



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 19, 2024 – 04:29 PM EST

PDB ID : 9DL3
Title : Structure of proline utilization A complexed with quinoline-2-carboxylic acid
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-09-10
Resolution : 1.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

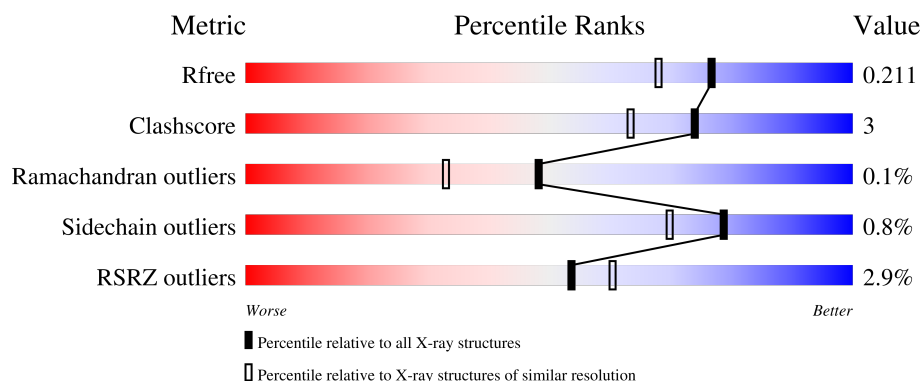
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

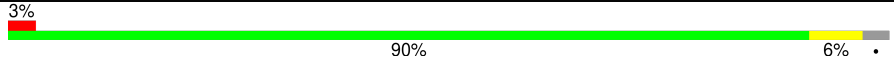
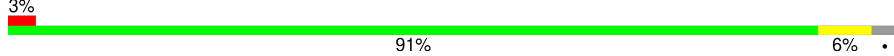
The reported resolution of this entry is 1.77 Å.

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}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	1235	
1	B	1235	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20478 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.

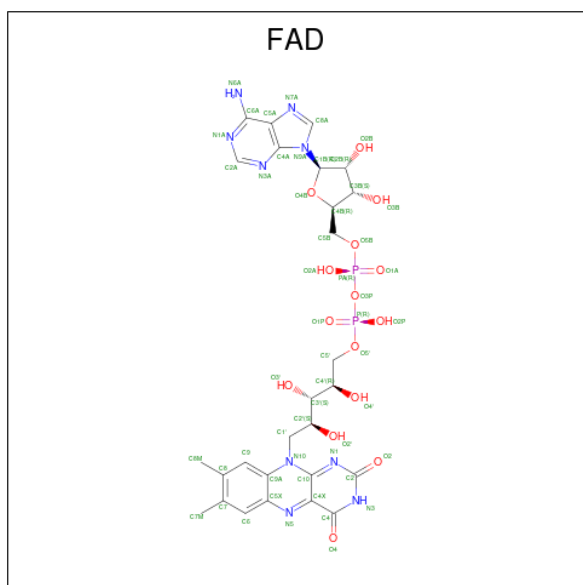
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1195	Total	C	N	O	S	0	12	0
			8845	5574	1577	1660	34			
1	B	1202	Total	C	N	O	S	0	21	0
			8941	5634	1599	1674	34			

There are 4 discrepancies between the modelled and reference sequences:

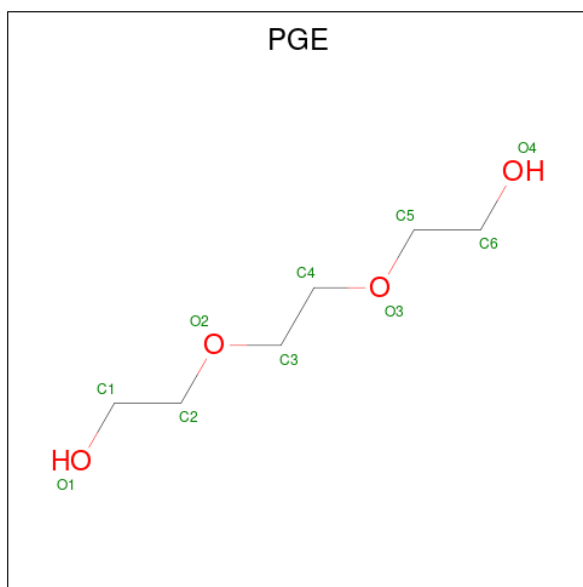
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

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



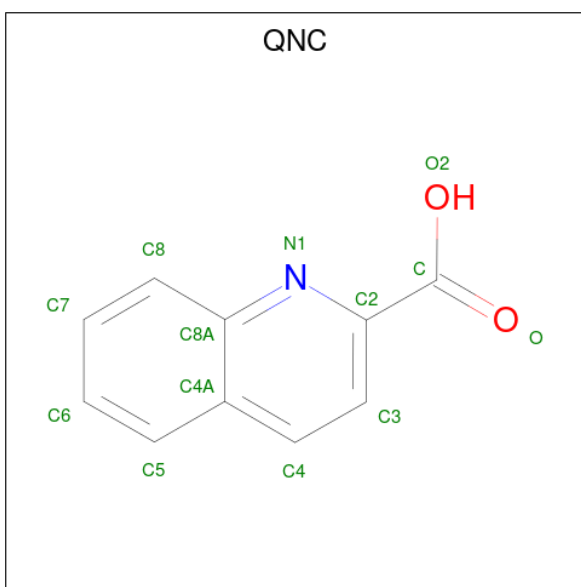
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			106	54	18	30	4	
2	B	1	Total	C	N	O	P	
			106	54	18	30	4	

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



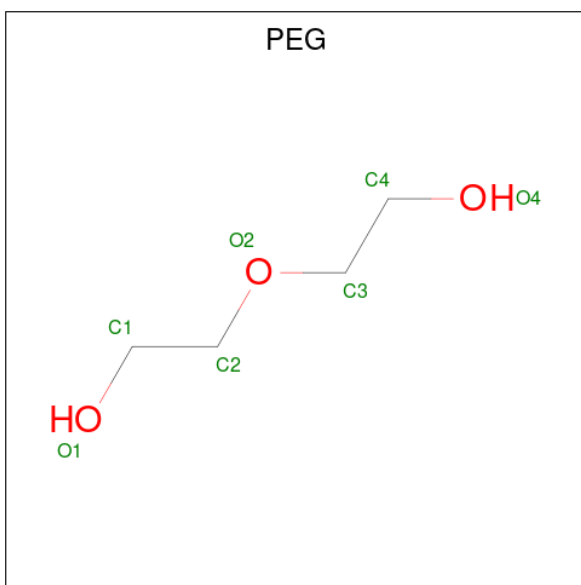
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			10	6	4	0	0
3	A	1	Total	C	O		
			10	6	4	0	0
3	A	1	Total	C	O		
			10	6	4	0	0
3	A	1	Total	C	O		
			10	6	4	0	0
3	B	1	Total	C	O		
			10	6	4	0	0
3	B	1	Total	C	O		
			10	6	4	0	0

- Molecule 4 is quinoline-2-carboxylic acid (three-letter code: QNC) (formula: $C_{10}H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



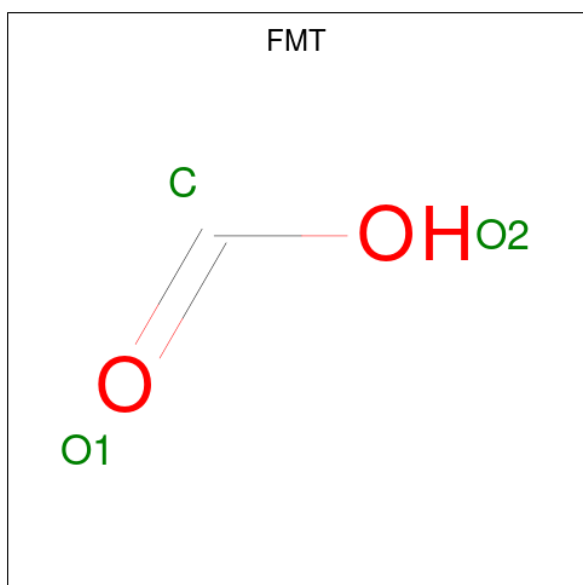
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	10	1	2		
4	A	1	Total	C	N	O	0	0
			13	10	1	2		
4	B	1	Total	C	N	O	0	0
			13	10	1	2		
4	B	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



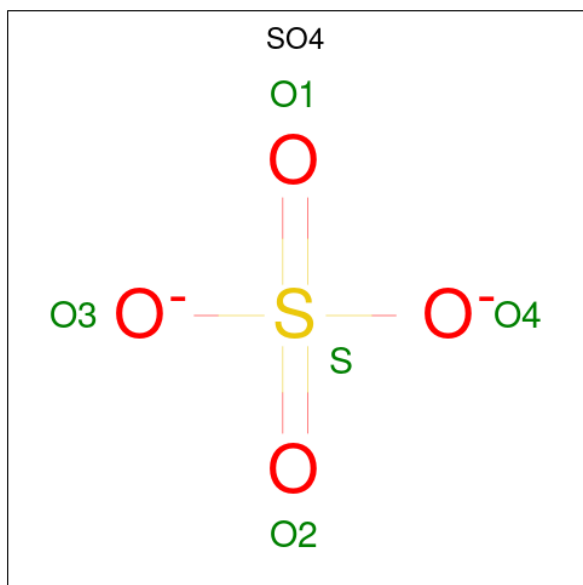
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

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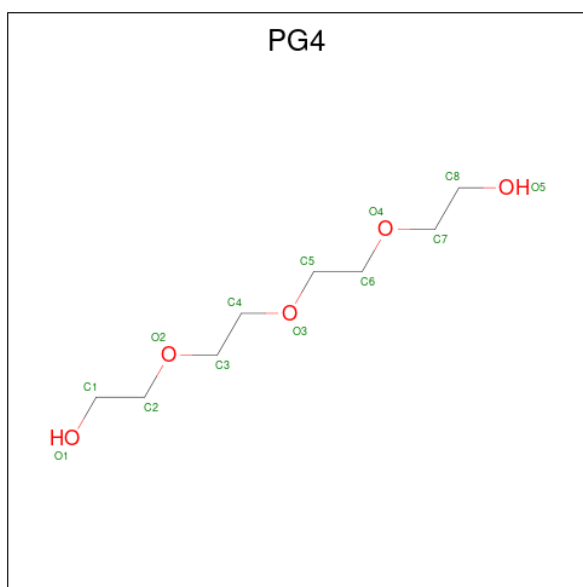
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1121	Total	O	0	3
			1121	1121		
10	B	1093	Total	O	0	0
			1093	1093		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.96Å 102.33Å 127.06Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	48.53 – 1.77 48.53 – 1.77	Depositor EDS
% Data completeness (in resolution range)	86.6 (48.53-1.77) 95.4 (48.53-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.177 , 0.213 0.176 , 0.211	Depositor DCC
R_{free} test set	4968 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20478	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: MG, SO4, QNC, FAD, PG4, FMT, PEG, PGE

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	0.34	0/9037	0.59	0/12310
1	B	0.35	0/9145	0.60	0/12455
All	All	0.35	0/18182	0.60	0/24765

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	8845	0	8807	58	0
1	B	8941	0	8918	43	0
2	A	106	0	62	8	0
2	B	106	0	62	5	0
3	A	40	0	56	5	0
3	B	20	0	28	2	0
4	A	26	0	12	0	0
4	B	26	0	12	1	0
5	A	35	0	50	6	0
5	B	35	0	50	6	0
6	A	6	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	3	0	0
7	A	25	0	0	1	0
7	B	30	0	0	1	0
8	A	1	0	0	0	0
9	B	13	0	18	0	0
10	A	1121	0	0	9	0
10	B	1093	0	0	10	0
All	All	20478	0	18080	109	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 3.

The worst 5 of 109 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:999:ASN:HD21	5:B:2006:PEG:H22	1.43	0.83
1:A:473:TYR:HB2	2:A:2001[B]:FAD:HM72	1.60	0.83
1:B:539:GLU:OE1	10:B:2101:HOH:O	2.00	0.79
1:B:473:TYR:HB2	2:B:2001[B]:FAD:HM72	1.66	0.78
1:A:673:ARG:HH11	5:A:2009:PEG:H12	1.50	0.76

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	1199/1235 (97%)	1177 (98%)	22 (2%)	0	100	100
1	B	1216/1235 (98%)	1190 (98%)	23 (2%)	3 (0%)	44	29
All	All	2415/2470 (98%)	2367 (98%)	45 (2%)	3 (0%)	48	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ASN
1	B	485	TYR
1	B	132	SER

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	882/951 (93%)	874 (99%)	8 (1%)	75	65
1	B	891/951 (94%)	884 (99%)	7 (1%)	79	70
All	All	1773/1902 (93%)	1758 (99%)	15 (1%)	79	70

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	ARG
1	B	342	TYR
1	B	39	TYR
1	B	590	ARG
1	B	223	LEU

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

Mol	Chain	Res	Type
1	A	298	ASN
1	A	304	ASN
1	B	304	ASN

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 ⓘ

Of 42 ligands modelled in this entry, 1 is monoatomic - leaving 41 for Mogul analysis.

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	PEG	B	2007	-	6,6,6	0.25	0	5,5,5	0.28	0
6	FMT	B	2013	-	2,2,2	0.64	0	1,1,1	0.02	0
3	PGE	B	2002	-	9,9,9	0.33	0	8,8,8	0.44	0
4	QNC	A	2004	-	14,14,14	1.20	2 (14%)	19,19,19	1.12	1 (5%)
7	SO4	B	2016	-	4,4,4	0.45	0	6,6,6	0.19	0
4	QNC	B	2004	-	14,14,14	1.14	2 (14%)	19,19,19	0.99	1 (5%)
7	SO4	A	2016	-	4,4,4	0.65	0	6,6,6	0.18	0
7	SO4	A	2019	-	4,4,4	0.66	0	6,6,6	0.31	0
2	FAD	B	2001[A]	-	54,58,58	2.26	15 (27%)	71,89,89	1.66	14 (19%)
3	PGE	A	2007	-	9,9,9	0.38	0	8,8,8	0.72	0
4	QNC	A	2003	8	14,14,14	1.06	1 (7%)	19,19,19	0.96	2 (10%)
7	SO4	B	2017	-	4,4,4	0.69	0	6,6,6	0.14	0
5	PEG	A	2006	-	6,6,6	0.26	0	5,5,5	0.31	0
3	PGE	A	2010	-	9,9,9	0.31	0	8,8,8	0.58	0
6	FMT	B	2012	-	2,2,2	0.63	0	1,1,1	0.12	0
4	QNC	B	2005	-	14,14,14	1.08	1 (7%)	19,19,19	0.97	1 (5%)
7	SO4	B	2015	-	4,4,4	0.67	0	6,6,6	0.15	0
2	FAD	A	2001[B]	-	54,58,58	2.48	17 (31%)	71,89,89	1.71	16 (22%)
5	PEG	B	2006	-	6,6,6	0.24	0	5,5,5	0.31	0
3	PGE	A	2005	-	9,9,9	0.33	0	8,8,8	0.50	0
5	PEG	B	2010	-	6,6,6	0.24	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	2018	-	4,4,4	0.67	0	6,6,6	0.10	0
3	PGE	A	2002	-	9,9,9	0.32	0	8,8,8	0.50	0
3	PGE	B	2003	-	9,9,9	0.31	0	8,8,8	0.57	0
7	SO4	B	2019	-	4,4,4	0.67	0	6,6,6	0.14	0
2	FAD	A	2001[A]	-	54,58,58	2.30	15 (27%)	71,89,89	1.72	15 (21%)
7	SO4	A	2017	-	4,4,4	0.65	0	6,6,6	0.24	0
5	PEG	A	2012	-	6,6,6	0.24	0	5,5,5	0.25	0
5	PEG	B	2011	-	6,6,6	0.25	0	5,5,5	0.18	0
9	PG4	B	2008	-	12,12,12	0.34	0	11,11,11	0.43	0
6	FMT	A	2008	-	2,2,2	0.60	0	1,1,1	0.23	0
7	SO4	B	2020	-	4,4,4	0.68	0	6,6,6	0.18	0
5	PEG	A	2014	-	6,6,6	0.27	0	5,5,5	0.27	0
5	PEG	B	2009	-	6,6,6	0.35	0	5,5,5	0.38	0
5	PEG	A	2009	-	6,6,6	0.26	0	5,5,5	0.25	0
2	FAD	B	2001[B]	-	54,58,58	2.45	17 (31%)	71,89,89	1.68	17 (23%)
7	SO4	A	2015	-	4,4,4	0.60	0	6,6,6	0.17	0
7	SO4	B	2018	-	4,4,4	0.66	0	6,6,6	0.11	0
6	FMT	A	2011	-	2,2,2	0.69	0	1,1,1	0.10	0
5	PEG	A	2013	-	6,6,6	0.24	0	5,5,5	0.23	0
6	FMT	B	2014	-	2,2,2	0.61	0	1,1,1	0.22	0

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	PEG	B	2007	-	-	1/4/4/4	-
3	PGE	B	2002	-	-	0/7/7/7	-
4	QNC	A	2004	-	-	0/4/4/4	0/2/2/2
4	QNC	B	2004	-	-	0/4/4/4	0/2/2/2
2	FAD	B	2001[A]	-	-	7/30/50/50	0/6/6/6
3	PGE	A	2007	-	-	4/7/7/7	-
4	QNC	A	2003	8	-	0/4/4/4	0/2/2/2
5	PEG	A	2006	-	-	2/4/4/4	-
3	PGE	A	2010	-	-	5/7/7/7	-
4	QNC	B	2005	-	-	0/4/4/4	0/2/2/2
2	FAD	A	2001[B]	-	-	10/30/50/50	0/6/6/6
5	PEG	B	2006	-	-	3/4/4/4	-
3	PGE	A	2005	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	2010	-	-	4/4/4/4	-
3	PGE	A	2002	-	-	2/7/7/7	-
3	PGE	B	2003	-	-	2/7/7/7	-
2	FAD	A	2001[A]	-	-	6/30/50/50	0/6/6/6
5	PEG	A	2012	-	-	3/4/4/4	-
5	PEG	B	2011	-	-	0/4/4/4	-
9	PG4	B	2008	-	-	6/10/10/10	-
5	PEG	A	2014	-	-	3/4/4/4	-
5	PEG	B	2009	-	-	2/4/4/4	-
5	PEG	A	2009	-	-	3/4/4/4	-
2	FAD	B	2001[B]	-	-	6/30/50/50	0/6/6/6
5	PEG	A	2013	-	-	0/4/4/4	-

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001[B]	FAD	PA-O3P	-10.60	1.48	1.59
2	B	2001[B]	FAD	PA-O3P	-10.09	1.48	1.59
2	A	2001[A]	FAD	PA-O3P	-9.09	1.49	1.59
2	B	2001[A]	FAD	PA-O3P	-7.86	1.51	1.59
2	A	2001[A]	FAD	O4-C4	7.33	1.37	1.23

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001[A]	FAD	N3A-C2A-N1A	-6.45	119.92	128.67
2	B	2001[B]	FAD	N3A-C2A-N1A	-6.40	119.99	128.67
2	B	2001[A]	FAD	N3A-C2A-N1A	-6.39	119.99	128.67
2	A	2001[B]	FAD	N3A-C2A-N1A	-6.20	120.26	128.67
2	A	2001[B]	FAD	O2P-P-O3P	-4.86	94.14	107.27

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001[A]	FAD	P-O3P-PA-O5B
2	A	2001[A]	FAD	N10-C1'-C2'-O2'
2	A	2001[A]	FAD	N10-C1'-C2'-C3'
2	A	2001[A]	FAD	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	A	2001[B]	FAD	C5B-O5B-PA-O3P

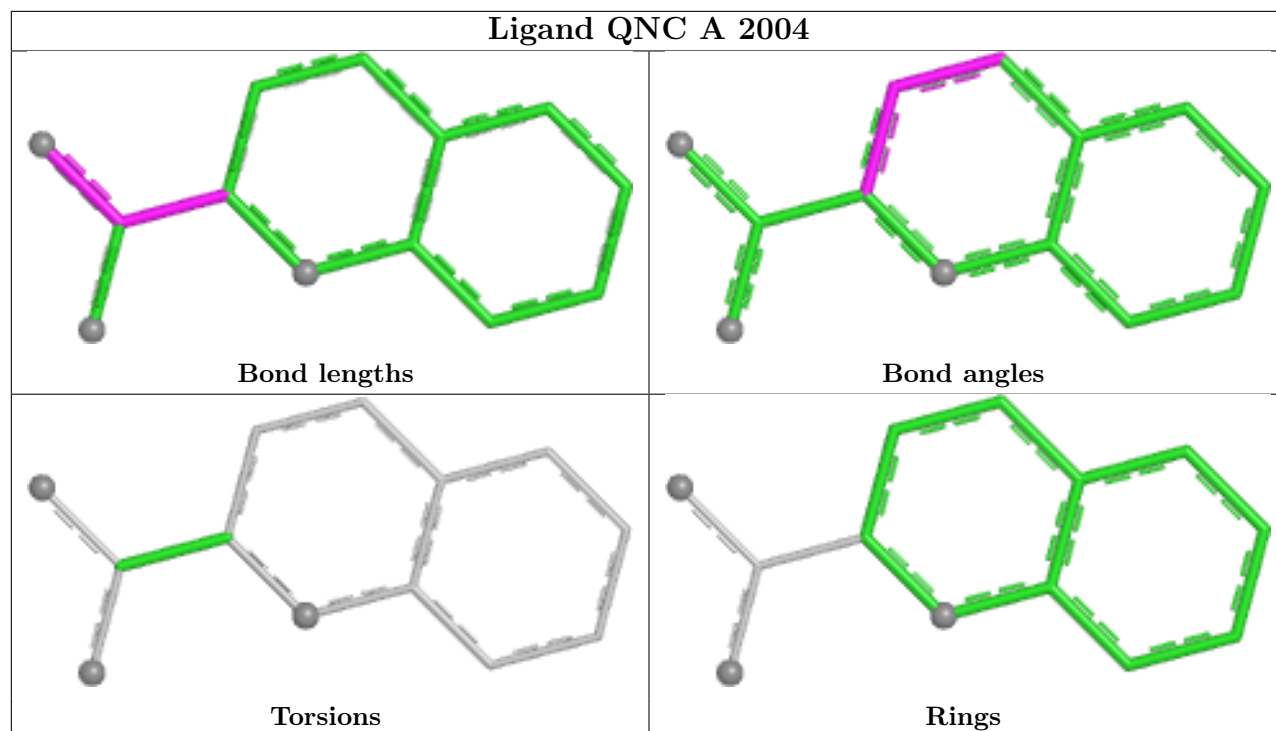
There are no ring outliers.

20 monomers are involved in 36 short contacts:

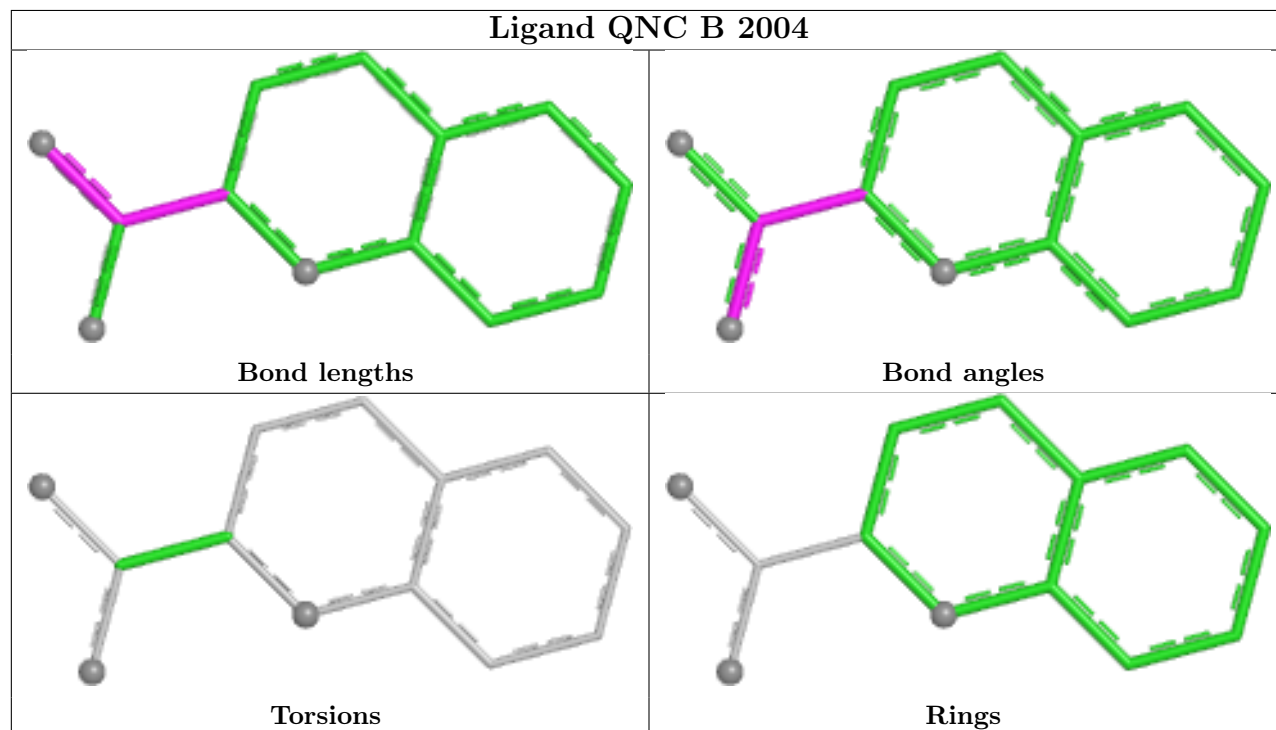
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2007	PEG	1	0
2	B	2001[A]	FAD	4	0
3	A	2007	PGE	2	0
7	B	2017	SO4	1	0
4	B	2005	QNC	1	0
2	A	2001[B]	FAD	4	0
5	B	2006	PEG	3	0
3	A	2005	PGE	1	0
5	B	2010	PEG	1	0
3	A	2002	PGE	2	0
3	B	2003	PGE	2	0
2	A	2001[A]	FAD	4	0
7	A	2017	SO4	1	0
5	A	2012	PEG	1	0
5	A	2014	PEG	2	0
5	B	2009	PEG	1	0
5	A	2009	PEG	2	0
2	B	2001[B]	FAD	1	0
6	A	2011	FMT	1	0
5	A	2013	PEG	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.

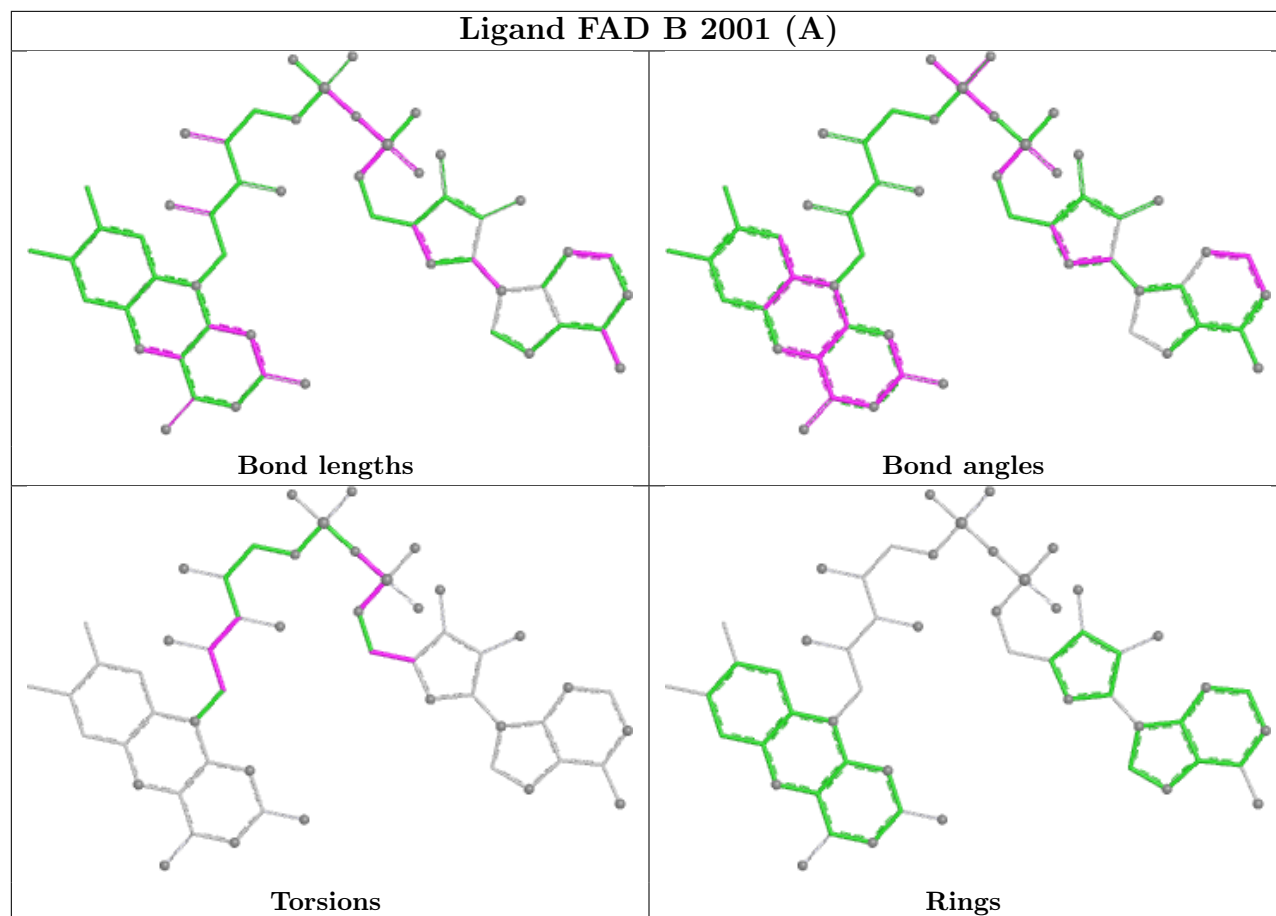
Ligand QNC A 2004



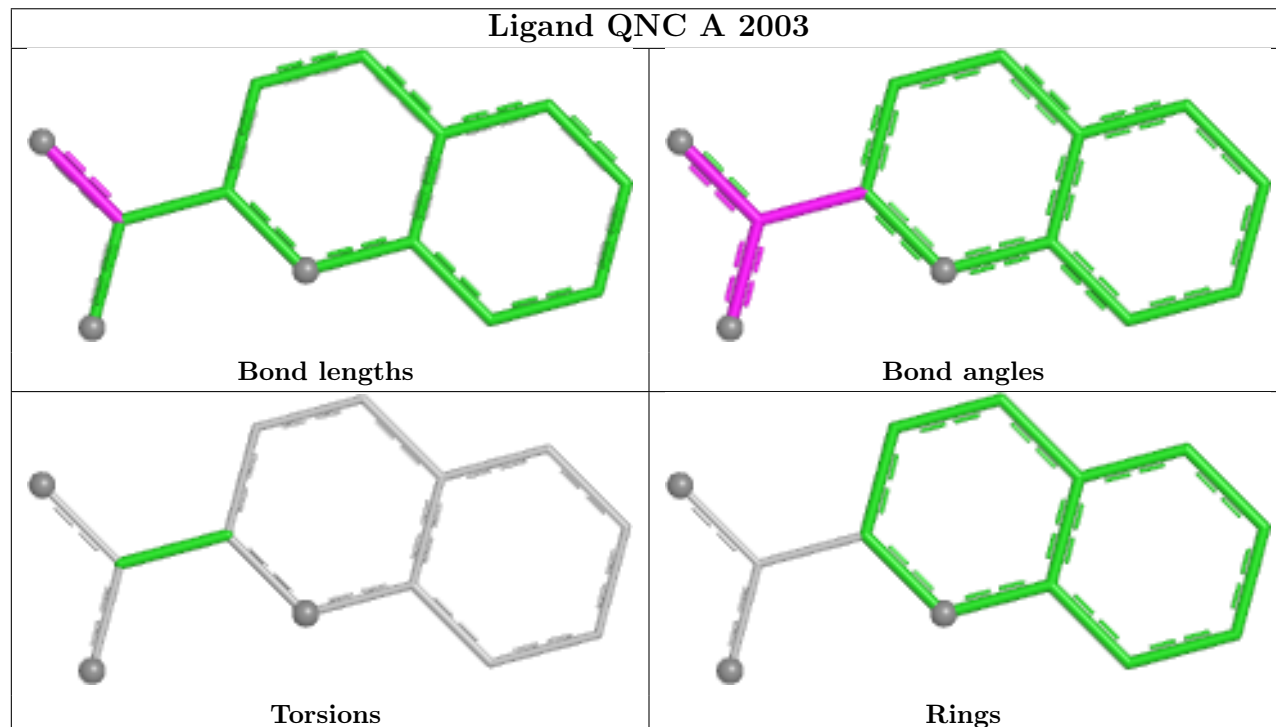
Ligand QNC B 2004

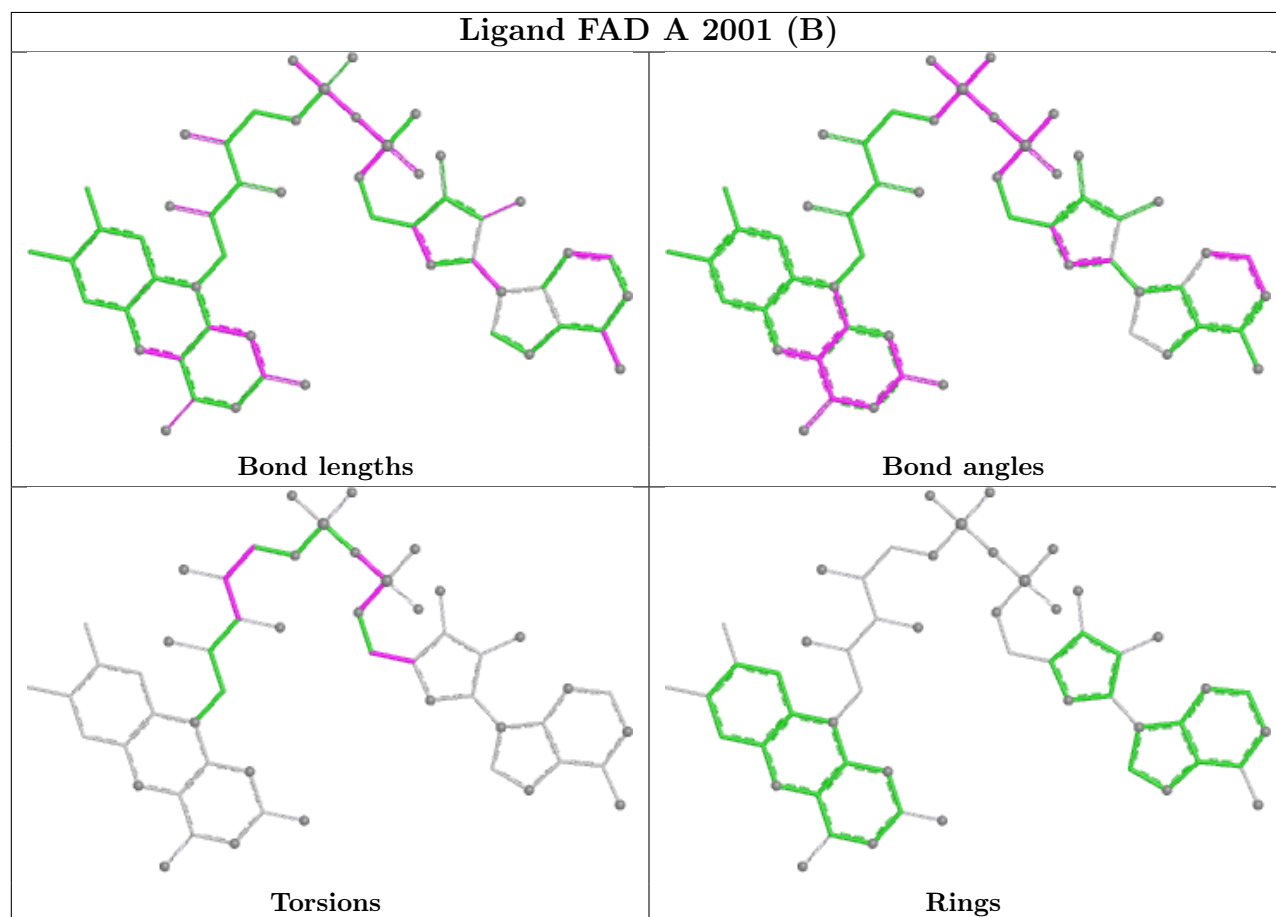
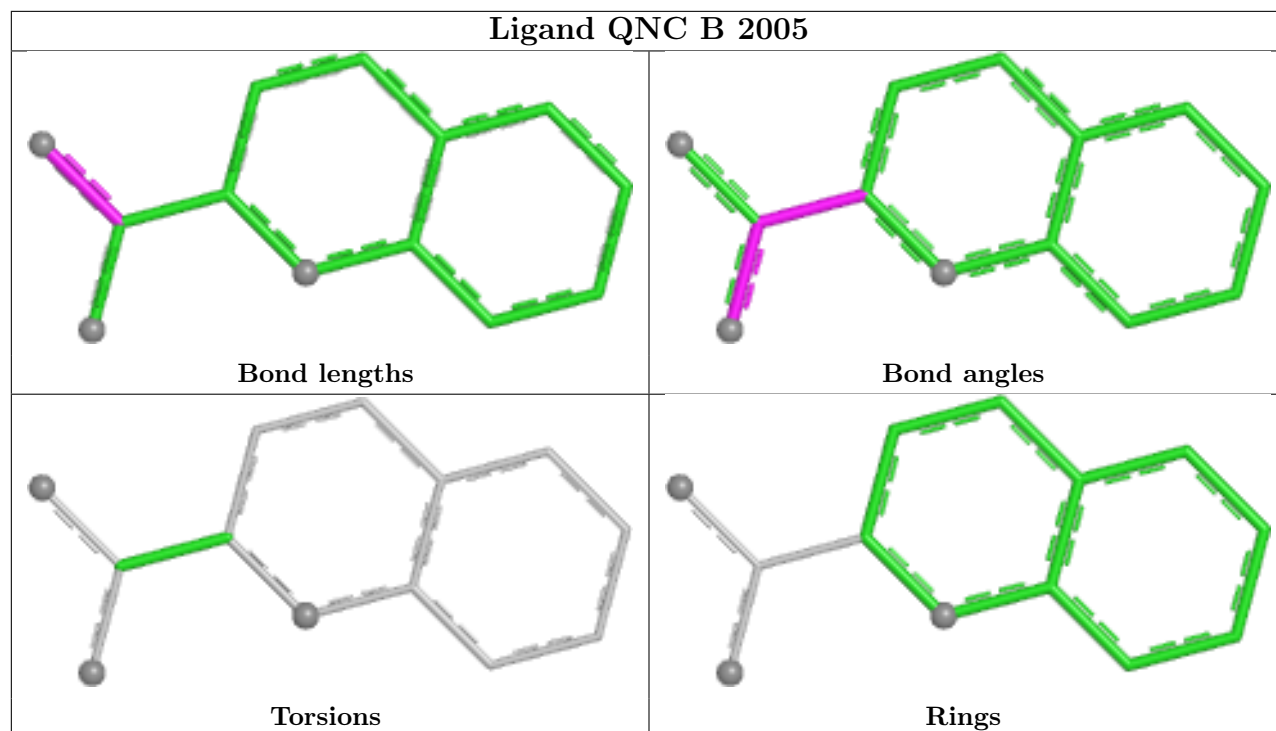


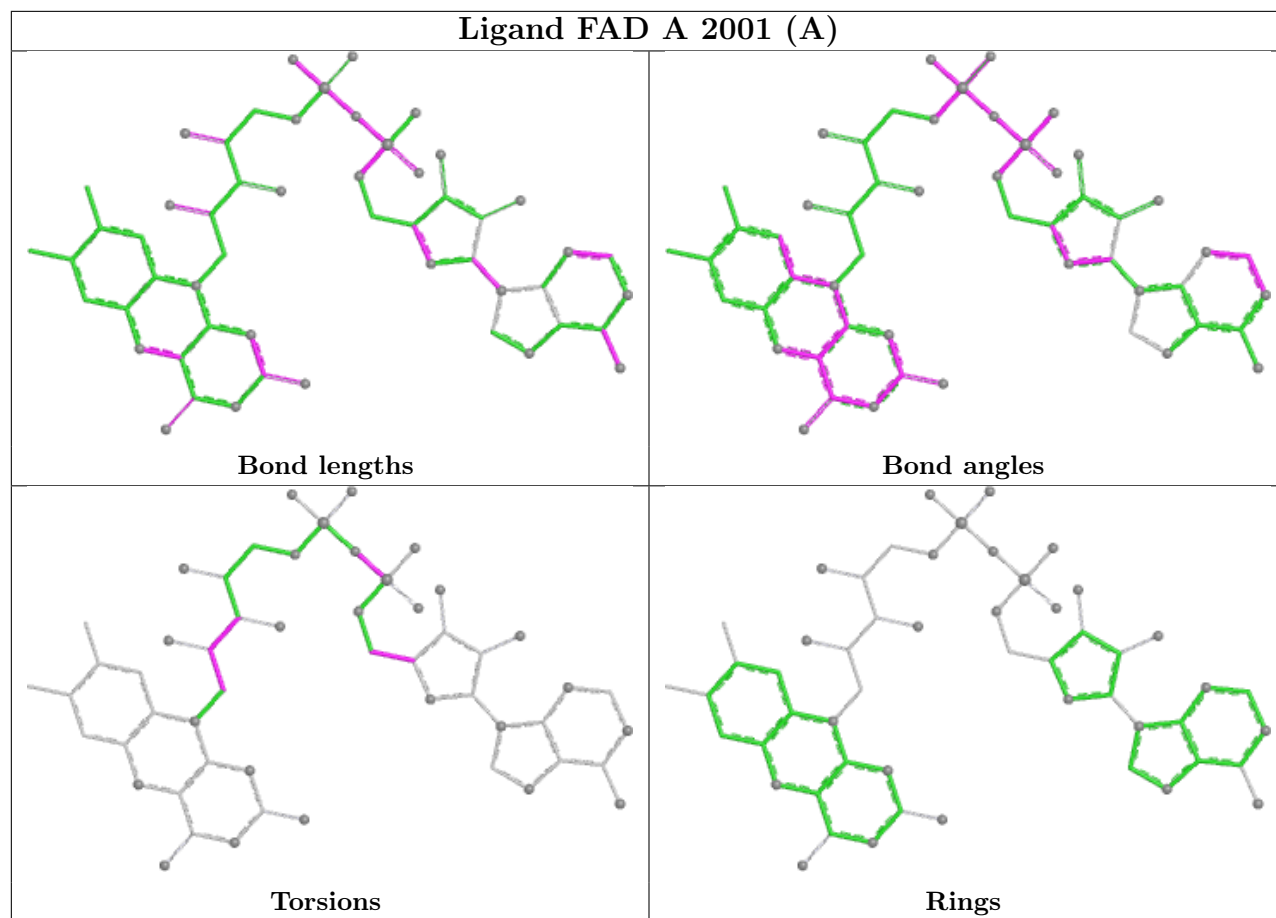
Ligand FAD B 2001 (A)

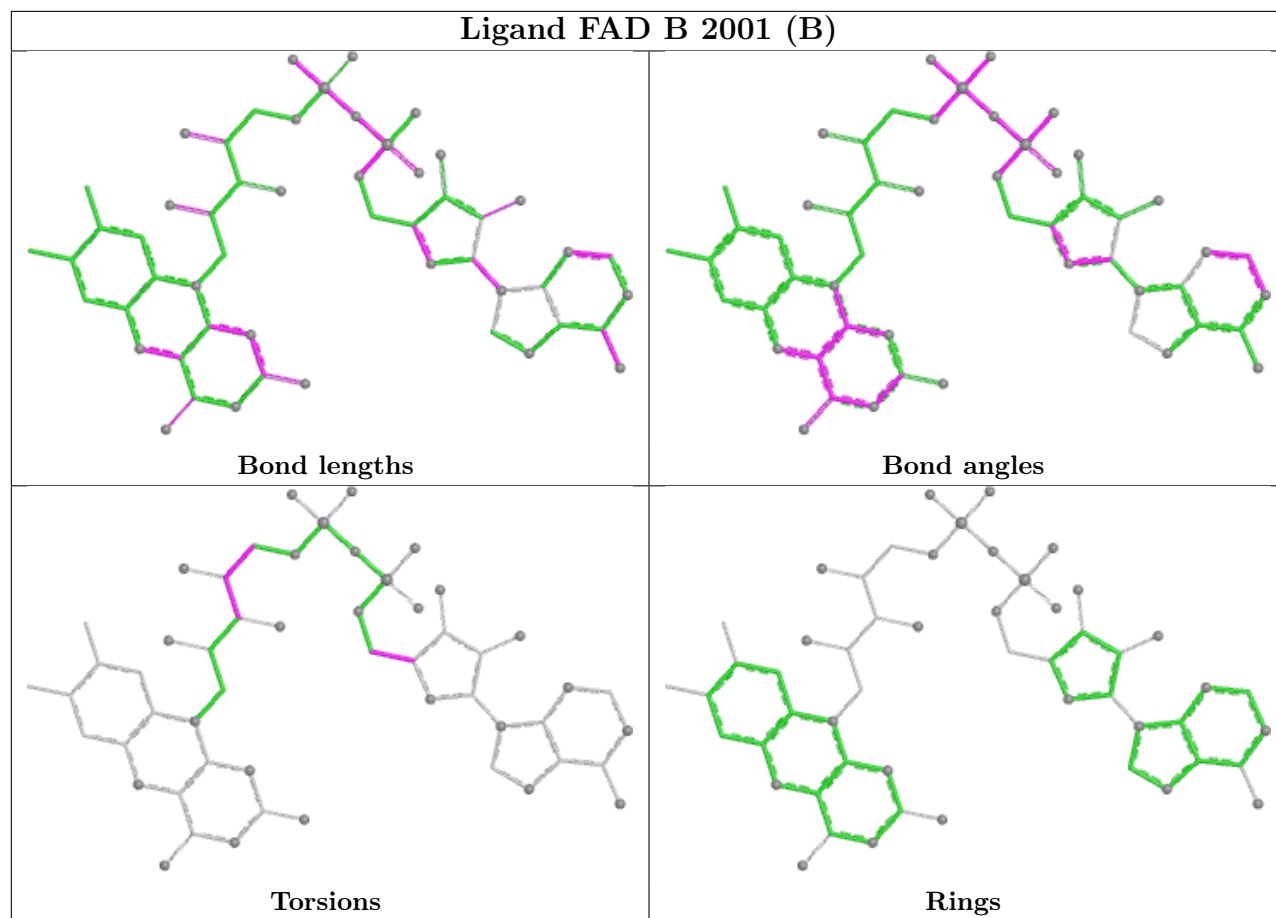


Ligand QNC A 2003









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	1195/1235 (96%)	-0.13	37 (3%)	51	58	9, 21, 43, 84	12 (1%)
1	B	1202/1235 (97%)	-0.18	32 (2%)	56	62	9, 20, 37, 72	21 (1%)
All	All	2397/2470 (97%)	-0.15	69 (2%)	54	60	9, 21, 39, 84	33 (1%)

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	ALA	6.2
1	A	526	VAL	5.5
1	B	486	LEU	5.3
1	B	491	LEU	5.0
1	A	525	PRO	5.0

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.

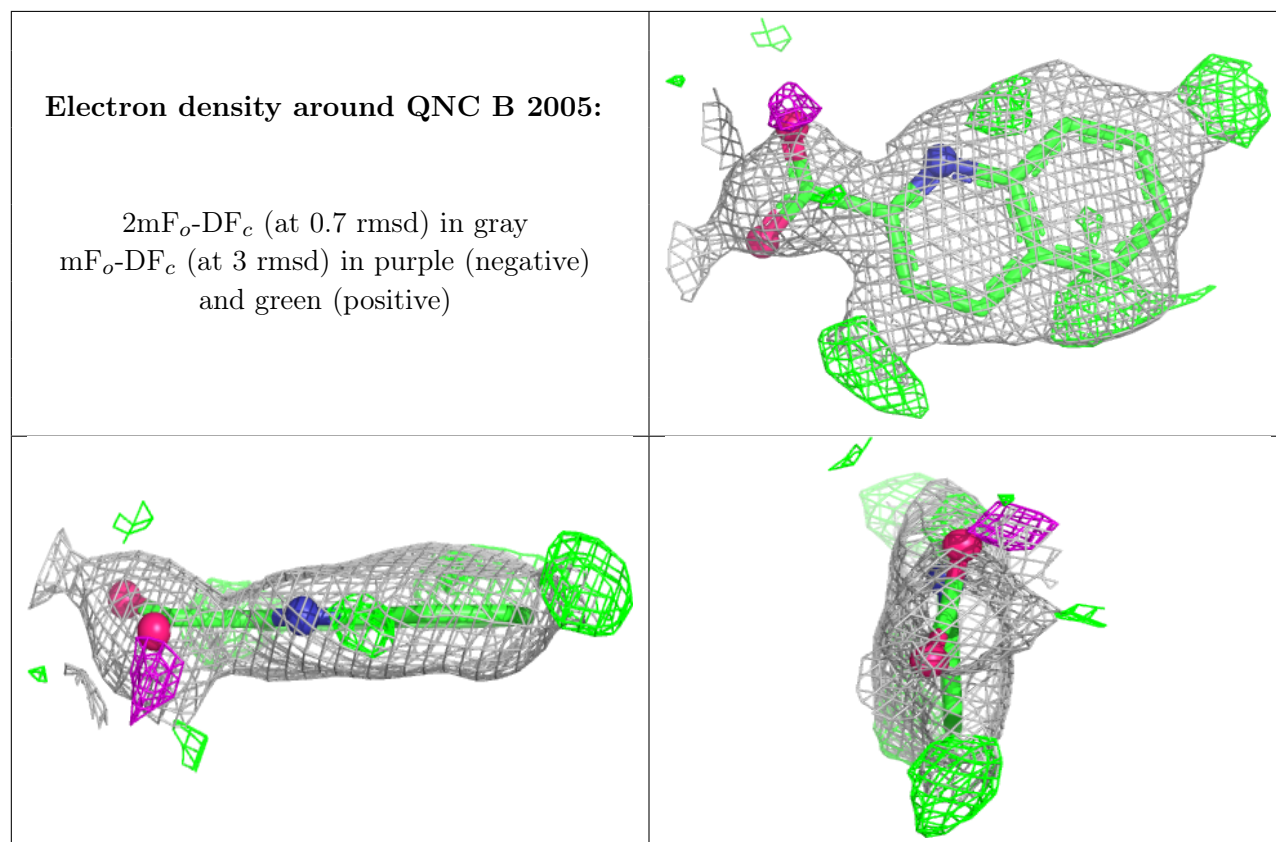
6.4 Ligands [i](#)

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, 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
6	FMT	B	2012	3/3	0.74	0.15	33,33,36,37	3
4	QNC	B	2005	13/13	0.75	0.18	29,33,38,39	13
3	PGE	A	2007	10/10	0.75	0.16	26,35,39,48	0
5	PEG	B	2010	7/7	0.76	0.16	30,37,42,44	0
3	PGE	A	2010	10/10	0.76	0.17	35,42,50,50	0
5	PEG	B	2009	7/7	0.77	0.17	22,34,39,47	0
3	PGE	B	2003	10/10	0.78	0.13	33,42,46,48	0
5	PEG	A	2013	7/7	0.80	0.16	28,38,47,50	0
5	PEG	A	2006	7/7	0.82	0.13	31,40,44,48	0
3	PGE	A	2005	10/10	0.83	0.13	33,43,47,50	0
6	FMT	A	2008	3/3	0.84	0.18	36,36,38,42	0
6	FMT	B	2014	3/3	0.84	0.12	40,40,44,46	0
5	PEG	B	2007	7/7	0.86	0.12	29,31,37,41	0
4	QNC	B	2004	13/13	0.86	0.12	22,25,32,36	13
5	PEG	B	2006	7/7	0.86	0.12	28,34,41,42	0
9	PG4	B	2008	13/13	0.86	0.13	26,34,40,41	0
5	PEG	A	2012	7/7	0.87	0.11	33,36,42,43	0
4	QNC	A	2004	13/13	0.87	0.12	22,27,34,34	13
5	PEG	A	2009	7/7	0.88	0.12	31,32,38,41	0
7	SO4	B	2018	5/5	0.88	0.11	34,40,43,45	5
5	PEG	B	2011	7/7	0.88	0.10	34,39,41,44	0
5	PEG	A	2014	7/7	0.89	0.11	23,31,39,45	0
7	SO4	A	2018	5/5	0.89	0.10	41,45,51,58	5
3	PGE	A	2002	10/10	0.91	0.09	24,28,38,40	0
2	FAD	A	2001[A]	53/53	0.91	0.09	17,25,31,33	53
7	SO4	B	2019	5/5	0.91	0.10	28,32,37,40	5
7	SO4	B	2020	5/5	0.91	0.09	37,37,42,43	5
2	FAD	A	2001[B]	53/53	0.91	0.09	18,25,30,33	53
7	SO4	A	2017	5/5	0.92	0.11	19,29,35,35	5
4	QNC	A	2003	13/13	0.92	0.08	21,25,28,29	13
3	PGE	B	2002	10/10	0.93	0.08	26,33,42,42	0
7	SO4	A	2016	5/5	0.93	0.08	37,39,44,48	5
7	SO4	A	2019	5/5	0.94	0.10	26,34,38,42	5
7	SO4	B	2017	5/5	0.94	0.11	21,24,30,31	5
7	SO4	B	2015	5/5	0.95	0.09	27,29,34,41	5
6	FMT	B	2013	3/3	0.96	0.11	8,8,26,29	0
2	FAD	B	2001[A]	53/53	0.96	0.07	14,18,21,22	53
2	FAD	B	2001[B]	53/53	0.96	0.07	15,18,21,21	53
6	FMT	A	2011	3/3	0.97	0.06	13,13,32,34	0
8	MG	A	2020	1/1	0.98	0.06	28,28,28,28	0
7	SO4	A	2015	5/5	0.98	0.05	20,20,23,24	0
7	SO4	B	2016	5/5	0.99	0.04	14,17,19,19	0

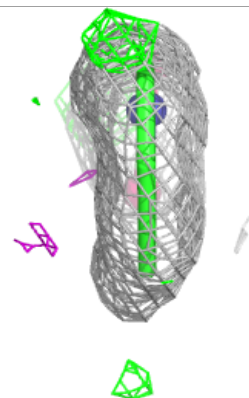
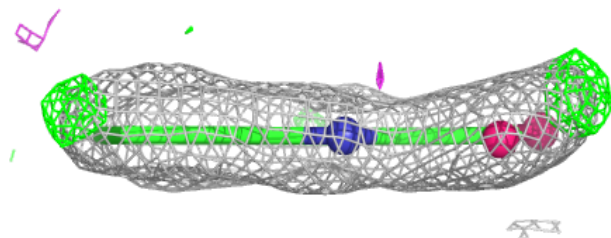
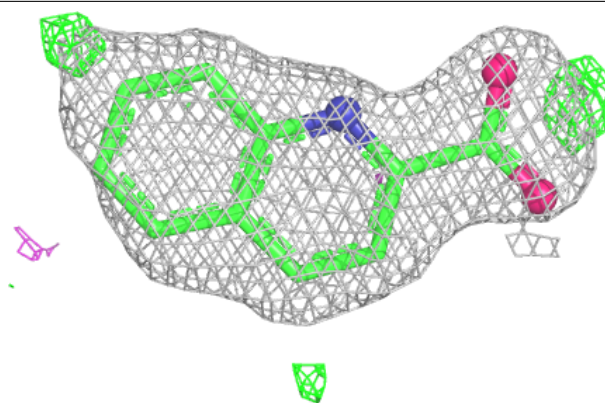
The following is a graphical depiction of the model fit to experimental electron density of all

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.

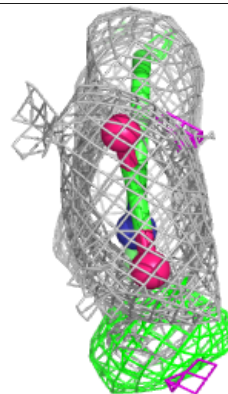
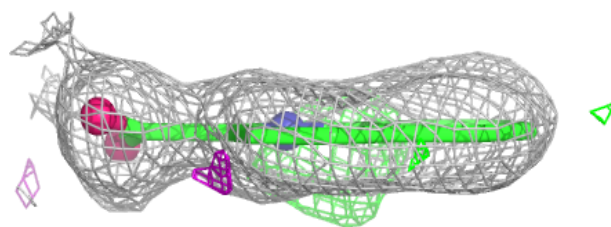
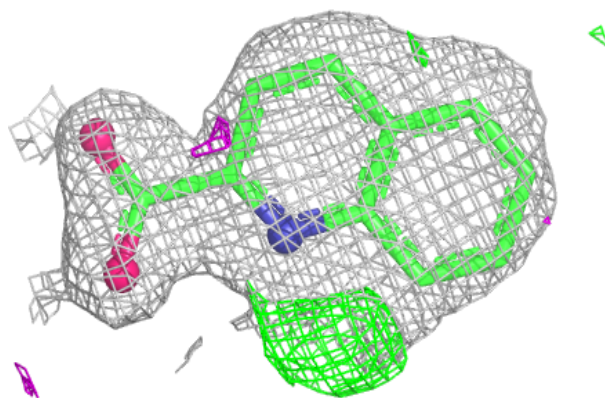


Electron density around QNC B 2004:

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

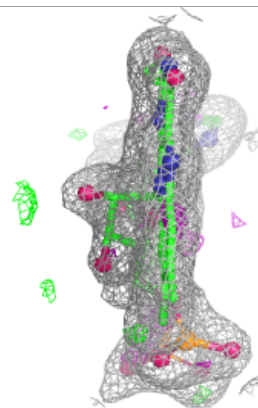
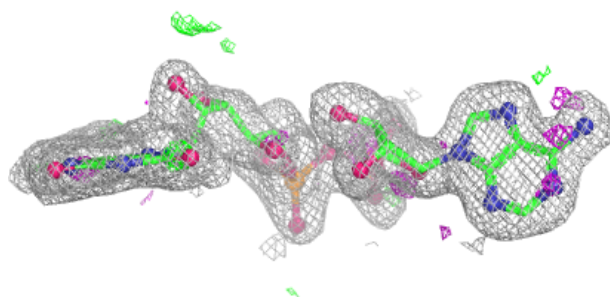
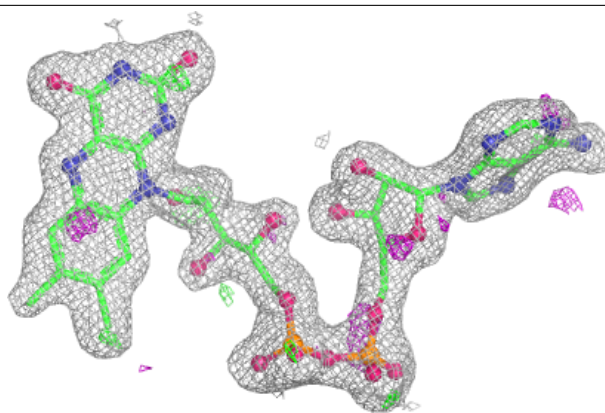
**Electron density around QNC A 2004:**

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

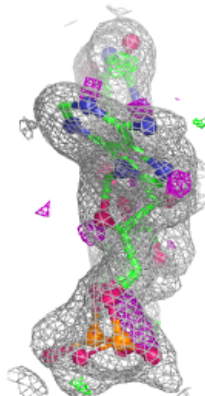
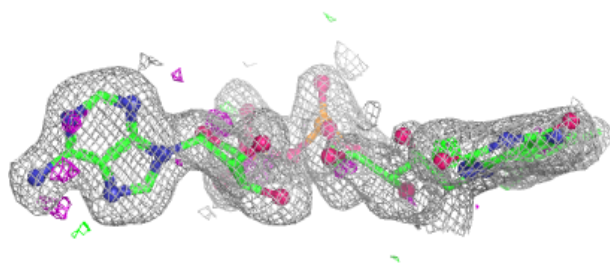
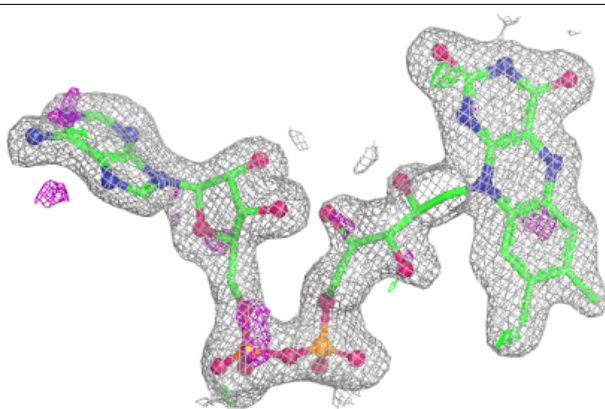


Electron density around FAD A 2001 (A):

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

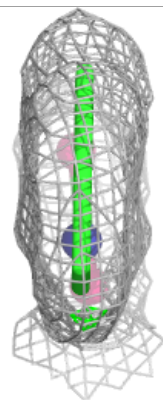
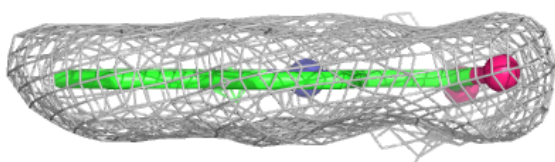
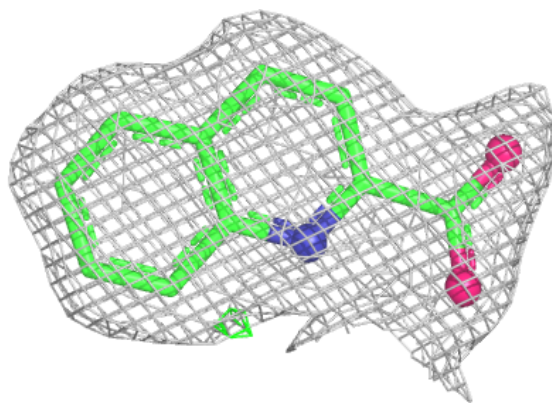
**Electron density around FAD A 2001 (B):**

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and green (positive)

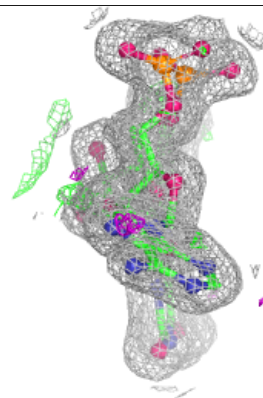
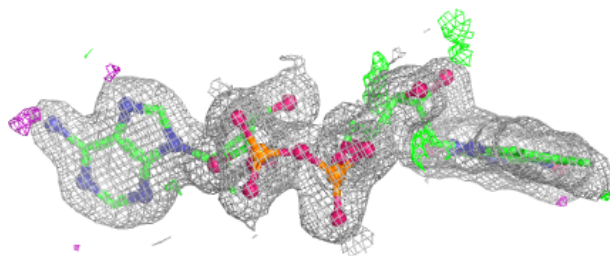
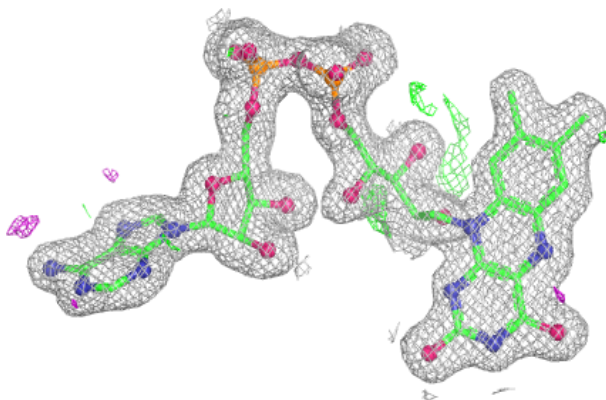


Electron density around QNC A 2003:

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

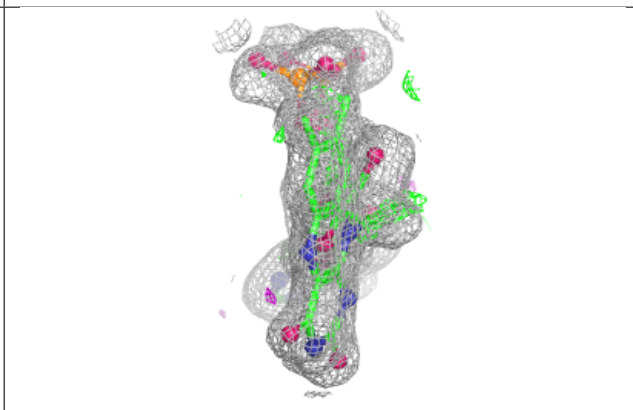
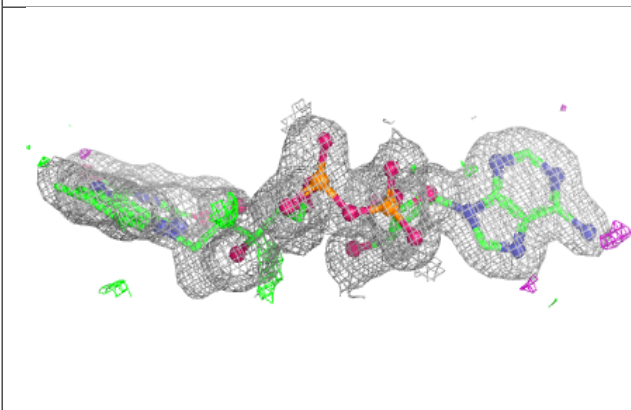
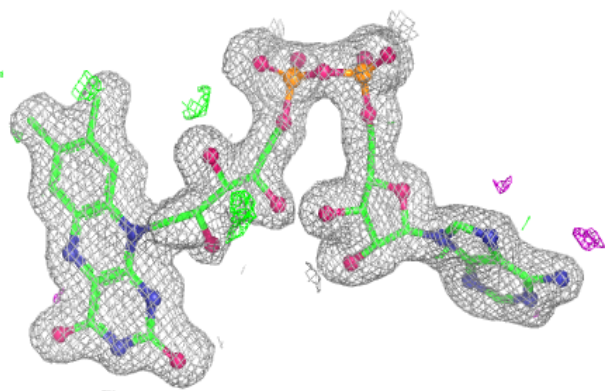
**Electron density around FAD B 2001 (A):**

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



Electron density around FAD B 2001 (B):

$2mF_o - DF_c$ (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.