



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:42 am BST

PDB ID : 6J7I
Title : Fusion protein of heme oxygenase-1 and NADPH cytochrome P450 reductase (15aa)
Authors : Sugishima, M.; Sato, H.; Wada, K.; Yamamoto, K.
Deposited on : 2019-01-18
Resolution : 3.30 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 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

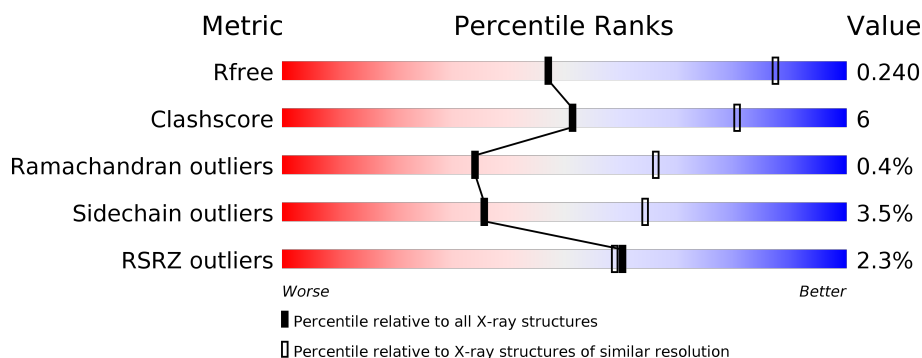
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	873	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 7%</div> </div> </div>
1	B	873	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13329 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	814	Total	C	N	O	S	0	0	0
			6530	4156	1118	1227	29			
1	B	815	Total	C	N	O	S	0	0	0
			6545	4162	1122	1232	29			

There are 54 discrepancies between the modelled and reference sequences:

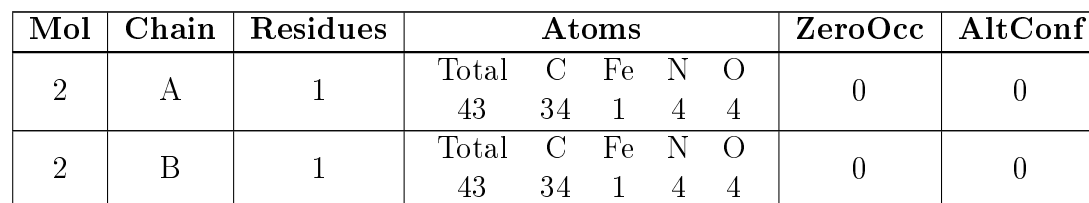
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P06762
A	-18	GLY	-	expression tag	UNP P06762
A	-17	SER	-	expression tag	UNP P06762
A	-16	SER	-	expression tag	UNP P06762
A	-15	HIS	-	expression tag	UNP P06762
A	-14	HIS	-	expression tag	UNP P06762
A	-13	HIS	-	expression 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	236	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	236	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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # FAD

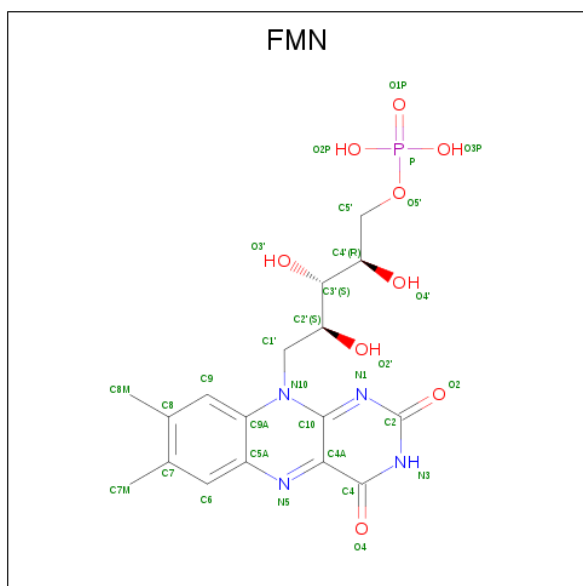
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

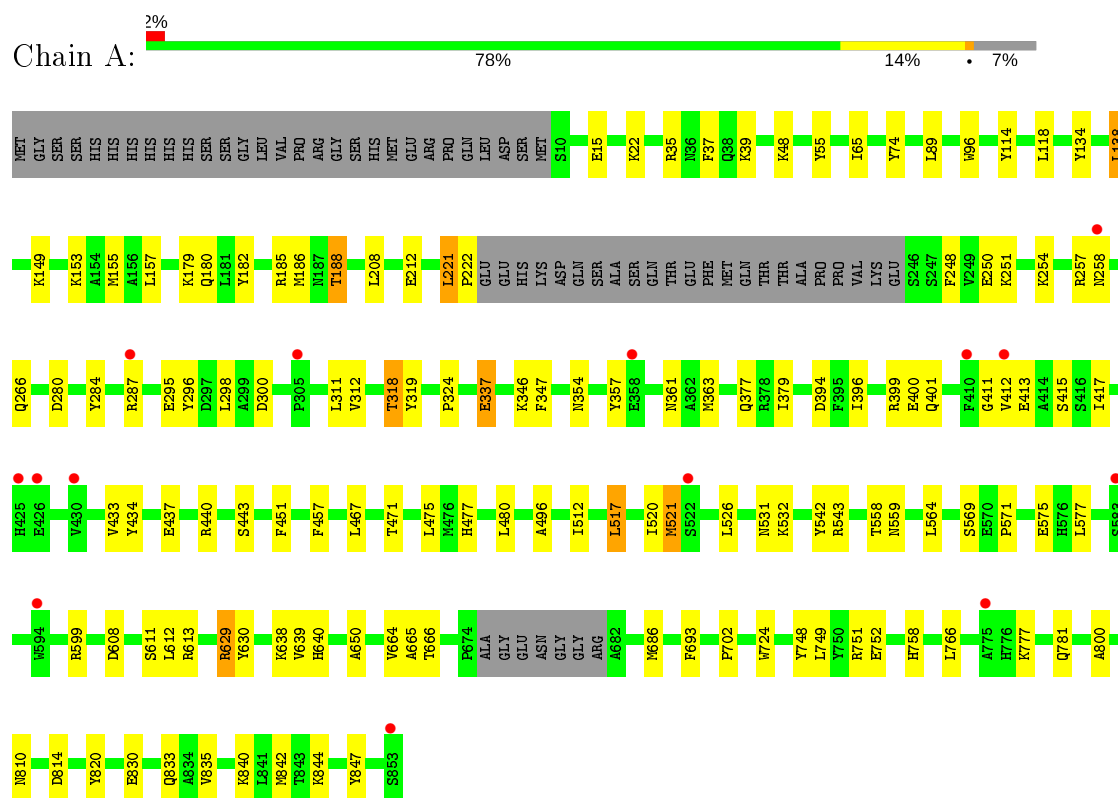


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

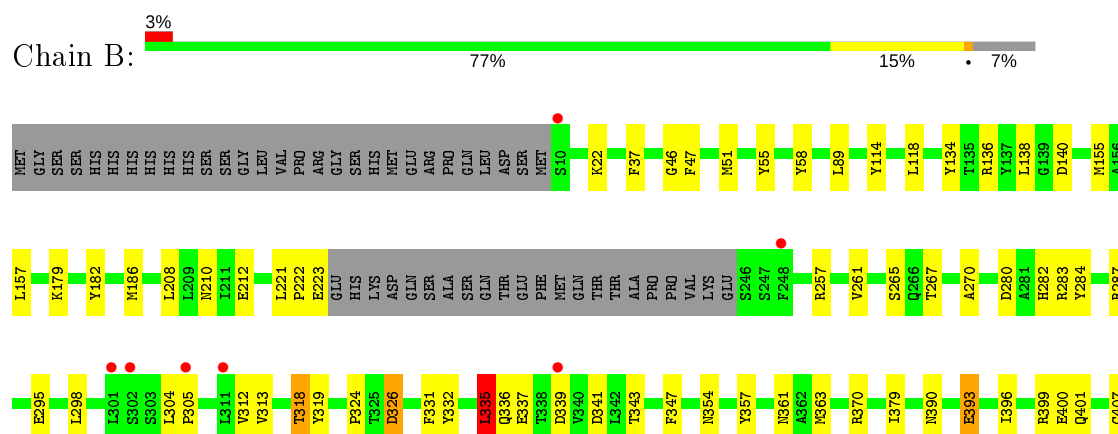
3 Residue-property plots [i](#)

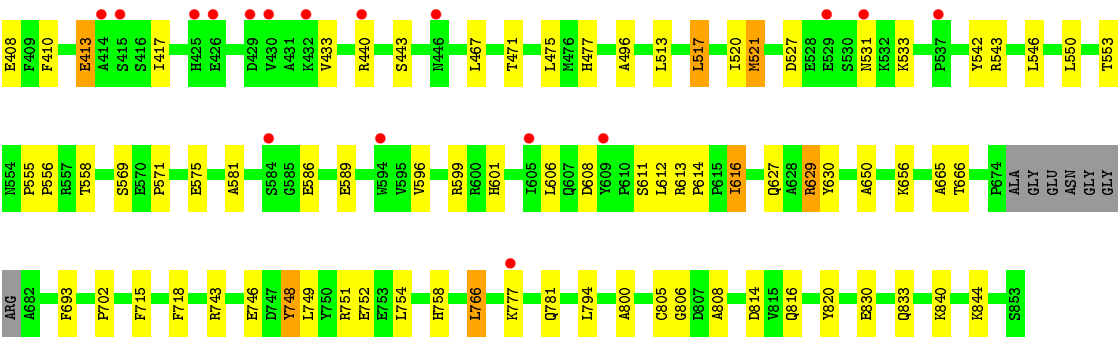
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.77Å 158.10Å 188.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.04 – 3.30 40.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (40.04-3.30) 89.5 (40.04-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.192 , 0.241 0.192 , 0.240	Depositor DCC
R_{free} test set	1973 reflections (5.81%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.6	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	0.91	EDS
Total number of atoms	13329	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/6690	0.44	0/9058
1	B	0.26	0/6706	0.44	1/9081 (0.0%)
All	All	0.27	0/13396	0.44	1/18139 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	335	LEU	CA-CB-CG	5.71	128.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	527	ASP	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6530	0	6342	72	0
1	B	6545	0	6344	81	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	53	0	30	1	0
3	B	53	0	30	0	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
All	All	13329	0	12844	147	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 6.

All (147) 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:265:SER:HB2	1:B:270:ALA:HB3	1.73	0.70
1:B:257:ARG:HG2	1:B:287:ARG:HG2	1.74	0.69
1:B:440:ARG:HG3	1:B:443:SER:HB3	1.75	0.69
1:B:138:LEU:HD13	1:B:179:LYS:HG2	1.76	0.68
1:A:138:LEU:HD13	1:A:179:LYS:HG2	1.76	0.67
1:B:571:PRO:O	1:B:575:GLU:HB2	1.95	0.66
1:A:810:ASN:HB3	1:B:336:GLN:HE22	1.60	0.65
1:B:569:SER:H	1:B:611:SER:HB3	1.62	0.65
1:A:569:SER:H	1:A:611:SER:HB3	1.62	0.65
1:A:346:LYS:NZ	1:A:377:GLN:OE1	2.31	0.64
1:B:282:HIS:HB3	1:B:283:ARG:HH21	1.62	0.64
1:A:517:LEU:HB3	1:A:543:ARG:HB2	1.79	0.64
1:A:810:ASN:OD1	1:B:332:TYR:OH	2.16	0.63
1:B:781:GLN:HG2	1:B:814:ASP:HB3	1.82	0.62
1:A:512:ILE:O	1:A:613:ARG:NH1	2.33	0.61
1:B:280:ASP:OD2	1:B:399:ARG:NH1	2.30	0.61
1:B:629:ARG:HD3	1:B:665:ALA:HB2	1.82	0.61
1:B:751:ARG:NH1	1:B:752:GLU:OE2	2.34	0.61
1:A:433:VAL:HG21	1:A:520:ILE:HD13	1.82	0.59
1:A:250:GLU:O	1:A:254:LYS:HG2	2.01	0.59
1:A:629:ARG:HD3	1:A:665:ALA:HB2	1.84	0.58
1:B:58:TYR:OH	1:B:140:ASP:OD2	2.19	0.57
1:B:546:LEU:HD12	1:B:550:LEU:HD12	1.87	0.57
1:B:513:LEU:HD23	1:B:616:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:PRO:HG2	1:B:800:ALA:HB2	1.86	0.57
1:B:331:PHE:O	1:B:335:LEU:HD23	2.05	0.56
1:B:433:VAL:HG21	1:B:520:ILE:HD13	1.87	0.56
1:A:612:LEU:O	1:A:613:ARG:NE	2.33	0.56
1:B:612:LEU:O	1:B:613:ARG:NE	2.38	0.56
1:A:55:TYR:HA	1:A:89:LEU:HD13	1.88	0.55
1:A:781:GLN:HG2	1:A:814:ASP:HB3	1.88	0.55
1:A:149:LYS:O	1:A:153:LYS:HG2	2.06	0.55
1:B:55:TYR:HA	1:B:89:LEU:HD13	1.90	0.54
1:B:324:PRO:HB3	1:B:363:MET:SD	2.47	0.54
1:A:475:LEU:HD22	1:A:749:LEU:HD21	1.90	0.54
1:A:182:TYR:O	1:A:186:MET:HG3	2.08	0.54
1:B:475:LEU:HD22	1:B:749:LEU:HD21	1.90	0.54
1:B:326:ASP:N	1:B:326:ASP:OD1	2.39	0.53
1:A:577:LEU:HD11	1:A:612:LEU:HD21	1.89	0.53
1:A:702:PRO:HG2	1:A:800:ALA:HB2	1.89	0.53
1:A:280:ASP:OD2	1:A:399:ARG:HD2	2.09	0.53
1:A:564:LEU:HB3	1:A:612:LEU:HD11	1.91	0.53
1:A:842:MET:HG2	1:A:847:TYR:HB3	1.90	0.53
1:A:180:GLN:NE2	1:A:842:MET:O	2.31	0.52
1:A:295:GLU:OE1	1:A:295:GLU:N	2.38	0.52
1:B:221:LEU:O	1:B:223:GLU:N	2.43	0.52
1:B:396:ILE:O	1:B:400:GLU:HB2	2.09	0.52
1:B:513:LEU:HD11	1:B:614:PRO:HD2	1.92	0.51
1:B:586:GLU:O	1:B:589:GLU:HB2	2.11	0.51
1:B:390:ASN:HB3	1:B:393:GLU:HB2	1.93	0.50
1:A:440:ARG:HG3	1:A:443:SER:HB3	1.93	0.50
1:A:296:TYR:O	1:A:298:LEU:HD22	2.12	0.50
1:B:341:ASP:OD1	1:B:343:THR:OG1	2.19	0.50
1:A:48:LYS:HG2	1:A:96:TRP:HB3	1.94	0.49
1:A:257:ARG:HG2	1:A:287:ARG:HG2	1.94	0.49
1:A:751:ARG:NH1	1:A:752:GLU:OE2	2.45	0.49
1:A:820:TYR:CZ	1:A:835:VAL:HG23	2.48	0.49
1:B:318:THR:HG21	1:B:361:ASN:HA	1.95	0.49
1:A:221:LEU:N	1:A:222:PRO:HD2	2.28	0.49
1:B:284:TYR:HA	1:B:417:ILE:HD13	1.93	0.49
1:A:248:PHE:CE1	1:A:300:ASP:HB2	2.48	0.49
1:B:401:GLN:HG2	1:B:558:THR:HB	1.95	0.49
1:B:521:MET:HG2	1:B:542:TYR:CZ	2.48	0.49
1:A:354:ASN:HB3	1:A:357:TYR:HD1	1.76	0.49
1:A:22:LYS:HE2	1:B:833:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:O	1:A:188:THR:HG22	2.13	0.48
1:A:569:SER:N	1:A:611:SER:HB3	2.25	0.48
1:B:182:TYR:O	1:B:186:MET:HG3	2.12	0.48
1:B:261:VAL:HG13	1:B:313:VAL:HB	1.96	0.48
1:A:411:GLY:O	1:A:413:GLU:N	2.38	0.48
1:A:248:PHE:HA	1:A:251:LYS:HB3	1.95	0.48
1:B:467:LEU:HD11	1:B:477:HIS:HB2	1.96	0.47
1:B:754:LEU:HB3	1:B:766:LEU:HD11	1.95	0.47
1:A:134:TYR:HB2	1:A:186:MET:HE1	1.96	0.47
1:A:318:THR:HG21	1:A:361:ASN:HA	1.97	0.47
1:B:596:VAL:O	1:B:599:ARG:HD2	2.15	0.47
1:A:531:ASN:OD1	1:A:531:ASN:N	2.47	0.46
1:B:304:LEU:N	1:B:305:PRO:HD2	2.30	0.46
1:B:136:ARG:NH1	1:B:210:ASN:OD1	2.48	0.46
1:B:354:ASN:HB3	1:B:357:TYR:HD1	1.81	0.46
1:B:531:ASN:N	1:B:531:ASN:OD1	2.48	0.46
1:B:47:PHE:O	1:B:51:MET:HG2	2.16	0.46
1:A:354:ASN:HB3	1:A:357:TYR:CD1	2.50	0.46
1:A:571:PRO:O	1:A:575:GLU:HB2	2.15	0.46
1:A:434:TYR:HD1	1:A:437:GLU:HG2	1.81	0.46
1:A:324:PRO:HB3	1:A:363:MET:SD	2.56	0.45
1:A:451:PHE:CG	1:A:457:PHE:HB2	2.50	0.45
1:B:298:LEU:HD22	1:B:331:PHE:CE1	2.51	0.45
1:A:312:VAL:O	1:A:347:PHE:HA	2.17	0.45
1:B:533:LYS:HA	1:B:533:LYS:HD3	1.80	0.45
1:A:337:GLU:O	1:B:777:LYS:NZ	2.45	0.45
1:A:400:GLU:O	1:A:559:ASN:HB3	2.17	0.45
1:A:496:ALA:HB2	1:A:630:TYR:CE2	2.52	0.45
1:B:816:GLN:HG2	1:B:820:TYR:CZ	2.51	0.45
1:A:396:ILE:O	1:A:400:GLU:HB2	2.17	0.45
1:B:134:TYR:HB2	1:B:186:MET:HE1	1.99	0.45
1:A:480:LEU:HD23	1:A:686:MET:HG2	1.98	0.44
1:A:346:LYS:HG3	1:A:379:ILE:HD11	2.00	0.44
1:A:15:GLU:OE1	1:A:844:LYS:HE2	2.18	0.44
1:B:282:HIS:NE2	1:B:287:ARG:HG3	2.33	0.44
1:B:627:GLN:O	1:B:629:ARG:NE	2.50	0.44
1:B:46:GLY:HA3	1:B:221:LEU:HD11	2.00	0.43
1:B:612:LEU:HA	1:B:612:LEU:HD23	1.82	0.43
1:A:639:VAL:HG23	1:A:640:HIS:ND1	2.33	0.43
1:A:650:ALA:HA	1:A:666:THR:HB	1.99	0.43
1:A:840:LYS:O	1:A:844:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:O	1:A:39:LYS:HG2	2.18	0.43
1:B:805:CYS:SG	1:B:806:GLY:N	2.91	0.43
1:A:467:LEU:HD11	1:A:477:HIS:HB2	2.00	0.43
1:A:526:LEU:HA	1:A:526:LEU:HD23	1.83	0.43
1:B:134:TYR:HB2	1:B:186:MET:CE	2.48	0.43
1:B:496:ALA:HB2	1:B:630:TYR:CE2	2.53	0.43
1:B:650:ALA:HA	1:B:666:THR:HB	2.01	0.43
1:A:417:ILE:H	1:A:417:ILE:HD12	1.84	0.43
1:A:65:ILE:HG23	1:A:74:TYR:CE2	2.54	0.43
1:A:401:GLN:HG2	1:A:558:THR:HB	2.01	0.43
1:A:521:MET:HG2	1:A:542:TYR:CZ	2.54	0.43
1:B:407:CYS:O	1:B:413:GLU:HG3	2.19	0.43
1:B:715:PHE:O	1:B:718:PHE:HB2	2.18	0.42
1:B:830:GLU:HG2	1:B:833:GLN:OE1	2.19	0.42
1:A:629:ARG:NH1	3:A:902:FAD:O1P	2.51	0.42
1:B:743:ARG:NH1	1:B:746:GLU:HB2	2.34	0.42
1:B:569:SER:N	1:B:611:SER:HB3	2.33	0.42
1:A:629:ARG:NH1	1:A:664:VAL:HB	2.35	0.42
1:B:335:LEU:HD12	1:B:370:ARG:HG2	2.00	0.42
1:B:134:TYR:O	1:B:138:LEU:HB2	2.19	0.42
1:B:558:THR:HG23	1:B:581:ALA:HA	2.01	0.42
1:B:208:LEU:O	1:B:212:GLU:HG2	2.20	0.41
1:B:748:TYR:CD2	1:B:751:ARG:HG3	2.55	0.41
1:A:532:LYS:H	1:A:532:LYS:HG2	1.61	0.41
1:B:656:LYS:H	1:B:656:LYS:HG2	1.62	0.41
1:A:134:TYR:HB2	1:A:186:MET:CE	2.50	0.41
1:B:267:THR:HG22	1:B:319:TYR:OH	2.20	0.41
1:B:312:VAL:O	1:B:347:PHE:HA	2.21	0.41
1:B:517:LEU:HB3	1:B:543:ARG:HB2	2.03	0.41
1:B:840:LYS:HA	1:B:840:LYS:HD2	1.86	0.41
1:B:840:LYS:O	1:B:844:LYS:HG3	2.20	0.41
1:A:266:GLN:HB2	1:A:319:TYR:CZ	2.56	0.41
1:A:638:LYS:HD3	1:A:724:TRP:CZ3	2.56	0.41
1:B:555:PRO:HA	1:B:556:PRO:HD3	1.85	0.41
1:B:553:THR:O	1:B:601:HIS:HB3	2.21	0.41
1:A:833:GLN:NE2	1:B:22:LYS:HE2	2.36	0.40
1:B:298:LEU:HD13	1:B:331:PHE:CD1	2.56	0.40
1:A:208:LEU:O	1:A:212:GLU:HG2	2.22	0.40
1:A:777:LYS:NZ	1:B:337:GLU:O	2.39	0.40
1:B:513:LEU:HD12	1:B:513:LEU:HA	1.79	0.40
1:B:513:LEU:HD13	1:B:606:LEU:HD13	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	808/873 (93%)	757 (94%)	48 (6%)	3 (0%)	34	66
1	B	809/873 (93%)	758 (94%)	48 (6%)	3 (0%)	34	66
All	All	1617/1746 (93%)	1515 (94%)	96 (6%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	VAL
1	B	808	ALA
1	B	413	GLU
1	A	415	SER
1	B	222	PRO
1	A	221	LEU

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	692/748 (92%)	668 (96%)	24 (4%)	36	64
1	B	694/748 (93%)	669 (96%)	25 (4%)	35	63
All	All	1386/1496 (93%)	1337 (96%)	49 (4%)	36	64

All (49) 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	138	LEU
1	A	155	MET
1	A	157	LEU
1	A	188	THR
1	A	258	ASN
1	A	284	TYR
1	A	311	LEU
1	A	318	THR
1	A	337	GLU
1	A	394	ASP
1	A	471	THR
1	A	517	LEU
1	A	521	MET
1	A	599	ARG
1	A	608	ASP
1	A	629	ARG
1	A	693	PHE
1	A	748	TYR
1	A	758	HIS
1	A	766	LEU
1	A	830	GLU
1	B	37	PHE
1	B	114	TYR
1	B	118	LEU
1	B	155	MET
1	B	157	LEU
1	B	295	GLU
1	B	318	THR
1	B	326	ASP
1	B	335	LEU
1	B	339	ASP
1	B	379	ILE
1	B	393	GLU
1	B	408	GLU
1	B	410	PHE
1	B	471	THR
1	B	517	LEU
1	B	521	MET
1	B	608	ASP

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Mol	Chain	Res	Type
1	B	616	ILE
1	B	629	ARG
1	B	693	PHE
1	B	748	TYR
1	B	758	HIS
1	B	766	LEU
1	B	794	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	401	GLN
1	A	816	GLN
1	B	559	ASN
1	B	645	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
4	FMN	B	903	-	31,33,33	1.31	4 (12%)	40,50,50	2.32	8 (20%)
4	FMN	A	903	-	31,33,33	1.29	4 (12%)	40,50,50	2.45	9 (22%)
2	HEM	A	901	1	27,50,50	0.92	1 (3%)	17,82,82	1.39	3 (17%)
2	HEM	B	901	1	27,50,50	0.94	1 (3%)	17,82,82	1.48	3 (17%)
3	FAD	A	902	-	51,58,58	4.63	18 (35%)	60,89,89	2.64	12 (20%)
3	FAD	B	902	-	51,58,58	4.65	18 (35%)	60,89,89	2.69	13 (21%)

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
4	FMN	B	903	-	-	0/18/18/18	0/3/3/3
4	FMN	A	903	-	-	0/18/18/18	0/3/3/3
2	HEM	A	901	1	-	0/6/54/54	-
2	HEM	B	901	1	-	0/6/54/54	-
3	FAD	A	902	-	-	4/30/50/50	0/6/6/6
3	FAD	B	902	-	-	6/30/50/50	0/6/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	FAD	O4B-C1B	15.25	1.62	1.41
3	B	902	FAD	O4B-C1B	15.24	1.62	1.41
3	B	902	FAD	C2B-C1B	-14.87	1.31	1.53
3	A	902	FAD	C2B-C1B	-14.84	1.31	1.53
3	B	902	FAD	C10-N1	10.54	1.46	1.33
3	A	902	FAD	C10-N1	10.31	1.46	1.33
3	A	902	FAD	C4X-N5	8.74	1.45	1.33
3	A	902	FAD	C5X-N5	8.67	1.49	1.35
3	B	902	FAD	C4X-N5	8.62	1.45	1.33
3	B	902	FAD	C5X-N5	8.53	1.49	1.35
3	B	902	FAD	C9A-N10	8.33	1.49	1.38
3	A	902	FAD	C9A-N10	8.19	1.49	1.38
3	A	902	FAD	C4-N3	7.75	1.46	1.33
3	B	902	FAD	C4-N3	7.49	1.46	1.33
3	B	902	FAD	C4X-C10	6.90	1.45	1.38
3	A	902	FAD	C4X-C10	6.70	1.45	1.38
3	B	902	FAD	O4B-C4B	-6.42	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	FAD	O4B-C4B	-6.34	1.30	1.45
3	B	902	FAD	C4-C4X	5.94	1.51	1.41
3	A	902	FAD	C4-C4X	5.90	1.51	1.41
3	A	902	FAD	C2-N3	5.88	1.49	1.38
3	B	902	FAD	C2-N3	5.73	1.49	1.38
3	B	902	FAD	C2-N1	5.25	1.48	1.38
3	A	902	FAD	C2-N1	5.07	1.48	1.38
3	B	902	FAD	C6A-N6A	3.15	1.45	1.34
3	A	902	FAD	C6A-N6A	3.13	1.45	1.34
2	B	901	HEM	C3B-C2B	-3.06	1.36	1.40
3	B	902	FAD	O3B-C3B	-3.01	1.35	1.43
3	B	902	FAD	O2B-C2B	2.99	1.50	1.43
3	A	902	FAD	O2B-C2B	2.96	1.49	1.43
2	A	901	HEM	C3B-C2B	-2.92	1.36	1.40
3	A	902	FAD	O3B-C3B	-2.92	1.36	1.43
4	B	903	FMN	C4A-C10	-2.66	1.36	1.38
4	A	903	FMN	C4A-C10	-2.63	1.36	1.38
3	A	902	FAD	C5A-C4A	-2.63	1.34	1.40
3	B	902	FAD	C5A-C4A	-2.58	1.34	1.40
4	A	903	FMN	C9A-C5A	-2.50	1.37	1.42
4	B	903	FMN	C9A-C5A	-2.47	1.37	1.42
3	B	902	FAD	C2A-N3A	2.41	1.36	1.32
4	A	903	FMN	C9A-N10	-2.36	1.35	1.38
3	B	902	FAD	O4-C4	-2.34	1.18	1.24
4	B	903	FMN	C9A-N10	-2.30	1.35	1.38
3	A	902	FAD	C2A-N3A	2.28	1.35	1.32
4	B	903	FMN	O4-C4	-2.25	1.18	1.24
3	A	902	FAD	O4-C4	-2.25	1.18	1.24
4	A	903	FMN	O4-C4	-2.19	1.19	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	FAD	C5A-C6A-N6A	12.57	139.46	120.35
3	A	902	FAD	C5A-C6A-N6A	12.32	139.08	120.35
4	A	903	FMN	C1'-N10-C9A	10.77	126.77	118.29
4	B	903	FMN	C1'-N10-C9A	10.10	126.24	118.29
3	B	902	FAD	N6A-C6A-N1A	-8.75	100.41	118.57
3	A	902	FAD	N6A-C6A-N1A	-8.60	100.73	118.57
4	A	903	FMN	C4-N3-C2	5.75	120.00	115.14
3	A	902	FAD	C4-N3-C2	5.67	119.93	115.14
4	B	903	FMN	C4-N3-C2	5.62	119.89	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	FAD	N3A-C2A-N1A	-5.58	119.96	128.68
4	A	903	FMN	C1'-N10-C10	-5.57	113.42	118.41
3	B	902	FAD	N3A-C2A-N1A	-5.48	120.11	128.68
3	B	902	FAD	C4-N3-C2	5.48	119.77	115.14
3	B	902	FAD	C7M-C7-C8	5.04	131.06	120.74
4	B	903	FMN	C1'-N10-C10	-4.92	114.00	118.41
3	B	902	FAD	C7M-C7-C6	-4.86	108.71	120.34
3	A	902	FAD	C7M-C7-C8	4.26	129.47	120.74
3	A	902	FAD	C7M-C7-C6	-4.26	110.16	120.34
4	A	903	FMN	C4A-N5-C5A	3.57	120.34	116.77
3	A	902	FAD	C3B-C2B-C1B	3.57	106.35	100.98
3	B	902	FAD	C5X-C9A-N10	3.52	120.27	117.72
3	B	902	FAD	P-O3P-PA	-3.51	120.79	132.83
3	A	902	FAD	C5X-C9A-N10	3.47	120.23	117.72
2	B	901	HEM	CAA-CBA-CGA	-3.46	106.87	112.67
3	B	902	FAD	C3B-C2B-C1B	3.45	106.17	100.98
3	A	902	FAD	P-O3P-PA	-3.40	121.17	132.83
4	B	903	FMN	C4A-N5-C5A	3.13	119.90	116.77
3	B	902	FAD	C4X-N5-C5X	2.97	119.74	116.77
3	A	902	FAD	C4X-N5-C5X	2.86	119.62	116.77
3	A	902	FAD	C1'-N10-C9A	2.84	120.53	118.29
4	B	903	FMN	C5A-C9A-N10	2.80	119.74	117.72
3	A	902	FAD	C4X-C4-N3	-2.78	119.64	123.43
2	A	901	HEM	CAA-CBA-CGA	-2.76	108.04	112.67
4	B	903	FMN	C7M-C7-C6	-2.71	113.86	120.34
2	B	901	HEM	CAD-CBD-CGD	-2.69	108.15	112.67
3	B	902	FAD	C4X-C4-N3	-2.68	119.76	123.43
4	A	903	FMN	C4A-C4-N3	-2.62	119.85	123.43
4	B	903	FMN	C7M-C7-C8	2.60	126.06	120.74
4	A	903	FMN	C7M-C7-C6	-2.59	114.16	120.34
4	A	903	FMN	C7M-C7-C8	2.55	125.96	120.74
4	A	903	FMN	C5A-C9A-N10	2.54	119.56	117.72
4	B	903	FMN	C4A-C4-N3	-2.50	120.01	123.43
2	B	901	HEM	CMC-C2C-C3C	2.43	129.22	124.68
4	A	903	FMN	C10-C4A-N5	-2.39	119.60	121.26
3	B	902	FAD	C1'-N10-C9A	2.28	120.09	118.29
2	A	901	HEM	CMC-C2C-C3C	2.25	128.89	124.68
2	A	901	HEM	CAD-CBD-CGD	-2.15	109.06	112.67
3	B	902	FAD	C4'-C3'-C2'	-2.03	109.14	113.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

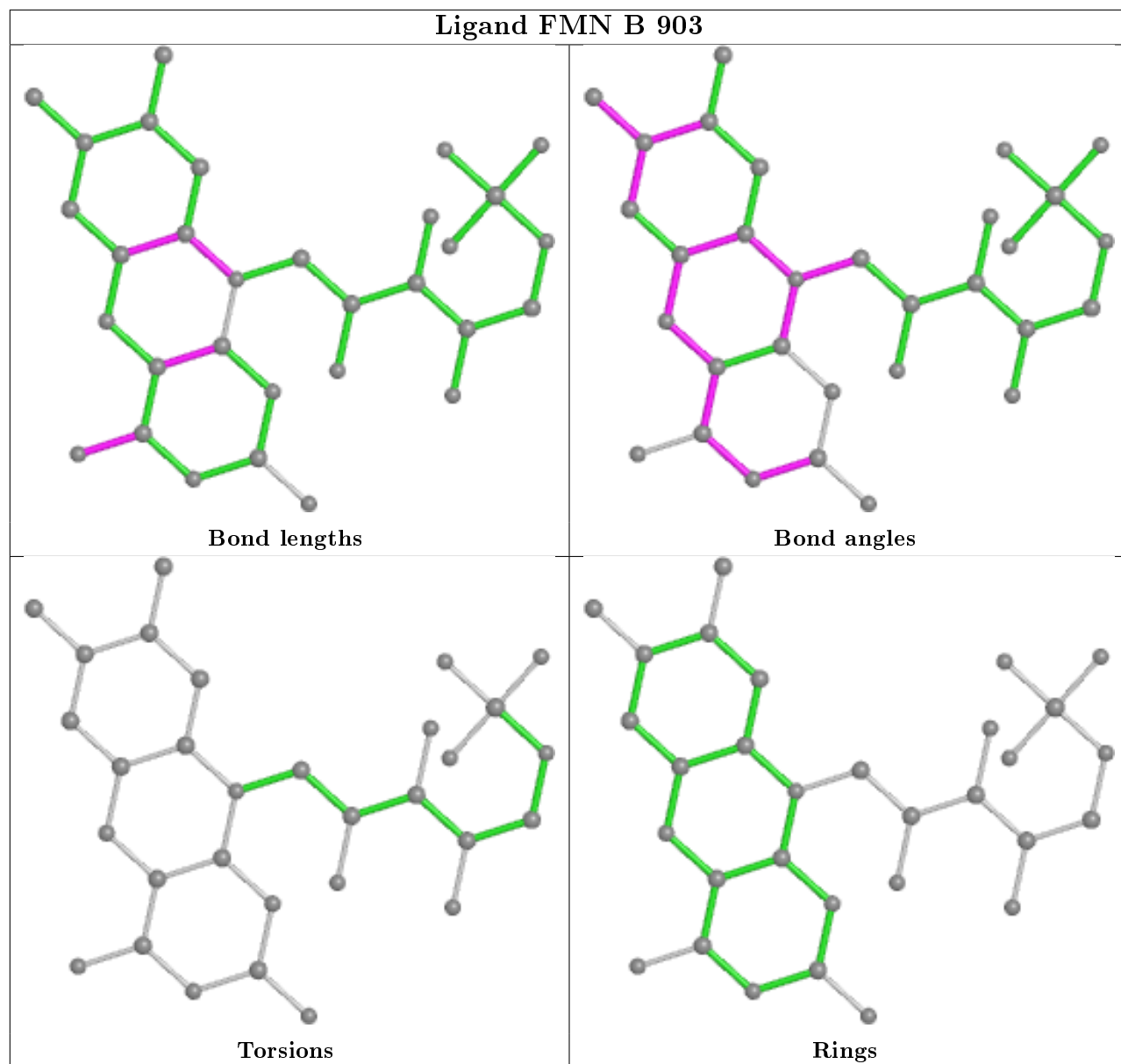
Mol	Chain	Res	Type	Atoms
3	A	902	FAD	C5B-O5B-PA-O3P
3	A	902	FAD	C3B-C4B-C5B-O5B
3	B	902	FAD	C5B-O5B-PA-O3P
3	B	902	FAD	C3B-C4B-C5B-O5B
3	A	902	FAD	O4B-C4B-C5B-O5B
3	B	902	FAD	O4B-C4B-C5B-O5B
3	B	902	FAD	O2'-C2'-C3'-C4'
3	A	902	FAD	C5B-O5B-PA-O2A
3	B	902	FAD	C5B-O5B-PA-O2A
3	B	902	FAD	O2'-C2'-C3'-O3'

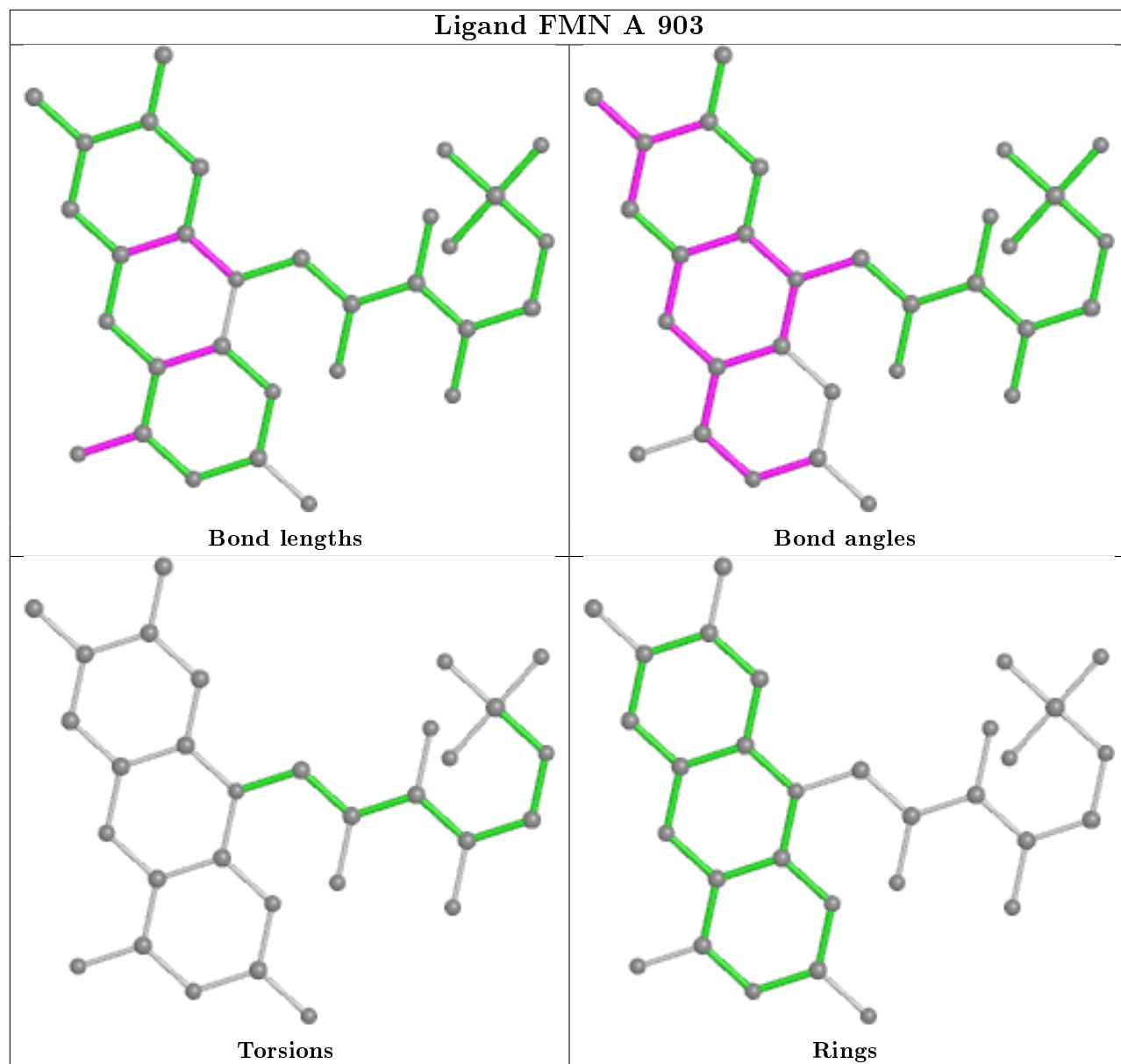
There are no ring outliers.

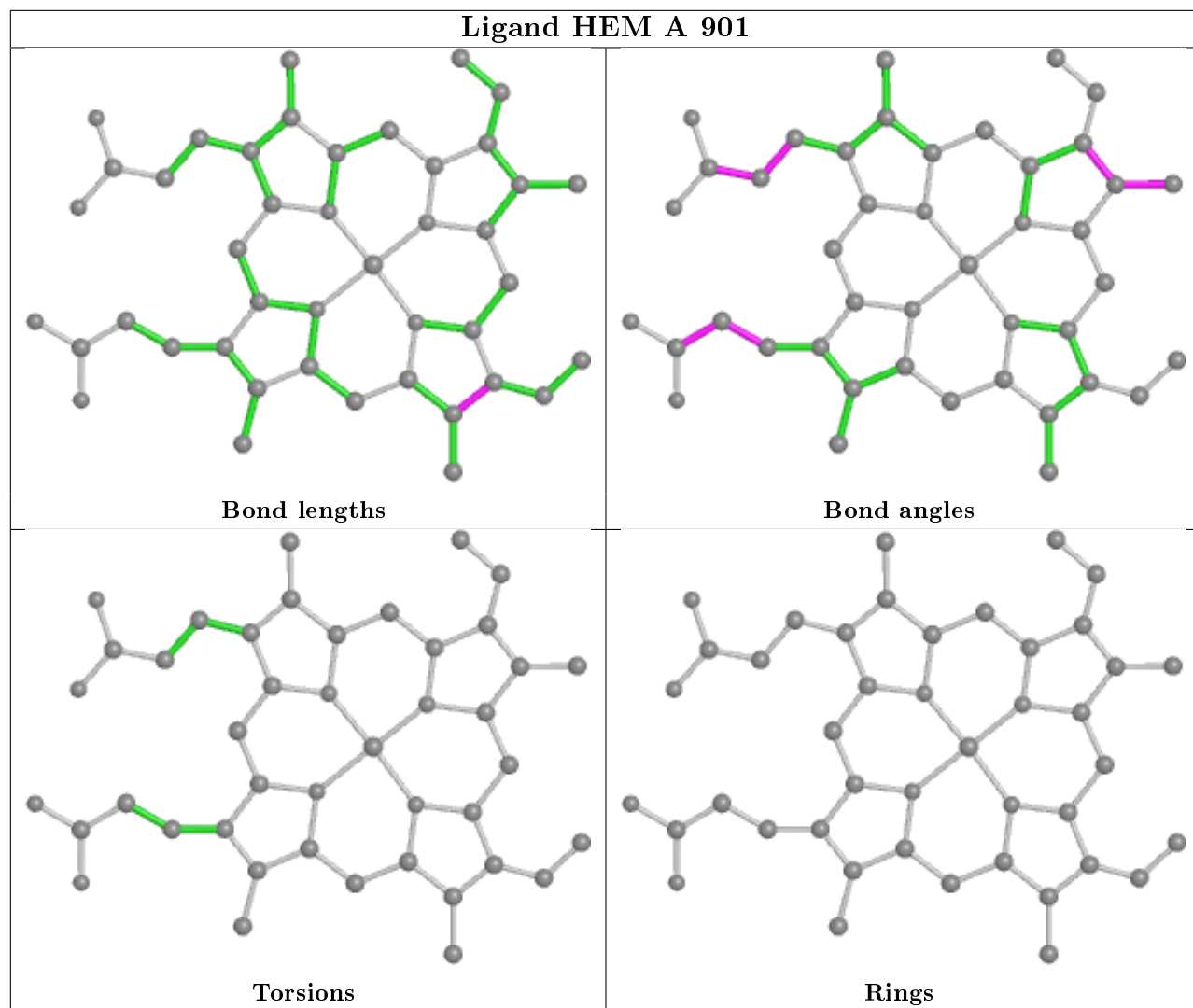
1 monomer is involved in 1 short contact:

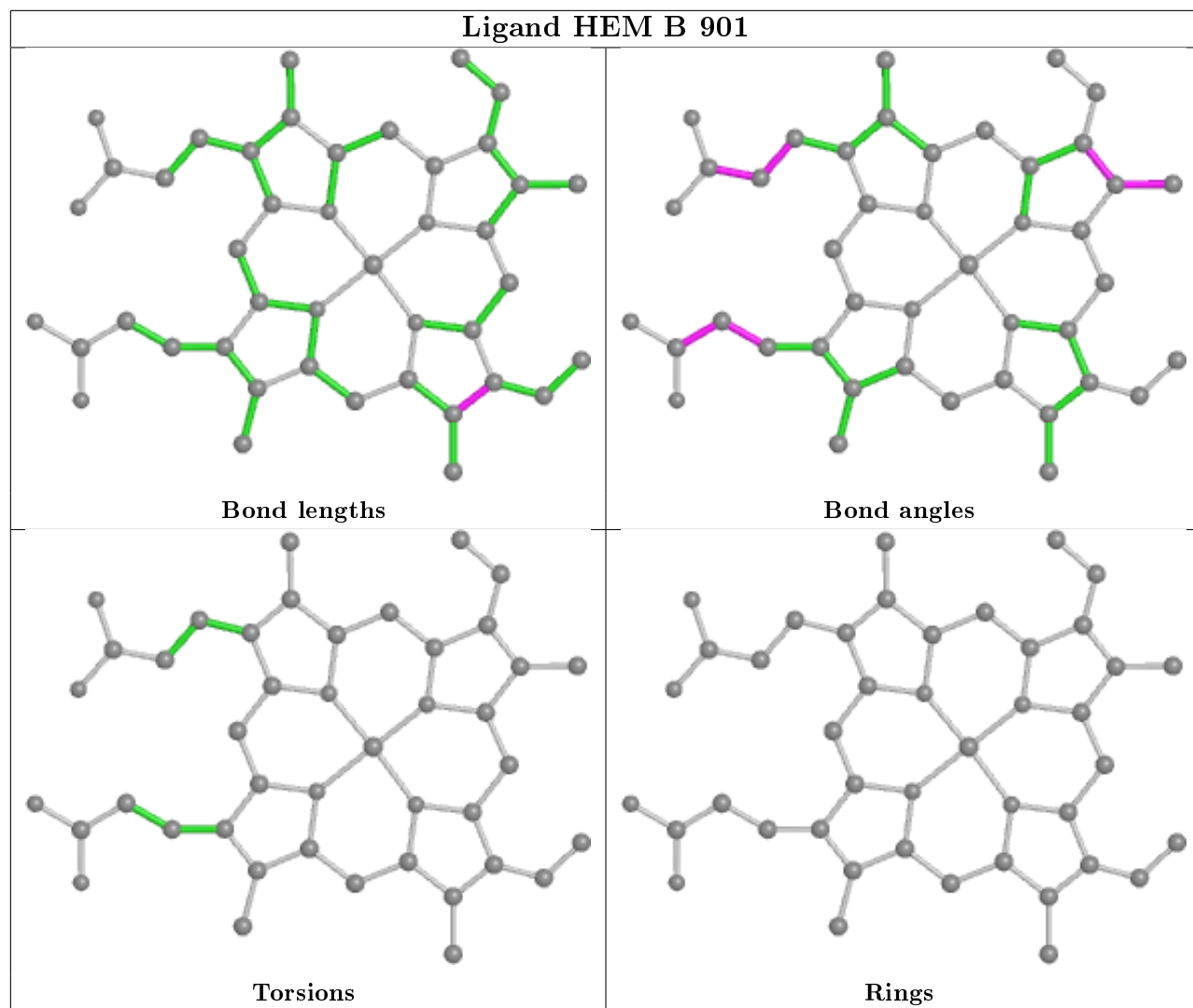
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	FAD	1	0

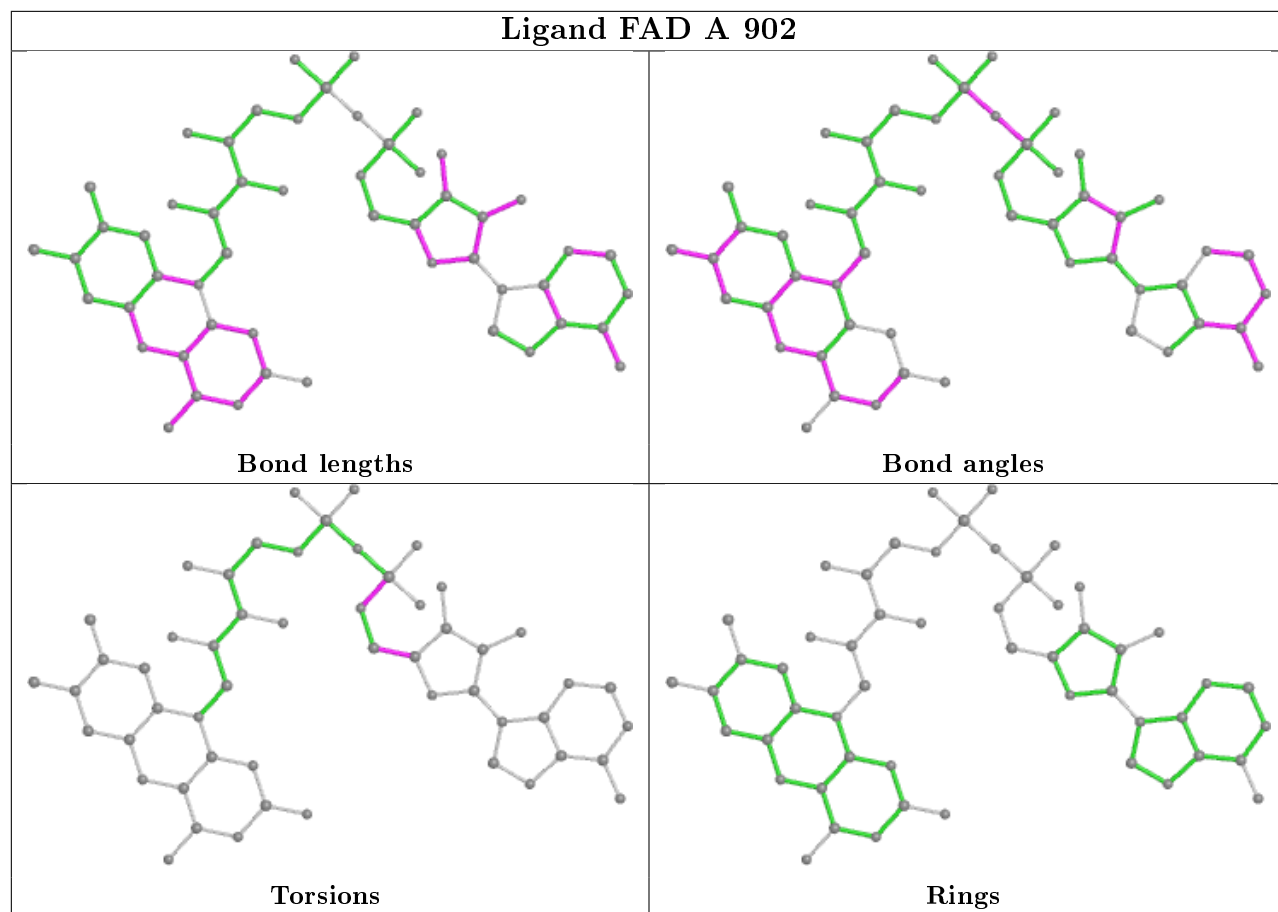
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

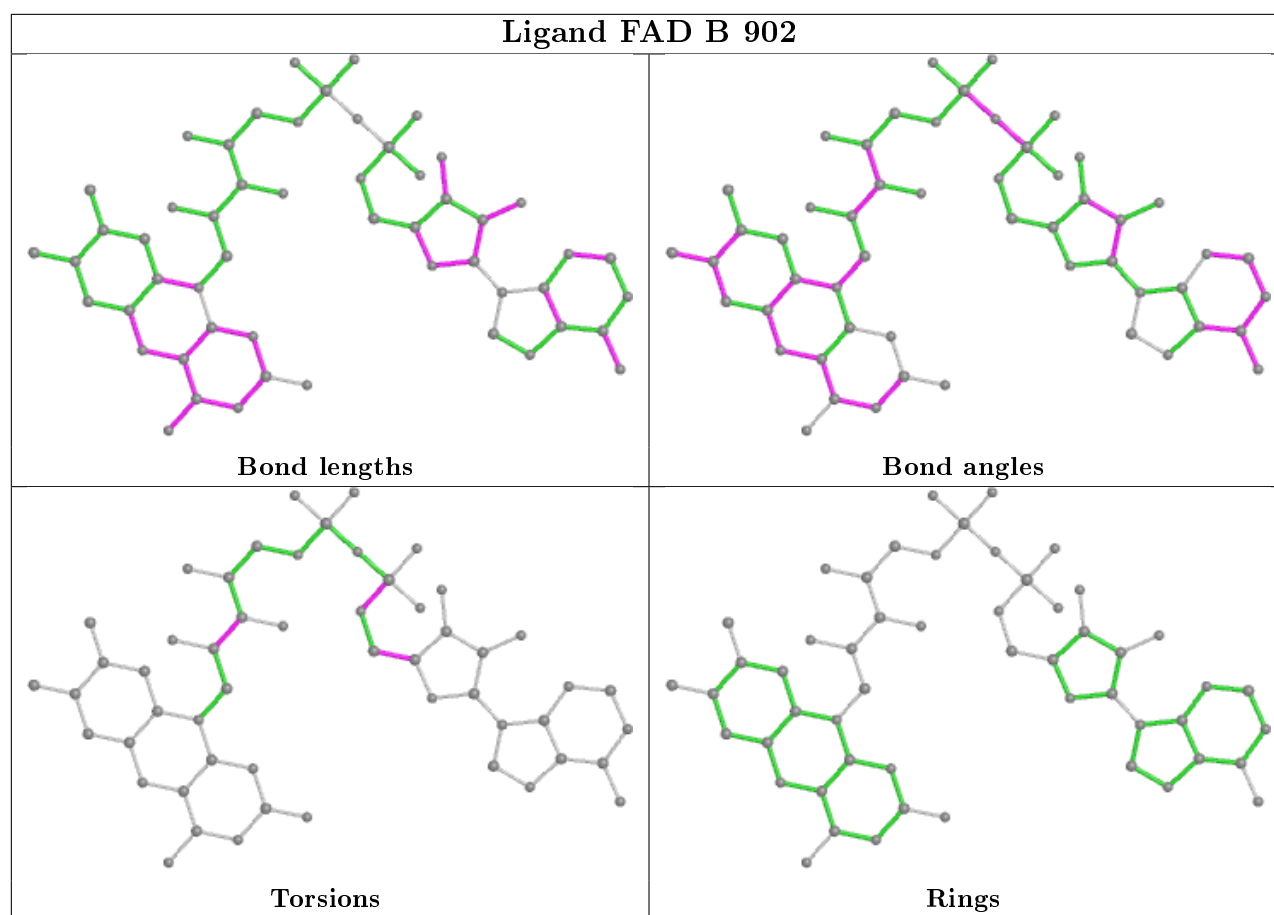












5.7 Other polymers [i](#)

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	814/873 (93%)	0.02	14 (1%) 70 68	22, 59, 113, 173	0
1	B	815/873 (93%)	0.04	24 (2%) 51 50	22, 61, 118, 190	0
All	All	1629/1746 (93%)	0.03	38 (2%) 60 59	22, 60, 116, 190	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	SER	5.2
1	A	583	SER	5.0
1	A	426	GLU	4.2
1	A	775	ALA	3.9
1	B	10	SER	3.6
1	B	414	ALA	3.1
1	A	412	VAL	3.1
1	B	426	GLU	3.0
1	B	429	ASP	2.9
1	A	853	SER	2.9
1	B	777	LYS	2.6
1	A	287	ARG	2.6
1	B	301	LEU	2.5
1	A	425	HIS	2.4
1	B	339	ASP	2.4
1	B	440	ARG	2.4
1	A	305	PRO	2.4
1	B	311	LEU	2.3
1	A	258	ASN	2.3
1	B	446	ASN	2.3
1	B	430	VAL	2.3
1	A	410	PHE	2.2
1	A	522	SER	2.2
1	A	358	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	529	GLU	2.2
1	B	605	ILE	2.2
1	B	305	PRO	2.2
1	B	531	ASN	2.2
1	B	609	TYR	2.1
1	B	432	LYS	2.1
1	B	302	SER	2.1
1	B	594	TRP	2.1
1	A	594	TRP	2.1
1	B	584	SER	2.1
1	B	425	HIS	2.0
1	B	248	PHE	2.0
1	A	430	VAL	2.0
1	B	537	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

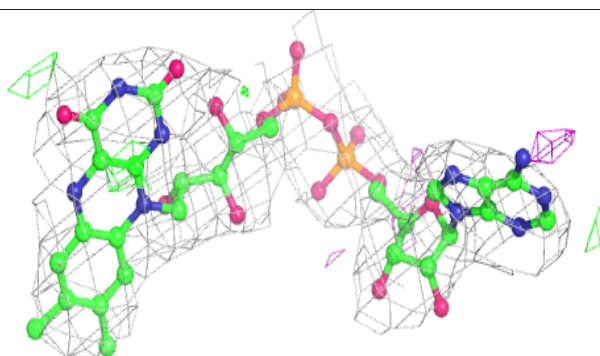
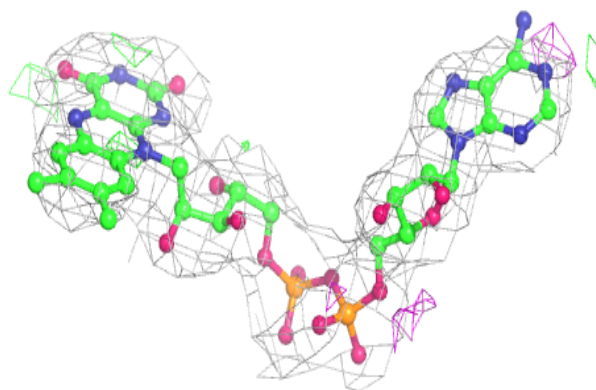
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FAD	A	902	53/53	0.92	0.26	26,43,70,74	0
3	FAD	B	902	53/53	0.95	0.19	36,48,74,79	0
4	FMN	A	903	31/31	0.96	0.22	31,52,61,62	0
2	HEM	B	901	43/43	0.96	0.23	15,39,57,73	0
2	HEM	A	901	43/43	0.97	0.24	7,23,66,83	0
4	FMN	B	903	31/31	0.97	0.19	33,46,54,56	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.

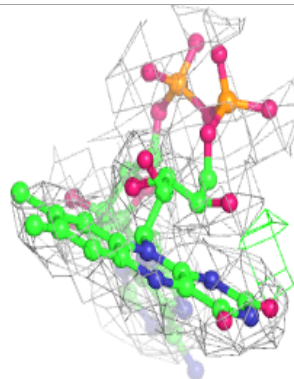
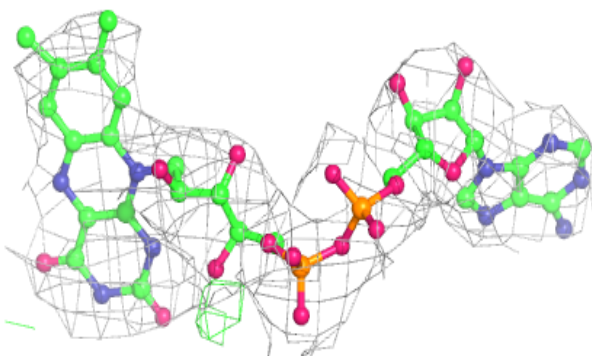
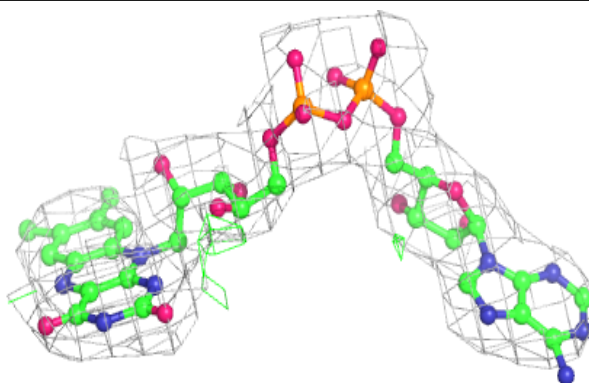
Electron density around FAD A 902:

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



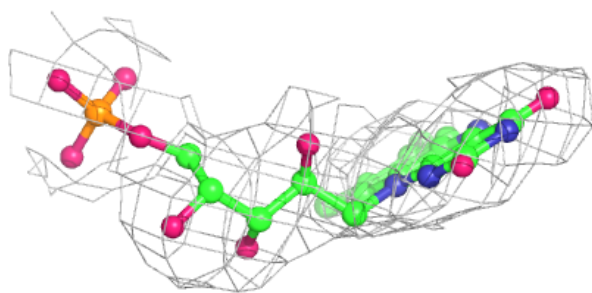
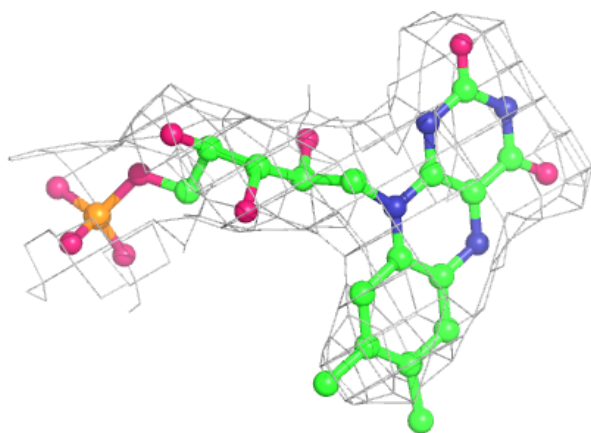
Electron density around FAD B 902:

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



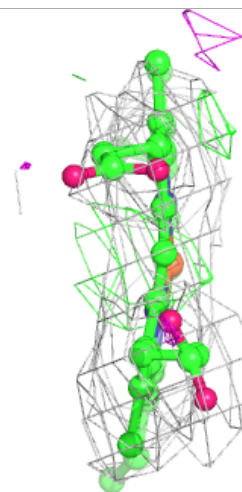
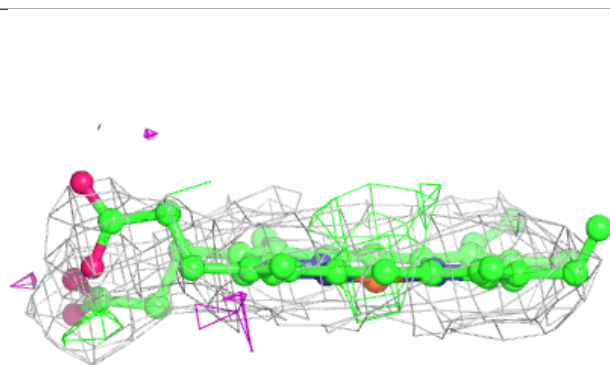
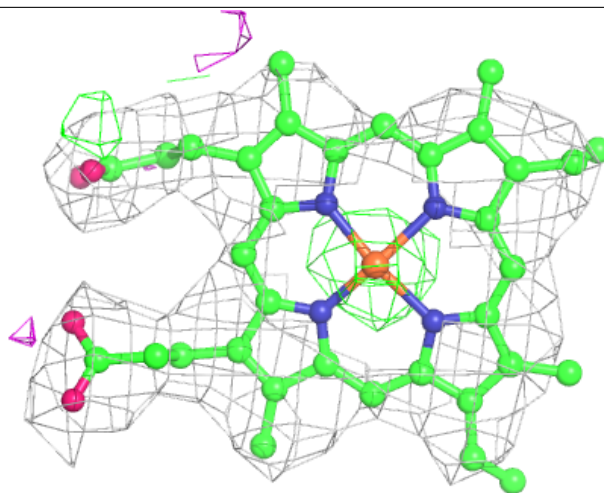
Electron density around FMN A 903:

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



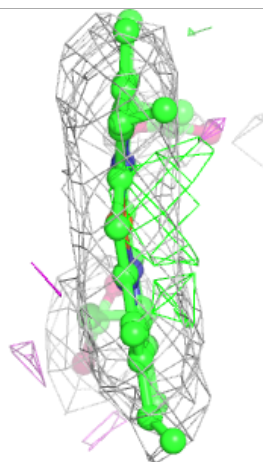
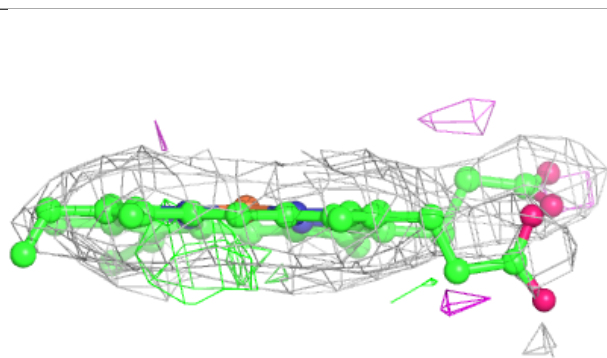
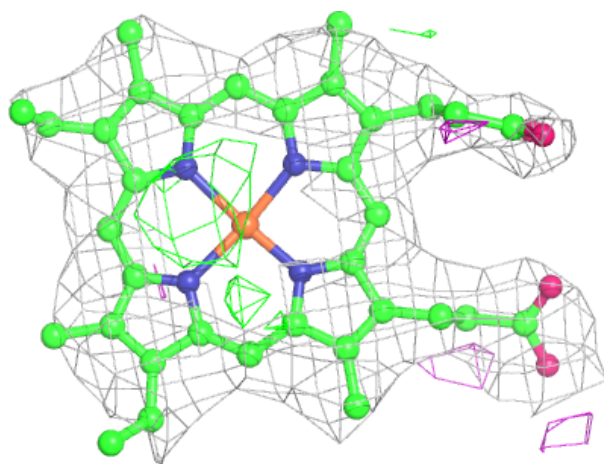
Electron density around HEM B 901:

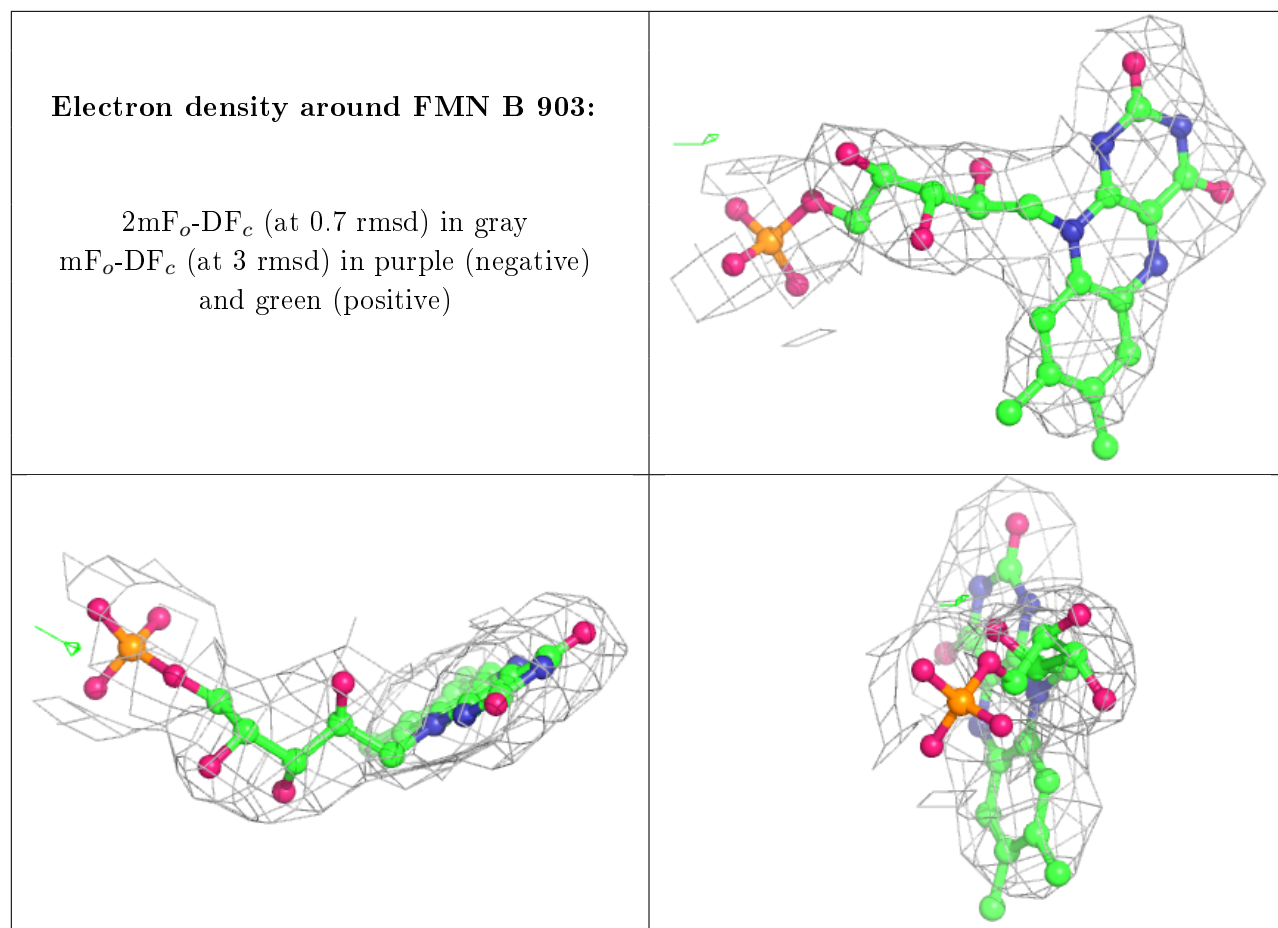
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.