wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 06:58 AM EDT

PDB ID	:	4ZGS
Title	:	Identification of the pyruvate reductase of Chlamydomonas reinhardtii
Authors	:	Burgess, S.J.; Hussein, T.; Yeoman, J.A.; Iamshanova, O.; Boehm, M.; Bundy, J.; Bialek, W.; Murray, J.W.; Nixon, P.J.
Deposited on	:	2015-04-23
Resolution	:	2.46 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

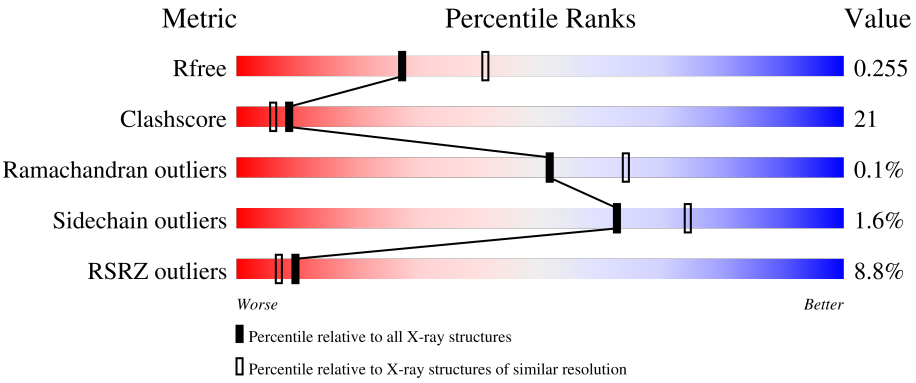
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	% 59% 30% • 10%
1	B	386	13% 54% 33% • 12%
1	C	386	12% 55% 33% • 11%
1	D	386	6% 59% 29% • 10%
1	E	386	7% 59% 28% • 11%

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Mol	Chain	Length	Quality of chain
1	F	386	10% 62% 25% 11%
1	G	386	8% 57% 31% 11%
1	H	386	6% 63% 25% 11%

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
2	NAD	B	1000	-	-	-	X
2	NAD	C	1000	-	-	-	X
2	NAD	F	1000	-	-	-	X
2	NAD	H	1000	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21903 atoms, of which 208 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 Putative D-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2661	1695	459	492	15			
1	B	338	Total	C	N	O	S	0	0	0
			2599	1657	449	478	15			
1	C	342	Total	C	N	O	S	0	0	0
			2633	1677	454	487	15			
1	D	346	Total	C	N	O	S	0	0	0
			2664	1697	458	494	15			
1	E	344	Total	C	N	O	S	0	0	0
			2648	1687	456	490	15			
1	F	343	Total	C	N	O	S	0	0	0
			2640	1682	455	488	15			
1	G	343	Total	C	N	O	S	0	0	0
			2640	1682	455	488	15			
1	H	343	Total	C	N	O	S	0	0	0
			2640	1681	455	489	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B0LUZ5
A	379	LEU	-	expression tag	UNP B0LUZ5
A	380	GLU	-	expression tag	UNP B0LUZ5
A	381	HIS	-	expression tag	UNP B0LUZ5
A	382	HIS	-	expression tag	UNP B0LUZ5
A	383	HIS	-	expression tag	UNP B0LUZ5
A	384	HIS	-	expression tag	UNP B0LUZ5
A	385	HIS	-	expression tag	UNP B0LUZ5
A	386	HIS	-	expression tag	UNP B0LUZ5
B	1	MET	-	initiating methionine	UNP B0LUZ5
B	379	LEU	-	expression tag	UNP B0LUZ5
B	380	GLU	-	expression tag	UNP B0LUZ5
B	381	HIS	-	expression tag	UNP B0LUZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	expression tag	UNP B0LUZ5
B	383	HIS	-	expression tag	UNP B0LUZ5
B	384	HIS	-	expression tag	UNP B0LUZ5
B	385	HIS	-	expression tag	UNP B0LUZ5
B	386	HIS	-	expression tag	UNP B0LUZ5
C	1	MET	-	initiating methionine	UNP B0LUZ5
C	379	LEU	-	expression tag	UNP B0LUZ5
C	380	GLU	-	expression tag	UNP B0LUZ5
C	381	HIS	-	expression tag	UNP B0LUZ5
C	382	HIS	-	expression tag	UNP B0LUZ5
C	383	HIS	-	expression tag	UNP B0LUZ5
C	384	HIS	-	expression tag	UNP B0LUZ5
C	385	HIS	-	expression tag	UNP B0LUZ5
C	386	HIS	-	expression tag	UNP B0LUZ5
D	1	MET	-	initiating methionine	UNP B0LUZ5
D	379	LEU	-	expression tag	UNP B0LUZ5
D	380	GLU	-	expression tag	UNP B0LUZ5
D	381	HIS	-	expression tag	UNP B0LUZ5
D	382	HIS	-	expression tag	UNP B0LUZ5
D	383	HIS	-	expression tag	UNP B0LUZ5
D	384	HIS	-	expression tag	UNP B0LUZ5
D	385	HIS	-	expression tag	UNP B0LUZ5
D	386	HIS	-	expression tag	UNP B0LUZ5
E	1	MET	-	initiating methionine	UNP B0LUZ5
E	379	LEU	-	expression tag	UNP B0LUZ5
E	380	GLU	-	expression tag	UNP B0LUZ5
E	381	HIS	-	expression tag	UNP B0LUZ5
E	382	HIS	-	expression tag	UNP B0LUZ5
E	383	HIS	-	expression tag	UNP B0LUZ5
E	384	HIS	-	expression tag	UNP B0LUZ5
E	385	HIS	-	expression tag	UNP B0LUZ5
E	386	HIS	-	expression tag	UNP B0LUZ5
F	1	MET	-	initiating methionine	UNP B0LUZ5
F	379	LEU	-	expression tag	UNP B0LUZ5
F	380	GLU	-	expression tag	UNP B0LUZ5
F	381	HIS	-	expression tag	UNP B0LUZ5
F	382	HIS	-	expression tag	UNP B0LUZ5
F	383	HIS	-	expression tag	UNP B0LUZ5
F	384	HIS	-	expression tag	UNP B0LUZ5
F	385	HIS	-	expression tag	UNP B0LUZ5
F	386	HIS	-	expression tag	UNP B0LUZ5
G	1	MET	-	initiating methionine	UNP B0LUZ5

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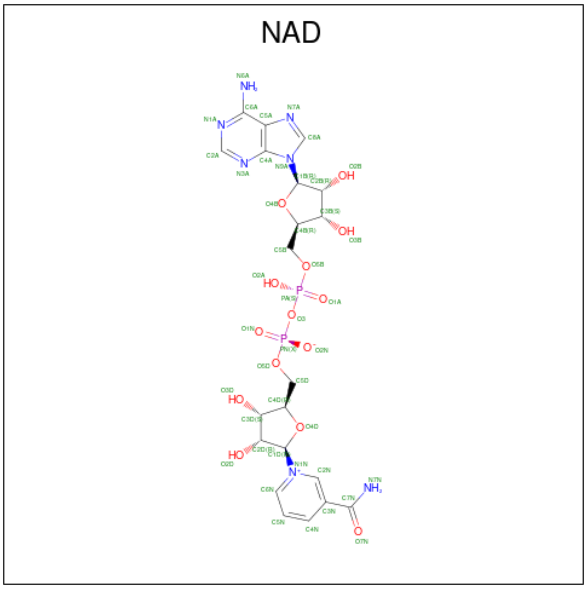
Chain	Residue	Modelled	Actual	Comment	Reference
G	379	LEU	-	expression tag	UNP B0LUZ5
G	380	GLU	-	expression tag	UNP B0LUZ5
G	381	HIS	-	expression tag	UNP B0LUZ5
G	382	HIS	-	expression tag	UNP B0LUZ5
G	383	HIS	-	expression tag	UNP B0LUZ5
G	384	HIS	-	expression tag	UNP B0LUZ5
G	385	HIS	-	expression tag	UNP B0LUZ5
G	386	HIS	-	expression tag	UNP B0LUZ5
H	1	MET	-	initiating methionine	UNP B0LUZ5
H	379	LEU	-	expression tag	UNP B0LUZ5
H	380	GLU	-	expression tag	UNP B0LUZ5
H	381	HIS	-	expression tag	UNP B0LUZ5
H	382	HIS	-	expression tag	UNP B0LUZ5
H	383	HIS	-	expression tag	UNP B0LUZ5
H	384	HIS	-	expression tag	UNP B0LUZ5
H	385	HIS	-	expression tag	UNP B0LUZ5
H	386	HIS	-	expression tag	UNP B0LUZ5

- 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	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	F	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	G	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	H	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

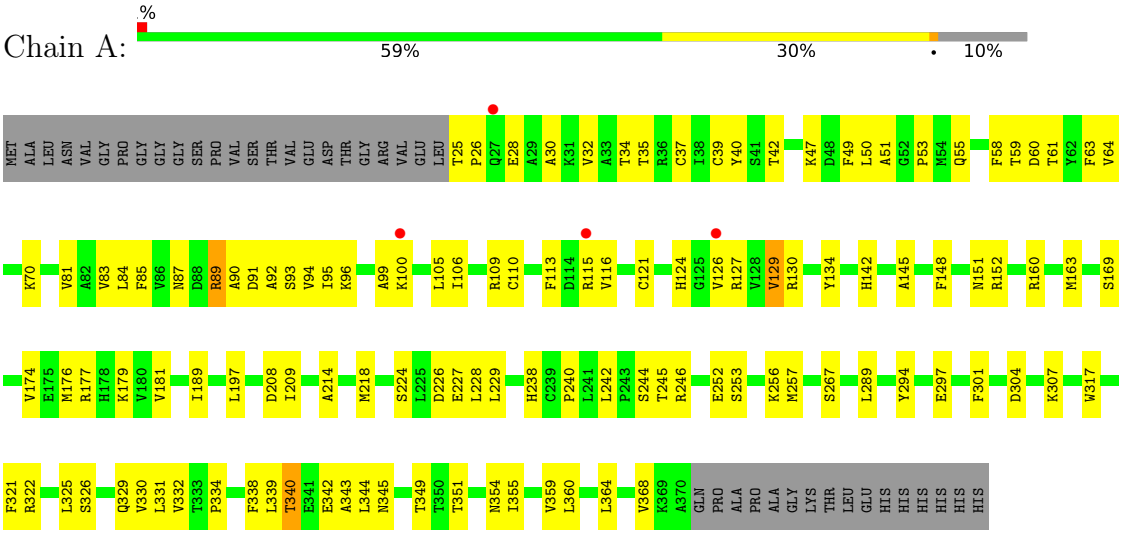
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	33	Total	O	0	0
			33	33		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		
3	E	33	Total	O	0	0
			33	33		
3	F	21	Total	O	0	0
			21	21		
3	G	20	Total	O	0	0
			20	20		
3	H	29	Total	O	0	0
			29	29		

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.

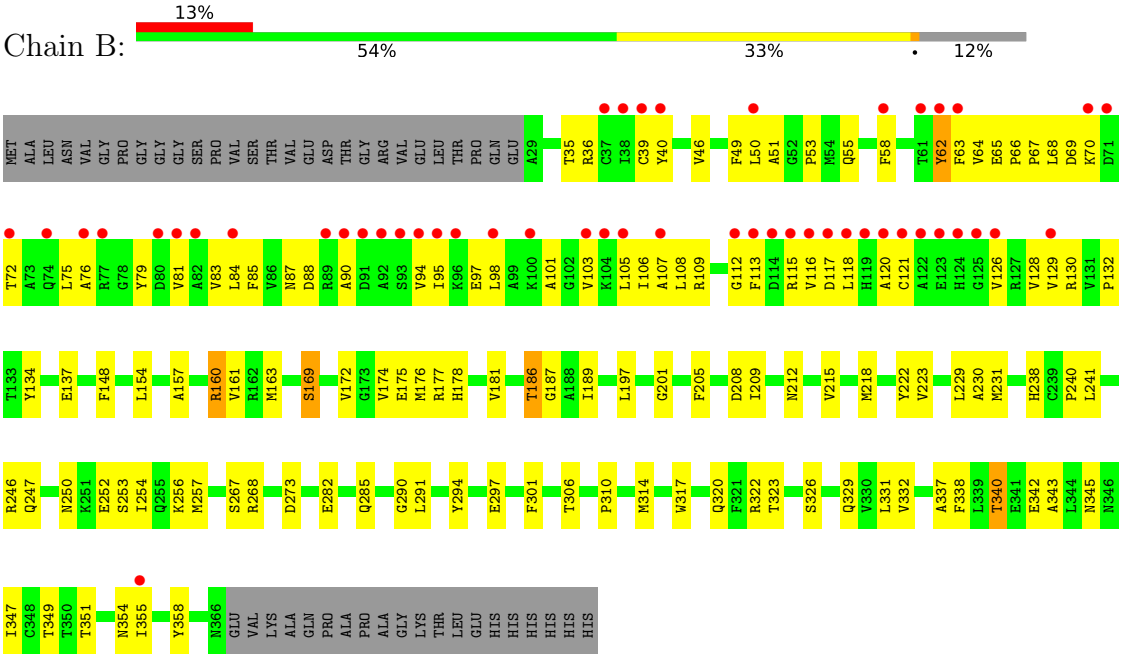
• Molecule 1: Putative D-lactate dehydrogenase

Chain A:



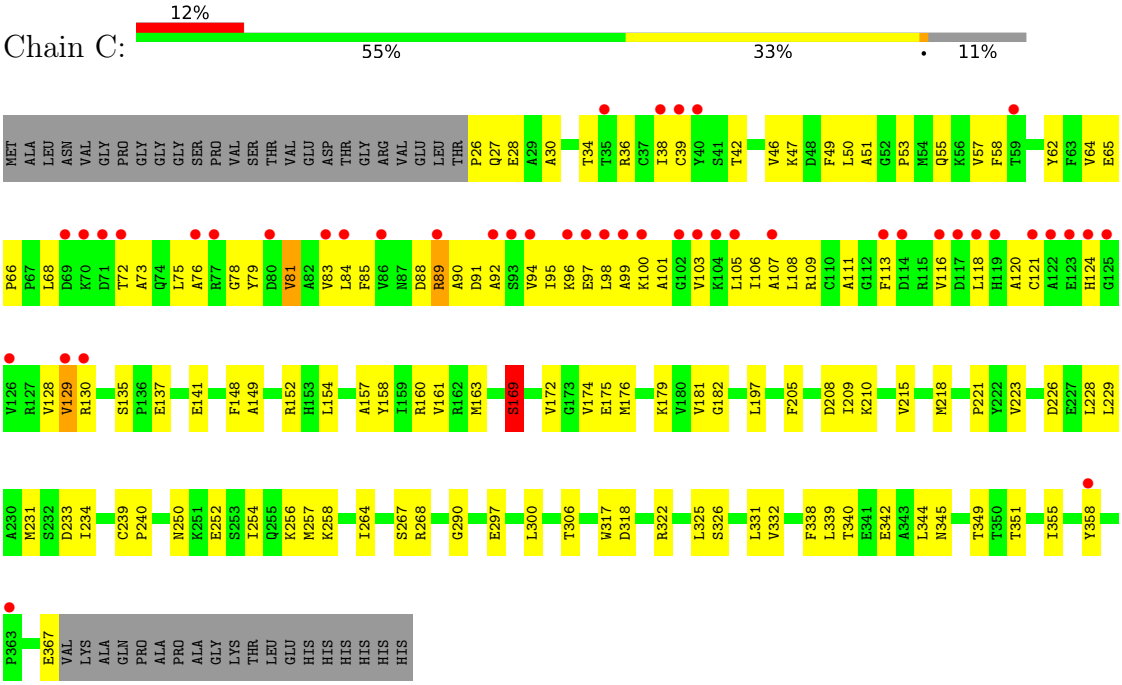
• Molecule 1: Putative D-lactate dehydrogenase

Chain B:



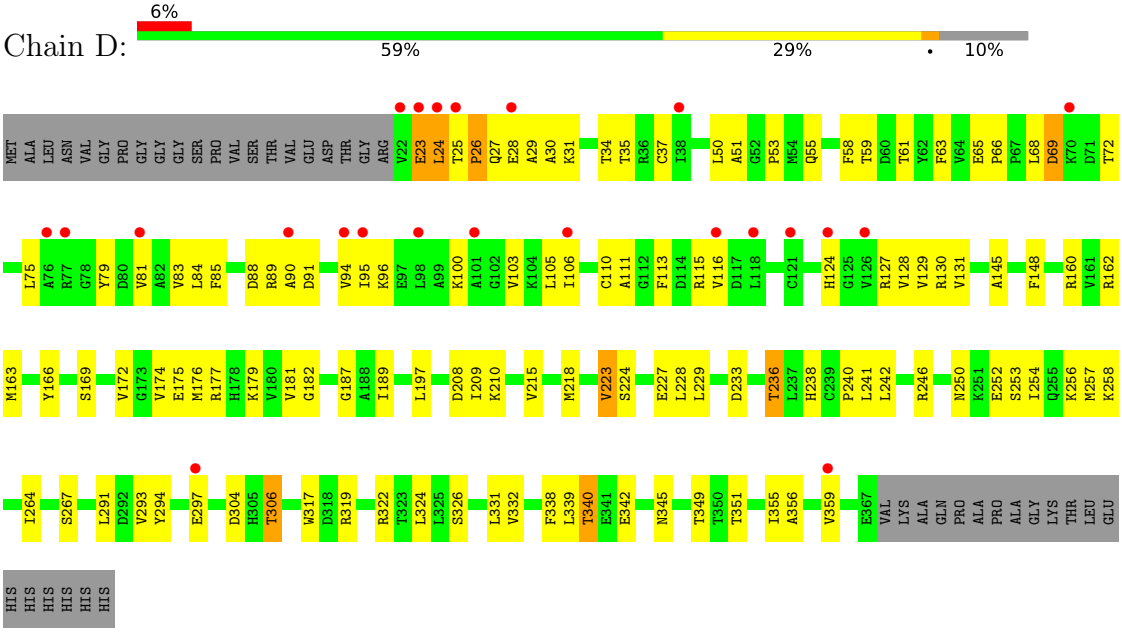
• Molecule 1: Putative D-lactate dehydrogenase

Chain C:



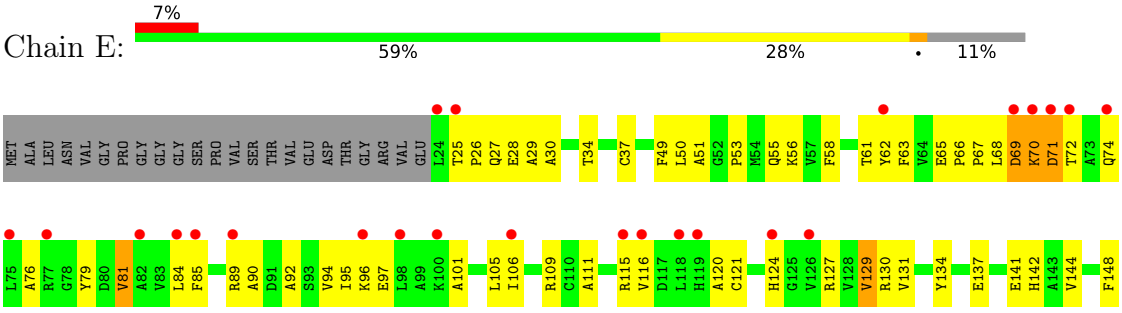
• Molecule 1: Putative D-lactate dehydrogenase

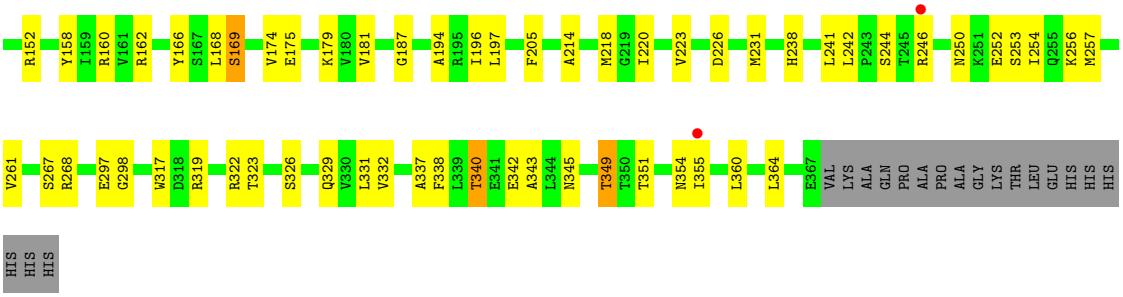
Chain D:



• Molecule 1: Putative D-lactate dehydrogenase

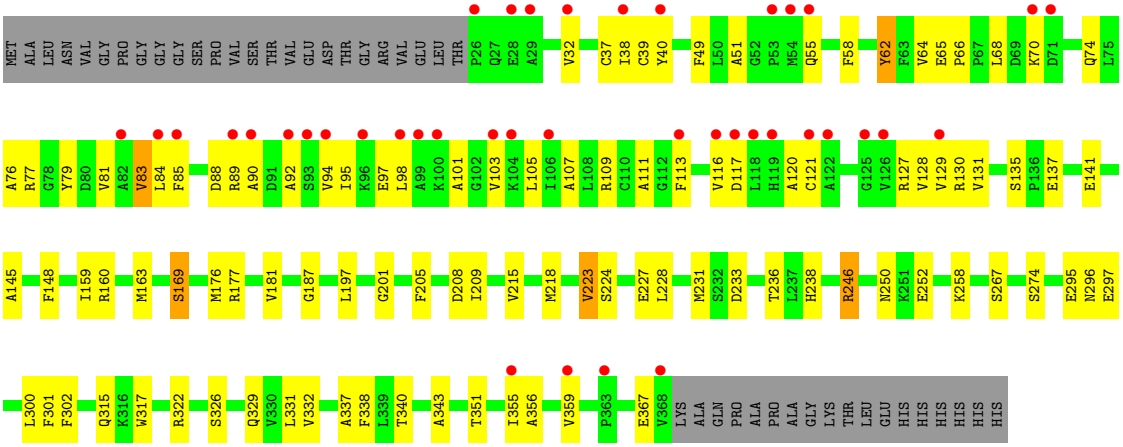
Chain E:





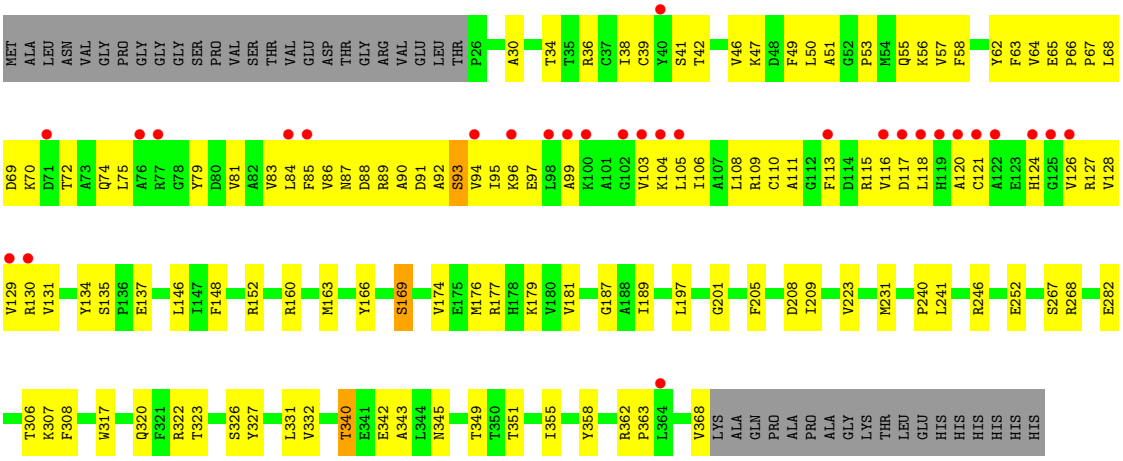
• Molecule 1: Putative D-lactate dehydrogenase

Chain F:



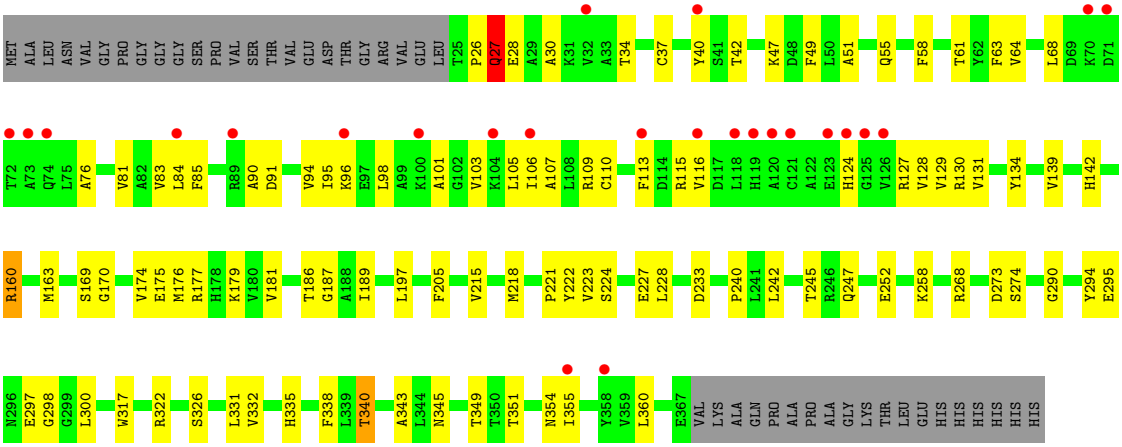
• Molecule 1: Putative D-lactate dehydrogenase

Chain G:



• Molecule 1: Putative D-lactate dehydrogenase

Chain H:


MET ALA LEU ASN VAL GLY PRO GLY GLY GLY SER PRO VAL SER THR VAL GLU ASP THR GLY ARG VAL GLU LEU T25 P26 Q27 E28 A29 A30 K31 V32 A33 T34 C37 Y40 S41 T42 K47 D48 F49 L50 A51 Q55 F58 T61 Y62 F63 V64 L68 D69 K70 D71
T72 A73 Q74 L75 A76 V81 A82 V83 L84 F85 R89 A90 D91 V94 I95 K96 E97 L98 A99 K100 A101 G102 V103 K104 L105 I106 A107 L108 R109 C110 F113 D114 R115 V116 D117 L118 H119 A120 C121 A122 E123 H124 G125 V126 R127 V128 V129 R130 V131 Y134 V139 H142
R160 M163 S169 G170 V174 E175 M176 R177 H178 K179 V180 V181 T186 G187 A188 I189 L197 F205 V215 M218 P221 Y222 V223 S224 E227 L228 D233 P240 L241 L242 T245 R246 Q247 E252 K258 R268 D273 S274 G290 Y294 E295
N296 E297 G298 G299 L300 W317 R322 S326 L331 V332 H335 F338 L339 T340 A343 L344 N345 T349 T350 T351 N354 I355 Y358 V359 L360 E367 VAL LYS ALA GLN PRO ALA PRO ALA GLY LYS THR LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.76Å 110.92Å 193.16Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	66.84 – 2.46 66.84 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.5 (66.84-2.46) 89.9 (66.84-2.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.254 0.205 , 0.255	Depositor DCC
R_{free} test set	6341 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21903	wwPDB-VP
Average B, all atoms (Å^2)	73.0	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 36.33 % 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 5.0818e-04. 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: 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	0.55	0/2710	0.75	1/3679 (0.0%)
1	B	0.52	0/2647	0.73	2/3593 (0.1%)
1	C	0.51	0/2682	0.73	2/3640 (0.1%)
1	D	0.51	0/2713	0.71	1/3684 (0.0%)
1	E	0.51	0/2697	0.72	2/3662 (0.1%)
1	F	0.53	0/2689	0.73	1/3650 (0.0%)
1	G	0.56	0/2689	0.76	1/3650 (0.0%)
1	H	0.51	0/2689	0.71	2/3651 (0.1%)
All	All	0.52	0/21516	0.73	12/29209 (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	1
1	C	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	SER	C-N-CA	7.24	137.50	122.30
1	F	169	SER	C-N-CA	7.08	137.16	122.30
1	G	169	SER	C-N-CA	6.87	136.72	122.30
1	B	169	SER	C-N-CA	6.84	136.66	122.30
1	H	169	SER	C-N-CA	6.18	135.27	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Peptide
1	C	89	ARG	Peptide
1	E	71	ASP	Peptide

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	2661	0	2707	107	0
1	B	2599	0	2646	137	0
1	C	2633	0	2674	134	0
1	D	2664	0	2706	109	0
1	E	2648	0	2691	112	0
1	F	2640	0	2683	106	0
1	G	2640	0	2683	142	0
1	H	2640	0	2680	89	0
2	A	44	26	26	6	0
2	B	44	26	26	8	0
2	C	44	26	26	6	0
2	D	44	26	26	5	0
2	E	44	26	26	3	0
2	F	44	26	26	4	0
2	G	44	26	26	9	0
2	H	44	26	26	5	0
3	A	30	0	0	3	0
3	B	33	0	0	6	0
3	C	25	0	0	1	0
3	D	27	0	0	3	0
3	E	33	0	0	3	0
3	F	21	0	0	2	0
3	G	20	0	0	1	0
3	H	29	0	0	2	0
All	All	21695	208	21678	889	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 21.

The worst 5 of 889 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:C:89:ARG:HB3	1:C:90:ALA:HA	1.21	1.16
1:F:38:ILE:HG22	1:F:62:TYR:HB3	1.18	1.15
1:E:70:LYS:HB3	1:E:71:ASP:HB2	1.31	1.12
1:C:106:ILE:HD11	1:C:128:VAL:HG13	1.31	1.09
1:G:89:ARG:HG3	1:G:115:ARG:HE	1.17	1.04

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	344/386 (89%)	336 (98%)	8 (2%)	0	100	100
1	B	336/386 (87%)	329 (98%)	7 (2%)	0	100	100
1	C	340/386 (88%)	331 (97%)	9 (3%)	0	100	100
1	D	344/386 (89%)	335 (97%)	7 (2%)	2 (1%)	25	29
1	E	342/386 (89%)	333 (97%)	9 (3%)	0	100	100
1	F	341/386 (88%)	335 (98%)	6 (2%)	0	100	100
1	G	341/386 (88%)	331 (97%)	10 (3%)	0	100	100
1	H	341/386 (88%)	334 (98%)	5 (2%)	2 (1%)	25	29
All	All	2729/3088 (88%)	2664 (98%)	61 (2%)	4 (0%)	51	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	LEU
1	H	27	GLN
1	H	26	PRO

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Mol	Chain	Res	Type
1	D	26	PRO

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	287/318 (90%)	285 (99%)	2 (1%)	84	90
1	B	280/318 (88%)	275 (98%)	5 (2%)	59	71
1	C	284/318 (89%)	281 (99%)	3 (1%)	73	82
1	D	288/318 (91%)	281 (98%)	7 (2%)	49	61
1	E	286/318 (90%)	279 (98%)	7 (2%)	49	61
1	F	285/318 (90%)	279 (98%)	6 (2%)	53	66
1	G	285/318 (90%)	281 (99%)	4 (1%)	67	77
1	H	285/318 (90%)	282 (99%)	3 (1%)	73	82
All	All	2280/2544 (90%)	2243 (98%)	37 (2%)	62	74

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	223	VAL
1	H	49	PHE
1	F	246	ARG
1	G	320	GLN
1	D	174	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	ASN
1	F	151	ASN
1	H	247	GLN
1	G	151	ASN

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Mol	Chain	Res	Type
1	B	354	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	C	1000	-	42,48,48	2.60	18 (42%)	50,73,73	1.56	9 (18%)
2	NAD	H	1000	-	42,48,48	2.62	17 (40%)	50,73,73	1.55	10 (20%)
2	NAD	B	1000	-	42,48,48	2.57	17 (40%)	50,73,73	1.52	9 (18%)
2	NAD	G	1000	-	42,48,48	2.55	17 (40%)	50,73,73	1.68	11 (22%)
2	NAD	A	1000	-	42,48,48	2.62	17 (40%)	50,73,73	1.55	11 (22%)
2	NAD	E	1000	-	42,48,48	2.63	17 (40%)	50,73,73	1.58	11 (22%)
2	NAD	D	1000	-	42,48,48	2.58	17 (40%)	50,73,73	1.60	8 (16%)
2	NAD	F	1000	-	42,48,48	2.59	17 (40%)	50,73,73	1.59	8 (16%)

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	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	H	1000	-	-	13/26/62/62	0/5/5/5
2	NAD	B	1000	-	-	11/26/62/62	0/5/5/5
2	NAD	G	1000	-	-	8/26/62/62	0/5/5/5
2	NAD	A	1000	-	-	12/26/62/62	0/5/5/5
2	NAD	E	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	D	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	F	1000	-	-	11/26/62/62	0/5/5/5

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NAD	O4B-C1B	6.60	1.50	1.41
2	H	1000	NAD	O4B-C1B	6.39	1.50	1.41
2	E	1000	NAD	O4B-C1B	6.30	1.49	1.41
2	D	1000	NAD	O4B-C1B	6.27	1.49	1.41
2	F	1000	NAD	O4B-C1B	6.21	1.49	1.41

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1000	NAD	C2A-N1A-C6A	5.48	128.13	118.75
2	C	1000	NAD	C2A-N1A-C6A	5.48	128.13	118.75
2	B	1000	NAD	C2A-N1A-C6A	5.45	128.08	118.75
2	E	1000	NAD	C2A-N1A-C6A	5.31	127.83	118.75
2	G	1000	NAD	C2A-N1A-C6A	5.28	127.79	118.75

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAD	O4B-C4B-C5B-O5B
2	A	1000	NAD	O4D-C1D-N1N-C2N
2	A	1000	NAD	O4D-C1D-N1N-C6N
2	B	1000	NAD	C5D-O5D-PN-O1N
2	B	1000	NAD	O4D-C1D-N1N-C2N

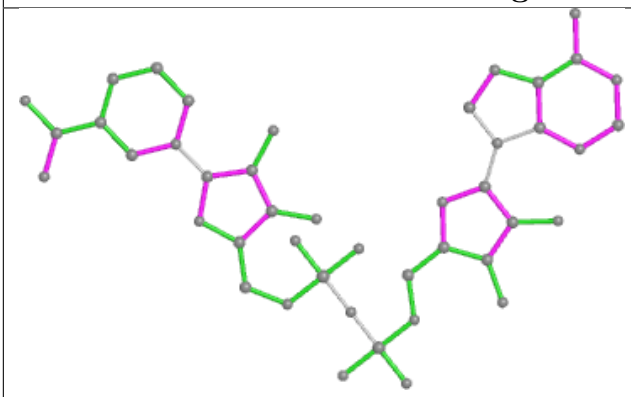
There are no ring outliers.

8 monomers are involved in 46 short contacts:

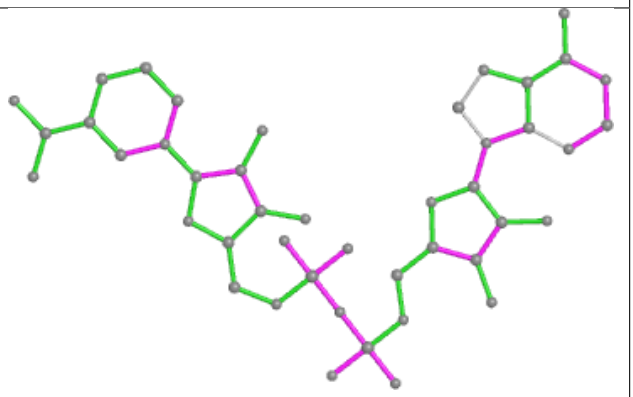
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	NAD	6	0
2	H	1000	NAD	5	0
2	B	1000	NAD	8	0
2	G	1000	NAD	9	0
2	A	1000	NAD	6	0
2	E	1000	NAD	3	0
2	D	1000	NAD	5	0
2	F	1000	NAD	4	0

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.

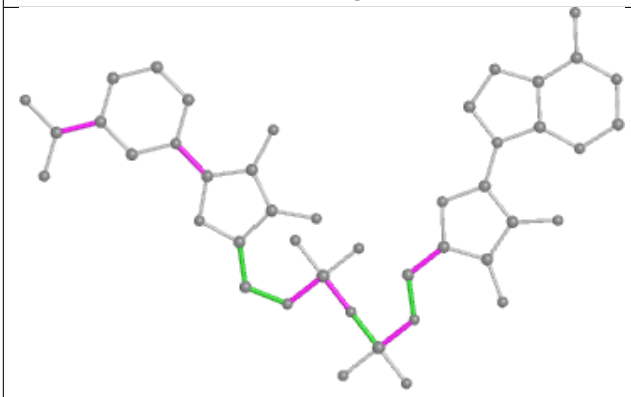
Ligand NAD C 1000



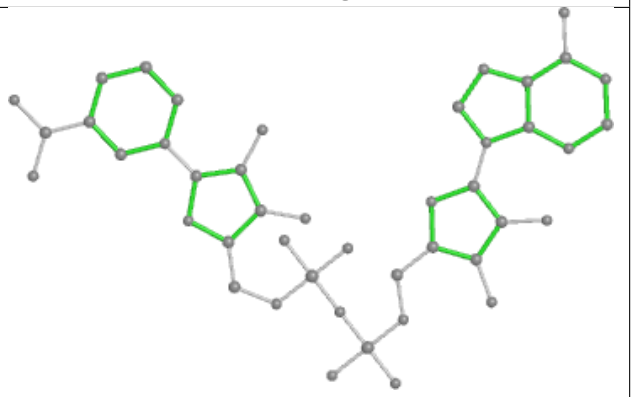
Bond lengths



Bond angles

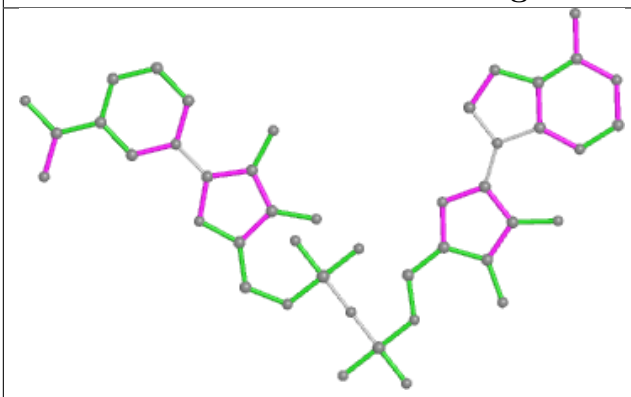


Torsions

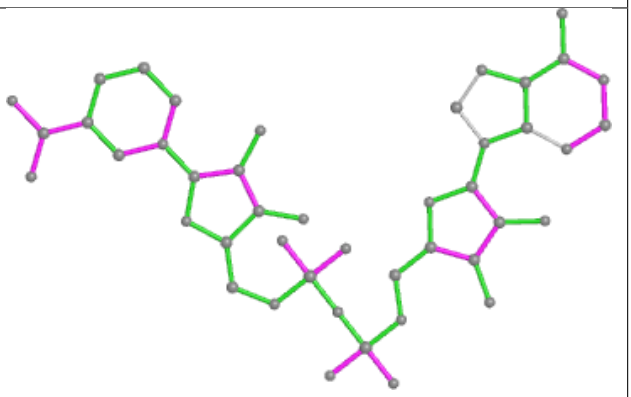


Rings

Ligand NAD H 1000



Bond lengths



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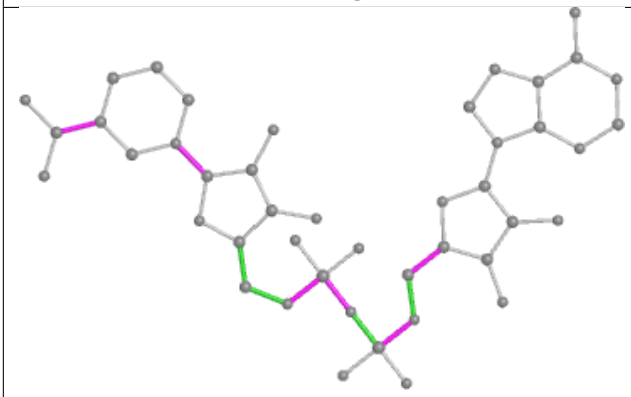
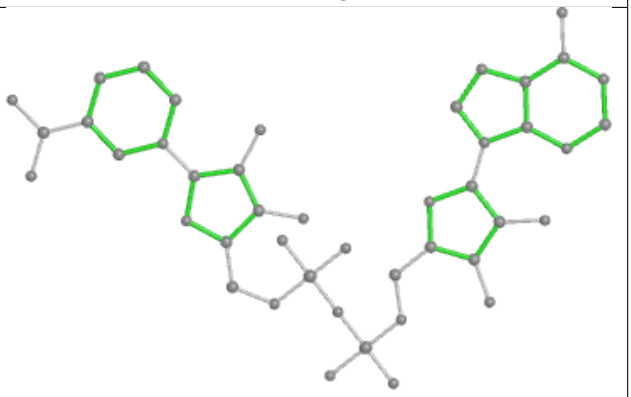
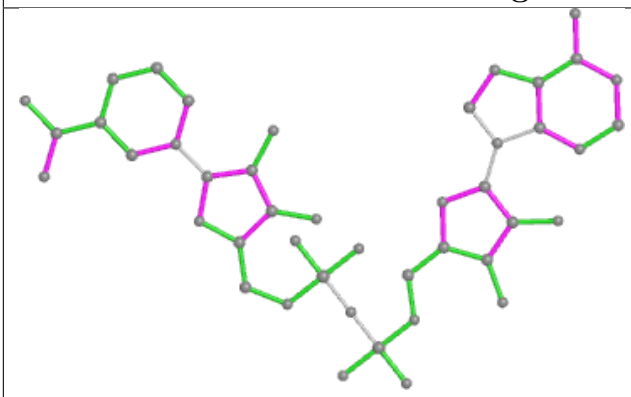


Torsions

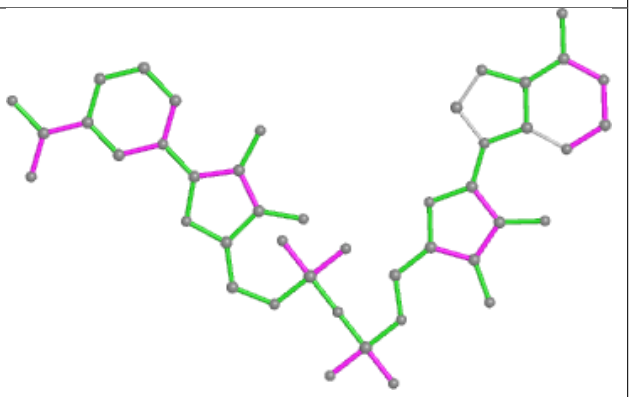


Rings

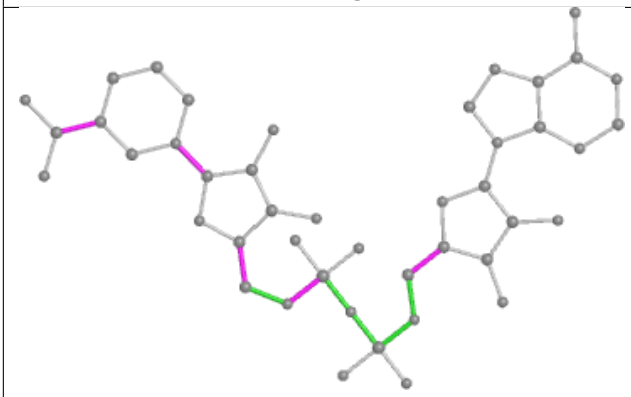
Ligand NAD B 1000



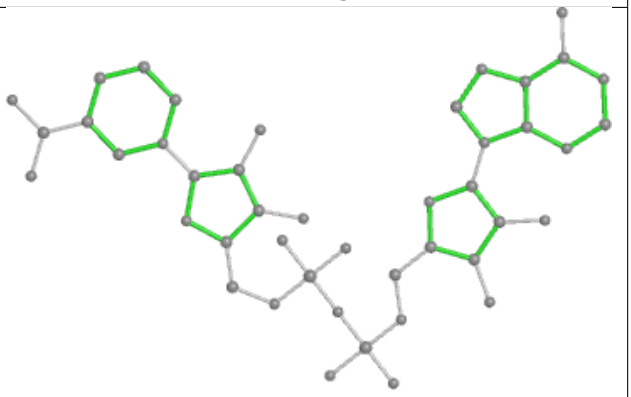
Bond lengths



Bond angles

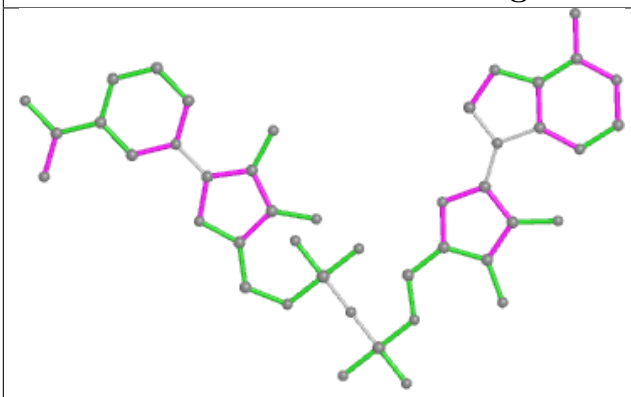


Torsions

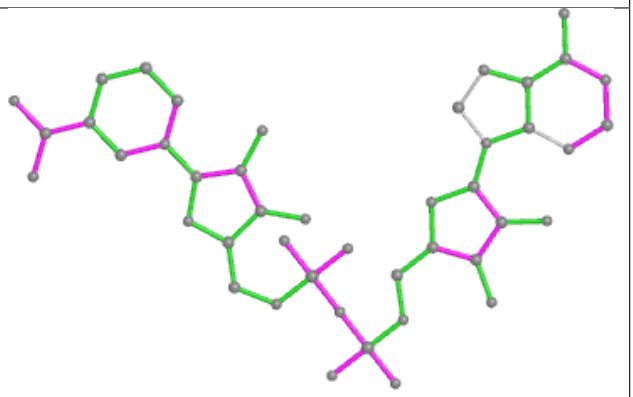


Rings

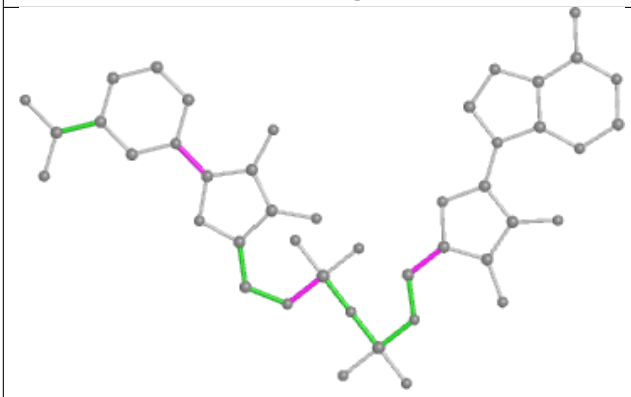
Ligand NAD G 1000



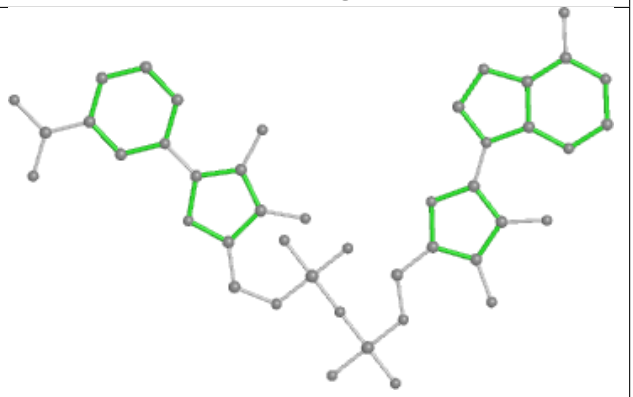
Bond lengths



Bond angles

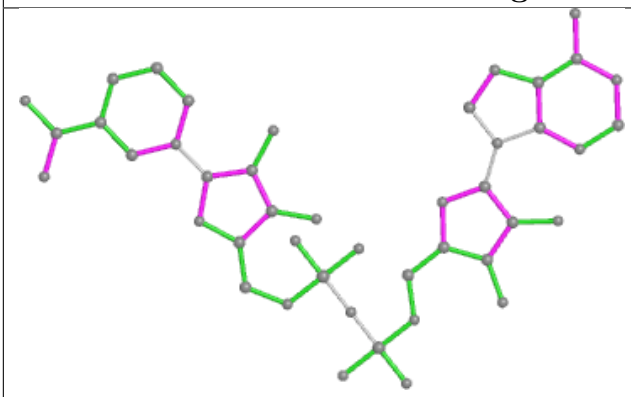


Torsions

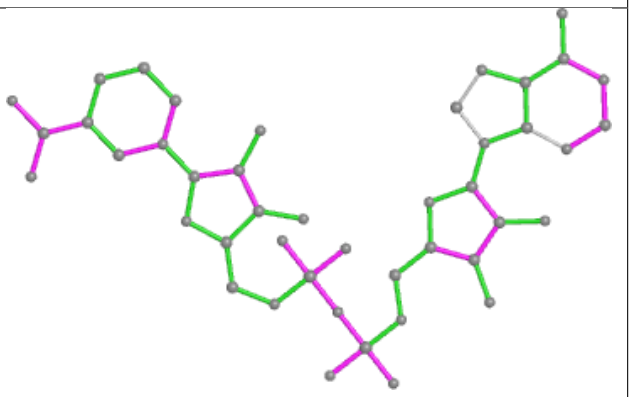


Rings

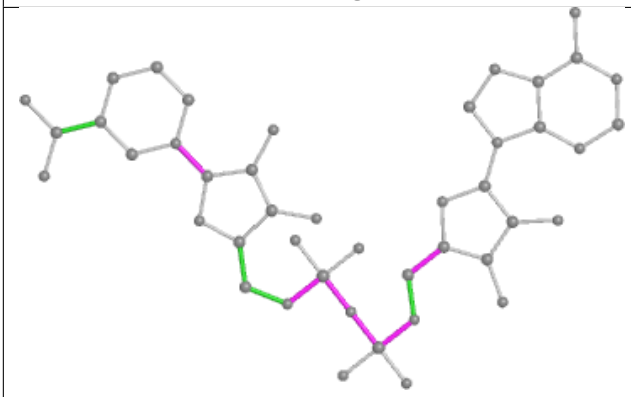
Ligand NAD A 1000



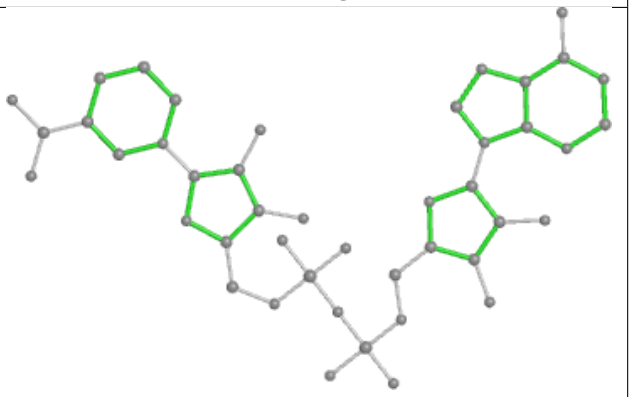
Bond lengths



Bond angles

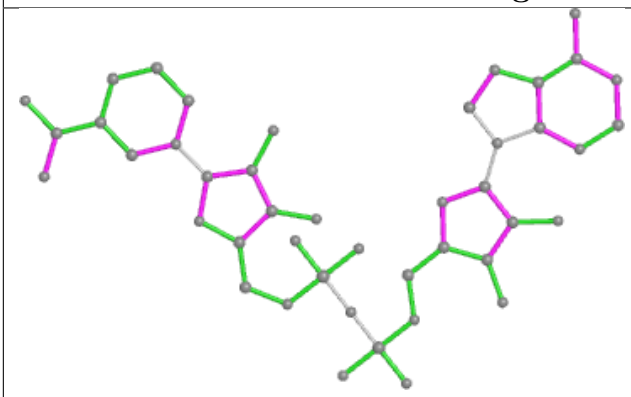


Torsions

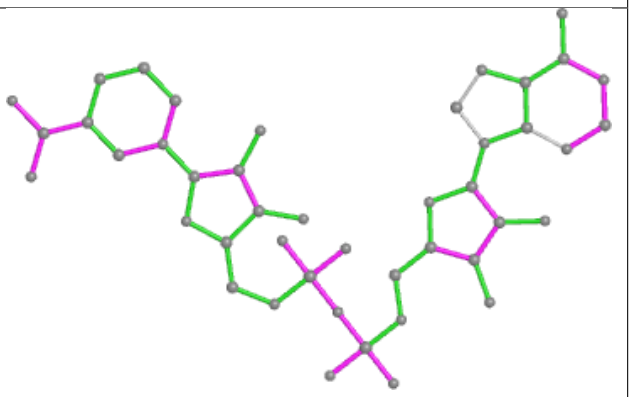


Rings

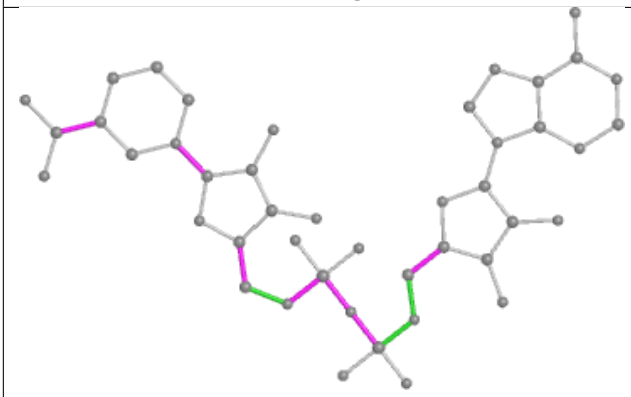
Ligand NAD E 1000



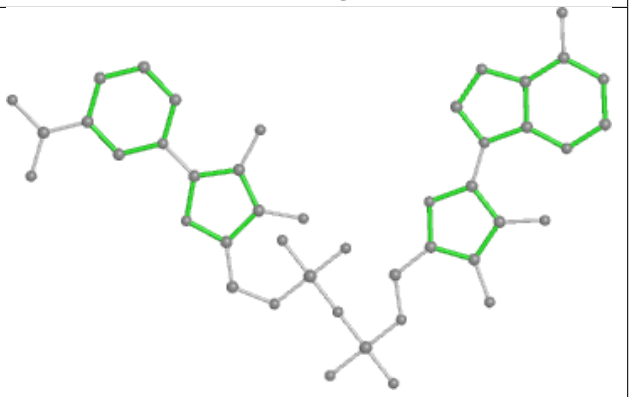
Bond lengths



Bond angles

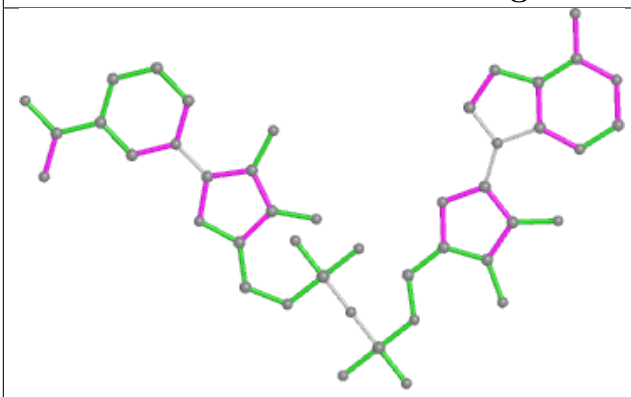


Torsions

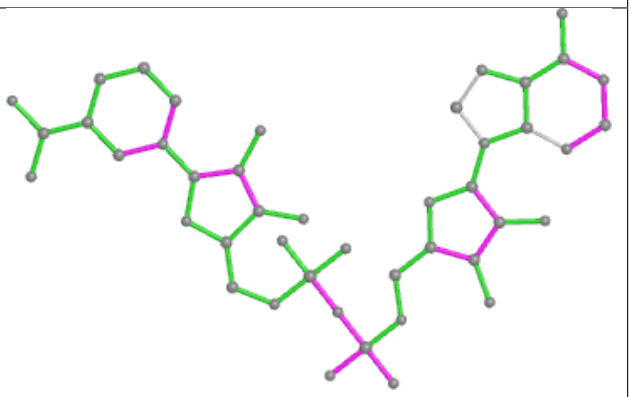


Rings

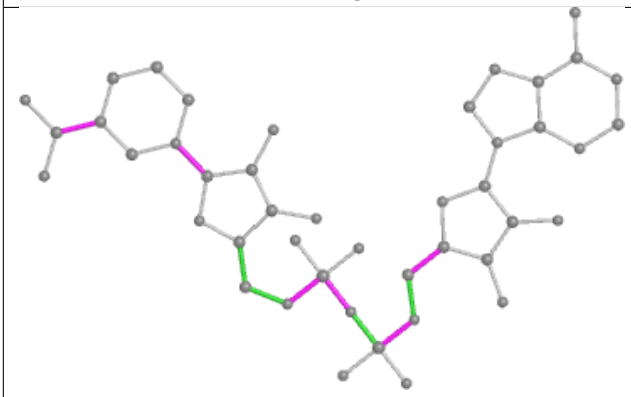
Ligand NAD D 1000



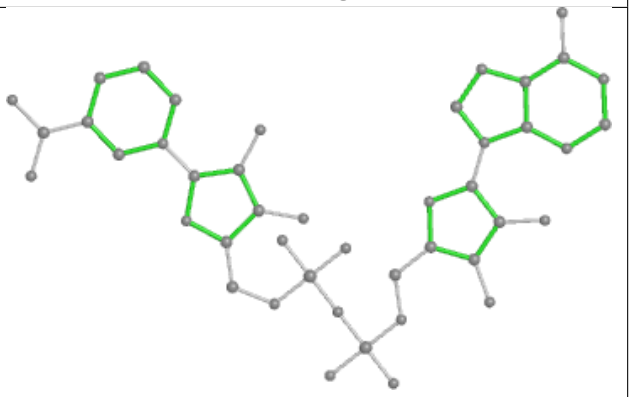
Bond lengths



Bond angles

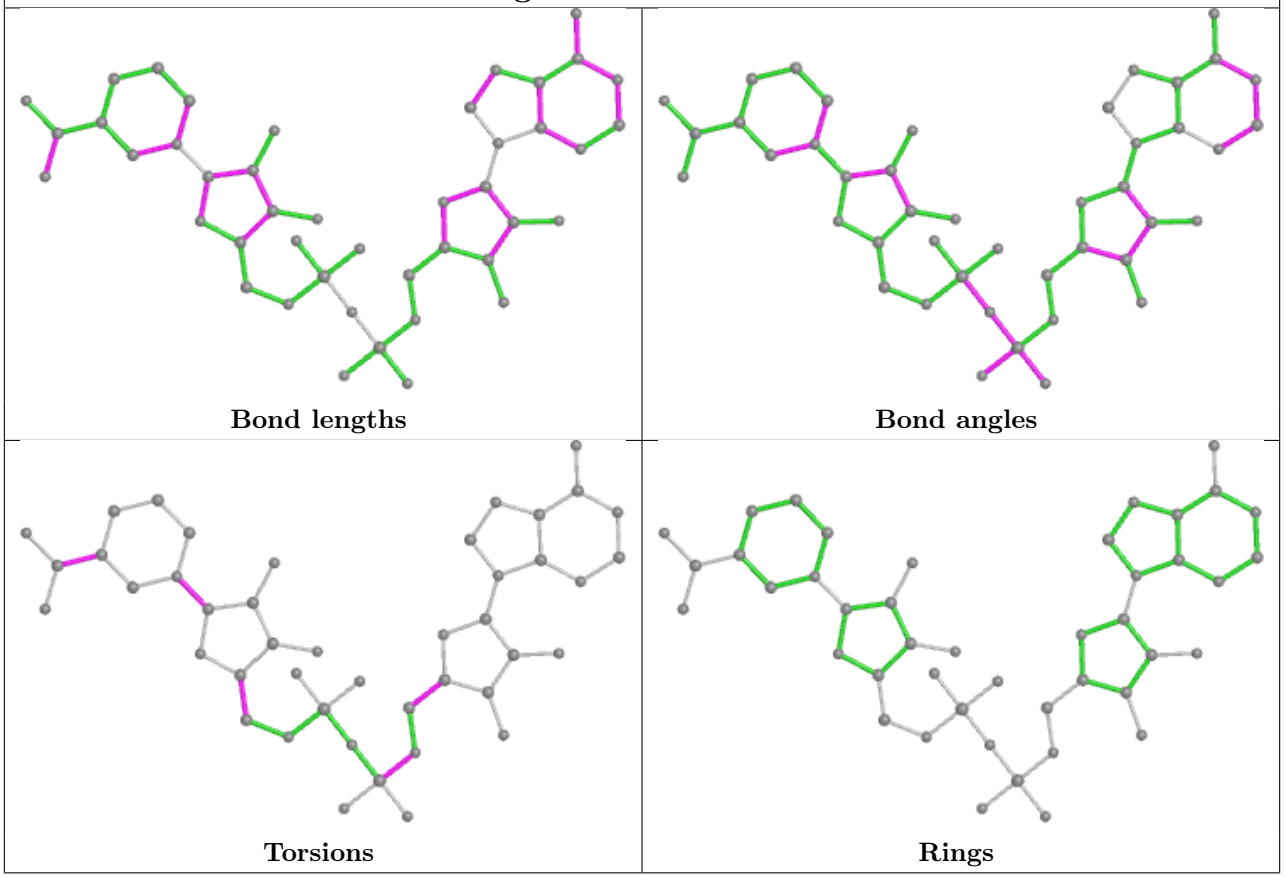


Torsions



Rings

Ligand NAD F 1000



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	346/386 (89%)	0.00	4 (1%) 79 77	30, 57, 95, 134	0
1	B	338/386 (87%)	0.58	50 (14%) 2 1	27, 61, 146, 199	0
1	C	342/386 (88%)	0.53	45 (13%) 3 2	32, 61, 160, 208	0
1	D	346/386 (89%)	0.21	23 (6%) 18 14	31, 58, 120, 175	0
1	E	344/386 (89%)	0.22	26 (7%) 13 10	30, 63, 133, 165	0
1	F	343/386 (88%)	0.43	40 (11%) 4 3	30, 58, 128, 170	0
1	G	343/386 (88%)	0.48	29 (8%) 10 8	29, 58, 163, 203	0
1	H	343/386 (88%)	0.36	25 (7%) 15 11	28, 59, 124, 173	0
All	All	2745/3088 (88%)	0.35	242 (8%) 10 7	27, 59, 138, 208	0

The worst 5 of 242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	CYS	12.3
1	C	98	LEU	10.4
1	G	98	LEU	9.1
1	G	94	VAL	8.0
1	B	93	SER	7.9

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)

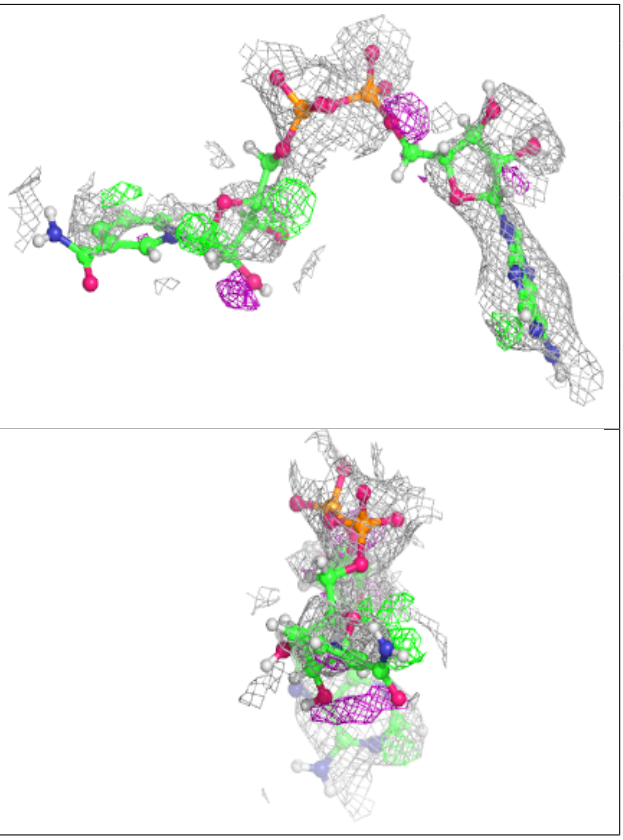
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAD	H	1000	44/44	0.63	0.42	161,163,197,199	0
2	NAD	B	1000	44/44	0.70	0.41	169,174,209,214	0
2	NAD	F	1000	44/44	0.73	0.43	172,177,213,216	0
2	NAD	D	1000	44/44	0.75	0.38	156,163,195,204	0
2	NAD	E	1000	44/44	0.75	0.35	153,176,211,218	0
2	NAD	C	1000	44/44	0.76	0.52	205,211,254,256	0
2	NAD	A	1000	44/44	0.77	0.36	157,163,196,197	0
2	NAD	G	1000	44/44	0.86	0.28	112,128,155,161	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.

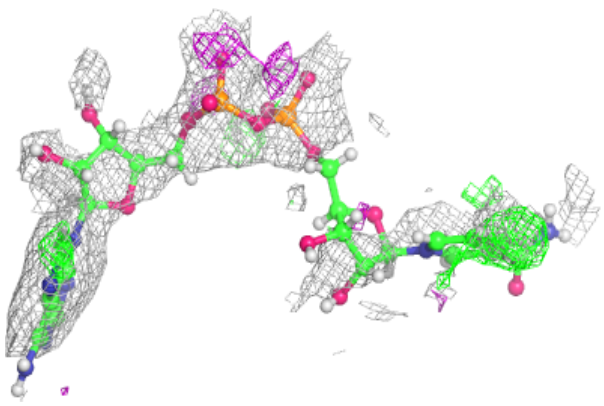
Electron density around NAD H 1000:

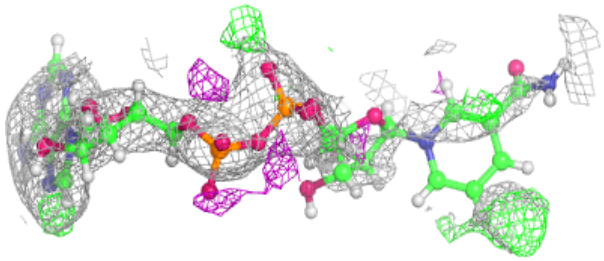
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

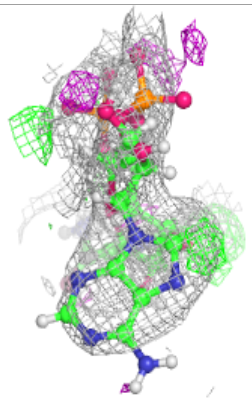


Electron density around NAD B 1000:

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

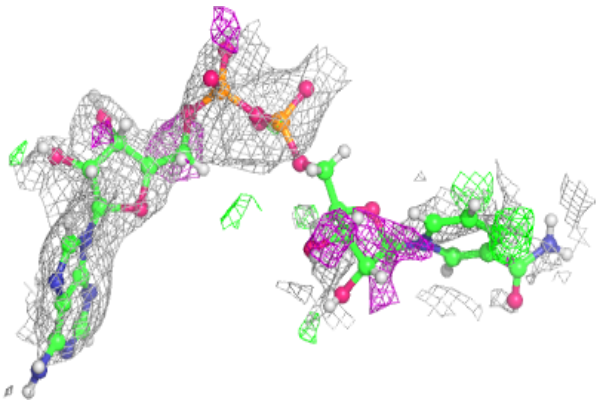


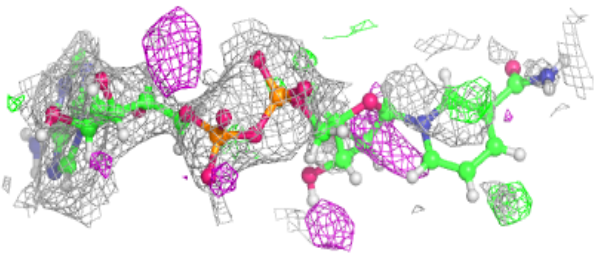


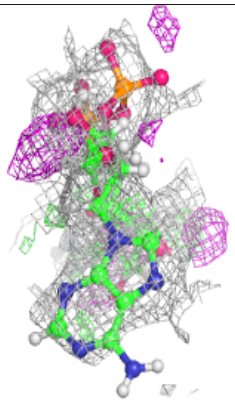


Electron density around NAD F 1000:

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

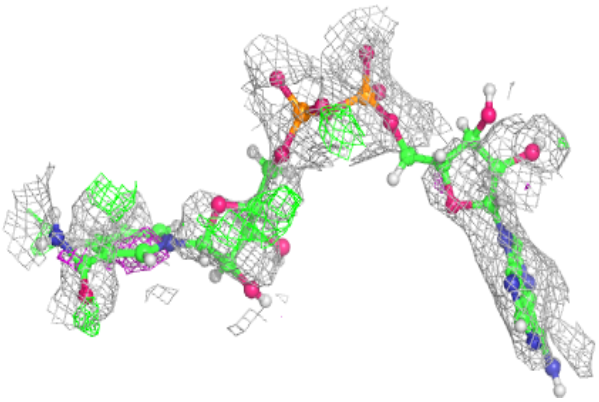


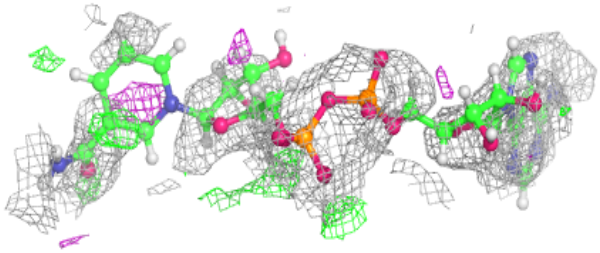


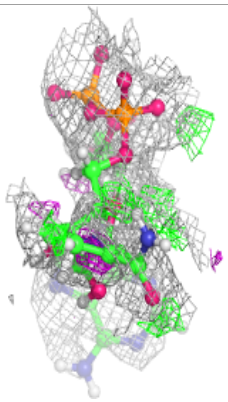


Electron density around NAD D 1000:

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

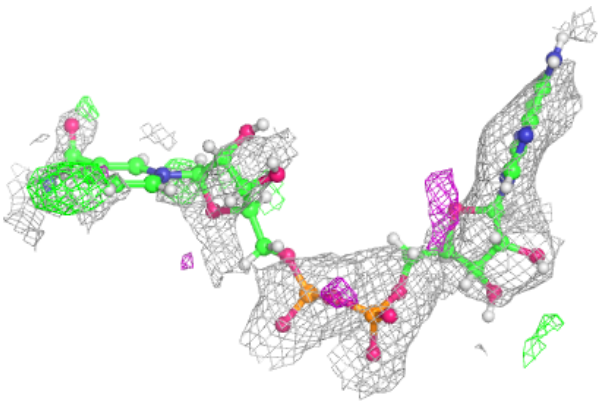


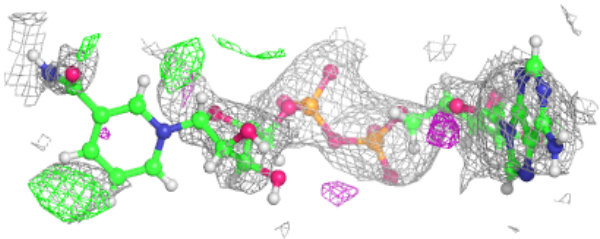


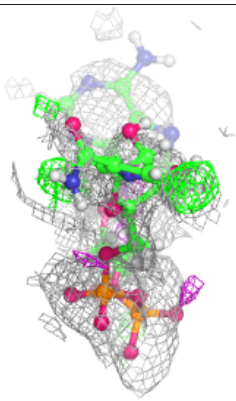


Electron density around NAD E 1000:

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

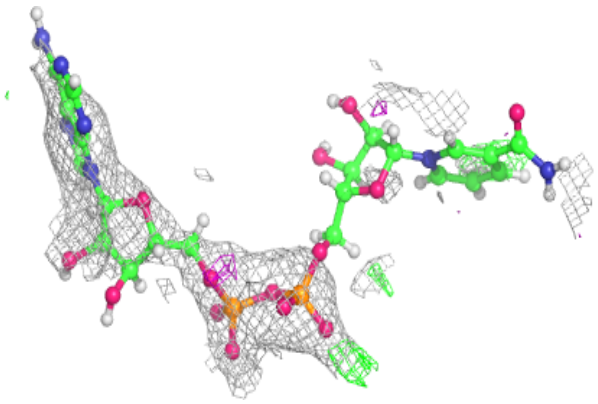


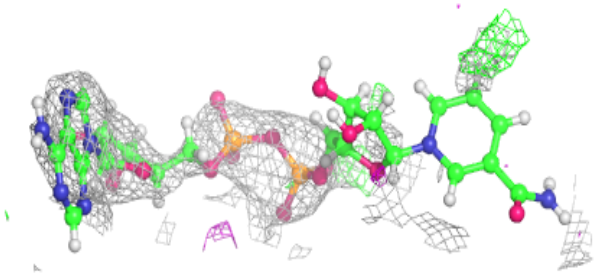


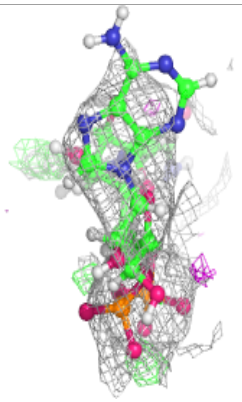


Electron density around NAD C 1000:

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

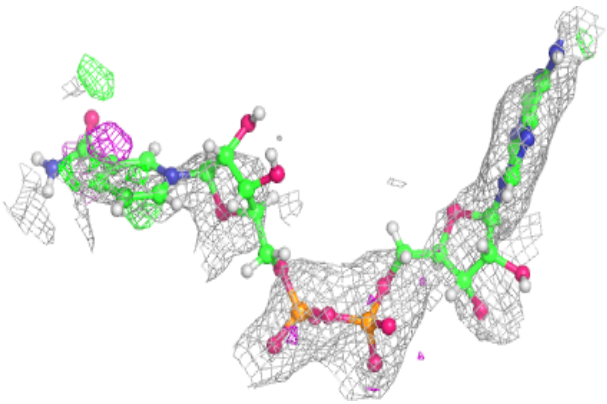


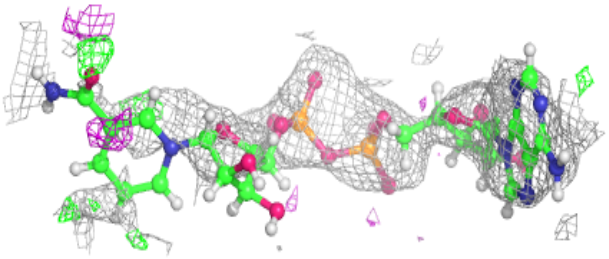


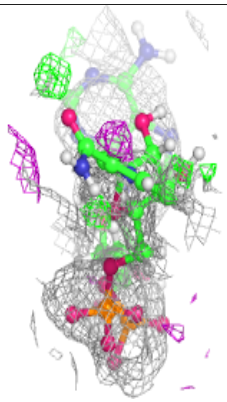


Electron density around NAD A 1000:

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

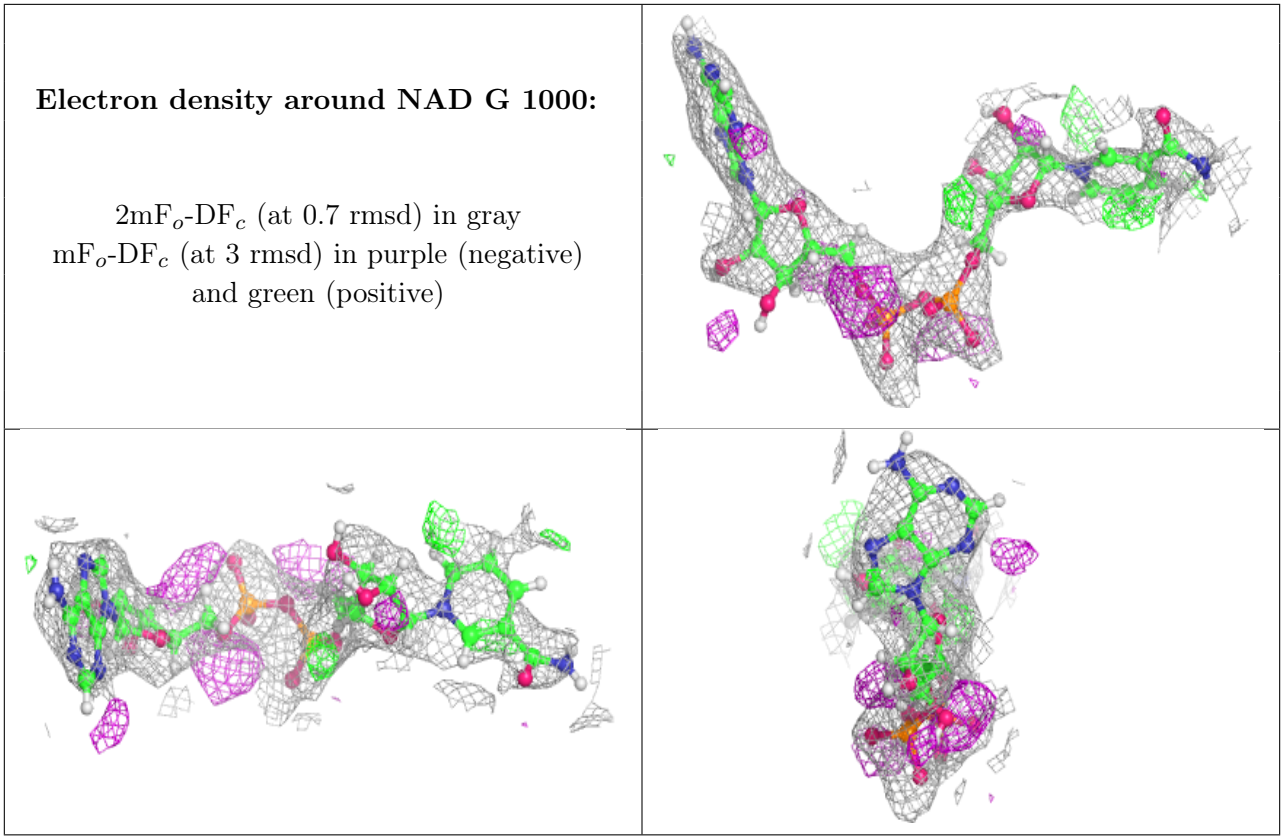






Electron density around NAD G 1000:

$2mF_o$-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.