



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:26 PM BST

PDB ID : 6QKR  
Title : 2-Naphthoyl-CoA Reductase-2-Naphthoyl-CoA complex(NCR-NCoA-soaked complex)  
Authors : Kayastha, K.; Ermler, U.  
Deposited on : 2019-01-30  
Resolution : 2.20 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

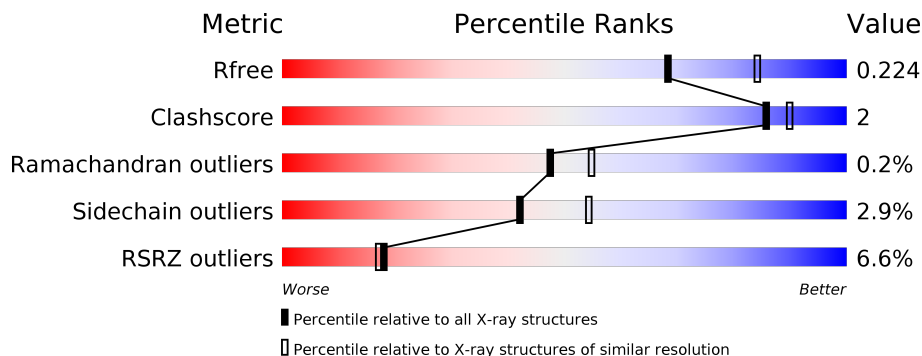
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	714	
1	B	714	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10716 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 NCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5064	3199	877	951	37	0	1	0
1	B	664	5104	3223	885	959	37	0	1	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	671	ARG	-	expression tag	UNP E1YD54
A	672	GLY	-	expression tag	UNP E1YD54
A	673	SER	-	expression tag	UNP E1YD54
A	674	LEU	-	expression tag	UNP E1YD54
A	675	GLU	-	expression tag	UNP E1YD54
A	676	VAL	-	expression tag	UNP E1YD54
A	677	ASP	-	expression tag	UNP E1YD54
A	678	LEU	-	expression tag	UNP E1YD54
A	679	GLN	-	expression tag	UNP E1YD54
A	680	GLY	-	expression tag	UNP E1YD54
A	681	ASP	-	expression tag	UNP E1YD54
A	682	HIS	-	expression tag	UNP E1YD54
A	683	GLY	-	expression tag	UNP E1YD54
A	684	LEU	-	expression tag	UNP E1YD54
A	685	SER	-	expression tag	UNP E1YD54
A	686	ALA	-	expression tag	UNP E1YD54
A	687	TRP	-	expression tag	UNP E1YD54
A	688	SER	-	expression tag	UNP E1YD54
A	689	HIS	-	expression tag	UNP E1YD54
A	690	PRO	-	expression tag	UNP E1YD54
A	691	GLN	-	expression tag	UNP E1YD54
A	692	PHE	-	expression tag	UNP E1YD54
A	693	GLU	-	expression tag	UNP E1YD54
A	694	LYS	-	expression tag	UNP E1YD54
A	695	GLY	-	expression tag	UNP E1YD54

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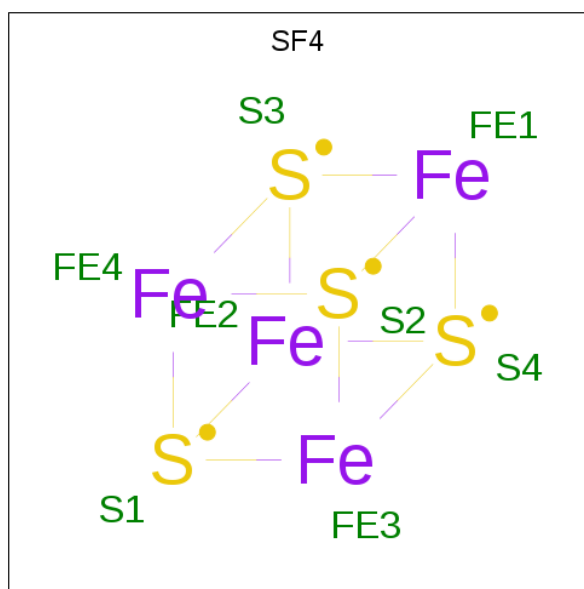
Chain	Residue	Modelled	Actual	Comment	Reference
A	696	GLY	-	expression tag	UNP E1YD54
A	697	GLY	-	expression tag	UNP E1YD54
A	698	SER	-	expression tag	UNP E1YD54
A	699	GLY	-	expression tag	UNP E1YD54
A	700	GLY	-	expression tag	UNP E1YD54
A	701	GLY	-	expression tag	UNP E1YD54
A	702	SER	-	expression tag	UNP E1YD54
A	703	GLY	-	expression tag	UNP E1YD54
A	704	GLY	-	expression tag	UNP E1YD54
A	705	GLY	-	expression tag	UNP E1YD54
A	706	SER	-	expression tag	UNP E1YD54
A	707	TRP	-	expression tag	UNP E1YD54
A	708	SER	-	expression tag	UNP E1YD54
A	709	HIS	-	expression tag	UNP E1YD54
A	710	PRO	-	expression tag	UNP E1YD54
A	711	GLN	-	expression tag	UNP E1YD54
A	712	PHE	-	expression tag	UNP E1YD54
A	713	GLU	-	expression tag	UNP E1YD54
A	714	LYS	-	expression tag	UNP E1YD54
B	671	ARG	-	expression tag	UNP E1YD54
B	672	GLY	-	expression tag	UNP E1YD54
B	673	SER	-	expression tag	UNP E1YD54
B	674	LEU	-	expression tag	UNP E1YD54
B	675	GLU	-	expression tag	UNP E1YD54
B	676	VAL	-	expression tag	UNP E1YD54
B	677	ASP	-	expression tag	UNP E1YD54
B	678	LEU	-	expression tag	UNP E1YD54
B	679	GLN	-	expression tag	UNP E1YD54
B	680	GLY	-	expression tag	UNP E1YD54
B	681	ASP	-	expression tag	UNP E1YD54
B	682	HIS	-	expression tag	UNP E1YD54
B	683	GLY	-	expression tag	UNP E1YD54
B	684	LEU	-	expression tag	UNP E1YD54
B	685	SER	-	expression tag	UNP E1YD54
B	686	ALA	-	expression tag	UNP E1YD54
B	687	TRP	-	expression tag	UNP E1YD54
B	688	SER	-	expression tag	UNP E1YD54
B	689	HIS	-	expression tag	UNP E1YD54
B	690	PRO	-	expression tag	UNP E1YD54
B	691	GLN	-	expression tag	UNP E1YD54
B	692	PHE	-	expression tag	UNP E1YD54
B	693	GLU	-	expression tag	UNP E1YD54

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Chain	Residue	Modelled	Actual	Comment	Reference
B	694	LYS	-	expression tag	UNP E1YD54
B	695	GLY	-	expression tag	UNP E1YD54
B	696	GLY	-	expression tag	UNP E1YD54
B	697	GLY	-	expression tag	UNP E1YD54
B	698	SER	-	expression tag	UNP E1YD54
B	699	GLY	-	expression tag	UNP E1YD54
B	700	GLY	-	expression tag	UNP E1YD54
B	701	GLY	-	expression tag	UNP E1YD54
B	702	SER	-	expression tag	UNP E1YD54
B	703	GLY	-	expression tag	UNP E1YD54
B	704	GLY	-	expression tag	UNP E1YD54
B	705	GLY	-	expression tag	UNP E1YD54
B	706	SER	-	expression tag	UNP E1YD54
B	707	TRP	-	expression tag	UNP E1YD54
B	708	SER	-	expression tag	UNP E1YD54
B	709	HIS	-	expression tag	UNP E1YD54
B	710	PRO	-	expression tag	UNP E1YD54
B	711	GLN	-	expression tag	UNP E1YD54
B	712	PHE	-	expression tag	UNP E1YD54
B	713	GLU	-	expression tag	UNP E1YD54
B	714	LYS	-	expression tag	UNP E1YD54

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	60	32	7	17	3	1	0	0
5	B	1	60	32	7	17	3	1	0	0

- Molecule 6 is water.

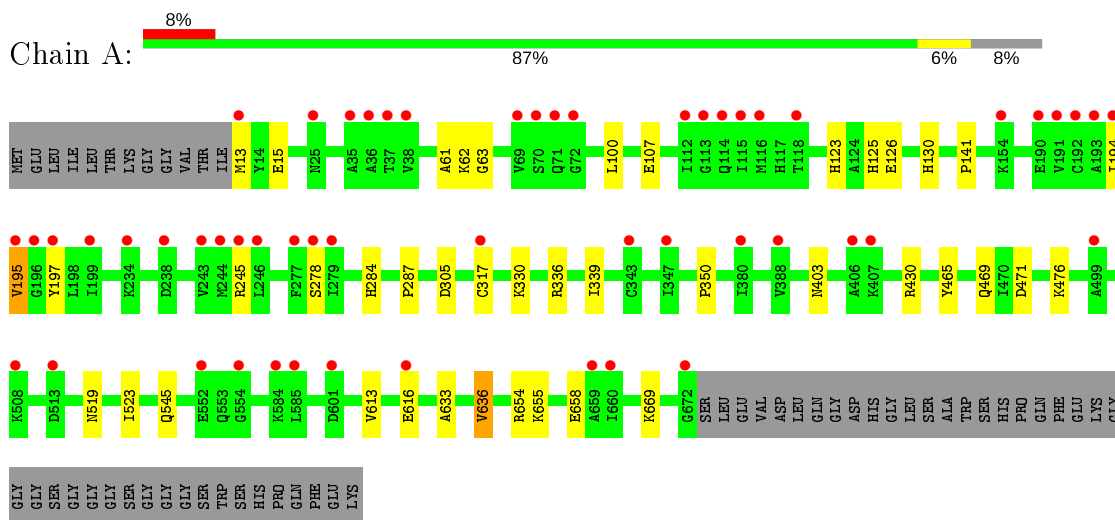
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	96	Total	O	0	0
			96	96		



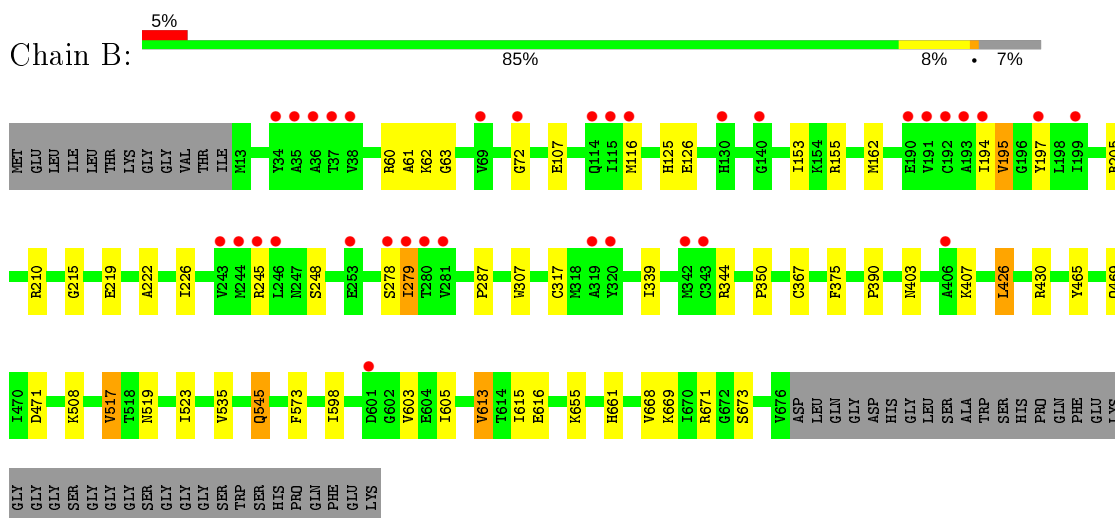
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NCR



- Molecule 1: NCR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.67Å 86.05Å 96.90Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	30.24 - 2.20 30.24 - 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.24-2.20) 99.1 (30.24-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.20Å)	Xtrriage
Refinement program	PHENIX, BUSTER	Depositor
R, $R_{free}$	0.178 , 0.218 0.182 , 0.224	Depositor DCC
$R_{free}$ test set	3405 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, SF4, J5H, 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	0.50	0/5160	0.67	2/6967 (0.0%)
1	B	0.51	0/5197	0.66	1/7017 (0.0%)
All	All	0.51	0/10357	0.66	3/13984 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ILE	C-N-CA	5.11	134.48	121.70
1	A	636	VAL	N-CA-C	-5.04	97.39	111.00
1	A	194	ILE	C-N-CA	5.03	134.27	121.70

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	5064	0	5096	16	0
1	B	5104	0	5138	29	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	A	60	0	0	3	0
5	B	60	0	0	2	0
6	A	148	0	0	1	0
6	B	96	0	0	0	0
All	All	10716	0	10334	45	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 2.

All (45) 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:248:SER:HB3	1:B:279:ILE:HG23	1.75	0.67
1:B:279:ILE:HD11	1:B:307:TRP:CE3	2.33	0.64
1:B:279:ILE:HD11	1:B:307:TRP:CZ3	2.32	0.64
1:A:125[B]:HIS:CD2	1:A:126:GLU:HG3	2.32	0.64
1:A:305:ASP:OD1	1:A:336:ARG:HD2	2.00	0.61
1:A:287:PRO:HA	5:A:804:J5H:N1	2.20	0.55
1:B:222:ALA:O	1:B:226:ILE:HG12	2.11	0.50
1:B:162:MET:O	1:B:210:ARG:NH2	2.45	0.50
1:A:284:HIS:HE1	5:A:804:J5H:CBT	2.25	0.49
1:B:210:ARG:HB2	1:B:215:GLY:HA3	1.95	0.49
1:B:197:TYR:OH	5:B:804:J5H:CAU	2.62	0.48
1:A:403:ASN:O	1:A:430:ARG:HD2	2.12	0.48
1:B:248:SER:CB	1:B:279:ILE:HG23	2.44	0.48
1:B:426:LEU:HD22	1:B:668:VAL:HG13	1.96	0.47
1:B:403:ASN:O	1:B:430:ARG:HD2	2.14	0.47
1:B:517:VAL:HG12	1:B:598:ILE:HG21	1.97	0.47
1:B:72:GLY:HA3	1:B:116:MET:HB3	1.97	0.46
1:B:317:CYS:HB3	1:B:339:ILE:HB	1.96	0.46
1:A:123:HIS:HE1	6:A:981:HOH:O	1.99	0.46
1:B:125[B]:HIS:CD2	1:B:126:GLU:HG3	2.51	0.44
1:A:654:ARG:HD2	1:A:658:GLU:HG2	1.99	0.44
1:B:519:ASN:O	1:B:523:ILE:HG12	2.18	0.44
1:A:633:ALA:O	1:A:636:VAL:O	2.34	0.44
1:B:153:ILE:HD12	1:B:155:ARG:HB3	1.99	0.44
1:A:317:CYS:HB3	1:A:339:ILE:HB	1.99	0.44
1:A:519:ASN:O	1:A:523:ILE:HG12	2.17	0.44
1:B:375:PHE:HB3	1:B:573:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:PRO:HA	5:B:804:J5H:N1	2.33	0.43
1:B:671:ARG:HD3	1:B:671:ARG:HA	1.90	0.43
1:B:545:GLN:HE21	1:B:545:GLN:HB2	1.64	0.43
1:A:245:ARG:HG2	1:A:278:SER:HB3	2.00	0.43
1:B:245:ARG:HG2	1:B:278:SER:HB3	2.01	0.43
1:A:63:GLY:HA3	1:A:350:PRO:O	2.20	0.42
1:B:605:ILE:HG13	1:B:613:VAL:HG13	2.00	0.42
1:B:63:GLY:HA3	1:B:350:PRO:O	2.19	0.42
1:A:197:TYR:OH	5:A:804:J5H:CAU	2.68	0.42
1:B:465:TYR:O	1:B:469:GLN:HG2	2.19	0.41
1:B:344:ARG:HB3	1:B:367:CYS:SG	2.61	0.41
1:A:61:ALA:HB1	1:A:107:GLU:HB2	2.03	0.41
1:B:116:MET:HE2	1:B:197:TYR:CE2	2.56	0.41
1:A:130:HIS:HA	1:A:141:PRO:HG3	2.03	0.40
1:B:61:ALA:HB1	1:B:107:GLU:HB2	2.02	0.40
1:B:535:VAL:HG21	1:B:615:ILE:HG22	2.02	0.40
1:A:465:TYR:O	1:A:469:GLN:HG2	2.22	0.40
1:B:390:PRO:HA	1:B:661:HIS:CE1	2.56	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	659/714 (92%)	638 (97%)	20 (3%)	1 (0%)	47	55
1	B	663/714 (93%)	643 (97%)	19 (3%)	1 (0%)	47	55
All	All	1322/1428 (93%)	1281 (97%)	39 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	VAL
1	B	195	VAL

### 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	532/572 (93%)	519 (98%)	13 (2%)	49 62
1	B	537/572 (94%)	519 (97%)	18 (3%)	37 47
All	All	1069/1144 (93%)	1038 (97%)	31 (3%)	42 54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	15	GLU
1	A	62	LYS
1	A	100	LEU
1	A	195	VAL
1	A	330	LYS
1	A	471	ASP
1	A	476	LYS
1	A	545	GLN
1	A	613	VAL
1	A	616	GLU
1	A	655	LYS
1	A	669	LYS
1	B	60	ARG
1	B	62	LYS
1	B	195	VAL
1	B	205	ARG
1	B	219	GLU
1	B	279	ILE
1	B	407	LYS
1	B	426	LEU
1	B	471	ASP

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Mol	Chain	Res	Type
1	B	508	LYS
1	B	517	VAL
1	B	545	GLN
1	B	603	VAL
1	B	613	VAL
1	B	616	GLU
1	B	655	LYS
1	B	669	LYS
1	B	673	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	284	HIS
1	A	545	GLN
1	B	545	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	FMN	A	803	-	31,33,33	1.71	5 (16%)	40,50,50	2.59	6 (15%)
2	SF4	A	801	1	0,12,12	0.00	-	-		
3	FAD	B	802	-	51,58,58	1.40	5 (9%)	60,89,89	2.15	8 (13%)
4	FMN	B	803	-	31,33,33	1.84	5 (16%)	40,50,50	2.63	6 (15%)
5	J5H	B	804	-	56,64,64	2.96	15 (26%)	72,95,95	1.23	8 (11%)
5	J5H	A	804	-	56,64,64	2.95	16 (28%)	72,95,95	1.29	6 (8%)
3	FAD	A	802	-	51,58,58	1.52	5 (9%)	60,89,89	2.14	8 (13%)
2	SF4	B	801	1	0,12,12	0.00	-	-		

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	803	-	-	1/18/18/18	0/3/3/3
2	SF4	A	801	1	-	-	0/6/5/5
3	FAD	B	802	-	-	2/30/50/50	0/6/6/6
4	FMN	B	803	-	-	1/18/18/18	0/3/3/3
5	J5H	B	804	-	-	9/51/71/71	0/5/5/5
5	J5H	A	804	-	-	6/51/71/71	0/5/5/5
3	FAD	A	802	-	-	1/30/50/50	0/6/6/6
2	SF4	B	801	1	-	-	0/6/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	J5H	C2'-C3'	-10.78	1.28	1.52
5	A	804	J5H	C2'-C3'	-10.63	1.29	1.52
5	A	804	J5H	C2'-C1'	9.10	1.67	1.53
5	B	804	J5H	C2'-C1'	9.05	1.67	1.53
3	A	802	FAD	C4X-C10	8.32	1.47	1.38
4	B	803	FMN	C4A-C10	7.72	1.46	1.38
5	B	804	J5H	O4'-C1'	-7.48	1.30	1.41
5	A	804	J5H	O4'-C1'	-7.47	1.30	1.41
5	A	804	J5H	CBP-NBH	7.22	1.49	1.33
5	B	804	J5H	CBP-NBH	7.11	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	J5H	CBQ-NBI	7.01	1.48	1.33
4	A	803	FMN	C4A-C10	6.87	1.45	1.38
3	B	802	FAD	C4X-C10	6.87	1.45	1.38
5	B	804	J5H	CBQ-NBI	6.86	1.48	1.33
5	A	804	J5H	O4'-C4'	4.73	1.55	1.45
5	B	804	J5H	O4'-C4'	4.54	1.55	1.45
5	B	804	J5H	CBR-SBO	4.01	1.84	1.76
5	A	804	J5H	CBR-SBO	3.94	1.84	1.76
4	B	803	FMN	C4-C4A	3.44	1.47	1.41
5	B	804	J5H	PCG-O3'	3.38	1.65	1.59
3	B	802	FAD	C9A-N10	3.31	1.43	1.38
3	B	802	FAD	C4-N3	3.27	1.38	1.33
4	B	803	FMN	C4-N3	3.22	1.38	1.33
4	B	803	FMN	C9A-N10	3.19	1.42	1.38
3	B	802	FAD	C4-C4X	3.17	1.46	1.41
4	A	803	FMN	C4-N3	3.15	1.38	1.33
5	A	804	J5H	PCG-O3'	3.12	1.65	1.59
4	A	803	FMN	C9A-N10	3.03	1.42	1.38
4	A	803	FMN	C4-C4A	2.98	1.46	1.41
3	A	802	FAD	C4-N3	2.97	1.38	1.33
5	A	804	J5H	C5'-C4'	-2.95	1.42	1.51
3	A	802	FAD	C4-C4X	2.94	1.46	1.41
5	B	804	J5H	PCH-O5'	2.87	1.70	1.59
5	A	804	J5H	PCH-O5'	2.87	1.70	1.59
4	A	803	FMN	C5A-N5	2.87	1.40	1.35
3	A	802	FAD	C9A-N10	2.86	1.42	1.38
5	B	804	J5H	C5'-C4'	-2.84	1.42	1.51
5	A	804	J5H	C6-N6	2.76	1.44	1.34
5	B	804	J5H	C6-N6	2.71	1.43	1.34
5	B	804	J5H	C3'-C4'	2.51	1.59	1.52
5	B	804	J5H	OAE-CBQ	-2.44	1.18	1.23
5	A	804	J5H	C3'-C4'	2.40	1.59	1.52
4	B	803	FMN	C5A-N5	2.33	1.39	1.35
5	B	804	J5H	CBU-CBR	2.32	1.54	1.49
5	B	804	J5H	CBT-CBU	2.23	1.41	1.37
3	A	802	FAD	C5X-N5	2.21	1.39	1.35
3	B	802	FAD	C5X-N5	2.19	1.39	1.35
5	A	804	J5H	CBU-CBR	2.17	1.53	1.49
5	A	804	J5H	PCI-OBK	2.09	1.67	1.59
5	A	804	J5H	O2'-C2'	2.05	1.47	1.43
5	A	804	J5H	CBT-CBU	2.01	1.41	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	FMN	C4-N3-C2	12.78	125.93	115.14
4	A	803	FMN	C4-N3-C2	12.72	125.88	115.14
3	A	802	FAD	C4-N3-C2	12.42	125.63	115.14
3	B	802	FAD	C4-N3-C2	12.40	125.61	115.14
4	A	803	FMN	C4A-C4-N3	-6.89	114.00	123.43
4	B	803	FMN	C4A-C4-N3	-6.86	114.05	123.43
3	B	802	FAD	C4X-C4-N3	-6.78	114.16	123.43
3	A	802	FAD	C4X-C4-N3	-6.74	114.21	123.43
5	A	804	J5H	N3-C2-N1	-4.83	121.13	128.68
5	B	804	J5H	N3-C2-N1	-4.82	121.14	128.68
3	B	802	FAD	C10-C4X-N5	4.43	124.32	121.26
4	B	803	FMN	C10-C4A-N5	4.23	124.18	121.26
3	A	802	FAD	C10-C4X-N5	4.07	124.07	121.26
4	A	803	FMN	C10-C4A-N5	4.00	124.02	121.26
3	B	802	FAD	C4-C4X-C10	-3.69	117.51	119.95
4	B	803	FMN	C4-C4A-C10	-3.60	117.57	119.95
3	A	802	FAD	C4-C4X-C10	-3.46	117.66	119.95
5	B	804	J5H	CBA-SBO-CBR	3.37	104.04	99.80
4	B	803	FMN	C4A-C10-N10	-3.30	116.91	120.30
4	A	803	FMN	C4-C4A-C10	-3.28	117.78	119.95
3	A	802	FAD	C4X-C10-N10	-3.23	116.98	120.30
3	B	802	FAD	C4X-C10-N10	-3.14	117.08	120.30
4	A	803	FMN	C4A-C10-N10	-3.05	117.17	120.30
5	A	804	J5H	C3'-C2'-C1'	3.02	106.57	99.89
3	A	802	FAD	C1'-N10-C9A	2.96	120.62	118.29
5	A	804	J5H	CAT-CBU-CBT	2.95	122.74	119.23
4	B	803	FMN	C1'-N10-C9A	2.81	120.50	118.29
5	B	804	J5H	C3'-C2'-C1'	2.68	105.82	99.89
3	B	802	FAD	C1'-N10-C9A	2.46	120.23	118.29
3	A	802	FAD	C4'-C3'-C2'	2.46	118.48	113.36
3	B	802	FAD	C4'-C3'-C2'	2.41	118.38	113.36
5	B	804	J5H	PCH-OBN-PCI	-2.39	124.61	132.83
3	A	802	FAD	C5A-C6A-N6A	2.36	123.94	120.35
5	B	804	J5H	OAD-CBP-CBB	-2.34	117.73	122.02
5	A	804	J5H	CAW-CAT-CBU	-2.34	118.15	120.79
4	A	803	FMN	C1'-N10-C9A	2.29	120.09	118.29
3	B	802	FAD	C5A-C6A-N6A	2.28	123.82	120.35
5	B	804	J5H	CAT-CBU-CBT	2.15	121.79	119.23
5	A	804	J5H	C4-C5-N7	-2.15	107.16	109.40
5	B	804	J5H	C4-C5-N7	-2.05	107.26	109.40
5	A	804	J5H	OAD-CBP-CBB	-2.02	118.33	122.02
5	B	804	J5H	OBK-CBD-CCF	-2.01	107.31	110.55

There are no chirality outliers.

All (20) torsion outliers are listed below:

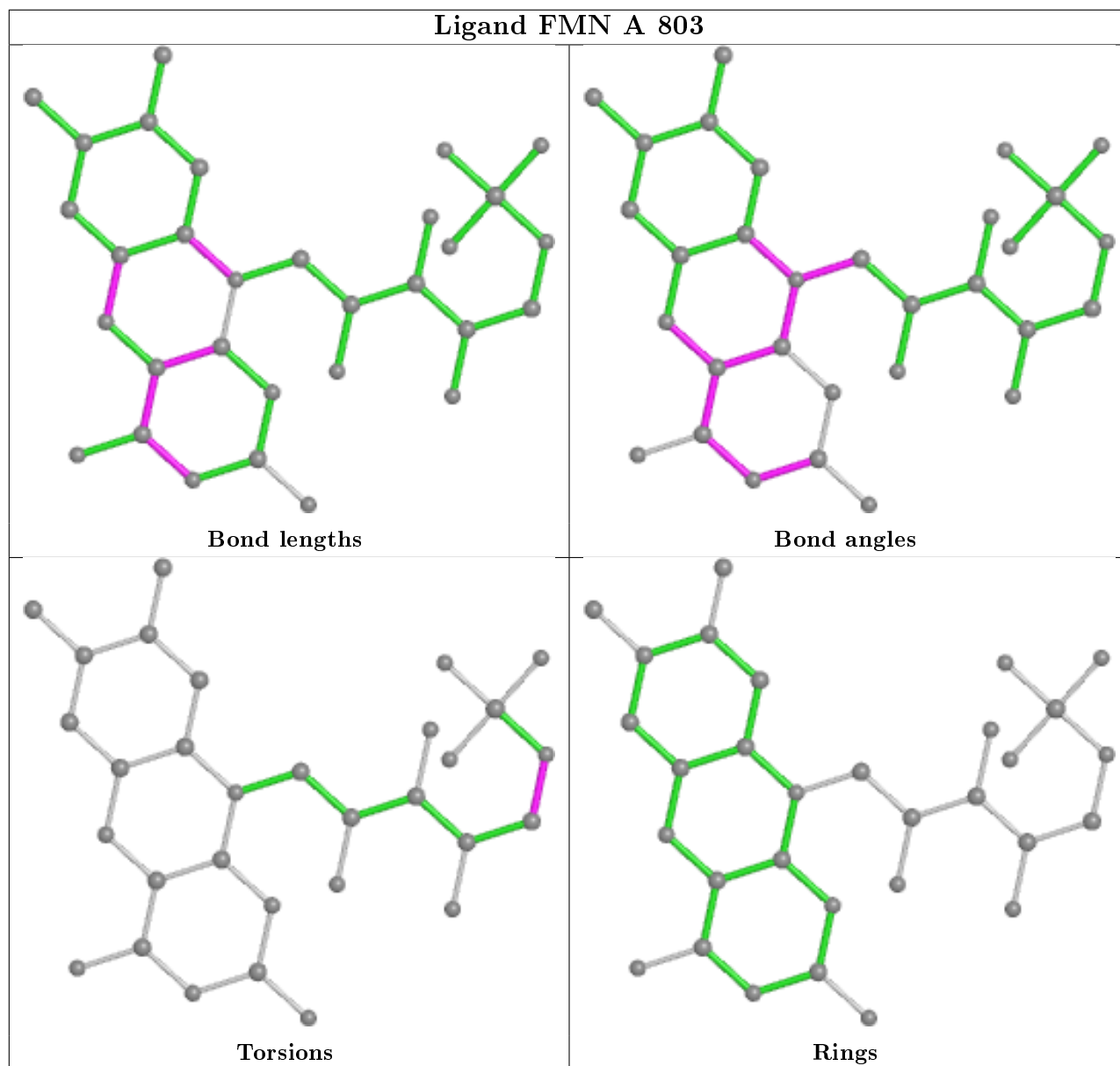
Mol	Chain	Res	Type	Atoms
5	B	804	J5H	CBU-CBR-SBO-CBA
5	B	804	J5H	OAF-CBR-SBO-CBA
5	B	804	J5H	NBI-CAZ-CBB-CBP
5	B	804	J5H	C5'-O5'-PCH-OAO
5	A	804	J5H	CBU-CBR-SBO-CBA
5	A	804	J5H	OAF-CBR-SBO-CBA
5	A	804	J5H	O4'-C4'-C5'-O5'
5	B	804	J5H	O4'-C4'-C5'-O5'
5	B	804	J5H	C3'-C4'-C5'-O5'
5	A	804	J5H	NBI-CAZ-CBB-CBP
4	B	803	FMN	C4'-C5'-O5'-P
5	B	804	J5H	C5'-O5'-PCH-OBN
4	A	803	FMN	C4'-C5'-O5'-P
5	B	804	J5H	C5'-O5'-PCH-OAH
5	A	804	J5H	C3'-C4'-C5'-O5'
3	B	802	FAD	PA-O3P-P-O5'
3	A	802	FAD	O4B-C4B-C5B-O5B
5	A	804	J5H	PCI-OBN-PCH-OAH
3	B	802	FAD	O4B-C4B-C5B-O5B
5	B	804	J5H	C4'-C3'-O3'-PCG

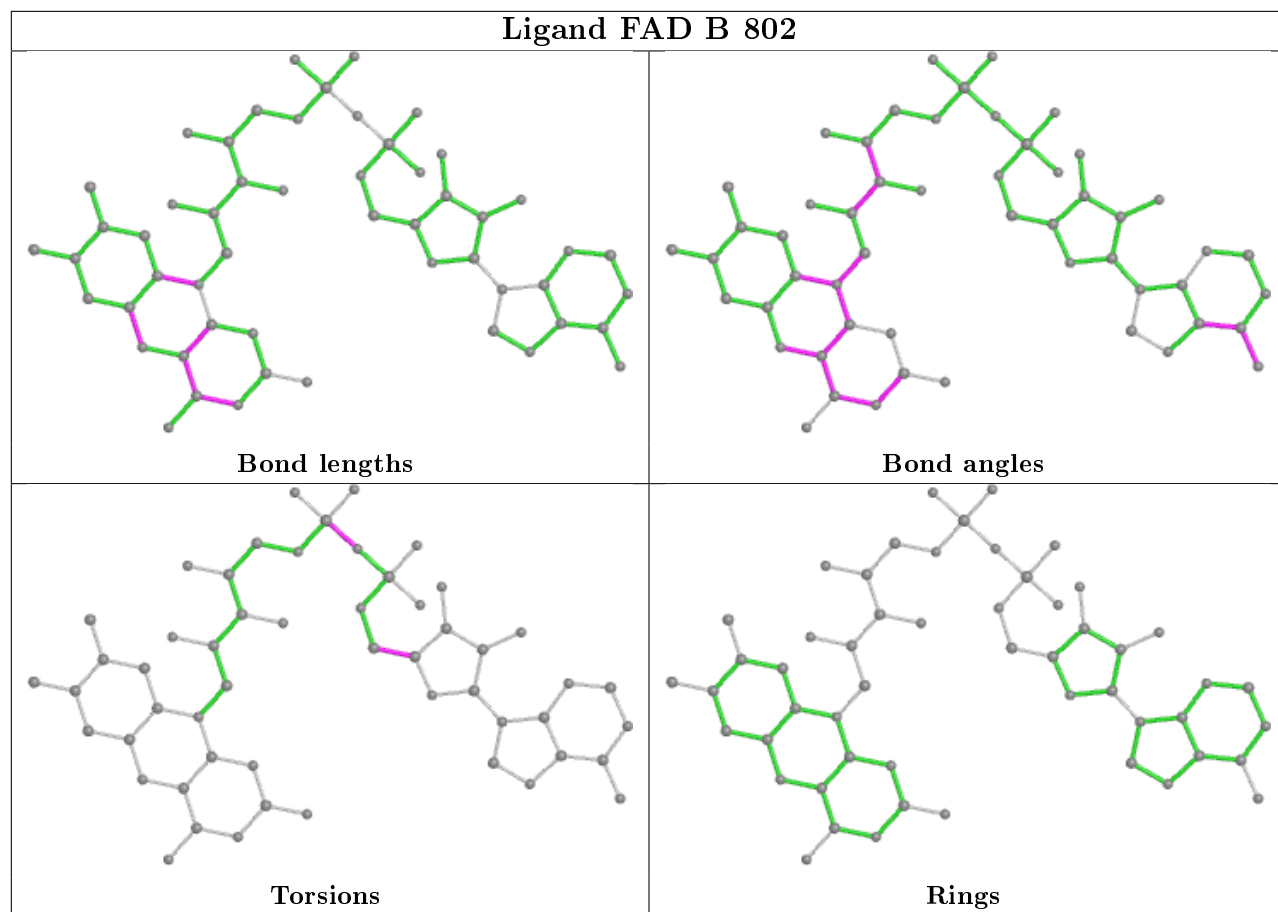
There are no ring outliers.

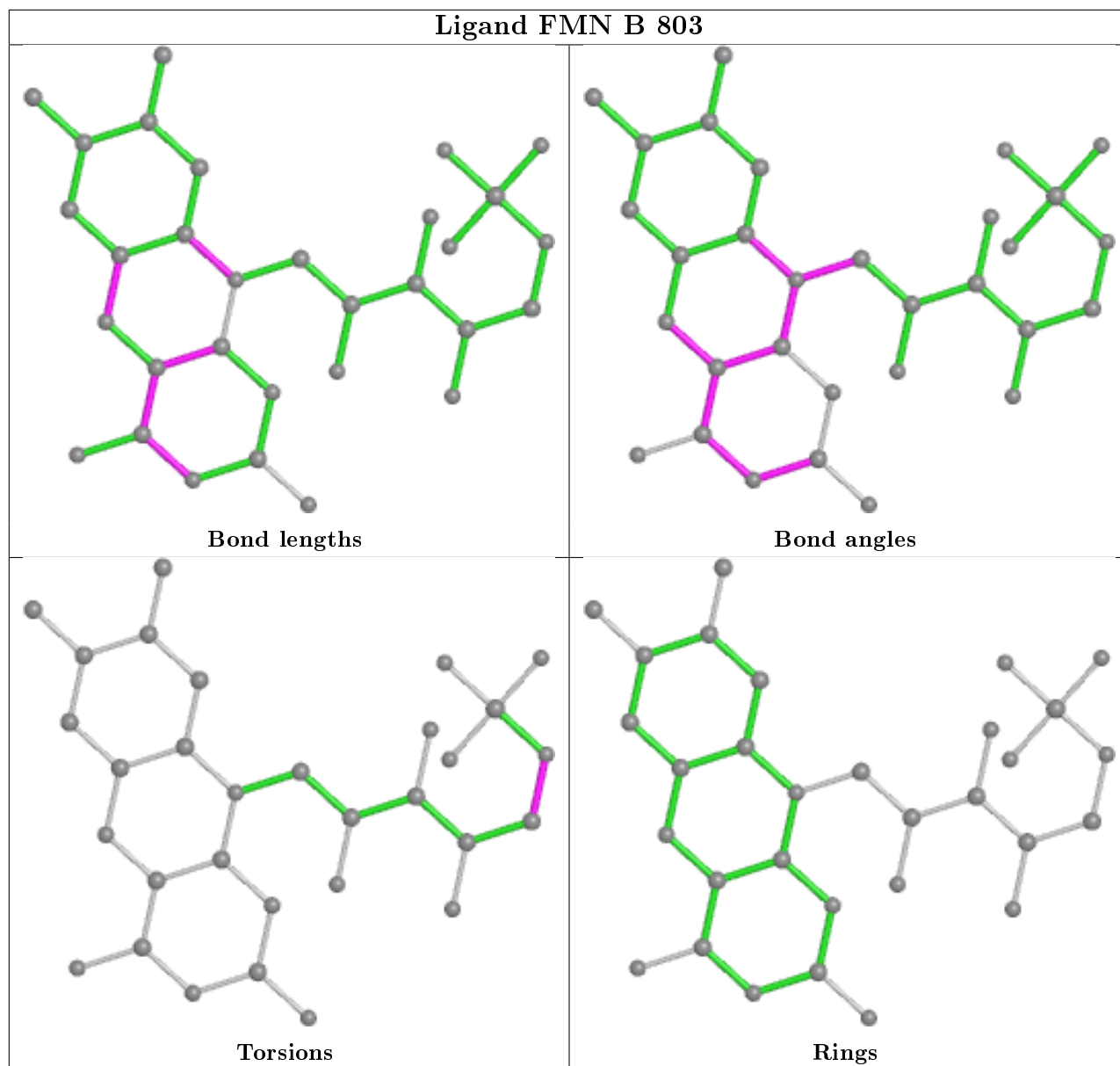
2 monomers are involved in 5 short contacts:

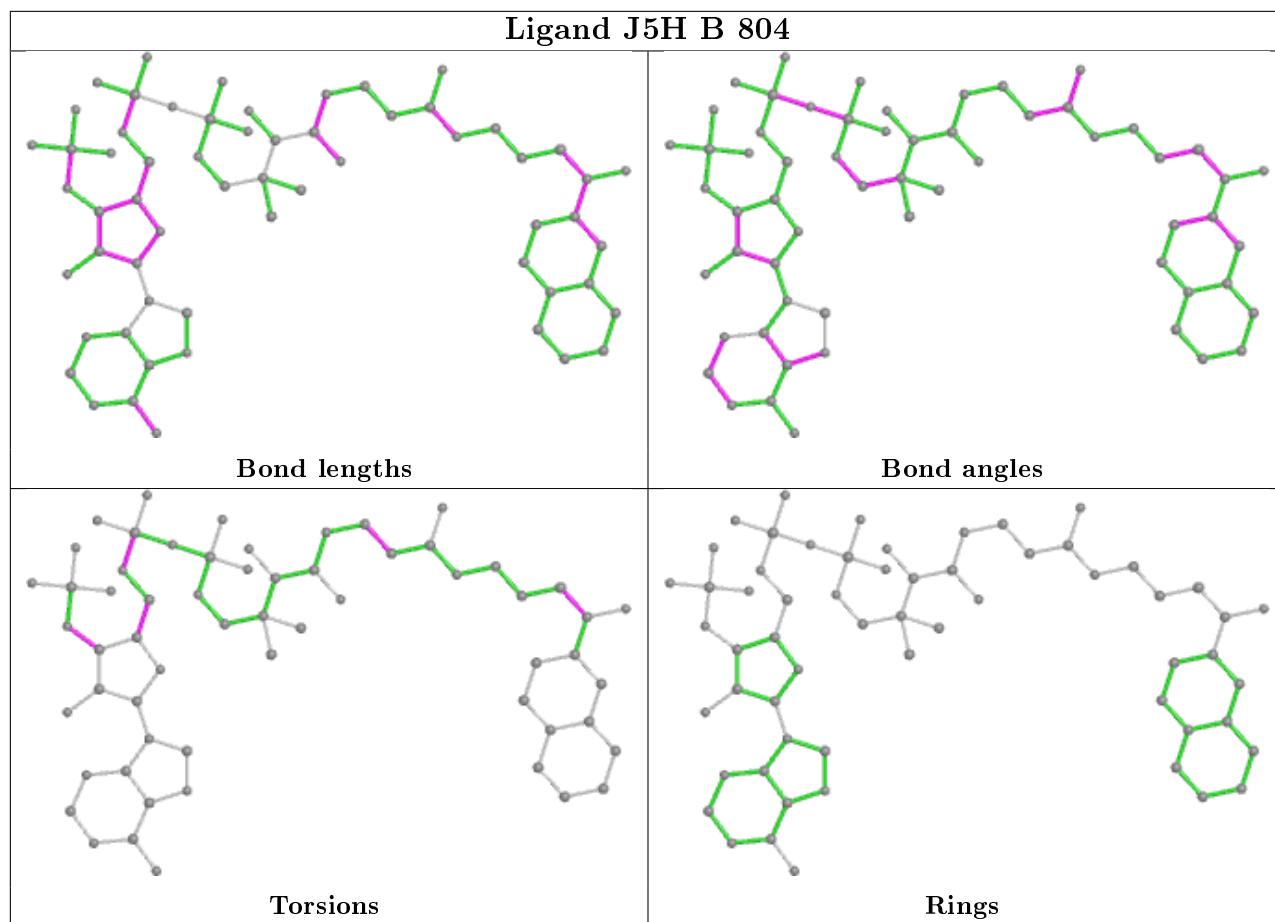
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	J5H	2	0
5	A	804	J5H	3	0

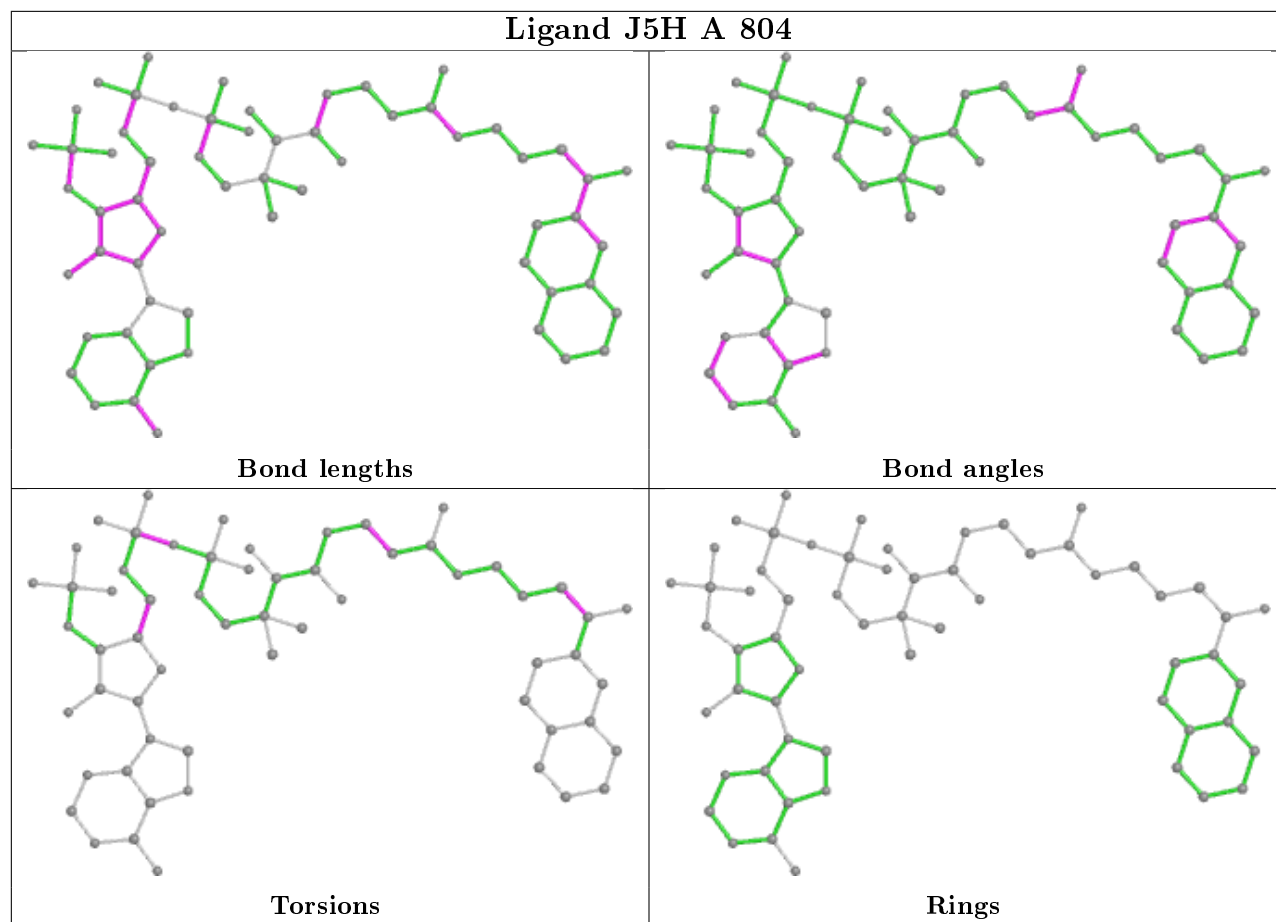
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



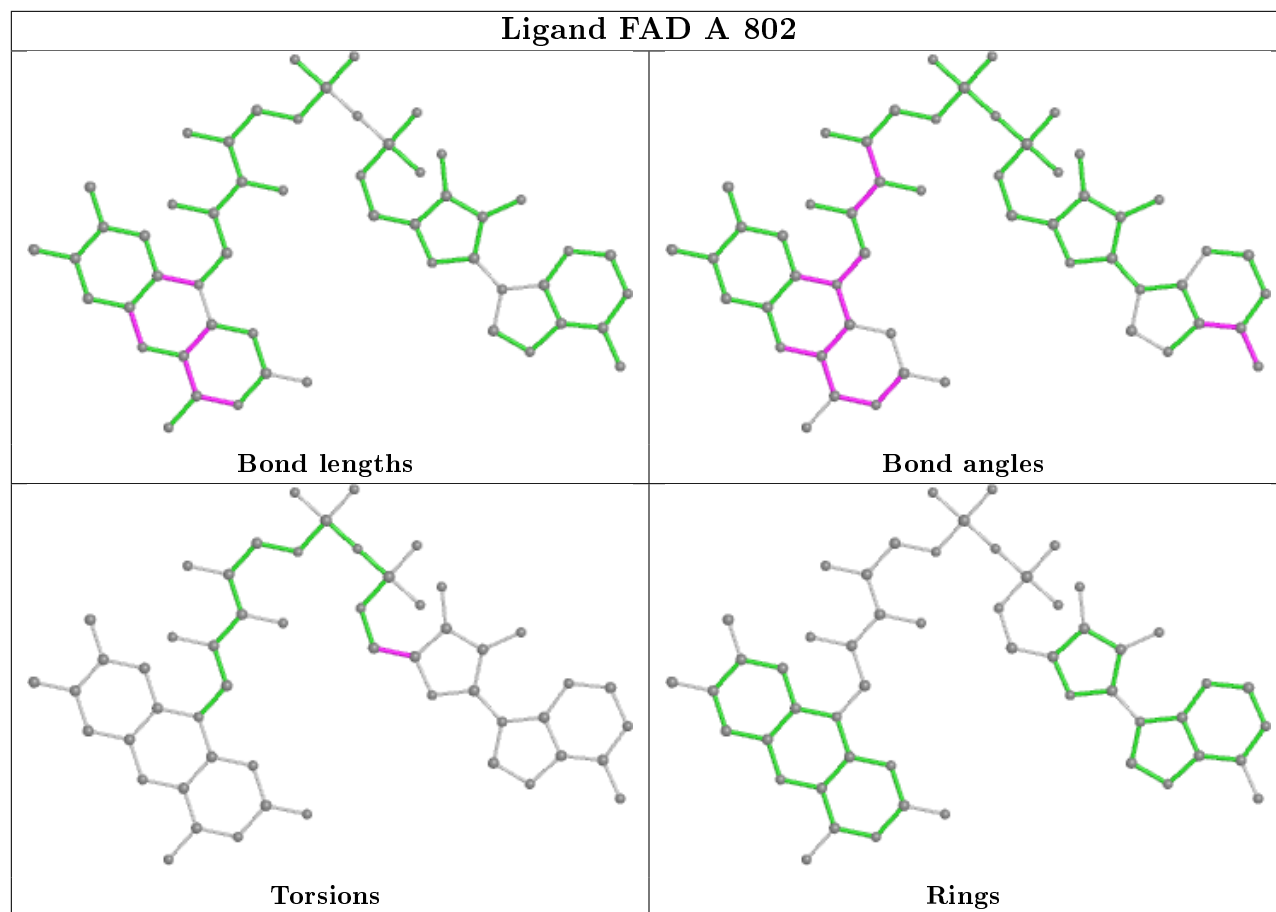












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	660/714 (92%)	0.20	54 (8%) <b>11</b> <b>10</b>	45, 62, 86, 105	0
1	B	664/714 (92%)	0.06	34 (5%) <b>28</b> <b>26</b>	41, 59, 85, 111	0
All	All	1324/1428 (92%)	0.13	88 (6%) <b>18</b> <b>17</b>	41, 60, 86, 111	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	6.7
1	A	191	VAL	5.7
1	A	245	ARG	5.3
1	B	406	ALA	5.1
1	A	192	CYS	5.1
1	A	36	ALA	4.9
1	B	192	CYS	4.7
1	B	35	ALA	4.7
1	A	244	MET	4.6
1	B	199	ILE	4.5
1	B	245	ARG	4.4
1	A	672	GLY	4.4
1	A	508	LYS	4.2
1	A	72	GLY	4.2
1	B	191	VAL	4.2
1	A	197	TYR	4.2
1	A	69	VAL	3.9
1	A	116	MET	3.9
1	B	36	ALA	3.9
1	A	70	SER	3.8
1	A	343	CYS	3.8
1	B	193	ALA	3.8
1	A	246	LEU	3.7
1	A	115	ILE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	199	ILE	3.7
1	A	193	ALA	3.7
1	A	278	SER	3.5
1	A	35	ALA	3.5
1	A	406	ALA	3.4
1	B	197	TYR	3.4
1	A	37	THR	3.4
1	A	317	CYS	3.4
1	B	343	CYS	3.3
1	A	195	VAL	3.3
1	A	407	LYS	3.2
1	B	69	VAL	3.2
1	A	38	VAL	3.2
1	B	243	VAL	3.1
1	B	244	MET	3.1
1	A	279	ILE	3.1
1	B	34	TYR	3.1
1	B	115	ILE	3.1
1	B	194	ILE	3.1
1	A	243	VAL	3.0
1	B	37	THR	3.0
1	B	278	SER	2.9
1	A	552	GLU	2.9
1	A	25	ASN	2.9
1	B	116	MET	2.9
1	A	114	GLN	2.9
1	A	660	ILE	2.8
1	B	130	HIS	2.8
1	A	659	ALA	2.8
1	B	190	GLU	2.8
1	B	279	ILE	2.7
1	A	196	GLY	2.7
1	A	118	THR	2.7
1	B	72	GLY	2.6
1	B	280	THR	2.6
1	B	601	ASP	2.6
1	A	585	LEU	2.6
1	A	584	LYS	2.5
1	A	380	ILE	2.5
1	A	112	ILE	2.5
1	A	277	PHE	2.5
1	B	38	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	2.5
1	A	234	LYS	2.4
1	B	319	ALA	2.4
1	B	342	MET	2.4
1	B	281	VAL	2.4
1	A	347	ILE	2.3
1	A	113	GLY	2.3
1	A	13	MET	2.3
1	A	601	ASP	2.3
1	A	554	GLY	2.3
1	A	499	ALA	2.2
1	A	154	LYS	2.2
1	A	388	VAL	2.2
1	A	71	GLN	2.2
1	A	190	GLU	2.2
1	A	238	ASP	2.2
1	B	253	GLU	2.2
1	B	246	LEU	2.2
1	B	320	TYR	2.1
1	A	513	ASP	2.1
1	A	616	GLU	2.1
1	B	114	GLN	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 monosaccharides 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, 95<sup>th</sup> 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.

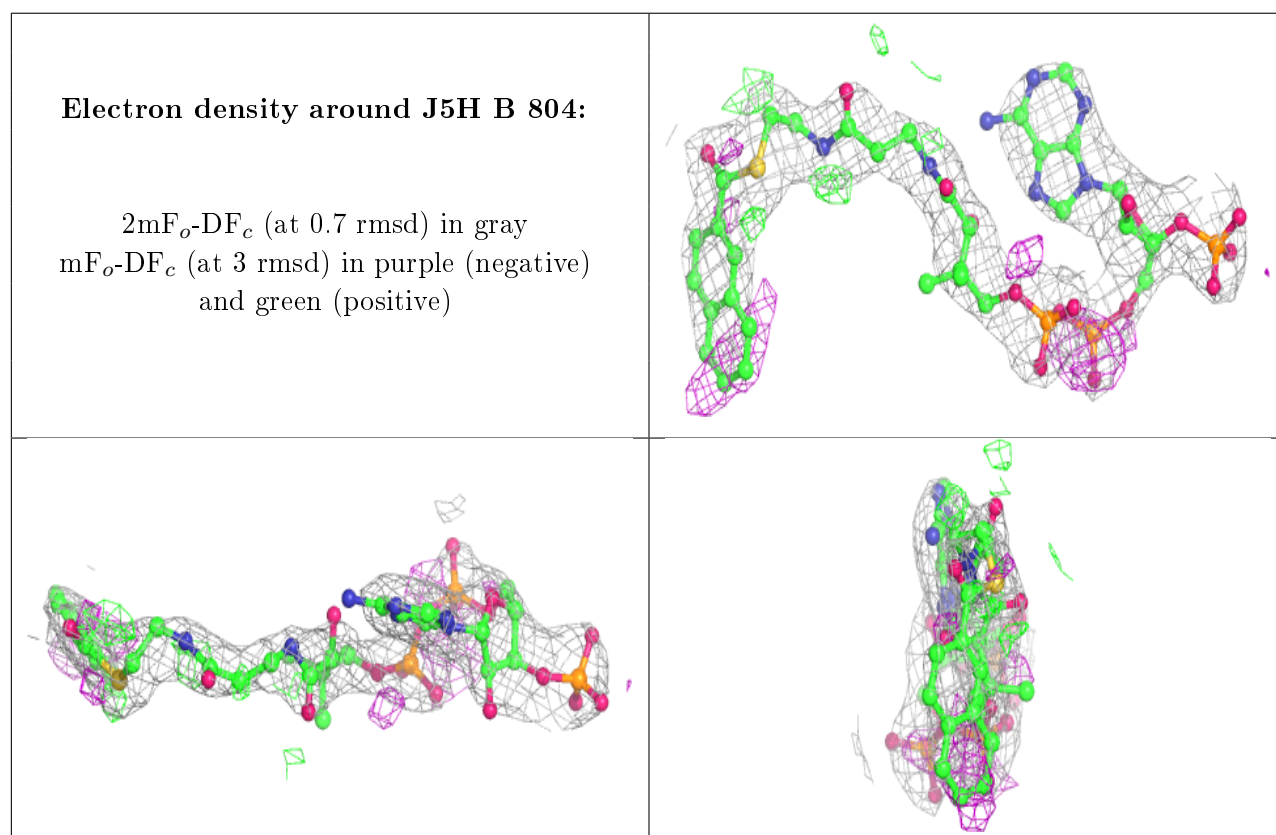
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	J5H	B	804	60/60	0.77	0.30	63,92,126,128	0

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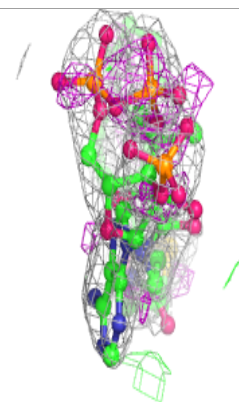
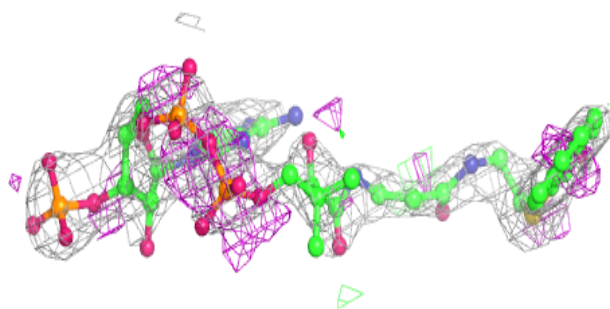
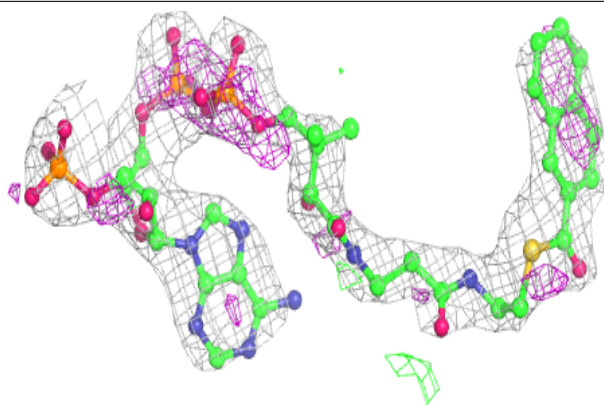
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	J5H	A	804	60/60	0.80	0.30	60,86,115,116	0
2	SF4	A	801	8/8	0.89	0.09	56,60,65,83	0
2	SF4	B	801	8/8	0.91	0.08	53,55,61,80	0
3	FAD	B	802	53/53	0.97	0.12	42,49,55,57	0
4	FMN	A	803	31/31	0.97	0.29	42,47,49,51	0
3	FAD	A	802	53/53	0.98	0.13	43,49,52,58	0
4	FMN	B	803	31/31	0.98	0.35	40,44,47,48	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.

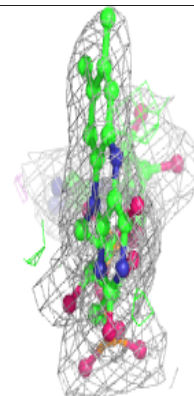
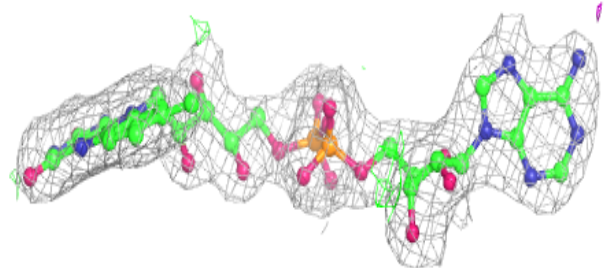
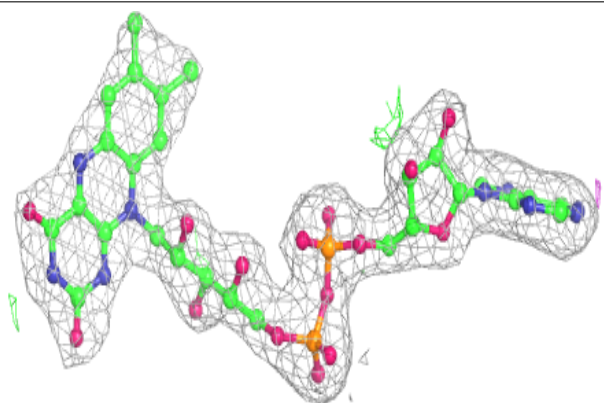


**Electron density around J5H A 804:**

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

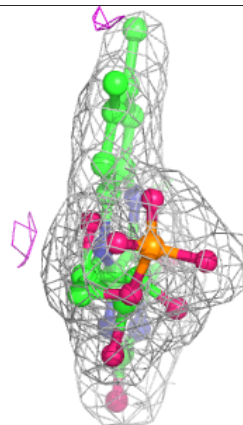
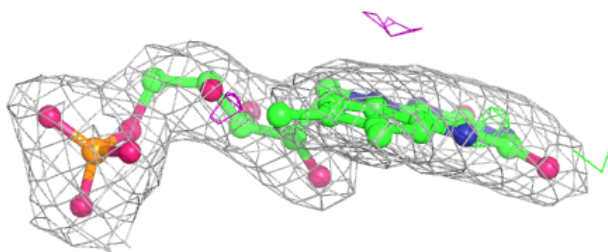
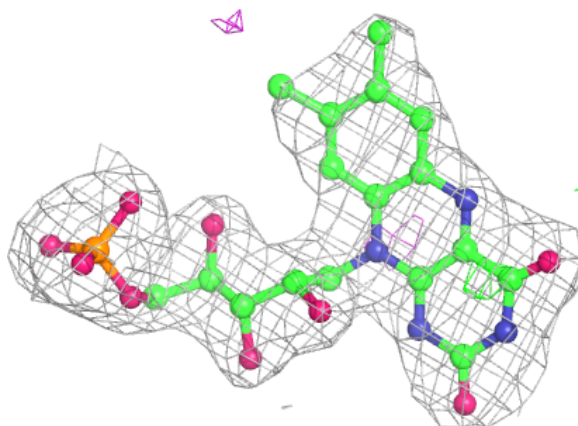
**Electron density around FAD B 802:**

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

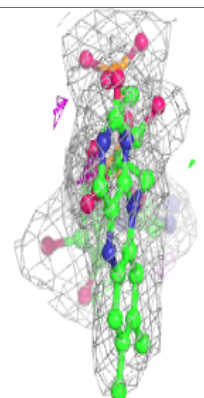
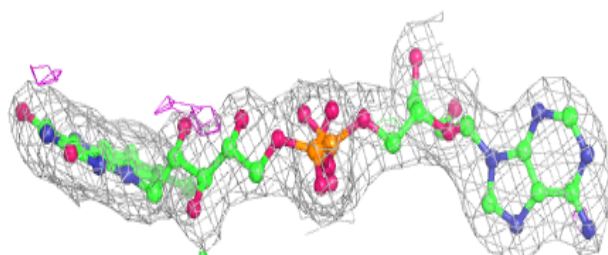
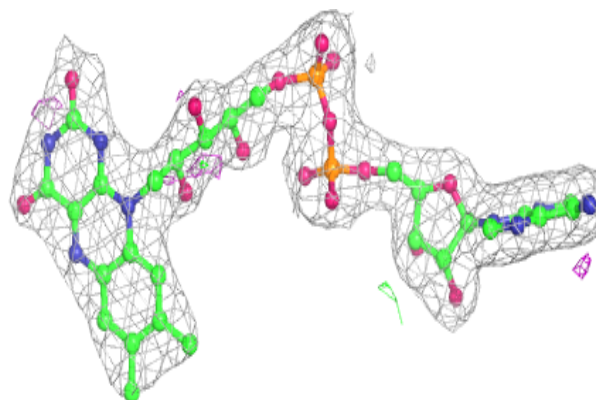


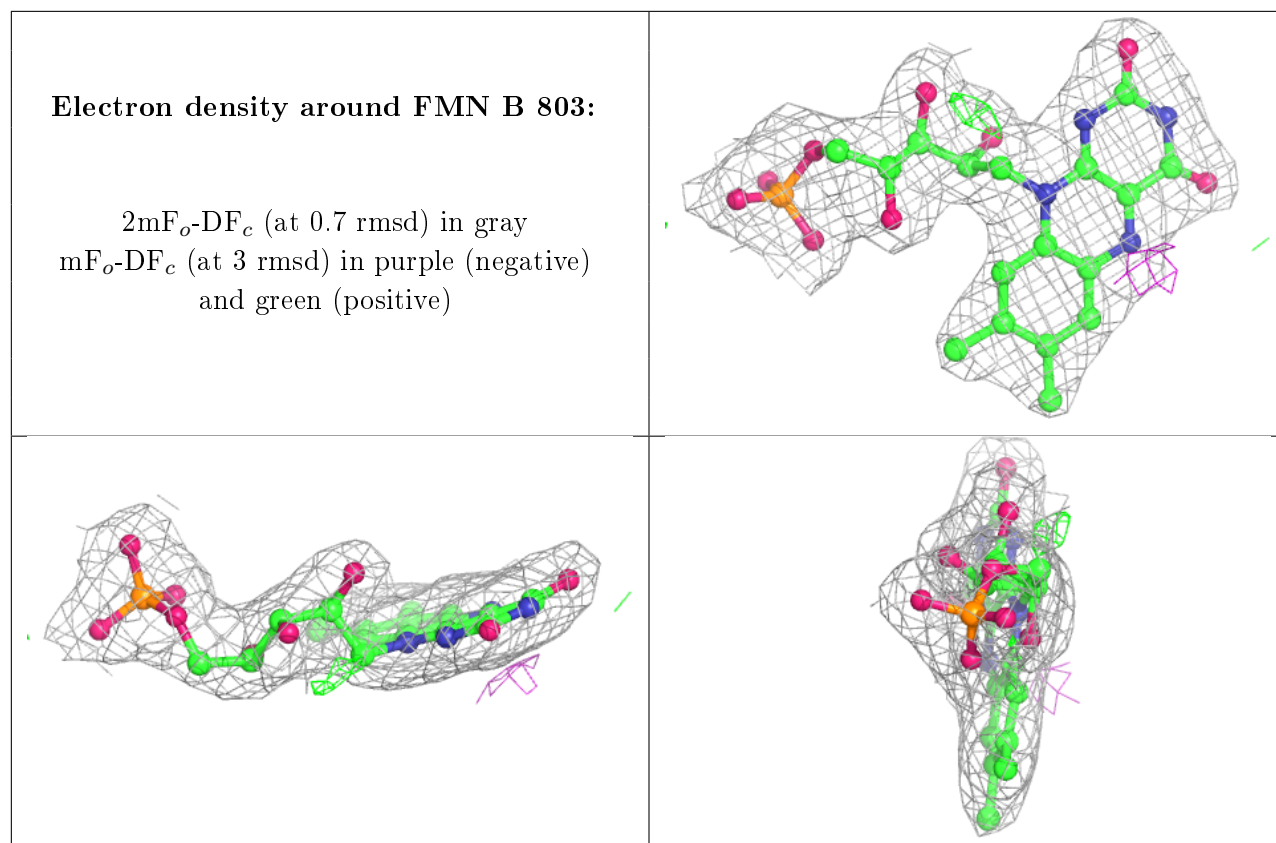
**Electron density around FMN A 803:**

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

**Electron density around FAD A 802:**

$2mF_o-DF_c$  (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.