Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:51 AM EDT

PDB ID	:	4G6H
Title	:	Crystal structure of NDH with NADH
Authors	:	Li, W.; Feng, Y.; Ge, J.; Yang, M.
Deposited on	:	2012-07-19
Resolution	:	2.26 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:

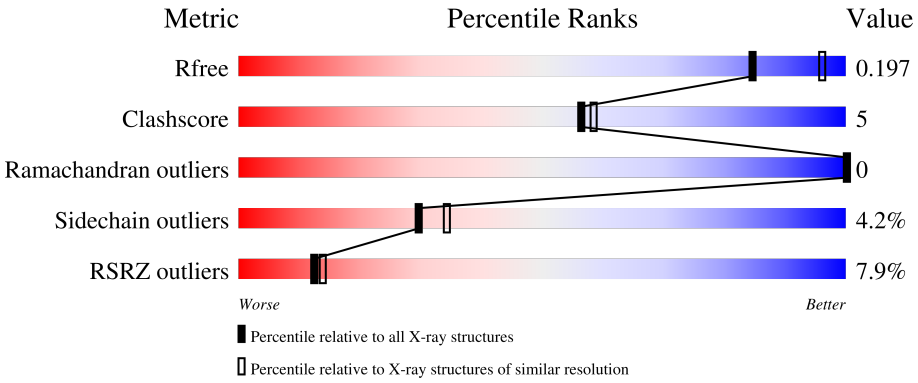
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	502	7% 82% 11% • 6%
1	B	502	8% 81% 13% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8221 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.

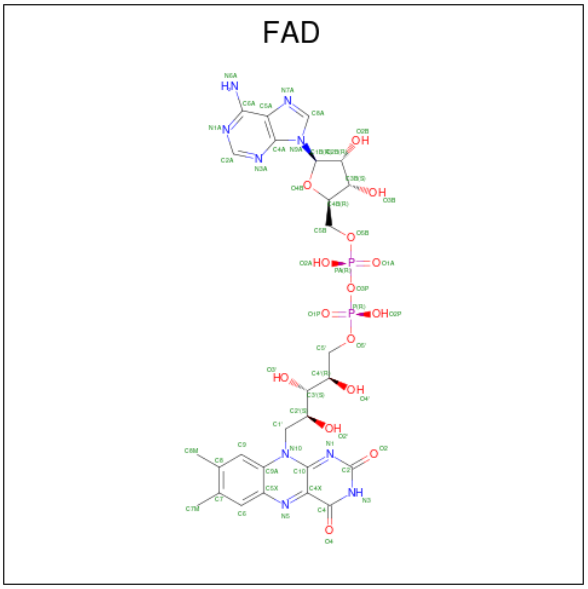
- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3738	2415	635	683	5			
1	B	472	Total	C	N	O	S	0	0	0
			3738	2415	635	683	5			

There are 24 discrepancies between the modelled and reference sequences:

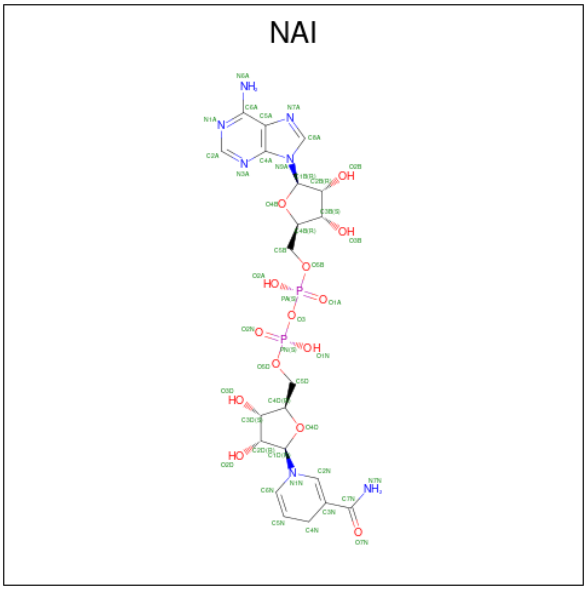
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP P32340
A	13	ARG	-	expression tag	UNP P32340
A	14	GLY	-	expression tag	UNP P32340
A	15	SER	-	expression tag	UNP P32340
A	16	HIS	-	expression tag	UNP P32340
A	17	HIS	-	expression tag	UNP P32340
A	18	HIS	-	expression tag	UNP P32340
A	19	HIS	-	expression tag	UNP P32340
A	20	HIS	-	expression tag	UNP P32340
A	21	HIS	-	expression tag	UNP P32340
A	22	GLY	-	expression tag	UNP P32340
A	23	SER	-	expression tag	UNP P32340
B	12	MET	-	expression tag	UNP P32340
B	13	ARG	-	expression tag	UNP P32340
B	14	GLY	-	expression tag	UNP P32340
B	15	SER	-	expression tag	UNP P32340
B	16	HIS	-	expression tag	UNP P32340
B	17	HIS	-	expression tag	UNP P32340
B	18	HIS	-	expression tag	UNP P32340
B	19	HIS	-	expression tag	UNP P32340
B	20	HIS	-	expression tag	UNP P32340
B	21	HIS	-	expression tag	UNP P32340
B	22	GLY	-	expression tag	UNP P32340
B	23	SER	-	expression tag	UNP P32340

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	B	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

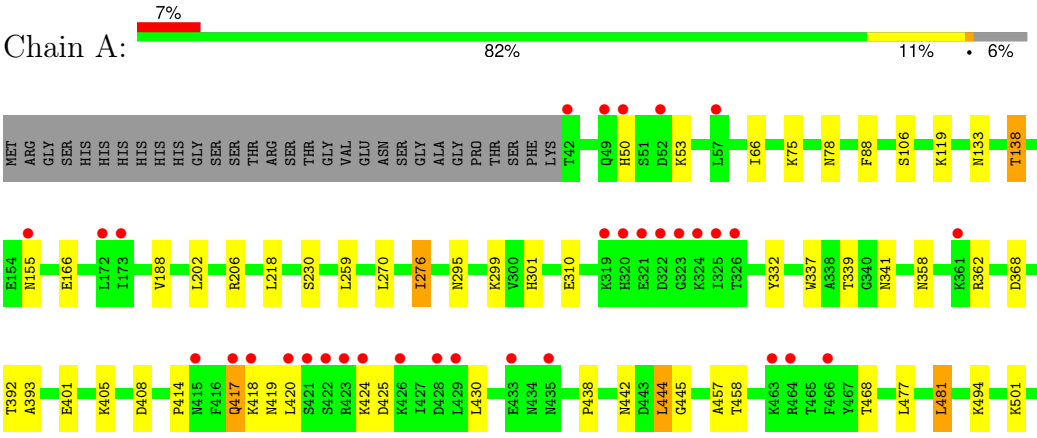
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	275	Total	O	0	0
			275	275		
5	B	270	Total	O	0	0
			270	270		

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.

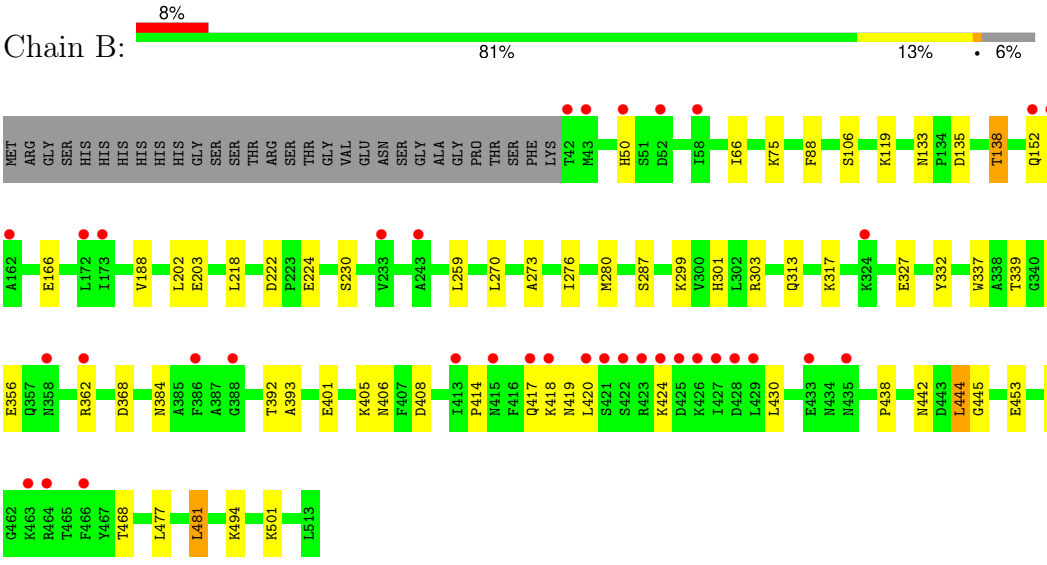
• Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial

Chain A:



• Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.19Å 229.59Å 111.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.26 29.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.15-2.26) 99.9 (29.89-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.193 , 0.225 0.195 , 0.197	Depositor DCC
R_{free} test set	3871 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8221	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, MG, NAI

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	0.51	0/3824	0.65	3/5177 (0.1%)
1	B	0.53	1/3824 (0.0%)	0.66	3/5177 (0.1%)
All	All	0.52	1/7648 (0.0%)	0.66	6/10354 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CG-CD	5.16	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	362	ARG	NE-CZ-NH1	-13.09	113.76	120.30
1	B	362	ARG	NE-CZ-NH2	12.55	126.58	120.30
1	A	362	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	362	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	B	362	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	362	ARG	CD-NE-CZ	5.86	131.81	123.60

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	3738	0	3803	32	0
1	B	3738	0	3803	32	1
2	A	53	0	31	3	0
2	B	53	0	31	3	0
3	A	44	0	27	10	0
3	B	44	0	27	7	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	275	0	0	15	0
5	B	270	0	0	10	0
All	All	8221	0	7722	77	1

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 5.

All (77) 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:A:419:ASN:O	5:A:729:HOH:O	1.88	0.91
1:A:392:THR:HG22	3:A:602:NAI:H5N	1.62	0.81
1:B:392:THR:HG22	3:B:604:NAI:H5N	1.62	0.81
1:A:341:ASN:ND2	3:A:602:NAI:O3D	2.16	0.78
1:B:406:ASN:OD1	5:B:935:HOH:O	2.01	0.78
3:A:602:NAI:O2A	5:A:815:HOH:O	2.02	0.77
1:B:368:ASP:HB3	1:B:438:PRO:HB3	1.68	0.76
1:A:425:ASP:OD1	5:A:945:HOH:O	2.02	0.75
1:A:295:ASN:OD1	5:A:784:HOH:O	2.04	0.75
1:B:224:GLU:OE1	5:B:894:HOH:O	2.08	0.71
1:A:138:THR:HG21	1:A:166:GLU:OE1	1.90	0.71
1:B:222:ASP:O	5:B:742:HOH:O	2.07	0.71
1:B:453:GLU:OE1	5:B:881:HOH:O	2.08	0.71
1:A:438:PRO:O	5:A:808:HOH:O	2.08	0.70
1:B:138:THR:HG21	1:B:166:GLU:OE1	1.93	0.68
1:A:368:ASP:HB3	1:A:438:PRO:HB3	1.75	0.68
3:B:604:NAI:O2A	5:B:831:HOH:O	2.12	0.67
1:A:75:LYS:HE3	1:A:119:LYS:HD2	1.77	0.66
1:B:75:LYS:HE3	1:B:119:LYS:HD2	1.77	0.66
1:B:152:GLN:HB2	1:B:153:PRO:HD3	1.79	0.65
1:A:152:GLN:HB2	1:A:153:PRO:HD3	1.80	0.63
1:B:341:ASN:ND2	3:B:604:NAI:O3D	2.31	0.63
1:A:310:GLU:OE2	5:A:898:HOH:O	2.16	0.61
1:A:358:ASN:ND2	5:A:910:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:HB2	1:B:138:THR:HG22	1.83	0.60
1:A:133:ASN:HB2	1:A:138:THR:HG22	1.84	0.60
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.84	0.60
1:B:313:GLN:OE1	5:B:968:HOH:O	2.16	0.60
3:A:602:NAI:H2D	5:A:774:HOH:O	2.02	0.60
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.85	0.59
1:B:419:ASN:ND2	1:B:424:LYS:O	2.37	0.57
3:A:602:NAI:H3D	5:A:774:HOH:O	2.05	0.56
1:A:299:LYS:HD3	1:A:301:HIS:NE2	2.21	0.56
3:A:602:NAI:C2D	5:A:774:HOH:O	2.54	0.55
1:A:417:GLN:NE2	5:A:919:HOH:O	1.91	0.55
1:B:299:LYS:HD3	1:B:301:HIS:NE2	2.22	0.54
1:B:106:SER:HA	1:B:494:LYS:HE3	1.89	0.54
1:A:337:TRP:HE1	1:A:339:THR:HG1	1.56	0.53
1:A:419:ASN:ND2	1:A:424:LYS:O	2.40	0.52
3:A:602:NAI:C3D	5:A:774:HOH:O	2.59	0.50
3:B:604:NAI:C3D	5:B:888:HOH:O	2.59	0.50
1:B:66:ILE:HG13	1:B:88:PHE:HB2	1.96	0.47
1:B:445:GLY:HA3	1:B:458:THR:O	2.13	0.47
1:A:106:SER:HA	1:A:494:LYS:HE3	1.96	0.47
2:A:601:FAD:C10	3:A:602:NAI:H42N	2.44	0.47
1:B:401:GLU:O	1:B:405:LYS:HG2	2.15	0.46
1:B:337:TRP:HE1	1:B:339:THR:HG1	1.63	0.46
1:A:401:GLU:O	1:A:405:LYS:HG2	2.15	0.46
1:A:206:ARG:HD2	5:A:924:HOH:O	2.16	0.46
1:A:393:ALA:HB2	2:A:601:FAD:H2'	1.97	0.46
1:A:66:ILE:HG13	1:A:88:PHE:HB2	1.98	0.46
1:A:230:SER:OG	1:A:332:TYR:HA	2.17	0.44
1:B:135:ASP:N	5:B:916:HOH:O	2.34	0.44
1:A:405:LYS:O	1:A:408:ASP:HB2	2.18	0.43
3:A:602:NAI:H1D	5:A:770:HOH:O	2.18	0.43
1:A:206:ARG:NH1	5:A:924:HOH:O	1.88	0.43
3:B:604:NAI:O1A	5:B:868:HOH:O	2.21	0.43
1:B:457:ALA:O	1:B:468:THR:HA	2.19	0.43
1:A:445:GLY:HA3	1:A:458:THR:O	2.19	0.43
1:A:442:ASN:O	1:A:444:LEU:HD13	2.19	0.42
1:B:230:SER:OG	1:B:332:TYR:HA	2.19	0.42
1:B:356:GLU:OE1	1:B:356:GLU:N	2.44	0.42
1:B:414:PRO:O	1:B:418:LYS:HG3	2.20	0.42
1:A:414:PRO:O	1:A:418:LYS:HG3	2.20	0.41
1:B:133:ASN:ND2	5:B:963:HOH:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ALA:HB2	2:B:605:FAD:H2'	2.02	0.41
1:B:354:ILE:HA	1:B:355:PRO:HD3	1.93	0.41
3:B:604:NAI:H42N	2:B:605:FAD:C10	2.51	0.41
1:A:276:ILE:H	1:A:276:ILE:HD13	1.85	0.41
1:B:317:LYS:HG2	1:B:327:GLU:HG2	2.03	0.41
1:B:273:ALA:O	1:B:303:ARG:HA	2.21	0.41
3:B:604:NAI:H42N	2:B:605:FAD:C4X	2.51	0.40
2:A:601:FAD:C4X	3:A:602:NAI:H42N	2.51	0.40
1:B:405:LYS:O	1:B:408:ASP:HB2	2.21	0.40
1:B:442:ASN:O	1:B:444:LEU:HD13	2.21	0.40
1:A:53:LYS:HD2	1:A:78:ASN:OD1	2.22	0.40
1:A:457:ALA:O	1:A:468:THR:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:SER:OG	1:B:287:SER:OG[3_454]	2.19	0.01

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	470/502 (94%)	457 (97%)	13 (3%)	0	100	100
1	B	470/502 (94%)	455 (97%)	15 (3%)	0	100	100
All	All	940/1004 (94%)	912 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	403/427 (94%)	386 (96%)	17 (4%)	30	34
1	B	403/427 (94%)	386 (96%)	17 (4%)	30	34
All	All	806/854 (94%)	772 (96%)	34 (4%)	30	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	138	THR
1	A	150	LEU
1	A	155	ASN
1	A	188	VAL
1	A	202	LEU
1	A	218	LEU
1	A	259	LEU
1	A	270	LEU
1	A	276	ILE
1	A	384	ASN
1	A	417	GLN
1	A	420	LEU
1	A	430	LEU
1	A	444	LEU
1	A	481	LEU
1	A	501	LYS
1	B	50	HIS
1	B	138	THR
1	B	155	ASN
1	B	188	VAL
1	B	202	LEU
1	B	218	LEU
1	B	259	LEU
1	B	270	LEU
1	B	276	ILE
1	B	280	MET

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Mol	Chain	Res	Type
1	B	384	ASN
1	B	417	GLN
1	B	420	LEU
1	B	430	LEU
1	B	444	LEU
1	B	481	LEU
1	B	501	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	B	341	ASN

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)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\|>2$
3	NAI	A	602	-	43,48,48	1.36	3 (6%)	50,73,73	1.12	3 (6%)
3	NAI	B	604	-	43,48,48	1.35	3 (6%)	50,73,73	1.14	3 (6%)
2	FAD	B	605	-	54,58,58	1.25	6 (11%)	71,89,89	1.54	11 (15%)
2	FAD	A	601	-	54,58,58	1.17	4 (7%)	71,89,89	1.70	17 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	A	602	-	-	11/25/72/72	0/5/5/5
3	NAI	B	604	-	-	11/25/72/72	0/5/5/5
2	FAD	B	605	-	-	2/30/50/50	0/6/6/6
2	FAD	A	601	-	-	3/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAI	C4N-C3N	-5.83	1.39	1.50
3	B	604	NAI	C4N-C3N	-5.78	1.39	1.50
2	B	605	FAD	C4X-N5	3.87	1.39	1.30
3	B	604	NAI	C4N-C5N	-3.83	1.39	1.49
2	A	601	FAD	C2A-N3A	3.80	1.38	1.32
3	A	602	NAI	C4N-C5N	-3.76	1.39	1.49
2	B	605	FAD	C2A-N3A	3.64	1.37	1.32
2	B	605	FAD	C10-N1	3.15	1.39	1.33
2	A	601	FAD	C4X-N5	3.11	1.37	1.30
2	B	605	FAD	C2A-N1A	2.84	1.39	1.33
2	A	601	FAD	C2A-N1A	2.76	1.38	1.33
2	B	605	FAD	PA-O3P	2.58	1.62	1.59
2	A	601	FAD	C10-N1	2.38	1.38	1.33
2	B	605	FAD	P-O3P	2.18	1.61	1.59
3	A	602	NAI	C6N-C5N	2.06	1.39	1.33
3	B	604	NAI	C6N-C5N	2.06	1.39	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	N3A-C2A-N1A	-7.33	118.72	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	605	FAD	N3A-C2A-N1A	-6.93	119.27	128.67
2	A	601	FAD	C4-N3-C2	-3.71	119.05	125.64
3	B	604	NAI	N3A-C2A-N1A	-3.71	123.64	128.67
3	A	602	NAI	N3A-C2A-N1A	-3.68	123.68	128.67
2	A	601	FAD	C4'-C3'-C2'	-3.64	107.50	113.57
2	B	605	FAD	C9A-C5X-N5	-3.29	118.96	122.45
2	B	605	FAD	C5X-C9A-N10	3.20	120.86	117.97
2	A	601	FAD	O3P-PA-O1A	-2.99	101.71	110.70
3	B	604	NAI	C4A-C5A-N7A	-2.77	106.42	109.34
3	A	602	NAI	C4A-C5A-N7A	-2.74	106.44	109.34
2	A	601	FAD	C4X-C10-N10	2.73	120.39	116.48
2	B	605	FAD	C4-N3-C2	-2.67	120.90	125.64
2	A	601	FAD	O4-C4-C4X	-2.66	119.50	126.53
2	B	605	FAD	C4'-C3'-C2'	-2.65	109.15	113.57
2	A	601	FAD	C1B-N9A-C4A	-2.63	122.03	126.64
2	A	601	FAD	C9A-C5X-N5	-2.59	119.70	122.45
3	B	604	NAI	C3D-C2D-C1D	2.58	106.33	101.46
2	A	601	FAD	O3'-C3'-C2'	2.54	114.69	108.93
2	A	601	FAD	C4-C4X-C10	2.53	121.28	116.93
2	A	601	FAD	C5X-C9A-N10	2.53	120.26	117.97
2	A	601	FAD	C4B-O4B-C1B	-2.43	107.70	109.92
2	A	601	FAD	C4X-C4-N3	2.42	119.42	113.25
2	B	605	FAD	C4X-C4-N3	2.37	119.30	113.25
2	B	605	FAD	O4-C4-C4X	-2.36	120.30	126.53
2	A	601	FAD	C10-C4X-N5	-2.35	120.00	124.81
3	A	602	NAI	C3D-C2D-C1D	2.22	105.66	101.46
2	B	605	FAD	O5'-C5'-C4'	-2.20	103.49	109.36
2	A	601	FAD	O2-C2-N1	-2.19	118.17	121.80
2	B	605	FAD	C4-C4X-C10	2.19	120.68	116.93
2	B	605	FAD	C4B-O4B-C1B	-2.18	107.93	109.92
2	A	601	FAD	O5'-C5'-C4'	-2.13	103.68	109.36
2	B	605	FAD	C4A-C5A-N7A	-2.10	107.12	109.34
2	A	601	FAD	C4X-C10-N1	-2.04	119.59	124.59

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAI	C5B-O5B-PA-O1A
3	B	604	NAI	PA-O3-PN-O5D
3	B	604	NAI	C5D-O5D-PN-O2N
3	B	604	NAI	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
3	A	602	NAI	C4D-C5D-O5D-PN
3	A	602	NAI	O4B-C4B-C5B-O5B
3	A	602	NAI	C3B-C4B-C5B-O5B
3	A	602	NAI	PN-O3-PA-O1A
3	A	602	NAI	PA-O3-PN-O5D
3	A	602	NAI	C5B-O5B-PA-O2A
3	A	602	NAI	C5B-O5B-PA-O3
3	B	604	NAI	C5B-O5B-PA-O1A
3	B	604	NAI	O4B-C4B-C5B-O5B
3	A	602	NAI	PN-O3-PA-O2A
3	B	604	NAI	PN-O3-PA-O1A
2	A	601	FAD	O3'-C3'-C4'-C5'
3	B	604	NAI	O4D-C1D-N1N-C2N
3	A	602	NAI	O4D-C1D-N1N-C2N
3	B	604	NAI	C2N-C3N-C7N-N7N
3	B	604	NAI	PN-O3-PA-O2A
2	B	605	FAD	O3'-C3'-C4'-C5'
3	A	602	NAI	C2D-C1D-N1N-C2N
3	B	604	NAI	C2D-C1D-N1N-C2N
2	A	601	FAD	O3'-C3'-C4'-O4'
2	B	605	FAD	O3'-C3'-C4'-O4'
3	B	604	NAI	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

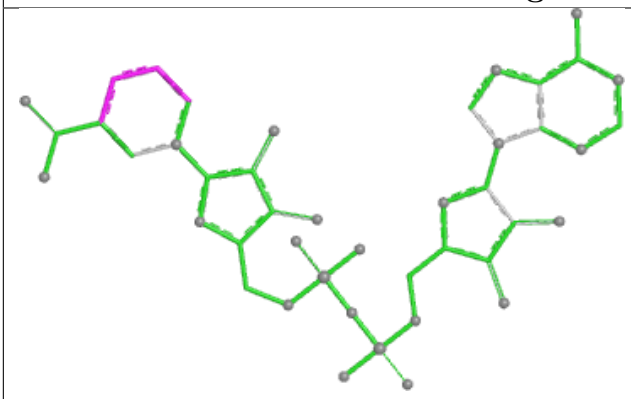
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAI	10	0
3	B	604	NAI	7	0
2	B	605	FAD	3	0
2	A	601	FAD	3	0

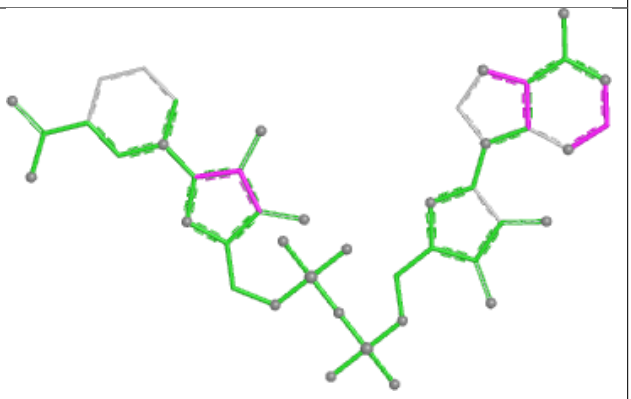
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

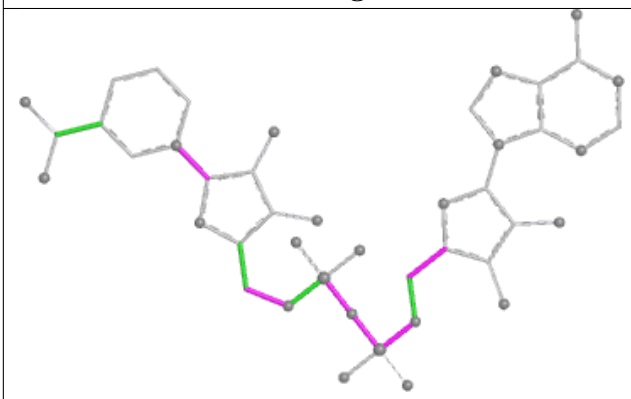
Ligand NAI A 602



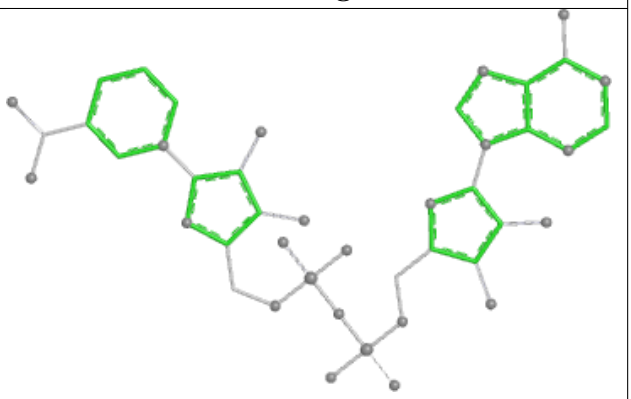
Bond lengths



Bond angles

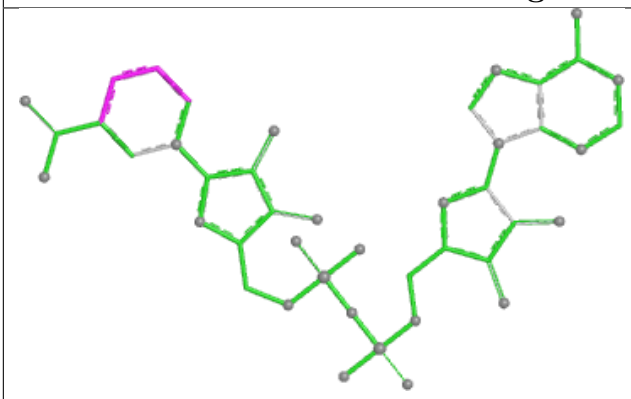


Torsions

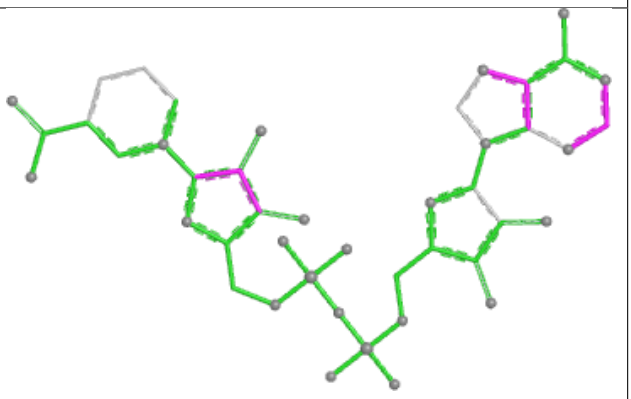


Rings

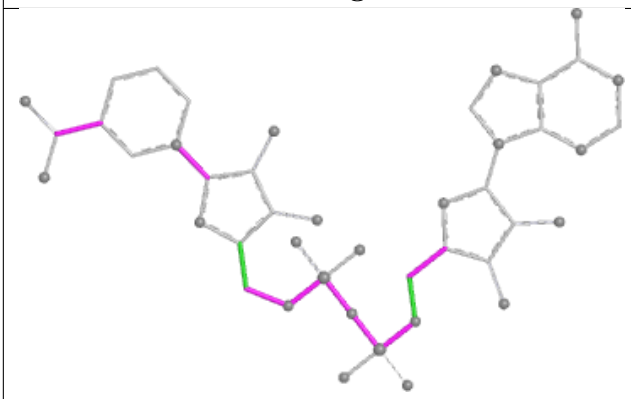
Ligand NAI B 604



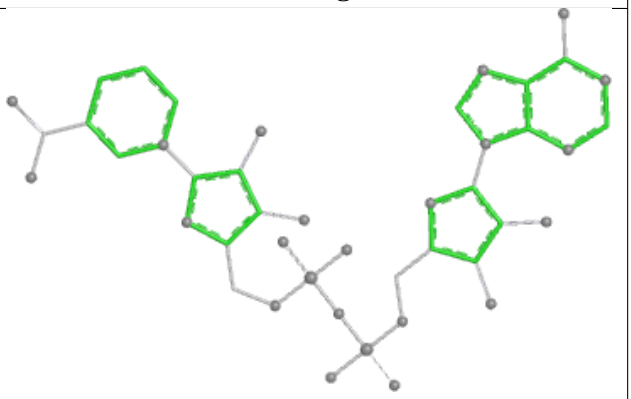
Bond lengths



Bond angles

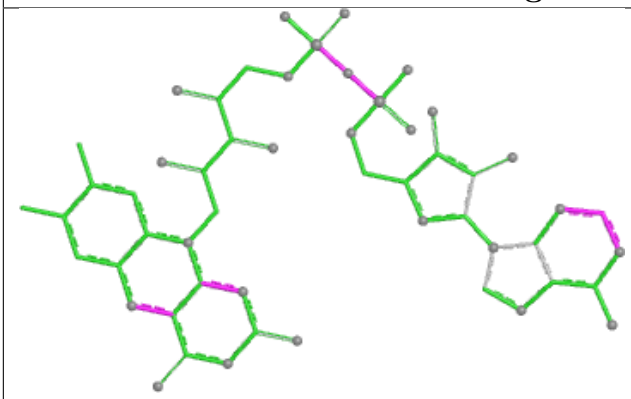


Torsions

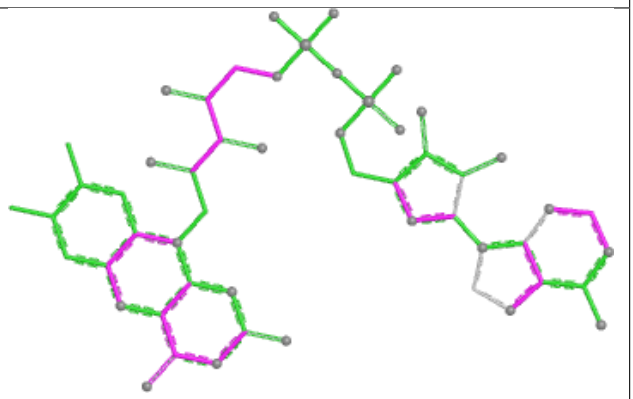


Rings

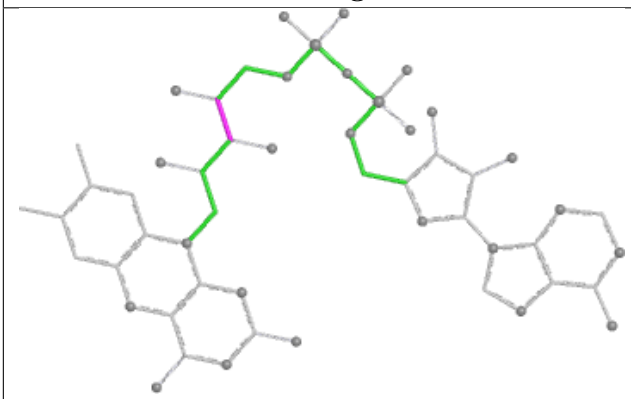
Ligand FAD B 605



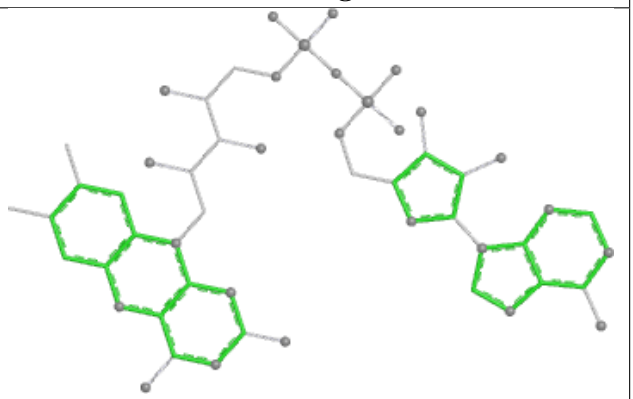
Bond lengths



Bond angles

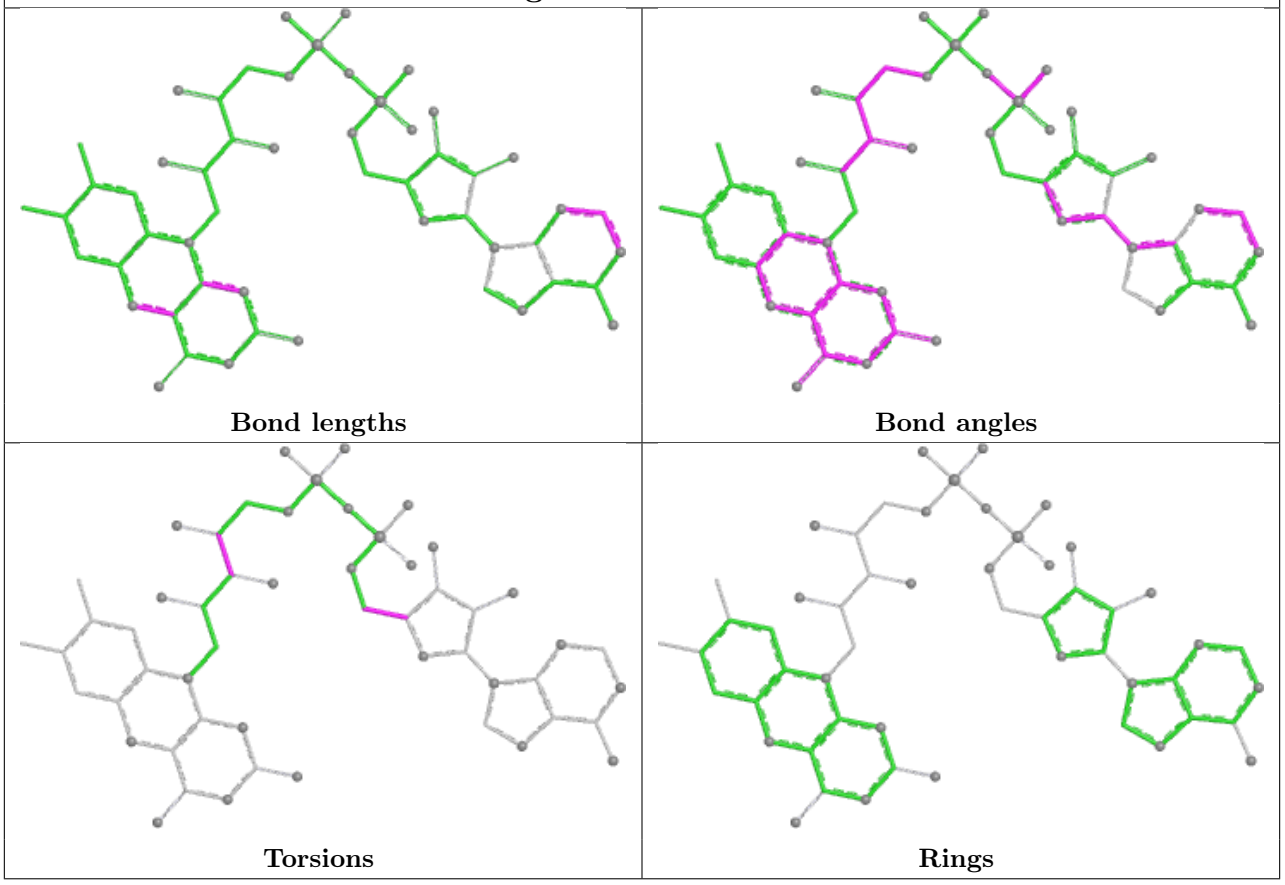


Torsions



Rings

Ligand FAD A 601



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^{th} 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	472/502 (94%)	0.02	36 (7%)	13	15	20, 34, 75, 103	0
1	B	472/502 (94%)	0.10	39 (8%)	11	12	20, 35, 76, 103	0
All	All	944/1004 (94%)	0.06	75 (7%)	12	14	20, 35, 76, 103	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	GLN	8.7
1	B	423	ARG	7.7
1	B	463	LYS	7.3
1	A	152	GLN	7.2
1	B	420	LEU	5.7
1	B	421	SER	5.2
1	A	324	LYS	5.2
1	B	422	SER	5.1
1	A	50	HIS	5.1
1	B	424	LYS	5.0
1	B	358	ASN	4.9
1	A	42	THR	4.7
1	B	42	THR	4.4
1	A	418	LYS	4.4
1	A	433	GLU	4.4
1	A	155	ASN	4.2
1	B	162	ALA	4.2
1	B	425	ASP	4.2
1	A	49	GLN	4.2
1	B	427	ILE	4.0
1	B	52	ASP	4.0
1	B	429	LEU	3.9
1	A	322	ASP	3.7
1	A	463	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	424	LYS	3.7
1	B	426	LYS	3.6
1	A	326	THR	3.6
1	A	52	ASP	3.5
1	A	423	ARG	3.5
1	A	321	GLU	3.4
1	B	155	ASN	3.4
1	A	417	GLN	3.3
1	A	429	LEU	3.3
1	B	362	ARG	3.2
1	B	153	PRO	3.2
1	A	421	SER	3.2
1	B	435	ASN	3.2
1	B	433	GLU	3.2
1	A	422	SER	3.1
1	A	320	HIS	3.0
1	A	319	LYS	2.9
1	A	426	LYS	2.9
1	A	464	ARG	2.9
1	A	378	ILE	2.8
1	A	153	PRO	2.8
1	B	418	LYS	2.8
1	B	415	ASN	2.8
1	A	323	GLY	2.8
1	A	466	PHE	2.8
1	A	428	ASP	2.8
1	B	428	ASP	2.7
1	A	172	LEU	2.7
1	B	417	GLN	2.7
1	B	464	ARG	2.6
1	A	420	LEU	2.5
1	B	386	PHE	2.5
1	A	57	LEU	2.4
1	B	172	LEU	2.4
1	A	415	ASN	2.3
1	B	413	ILE	2.3
1	B	388	GLY	2.3
1	B	43	MET	2.3
1	B	50	HIS	2.3
1	B	243	ALA	2.3
1	B	58	ILE	2.2
1	A	325	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	466	PHE	2.2
1	A	435	ASN	2.2
1	B	324	LYS	2.2
1	B	461	SER	2.2
1	A	361	LYS	2.1
1	A	173	ILE	2.1
1	B	355	PRO	2.1
1	B	233	VAL	2.0
1	B	173	ILE	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)

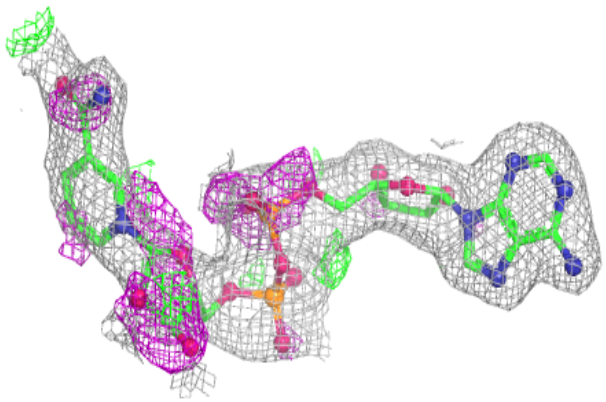
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

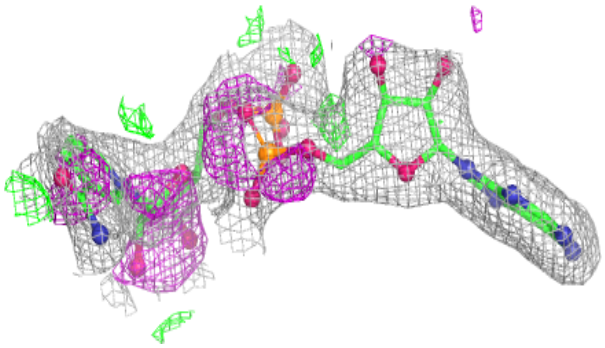
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	605	1/1	0.80	0.12	71,71,71,71	0
4	MG	B	601	1/1	0.81	0.34	81,81,81,81	0
3	NAI	A	602	44/44	0.92	0.14	34,44,60,66	0
3	NAI	B	604	44/44	0.92	0.14	26,42,63,65	0
4	MG	B	603	1/1	0.93	0.12	50,50,50,50	0
4	MG	A	604	1/1	0.96	0.09	46,46,46,46	0
4	MG	A	603	1/1	0.96	0.11	34,34,34,34	0
2	FAD	B	605	53/53	0.98	0.14	21,28,33,41	0
2	FAD	A	601	53/53	0.98	0.12	17,23,31,35	0
4	MG	B	602	1/1	0.99	0.15	20,20,20,20	0

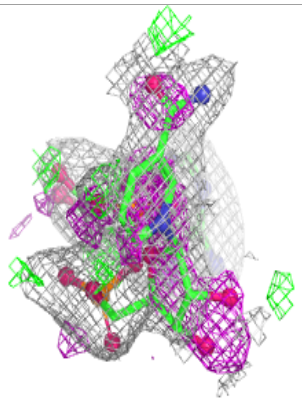
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI A 602:

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

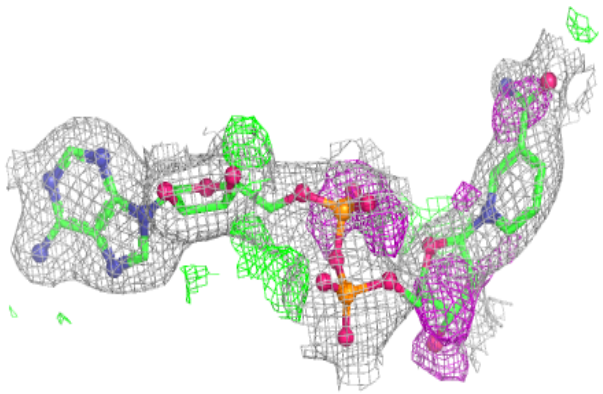


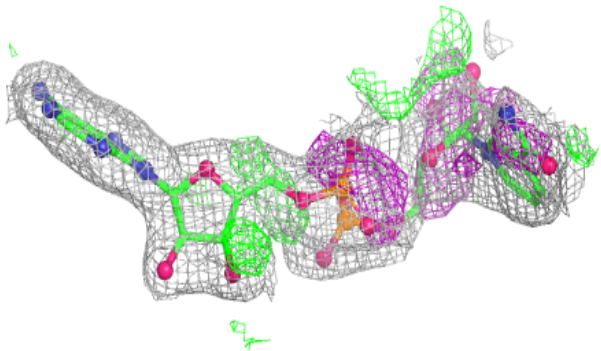


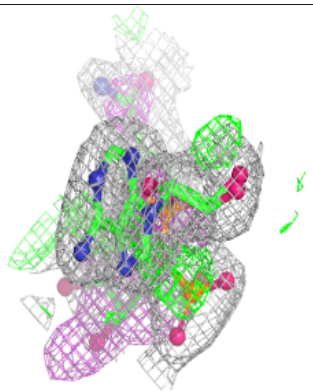


Electron density around NAI B 604:

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

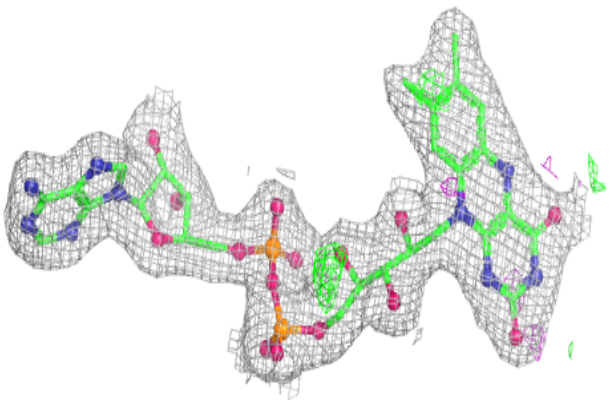


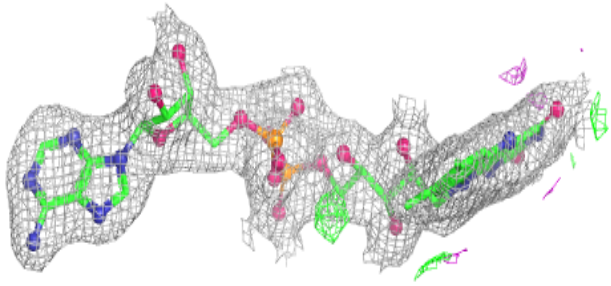


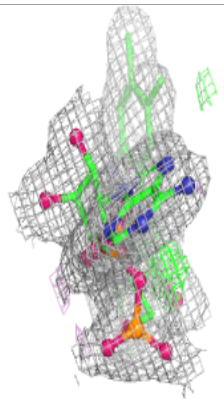


Electron density around FAD B 605:

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

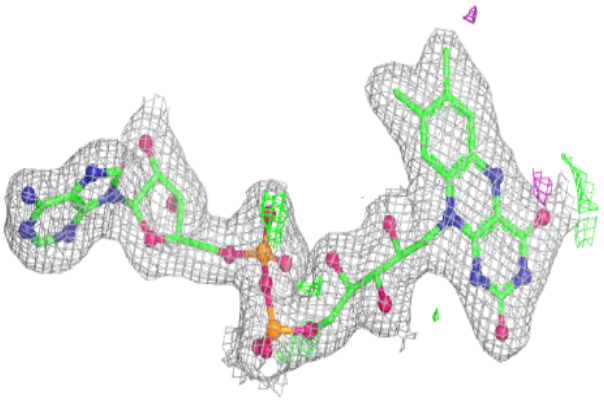


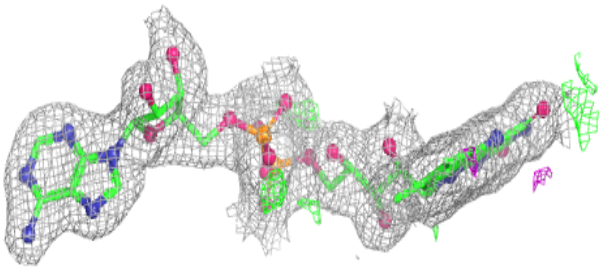


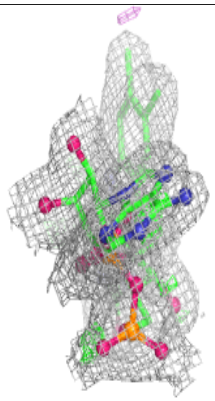


Electron density around FAD A 601:

$2mF_o$-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.