



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 18, 2019 – 07:31 PM EDT

PDB ID : 6A7X
Title : Rat Xanthine oxidoreductase, D428A variant, NAD bound form
Authors : Okamoto, K.; Kawaguchi, Y.
Deposited on : 2018-07-05
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

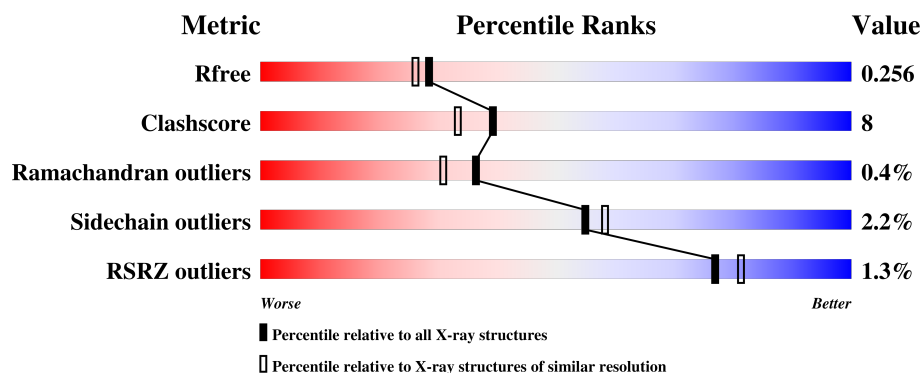
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	111664	1287 (2.16-2.16)
Clashscore	122126	1390 (2.16-2.16)
Ramachandran outliers	120053	1368 (2.16-2.16)
Sidechain outliers	120020	1367 (2.16-2.16)
RSRZ outliers	108989	1262 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1331	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	B	1331	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	URC	B	3004	-	X	-	-
5	FES	B	3001	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21778 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.

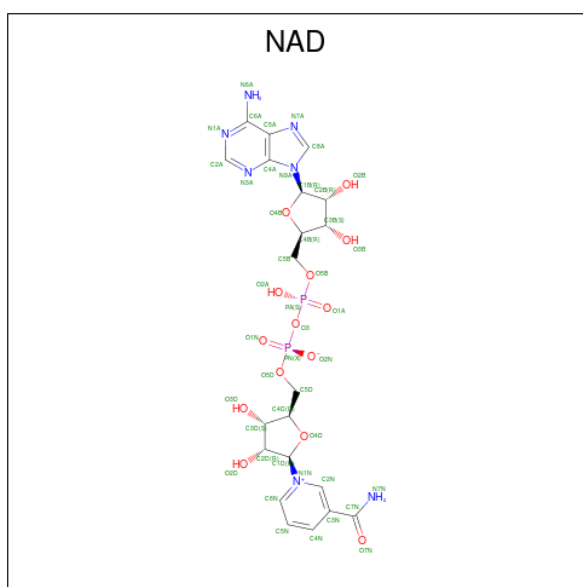
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1295	Total	C	N	O	S	0	0	0
			10013	6348	1724	1876	65			
1	B	1291	Total	C	N	O	S	0	0	0
			9968	6319	1716	1869	64			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	ALA	ASP	engineered mutation	UNP P22985
B	428	ALA	ASP	engineered mutation	UNP P22985

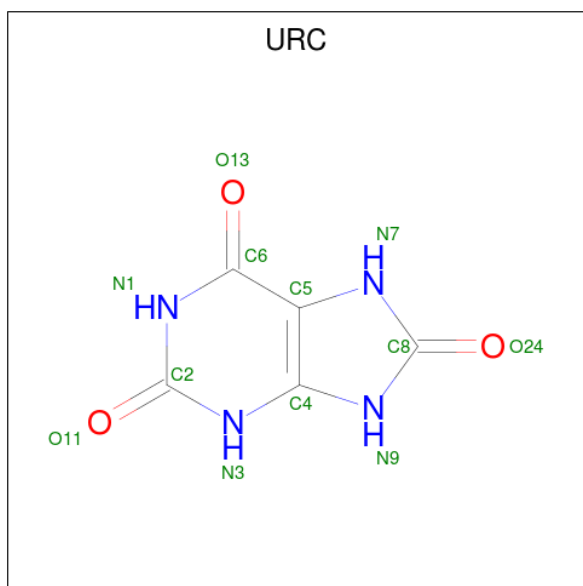
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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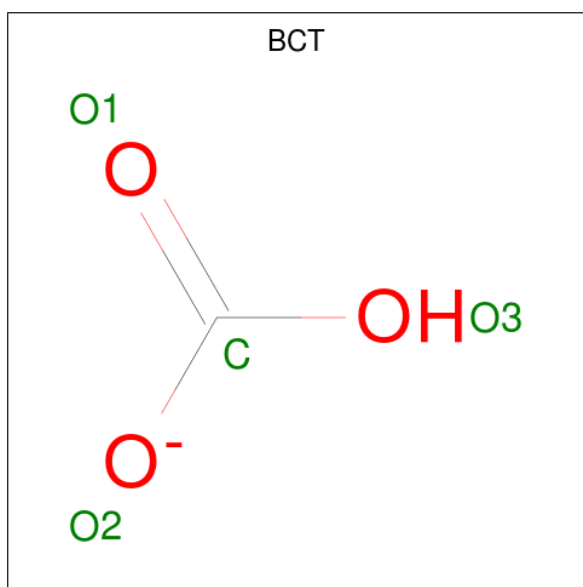
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	
			23	10	5	7	1	
							0	0

- Molecule 3 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



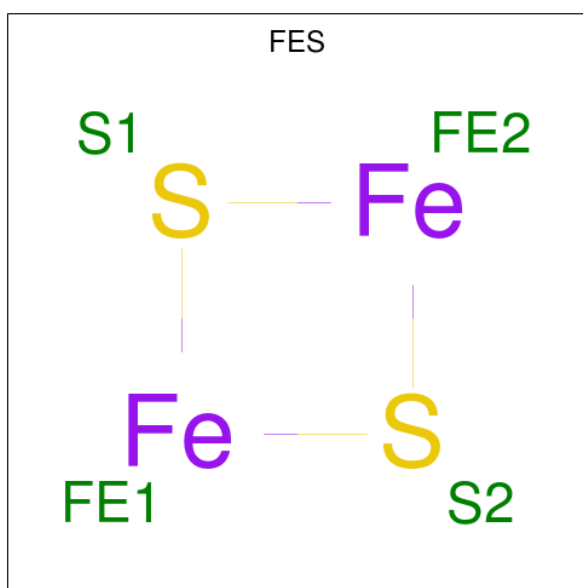
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			12	5	4	3	0	0
3	B	1	Total	C	N	O		
			12	5	4	3	0	0

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



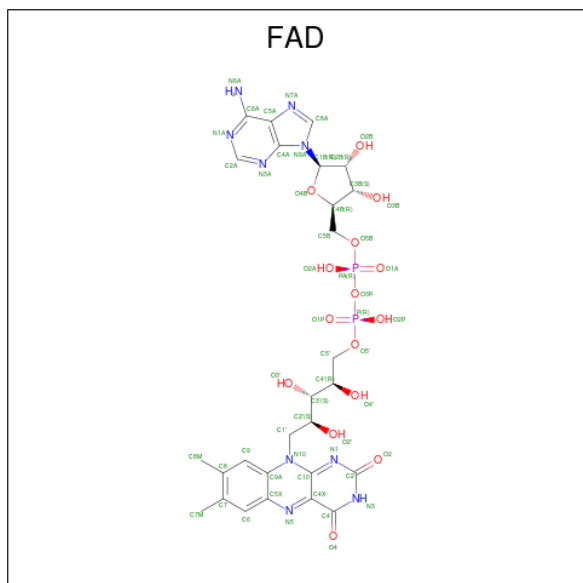
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		

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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

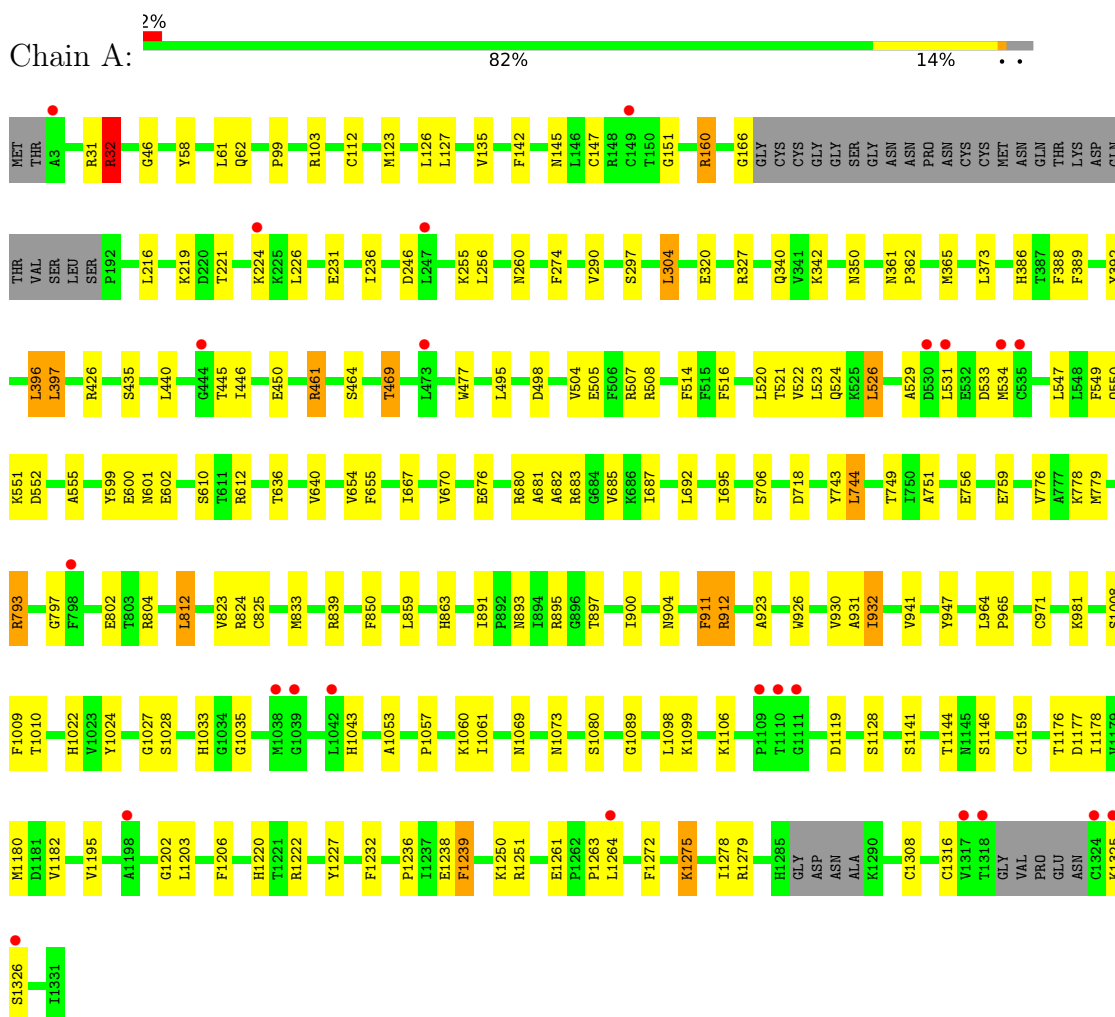
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	721	Total O 721 721	0	0
7	B	872	Total O 872 872	0	0

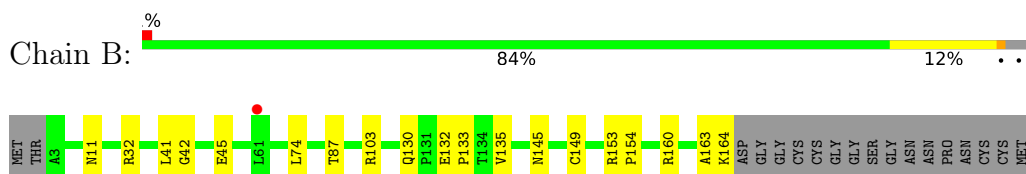
3 Residue-property plots

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

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase



TRP	GLN
SER	THR
VAL	VAL
ARG	SER
ILE	LEU
	SER
	P192
	S193
	L194
	F200
	I210
	F211
	L216
	R217
	L218
	K219
	K224
	E231
	R232
	M241
	Q250
	D253
	T261
	M267
	L273
	I296
	E314
	K317
	Q340
	N350
	I357
	A366
	R376
	R383
	H386
	K394
	R425
	D429
	I430
	R438
	R461
	L466
	K467
	T468
	T469
	P470
	K471
	Q472
	L473
	S474
	K475
	E480
	Q483
	S513
	F516
	L520
	K537
	L538
	D539
	L547
	K565
	M584
	R606
	N650
	D658
	V670
	E676
	A681
	T695
	T696
	T697
	N703
	G709
	I714
	A726
	E740
	H741
	F742
	L743
	L744
	E745
	T746
	T749
	I750
	A751
	E756
	K778
	N785
	R786
	V791
	K792
	R793
	G797
	T806
	S809
	T810
	A811
	L812
	V823
	R824
	M833
	L843
	H863
	G867
	E871
	S874
	R875
	L882
	M885
	D886
	N887
	R899
	I900
	C901
	N904
	A910
	F911
	R912
	P917
	M927
	C934
	G935
	L936
	R942
	H954
	F955
	C967
	S975
	R980
	F987
	K994
	K995
	R996
	S1008
	V1021
	H1022
	V1023
	Y1024
	H1033
	H1043
	P1057
	K1060
	I1061
	H1062
	T1066
	V1071
	P1072
	N1073
	A1081
	D1084
	G1089
	L1101
	E1102
	P1103
	F1104
	K1105
	K1106
	T1110
	G1111
	A1120
	V1125
	N1145
	R1175
	L1203
	M1208
	T1221
	Y1227
	P1236
	I1237
	E1238
	F1239
	N1249
	K1250
	I1253
	Y1254
	A1255
	E1261
	P1262
	K1275
	A1280
	Q1284
	H1285
	G1286
	D1287
	N1288
	A1289
	V1320
	PRO
	GLU
	ASN
	CYS
	LYS
	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.14Å 137.79Å 222.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.63 – 2.15 41.60 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.63-2.15) 99.4 (41.60-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.195 , 0.255 0.200 , 0.256	Depositor DCC
R_{free} test set	8171 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	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	0.95	EDS
Total number of atoms	21778	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: BCT, FAD, FES, NAD, URC

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	0.49	0/10223	0.65	2/13829 (0.0%)
1	B	0.50	0/10178	0.66	0/13773
All	All	0.49	0/20401	0.66	2/27602 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	6
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	793	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	507	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	804	ARG	Sidechain

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	10013	0	10029	173	0
1	B	9968	0	9983	155	0
2	A	27	0	12	0	0
2	B	23	0	12	0	0
3	A	12	0	4	1	0
3	B	12	0	4	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	8	0	0	1	0
5	B	8	0	0	3	0
6	A	53	0	31	2	0
6	B	53	0	31	0	0
7	A	721	0	0	86	0
7	B	872	0	0	89	0
All	All	21778	0	20106	323	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 8.

The worst 5 of 323 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:1089:GLY:HA3	7:B:3663:HOH:O	1.29	1.32
1:A:1089:GLY:HA3	7:A:1831:HOH:O	1.26	1.28
1:B:812:LEU:HB2	7:B:3348:HOH:O	1.42	1.18
1:B:366:ALA:HB1	7:B:3120:HOH:O	1.49	1.12
1:A:123:MET:SD	7:A:2164:HOH:O	2.10	1.09

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	1287/1331 (97%)	1239 (96%)	43 (3%)	5 (0%)	36	31
1	B	1287/1331 (97%)	1244 (97%)	38 (3%)	5 (0%)	36	31
All	All	2574/2662 (97%)	2483 (96%)	81 (3%)	10 (0%)	36	31

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	797	GLY
1	B	912	ARG

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	1094/1123 (97%)	1061 (97%)	33 (3%)	44	43
1	B	1088/1123 (97%)	1072 (98%)	16 (2%)	67	72
All	All	2182/2246 (97%)	2133 (98%)	49 (2%)	55	58

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	812	LEU

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Mol	Chain	Res	Type
1	A	1106	LYS
1	B	899	ARG
1	A	932	ILE
1	A	1119	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1284	GLN
1	B	111	GLN
1	B	1062	HIS
1	B	11	ASN
1	B	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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
2	NAD	A	1401	-	24,29,48	1.49	5 (20%)	25,45,73	1.52	3 (12%)
3	URC	A	1402	-	13,13,13	3.98	4 (30%)	13,19,19	4.70	9 (69%)
4	BCT	A	1403	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FES	A	1404	1,7	0,4,4	0.00	-	-	-	-
5	FES	A	1405	1	0,4,4	0.00	-	-	-	-
6	FAD	A	1406	-	50,58,58	1.84	6 (12%)	58,89,89	2.03	11 (18%)
5	FES	B	3001	1	0,4,4	0.00	-	-	-	-
5	FES	B	3002	1,7	0,4,4	0.00	-	-	-	-
2	NAD	B	3003	-	21,25,48	1.28	2 (9%)	23,38,73	1.35	4 (17%)
3	URC	B	3004	-	13,13,13	4.26	5 (38%)	13,19,19	5.33	9 (69%)
4	BCT	B	3005	-	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	B	3006	-	50,58,58	1.82	7 (14%)	58,89,89	2.40	14 (24%)

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
2	NAD	A	1401	-	-	6/12/32/62	0/3/3/5
3	URC	A	1402	-	-	-	0/2/2/2
5	FES	A	1404	1,7	-	-	0/1/1/1
5	FES	A	1405	1	-	-	0/1/1/1
6	FAD	A	1406	-	-	3/30/50/50	0/6/6/6
5	FES	B	3001	1	-	-	0/1/1/1
5	FES	B	3002	1,7	-	-	0/1/1/1
2	NAD	B	3003	-	-	0/6/26/62	0/3/3/5
3	URC	B	3004	-	-	-	0/2/2/2
6	FAD	B	3006	-	-	6/30/50/50	0/6/6/6

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3004	URC	C4-N3	-11.32	1.33	1.46
3	A	1402	URC	C4-N3	-10.19	1.34	1.46
6	A	1406	FAD	C4X-C10	9.39	1.48	1.38
6	B	3006	FAD	C4X-C10	8.47	1.47	1.38
3	A	1402	URC	C4-N9	-7.61	1.35	1.44

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3004	URC	C4-N9-C8	-10.83	105.53	112.89
6	B	3006	FAD	C4-N3-C2	9.22	122.93	115.14
3	B	3004	URC	C5-C4-N9	9.04	106.83	102.64
3	A	1402	URC	C4-N9-C8	-8.99	106.78	112.89
6	A	1406	FAD	C4-N3-C2	8.98	122.72	115.14

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	NAD	C5B-O5B-PA-O1A
6	A	1406	FAD	N10-C1'-C2'-O2'
6	A	1406	FAD	N10-C1'-C2'-C3'
6	B	3006	FAD	N10-C1'-C2'-O2'
6	B	3006	FAD	N10-C1'-C2'-C3'

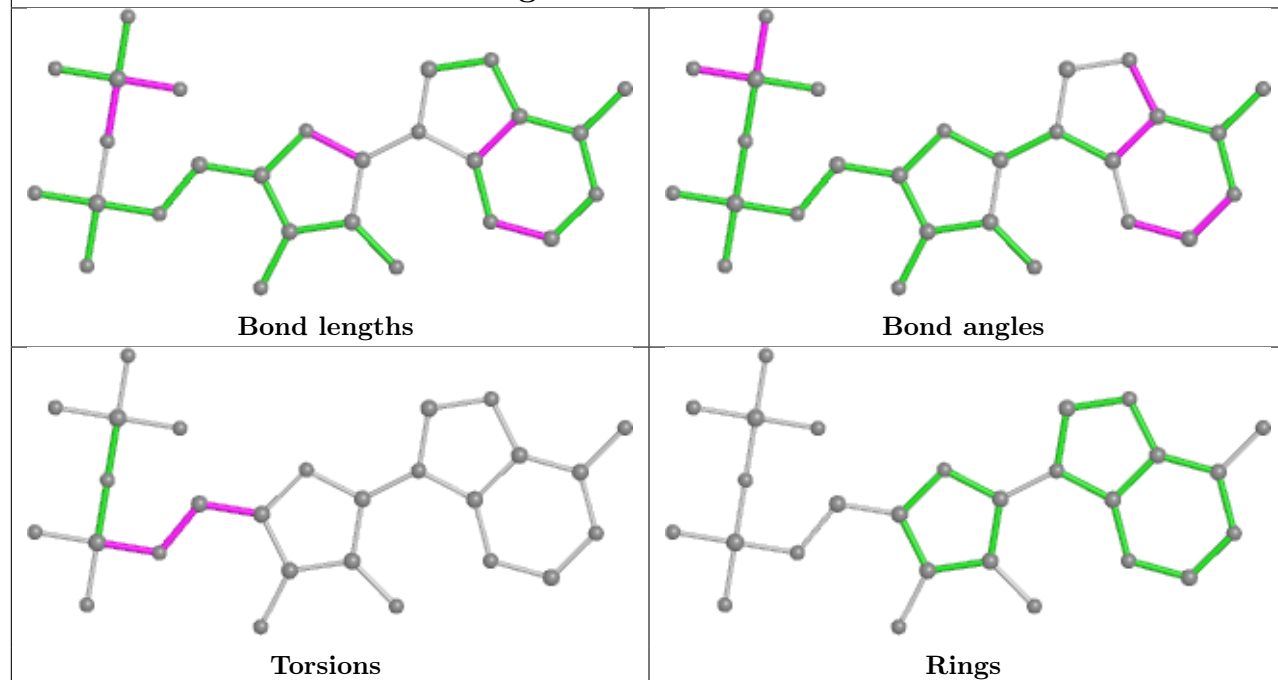
There are no ring outliers.

5 monomers are involved in 7 short contacts:

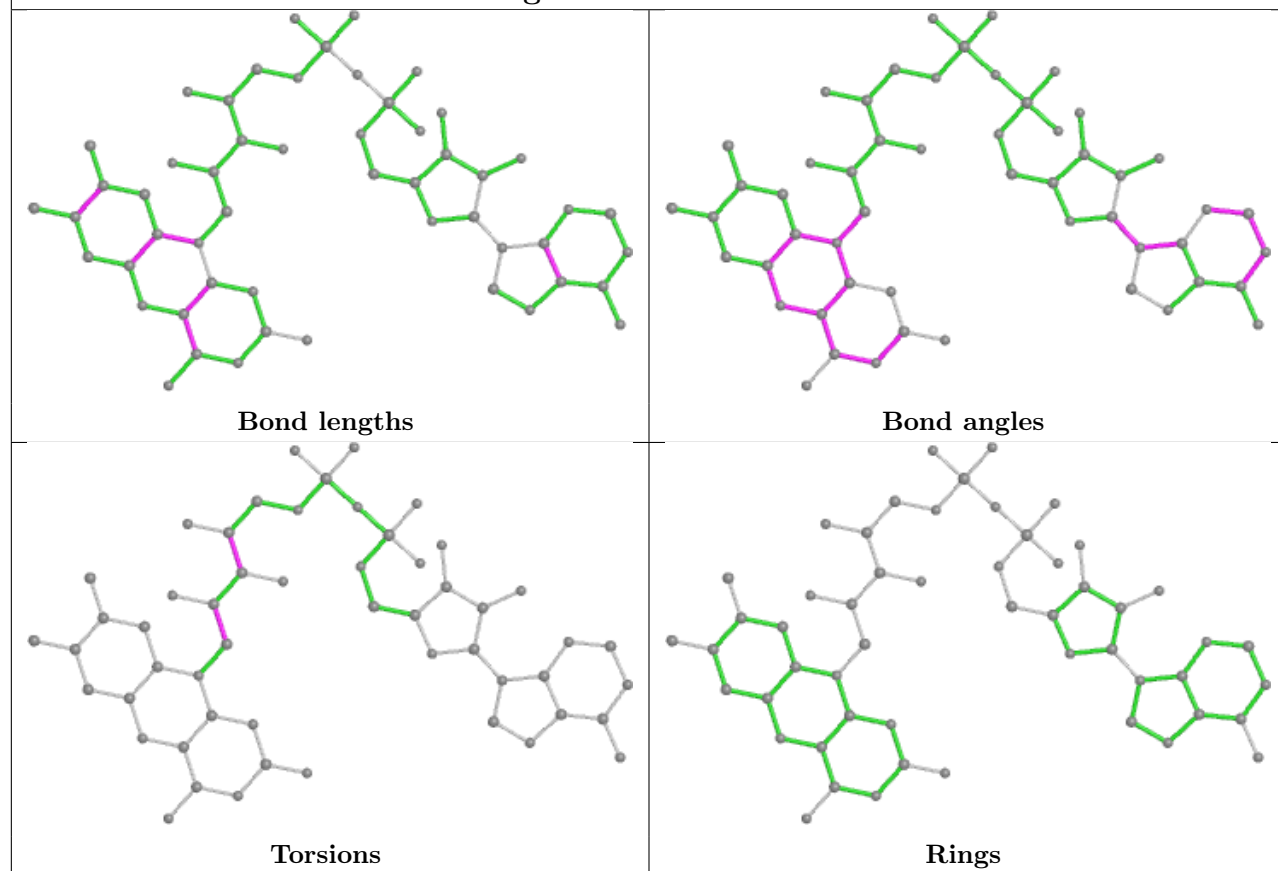
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	URC	1	0
5	A	1404	FES	1	0
6	A	1406	FAD	2	0
5	B	3001	FES	2	0
5	B	3002	FES	1	0

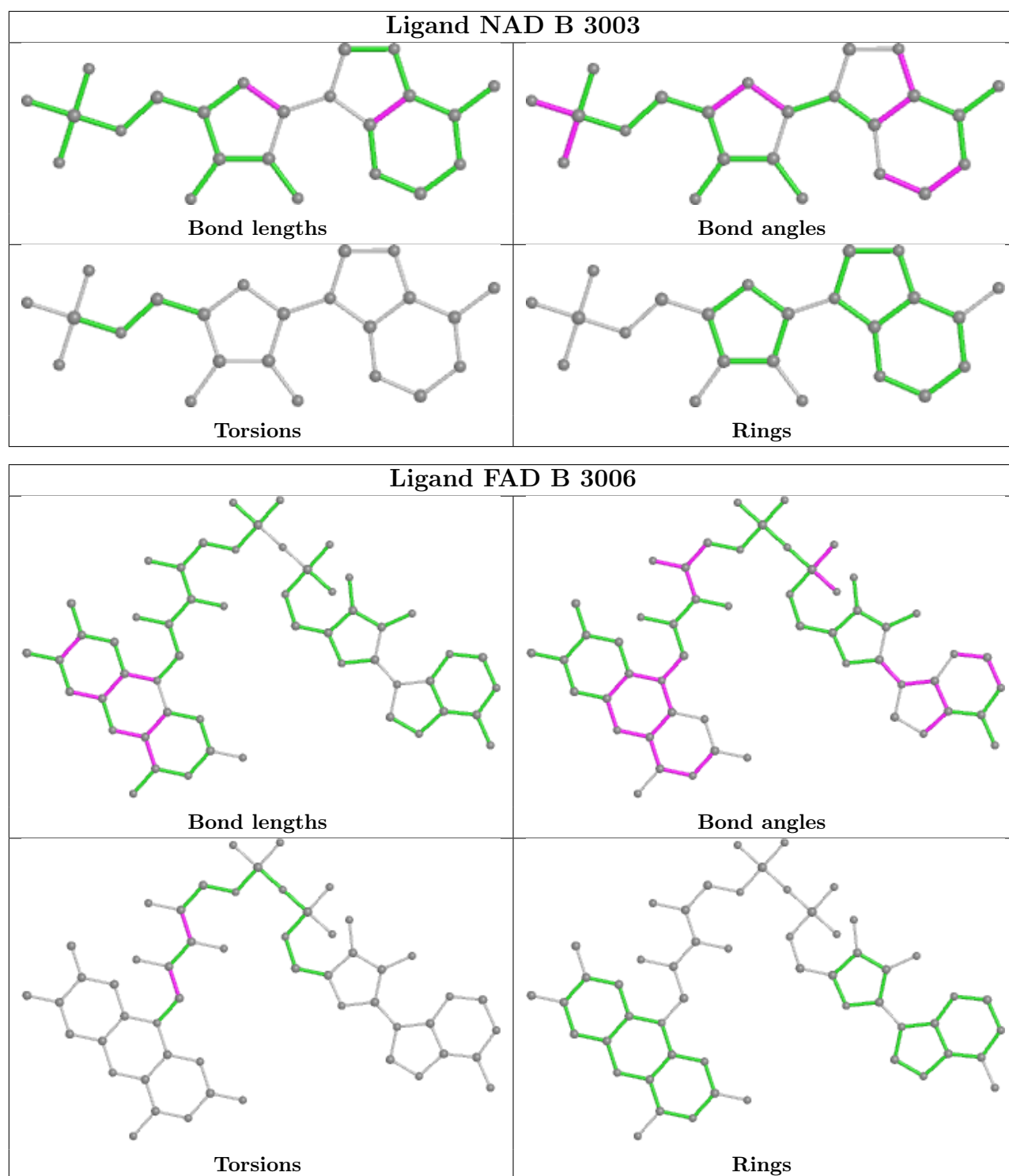
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NAD A 1401



Ligand FAD A 1406





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1295/1331 (97%)	-0.08	24 (1%) 66 73	26, 41, 69, 123	0
1	B	1291/1331 (96%)	-0.31	10 (0%) 86 89	24, 35, 59, 102	0
All	All	2586/2662 (97%)	-0.20	34 (1%) 77 81	24, 38, 66, 123	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1324	CYS	8.3
1	B	1111	GLY	4.5
1	A	3	ALA	4.5
1	B	1287	ASP	4.3
1	A	1326	SER	3.6

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](#)

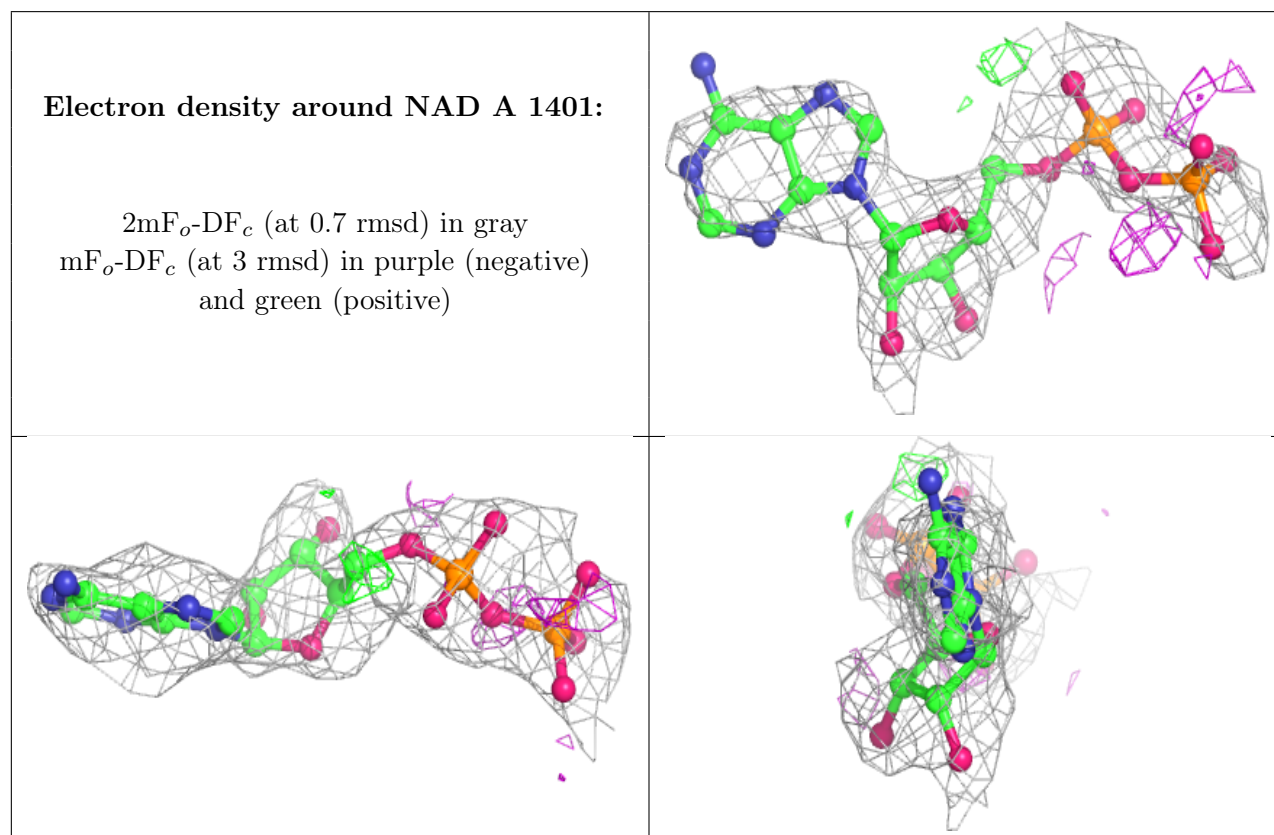
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

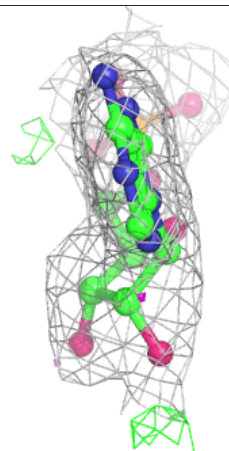
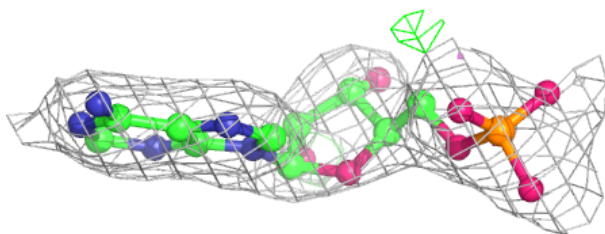
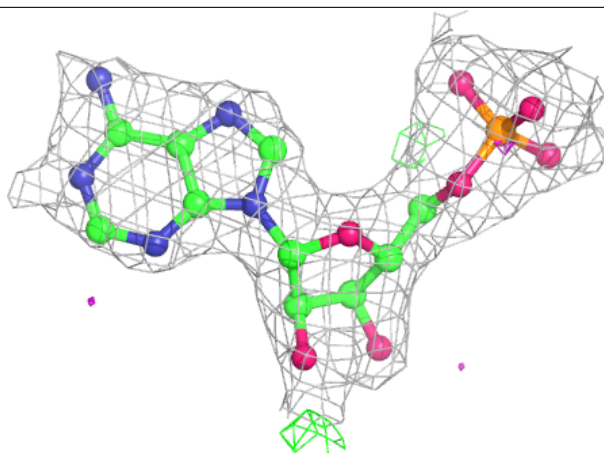
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	A	1401	27/44	0.77	0.19	72,96,117,123	0
2	NAD	B	3003	23/44	0.87	0.15	55,60,76,89	0
3	URC	A	1402	12/12	0.91	0.13	40,45,46,47	0
6	FAD	A	1406	53/53	0.96	0.12	34,40,44,46	0
3	URC	B	3004	12/12	0.96	0.12	35,36,40,41	0
6	FAD	B	3006	53/53	0.97	0.12	26,30,33,34	0
4	BCT	A	1403	4/4	0.98	0.14	37,41,45,45	0
5	FES	B	3001	4/4	0.98	0.06	41,45,45,52	0
4	BCT	B	3005	4/4	0.98	0.10	32,34,36,38	0
5	FES	A	1405	4/4	0.98	0.08	38,43,44,50	0
5	FES	A	1404	4/4	0.99	0.07	29,31,33,33	0
5	FES	B	3002	4/4	0.99	0.08	28,28,29,30	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.

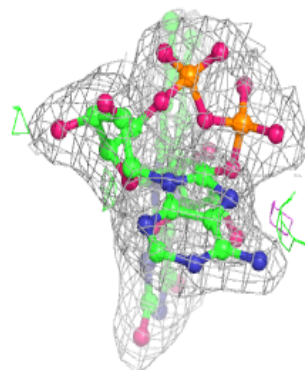
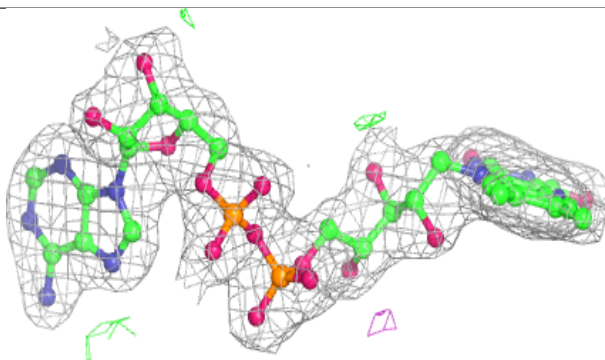
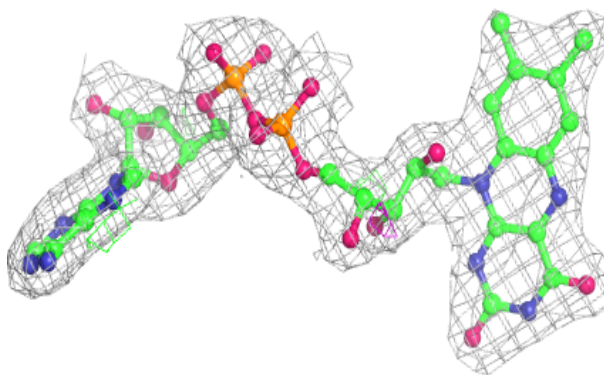


Electron density around NAD B 3003:

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

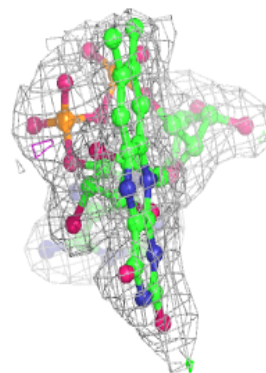
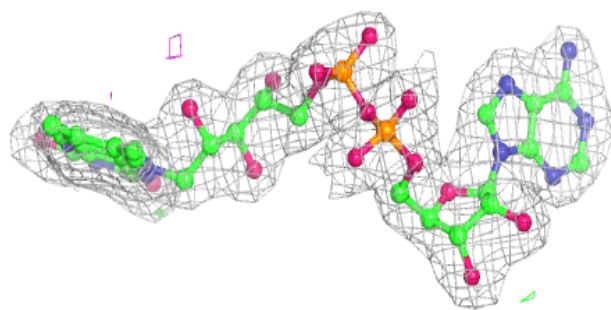
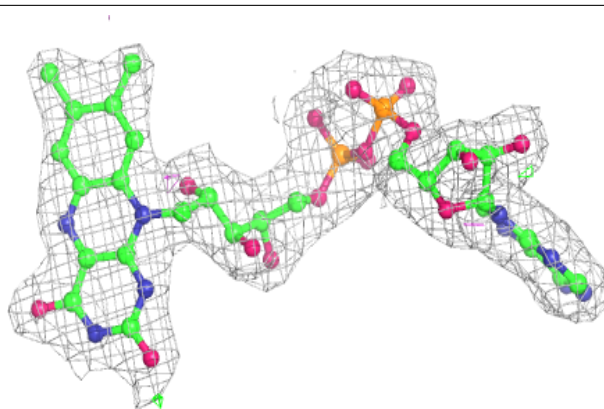
**Electron density around FAD A 1406:**

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



Electron density around FAD B 3006:

$2mF_o - DF_c$ (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.