wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 05:04 PM BST

PDB ID	:	5K4Y
Title	:	Three-dimensional structure of L-threonine 3-dehydrogenase from Trypanosoma brucei refined to 1.77 angstroms
Authors	:	Adjogatse, E.A.; Erskine, P.T.; Cooper, J.B.
Deposited on	:	2016-05-22
Resolution	:	1.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

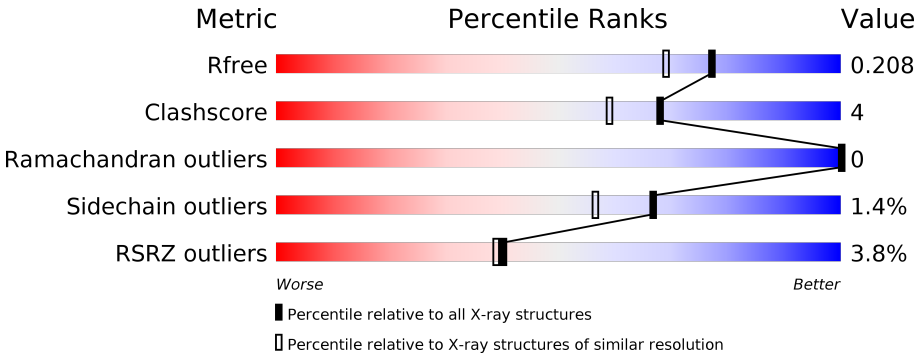
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	3% 91% 9%
1	B	320	4% 93% 7%
1	C	320	3% 96%
1	D	320	4% 89% 10%
1	E	320	4% 90% 9%
1	F	320	4% 90% 8%

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	ACT	C	3402	-	-	X	-
3	ACT	F	6403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16948 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.

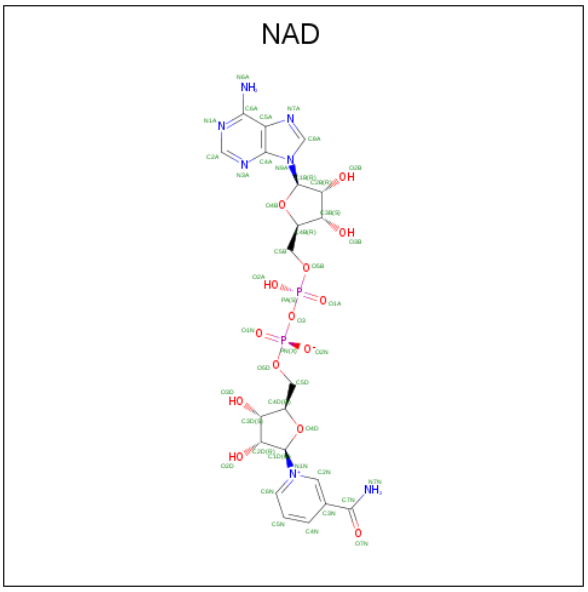
- Molecule 1 is a protein called L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	4	0
			2521	1608	417	477	19			
1	B	320	Total	C	N	O	S	0	3	0
			2518	1606	418	474	20			
1	C	320	Total	C	N	O	S	0	4	0
			2525	1611	420	475	19			
1	D	320	Total	C	N	O	S	0	12	0
			2564	1636	426	482	20			
1	E	319	Total	C	N	O	S	0	5	0
			2524	1611	420	474	19			
1	F	320	Total	C	N	O	S	0	8	0
			2540	1623	421	475	21			

There are 6 discrepancies between the modelled and reference sequences:

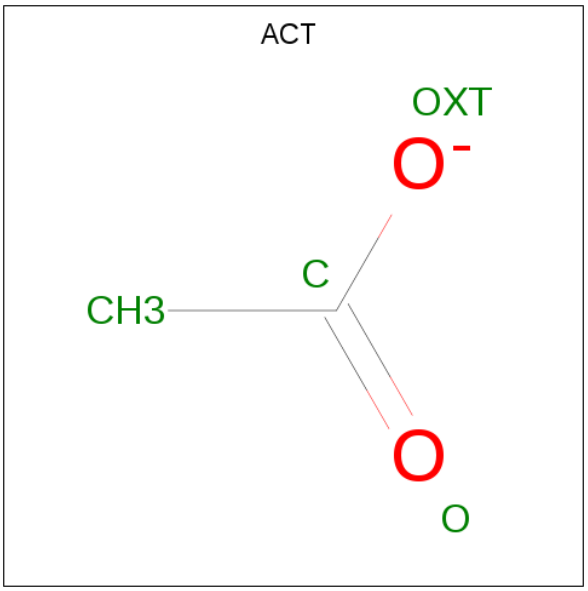
Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	MET	-	initiating methionine	UNP Q7YW97
B	2002	MET	-	initiating methionine	UNP Q7YW97
C	3002	MET	-	initiating methionine	UNP Q7YW97
D	4002	MET	-	initiating methionine	UNP Q7YW97
E	5002	MET	-	initiating methionine	UNP Q7YW97
F	6002	MET	-	initiating 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 ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

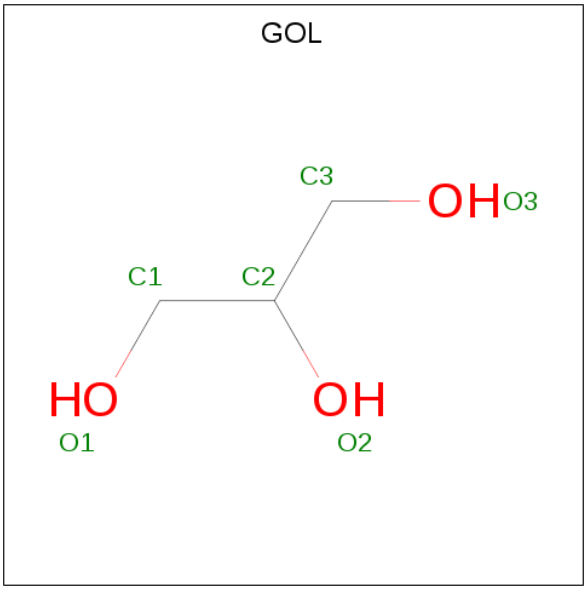
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Cl 2 2	0	0
4	E	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Na 2 2	0	0
5	E	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	249	Total O 249 249	0	0
7	B	240	Total O 240 240	0	0

Continued on next page...

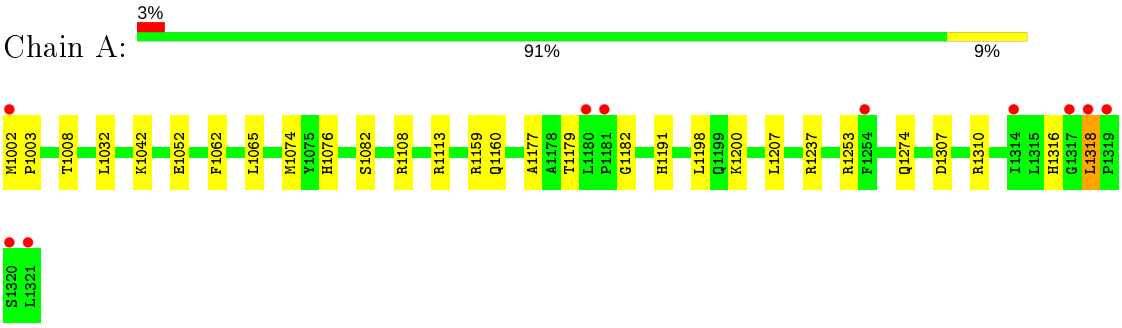
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	270	Total O 270 270	0	0
7	D	231	Total O 231 231	0	0
7	E	219	Total O 219 219	0	0
7	F	239	Total O 239 239	0	0

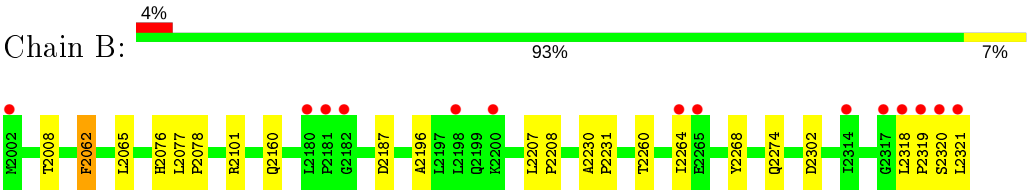
3 Residue-property plots (i)

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.

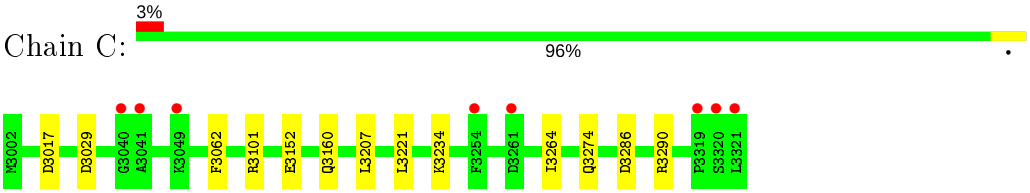
- Molecule 1: L-threonine 3-dehydrogenase



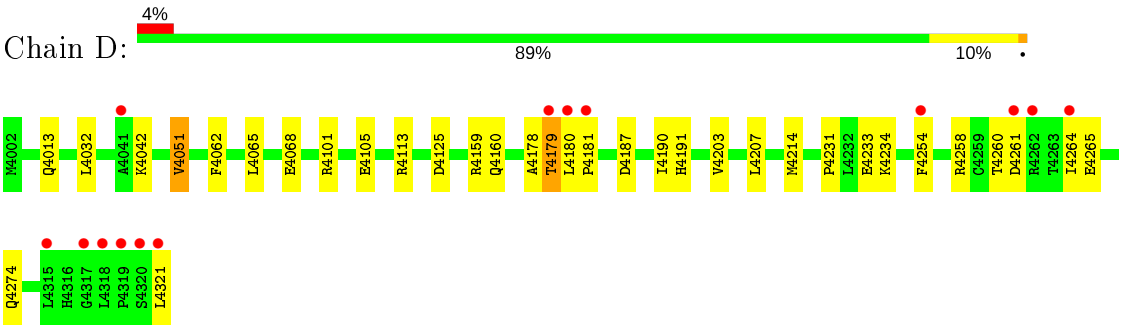
- Molecule 1: L-threonine 3-dehydrogenase



- Molecule 1: L-threonine 3-dehydrogenase

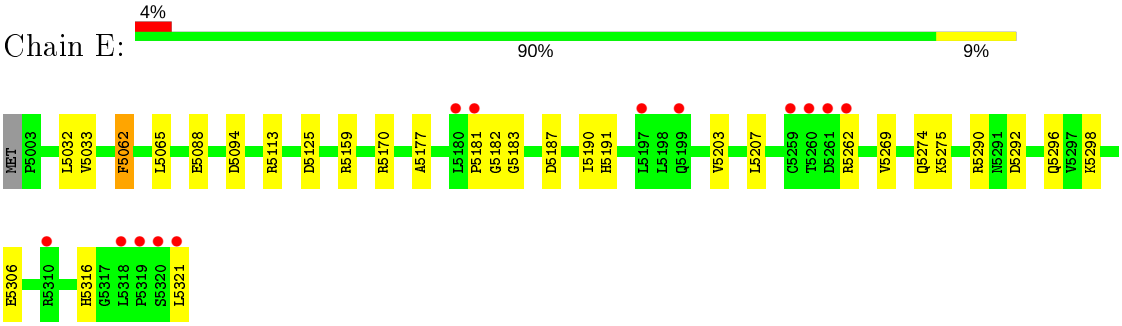


- Molecule 1: L-threonine 3-dehydrogenase



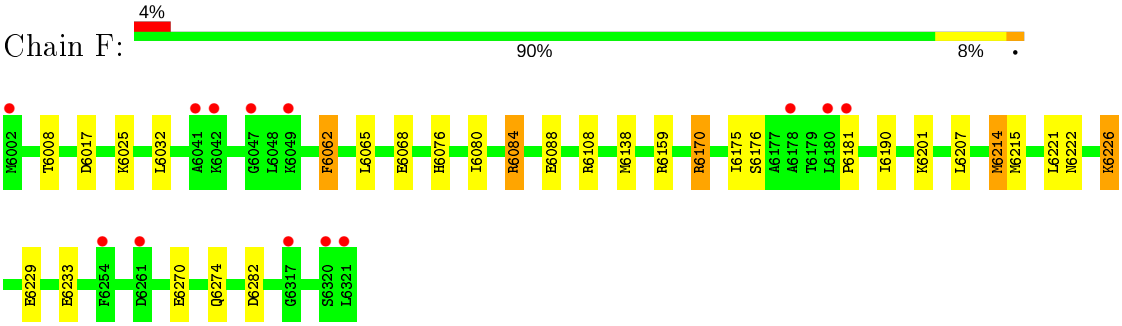
• Molecule 1: L-threonine 3-dehydrogenase

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	133.45Å 278.63Å 56.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 1.77 39.03 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-1.77) 99.8 (39.03-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.161 , 0.201 0.172 , 0.208	Depositor DCC
R_{free} test set	10231 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 28.53 % 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 1.8140e-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, ACT, NA, NAD, CL

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	0.98	1/2589 (0.0%)	1.07	6/3512 (0.2%)
1	B	0.96	0/2580	1.00	4/3499 (0.1%)
1	C	1.02	1/2590 (0.0%)	0.97	0/3514
1	D	1.01	2/2639 (0.1%)	1.01	9/3579 (0.3%)
1	E	0.94	0/2592	1.01	10/3513 (0.3%)
1	F	0.99	0/2620	1.05	12/3550 (0.3%)
All	All	0.98	4/15610 (0.0%)	1.02	41/21167 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4233	GLU	CD-OE2	6.35	1.32	1.25
1	D	4214	MET	SD-CE	-6.35	1.42	1.77
1	A	1237	ARG	CD-NE	-6.27	1.35	1.46
1	C	3152	GLU	CD-OE1	5.17	1.31	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1237	ARG	NE-CZ-NH1	18.32	129.46	120.30
1	A	1237	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	F	6084	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	E	5094	ASP	CB-CG-OD1	9.54	126.88	118.30
1	A	1108	ARG	NE-CZ-NH1	-8.46	116.07	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2535	19	0
1	B	2518	0	2533	15	0
1	C	2525	0	2545	10	0
1	D	2564	0	2592	24	0
1	E	2524	0	2549	14	0
1	F	2540	0	2579	29	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	3	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	3	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	6	0	8	2	0
7	A	249	0	0	8	0
7	B	240	0	0	5	0
7	C	270	0	0	10	0
7	D	231	0	0	5	0
7	E	219	0	0	7	0
7	F	239	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16948	0	15515	117	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 117 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:5191:HIS:NE2	7:E:5501:HOH:O	1.81	1.13
1:A:1160[A]:GLN:HG3	7:A:1590:HOH:O	1.61	0.99
1:D:4187:ASP:HB2	7:D:4538:HOH:O	1.66	0.94
1:A:1160[A]:GLN:OE1	7:A:1501:HOH:O	1.87	0.91
1:D:4187:ASP:CB	7:D:4538:HOH:O	2.20	0.89

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	322/320 (101%)	316 (98%)	6 (2%)	0	100	100
1	B	321/320 (100%)	317 (99%)	4 (1%)	0	100	100
1	C	322/320 (101%)	315 (98%)	7 (2%)	0	100	100
1	D	330/320 (103%)	321 (97%)	9 (3%)	0	100	100
1	E	322/320 (101%)	317 (98%)	5 (2%)	0	100	100
1	F	326/320 (102%)	321 (98%)	5 (2%)	0	100	100
All	All	1943/1920 (101%)	1907 (98%)	36 (2%)	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	281/277 (101%)	276 (98%)	5 (2%)	59	45
1	B	280/277 (101%)	278 (99%)	2 (1%)	84	79
1	C	281/277 (101%)	279 (99%)	2 (1%)	84	79
1	D	286/277 (103%)	277 (97%)	9 (3%)	40	22
1	E	281/277 (101%)	276 (98%)	5 (2%)	59	45
1	F	285/277 (103%)	283 (99%)	2 (1%)	84	79
All	All	1694/1662 (102%)	1669 (98%)	25 (2%)	67	53

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4062	PHE
1	D	4160[A]	GLN
1	F	6062	PHE
1	D	4068	GLU
1	D	4160[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4191	HIS
1	D	4274	GLN
1	E	5311	GLN
1	C	3222	ASN
1	C	3274	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)

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	ACT	D	4402	-	1,3,3	1.85	0	0,3,3	0.00	-
3	ACT	A	1402	-	1,3,3	2.39	1 (100%)	0,3,3	0.00	-
2	NAD	D	4401	-	42,48,48	1.64	7 (16%)	50,73,73	1.41	9 (18%)
3	ACT	B	2402	-	1,3,3	0.16	0	0,3,3	0.00	-
2	NAD	F	6401	-	42,48,48	1.86	5 (11%)	50,73,73	1.41	6 (12%)
3	ACT	C	3402	-	1,3,3	7.90	1 (100%)	0,3,3	0.00	-
6	GOL	F	6402	-	5,5,5	0.65	0	5,5,5	2.09	2 (40%)
2	NAD	C	3401	-	42,48,48	1.76	9 (21%)	50,73,73	1.61	9 (18%)
2	NAD	E	5401	-	42,48,48	1.57	10 (23%)	50,73,73	1.57	10 (20%)
2	NAD	B	2401	-	42,48,48	1.57	4 (9%)	50,73,73	1.74	11 (22%)
2	NAD	A	1401	-	42,48,48	1.44	4 (9%)	50,73,73	1.41	7 (14%)
3	ACT	F	6403	-	1,3,3	4.89	1 (100%)	0,3,3	0.00	-
3	ACT	E	5402	-	1,3,3	3.17	1 (100%)	0,3,3	0.00	-

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	C	3401	-	-	3/26/62/62	0/5/5/5
2	NAD	D	4401	-	-	3/26/62/62	0/5/5/5
2	NAD	F	6401	-	-	4/26/62/62	0/5/5/5
6	GOL	F	6402	-	-	3/4/4/4	-
2	NAD	E	5401	-	-	4/26/62/62	0/5/5/5
2	NAD	B	2401	-	-	2/26/62/62	0/5/5/5
2	NAD	A	1401	-	-	4/26/62/62	0/5/5/5

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6401	NAD	C2N-N1N	8.19	1.44	1.35
3	C	3402	ACT	CH3-C	-7.90	1.38	1.48
2	B	2401	NAD	C2N-N1N	5.47	1.41	1.35
3	F	6403	ACT	CH3-C	-4.89	1.42	1.48
2	A	1401	NAD	O4D-C1D	4.50	1.47	1.41

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3401	NAD	N3A-C2A-N1A	-6.03	119.26	128.68
2	A	1401	NAD	N3A-C2A-N1A	-5.37	120.29	128.68
2	B	2401	NAD	C6N-N1N-C2N	-4.74	117.65	121.97
2	E	5401	NAD	C2N-C3N-C4N	4.29	123.12	118.26
2	E	5401	NAD	O7N-C7N-C3N	-3.78	115.11	119.63

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

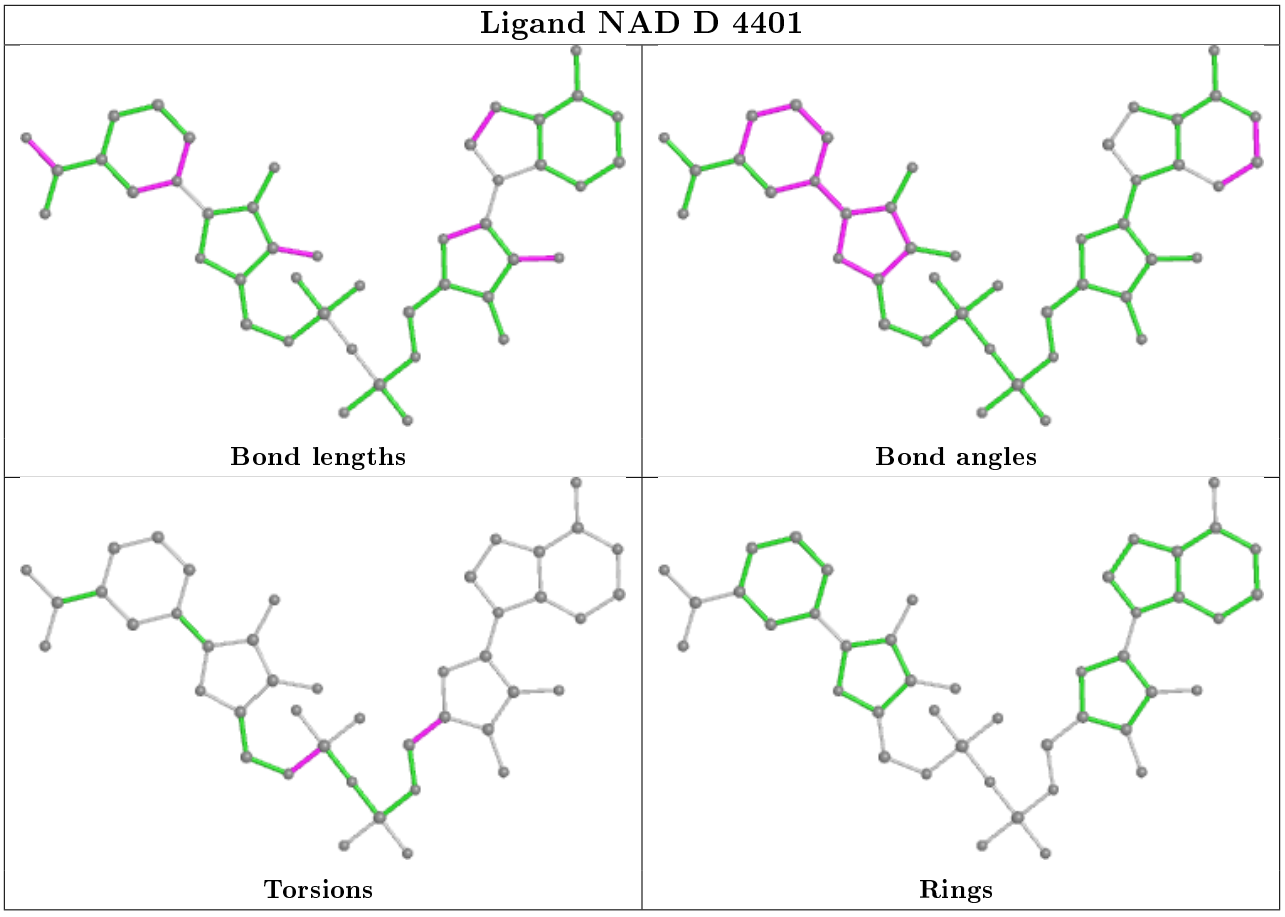
Mol	Chain	Res	Type	Atoms
2	E	5401	NAD	C5D-O5D-PN-O1N
6	F	6402	GOL	C1-C2-C3-O3
2	D	4401	NAD	C5D-O5D-PN-O1N
2	C	3401	NAD	C5D-O5D-PN-O1N
2	F	6401	NAD	C5D-O5D-PN-O1N

There are no ring outliers.

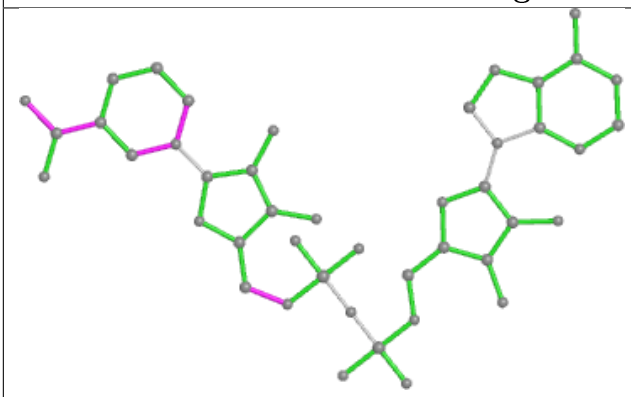
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3402	ACT	3	0
6	F	6402	GOL	2	0
3	F	6403	ACT	3	0

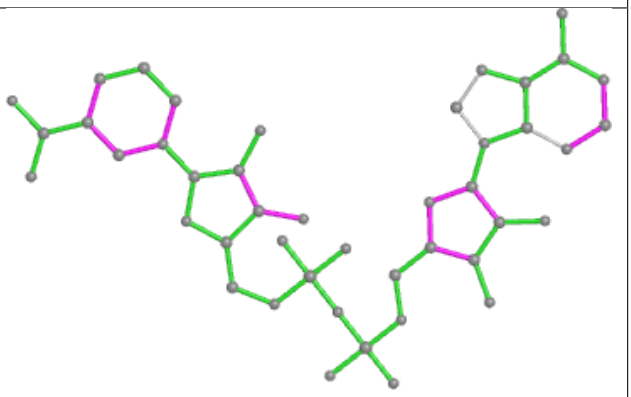
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



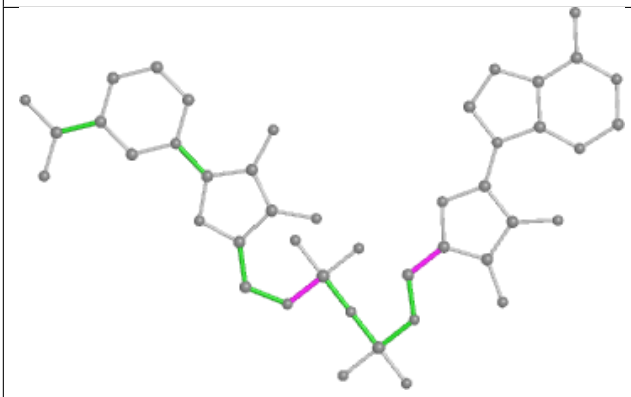
Ligand NAD F 6401



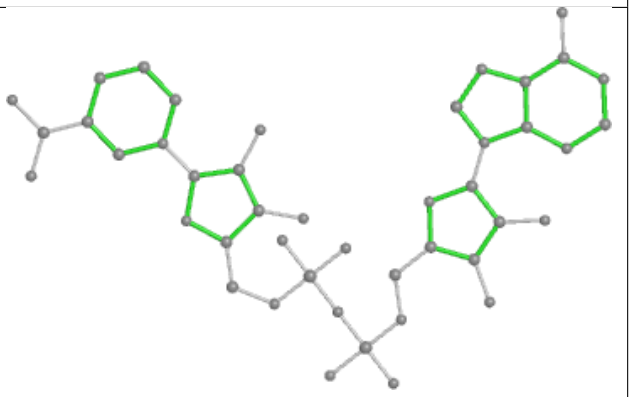
Bond lengths



Bond angles

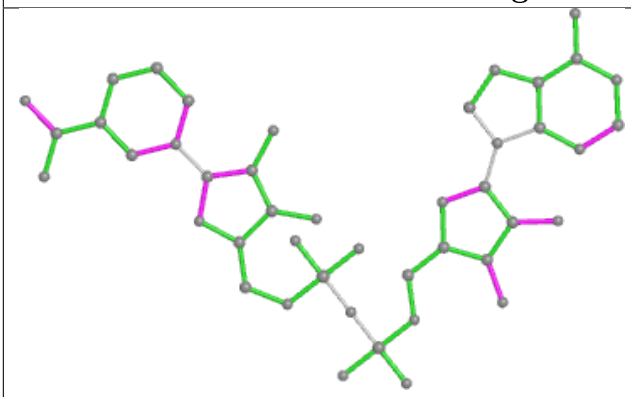


Torsions

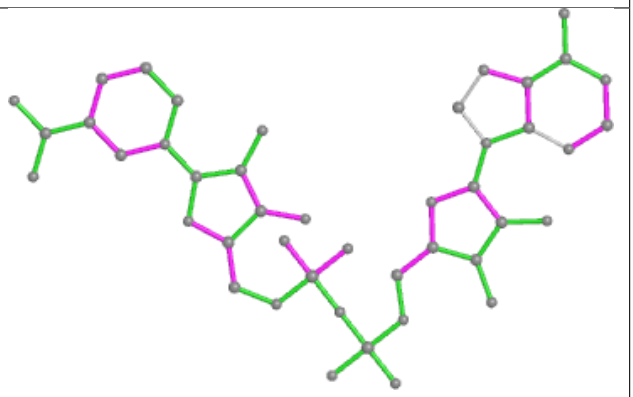


Rings

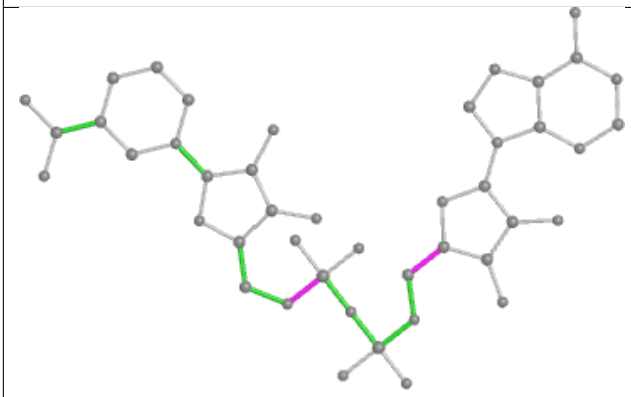
Ligand NAD C 3401



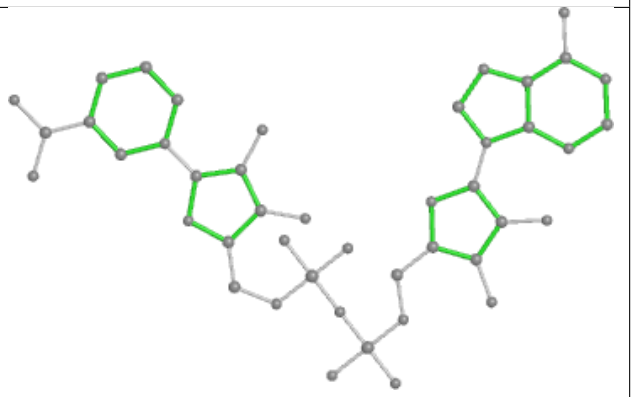
Bond lengths



Bond angles

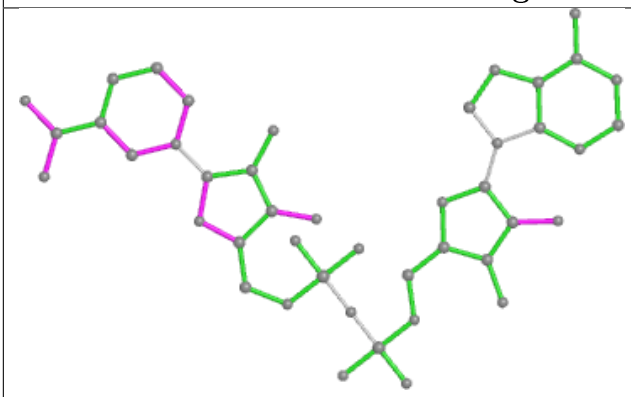


Torsions

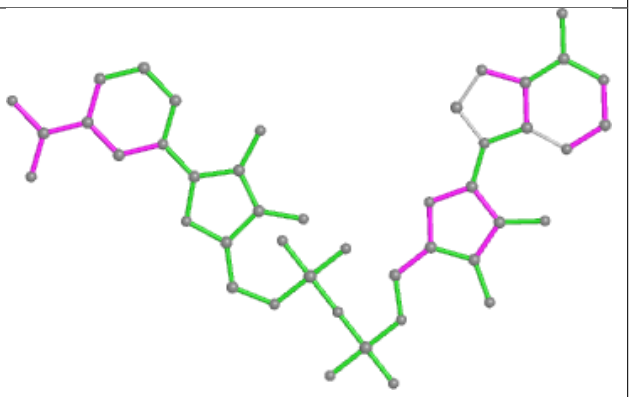


Rings

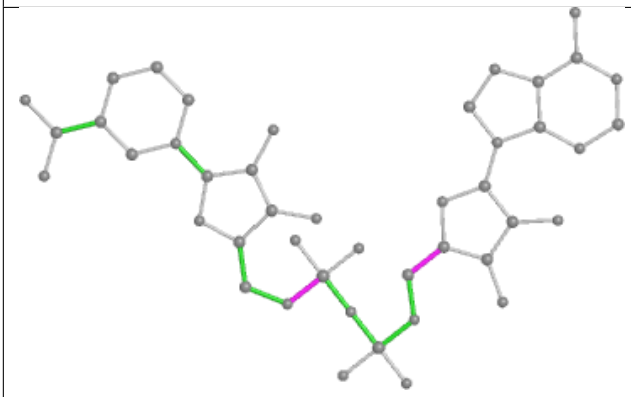
Ligand NAD E 5401



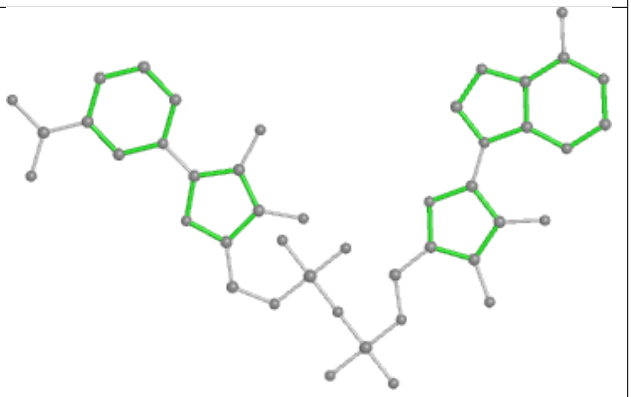
Bond lengths



Bond angles

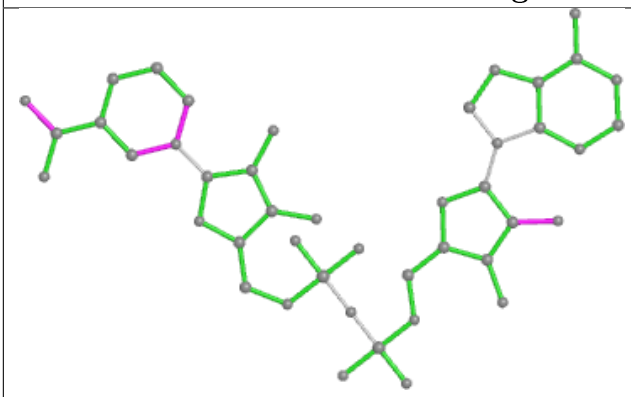


Torsions

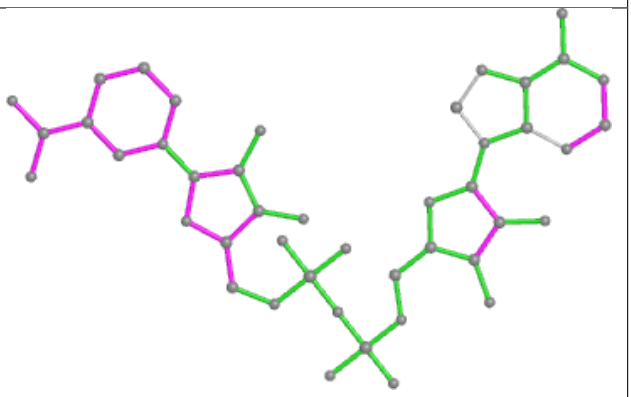


Rings

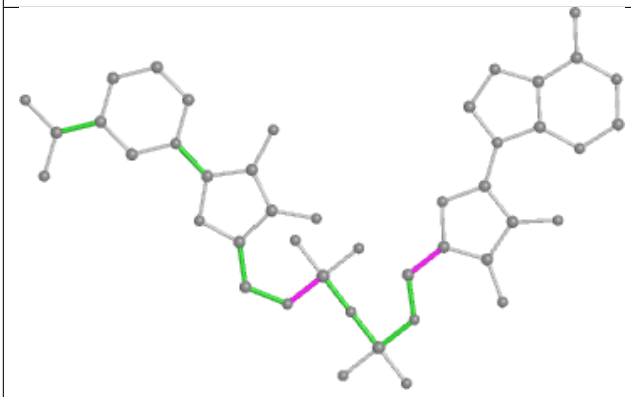
Ligand NAD B 2401



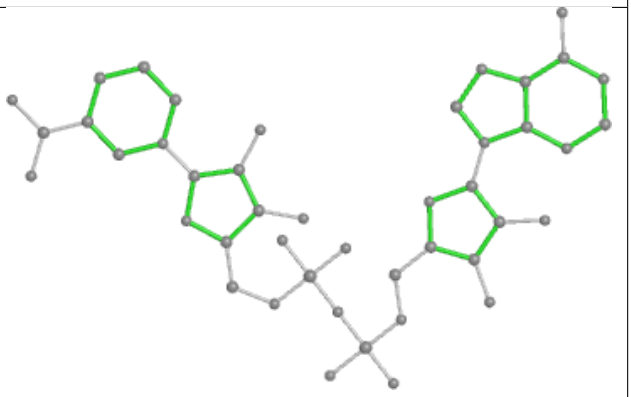
Bond lengths



Bond angles

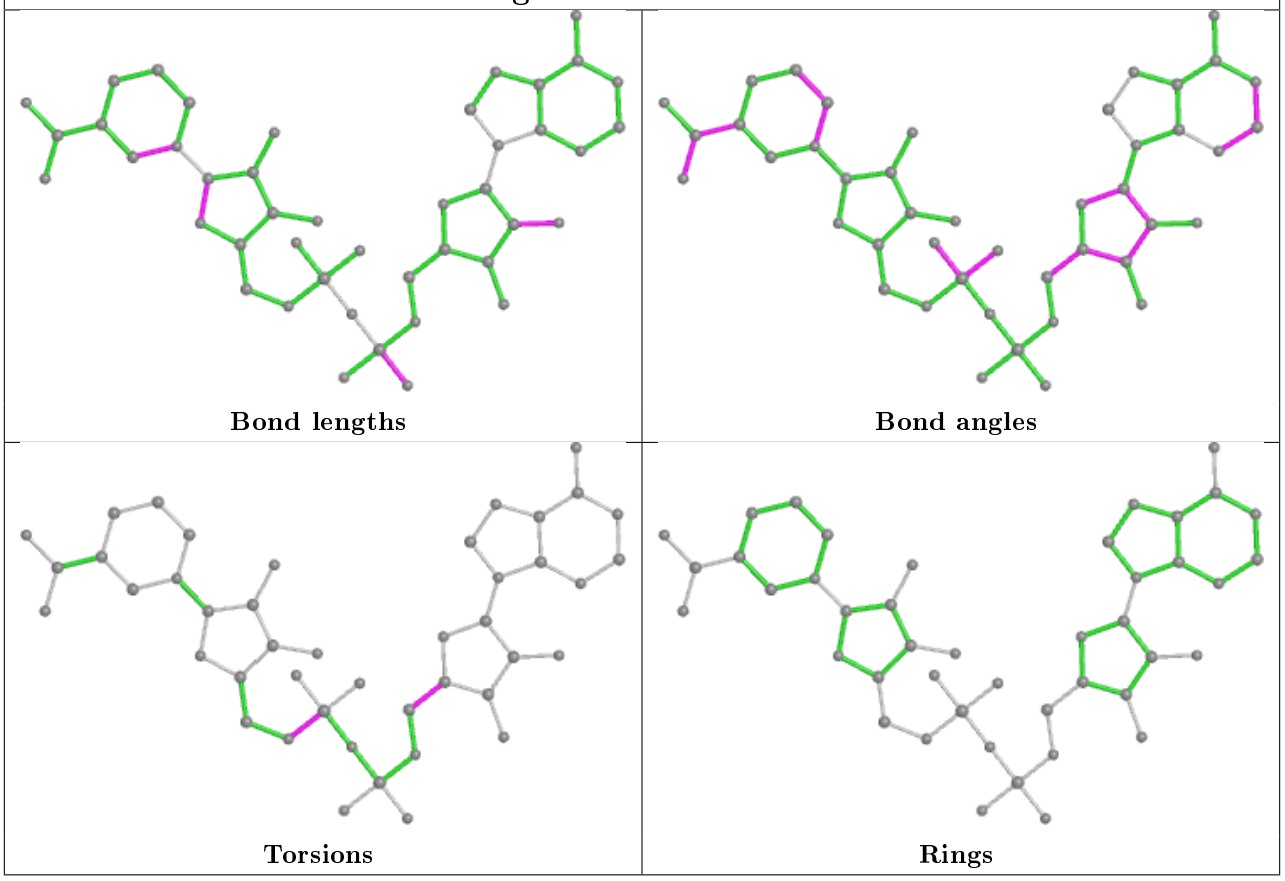


Torsions



Rings

Ligand NAD A 1401



5.7 Other polymers

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

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%)	-0.08	10 (3%) 49 47	7, 15, 35, 79	0
1	B	320/320 (100%)	-0.02	14 (4%) 34 32	7, 16, 43, 55	0
1	C	320/320 (100%)	-0.11	8 (2%) 57 56	7, 15, 34, 46	0
1	D	320/320 (100%)	-0.00	14 (4%) 34 32	7, 15, 40, 51	0
1	E	319/320 (99%)	0.04	13 (4%) 37 35	7, 17, 46, 72	0
1	F	320/320 (100%)	-0.06	13 (4%) 37 35	8, 16, 39, 56	0
All	All	1919/1920 (99%)	-0.04	72 (3%) 40 39	7, 16, 40, 79	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1321	LEU	11.0
1	E	5321	LEU	9.4
1	D	4321	LEU	5.8
1	F	6321	LEU	5.7
1	C	3041	ALA	5.6

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)

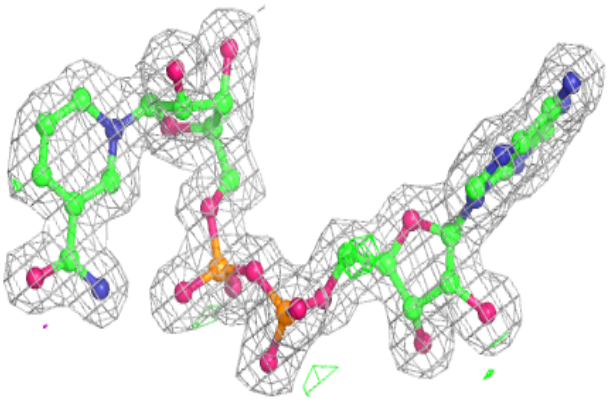
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

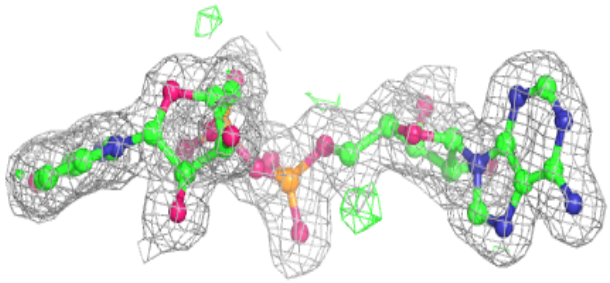
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	F	6402	6/6	0.87	0.25	13,15,17,21	6
3	ACT	C	3402	4/4	0.91	0.10	12,14,17,18	0
4	CL	D	4404	1/1	0.93	0.23	43,43,43,43	0
4	CL	E	5403	1/1	0.94	0.09	44,44,44,44	0
3	ACT	F	6403	4/4	0.94	0.09	13,15,17,20	0
4	CL	B	2403	1/1	0.95	0.09	35,35,35,35	0
3	ACT	E	5402	4/4	0.95	0.10	15,16,19,19	0
3	ACT	A	1402	4/4	0.96	0.10	14,16,16,19	0
5	NA	F	6405	1/1	0.96	0.07	27,27,27,27	0
4	CL	D	4403	1/1	0.96	0.06	32,32,32,32	0
5	NA	E	5404	1/1	0.97	0.13	32,32,32,32	0
3	ACT	D	4402	4/4	0.97	0.09	14,15,16,19	0
5	NA	B	2404	1/1	0.97	0.09	30,30,30,30	0
2	NAD	D	4401	44/44	0.98	0.07	8,11,12,13	0
4	CL	F	6404	1/1	0.98	0.05	27,27,27,27	0
2	NAD	C	3401	44/44	0.98	0.07	10,12,14,15	0
2	NAD	F	6401	44/44	0.98	0.06	9,12,15,16	0
2	NAD	E	5401	44/44	0.98	0.07	9,12,14,15	0
5	NA	D	4406	1/1	0.98	0.05	31,31,31,31	0
2	NAD	B	2401	44/44	0.98	0.07	10,11,13,15	0
2	NAD	A	1401	44/44	0.98	0.07	8,11,12,14	0
4	CL	A	1403	1/1	0.98	0.07	34,34,34,34	0
3	ACT	B	2402	4/4	0.98	0.07	15,16,18,20	0
5	NA	D	4405	1/1	0.99	0.05	29,29,29,29	0
4	CL	C	3403	1/1	0.99	0.04	21,21,21,21	0
5	NA	C	3404	1/1	0.99	0.03	24,24,24,24	0
5	NA	A	1404	1/1	0.99	0.06	27,27,27,27	0

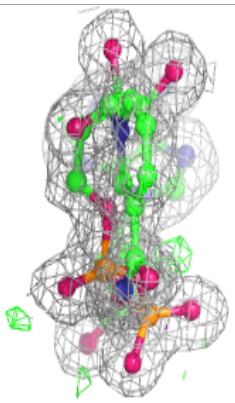
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

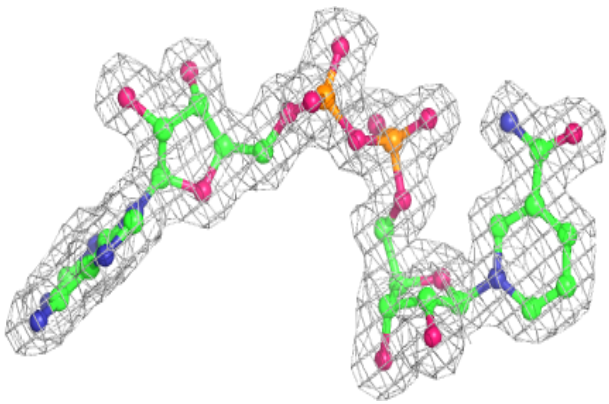


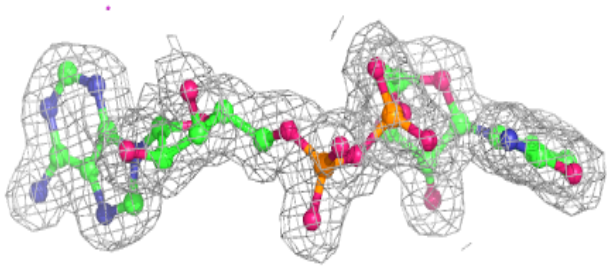


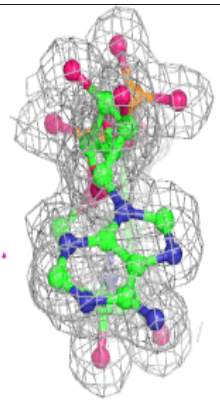


Electron density around NAD C 3401:

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

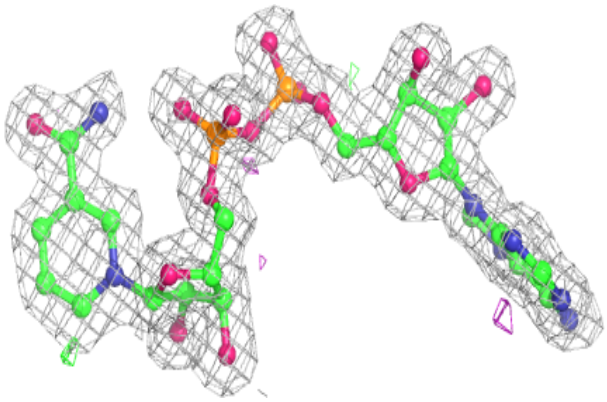


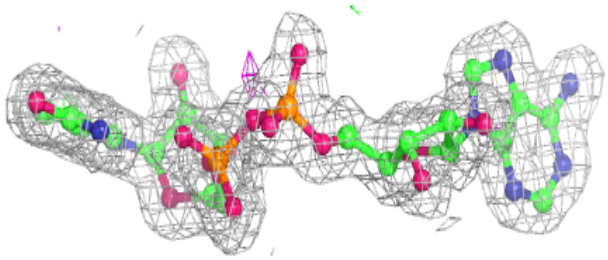


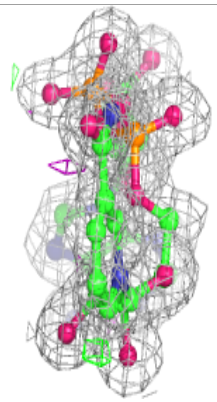


Electron density around NAD F 6401:

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

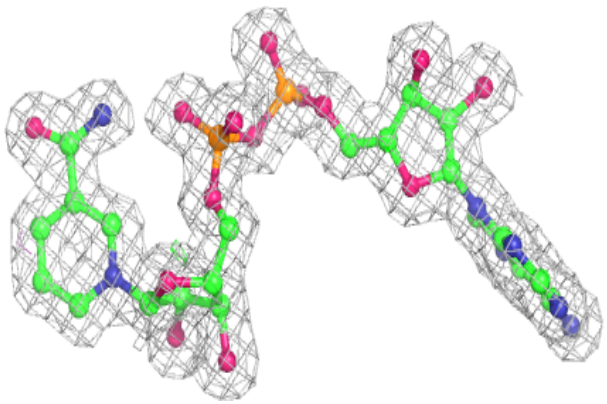


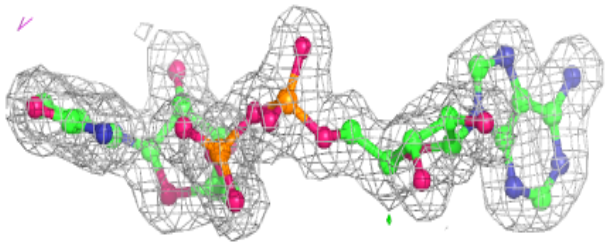


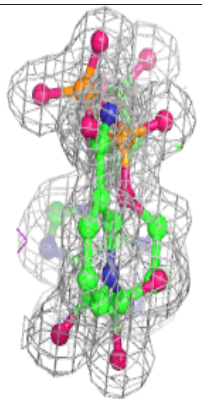


Electron density around NAD E 5401:

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

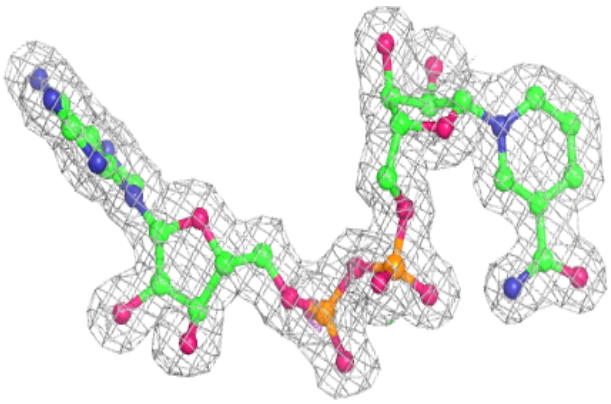


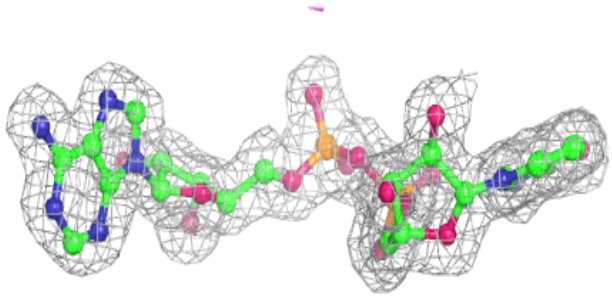


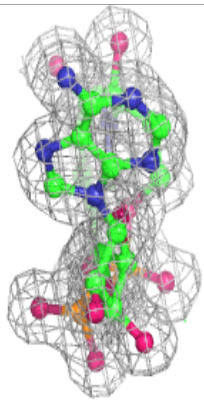


Electron density around NAD B 2401:

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

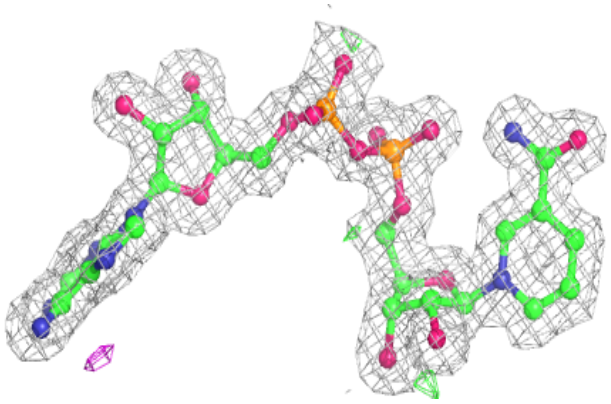


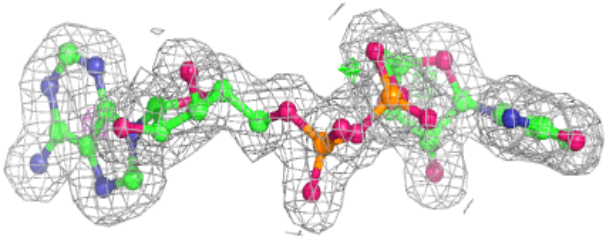


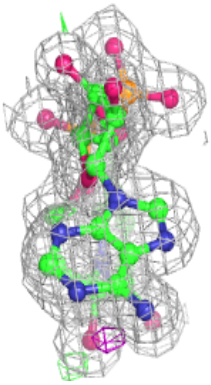


Electron density around NAD A 1401:

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







6.5 Other polymers (i)

There are no such residues in this entry.