wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 02:47 PM BST

PDB ID	:	5K4Q
Title	:	Three-dimensional structure of L-threonine 3-dehydrogenase from Trypanosoma brucei bound to NAD+ refined to 2.3 angstroms
Authors	:	Adjogatse, E.K.; Cooper, J.B.; Erskine, P.T.
Deposited on	:	2016-05-21
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

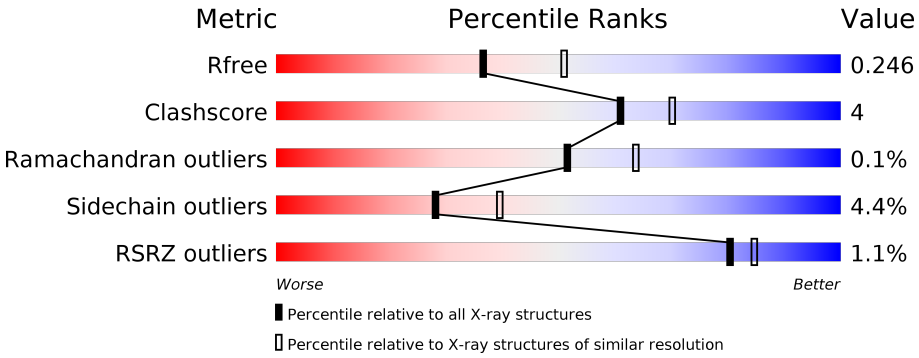
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	320	91% 8%
1	B	320	90% 9%
1	C	320	89% 10%
1	D	320	85% 14%
1	E	320	86% 12%
1	F	320	85% 14%

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	GOL	A	1402	-	-	X	-
3	GOL	C	3402	-	X	X	-
3	GOL	E	5402	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16257 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.

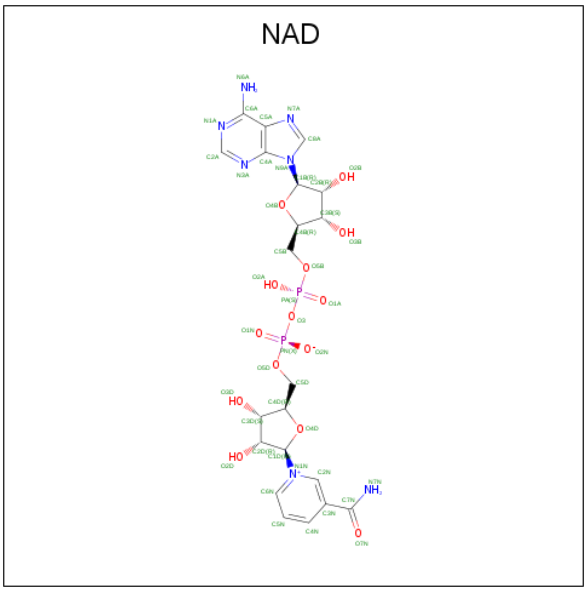
- Molecule 1 is a protein called L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2501	1595	416	471	19			
1	B	319	Total	C	N	O	S	0	1	0
			2502	1595	417	472	18			
1	C	319	Total	C	N	O	S	0	0	0
			2493	1590	415	470	18			
1	D	320	Total	C	N	O	S	0	0	0
			2501	1595	416	471	19			
1	E	319	Total	C	N	O	S	0	1	0
			2502	1596	417	471	18			
1	F	319	Total	C	N	O	S	0	2	0
			2505	1600	417	470	18			

There are 6 discrepancies between the modelled and reference sequences:

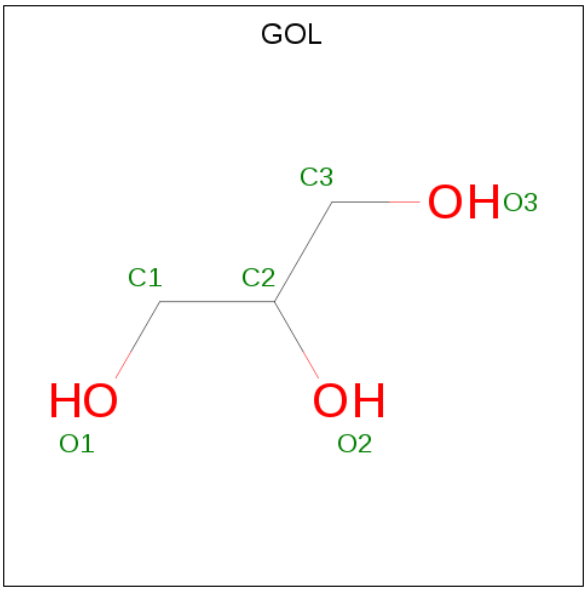
Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	MET	-	initiating methionine	UNP Q7YW97
B	2002	MET	-	initiating methionine	UNP Q7YW97
C	3002	MET	-	initiating methionine	UNP Q7YW97
D	4002	MET	-	initiating methionine	UNP Q7YW97
E	5002	MET	-	initiating methionine	UNP Q7YW97
F	6002	MET	-	initiating methionine	UNP Q7YW97

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



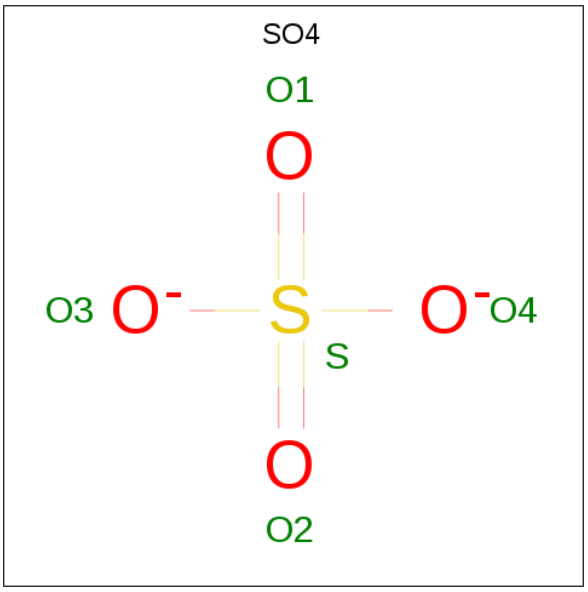
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

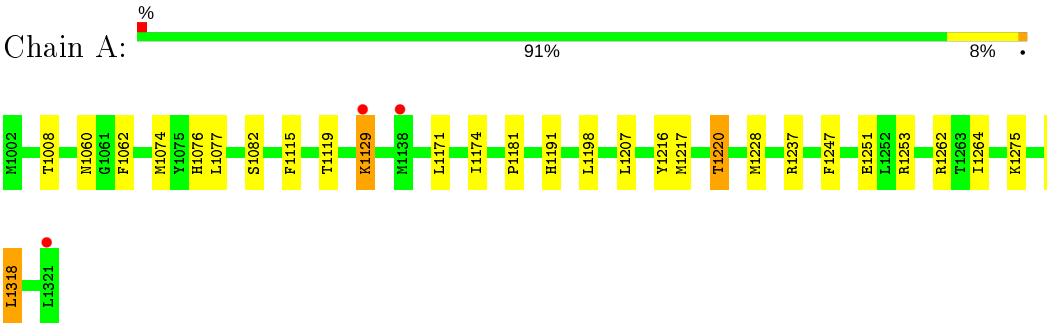
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	161	Total O 161 161	0	0
5	B	168	Total O 168 168	0	0
5	C	174	Total O 174 174	0	0
5	D	143	Total O 143 143	0	0
5	E	131	Total O 131 131	0	0
5	F	151	Total O 151 151	0	0

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.

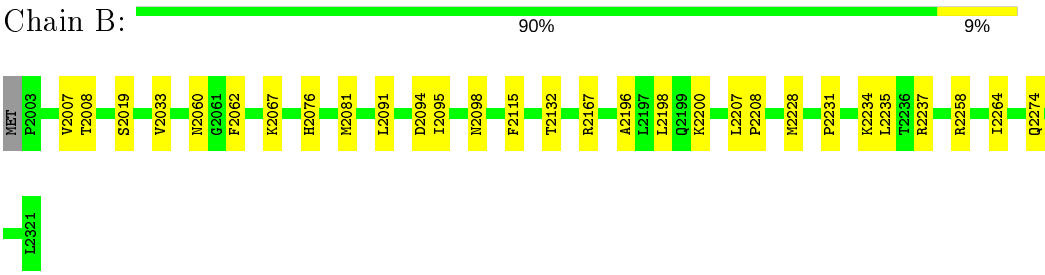
- Molecule 1: L-threonine 3-dehydrogenase

Chain A:



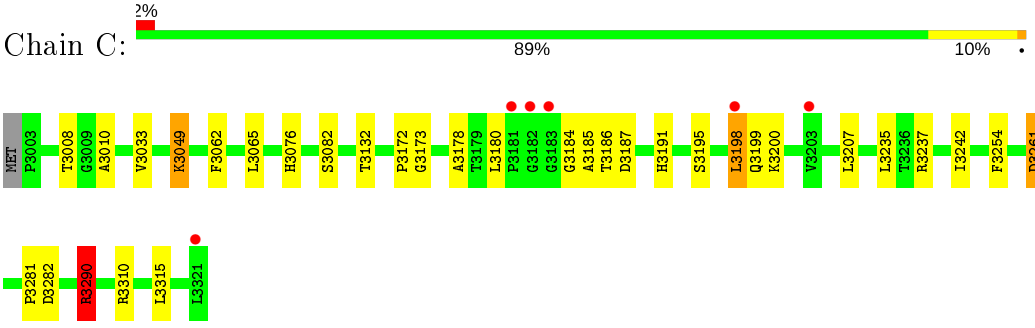
- Molecule 1: L-threonine 3-dehydrogenase

Chain B:



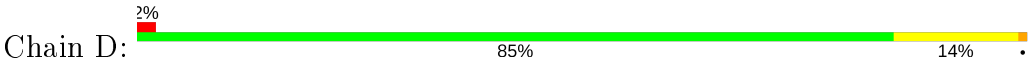
- Molecule 1: L-threonine 3-dehydrogenase

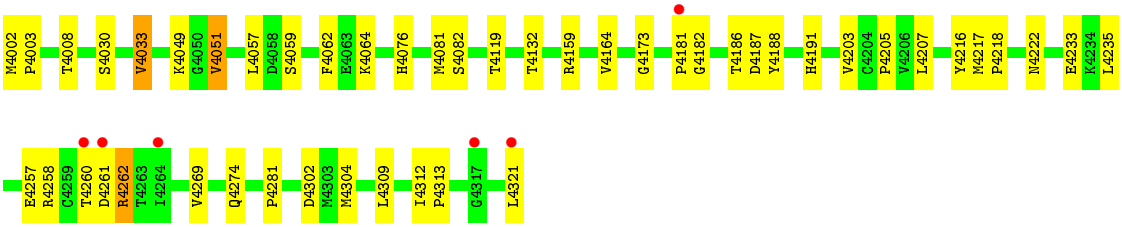
Chain C:



- Molecule 1: L-threonine 3-dehydrogenase

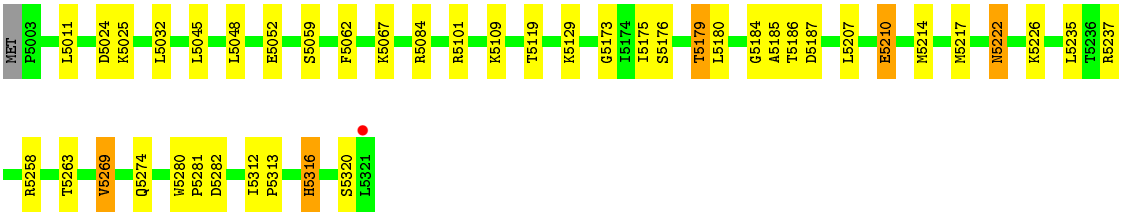
Chain D:





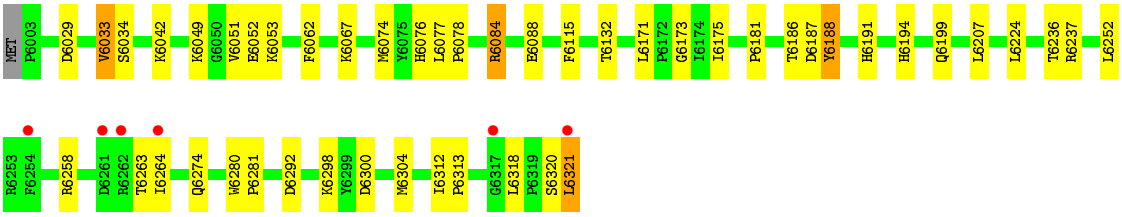
- Molecule 1: L-threonine 3-dehydrogenase

Chain E:



- Molecule 1: L-threonine 3-dehydrogenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.63Å 277.72Å 56.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.30 48.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.14-2.30) 99.2 (48.14-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.174 , 0.244 0.180 , 0.246	Depositor DCC
R_{free} test set	4653 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16257	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0728e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, SO4, NAD

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	0.74	0/2557	0.90	7/3469 (0.2%)
1	B	0.75	0/2558	0.82	0/3470
1	C	0.69	0/2549	0.87	4/3458 (0.1%)
1	D	0.72	0/2557	0.83	0/3469
1	E	0.68	1/2558 (0.0%)	0.83	4/3469 (0.1%)
1	F	0.74	0/2567	0.85	4/3480 (0.1%)
All	All	0.72	1/15346 (0.0%)	0.85	19/20815 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	5210	GLU	CD-OE2	6.62	1.32	1.25

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1237	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	C	3290	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	1237	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	E	5282	ASP	CB-CG-OD1	6.66	124.30	118.30
1	F	6084	ARG	NE-CZ-NH1	6.26	123.43	120.30

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	2501	0	2512	17	0
1	B	2502	0	2511	18	0
1	C	2493	0	2504	20	0
1	D	2501	0	2512	26	0
1	E	2502	0	2516	28	0
1	F	2505	0	2530	26	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
3	A	6	0	8	4	0
3	B	6	0	8	1	0
3	C	6	0	8	7	0
3	D	6	0	8	2	0
3	E	6	0	8	4	0
3	F	6	0	8	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	F	5	0	0	0	0
5	A	161	0	0	2	0
5	B	168	0	0	2	0
5	C	174	0	0	1	0
5	D	143	0	0	3	0
5	E	131	0	0	7	0
5	F	151	0	0	4	0
All	All	16257	0	15289	137	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 4.

The worst 5 of 137 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:E:5210:GLU:HG3	5:E:5502:HOH:O	1.52	1.08
1:E:5175:ILE:HD11	1:E:5214:MET:CE	2.01	0.89
1:E:5175:ILE:HD11	1:E:5214:MET:HE3	1.55	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4181:PRO:HB2	1:D:4191:HIS:CE1	2.11	0.84
1:E:5179:THR:OG1	5:E:5501:HOH:O	1.93	0.84

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	318/320 (99%)	312 (98%)	6 (2%)	0	100	100
1	B	318/320 (99%)	311 (98%)	7 (2%)	0	100	100
1	C	317/320 (99%)	308 (97%)	8 (2%)	1 (0%)	41	50
1	D	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
1	E	318/320 (99%)	304 (96%)	13 (4%)	1 (0%)	41	50
1	F	319/320 (100%)	313 (98%)	6 (2%)	0	100	100
All	All	1908/1920 (99%)	1857 (97%)	49 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3261	ASP
1	E	5320	SER

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	277/277 (100%)	268 (97%)	9 (3%)	39	54
1	B	277/277 (100%)	270 (98%)	7 (2%)	47	65
1	C	276/277 (100%)	263 (95%)	13 (5%)	26	37
1	D	277/277 (100%)	263 (95%)	14 (5%)	24	33
1	E	277/277 (100%)	261 (94%)	16 (6%)	20	27
1	F	278/277 (100%)	264 (95%)	14 (5%)	24	34
All	All	1662/1662 (100%)	1589 (96%)	73 (4%)	28	39

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4057	LEU
1	D	4235	LEU
1	F	6199	GLN
1	D	4119	THR
1	D	4262	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3199	GLN
1	C	3274	GLN
1	E	5278	ASN
1	B	2274	GLN
1	D	4274	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	F	6401	-	42,48,48	1.98	4 (9%)	50,73,73	1.52	8 (16%)
2	NAD	A	1401	-	42,48,48	2.03	7 (16%)	50,73,73	1.42	6 (12%)
3	GOL	A	1402	-	5,5,5	0.72	0	5,5,5	0.84	0
4	SO4	F	6403	-	4,4,4	0.38	0	6,6,6	0.19	0
3	GOL	E	5402	-	5,5,5	0.18	0	5,5,5	1.23	0
2	NAD	E	5401	-	42,48,48	1.83	7 (16%)	50,73,73	1.52	7 (14%)
2	NAD	D	4401	-	42,48,48	1.89	6 (14%)	50,73,73	1.70	11 (22%)
4	SO4	D	4404	-	4,4,4	0.41	0	6,6,6	0.22	0
2	NAD	B	2401	-	42,48,48	1.85	7 (16%)	50,73,73	1.46	6 (12%)
4	SO4	C	3403	-	4,4,4	0.36	0	6,6,6	0.13	0
3	GOL	C	3402	-	5,5,5	0.91	0	5,5,5	2.05	2 (40%)
4	SO4	D	4403	-	4,4,4	0.38	0	6,6,6	0.29	0
3	GOL	F	6402	-	5,5,5	0.30	0	5,5,5	1.00	0
3	GOL	B	2402	-	5,5,5	0.89	0	5,5,5	1.96	3 (60%)
4	SO4	B	2403	-	4,4,4	0.46	0	6,6,6	0.23	0
2	NAD	C	3401	-	42,48,48	1.53	4 (9%)	50,73,73	1.39	4 (8%)
3	GOL	D	4402	-	5,5,5	0.78	0	5,5,5	1.45	1 (20%)

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	F	6401	-	-	4/26/62/62	0/5/5/5
2	NAD	A	1401	-	-	1/26/62/62	0/5/5/5
3	GOL	A	1402	-	-	4/4/4/4	-
3	GOL	E	5402	-	-	2/4/4/4	-
2	NAD	E	5401	-	-	3/26/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	4401	-	-	1/26/62/62	0/5/5/5
2	NAD	B	2401	-	-	3/26/62/62	0/5/5/5
2	NAD	C	3401	-	-	4/26/62/62	0/5/5/5
3	GOL	C	3402	-	-	4/4/4/4	-
3	GOL	F	6402	-	-	4/4/4/4	-
3	GOL	B	2402	-	-	2/4/4/4	-
3	GOL	D	4402	-	-	0/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6401	NAD	C2N-N1N	7.48	1.44	1.35
2	A	1401	NAD	C2N-N1N	7.35	1.43	1.35
2	B	2401	NAD	O7N-C7N	6.78	1.37	1.24
2	F	6401	NAD	O7N-C7N	6.77	1.37	1.24
2	D	4401	NAD	C2N-N1N	6.45	1.42	1.35

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4401	NAD	C6N-N1N-C2N	-7.22	115.39	121.97
2	E	5401	NAD	N3A-C2A-N1A	-5.83	119.56	128.68
2	A	1401	NAD	N3A-C2A-N1A	-5.11	120.69	128.68
2	F	6401	NAD	N3A-C2A-N1A	-4.78	121.21	128.68
2	C	3401	NAD	C6N-N1N-C2N	-4.68	117.70	121.97

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

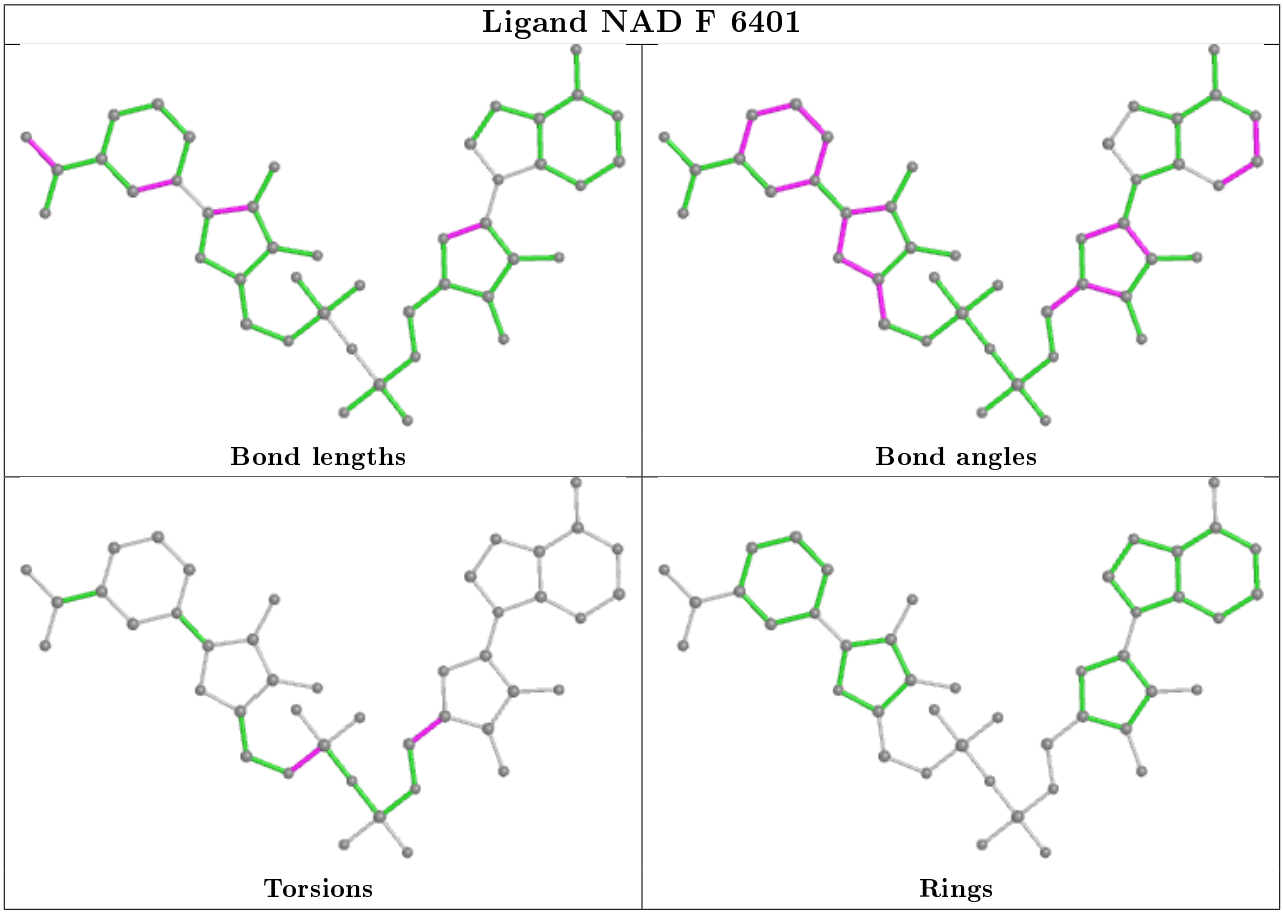
Mol	Chain	Res	Type	Atoms
3	E	5402	GOL	O1-C1-C2-C3
2	F	6401	NAD	C5D-O5D-PN-O1N
2	E	5401	NAD	C5D-O5D-PN-O1N
3	C	3402	GOL	O1-C1-C2-O2
3	C	3402	GOL	C1-C2-C3-O3

There are no ring outliers.

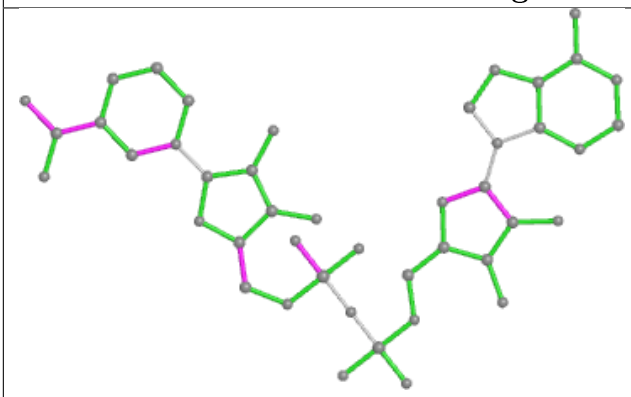
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	6401	NAD	1	0
2	A	1401	NAD	2	0
3	A	1402	GOL	4	0
3	E	5402	GOL	4	0
2	D	4401	NAD	1	0
3	C	3402	GOL	7	0
3	B	2402	GOL	1	0
3	D	4402	GOL	2	0

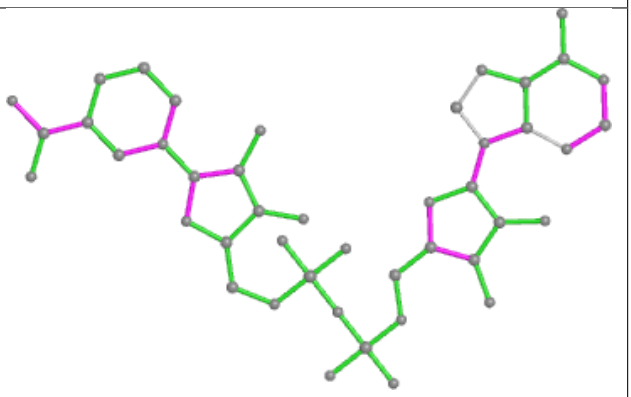
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



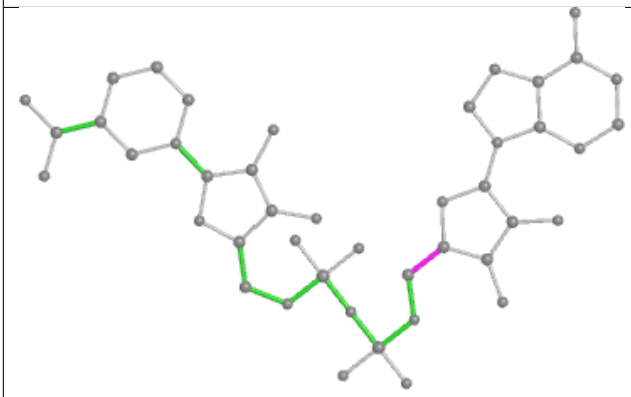
Ligand NAD A 1401



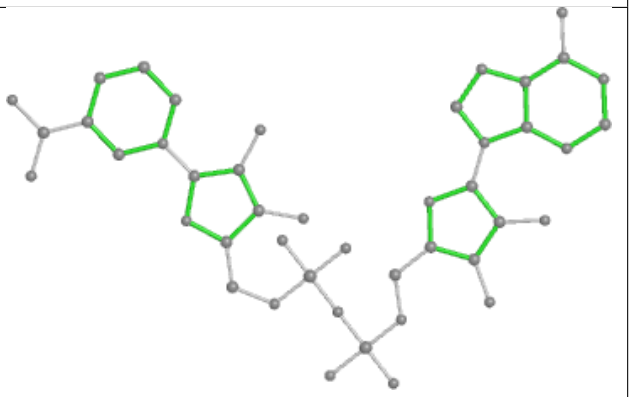
Bond lengths



Bond angles

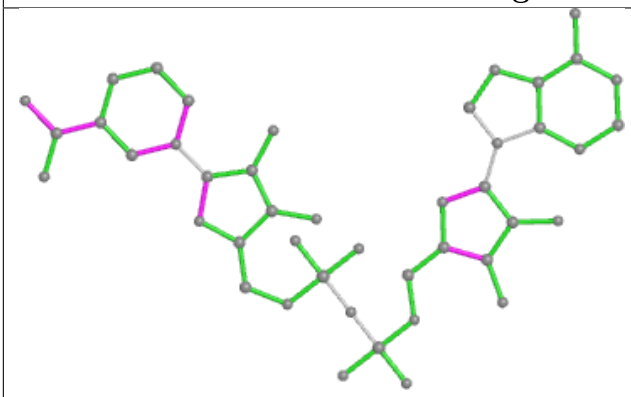


Torsions

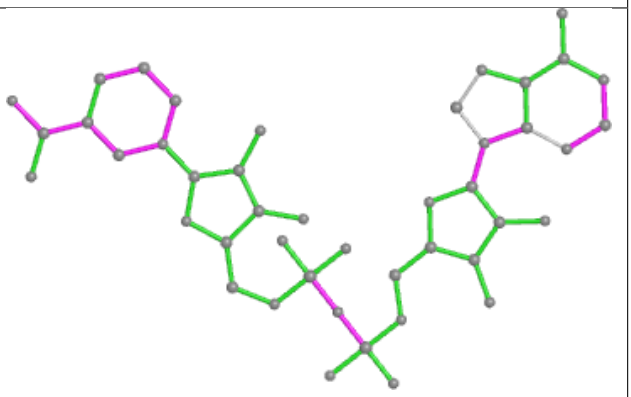


Rings

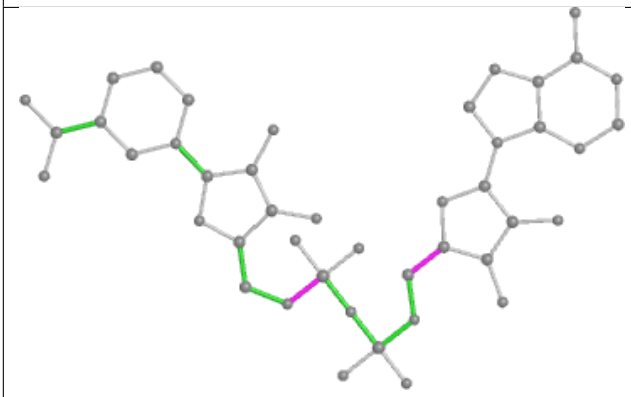
Ligand NAD E 5401



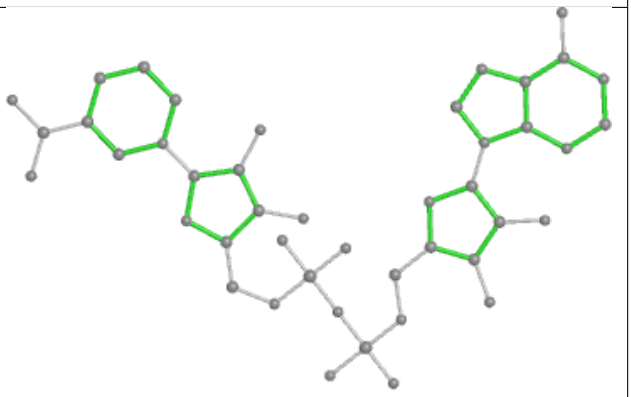
Bond lengths



Bond angles

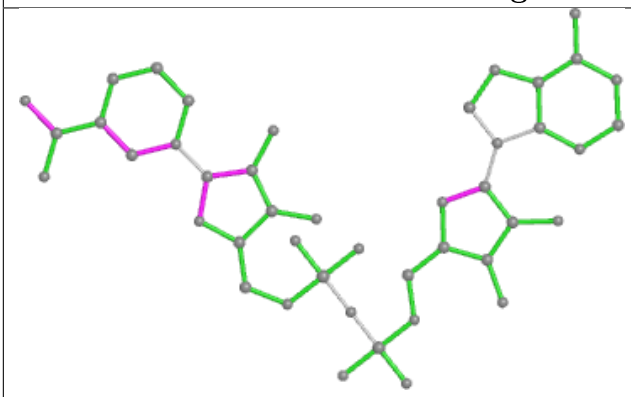


Torsions

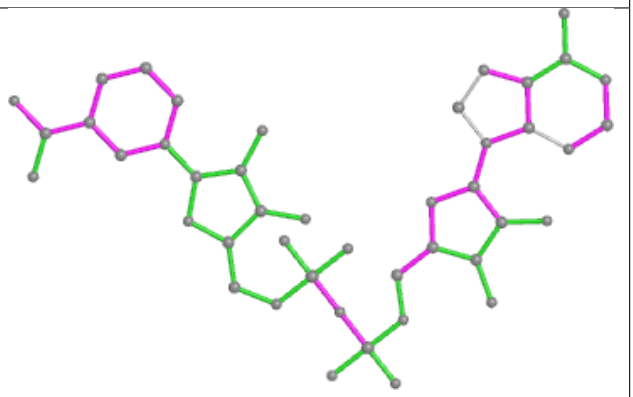


Rings

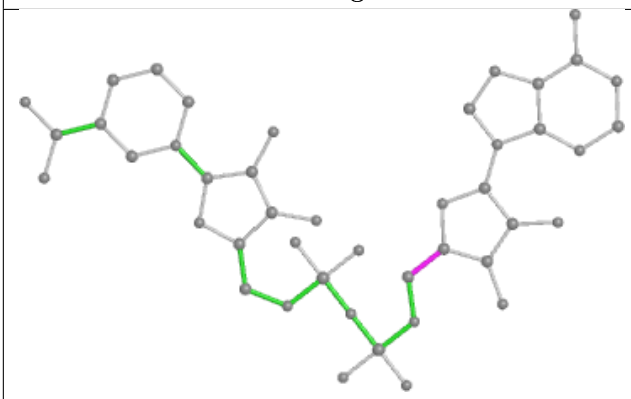
Ligand NAD D 4401



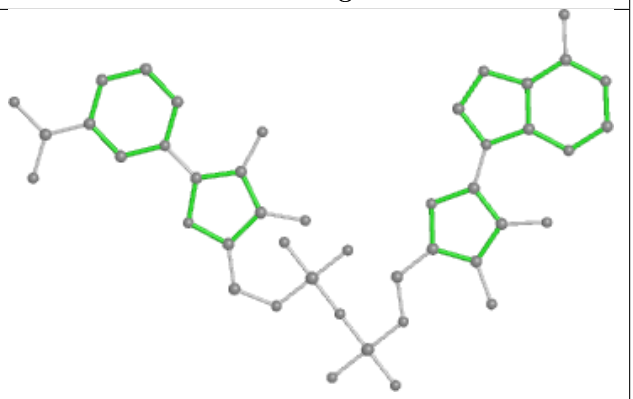
Bond lengths



Bond angles

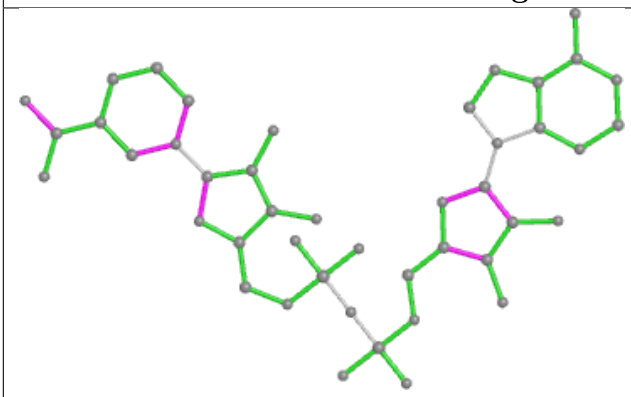


Torsions

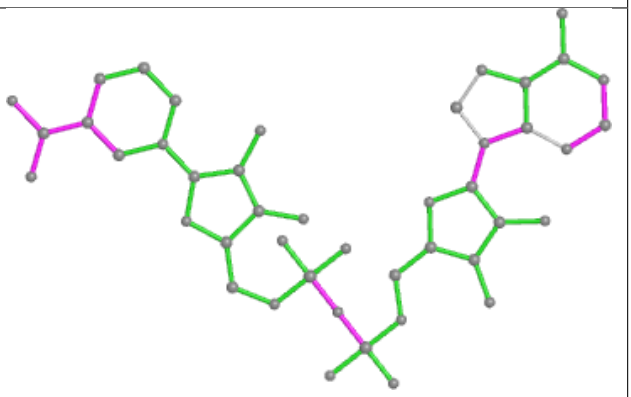


Rings

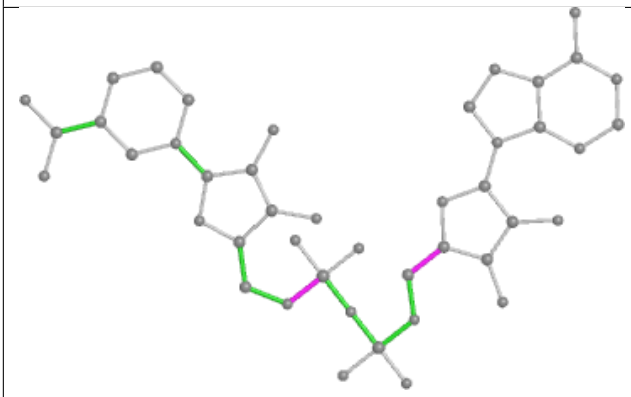
Ligand NAD B 2401



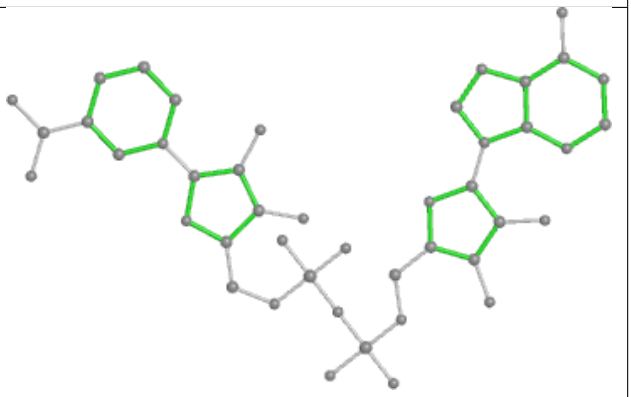
Bond lengths



Bond angles

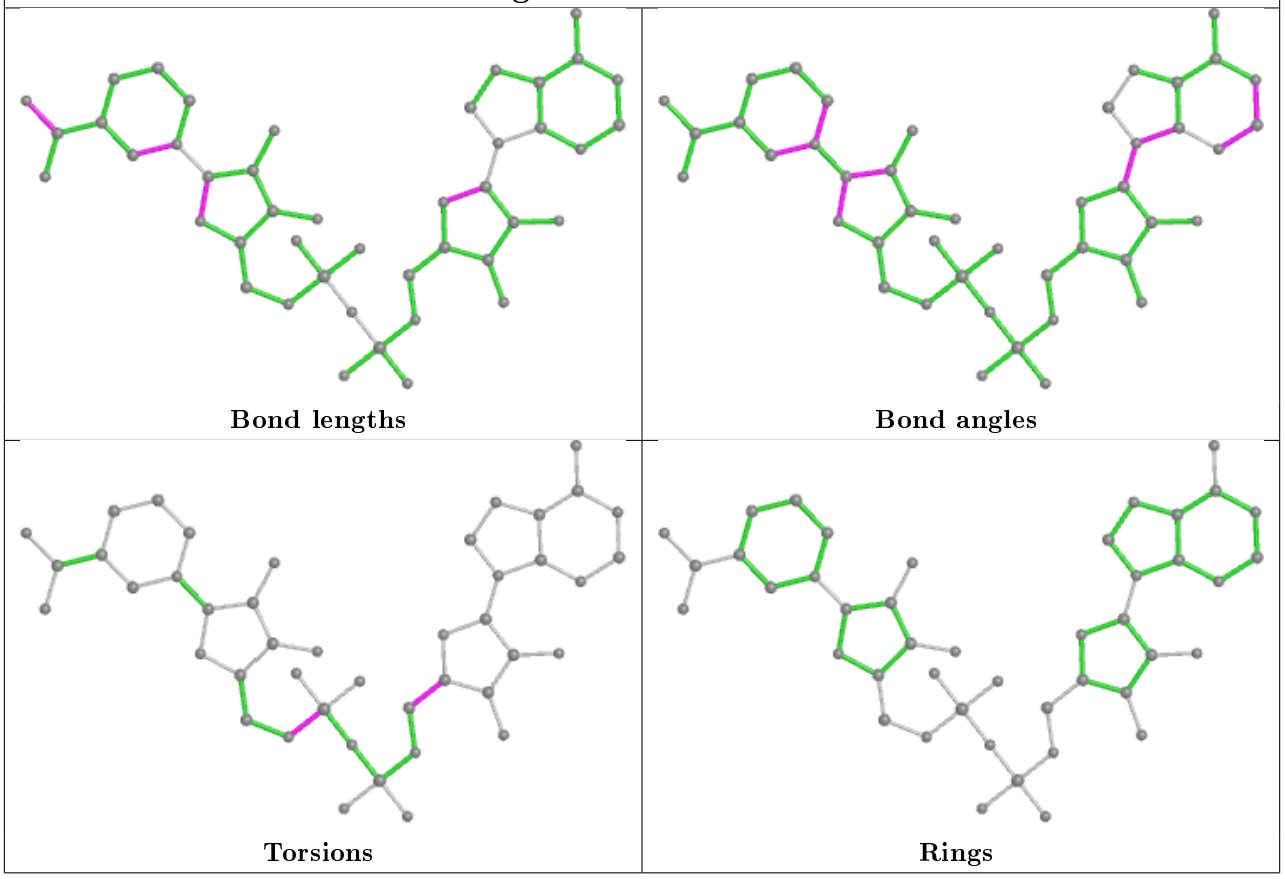


Torsions



Rings

Ligand NAD C 3401



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	320/320 (100%)	-0.45	3 (0%) 84 88	9, 19, 39, 66	4 (1%)
1	B	319/320 (99%)	-0.44	0 100 100	9, 20, 38, 55	1 (0%)
1	C	319/320 (99%)	-0.39	6 (1%) 66 73	10, 20, 46, 70	0
1	D	320/320 (100%)	-0.31	6 (1%) 66 73	10, 20, 45, 71	0
1	E	319/320 (99%)	-0.27	1 (0%) 94 96	8, 23, 50, 65	0
1	F	319/320 (99%)	-0.31	6 (1%) 66 73	9, 20, 43, 67	1 (0%)
All	All	1916/1920 (99%)	-0.36	22 (1%) 80 85	8, 20, 44, 71	6 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6321	LEU	5.6
1	D	4321	LEU	4.4
1	A	1129	LYS	4.0
1	C	3203	VAL	4.0
1	D	4181	PRO	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

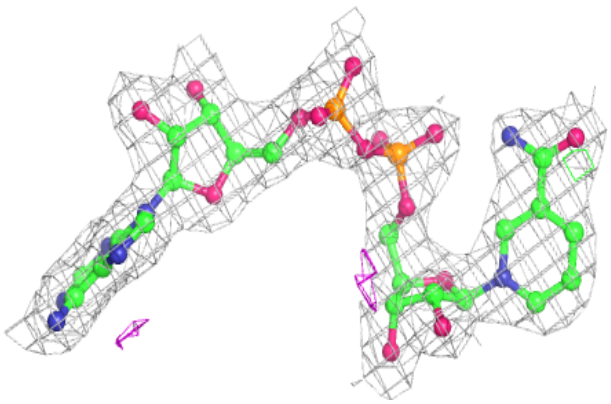
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

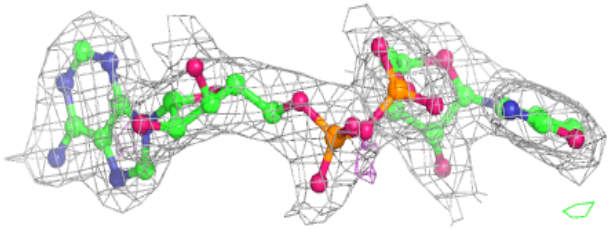
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1402	6/6	0.81	0.25	23,31,34,35	0
3	GOL	D	4402	6/6	0.83	0.20	25,30,35,36	0
3	GOL	B	2402	6/6	0.83	0.22	27,31,32,39	0
4	SO4	C	3403	5/5	0.86	0.24	83,88,88,88	0
3	GOL	E	5402	6/6	0.87	0.21	31,35,35,36	0
3	GOL	C	3402	6/6	0.90	0.19	27,29,30,34	0
3	GOL	F	6402	6/6	0.92	0.17	31,33,37,40	0
4	SO4	D	4404	5/5	0.93	0.27	63,64,68,75	0
4	SO4	F	6403	5/5	0.94	0.29	83,84,86,86	0
4	SO4	B	2403	5/5	0.95	0.17	59,59,63,65	0
4	SO4	D	4403	5/5	0.95	0.12	57,58,65,68	0
2	NAD	F	6401	44/44	0.97	0.09	10,17,19,20	0
2	NAD	B	2401	44/44	0.97	0.11	17,23,26,27	0
2	NAD	A	1401	44/44	0.97	0.10	17,20,24,27	0
2	NAD	E	5401	44/44	0.97	0.12	18,21,25,26	0
2	NAD	D	4401	44/44	0.98	0.09	10,15,16,18	0
2	NAD	C	3401	44/44	0.98	0.08	16,18,19,22	0

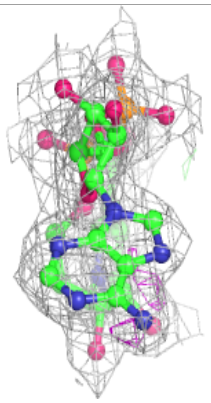
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD F 6401:

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

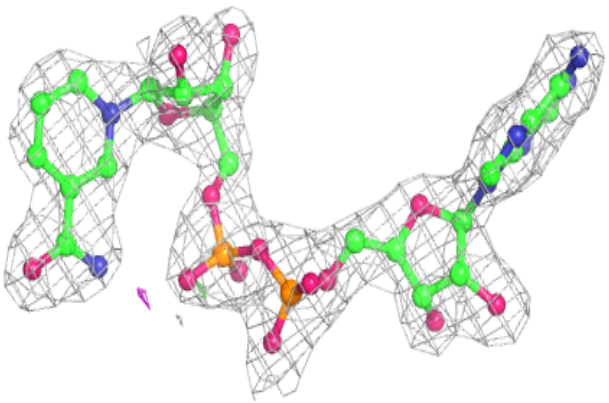


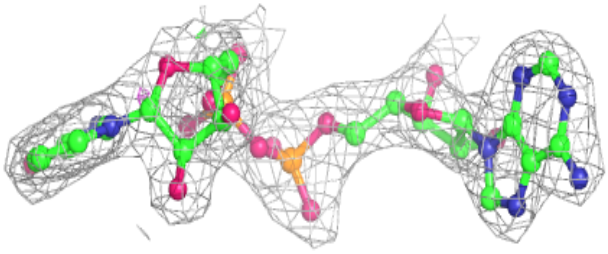


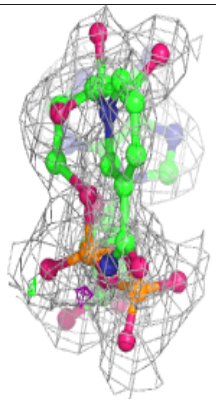


Electron density around NAD B 2401:

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

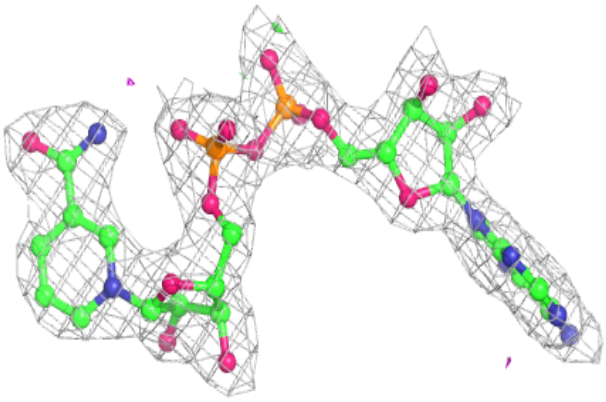


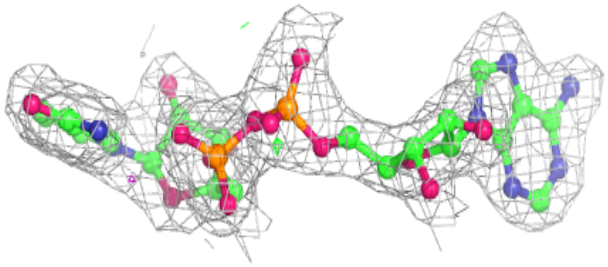


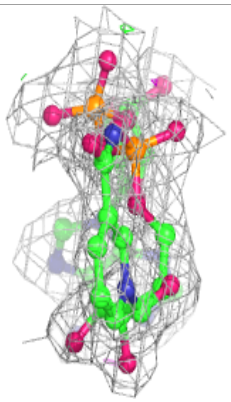


Electron density around NAD A 1401:

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

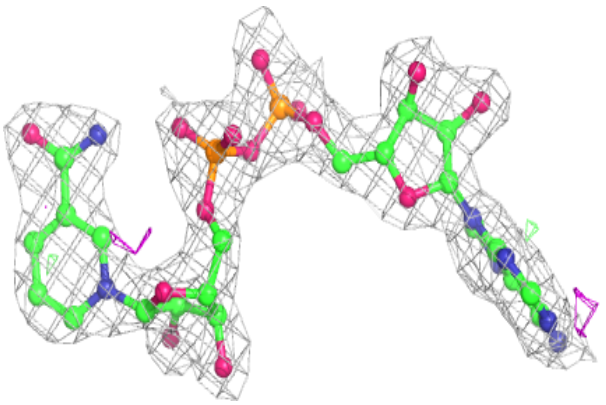


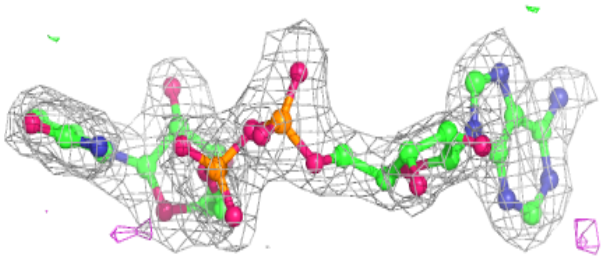


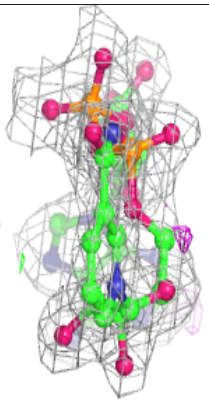


Electron density around NAD E 5401:

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

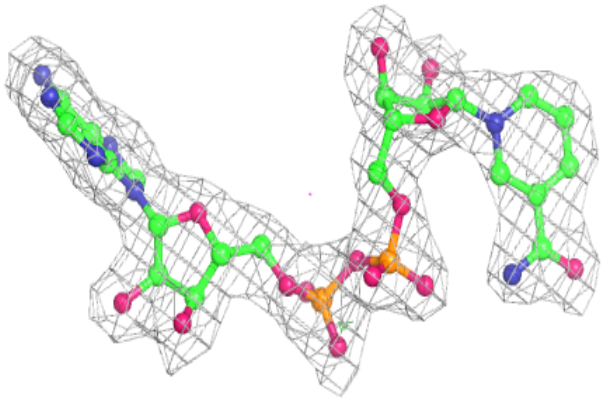


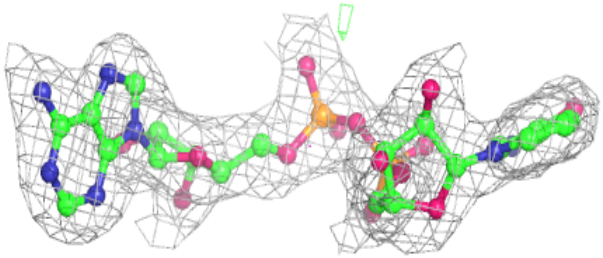


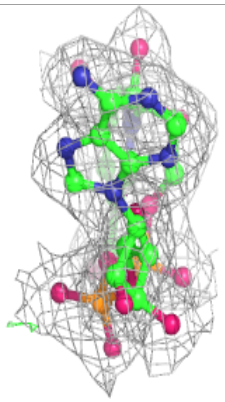


Electron density around NAD D 4401:

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

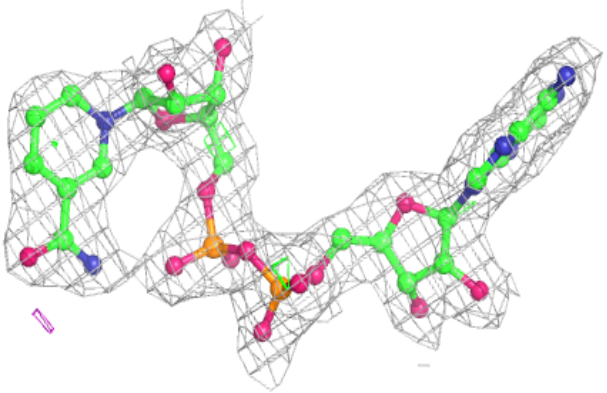


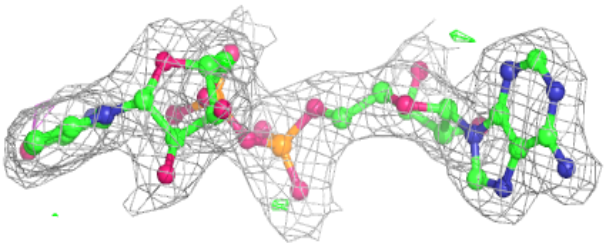


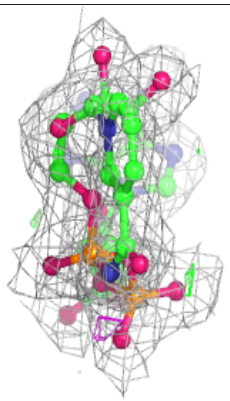


Electron density around NAD C 3401:

$2mF_o$-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.