O	2.33	0.61
1:B:352:ASN:HD21	1:B:354:THR:HG1	1.46	0.60
1:B:749:ARG:NH1	1:B:750:GLU:OE2	2.34	0.60
1:A:775:LYS:NZ	1:B:335:GLU:O	2.29	0.59
1:A:316:THR:HG21	1:A:359:ASN:HA	1.83	0.59
1:A:627:ARG:HD3	1:A:663:ALA:HB2	1.84	0.59
1:A:265:THR:OG1	3:A:902:FMN:O2P	2.19	0.59
1:B:567:SER:H	1:B:609:SER:HB3	1.68	0.59
1:B:366:ASP:OD1	1:B:376:ARG:NH1	2.28	0.59
1:A:749:ARG:NH1	1:A:750:GLU:OE2	2.36	0.59
1:A:779:GLN:HG2	1:A:812:ASP:HB3	1.84	0.59
1:B:752:LEU:HB3	1:B:764:LEU:HD11	1.86	0.58
1:B:473:LEU:HD22	1:B:747:LEU:HD21	1.85	0.58
1:A:473:LEU:HD22	1:A:747:LEU:HD21	1.85	0.57
1:A:138:LEU:HD13	1:A:179:LYS:HG2	1.86	0.57
1:A:180:GLN:NE2	1:A:840:MET:O	2.36	0.57
1:A:438:ARG:HG3	1:A:441:SER:HB3	1.87	0.56
1:B:463:ARG:NH1	5:B:1002:HOH:O	2.37	0.56
1:A:752:LEU:HB3	1:A:764:LEU:HD11	1.88	0.56
1:A:253:THR:O	1:A:285:ARG:NH2	2.37	0.56
1:A:263:SER:HB2	1:A:268:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:HD2	1:B:211:ILE:HD13	1.89	0.55
1:A:610:LEU:O	1:A:611:ARG:NE	2.38	0.55
1:B:431:VAL:HG21	1:B:518:ILE:HD13	1.88	0.55
1:A:459:VAL:HG21	1:A:670:LYS:HB3	1.89	0.54
1:A:648:ALA:HA	1:A:664:THR:HB	1.91	0.53
1:B:628:TYR:HE2	1:B:687:ARG:HD2	1.74	0.52
1:B:519:MET:HG2	1:B:540:TYR:CZ	2.44	0.52
1:B:478:LEU:HD23	1:B:684:MET:HG2	1.91	0.52
1:B:265:THR:OG1	3:B:902:FMN:O2P	2.22	0.52
1:A:825:GLY:O	1:A:827:MET:N	2.43	0.52
1:A:254:GLY:O	1:A:285:ARG:NE	2.34	0.51
1:B:305:ILE:HB	1:B:308:SER:HB3	1.92	0.51
1:A:807:ARG:NH1	1:B:334:GLN:O	2.44	0.51
1:B:347:VAL:HG11	1:B:366:ASP:HB2	1.92	0.51
1:B:459:VAL:HG21	1:B:670:LYS:HB3	1.94	0.50
1:A:332:TRP:HE3	1:A:333:LEU:HD12	1.77	0.49
1:B:610:LEU:O	1:B:611:ARG:NE	2.42	0.49
1:B:347:VAL:HG13	1:B:380:LEU:HD13	1.93	0.49
1:B:627:ARG:NH1	2:B:901:FAD:O1P	2.45	0.49
1:A:827:MET:HB3	1:A:831:GLN:HG3	1.95	0.49
1:A:627:ARG:NH1	2:A:901:FAD:O1P	2.46	0.49
1:B:666:TRP:HH2	1:B:682:VAL:HA	1.78	0.49
1:A:30:ASN:O	1:A:35:ARG:NH1	2.44	0.48
1:A:206:ALA:O	1:A:210:ASN:ND2	2.41	0.48
1:A:607:TYR:HB3	1:A:610:LEU:HD23	1.95	0.48
1:B:418:TYR:HD2	1:B:619:GLU:HG3	1.79	0.48
1:A:282:TYR:HA	1:A:415:ILE:HG21	1.96	0.47
1:B:648:ALA:HA	1:B:664:THR:HB	1.96	0.47
1:A:263:SER:H	1:A:325:ASN:HD21	1.62	0.47
1:A:377:ILE:O	1:A:581:SER:OG	2.24	0.47
1:A:720:ARG:HH11	1:A:730:VAL:HG13	1.78	0.47
1:B:277:LYS:O	1:B:281:ARG:NH1	2.40	0.47
1:B:825:GLY:O	1:B:827:MET:N	2.48	0.47
1:A:15:GLU:OE1	1:A:842:LYS:HE2	2.15	0.46
1:A:303:PRO:HD3	1:A:343:VAL:HG22	1.97	0.46
1:A:556:THR:HG23	1:A:579:ALA:HA	1.97	0.46
1:A:334:GLN:NE2	1:A:364:TYR:OH	2.46	0.46
1:A:567:SER:H	1:A:609:SER:HB3	1.79	0.46
1:A:814:GLN:HG2	1:A:818:TYR:CZ	2.50	0.46
1:B:322:PRO:HG3	1:B:330:TYR:CB	2.46	0.46
1:A:805:ASP:HB3	1:A:850:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:TYR:O	1:B:593:VAL:HG12	2.16	0.45
1:A:274:ARG:NH2	1:A:390:GLU:OE2	2.49	0.45
1:B:322:PRO:HB3	1:B:361:MET:SD	2.57	0.45
1:B:358:PHE:CE2	1:B:382:LEU:HB3	2.51	0.45
1:A:309:LEU:HD13	1:A:377:ILE:HD12	1.98	0.45
1:B:627:ARG:HD3	1:B:663:ALA:HB2	1.97	0.45
1:B:628:TYR:CE2	1:B:687:ARG:HD2	2.51	0.45
1:B:255:ARG:HD3	1:B:287:MET:HB3	1.98	0.45
1:B:699:THR:HG21	1:B:799:HIS:HD2	1.82	0.45
1:A:247:VAL:HG11	1:A:301:SER:O	2.17	0.45
1:A:807:ARG:HG2	1:A:808:ASN:ND2	2.33	0.44
1:B:138:LEU:HD13	1:B:179:LYS:HG2	1.98	0.44
1:A:399:GLN:HG3	1:A:556:THR:HB	1.98	0.44
1:A:627:ARG:NH1	1:A:662:VAL:HB	2.33	0.44
1:B:76:PRO:HG3	1:B:695:PHE:CE2	2.53	0.44
1:A:828:GLU:HB2	1:A:831:GLN:HG2	1.99	0.44
1:A:410:VAL:HG22	1:A:412:ALA:H	1.83	0.43
1:B:416:ARG:NH2	1:B:418:TYR:O	2.51	0.43
1:B:262:GLY:HA2	1:B:325:ASN:HD21	1.84	0.43
1:B:131:ALA:HB2	1:B:199:VAL:HG13	1.99	0.43
1:A:17:LEU:HD21	1:A:199:VAL:HG12	2.00	0.43
1:A:322:PRO:HB3	1:A:361:MET:SD	2.58	0.43
1:A:399:GLN:OE1	1:A:555:ARG:HB3	2.18	0.43
1:B:550:ILE:HG22	1:B:621:LEU:HD23	2.01	0.43
1:B:402:PRO:HG2	1:B:557:ASN:HA	2.00	0.43
1:A:48:LYS:HG2	1:A:96:TRP:HB3	2.01	0.43
1:B:30:ASN:O	1:B:35:ARG:NH1	2.51	0.43
1:B:670:LYS:HD3	1:B:670:LYS:HA	1.75	0.43
1:B:807:ARG:N	1:B:807:ARG:HD2	2.34	0.43
1:A:311:VAL:HA	1:A:346:ALA:O	2.18	0.43
1:B:217:LEU:O	1:B:221:LEU:HD23	2.19	0.43
1:B:64:GLU:HB3	1:B:122:GLY:HA3	2.01	0.43
1:A:27:ARG:HD2	1:A:211:ILE:HD13	2.01	0.42
1:A:511:LEU:HD11	1:A:612:PRO:HD2	2.01	0.42
1:A:575:LEU:HD11	1:A:610:LEU:HD21	2.00	0.42
1:B:263:SER:HB2	1:B:268:ALA:HB3	2.01	0.42
1:B:299:LEU:HD11	1:B:340:LEU:HD13	2.01	0.42
1:A:762:THR:HG22	1:A:763:GLN:HG3	2.00	0.42
1:B:264:GLN:HB2	1:B:317:TYR:CZ	2.55	0.42
1:A:332:TRP:CE3	1:A:333:LEU:HD12	2.54	0.42
1:A:367:GLN:HG3	1:A:368:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PRO:HA	1:A:554:PRO:HD3	1.90	0.42
1:B:567:SER:N	1:B:609:SER:HB3	2.33	0.42
1:B:20:ALA:HB1	1:B:204:LYS:HE3	2.02	0.41
1:B:654:LYS:HG2	1:B:654:LYS:H	1.63	0.41
1:B:182:TYR:O	1:B:186:MET:HG3	2.20	0.41
1:A:418:TYR:HD2	1:A:619:GLU:HG3	1.85	0.41
1:A:519:MET:HG2	1:A:540:TYR:CZ	2.54	0.41
1:A:558:VAL:HG12	1:A:620:LEU:HB3	2.02	0.41
1:B:756:HIS:HB2	1:B:764:LEU:HD12	2.02	0.41
1:A:35:ARG:O	1:A:39:LYS:HG2	2.21	0.41
1:A:395:THR:HG23	1:A:555:ARG:HH12	1.86	0.41
1:B:246:PHE:CE1	1:B:298:ASP:HB2	2.55	0.41
1:B:701:VAL:HG13	1:B:720:ARG:HH21	1.86	0.41
1:B:762:THR:HG22	1:B:763:GLN:HG3	2.01	0.41
1:B:734:LEU:HG	1:B:763:GLN:HB2	2.03	0.41
1:A:251:LYS:HE3	1:A:251:LYS:HB2	1.92	0.41
1:B:399:GLN:HG2	1:B:556:THR:HB	2.02	0.41
1:A:274:ARG:HG2	1:A:397:ARG:NH1	2.37	0.40
1:B:322:PRO:HG3	1:B:330:TYR:HB2	2.01	0.40
1:B:322:PRO:HA	1:B:361:MET:HG3	2.01	0.40
1:A:495:VAL:HG22	1:A:684:MET:HB3	2.04	0.40
1:A:65:ILE:HG23	1:A:74:TYR:CE2	2.56	0.40
1:B:114:TYR:HA	1:B:209:LEU:HD13	2.03	0.40
1:B:472:HIS:HB3	1:B:648:ALA:HB3	2.02	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	810/871 (93%)	754 (93%)	52 (6%)	4 (0%)	29 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	805/871 (92%)	747 (93%)	54 (7%)	4 (0%)	29	63
All	All	1615/1742 (93%)	1501 (93%)	106 (7%)	8 (0%)	29	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	B	222	PRO
1	A	808	ASN
1	B	680	ALA
1	A	826	PRO
1	B	221	LEU
1	B	826	PRO
1	A	221	LEU

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	695/746 (93%)	674 (97%)	21 (3%)	41	70
1	B	687/746 (92%)	664 (97%)	23 (3%)	38	68
All	All	1382/1492 (93%)	1338 (97%)	44 (3%)	39	69

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	114	TYR
1	A	118	LEU
1	A	130	VAL
1	A	155	MET
1	A	174	ASN
1	A	285	ARG
1	A	299	LEU

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Mol	Chain	Res	Type
1	A	316	THR
1	A	340	LEU
1	A	367	GLN
1	A	375	GLN
1	A	392	ASP
1	A	519	MET
1	A	627	ARG
1	A	691	PHE
1	A	746	TYR
1	A	756	HIS
1	A	764	LEU
1	A	779	GLN
1	A	831	GLN
1	B	37	PHE
1	B	114	TYR
1	B	118	LEU
1	B	155	MET
1	B	157	LEU
1	B	201	GLU
1	B	247	VAL
1	B	280	HIS
1	B	309	LEU
1	B	314	MET
1	B	368	ARG
1	B	469	THR
1	B	519	MET
1	B	525	ASP
1	B	561	GLU
1	B	573	GLU
1	B	627	ARG
1	B	691	PHE
1	B	746	TYR
1	B	756	HIS
1	B	764	LEU
1	B	779	GLN
1	B	807	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	814	GLN

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Mol	Chain	Res	Type
1	B	352	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	FMN	B	902	-	31,33,33	1.32	4 (12%)	40,50,50	2.38	8 (20%)
2	FAD	B	901	-	51,58,58	4.65	18 (35%)	60,89,89	2.68	12 (20%)
4	HEM	A	903	1,5	27,50,50	0.87	2 (7%)	17,82,82	1.26	2 (11%)
4	HEM	B	903	1,5	27,50,50	0.87	1 (3%)	17,82,82	1.22	1 (5%)
3	FMN	A	902	-	31,33,33	1.30	4 (12%)	40,50,50	2.37	8 (20%)
2	FAD	A	901	-	51,58,58	4.67	18 (35%)	60,89,89	2.67	12 (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	FMN	B	902	-	-	0/18/18/18	0/3/3/3
2	FAD	B	901	-	-	4/30/50/50	0/6/6/6
4	HEM	A	903	1,5	-	0/6/54/54	-
4	HEM	B	903	1,5	-	0/6/54/54	-
3	FMN	A	902	-	-	0/18/18/18	0/3/3/3
2	FAD	A	901	-	-	2/30/50/50	0/6/6/6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	O4B-C1B	15.34	1.62	1.41
2	B	901	FAD	O4B-C1B	15.25	1.62	1.41
2	A	901	FAD	C2B-C1B	-14.85	1.31	1.53
2	B	901	FAD	C2B-C1B	-14.77	1.31	1.53
2	B	901	FAD	C10-N1	10.48	1.46	1.33
2	A	901	FAD	C10-N1	10.44	1.46	1.33
2	A	901	FAD	C4X-N5	8.77	1.45	1.33
2	B	901	FAD	C4X-N5	8.69	1.45	1.33
2	A	901	FAD	C5X-N5	8.66	1.49	1.35
2	B	901	FAD	C5X-N5	8.61	1.49	1.35
2	A	901	FAD	C9A-N10	8.42	1.49	1.38
2	B	901	FAD	C9A-N10	8.42	1.49	1.38
2	A	901	FAD	C4-N3	7.65	1.46	1.33
2	B	901	FAD	C4-N3	7.61	1.46	1.33
2	A	901	FAD	C4X-C10	6.94	1.45	1.38
2	B	901	FAD	C4X-C10	6.82	1.45	1.38
2	B	901	FAD	O4B-C4B	-6.41	1.30	1.45
2	A	901	FAD	O4B-C4B	-6.37	1.30	1.45
2	A	901	FAD	C4-C4X	6.17	1.52	1.41
2	B	901	FAD	C4-C4X	6.00	1.51	1.41
2	A	901	FAD	C2-N3	5.84	1.49	1.38
2	B	901	FAD	C2-N3	5.74	1.49	1.38
2	B	901	FAD	C2-N1	5.24	1.48	1.38
2	A	901	FAD	C2-N1	5.15	1.48	1.38
2	A	901	FAD	C6A-N6A	3.14	1.45	1.34
2	B	901	FAD	C6A-N6A	3.13	1.45	1.34
2	A	901	FAD	O2B-C2B	2.98	1.50	1.43
2	B	901	FAD	O2B-C2B	2.98	1.50	1.43
2	A	901	FAD	O3B-C3B	-2.95	1.36	1.43
2	B	901	FAD	O3B-C3B	-2.92	1.36	1.43
3	B	902	FMN	C4A-C10	-2.71	1.36	1.38
3	A	902	FMN	C4A-C10	-2.62	1.36	1.38
2	B	901	FAD	C5A-C4A	-2.62	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C5A-C4A	-2.62	1.34	1.40
4	B	903	HEM	C3B-C2B	-2.59	1.36	1.40
4	A	903	HEM	C3B-C2B	-2.52	1.36	1.40
3	A	902	FMN	C9A-C5A	-2.50	1.37	1.42
3	B	902	FMN	C9A-C5A	-2.50	1.37	1.42
3	A	902	FMN	C9A-N10	-2.46	1.35	1.38
2	B	901	FAD	C2A-N3A	2.37	1.35	1.32
3	B	902	FMN	C9A-N10	-2.35	1.35	1.38
2	A	901	FAD	C2A-N3A	2.31	1.35	1.32
2	B	901	FAD	O4-C4	-2.24	1.18	1.24
3	A	902	FMN	O4-C4	-2.22	1.19	1.24
3	B	902	FMN	O4-C4	-2.22	1.19	1.24
2	A	901	FAD	O4-C4	-2.18	1.19	1.24
4	A	903	HEM	C4D-C3D	2.03	1.47	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	FAD	C5A-C6A-N6A	12.66	139.59	120.35
2	A	901	FAD	C5A-C6A-N6A	12.61	139.51	120.35
3	A	902	FMN	C1'-N10-C9A	10.49	126.55	118.29
3	B	902	FMN	C1'-N10-C9A	10.36	126.45	118.29
2	A	901	FAD	N6A-C6A-N1A	-8.82	100.26	118.57
2	B	901	FAD	N6A-C6A-N1A	-8.81	100.29	118.57
3	B	902	FMN	C4-N3-C2	5.70	119.96	115.14
3	A	902	FMN	C4-N3-C2	5.64	119.91	115.14
2	A	901	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	901	FAD	C4-N3-C2	5.55	119.83	115.14
2	A	901	FAD	C4-N3-C2	5.55	119.83	115.14
2	B	901	FAD	N3A-C2A-N1A	-5.51	120.07	128.68
3	B	902	FMN	C1'-N10-C10	-5.34	113.62	118.41
3	A	902	FMN	C1'-N10-C10	-5.18	113.77	118.41
2	B	901	FAD	C7M-C7-C8	4.77	130.51	120.74
2	A	901	FAD	C7M-C7-C8	4.70	130.37	120.74
2	B	901	FAD	C7M-C7-C6	-4.62	109.29	120.34
2	A	901	FAD	C7M-C7-C6	-4.57	109.42	120.34
2	B	901	FAD	C3B-C2B-C1B	3.65	106.47	100.98
3	B	902	FMN	C4A-N5-C5A	3.45	120.22	116.77
2	A	901	FAD	C3B-C2B-C1B	3.44	106.16	100.98
2	B	901	FAD	C5X-C9A-N10	3.34	120.13	117.72
2	A	901	FAD	C5X-C9A-N10	3.27	120.08	117.72
3	A	902	FMN	C4A-N5-C5A	3.23	120.00	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	FAD	C4X-N5-C5X	3.21	119.98	116.77
3	A	902	FMN	C5A-C9A-N10	3.14	119.99	117.72
2	B	901	FAD	P-O3P-PA	-3.05	122.38	132.83
2	A	901	FAD	C4X-N5-C5X	3.04	119.81	116.77
3	B	902	FMN	C5A-C9A-N10	2.97	119.87	117.72
2	A	901	FAD	C4X-C4-N3	-2.87	119.51	123.43
2	A	901	FAD	P-O3P-PA	-2.74	123.41	132.83
2	B	901	FAD	C4X-C4-N3	-2.74	119.69	123.43
2	A	901	FAD	C1'-N10-C9A	2.52	120.28	118.29
3	A	902	FMN	C4A-C4-N3	-2.52	119.98	123.43
4	B	903	HEM	CAA-CBA-CGA	-2.49	108.50	112.67
3	A	902	FMN	C7M-C7-C6	-2.47	114.42	120.34
4	A	903	HEM	CAA-CBA-CGA	-2.42	108.61	112.67
3	B	902	FMN	C7M-C7-C6	-2.41	114.57	120.34
3	B	902	FMN	C4A-C4-N3	-2.41	120.13	123.43
3	A	902	FMN	C7M-C7-C8	2.40	125.66	120.74
3	B	902	FMN	C7M-C7-C8	2.38	125.62	120.74
2	B	901	FAD	C1'-N10-C9A	2.38	120.17	118.29
4	A	903	HEM	CMC-C2C-C3C	2.02	128.46	124.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	FAD	C5'-O5'-P-O2P
2	B	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	C5'-O5'-P-O3P
2	B	901	FAD	C5'-O5'-P-O1P
2	A	901	FAD	C5'-O5'-P-O2P
2	B	901	FAD	O3'-C3'-C4'-C5'

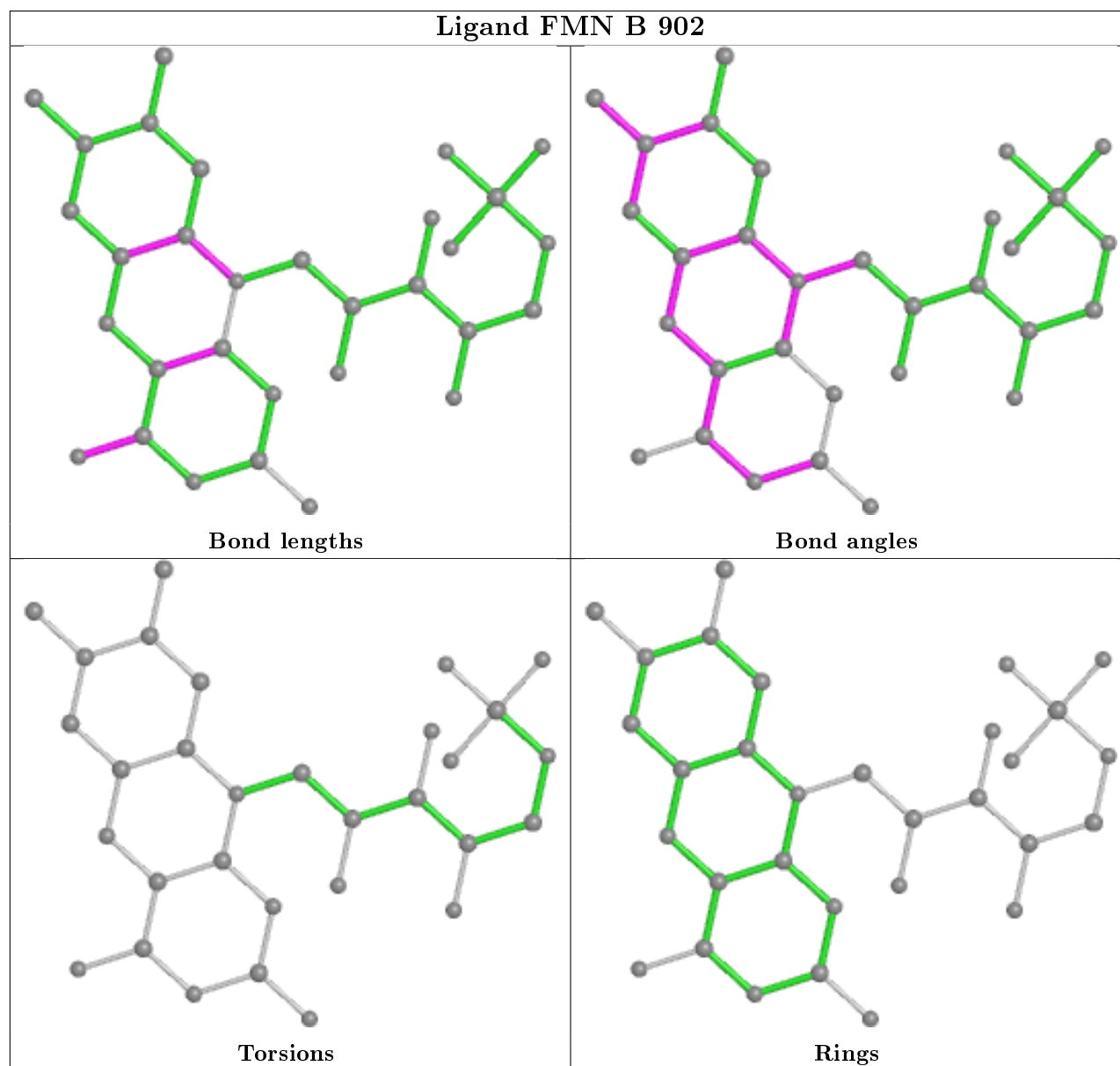
There are no ring outliers.

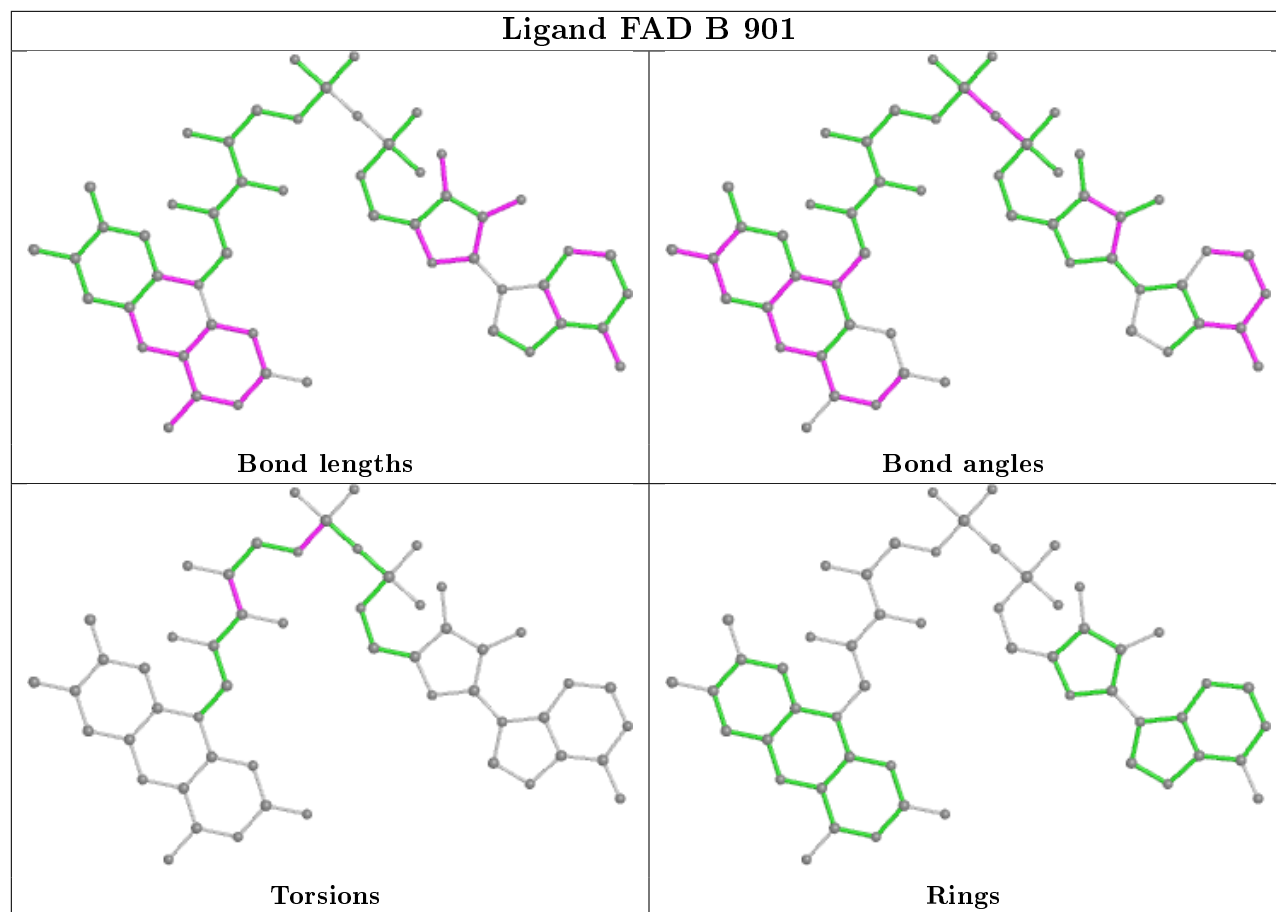
4 monomers are involved in 4 short contacts:

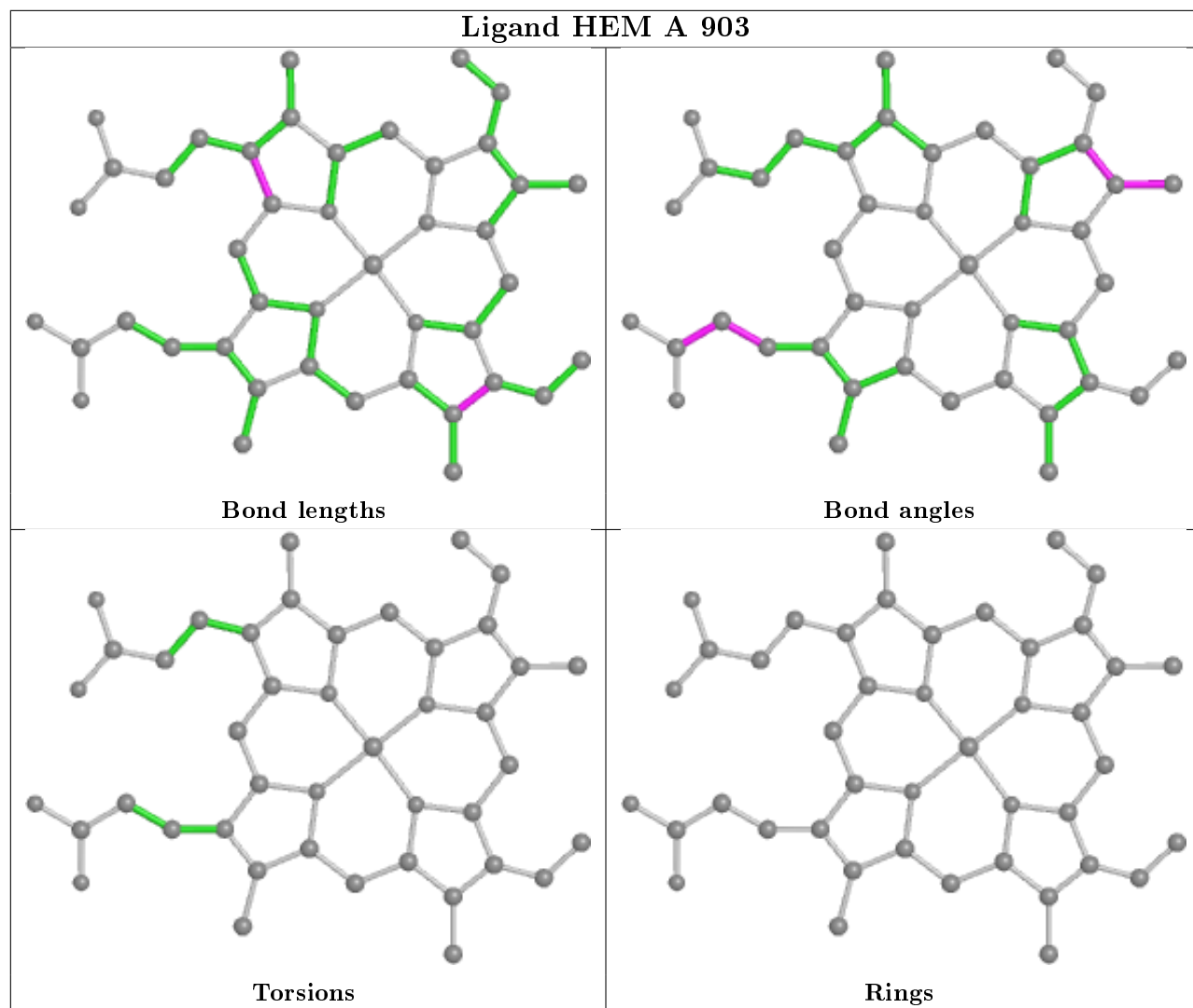
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	FMN	1	0
2	B	901	FAD	1	0
3	A	902	FMN	1	0
2	A	901	FAD	1	0

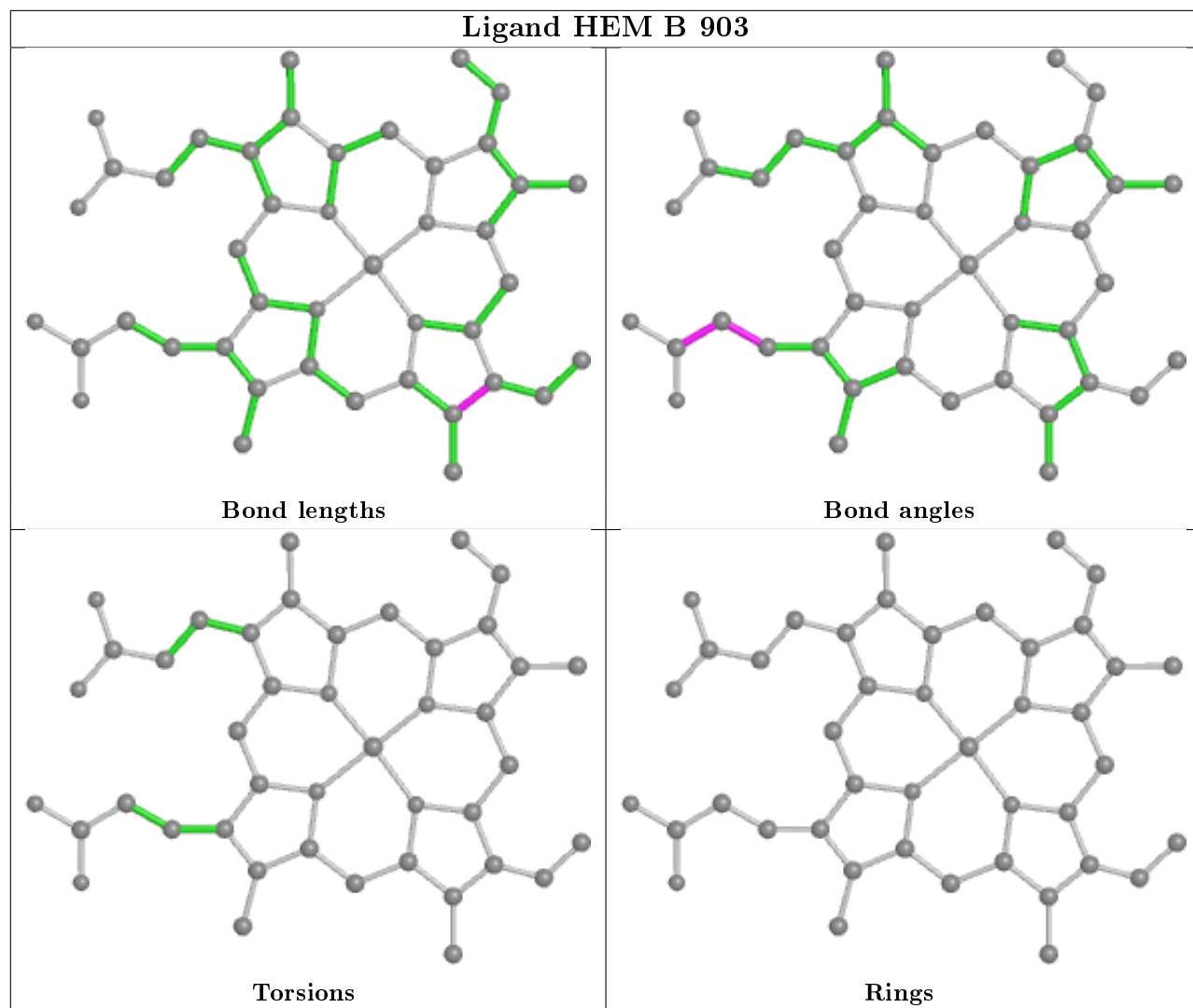
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

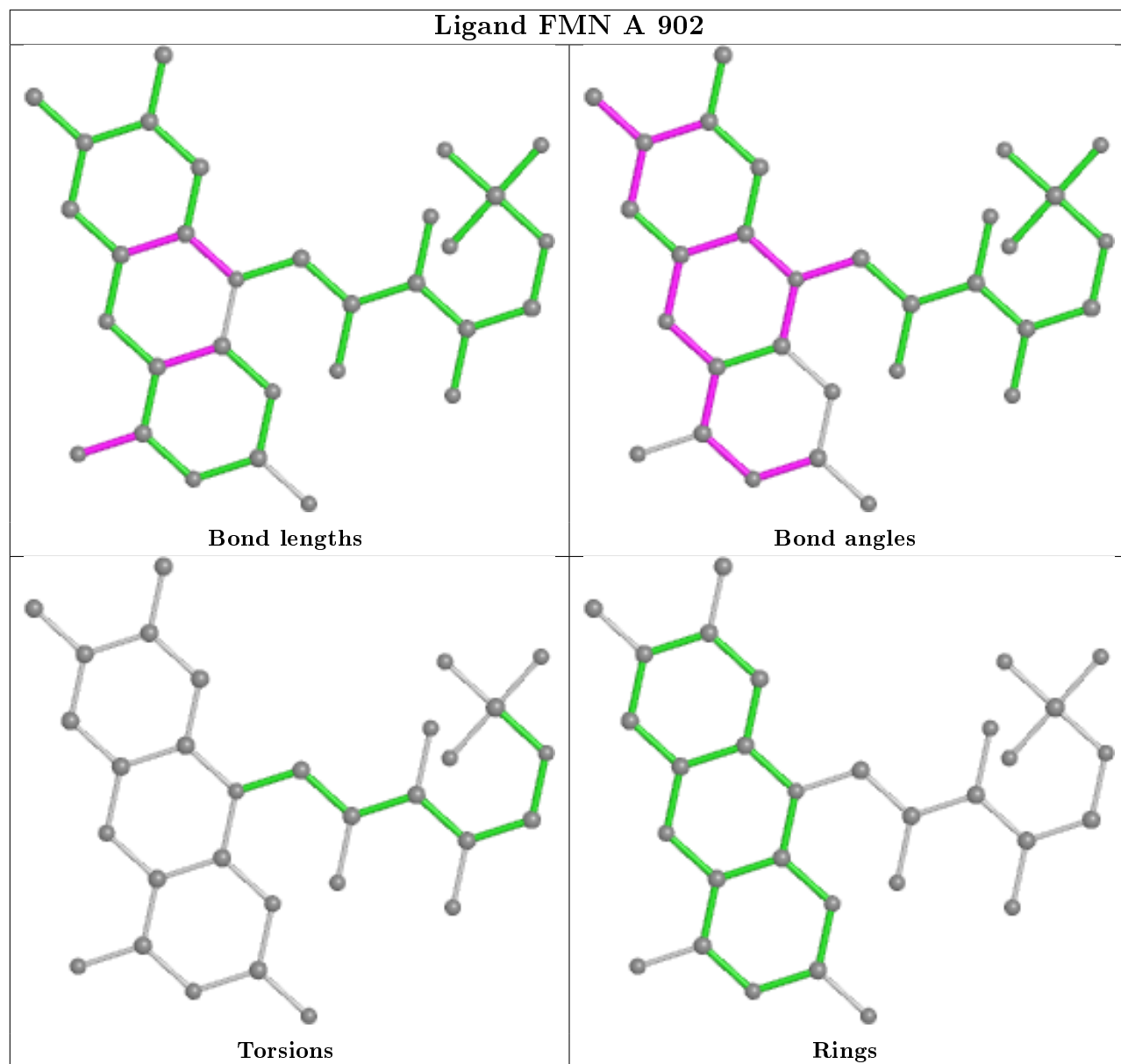
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

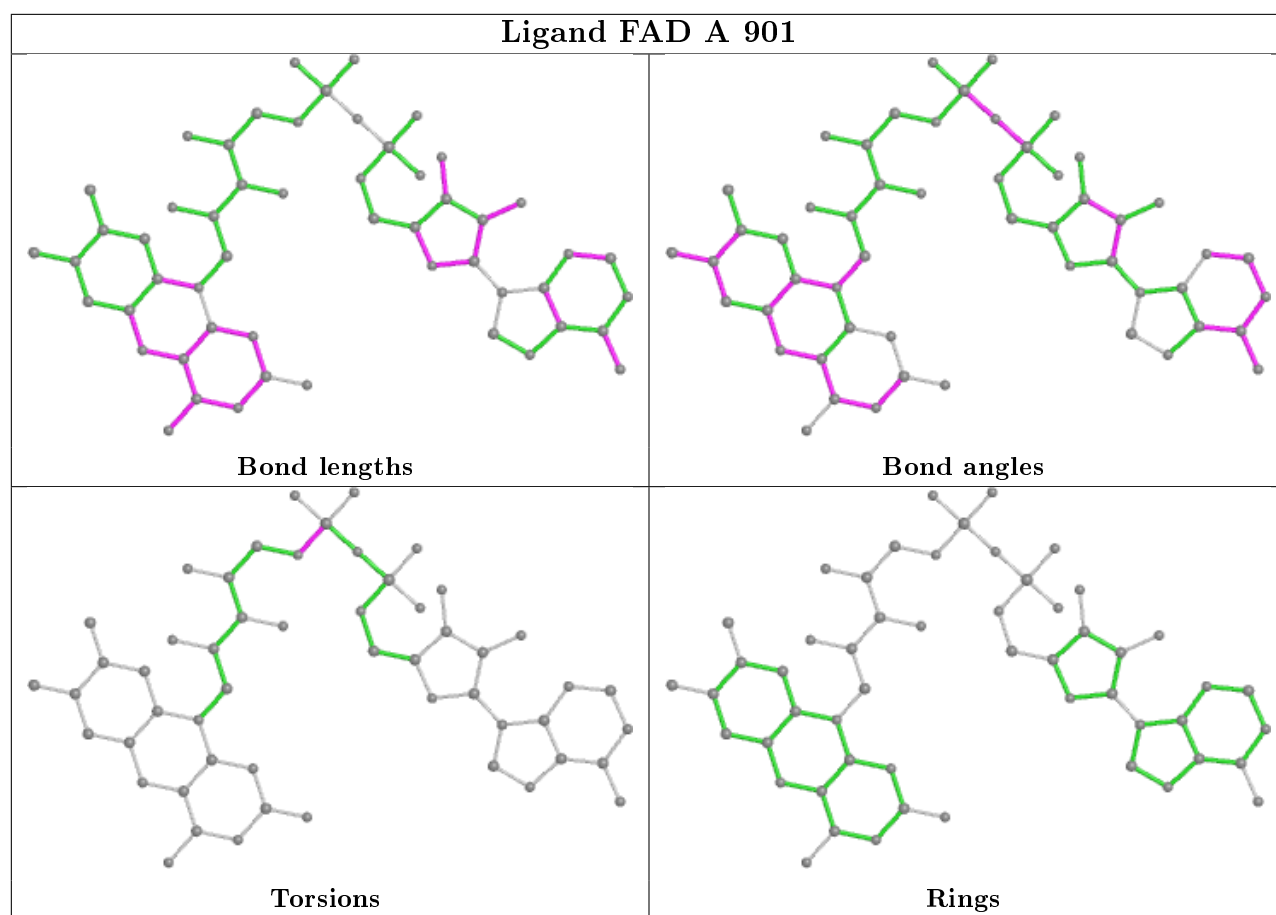












5.7 Other polymers [i](#)

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	816/871 (93%)	0.41	61 (7%) 14 14	74, 127, 188, 271	0
1	B	813/871 (93%)	0.55	68 (8%) 11 11	75, 123, 187, 230	0
All	All	1629/1742 (93%)	0.48	129 (7%) 12 12	74, 125, 187, 271	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	851	SER	5.4
1	B	309	LEU	5.4
1	A	543	ALA	5.1
1	A	775	LYS	5.1
1	B	246	PHE	4.7
1	B	592	TRP	4.6
1	A	412	ALA	4.5
1	B	578	MET	4.5
1	B	299	LEU	4.2
1	B	426	MET	4.2
1	B	377	ILE	4.1
1	B	259	VAL	4.0
1	B	296	LEU	3.9
1	A	424	GLU	3.9
1	B	257	ILE	3.9
1	A	681	LEU	3.9
1	B	599	HIS	3.9
1	A	377	ILE	3.8
1	B	431	VAL	3.8
1	B	679	ARG	3.7
1	A	344	LYS	3.6
1	B	603	ILE	3.6
1	A	309	LEU	3.5
1	A	593	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	10	SER	3.4
1	B	536	CYS	3.4
1	B	535	PRO	3.4
1	A	345	PHE	3.3
1	B	775	LYS	3.3
1	A	476	LEU	3.3
1	A	550	ILE	3.2
1	A	547	TYR	3.2
1	B	507	ILE	3.1
1	B	600	ILE	3.1
1	A	544	LEU	3.1
1	A	257	ILE	3.1
1	B	518	ILE	3.1
1	A	308	SER	3.1
1	A	404	VAL	3.0
1	B	581	SER	3.0
1	A	603	ILE	3.0
1	A	343	VAL	3.0
1	B	563	ALA	3.0
1	B	258	ILE	3.0
1	A	251	LYS	3.0
1	A	423	HIS	3.0
1	B	577	LYS	3.0
1	B	618	CYS	3.0
1	A	439	LEU	2.9
1	A	408	PHE	2.9
1	B	607	TYR	2.9
1	A	679	ARG	2.9
1	B	598	ARG	2.9
1	A	247	VAL	2.8
1	B	10	SER	2.8
1	A	430	LYS	2.8
1	B	420	LEU	2.8
1	B	521	LEU	2.7
1	A	540	TYR	2.7
1	B	421	VAL	2.7
1	B	519	MET	2.7
1	B	559	LEU	2.7
1	A	777	TYR	2.7
1	B	313	CYS	2.7
1	B	517	VAL	2.7
1	B	515	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	442	TYR	2.7
1	A	400	PHE	2.7
1	B	430	LYS	2.6
1	B	302	LEU	2.6
1	A	575	LEU	2.6
1	B	427	ASP	2.6
1	B	610	LEU	2.6
1	B	537	PRO	2.6
1	A	310	VAL	2.6
1	B	287	MET	2.6
1	A	369	LEU	2.5
1	B	423	HIS	2.5
1	B	562	LEU	2.5
1	A	285	ARG	2.5
1	A	556	THR	2.5
1	A	260	PHE	2.5
1	B	41	GLN	2.5
1	B	510	ILE	2.5
1	B	436	MET	2.5
1	A	256	ASN	2.4
1	A	646	ALA	2.4
1	A	312	PHE	2.4
1	B	275	LEU	2.4
1	A	600	ILE	2.4
1	B	294	TYR	2.4
1	A	598	ARG	2.3
1	B	684	MET	2.3
1	A	275	LEU	2.3
1	B	601	LEU	2.3
1	B	437	GLY	2.3
1	B	424	GLU	2.3
1	A	644	ILE	2.3
1	A	592	TRP	2.3
1	A	478	LEU	2.3
1	A	435	GLU	2.2
1	A	313	CYS	2.2
1	A	440	LYS	2.2
1	A	258	ILE	2.2
1	A	255	ARG	2.2
1	A	252	LYS	2.2
1	B	330	TYR	2.2
1	B	434	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	2.2
1	B	300	SER	2.1
1	A	428	VAL	2.1
1	B	332	TRP	2.1
1	B	422	VAL	2.1
1	A	41	GLN	2.1
1	A	604	LEU	2.1
1	A	745	ASP	2.1
1	B	566	ALA	2.1
1	A	411	GLU	2.1
1	A	321	ASP	2.1
1	B	337	ASP	2.1
1	B	312	PHE	2.1
1	B	511	LEU	2.1
1	A	347	VAL	2.1
1	B	776	VAL	2.1
1	B	807	ARG	2.0
1	A	560	TYR	2.0
1	B	346	ALA	2.0
1	B	526	GLU	2.0
1	B	401	TRP	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 carbohydrates 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.

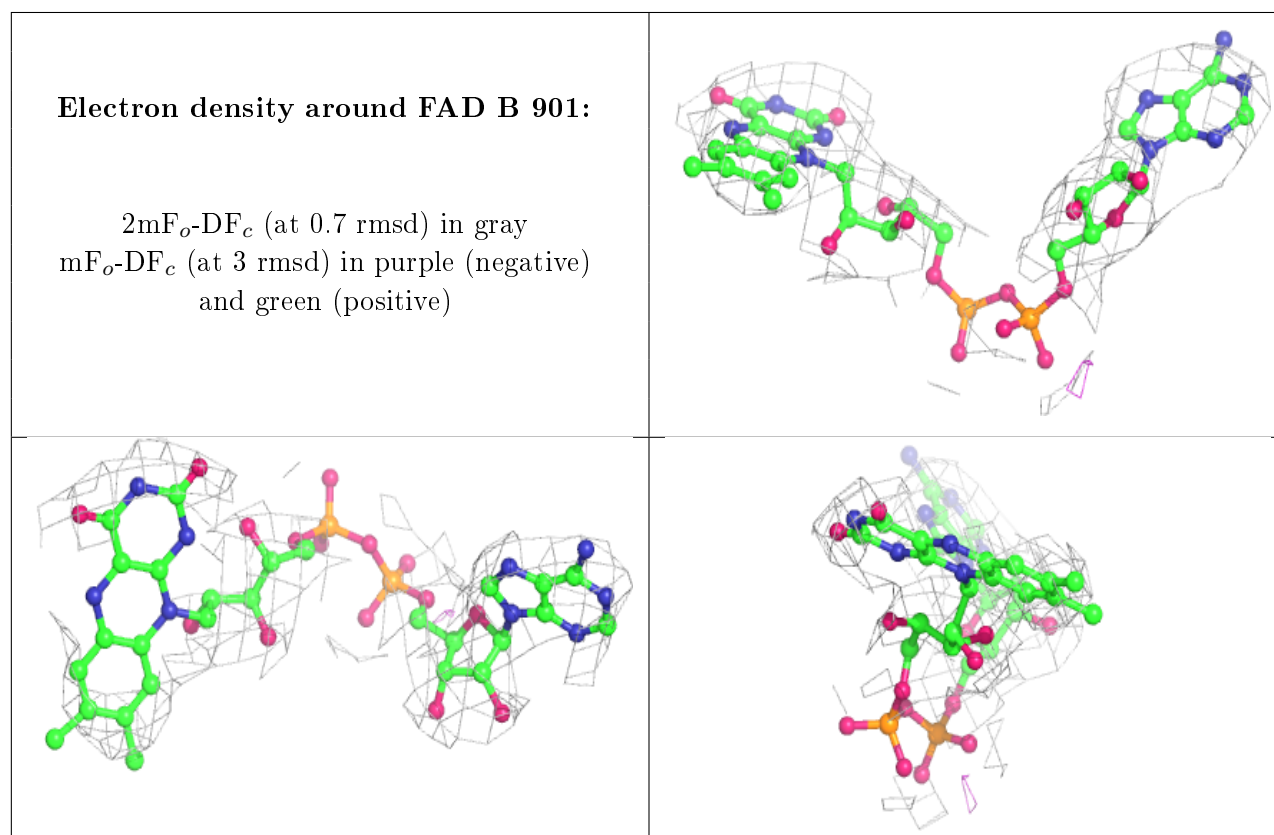
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	901	53/53	0.93	0.24	93,115,141,148	0
2	FAD	A	901	53/53	0.93	0.23	87,111,146,148	0

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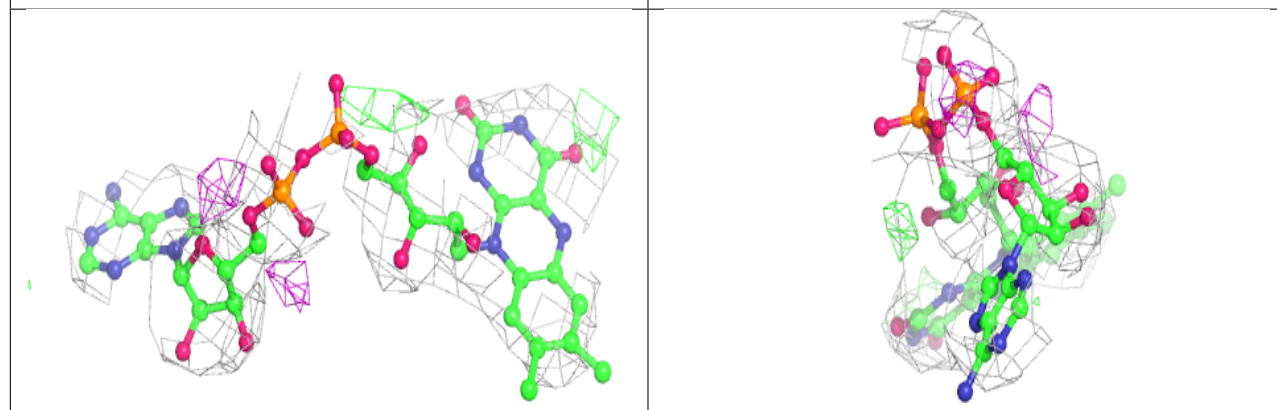
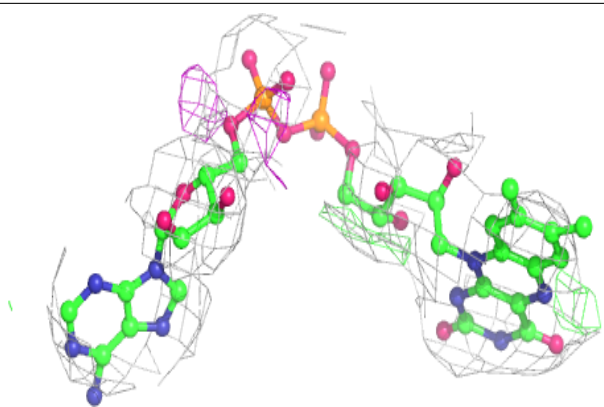
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMN	A	902	31/31	0.95	0.19	86,117,126,133	0
4	HEM	B	903	43/43	0.96	0.29	79,109,140,155	0
3	FMN	B	902	31/31	0.96	0.18	89,108,120,122	0
4	HEM	A	903	43/43	0.96	0.30	76,102,145,167	0

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.



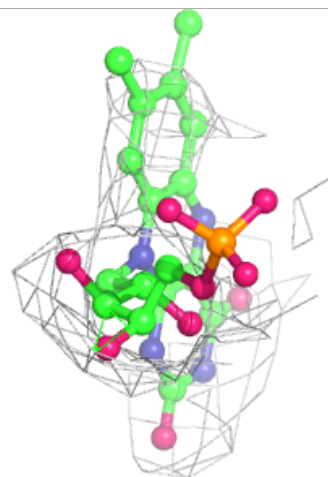
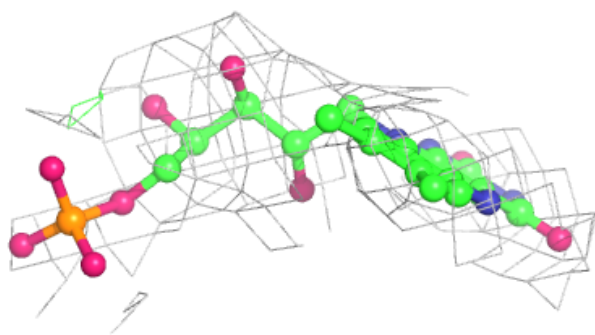
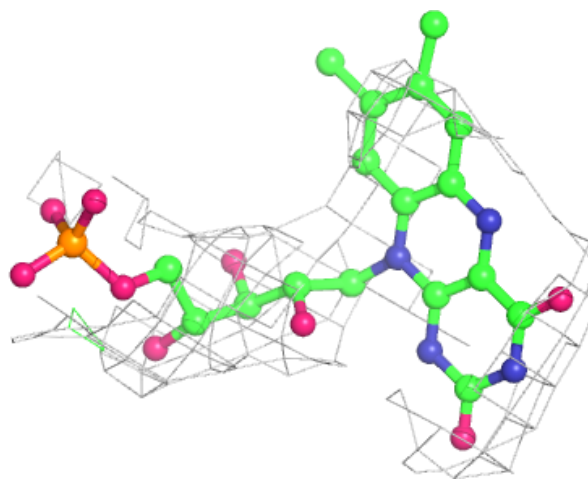
Electron density around FAD A 901:

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



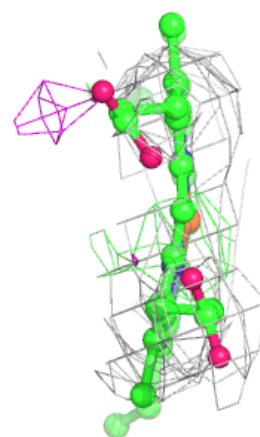
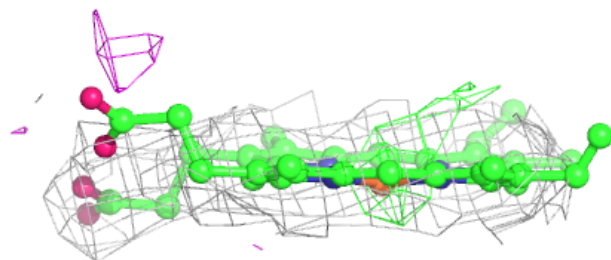
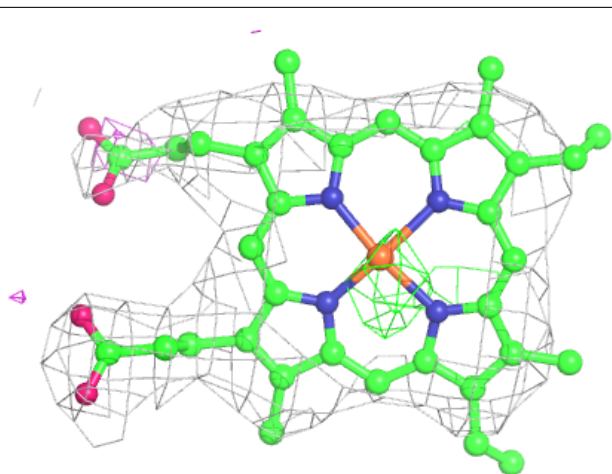
Electron density around FMN A 902:

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



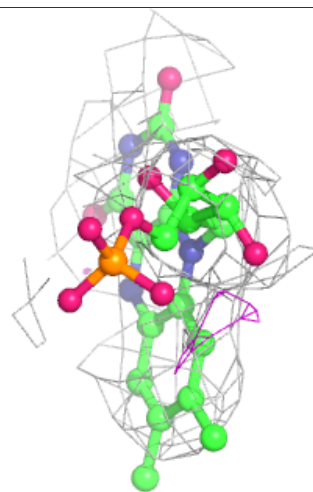
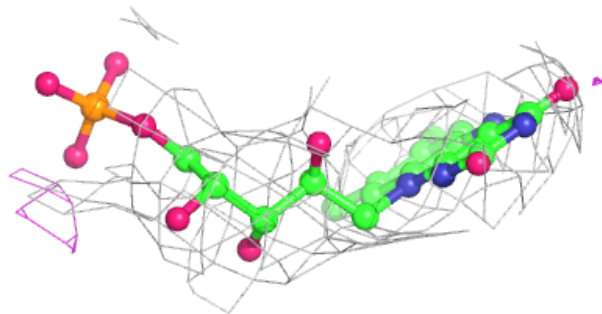
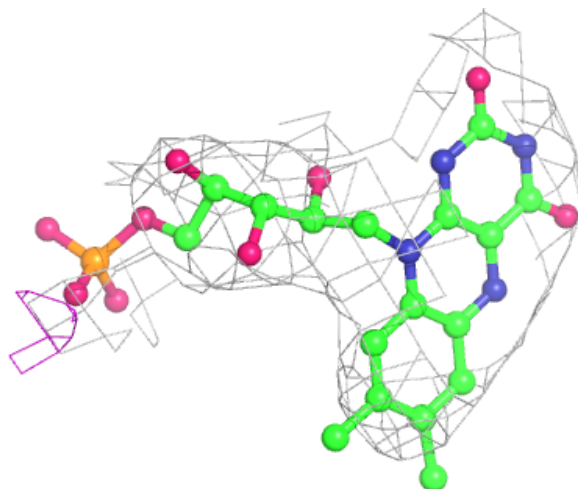
Electron density around HEM B 903:

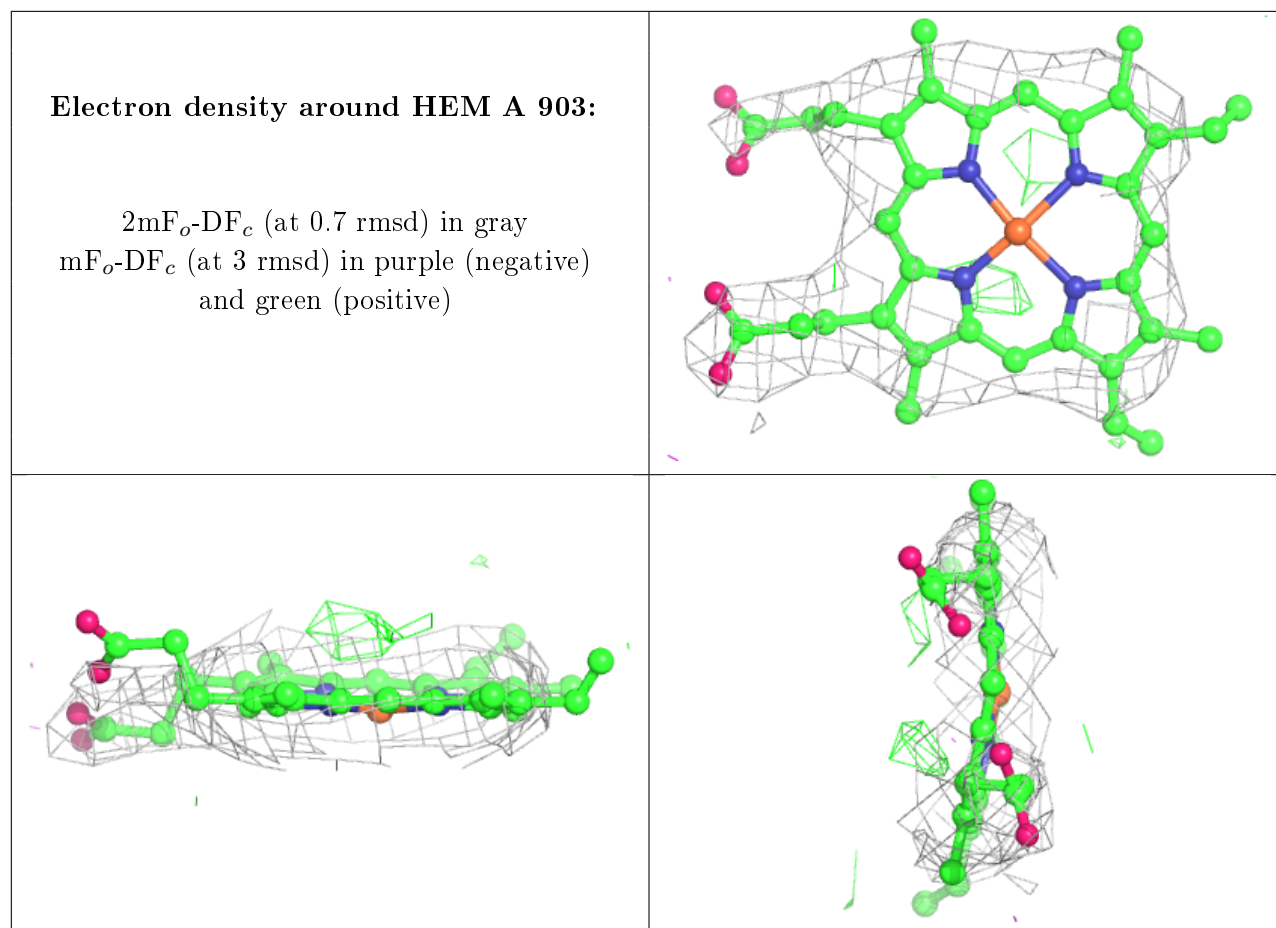
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 902:

$2mF_o-DF_c$ (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.