



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:57 PM UTC

PDB ID : 6QKR / pdb_00006qkr
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

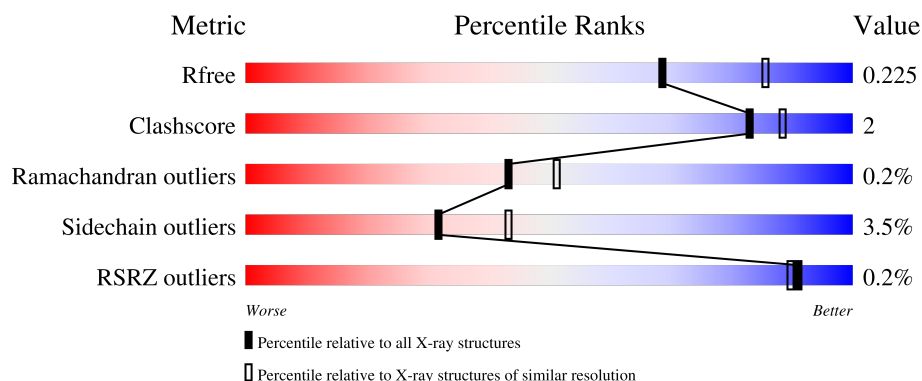
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	714	 84% 8% 8%
1	B	714	 82% 9% 7%

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
1	A	660	Total	C	N	O	S	0	1	0
			5064	3199	877	951	37			
1	B	664	Total	C	N	O	S	0	1	0
			5104	3223	885	959	37			

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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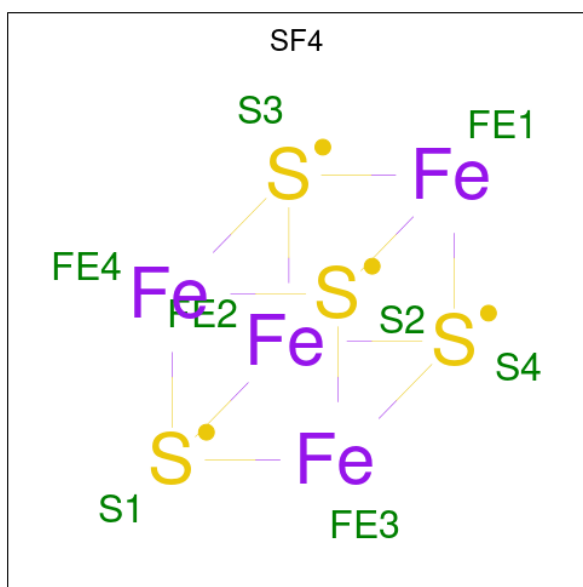
Chain	Residue	Modelled	Actual	Comment	Reference
A	696	GLY	-	expression tag	UNP E1YD54
A	697	GLY	-	expression tag	UNP E1YD54
A	698	SER	-	expression tag	UNP E1YD54
A	699	GLY	-	expression tag	UNP E1YD54
A	700	GLY	-	expression tag	UNP E1YD54
A	701	GLY	-	expression tag	UNP E1YD54
A	702	SER	-	expression tag	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 (CCD ID: SF4) (formula: Fe_4S_4).



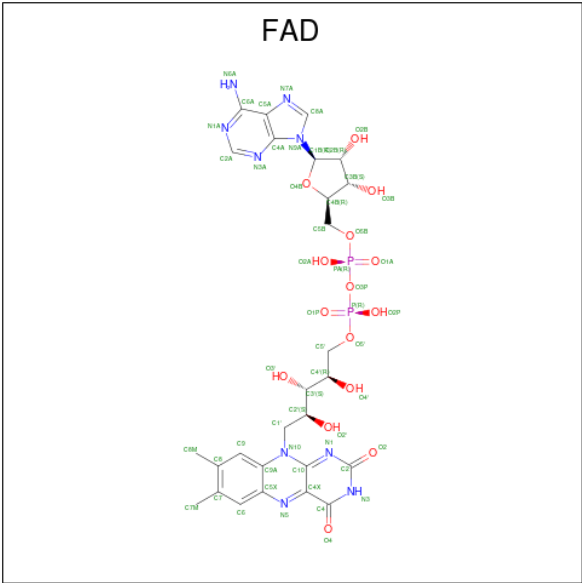
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

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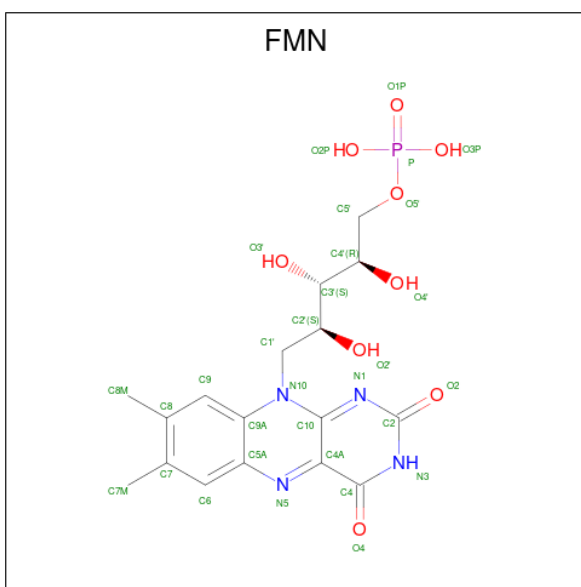
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	B	1	8	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



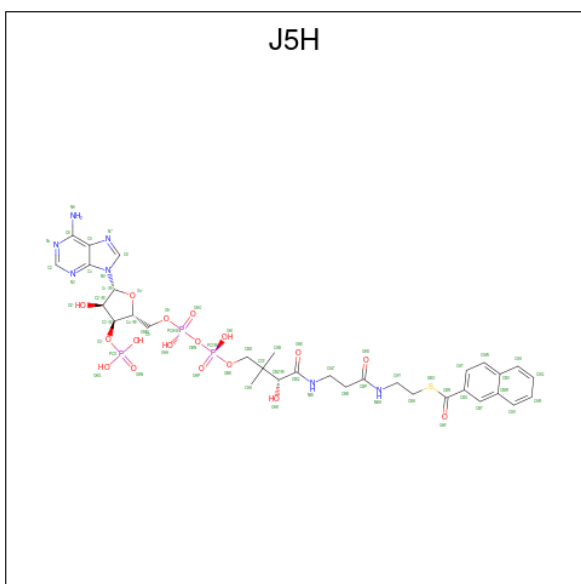
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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		

- Molecule 5 is {S}-[2-[3-[(2 {R})-4-[[[(2 {R}),3 {S},4 {R}),5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] naphthalene-2-carbothioate (CCD ID: J5H) (formula: C₃₂H₄₂N₇O₁₇P₃S).



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

- Molecule 6 is water.

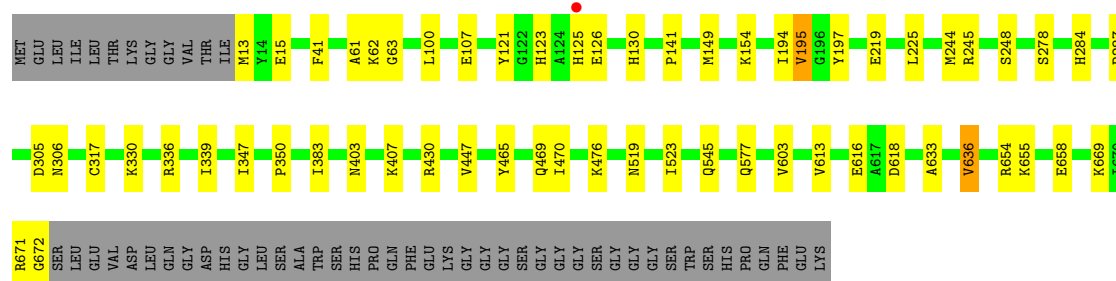
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	96	Total	O	0	0
			96	96		

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.

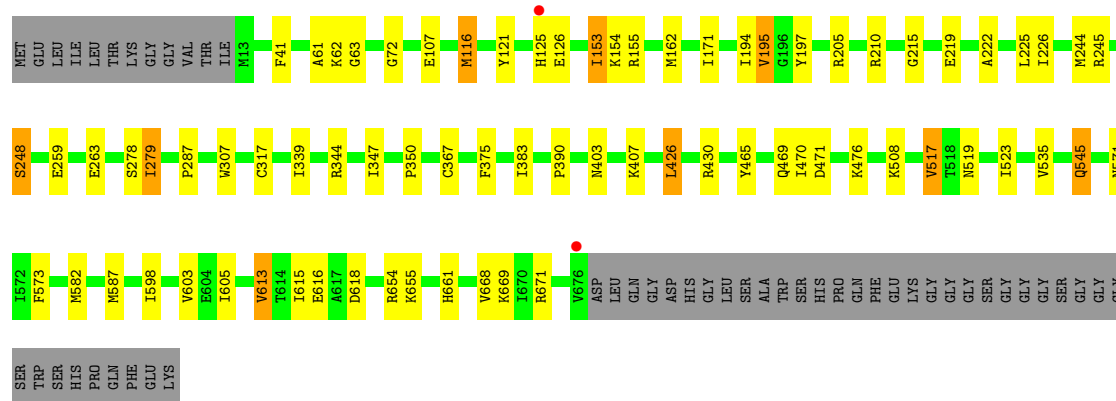
• Molecule 1: NCR

Chain A: 



• Molecule 1: NCR

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.0 (30.24-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.20Å)	Xtriage
Refinement program	PHENIX, BUSTER	Depositor
R, R_{free}	0.178 , 0.218 0.184 , 0.225	Depositor DCC
R_{free} test set	3405 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10716	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FMN, FAD, J5H

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	0.87	1/5160 (0.0%)	1.26	17/6967 (0.2%)
1	B	0.88	1/5197 (0.0%)	1.25	18/7017 (0.3%)
All	All	0.87	2/10357 (0.0%)	1.26	35/13984 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	MET	SD-CE	-9.70	1.55	1.79
1	A	149	MET	SD-CE	6.18	1.95	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	VAL	N-CA-C	-8.67	97.39	109.45
1	B	347	ILE	N-CA-C	-7.29	103.75	110.82
1	A	347	ILE	N-CA-C	-7.21	103.83	110.82
1	B	194	ILE	CA-C-N	6.95	134.48	121.97
1	B	194	ILE	C-N-CA	6.95	134.48	121.97
1	A	194	ILE	CA-C-N	6.83	134.27	121.97
1	A	194	ILE	C-N-CA	6.83	134.27	121.97
1	B	263	GLU	CB-CG-CD	6.27	123.26	112.60
1	A	248	SER	N-CA-C	-6.20	105.87	113.50
1	A	618	ASP	N-CA-C	-6.06	104.97	112.90
1	B	248	SER	N-CA-C	-5.78	106.39	113.50
1	A	470	ILE	CA-C-N	5.60	127.72	120.44
1	A	470	ILE	C-N-CA	5.60	127.72	120.44
1	B	41	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	671	ARG	N-CA-C	5.40	117.50	110.53
1	A	121	TYR	CA-C-N	5.33	125.04	119.92
1	A	121	TYR	C-N-CA	5.33	125.04	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	153	ILE	CA-C-N	5.27	127.60	120.38
1	B	153	ILE	C-N-CA	5.27	127.60	120.38
1	B	121	TYR	CA-C-N	5.23	125.07	120.10
1	B	121	TYR	C-N-CA	5.23	125.07	120.10
1	B	470	ILE	CA-C-N	5.22	127.54	120.65
1	B	470	ILE	C-N-CA	5.22	127.54	120.65
1	B	571	ASN	CA-C-N	5.22	127.89	120.53
1	B	571	ASN	C-N-CA	5.22	127.89	120.53
1	A	306	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	171	ILE	N-CA-C	-5.15	105.69	110.53
1	B	571	ASN	CA-CB-CG	5.14	117.74	112.60
1	B	618	ASP	N-CA-C	-5.14	105.31	112.45
1	B	194	ILE	N-CA-C	5.12	116.22	108.96
1	A	447	VAL	CA-C-N	5.03	127.52	120.28
1	A	447	VAL	C-N-CA	5.03	127.52	120.28
1	A	154	LYS	CA-C-N	5.00	127.23	120.38
1	A	154	LYS	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5064	0	5096	18	0
1	B	5104	0	5138	32	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
4	A	31	0	19	0	0
4	B	31	0	19	1	0
5	A	60	0	0	3	0
5	B	60	0	0	2	0
6	A	148	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	96	0	0	0	0
All	All	10716	0	10334	50	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 (50) 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:116:MET:HE2	1:B:197:TYR:CE2	2.30	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:B:116:MET:HE1	4:B:803:FMN:N3	2.19	0.58
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:225:LEU:HD21	1:A:244:MET:HE1	1.98	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:225:LEU:HD21	1:B:244:MET:HE1	1.99	0.44
1:B:375:PHE:HB3	1:B:573:PHE:CZ	2.53	0.43
1:B:287:PRO:HA	5:B:804:J5H:N1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ARG:HA	1:B:671:ARG:HD3	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:407:LYS:HG2	1:A:672:GLY:C	2.43	0.42
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:582:MET:HE3	1:B:587:MET:HE2	2.02	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: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

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	659/714 (92%)	638 (97%)	20 (3%)	1 (0%)	43	51
1	B	663/714 (93%)	643 (97%)	19 (3%)	1 (0%)	43	51
All	All	1322/1428 (93%)	1281 (97%)	39 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

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

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	532/572 (93%)	516 (97%)	16 (3%)	36	49
1	B	537/572 (94%)	516 (96%)	21 (4%)	28	39
All	All	1069/1144 (93%)	1032 (96%)	37 (4%)	32	43

All (37) 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	219	GLU
1	A	330	LYS
1	A	383	ILE
1	A	476	LYS
1	A	545	GLN
1	A	577	GLN
1	A	603	VAL
1	A	613	VAL
1	A	616	GLU
1	A	655	LYS
1	A	669	LYS
1	B	62	LYS
1	B	154	LYS
1	B	195	VAL
1	B	205	ARG
1	B	219	GLU
1	B	259	GLU

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Mol	Chain	Res	Type
1	B	279	ILE
1	B	383	ILE
1	B	407	LYS
1	B	426	LEU
1	B	471	ASP
1	B	476	LYS
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	654	ARG
1	B	655	LYS
1	B	669	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	306	ASN
1	A	480	ASN
1	B	26	HIS
1	B	480	ASN
1	B	577	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
5	J5H	B	804	-	62,64,64	2.99	20 (32%)	89,95,95	1.53	13 (14%)
2	SF4	A	801	1	0,12,12	-	-	-		
3	FAD	B	802	-	58,58,58	0.38	0	85,89,89	0.51	1 (1%)
4	FMN	A	803	-	33,33,33	0.37	0	48,50,50	0.53	0
2	SF4	B	801	1	0,12,12	-	-	-		
4	FMN	B	803	-	33,33,33	0.40	0	48,50,50	0.51	0
3	FAD	A	802	-	58,58,58	0.40	0	85,89,89	0.52	1 (1%)
5	J5H	A	804	-	62,64,64	2.98	19 (30%)	89,95,95	1.54	12 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	J5H	B	804	-	-	9/55/71/71	0/5/5/5
2	SF4	A	801	1	-	-	0/6/5/5
3	FAD	B	802	-	-	1/34/50/50	0/6/6/6
4	FMN	A	803	-	-	1/18/18/18	0/3/3/3
4	FMN	B	803	-	-	1/18/18/18	0/3/3/3
2	SF4	B	801	1	-	-	0/6/5/5
3	FAD	A	802	-	-	0/34/50/50	0/6/6/6
5	J5H	A	804	-	-	6/55/71/71	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	J5H	C2'-C3'	-11.01	1.28	1.53
5	A	804	J5H	C2'-C3'	-10.86	1.29	1.53
5	A	804	J5H	PCI-OBN	8.48	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	J5H	PCH-OBN	8.44	1.68	1.59
5	B	804	J5H	PCI-OBN	8.40	1.68	1.59
5	A	804	J5H	PCH-OBN	8.29	1.68	1.59
5	A	804	J5H	CBP-NBH	6.92	1.49	1.33
5	B	804	J5H	CBP-NBH	6.82	1.49	1.33
5	A	804	J5H	CBQ-NBI	6.53	1.48	1.33
5	B	804	J5H	CBQ-NBI	6.39	1.48	1.33
5	B	804	J5H	O4'-C1'	-4.92	1.30	1.42
5	A	804	J5H	O4'-C1'	-4.91	1.30	1.42
5	A	804	J5H	O4'-C4'	4.76	1.55	1.45
5	B	804	J5H	O4'-C4'	4.56	1.55	1.45
5	A	804	J5H	C2'-C1'	4.48	1.67	1.53
5	B	804	J5H	C2'-C1'	4.46	1.67	1.53
5	A	804	J5H	C6-N6	3.87	1.44	1.34
5	B	804	J5H	C6-N6	3.81	1.43	1.34
5	B	804	J5H	CBR-SBO	3.79	1.84	1.76
5	A	804	J5H	CBR-SBO	3.72	1.84	1.76
5	B	804	J5H	PCG-O3'	3.52	1.65	1.59
5	A	804	J5H	PCG-O3'	3.24	1.65	1.59
5	A	804	J5H	C5'-C4'	-3.05	1.42	1.51
5	B	804	J5H	PCH-O5'	2.95	1.70	1.59
5	A	804	J5H	PCH-O5'	2.95	1.70	1.59
5	B	804	J5H	C5'-C4'	-2.94	1.42	1.51
5	B	804	J5H	C3'-C4'	2.59	1.59	1.52
5	A	804	J5H	CBD-CCF	2.55	1.56	1.52
5	B	804	J5H	OAE-CBQ	-2.53	1.18	1.23
5	A	804	J5H	C3'-C4'	2.48	1.59	1.52
5	B	804	J5H	CBD-CCF	2.42	1.56	1.52
5	B	804	J5H	CBU-CBR	2.39	1.54	1.49
5	B	804	J5H	C8-N9	-2.27	1.33	1.37
5	A	804	J5H	CBU-CBR	2.24	1.53	1.49
5	B	804	J5H	C5-N7	-2.22	1.35	1.39
5	A	804	J5H	C5-N7	-2.22	1.35	1.39
5	A	804	J5H	C8-N9	-2.18	1.33	1.37
5	A	804	J5H	PCI-OBK	2.13	1.67	1.59
5	B	804	J5H	CBT-CBU	2.13	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	J5H	C5-C4-N3	-5.40	119.28	126.72
5	A	804	J5H	C5-C4-N3	-5.07	119.74	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	J5H	N1-C2-N3	-4.92	121.13	128.58
5	B	804	J5H	N1-C2-N3	-4.92	121.14	128.58
5	B	804	J5H	N3-C4-N9	4.28	134.44	127.17
5	A	804	J5H	N3-C4-N9	3.93	133.84	127.17
5	B	804	J5H	C2-N3-C4	3.66	120.76	111.83
5	B	804	J5H	CBA-SBO-CBR	3.56	104.04	99.85
5	A	804	J5H	C2-N3-C4	3.55	120.49	111.83
5	B	804	J5H	C5-N7-C8	3.31	108.65	103.45
5	A	804	J5H	C5-N7-C8	3.26	108.58	103.45
5	B	804	J5H	N9-C8-N7	-3.07	109.58	113.94
5	A	804	J5H	C3'-C2'-C1'	3.04	106.57	99.89
5	A	804	J5H	C4-C5-N7	-3.00	107.16	110.58
3	A	802	FAD	C4'-C3'-C2'	2.95	118.48	113.57
5	A	804	J5H	N9-C8-N7	-2.95	109.75	113.94
5	A	804	J5H	CAT-CBU-CBT	2.92	122.74	119.21
5	B	804	J5H	C4-C5-N7	-2.91	107.26	110.58
3	B	802	FAD	C4'-C3'-C2'	2.89	118.38	113.57
5	B	804	J5H	C3'-C2'-C1'	2.70	105.82	99.89
5	B	804	J5H	OAD-CBP-CBB	-2.36	117.73	122.02
5	B	804	J5H	C4-N9-C8	2.36	108.22	105.74
5	A	804	J5H	CAW-CAT-CBU	-2.22	118.15	120.78
5	A	804	J5H	C4-N9-C8	2.18	108.03	105.74
5	B	804	J5H	CAT-CBU-CBT	2.14	121.79	119.21
5	A	804	J5H	OAD-CBP-CBB	-2.04	118.33	122.02
5	B	804	J5H	OBK-CBD-CCF	-2.01	107.31	110.55

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	804	J5H	CBU-CBR-SBO-CBA
5	B	804	J5H	NBI-CAZ-CBB-CBP
5	B	804	J5H	C5'-O5'-PCH-OBN
5	B	804	J5H	C5'-O5'-PCH-OAO
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	CBU-CBR-SBO-CBA
5	A	804	J5H	OAF-CBR-SBO-CBA
5	B	804	J5H	OAF-CBR-SBO-CBA
5	A	804	J5H	NBI-CAZ-CBB-CBP
4	B	803	FMN	C4'-C5'-O5'-P

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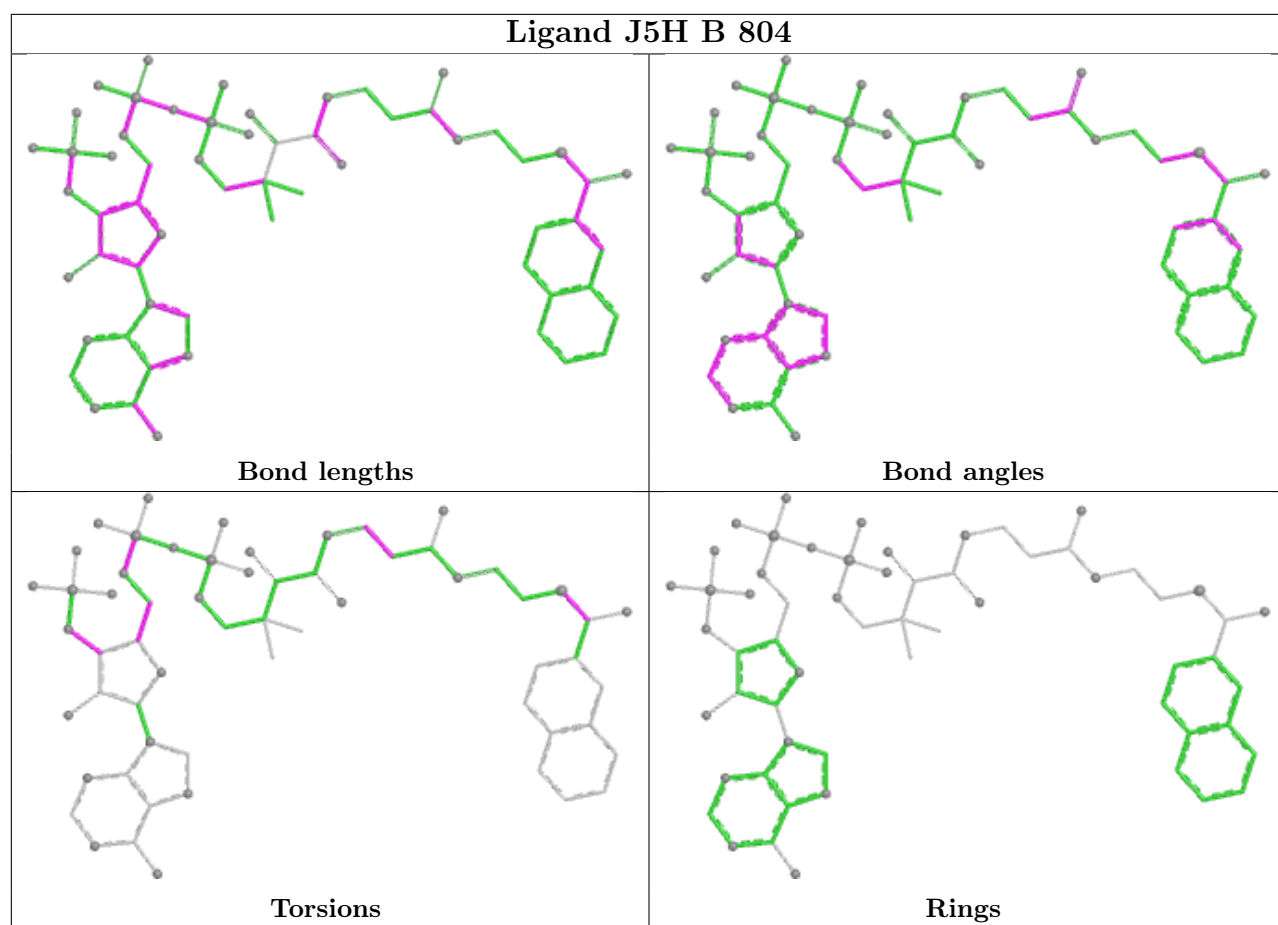
Mol	Chain	Res	Type	Atoms
5	B	804	J5H	C5'-O5'-PCH-OAH
4	A	803	FMN	C4'-C5'-O5'-P
5	A	804	J5H	C3'-C4'-C5'-O5'
3	B	802	FAD	PA-O3P-P-O5'
5	A	804	J5H	PCI-OBN-PCH-OAH
5	B	804	J5H	C4'-C3'-O3'-PCG

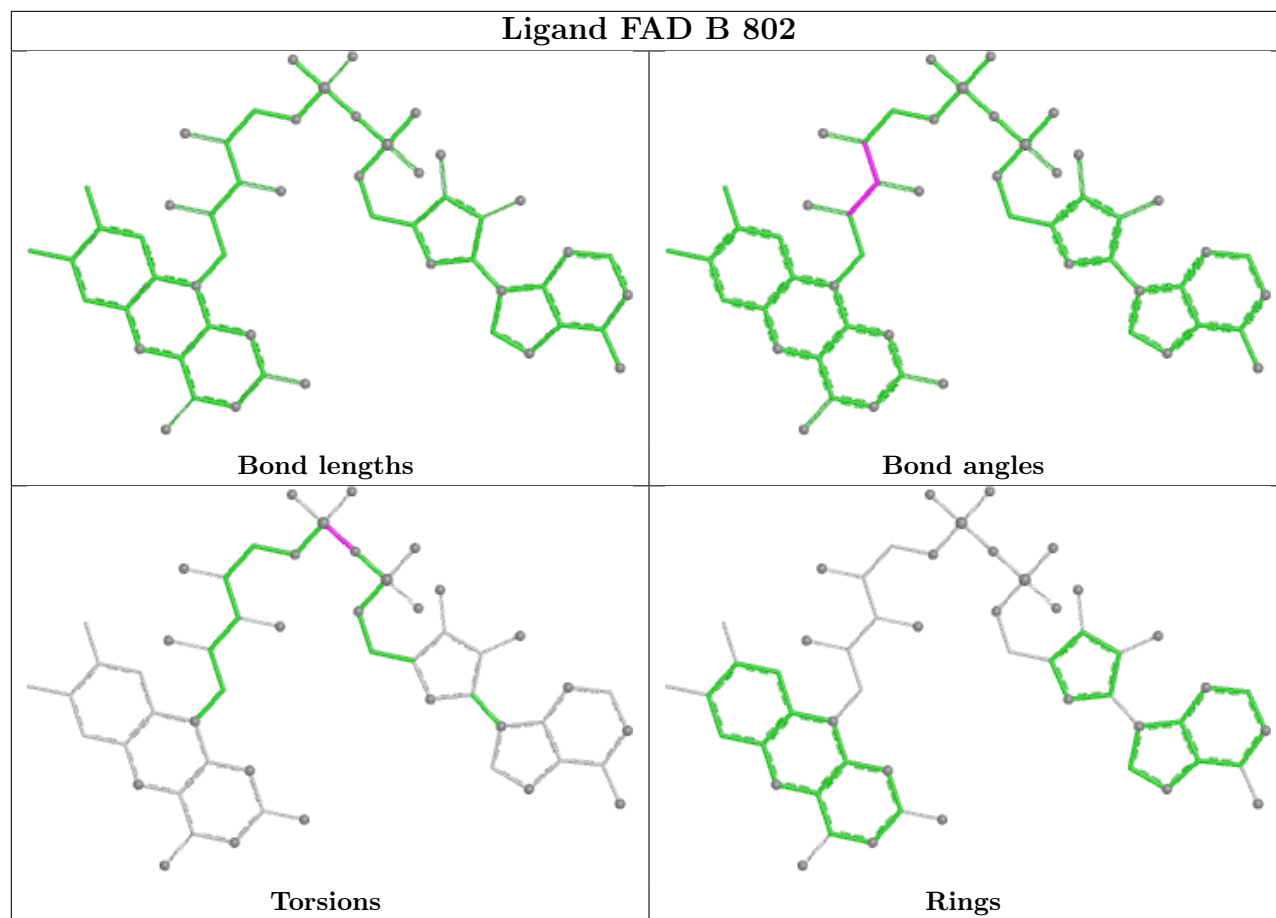
There are no ring outliers.

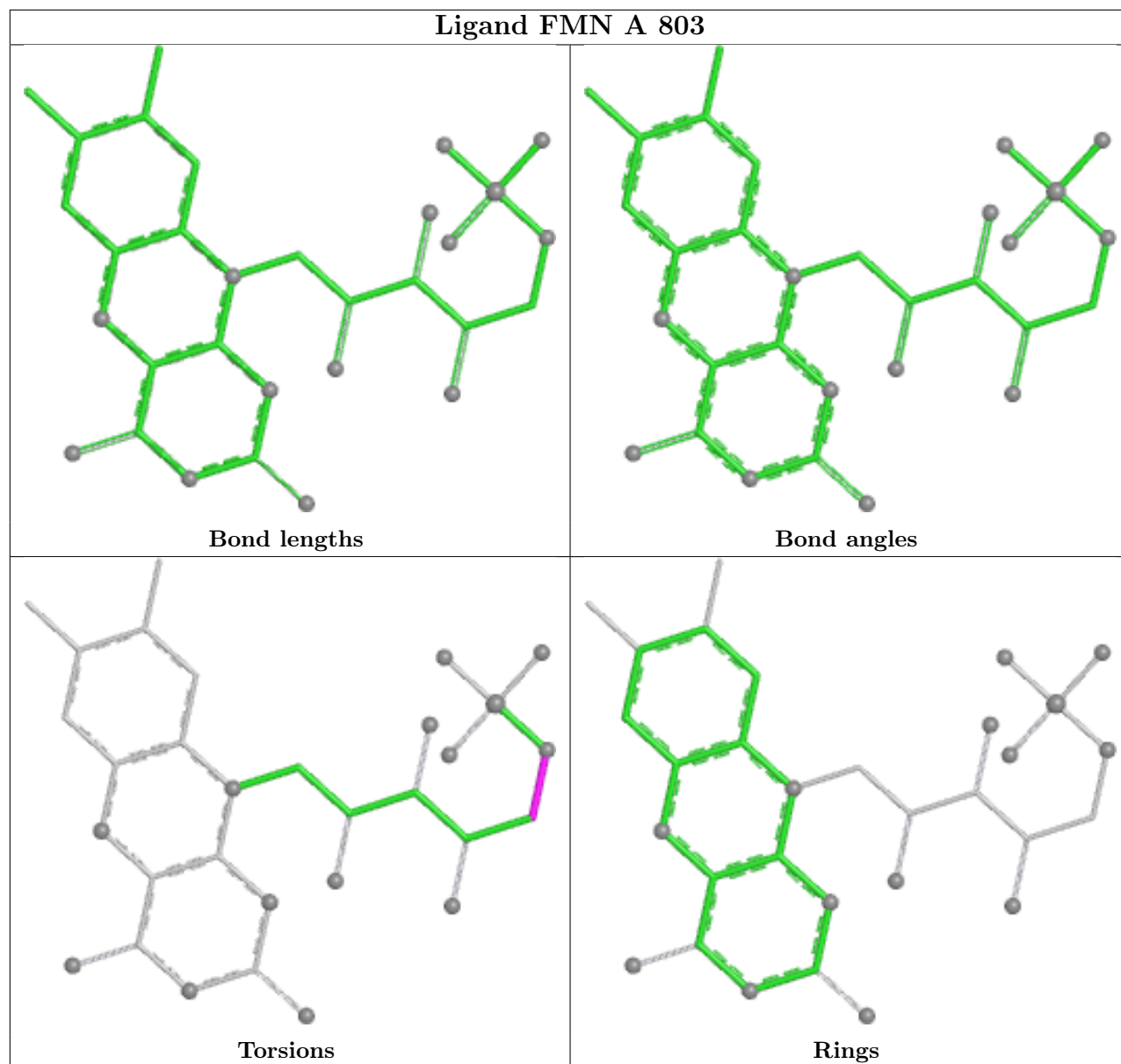
3 monomers are involved in 6 short contacts:

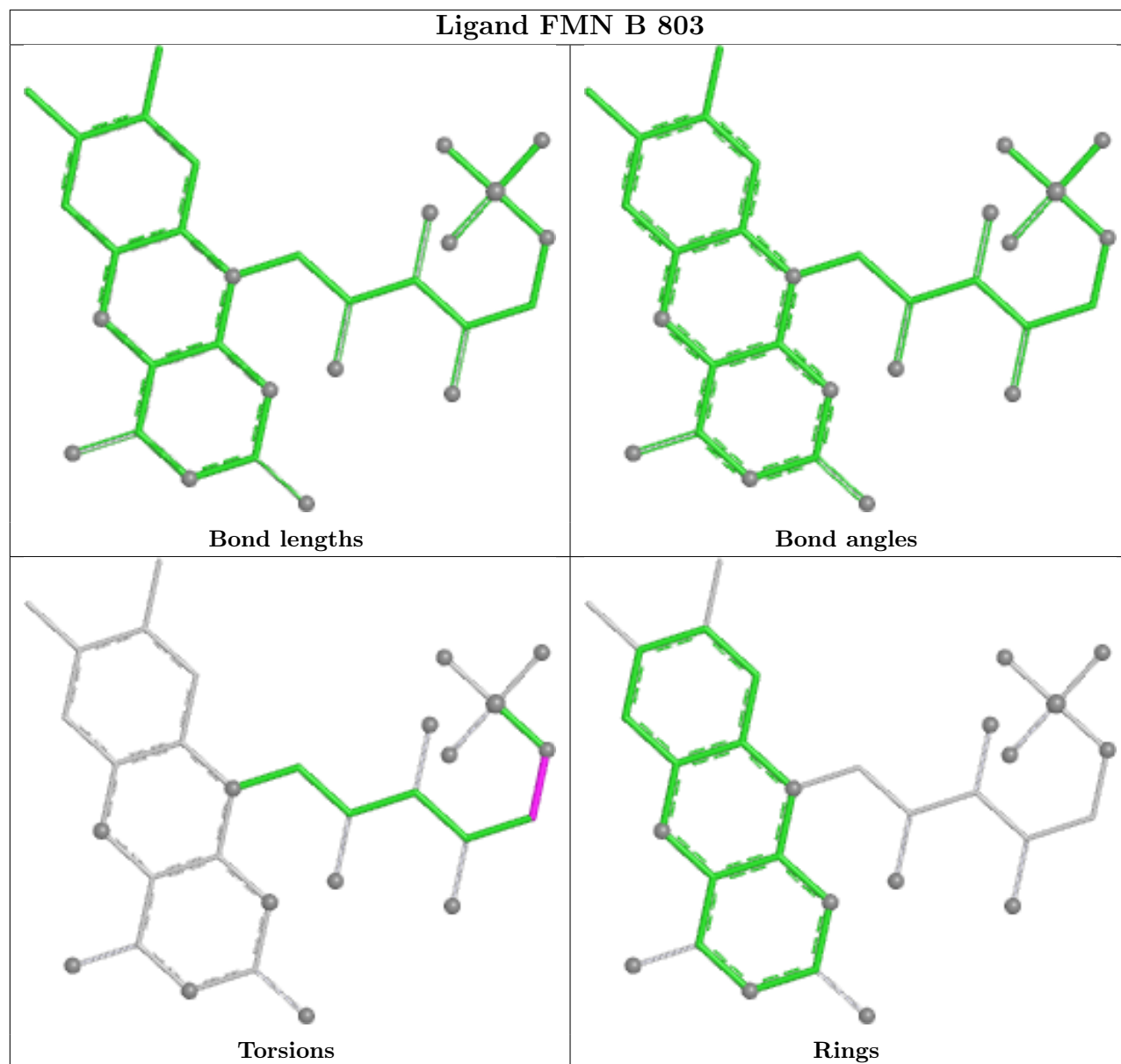
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	J5H	2	0
4	B	803	FMN	1	0
5	A	804	J5H	3	0

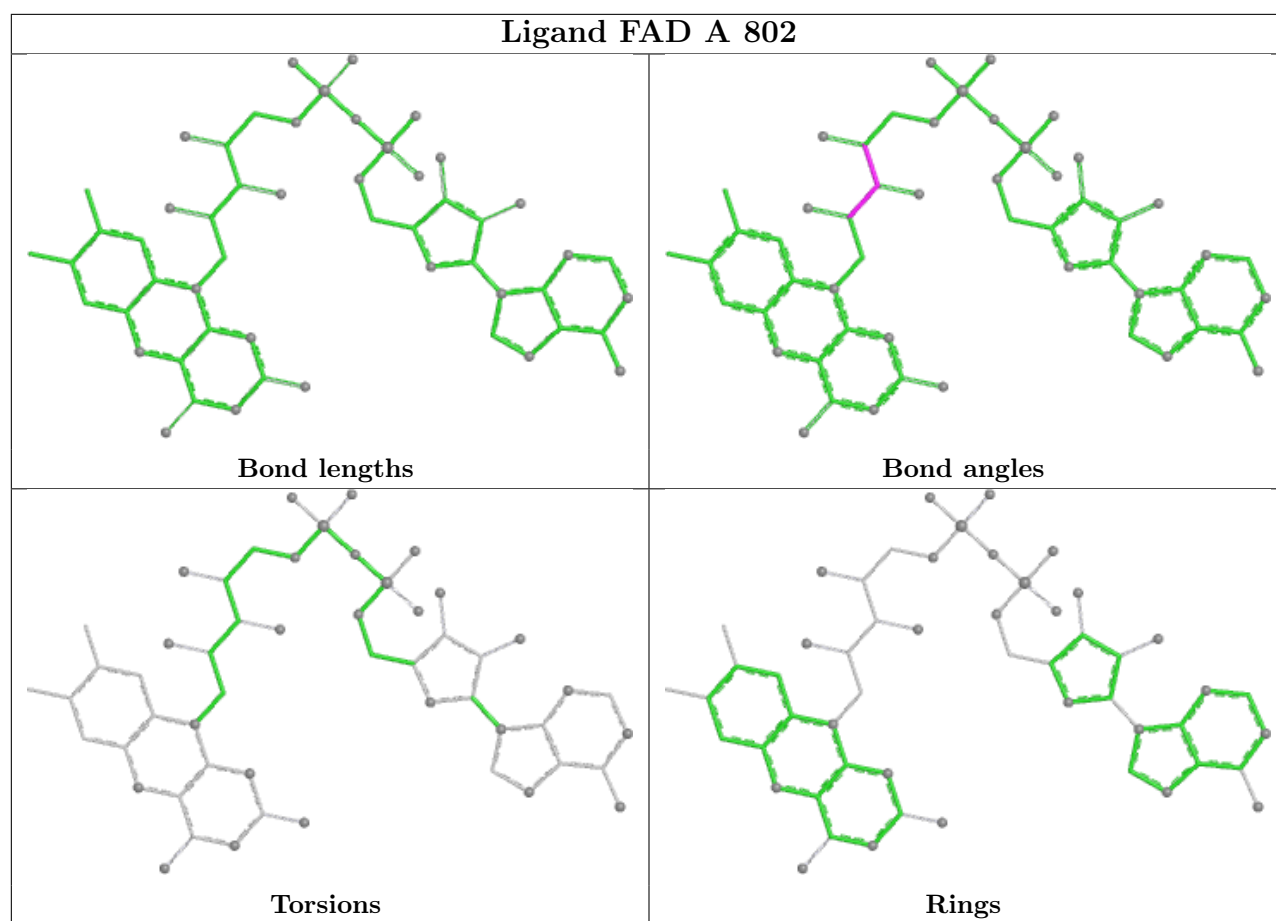
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

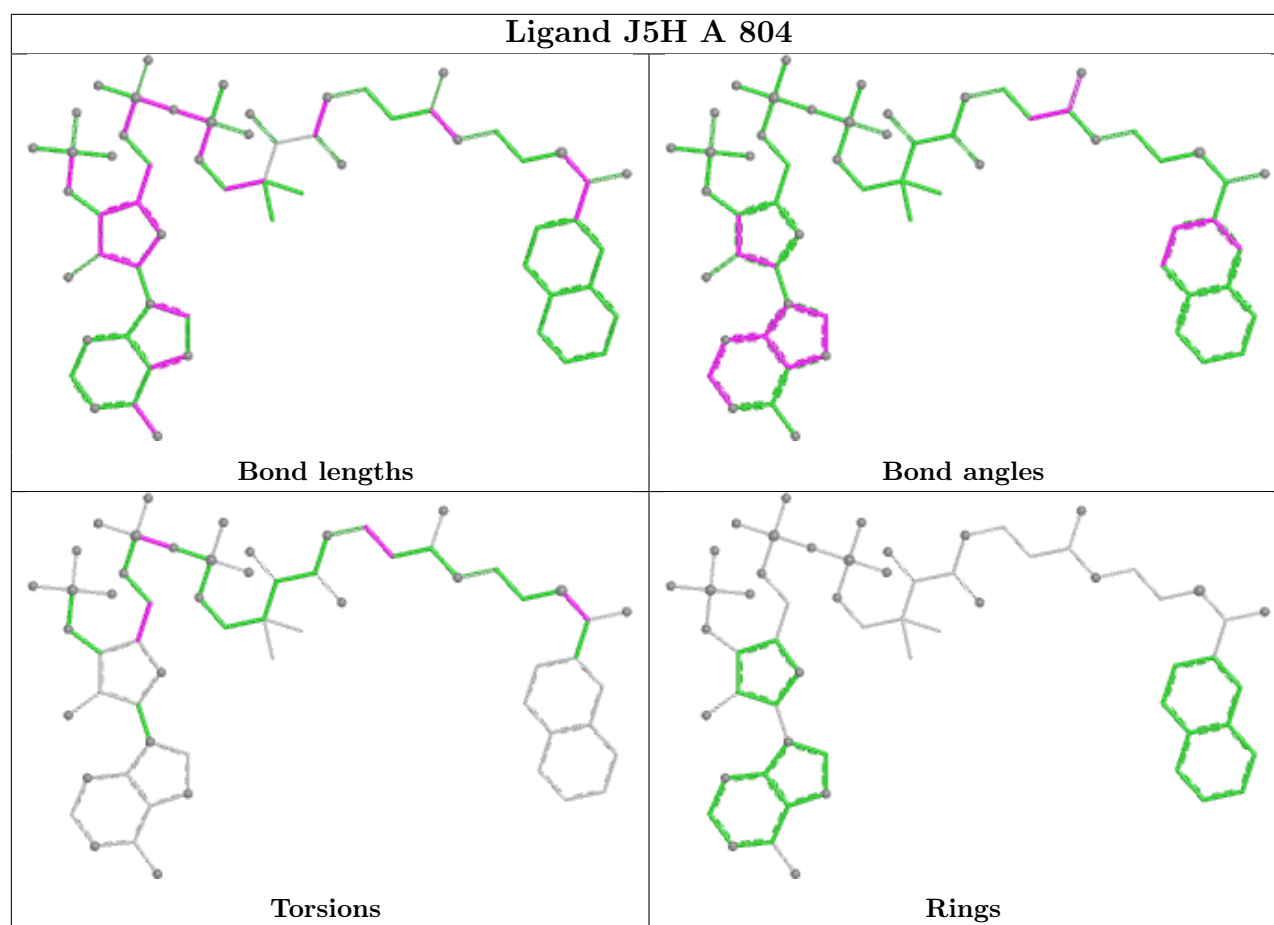












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	660/714 (92%)	-0.19	1 (0%) 91 90	41, 61, 86, 105	1 (0%)
1	B	664/714 (92%)	-0.26	2 (0%) 90 88	35, 58, 85, 111	1 (0%)
All	All	1324/1428 (92%)	-0.23	3 (0%) 91 90	35, 60, 86, 111	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	VAL	4.1
1	B	125[A]	HIS	2.9
1	A	125[A]	HIS	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	J5H	A	804	60/60	0.83	0.12	60,86,115,116	0
5	J5H	B	804	60/60	0.84	0.11	63,92,126,128	0

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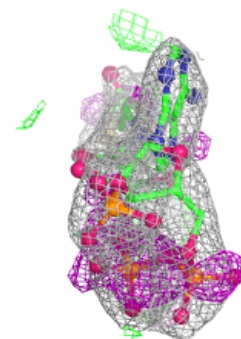
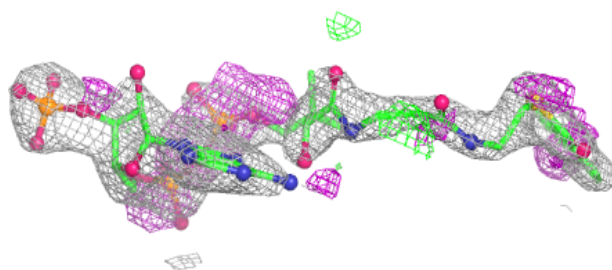
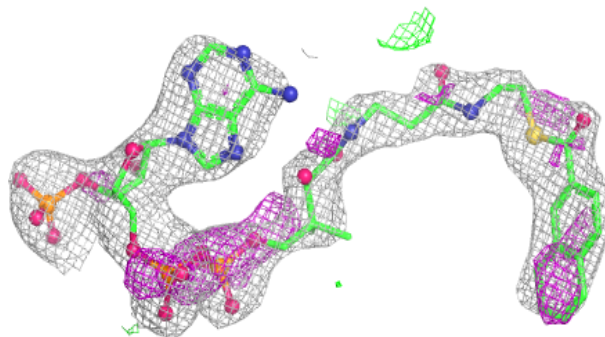
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	A	801	8/8	0.95	0.07	56,60,65,83	0
2	SF4	B	801	8/8	0.96	0.06	53,55,61,80	0
3	FAD	A	802	53/53	0.97	0.05	43,49,52,58	0
3	FAD	B	802	53/53	0.97	0.05	42,49,55,57	0
4	FMN	A	803	31/31	0.98	0.06	42,47,49,51	0
4	FMN	B	803	31/31	0.98	0.05	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.

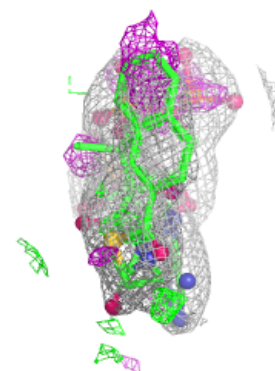
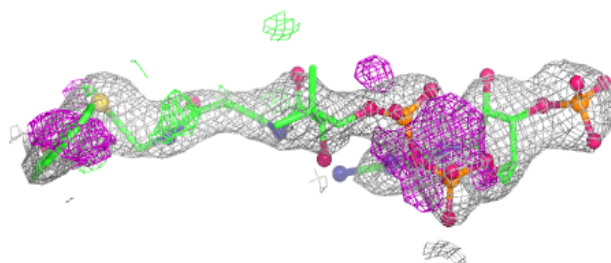
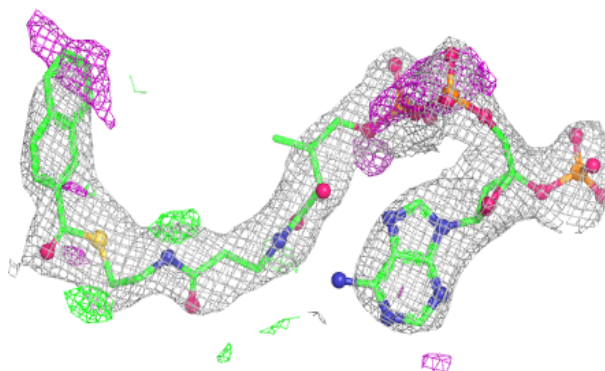
Electron density around J5H A 804:

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

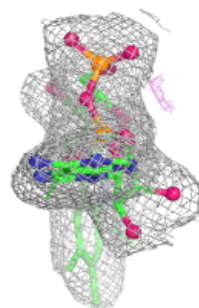
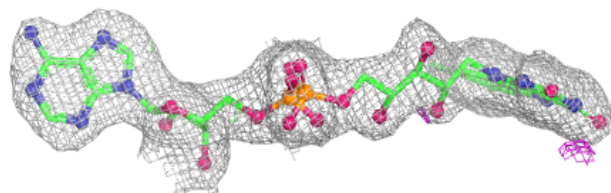
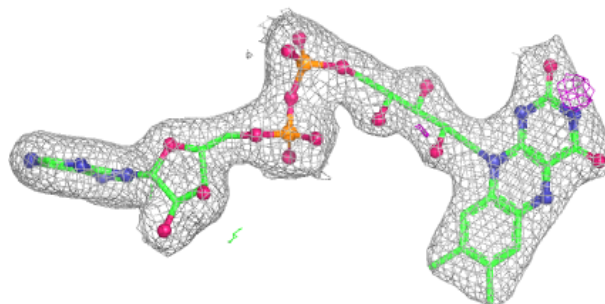


Electron density around J5H B 804:

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

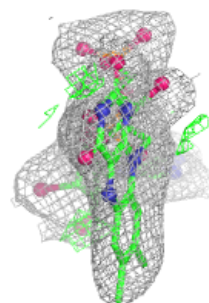
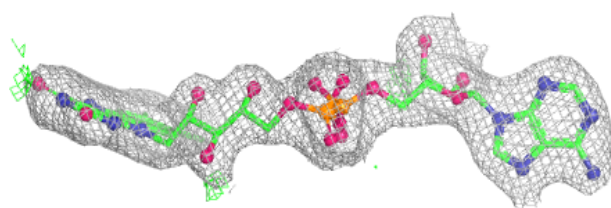
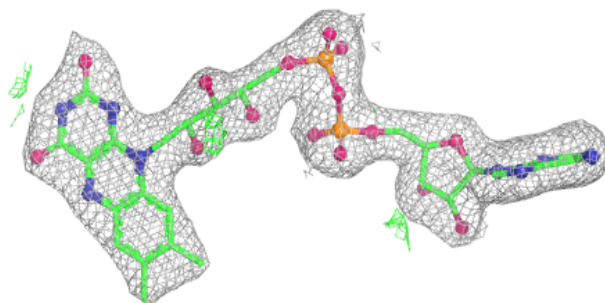
**Electron density around FAD A 802:**

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

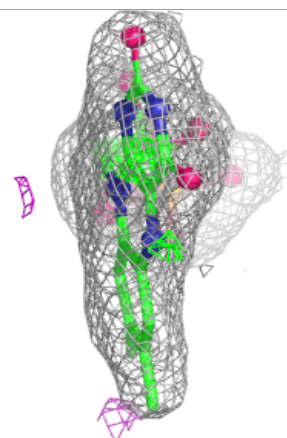
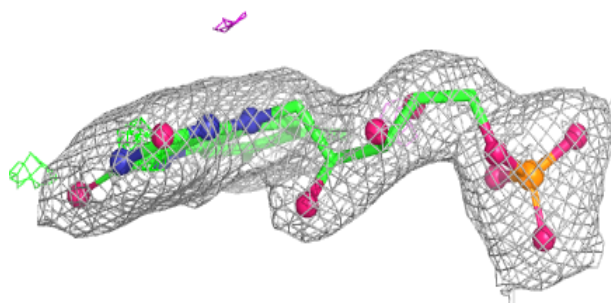
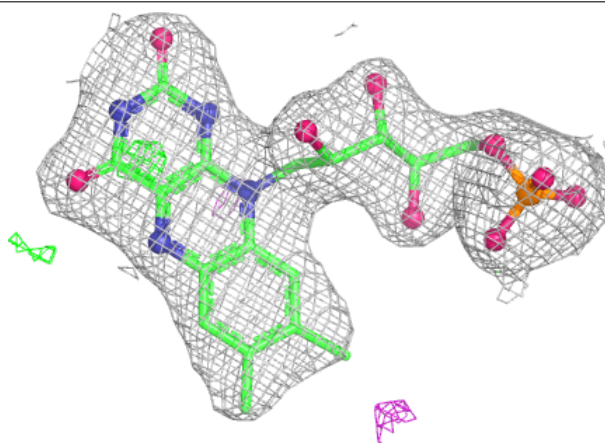


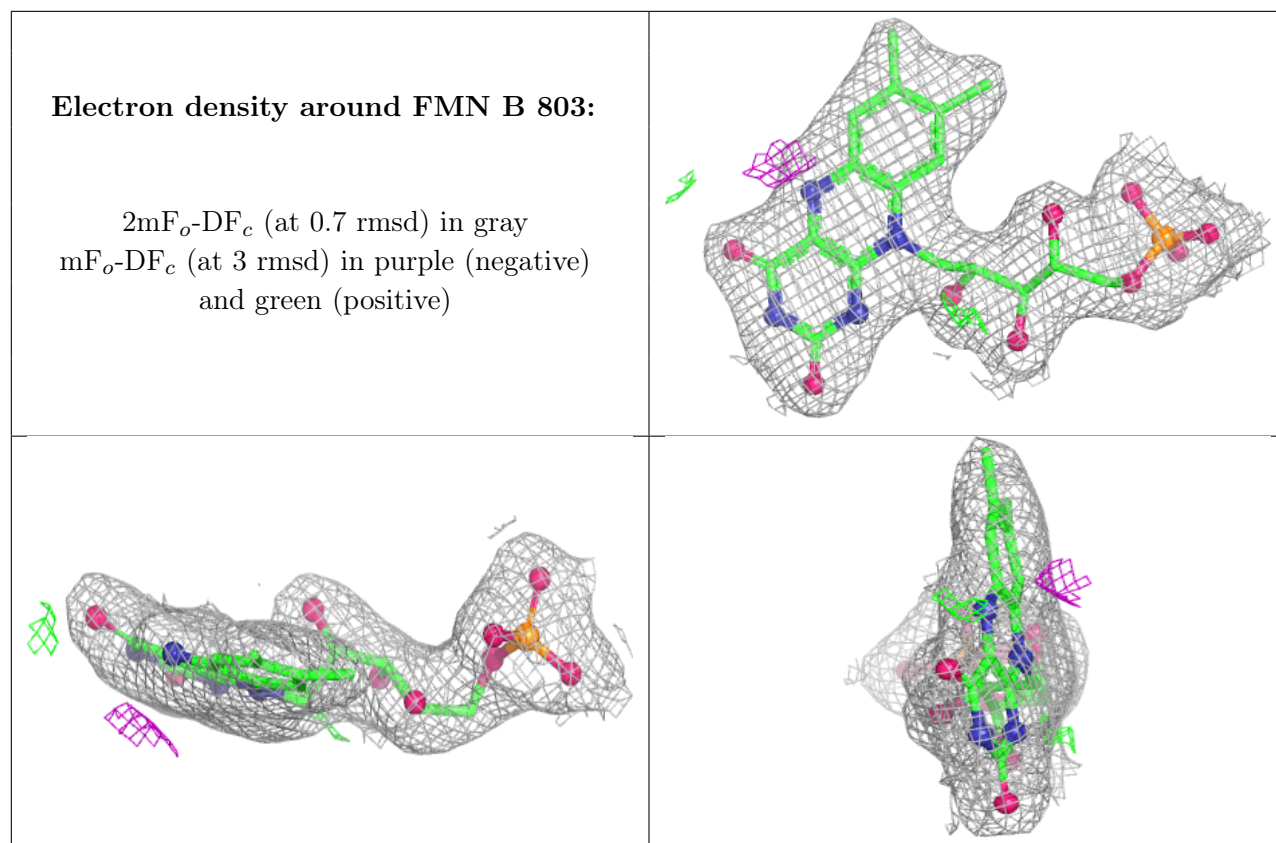
Electron density around FAD B 802:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.