



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:37 am BST

PDB ID : 6J7A
Title : Fusion protein of heme oxygenase-1 and NADPH cytochrome P450 reductase (17aa)
Authors : Sugishima, M.; Sato, H.; Wada, K.; Yamamoto, K.
Deposited on : 2019-01-17
Resolution : 3.27 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

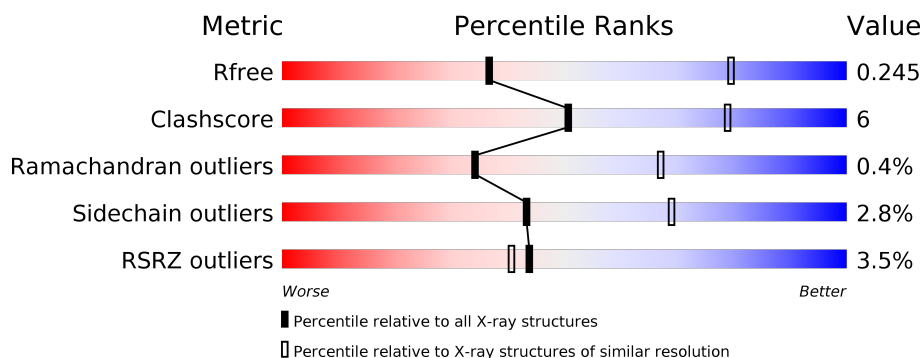
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	875	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>7%</div> </div> </div>
1	B	875	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13273 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	807	Total	C	N	O	S	0	0	0
			6486	4128	1110	1219	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	238	MET	-	linker	UNP P06762
A	?	-	THR	deletion	UNP P00388
A	?	-	GLY	deletion	UNP P00388

Continued on next page...

Continued from previous page...

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	238	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: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).



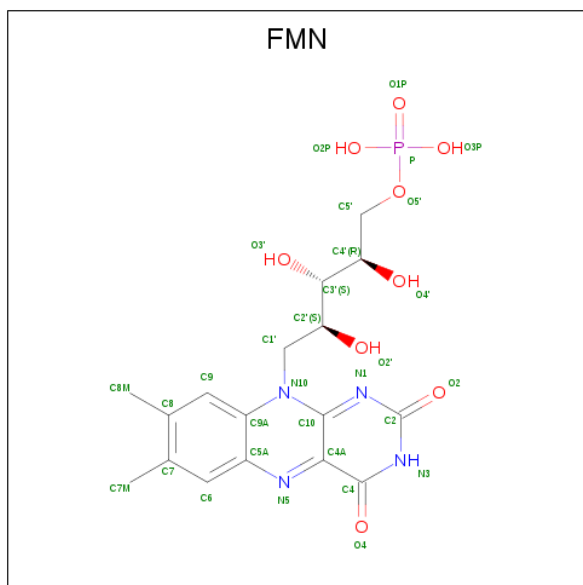
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

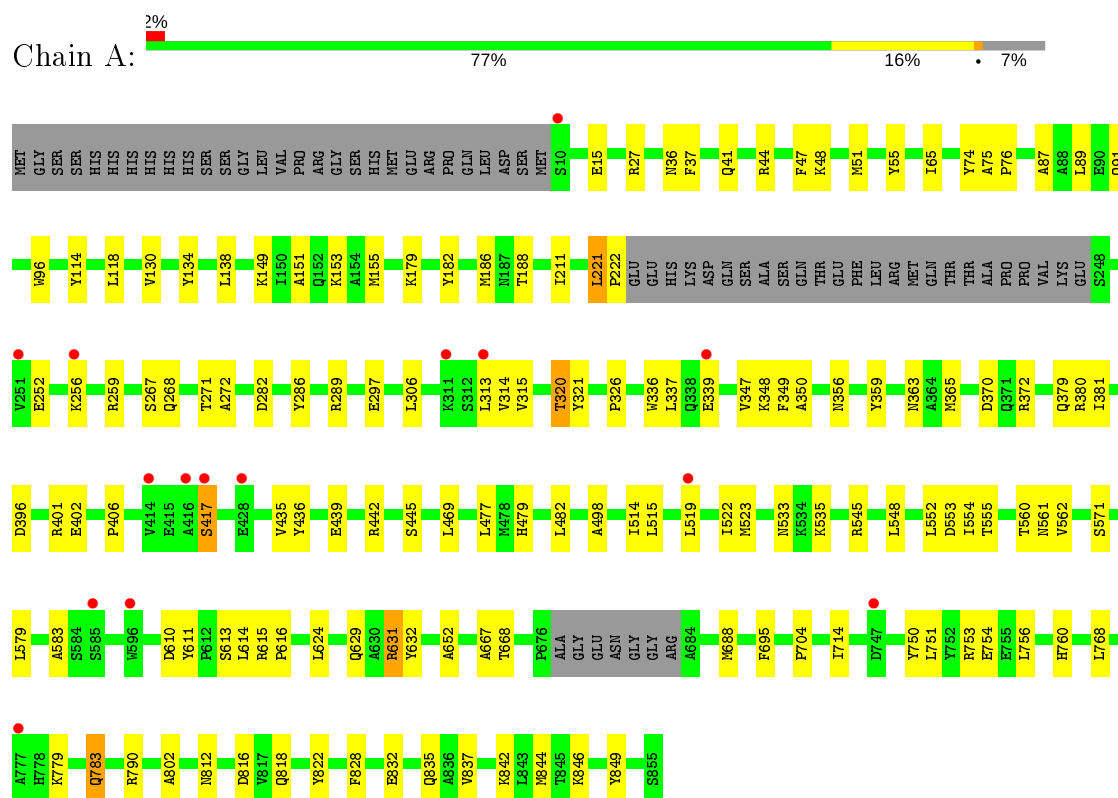
- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by author).



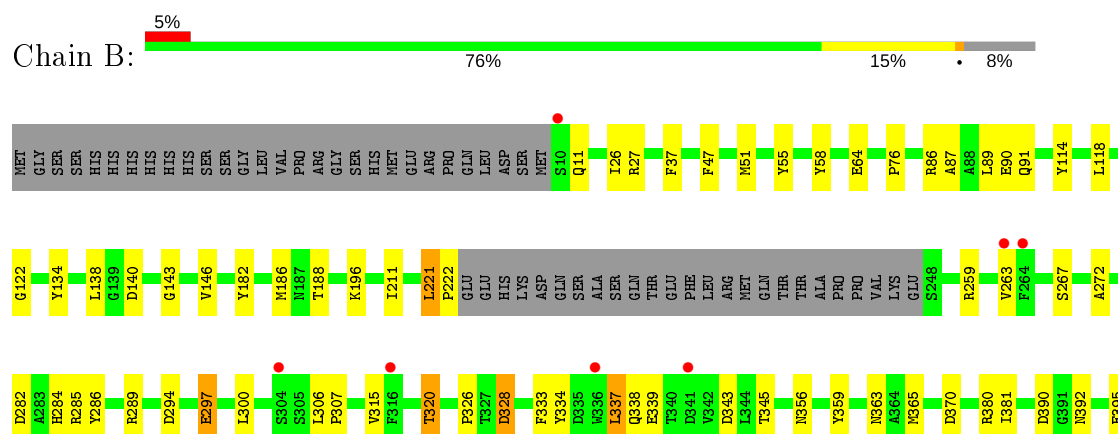
3 Residue-property plots [i](#)

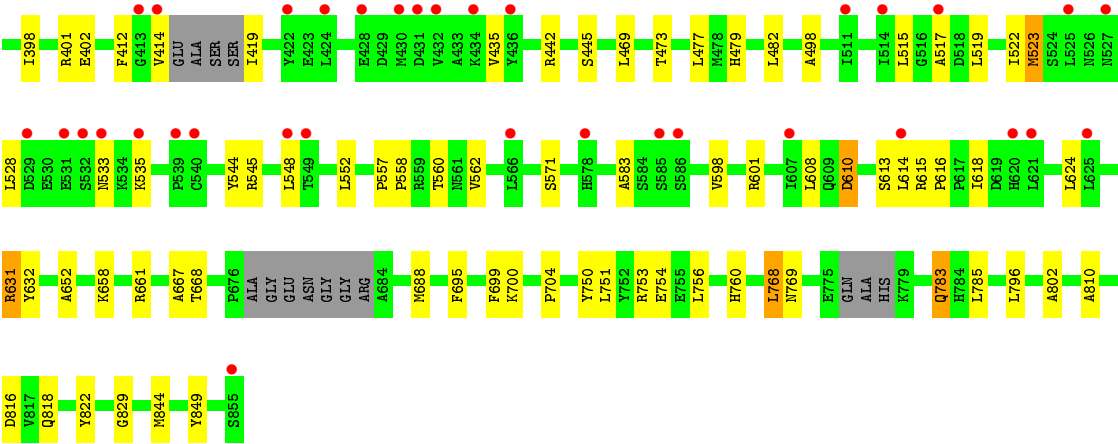
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	82.69Å 160.19Å 188.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.48 – 3.27 46.48 – 3.27	Depositor EDS
% Data completeness (in resolution range)	91.7 (46.48-3.27) 91.7 (46.48-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.228 , 0.246 0.228 , 0.245	Depositor DCC
R_{free} test set	1970 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13273	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.24	0/6690	0.41	0/9058
1	B	0.24	0/6644	0.42	1/8995 (0.0%)
All	All	0.24	0/13334	0.42	1/18053 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	LEU	CA-CB-CG	7.17	131.79	115.30

There are no chirality outliers.

There are no planarity outliers.

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	76	0
1	B	6486	0	6288	76	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	1	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	2	0	0	0	0
All	All	13273	0	12788	148	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 (148) 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:267:SER:HB2	1:B:272:ALA:HB3	1.76	0.67
1:A:348:LYS:NZ	1:A:379:GLN:OE1	2.29	0.66
1:A:519:LEU:HB3	1:A:545:ARG:HB2	1.77	0.65
1:A:631:ARG:HD3	1:A:667:ALA:HB2	1.78	0.65
1:B:259:ARG:HG2	1:B:289:ARG:HG2	1.79	0.65
1:B:515:LEU:HD11	1:B:616:PRO:HD2	1.79	0.65
1:A:482:LEU:HD23	1:A:688:MET:HG2	1.78	0.64
1:A:514:ILE:O	1:A:615:ARG:NH1	2.30	0.64
1:A:832:GLU:OE1	1:A:835:GLN:NE2	2.31	0.64
1:A:571:SER:H	1:A:613:SER:HB3	1.63	0.64
1:B:442:ARG:HG3	1:B:445:SER:HB3	1.79	0.62
1:B:756:LEU:HB3	1:B:768:LEU:HD11	1.81	0.62
1:B:631:ARG:NH1	3:B:902:FAD:O1P	2.33	0.62
1:A:614:LEU:O	1:A:615:ARG:NE	2.32	0.61
1:B:631:ARG:HD3	1:B:667:ALA:HB2	1.81	0.61
1:A:435:VAL:HG21	1:A:522:ILE:HD13	1.83	0.61
1:B:86:ARG:NH1	1:B:90:GLU:OE1	2.34	0.60
1:A:55:TYR:HA	1:A:89:LEU:HD13	1.84	0.59
1:B:783:GLN:HG2	1:B:816:ASP:HB3	1.83	0.59
1:B:328:ASP:N	1:B:328:ASP:OD1	2.34	0.58
1:B:614:LEU:O	1:B:615:ARG:NE	2.36	0.57
1:A:631:ARG:NH1	3:A:902:FAD:O1P	2.37	0.57
1:A:138:LEU:HD13	1:A:179:LYS:HG2	1.87	0.57
1:B:221:LEU:N	1:B:222:PRO:HD2	2.20	0.57
1:B:571:SER:H	1:B:613:SER:HB3	1.70	0.57
1:A:704:PRO:HG2	1:A:802:ALA:HB2	1.87	0.56
1:B:477:LEU:HD22	1:B:751:LEU:HD21	1.88	0.56
1:A:560:THR:HG23	1:A:583:ALA:HA	1.87	0.56
1:A:822:TYR:CZ	1:A:837:VAL:HG23	2.41	0.56
1:A:783:GLN:HG2	1:A:816:ASP:HB3	1.88	0.56
1:B:334:TYR:O	1:B:337:LEU:HD23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:ASN:OD1	1:B:334:TYR:OH	2.23	0.55
1:B:753:ARG:NH1	1:B:754:GLU:OE2	2.39	0.55
1:A:579:LEU:HD11	1:A:614:LEU:HD21	1.88	0.55
1:B:519:LEU:HB3	1:B:545:ARG:HB2	1.87	0.55
1:B:517:ALA:HB3	1:B:618:ILE:HG13	1.89	0.55
1:A:252:GLU:O	1:A:256:LYS:HG2	2.06	0.55
1:A:812:ASN:HB3	1:B:338:GLN:HE22	1.71	0.55
1:B:435:VAL:HG21	1:B:522:ILE:HD13	1.89	0.55
1:B:704:PRO:HG2	1:B:802:ALA:HB2	1.88	0.55
1:A:221:LEU:N	1:A:222:PRO:HD2	2.22	0.54
1:B:284:HIS:HB3	1:B:285:ARG:HH21	1.72	0.54
1:A:844:MET:HG2	1:A:849:TYR:HB3	1.90	0.54
1:A:149:LYS:NZ	1:A:271:THR:OG1	2.40	0.54
1:A:548:LEU:HD12	1:A:552:LEU:HD12	1.90	0.53
1:B:523:MET:HG2	1:B:544:TYR:CZ	2.44	0.53
1:B:652:ALA:HA	1:B:668:THR:HB	1.91	0.53
1:B:482:LEU:HD23	1:B:688:MET:HG2	1.90	0.53
1:A:562:VAL:HG12	1:A:624:LEU:HB3	1.91	0.52
1:B:469:LEU:HD11	1:B:479:HIS:HB2	1.92	0.52
1:A:477:LEU:HD22	1:A:751:LEU:HD21	1.92	0.51
1:A:611:TYR:HB3	1:A:614:LEU:HD23	1.93	0.51
1:A:842:LYS:HB3	1:A:846:LYS:HE3	1.93	0.51
1:B:11:GLN:O	1:B:196:LYS:NZ	2.31	0.51
1:B:55:TYR:HA	1:B:89:LEU:HD13	1.93	0.51
1:B:562:VAL:HG12	1:B:624:LEU:HB3	1.92	0.51
1:A:442:ARG:HG3	1:A:445:SER:HB3	1.93	0.50
1:A:571:SER:N	1:A:613:SER:HB3	2.25	0.50
1:B:598:VAL:O	1:B:601:ARG:HD2	2.12	0.49
1:B:560:THR:HG23	1:B:583:ALA:HA	1.93	0.49
1:A:370:ASP:OD1	1:A:380:ARG:NH1	2.45	0.49
1:A:832:GLU:OE2	1:B:26:ILE:HG12	2.12	0.49
1:B:58:TYR:OH	1:B:140:ASP:OD2	2.25	0.49
1:A:533:ASN:N	1:A:533:ASN:OD1	2.46	0.49
1:A:818:GLN:HG2	1:A:822:TYR:CZ	2.48	0.49
1:A:134:TYR:HB2	1:A:186:MET:HE1	1.95	0.48
1:A:469:LEU:HD11	1:A:479:HIS:HB2	1.95	0.48
1:B:182:TYR:O	1:B:186:MET:HG3	2.13	0.48
1:A:652:ALA:HA	1:A:668:THR:HB	1.95	0.48
1:A:714:ILE:HD11	1:A:756:LEU:HD11	1.95	0.48
1:A:282:ASP:OD2	1:A:401:ARG:HD2	2.13	0.48
1:B:87:ALA:O	1:B:91:GLN:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:HG21	1:A:363:ASN:HA	1.96	0.48
1:A:15:GLU:OE1	1:A:846:LYS:HE2	2.13	0.48
1:A:779:LYS:NZ	1:B:339:GLU:O	2.46	0.48
1:B:326:PRO:HB3	1:B:365:MET:SD	2.54	0.47
1:A:314:VAL:O	1:A:349:PHE:HA	2.14	0.47
1:A:515:LEU:HD11	1:A:616:PRO:HD2	1.95	0.47
1:B:263:VAL:HG13	1:B:315:VAL:HB	1.97	0.47
1:B:392:ASN:OD1	1:B:395:GLU:N	2.47	0.47
1:B:533:ASN:OD1	1:B:533:ASN:N	2.46	0.47
1:B:221:LEU:H	1:B:222:PRO:HD2	1.79	0.47
1:A:259:ARG:HG2	1:A:289:ARG:HG2	1.97	0.46
1:B:282:ASP:OD2	1:B:401:ARG:NH1	2.39	0.46
1:B:610:ASP:OD1	1:B:661:ARG:NH2	2.46	0.46
1:A:134:TYR:HB2	1:A:186:MET:CE	2.45	0.46
1:B:306:LEU:N	1:B:307:PRO:HD2	2.30	0.46
1:A:297:GLU:OE1	1:A:297:GLU:N	2.43	0.46
1:B:370:ASP:OD1	1:B:380:ARG:NH1	2.49	0.46
1:A:790:ARG:HB2	1:A:828:PHE:HE1	1.81	0.46
1:A:336:TRP:HE3	1:A:337:LEU:HD12	1.81	0.45
1:A:356:ASN:HB3	1:A:359:TYR:HD1	1.81	0.45
1:A:553:ASP:OD1	1:A:555:THR:OG1	2.34	0.45
1:A:753:ARG:NH1	1:A:754:GLU:OE2	2.49	0.45
1:A:629:GLN:O	1:A:631:ARG:NE	2.47	0.45
1:B:818:GLN:HG2	1:B:822:TYR:CZ	2.50	0.45
1:A:337:LEU:HD23	1:A:372:ARG:HG2	1.98	0.45
1:B:188:THR:HG23	1:B:700:LYS:HG3	1.99	0.45
1:B:300:LEU:HD22	1:B:333:PHE:CE1	2.52	0.45
1:B:134:TYR:O	1:B:138:LEU:HB2	2.17	0.44
1:B:844:MET:HG2	1:B:849:TYR:HB3	1.98	0.44
1:B:398:ILE:O	1:B:402:GLU:HB2	2.18	0.44
1:A:36:ASN:HB3	1:A:41:GLN:O	2.18	0.44
1:A:498:ALA:HB2	1:A:632:TYR:CE2	2.53	0.44
1:A:151:ALA:O	1:A:155:MET:HG3	2.17	0.44
1:A:182:TYR:O	1:A:186:MET:HG3	2.17	0.44
1:B:769:ASN:HB3	1:B:785:LEU:HD13	1.99	0.44
1:B:76:PRO:HG3	1:B:699:PHE:CE2	2.53	0.44
1:B:143:GLY:O	1:B:146:VAL:HG22	2.18	0.43
1:A:306:LEU:HD22	1:A:347:VAL:HG13	2.01	0.43
1:B:381:ILE:HA	1:B:381:ILE:HD13	1.85	0.43
1:A:75:ALA:HB3	1:A:76:PRO:HD3	2.00	0.43
1:A:44:ARG:HA	1:A:155:MET:CE	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:HD1	1:A:439:GLU:HG2	1.84	0.42
1:B:320:THR:HG21	1:B:363:ASN:HA	2.01	0.42
1:B:658:LYS:HG2	1:B:658:LYS:H	1.63	0.42
1:A:47:PHE:O	1:A:51:MET:HG2	2.19	0.42
1:B:64:GLU:HB3	1:B:122:GLY:HA3	2.01	0.42
1:B:515:LEU:HD13	1:B:608:LEU:HD13	2.01	0.42
1:A:348:LYS:HG3	1:A:381:ILE:HD11	2.01	0.42
1:A:268:GLN:HB2	1:A:321:TYR:CZ	2.54	0.42
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.90	0.42
1:B:528:LEU:HD23	1:B:528:LEU:HA	1.85	0.42
1:A:27:ARG:HD2	1:A:211:ILE:HD13	2.01	0.42
1:A:406:PRO:HG2	1:A:561:ASN:HA	2.00	0.42
1:B:134:TYR:HB2	1:B:186:MET:HE1	2.02	0.42
1:B:27:ARG:HD2	1:B:211:ILE:HD13	2.02	0.42
1:A:149:LYS:O	1:A:153:LYS:HG2	2.20	0.41
1:A:535:LYS:HA	1:A:535:LYS:HD3	1.87	0.41
1:B:282:ASP:OD2	1:B:401:ARG:HD2	2.19	0.41
1:B:343:ASP:OD1	1:B:345:THR:OG1	2.20	0.41
1:A:402:GLU:O	1:A:561:ASN:HB3	2.20	0.41
1:B:548:LEU:HD12	1:B:552:LEU:HD12	2.02	0.41
1:B:498:ALA:HB2	1:B:632:TYR:CE2	2.55	0.41
1:B:286:TYR:HA	1:B:419:ILE:HD13	2.02	0.41
1:B:557:PRO:HA	1:B:558:PRO:HD3	1.88	0.41
1:A:48:LYS:HG2	1:A:96:TRP:HB3	2.03	0.41
1:B:356:ASN:HB3	1:B:359:TYR:HD1	1.85	0.41
1:B:47:PHE:O	1:B:51:MET:HG2	2.20	0.41
1:B:535:LYS:HD3	1:B:535:LYS:HA	1.86	0.41
1:B:294:ASP:HB3	1:B:297:GLU:OE1	2.21	0.41
1:B:134:TYR:HB2	1:B:186:MET:CE	2.50	0.41
1:A:65:ILE:HG23	1:A:74:TYR:CE2	2.56	0.40
1:A:267:SER:HB2	1:A:272:ALA:HB3	2.02	0.40
1:A:326:PRO:HB3	1:A:365:MET:SD	2.61	0.40
1:A:87:ALA:O	1:A:91:GLN:HG2	2.21	0.40
1:B:515:LEU:HD23	1:B:618:ILE:HG12	2.02	0.40
1:A:315:VAL:HA	1:A:350:ALA:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	808/875 (92%)	761 (94%)	44 (5%)	3 (0%)	34	67
1	B	797/875 (91%)	753 (94%)	41 (5%)	3 (0%)	34	67
All	All	1605/1750 (92%)	1514 (94%)	85 (5%)	6 (0%)	34	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	810	ALA
1	A	417	SER
1	B	221	LEU
1	B	829	GLY
1	A	554	ILE
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	692/750 (92%)	673 (97%)	19 (3%)	44	70
1	B	688/750 (92%)	669 (97%)	19 (3%)	43	69
All	All	1380/1500 (92%)	1342 (97%)	38 (3%)	43	69

All (38) 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	188	THR
1	A	286	TYR
1	A	313	LEU
1	A	320	THR
1	A	339	GLU
1	A	396	ASP
1	A	417	SER
1	A	523	MET
1	A	610	ASP
1	A	631	ARG
1	A	695	PHE
1	A	750	TYR
1	A	760	HIS
1	A	768	LEU
1	A	783	GLN
1	B	37	PHE
1	B	114	TYR
1	B	118	LEU
1	B	297	GLU
1	B	320	THR
1	B	328	ASP
1	B	390	ASP
1	B	412	PHE
1	B	414	VAL
1	B	473	THR
1	B	523	MET
1	B	610	ASP
1	B	631	ARG
1	B	695	PHE
1	B	750	TYR
1	B	760	HIS
1	B	768	LEU
1	B	783	GLN
1	B	796	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	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	818	GLN
1	B	647	HIS
1	B	803	HIS
1	B	818	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	A	903	-	31,33,33	1.30	4 (12%)	40,50,50	2.39	8 (20%)
4	FMN	B	903	-	31,33,33	1.32	4 (12%)	40,50,50	2.37	8 (20%)
2	HEM	A	901	1	27,50,50	0.90	2 (7%)	17,82,82	1.34	2 (11%)
2	HEM	B	901	1	27,50,50	0.91	2 (7%)	17,82,82	1.28	2 (11%)
3	FAD	A	902	-	51,58,58	4.69	18 (35%)	60,89,89	2.64	11 (18%)
3	FAD	B	902	-	51,58,58	4.66	18 (35%)	60,89,89	2.69	14 (23%)

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	A	903	-	-	0/18/18/18	0/3/3/3
4	FMN	B	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	-	-	5/30/50/50	0/6/6/6
3	FAD	B	902	-	-	12/30/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	FAD	O4B-C1B	15.45	1.62	1.41
3	B	902	FAD	O4B-C1B	15.23	1.62	1.41
3	A	902	FAD	C2B-C1B	-14.90	1.31	1.53
3	B	902	FAD	C2B-C1B	-14.84	1.31	1.53
3	B	902	FAD	C10-N1	10.57	1.46	1.33
3	A	902	FAD	C10-N1	10.53	1.46	1.33
3	A	902	FAD	C4X-N5	8.85	1.46	1.33
3	B	902	FAD	C4X-N5	8.76	1.45	1.33
3	A	902	FAD	C5X-N5	8.68	1.49	1.35
3	B	902	FAD	C5X-N5	8.64	1.49	1.35
3	A	902	FAD	C9A-N10	8.40	1.49	1.38
3	B	902	FAD	C9A-N10	8.31	1.49	1.38
3	B	902	FAD	C4-N3	7.64	1.46	1.33
3	A	902	FAD	C4-N3	7.63	1.46	1.33
3	A	902	FAD	C4X-C10	6.97	1.45	1.38
3	B	902	FAD	C4X-C10	6.91	1.45	1.38
3	B	902	FAD	O4B-C4B	-6.41	1.30	1.45
3	A	902	FAD	O4B-C4B	-6.29	1.30	1.45
3	B	902	FAD	C4-C4X	6.17	1.52	1.41
3	A	902	FAD	C4-C4X	6.16	1.52	1.41
3	A	902	FAD	C2-N3	5.82	1.49	1.38
3	B	902	FAD	C2-N3	5.71	1.49	1.38
3	A	902	FAD	C2-N1	5.29	1.48	1.38
3	B	902	FAD	C2-N1	5.28	1.48	1.38
3	A	902	FAD	C6A-N6A	3.13	1.45	1.34
3	B	902	FAD	C6A-N6A	3.12	1.45	1.34
3	A	902	FAD	O2B-C2B	2.99	1.50	1.43
3	B	902	FAD	O2B-C2B	2.97	1.50	1.43
3	A	902	FAD	O3B-C3B	-2.94	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	FAD	O3B-C3B	-2.90	1.36	1.43
2	B	901	HEM	C3B-C2B	-2.87	1.36	1.40
2	A	901	HEM	C3B-C2B	-2.84	1.36	1.40
4	A	903	FMN	C4A-C10	-2.70	1.36	1.38
4	B	903	FMN	C4A-C10	-2.66	1.36	1.38
3	B	902	FAD	C5A-C4A	-2.60	1.34	1.40
3	A	902	FAD	C5A-C4A	-2.59	1.34	1.40
4	B	903	FMN	C9A-C5A	-2.50	1.37	1.42
4	A	903	FMN	C9A-C5A	-2.49	1.37	1.42
4	B	903	FMN	C9A-N10	-2.42	1.35	1.38
3	A	902	FAD	C2A-N3A	2.33	1.35	1.32
3	B	902	FAD	C2A-N3A	2.31	1.35	1.32
4	A	903	FMN	C9A-N10	-2.28	1.35	1.38
4	A	903	FMN	O4-C4	-2.24	1.18	1.24
4	B	903	FMN	O4-C4	-2.23	1.18	1.24
3	A	902	FAD	O4-C4	-2.23	1.18	1.24
3	B	902	FAD	O4-C4	-2.19	1.19	1.24
2	B	901	HEM	C4D-C3D	2.02	1.47	1.42
2	A	901	HEM	C4D-C3D	2.02	1.47	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	FAD	C5A-C6A-N6A	12.72	139.68	120.35
3	A	902	FAD	C5A-C6A-N6A	12.50	139.34	120.35
4	A	903	FMN	C1'-N10-C9A	10.56	126.61	118.29
4	B	903	FMN	C1'-N10-C9A	10.34	126.43	118.29
3	B	902	FAD	N6A-C6A-N1A	-8.84	100.22	118.57
3	A	902	FAD	N6A-C6A-N1A	-8.70	100.51	118.57
4	A	903	FMN	C4-N3-C2	5.65	119.91	115.14
4	B	903	FMN	C4-N3-C2	5.58	119.85	115.14
3	A	902	FAD	N3A-C2A-N1A	-5.53	120.04	128.68
3	A	902	FAD	C4-N3-C2	5.52	119.80	115.14
3	B	902	FAD	N3A-C2A-N1A	-5.49	120.10	128.68
3	B	902	FAD	C4-N3-C2	5.47	119.76	115.14
4	A	903	FMN	C1'-N10-C10	-5.28	113.68	118.41
4	B	903	FMN	C1'-N10-C10	-5.12	113.82	118.41
3	B	902	FAD	C7M-C7-C8	4.86	130.70	120.74
3	B	902	FAD	C7M-C7-C6	-4.68	109.16	120.34
3	A	902	FAD	C7M-C7-C8	4.59	130.15	120.74
3	A	902	FAD	C7M-C7-C6	-4.48	109.62	120.34
3	B	902	FAD	C3B-C2B-C1B	3.90	106.84	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	FAD	C5X-C9A-N10	3.41	120.19	117.72
4	B	903	FMN	C4A-N5-C5A	3.39	120.16	116.77
4	A	903	FMN	C4A-N5-C5A	3.38	120.15	116.77
3	B	902	FAD	C4X-N5-C5X	3.30	120.06	116.77
3	A	902	FAD	C3B-C2B-C1B	3.30	105.94	100.98
3	A	902	FAD	C4X-N5-C5X	3.25	120.02	116.77
2	A	901	HEM	CAD-CBD-CGD	-3.14	107.40	112.67
3	B	902	FAD	C5X-C9A-N10	3.14	119.99	117.72
4	B	903	FMN	C5A-C9A-N10	3.03	119.91	117.72
3	B	902	FAD	P-O3P-PA	-2.99	122.57	132.83
3	A	902	FAD	P-O3P-PA	-2.92	122.82	132.83
4	A	903	FMN	C5A-C9A-N10	2.90	119.82	117.72
3	B	902	FAD	C4X-C4-N3	-2.73	119.70	123.43
2	B	901	HEM	CAD-CBD-CGD	-2.72	108.11	112.67
3	A	902	FAD	C4X-C4-N3	-2.69	119.76	123.43
4	B	903	FMN	C7M-C7-C6	-2.68	113.92	120.34
4	B	903	FMN	C7M-C7-C8	2.68	126.23	120.74
4	A	903	FMN	C7M-C7-C6	-2.57	114.19	120.34
4	A	903	FMN	C4A-C4-N3	-2.53	119.97	123.43
4	A	903	FMN	C7M-C7-C8	2.52	125.91	120.74
4	B	903	FMN	C4A-C4-N3	-2.46	120.07	123.43
2	A	901	HEM	CAA-CBA-CGA	-2.45	108.56	112.67
2	B	901	HEM	CAA-CBA-CGA	-2.35	108.72	112.67
3	B	902	FAD	C1'-N10-C9A	2.16	119.99	118.29
3	B	902	FAD	C4'-C3'-C2'	-2.09	109.01	113.36
3	B	902	FAD	C10-C4X-N5	-2.02	119.86	121.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	FAD	C1'-C2'-C3'-C4'
3	B	902	FAD	C1'-C2'-C3'-C4'
3	B	902	FAD	O2'-C2'-C3'-O3'
3	B	902	FAD	O2'-C2'-C3'-C4'
3	B	902	FAD	O3'-C3'-C4'-C5'
3	A	902	FAD	O2'-C2'-C3'-C4'
3	B	902	FAD	C3B-C4B-C5B-O5B
3	B	902	FAD	C2'-C3'-C4'-O4'
3	A	902	FAD	O2'-C2'-C3'-O3'
3	B	902	FAD	C2'-C3'-C4'-C5'
3	B	902	FAD	O3'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

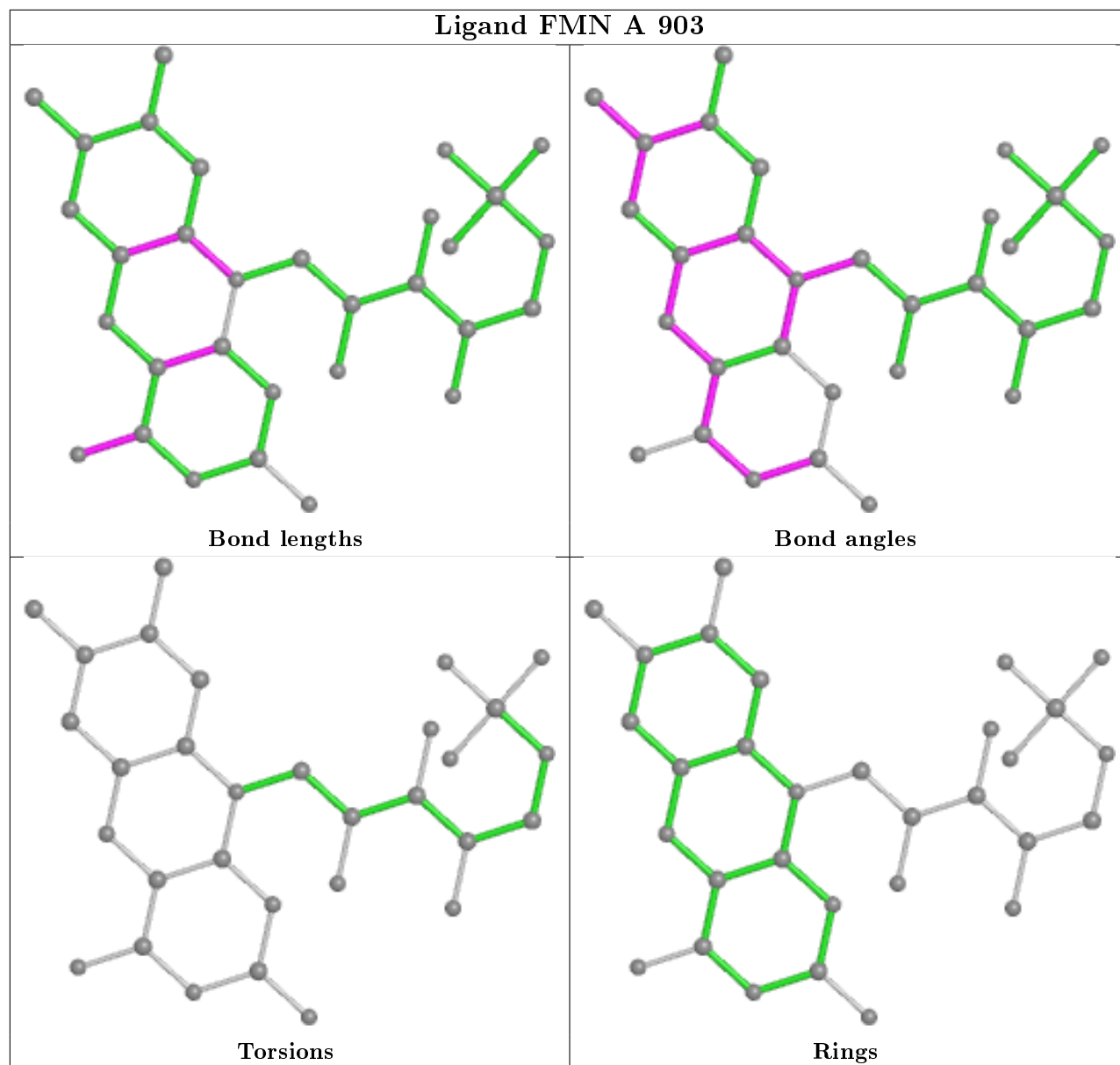
Mol	Chain	Res	Type	Atoms
3	B	902	FAD	O4B-C4B-C5B-O5B
3	B	902	FAD	C5'-O5'-P-O3P
3	A	902	FAD	PA-O3P-P-O2P
3	B	902	FAD	PA-O3P-P-O2P
3	B	902	FAD	C1'-C2'-C3'-O3'
3	A	902	FAD	O3'-C3'-C4'-C5'

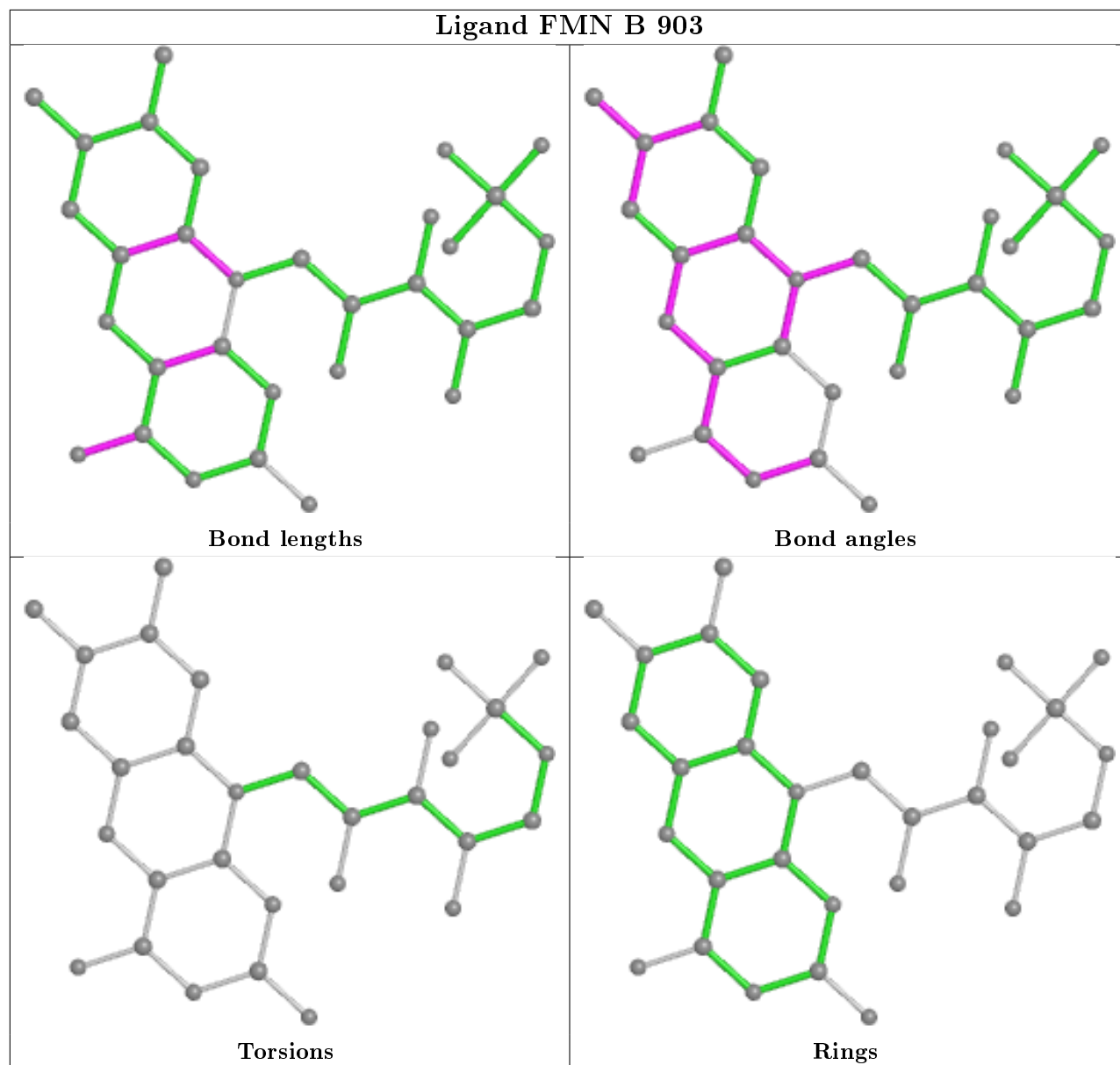
There are no ring outliers.

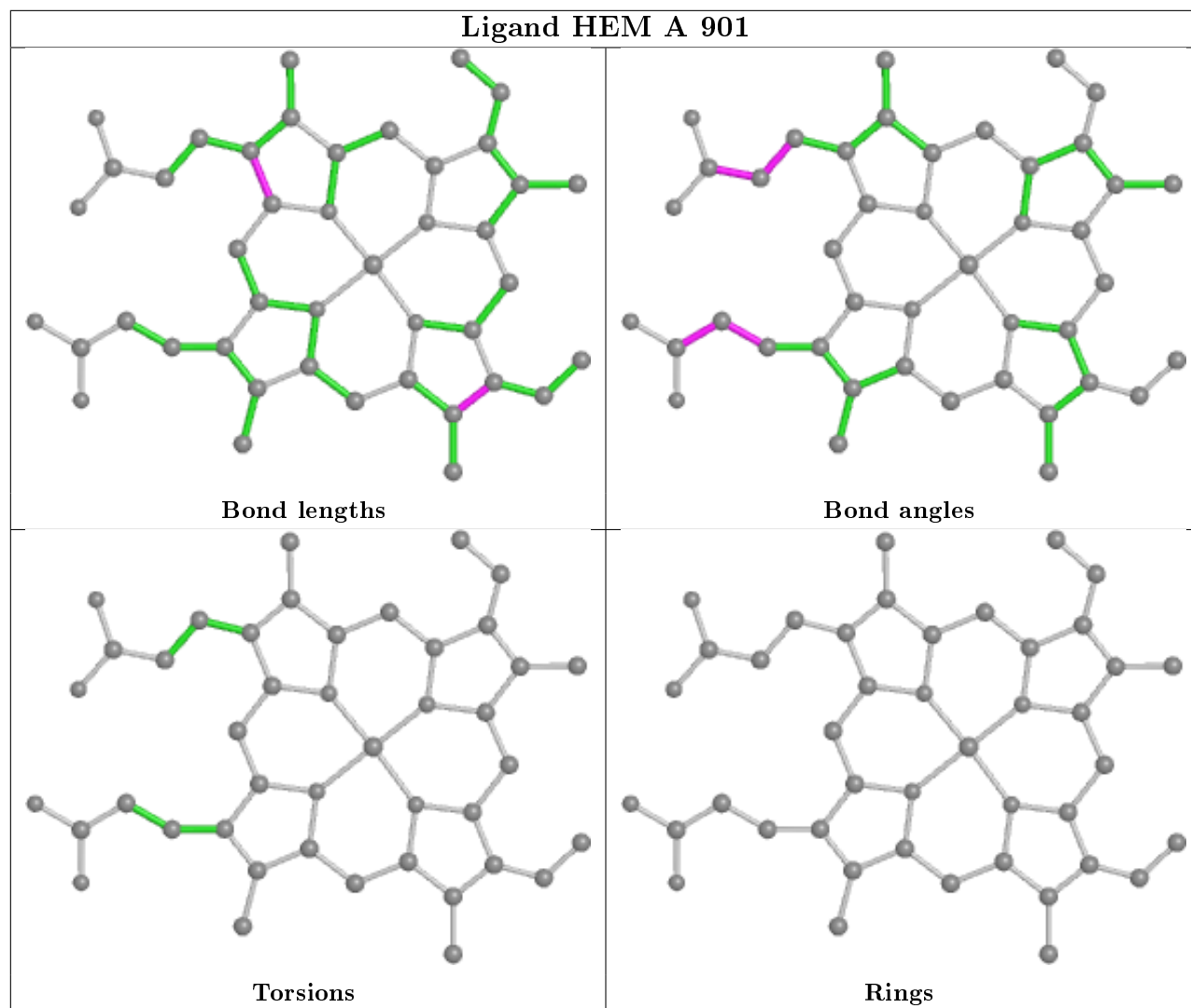
2 monomers are involved in 2 short contacts:

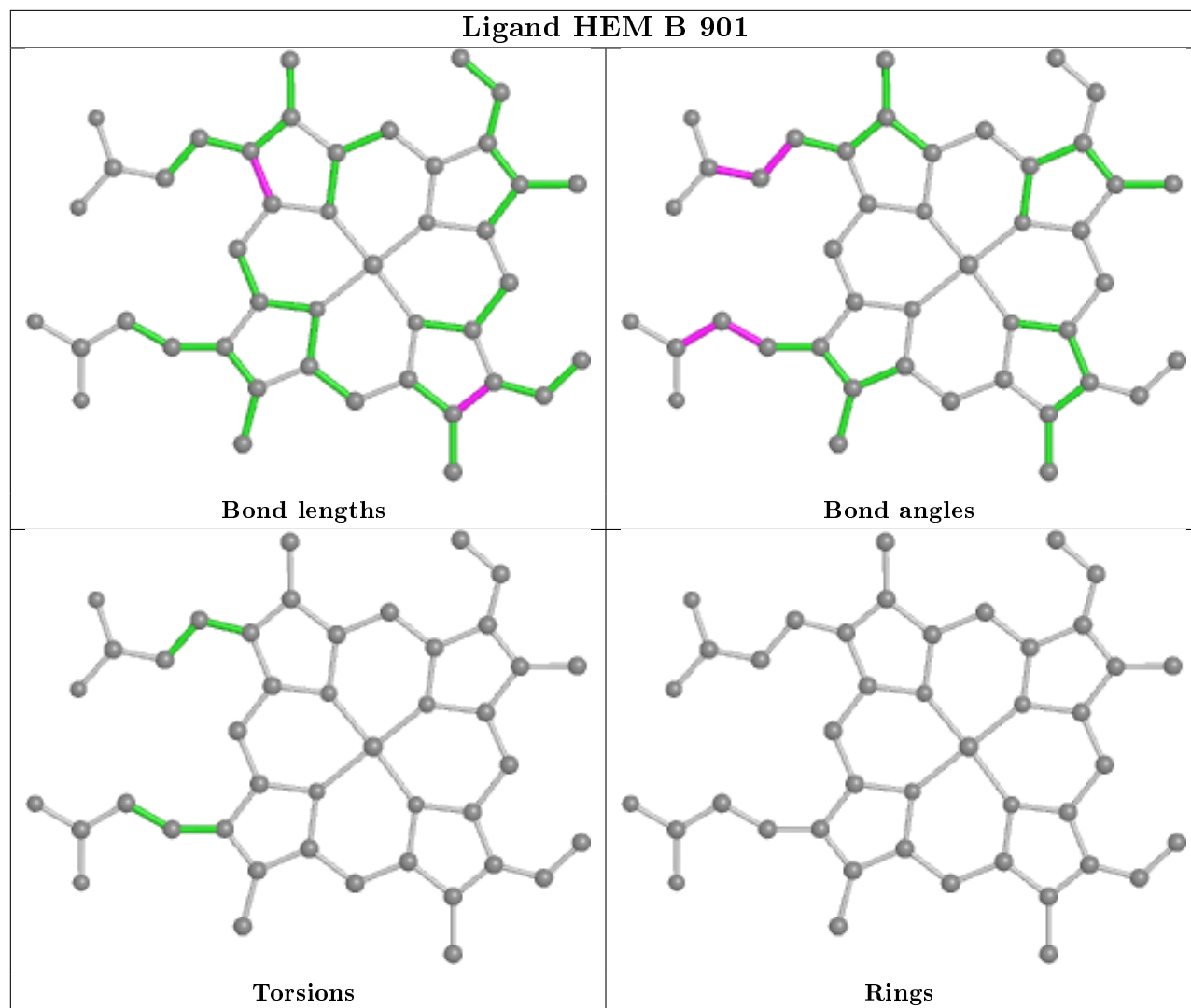
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	FAD	1	0
3	B	902	FAD	1	0

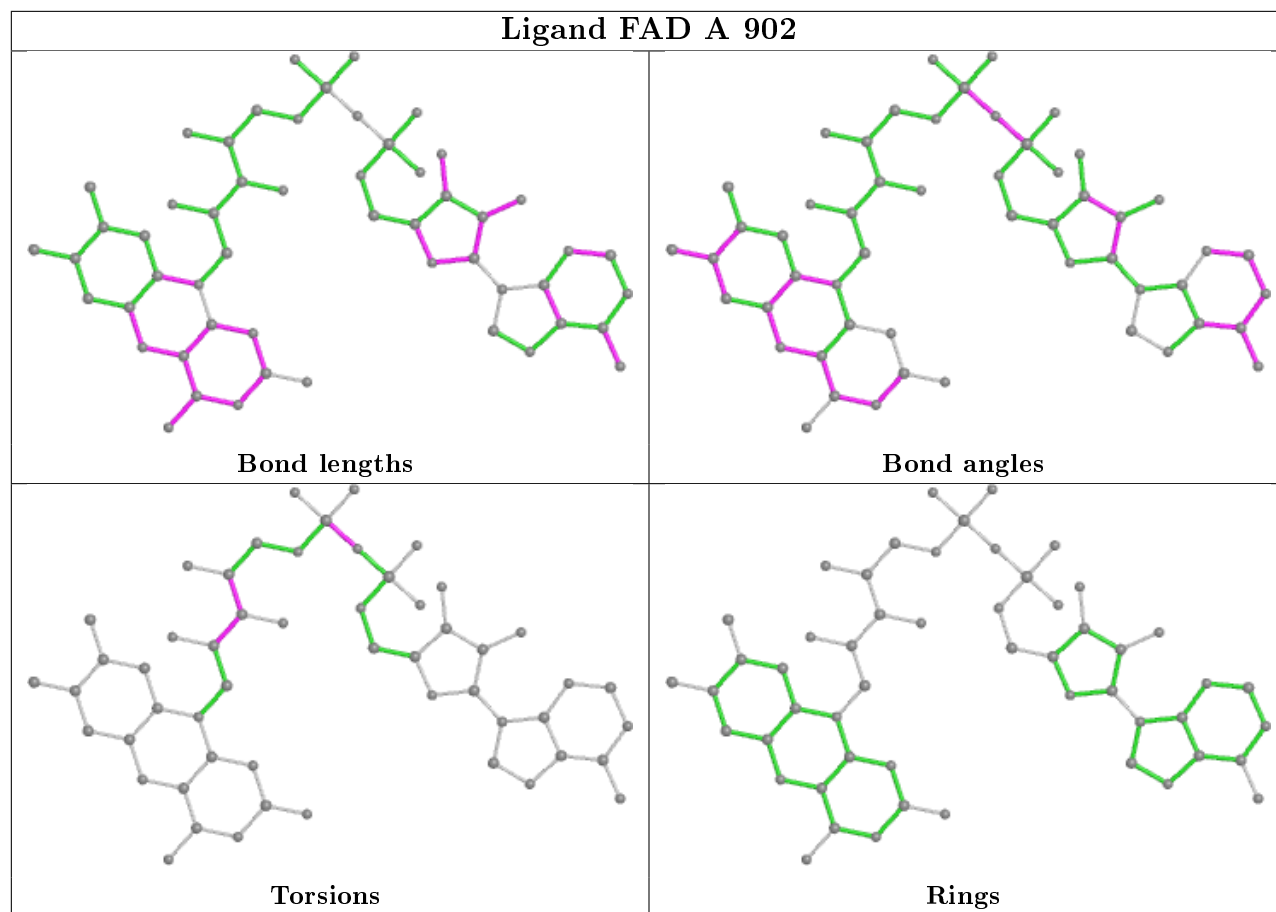
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

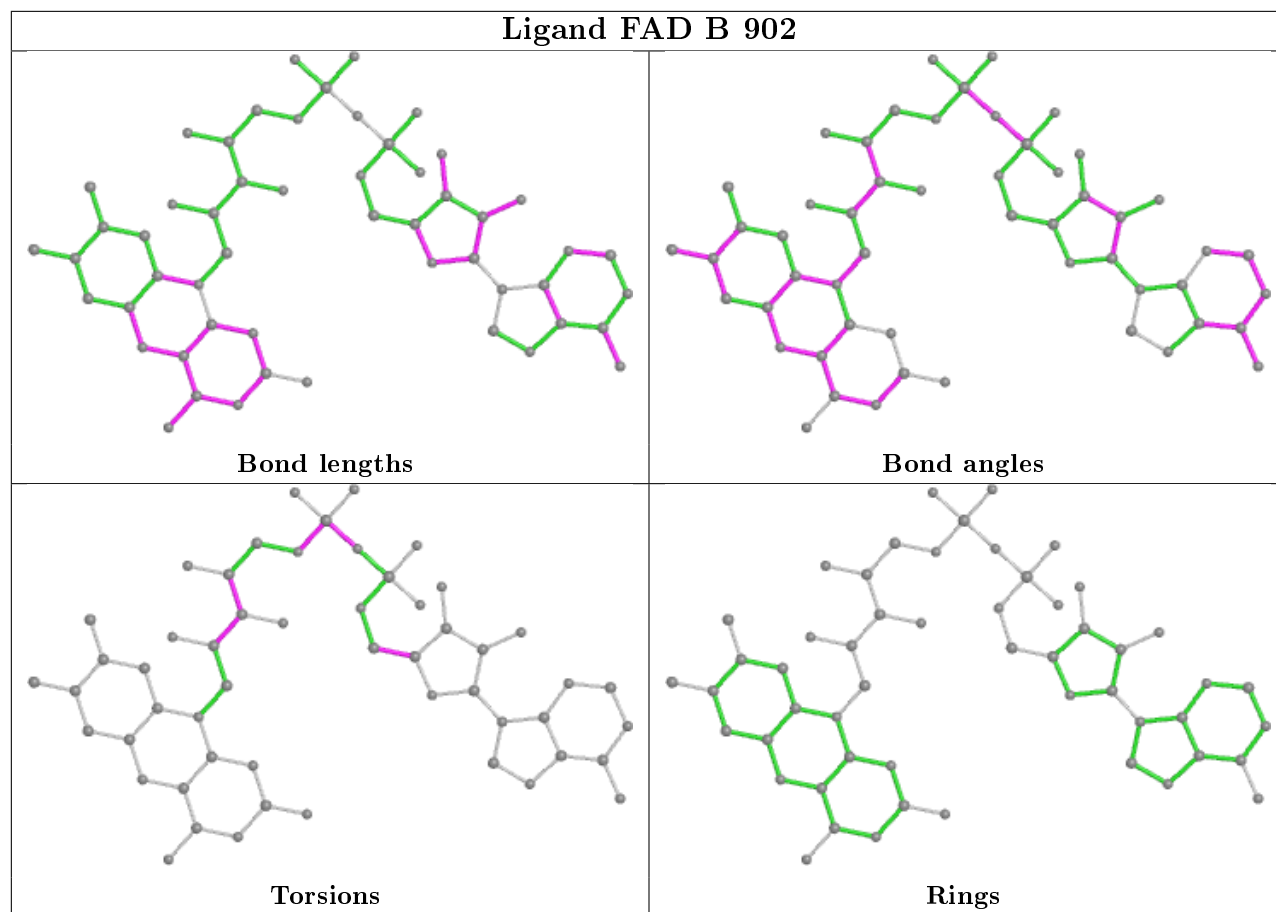












5.7 Other polymers [i](#)

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	814/875 (93%)	0.23	15 (1%) 68 65	22, 68, 121, 178	0
1	B	807/875 (92%)	0.36	41 (5%) 28 26	30, 72, 128, 171	0
All	All	1621/1750 (92%)	0.30	56 (3%) 44 40	22, 70, 125, 178	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	MET	3.9
1	B	525	LEU	3.6
1	B	10	SER	3.4
1	A	10	SER	3.4
1	A	256	LYS	3.4
1	B	531	GLU	3.4
1	B	413	GLY	3.4
1	A	251	VAL	3.4
1	A	416	ALA	3.3
1	B	586	SER	3.2
1	B	540	CYS	3.2
1	B	304	SER	3.2
1	B	549	THR	3.2
1	B	431	ASP	3.1
1	B	607	ILE	3.1
1	B	621	LEU	2.9
1	A	428	GLU	2.9
1	B	432	VAL	2.8
1	B	428	GLU	2.8
1	B	517	ALA	2.7
1	B	539	PRO	2.7
1	B	533	ASN	2.6
1	B	264	PHE	2.5
1	A	311	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	2.5
1	B	620	HIS	2.5
1	A	339	GLU	2.5
1	A	313	LEU	2.5
1	A	519	LEU	2.5
1	B	532	SER	2.5
1	B	527	ASN	2.4
1	B	578	HIS	2.4
1	B	514	ILE	2.4
1	B	341	ASP	2.3
1	A	585	SER	2.3
1	B	625	LEU	2.3
1	B	434	LYS	2.3
1	B	414	VAL	2.3
1	A	777	ALA	2.3
1	B	422	TYR	2.3
1	B	585	SER	2.2
1	A	417	SER	2.2
1	A	747	ASP	2.2
1	A	596	TRP	2.2
1	B	316	PHE	2.2
1	B	511	ILE	2.2
1	B	529	ASP	2.1
1	B	548	LEU	2.1
1	B	263	VAL	2.1
1	B	336	TRP	2.1
1	B	424	LEU	2.1
1	B	855	SER	2.1
1	B	535	LYS	2.0
1	B	436	TYR	2.0
1	B	614	LEU	2.0
1	B	566	LEU	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 ⓘ

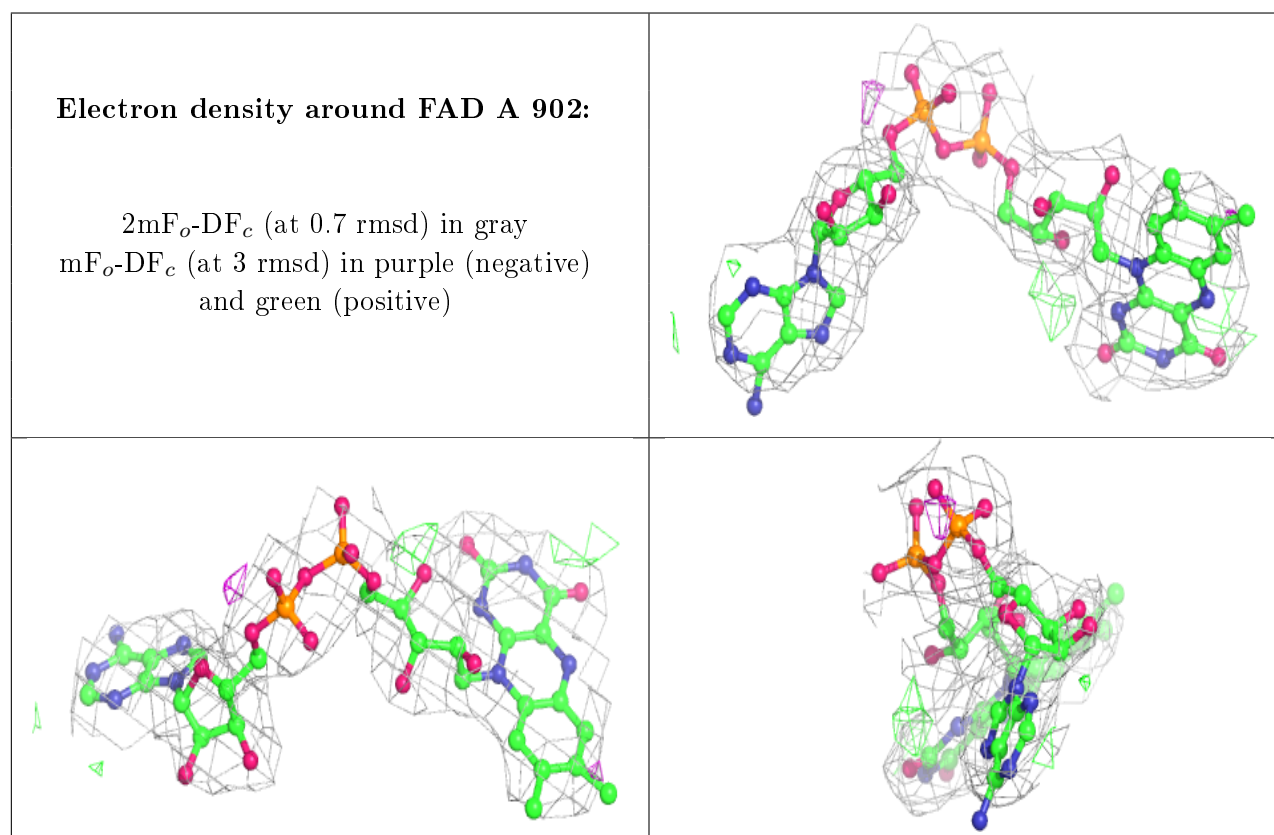
There are no carbohydrates in this entry.

6.4 Ligands [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.

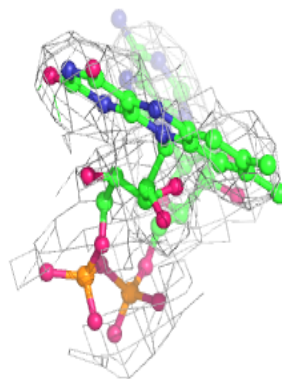
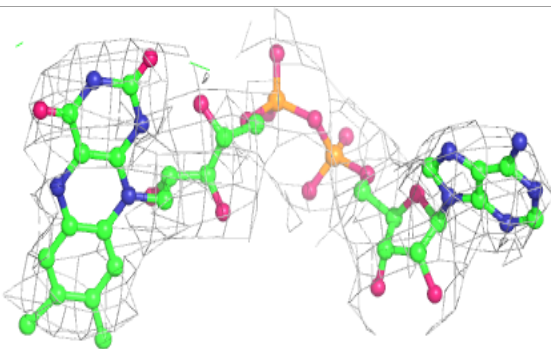
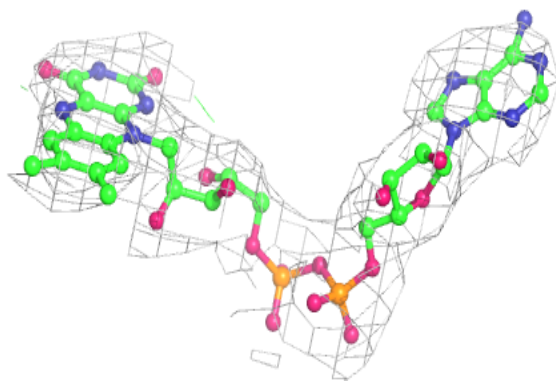
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	A	902	53/53	0.92	0.22	44,53,73,75	0
3	FAD	B	902	53/53	0.92	0.23	53,63,79,82	0
2	HEM	B	901	43/43	0.94	0.27	33,51,73,83	0
4	FMN	A	903	31/31	0.94	0.23	41,54,56,59	0
4	FMN	B	903	31/31	0.94	0.26	43,57,60,62	0
2	HEM	A	901	43/43	0.95	0.28	31,47,72,84	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.



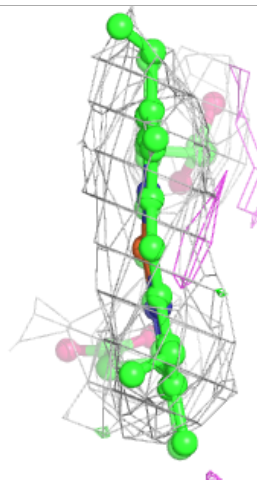
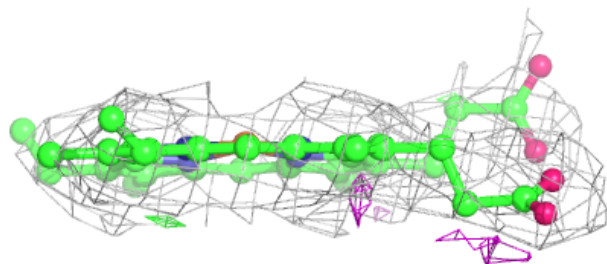
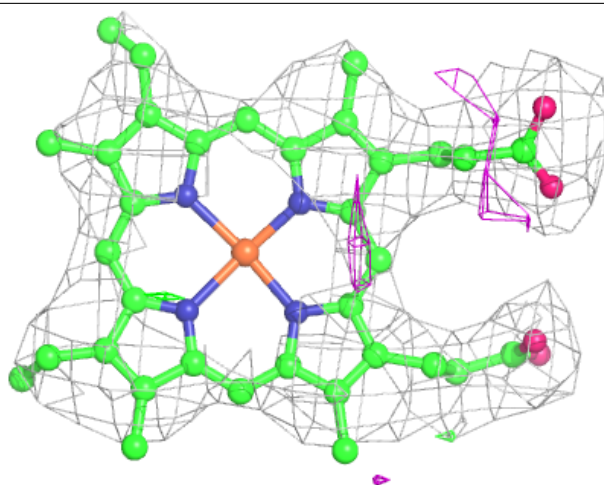
Electron density around FAD B 902:

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



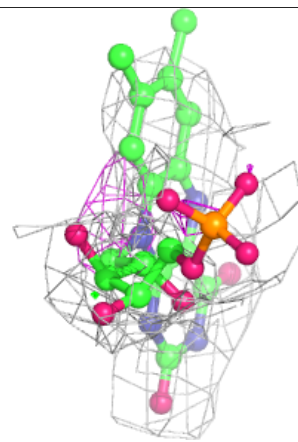
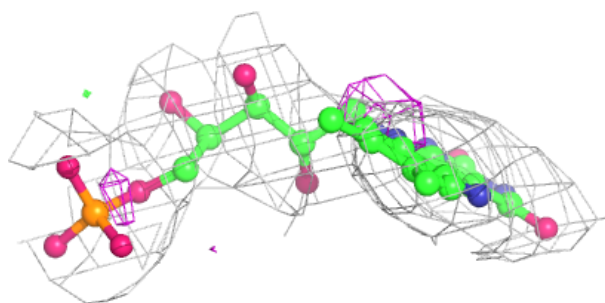
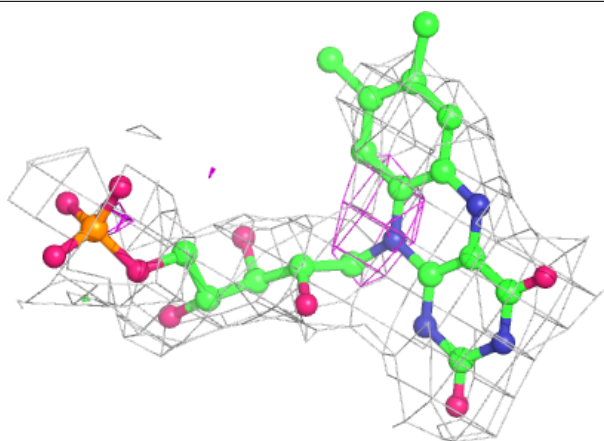
Electron density around HEM B 901:

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



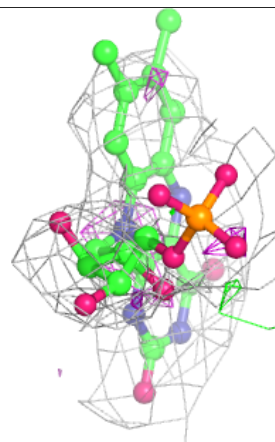
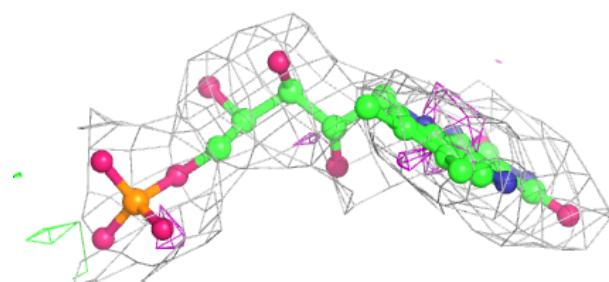
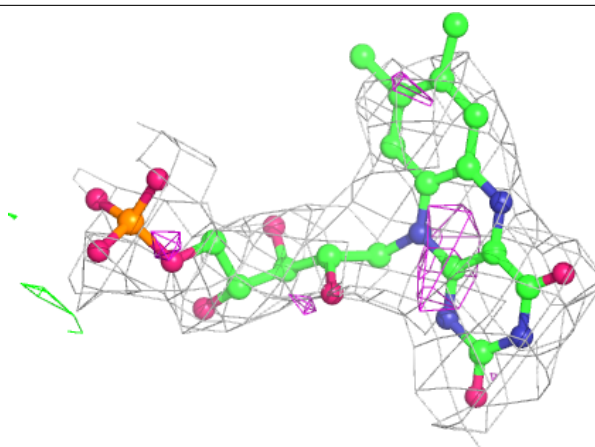
Electron density around FMN A 903:

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



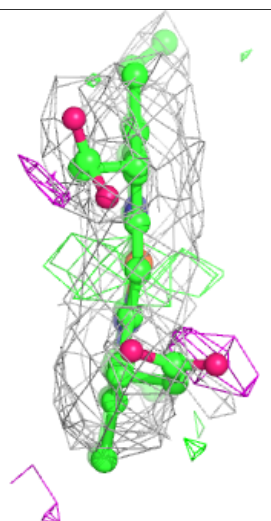
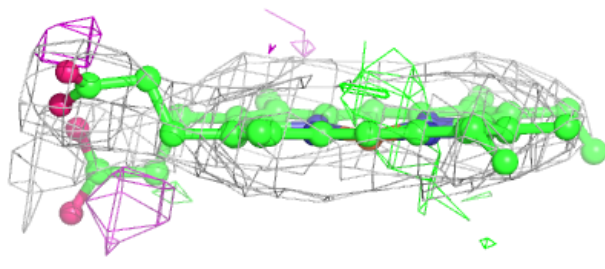
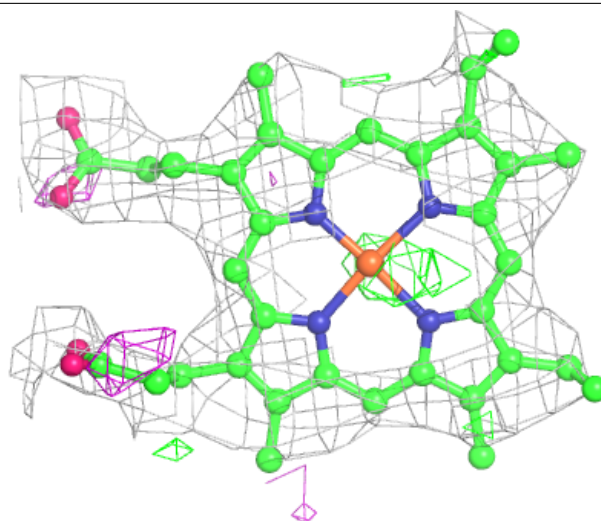
Electron density around FMN B 903:

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



Electron density around 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 ⓘ

There are no such residues in this entry.