wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 07:42 am BST

PDB ID	:	3HDH
Title	:	PIG HEART SHORT CHAIN L-3-HYDROXYACYL COA DEHYDROGENASE REVISITED: SEQUENCE ANALYSIS AND CRYSTAL STRUCTURE DETERMINATION
Authors	:	Barycki, J.J.; O'Brien, L.K.; Birktoft, J.J.; Strauss, A.W.; Banaszak, L.J.
Deposited on	:	1999-04-13
Resolution	:	2.80 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 (i)) were used in the production of this report:

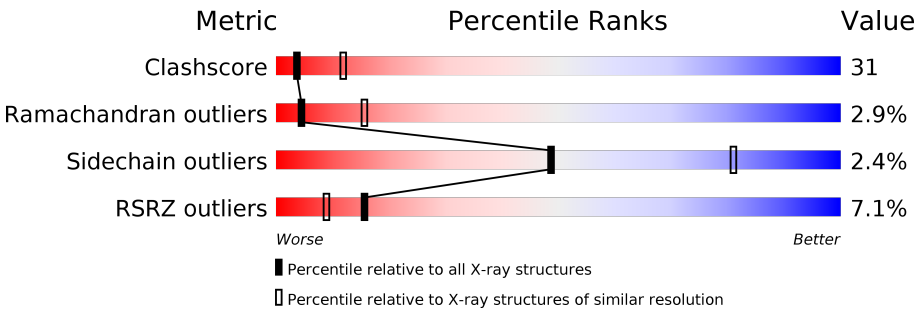
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	302	% 61% 33% • •
1	B	302	% 56% 37% • •
1	C	302	18% 35% 48% 5% 12%

2 Entry composition (i)

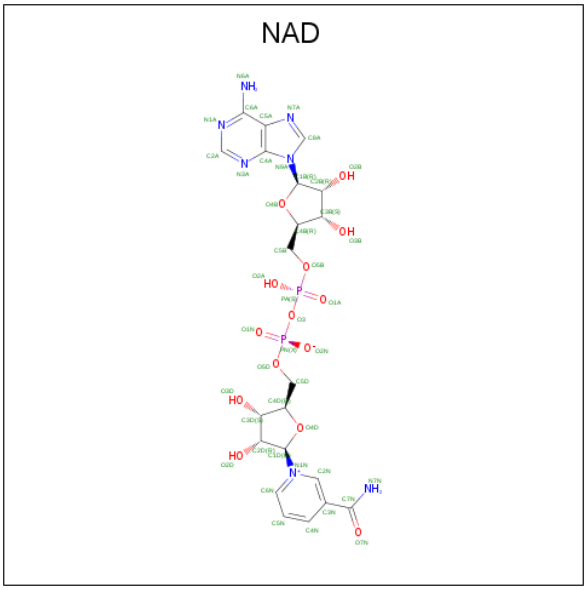
There are 3 unique types of molecules in this entry. The entry contains 6661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (L-3-HYDROXYACYL COA DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	2241	1434	373	426	8	0	0	0
			Total	C	N	O	S			
1	B	291	2237	1431	372	426	8	0	0	0
			Total	C	N	O	S			
1	C	265	2028	1298	339	385	6	0	0	0

- 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
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	B	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	C	1	44	21	7	14	2	0	0

- Molecule 3 is water.

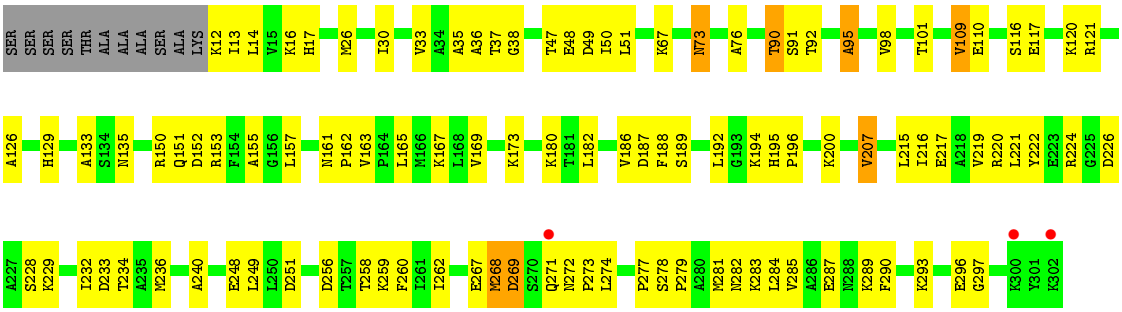
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	7	7	7	0	0
			Total	O		
3	B	16	16	16	0	0

3 Residue-property plots (i)

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

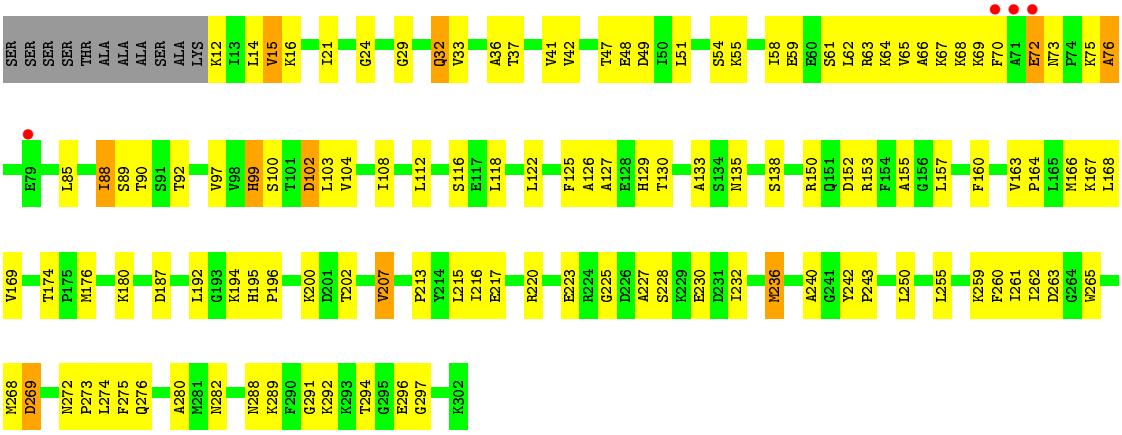
- Molecule 1: PROTEIN (L-3-HYDROXYACYL COA DEHYDROGENASE)

Chain A:



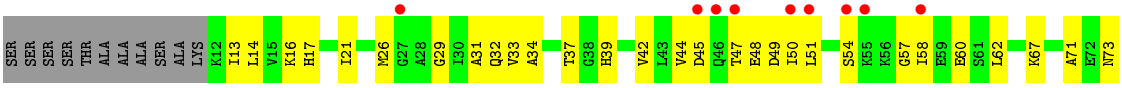
- Molecule 1: PROTEIN (L-3-HYDROXYACYL COA DEHYDROGENASE)

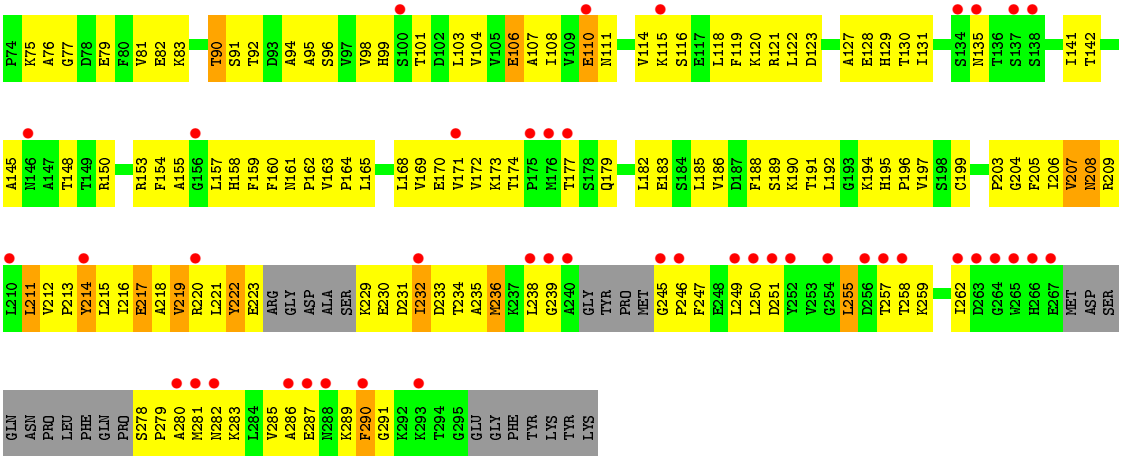
Chain B:



- Molecule 1: PROTEIN (L-3-HYDROXYACYL COA DEHYDROGENASE)

Chain C:




P74 K75 A76 G77 D78 E79 F80 V81 E82 K83
T90 S91 T92 D93 A94 A95 S96 V97 V98 H99 S100 T101 D102 L103 V104 V105 E106 A107 I108 V109 E110 N111
V114 K115 S116 E117 L118 F119 K120 R121 L122 D123
A127 E128 H129 T130 I131
S134 N135 T136 S137 S138
I141 T142
A145 N146 A147 T148 T149 R150
R153 F154 A155 G156 L157 H158 F159 F160 N161 P162 V163 P164 L165
L168 V169 E170 V171 V172 K173 T174 P175 M176 T177 S178 Q179
L182 E183 S184 L185 V186 D187 F188 S189 K190 T191 L192 G193 K194 H195 P196 V197 S198 C199
P203 G204 F205 I206 V207 N208 R209
L210 L211 V212 P213 Y214 L215 I216 E217 A218 V219 R220 L221 Y222 E223 ARG GLY ASP ALA SER K229 E230 D231 I232 D233 T234 A235 M236 R237 L238 G239 A240 GLY TYR PRO MET G245 P246 F247 E248 L249 L250 D251 Y252 V253 G254 L255 D256 T257 T258 K259
I262 D263 G264 W265 H266 E267 MET ASP SER
GLN ASN PRO LEU PHE GLN PRO S278 P279 A280 M281 N282 K283 L284 V285 A286 E287 N288 K289 F290 G291 K292 K293 T294 G295 GLU GLY PHE TYR LYS TYR LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	227.20Å 82.10Å 124.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.35 – 2.66	Depositor EDS
% Data completeness (in resolution range)	84.7 (20.00-2.80) 85.3 (29.35-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.287 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6661	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.42	0/2282	0.70	0/3080
1	B	0.42	0/2278	0.69	0/3076
1	C	0.52	0/2058	0.77	0/2775
All	All	0.45	0/6618	0.72	0/8931

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	222	TYR	Sidechain

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	2241	0	2298	105	0
1	B	2237	0	2287	132	0
1	C	2028	0	2101	196	1
2	A	44	0	25	2	0
2	B	44	0	25	2	0
2	C	44	0	26	4	0
3	A	7	0	0	1	0
3	B	16	0	0	2	0
All	All	6661	0	6762	420	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 420 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:47:THR:HG22	1:C:48:GLU:H	1.13	1.10
1:C:215:LEU:HD21	1:C:249:LEU:HD23	1.38	1.03
1:A:47:THR:HB	1:A:50:ILE:HG13	1.40	1.01
1:C:236:MET:HG2	1:C:246:PRO:HD3	1.43	1.00
1:C:231:ASP:HA	1:C:234:THR:HB	1.47	0.96

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLU:CG	1:C:217:GLU:CG[3_555]	2.06	0.14

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	289/302 (96%)	259 (90%)	21 (7%)	9 (3%)	4 14
1	B	289/302 (96%)	227 (78%)	52 (18%)	10 (4%)	3 12
1	C	257/302 (85%)	218 (85%)	34 (13%)	5 (2%)	8 26
All	All	835/906 (92%)	704 (84%)	107 (13%)	24 (3%)	4 15

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ASP
1	B	72	GLU
1	B	207	VAL
1	A	36	ALA
1	A	268	MET

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	247/254 (97%)	245 (99%)	2 (1%)	81 94
1	B	246/254 (97%)	241 (98%)	5 (2%)	55 84
1	C	225/254 (89%)	215 (96%)	10 (4%)	28 61
All	All	718/762 (94%)	701 (98%)	17 (2%)	49 81

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	THR
1	C	106	GLU
1	C	232	ILE
1	B	276	GLN
1	C	236	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	B	195	HIS
1	C	179	GLN
1	A	288	ASN
1	C	99	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	350	-	42,48,48	2.39	11 (26%)	50,73,73	2.53	17 (34%)
2	NAD	B	750	-	42,48,48	2.51	13 (30%)	50,73,73	2.51	16 (32%)
2	NAD	C	1150	-	42,48,48	2.73	15 (35%)	50,73,73	2.55	16 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	350	-	-	11/26/62/62	0/5/5/5
2	NAD	B	750	-	-	7/26/62/62	0/5/5/5
2	NAD	C	1150	-	-	5/26/62/62	0/5/5/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAD	C2A-N3A	7.22	1.43	1.32
2	C	1150	NAD	C2A-N3A	6.90	1.43	1.32
2	B	750	NAD	C2A-N3A	6.88	1.43	1.32
2	C	1150	NAD	C4N-C3N	6.46	1.50	1.39
2	C	1150	NAD	C7N-N7N	6.31	1.45	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1150	NAD	C2A-N1A-C6A	6.90	130.56	118.75
2	B	750	NAD	C2A-N1A-C6A	6.73	130.27	118.75
2	A	350	NAD	C2A-N1A-C6A	6.46	129.80	118.75
2	C	1150	NAD	C5N-C4N-C3N	-6.10	113.12	120.34
2	A	350	NAD	C5N-C4N-C3N	-6.00	113.25	120.34

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	350	NAD	O4D-C1D-N1N-C2N
2	A	350	NAD	O4D-C1D-N1N-C6N
2	A	350	NAD	C2D-C1D-N1N-C2N
2	A	350	NAD	C2D-C1D-N1N-C6N
2	B	750	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

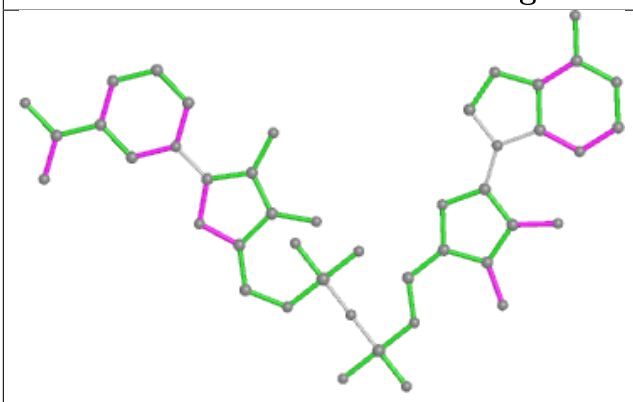
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	NAD	2	0
2	B	750	NAD	2	0
2	C	1150	NAD	4	0

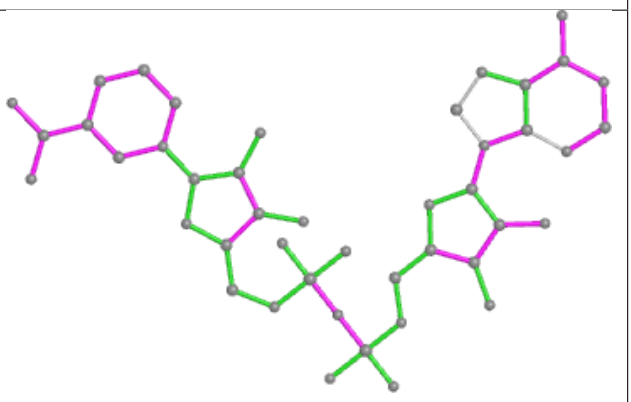
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

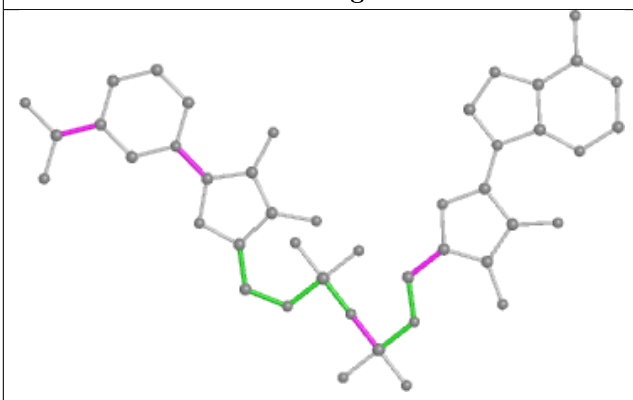
Ligand NAD A 350



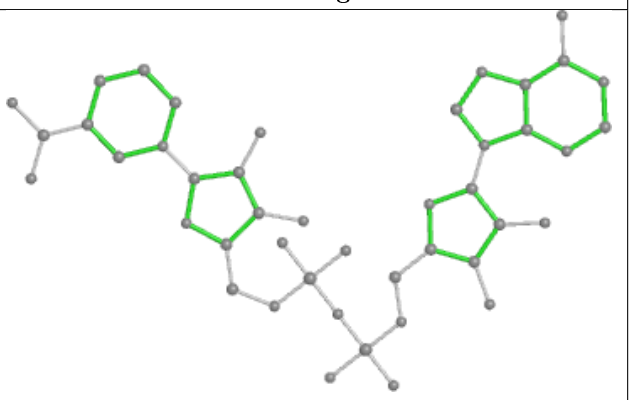
Bond lengths



Bond angles

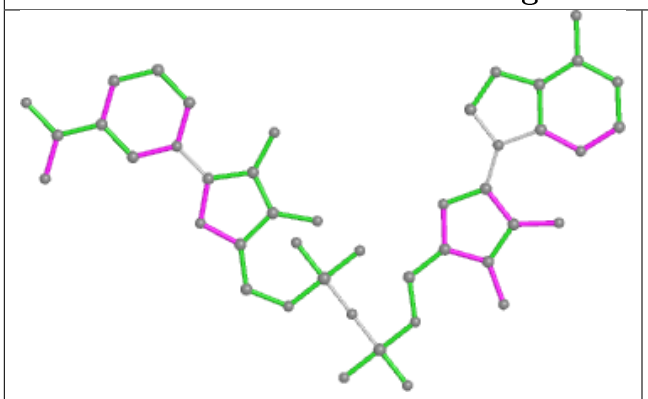


Torsions

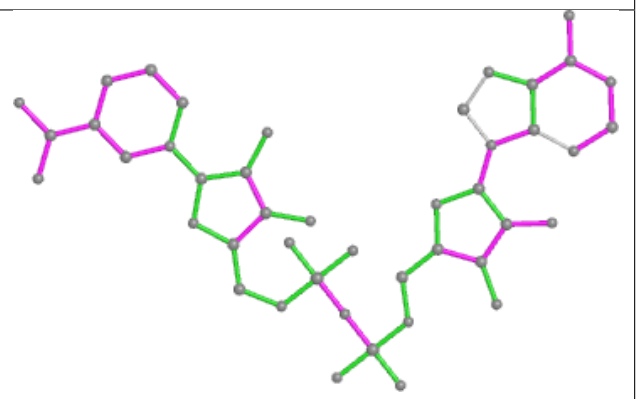


Rings

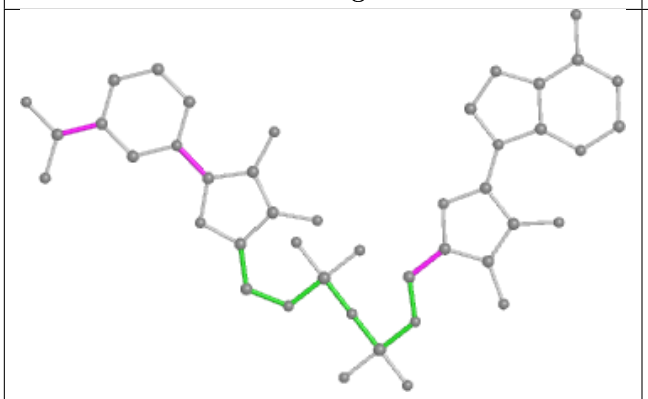
Ligand NAD B 750



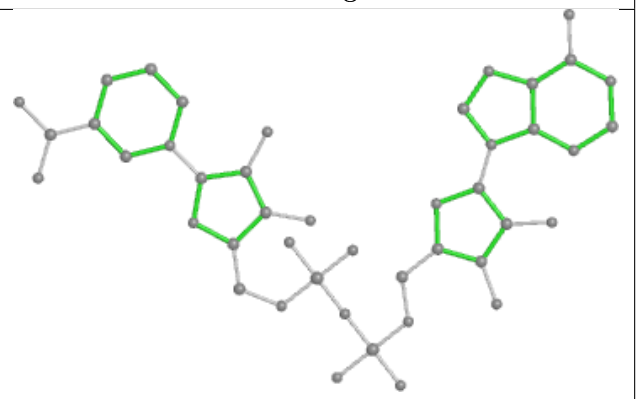
Bond lengths



Bond angles

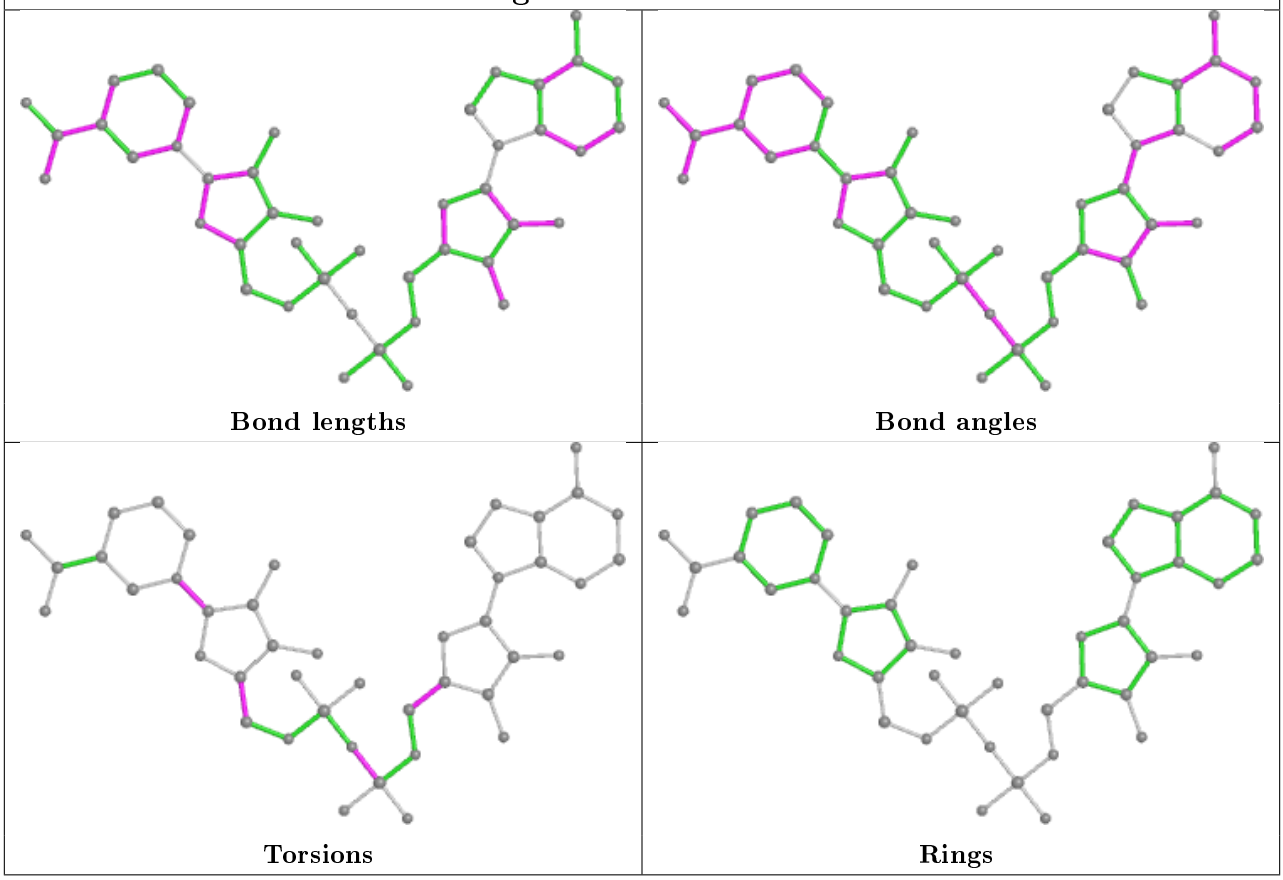


Torsions



Rings

Ligand NAD C 1150



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	291/302 (96%)	-0.54	3 (1%)	82	77	17, 42, 82, 99	0
1	B	291/302 (96%)	-0.27	4 (1%)	75	70	17, 53, 95, 100	0
1	C	265/302 (87%)	1.00	53 (20%)	1	0	26, 87, 100, 100	28 (10%)
All	All	847/906 (93%)	0.04	60 (7%)	16	9	17, 60, 99, 100	28 (3%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	ILE	7.0
1	C	288	ASN	6.4
1	C	258	THR	5.6
1	C	210	LEU	5.1
1	C	286	ALA	4.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

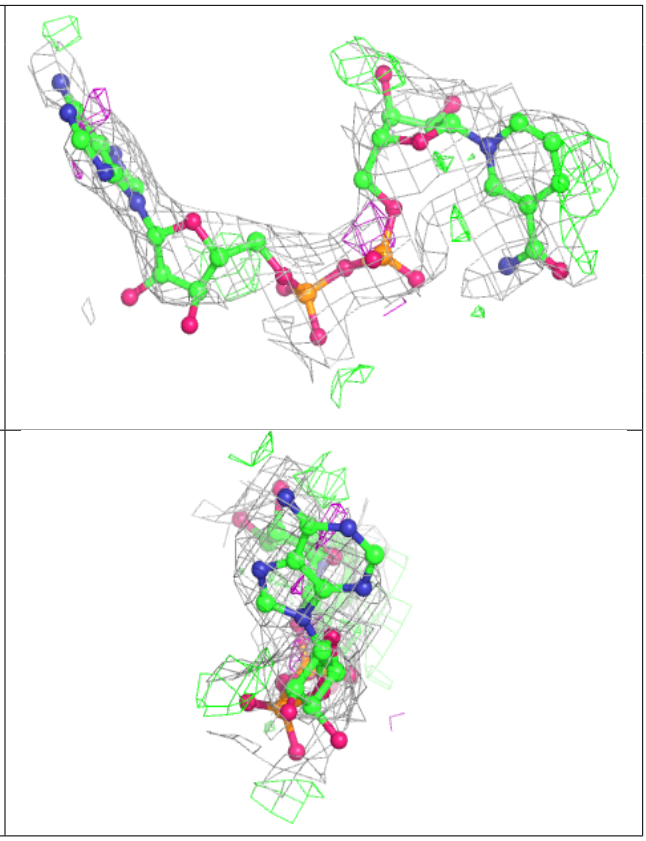
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	1150	44/44	0.60	0.33	81,99,100,100	0
2	NAD	B	750	44/44	0.92	0.17	53,68,77,81	0
2	NAD	A	350	44/44	0.96	0.16	32,65,70,82	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.

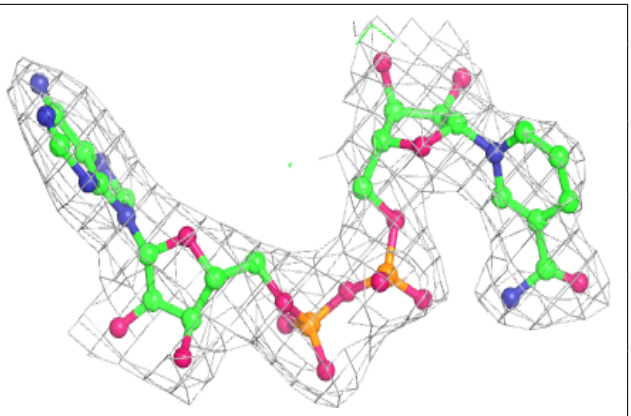
Electron density around NAD C 1150:

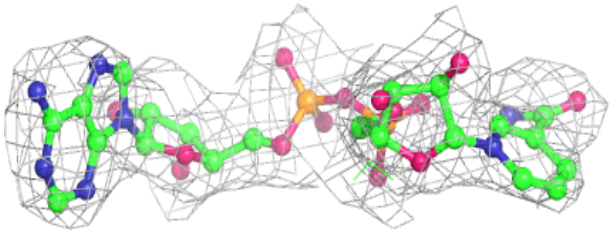
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

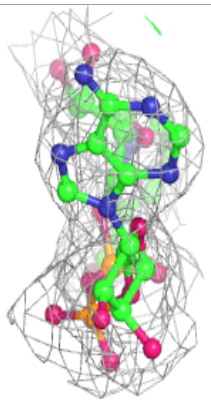


Electron density around NAD B 750:

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

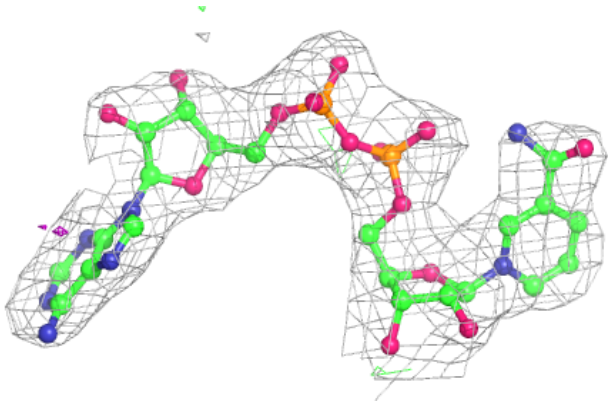


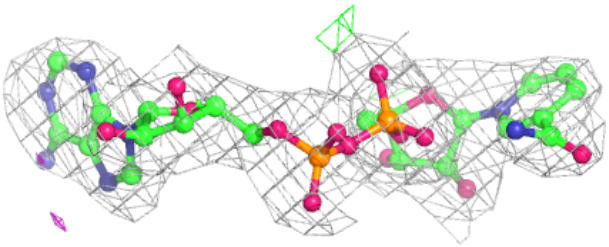


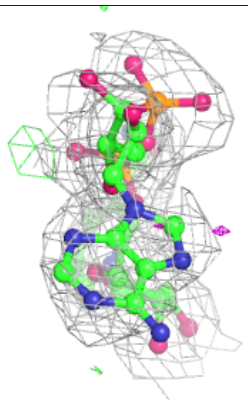


Electron density around NAD A 350:

$2mF_o$-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.