wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 05:44 PM EDT

PDB ID	:	1J0X
Title	:	Crystal structure of the rabbit muscle glyceraldehyde-3-phosphate dehydrogenase (GAPDH)
Authors	:	Cowan-Jacob, S.W.; Kaufmann, M.; Anselmo, A.N.; Stark, W.; Grutter, M.G.
Deposited on	:	2002-11-25
Resolution	:	2.40 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:

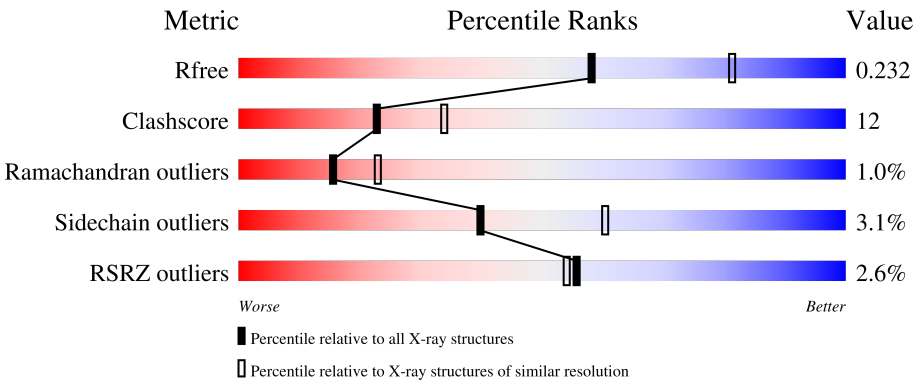
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

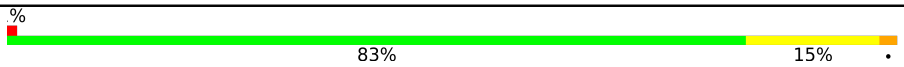
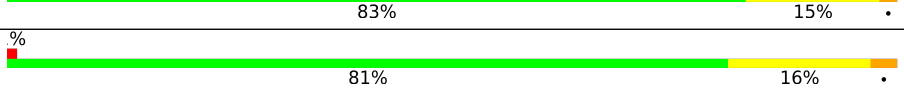
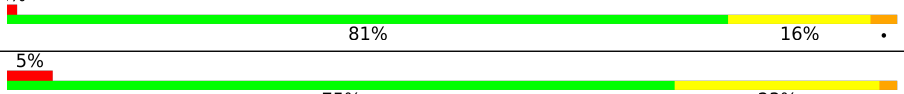
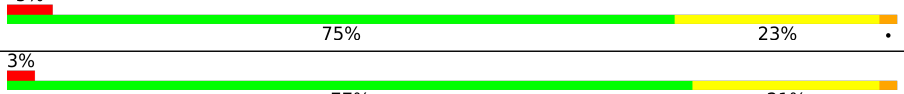
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	O	332	
1	P	332	
1	Q	332	
1	R	332	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10605 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 glyceraldehyde-3-phosphate dehydrogenase.

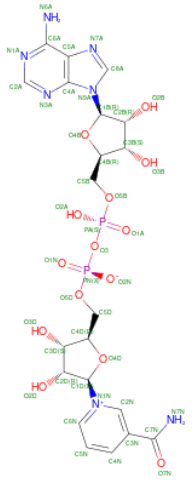
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	332	2511	1588	436	474	13	0	0	0
1	P	332	2511	1588	436	474	13	0	0	0
1	Q	332	2511	1588	436	474	13	0	0	0
1	R	332	2511	1588	436	474	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	123	ALA	UNK	SEE REMARK 999	UNP P46406
O	149	CSX	CYS	modified residue	UNP P46406
O	286	ASP	ALA	SEE REMARK 999	UNP P46406
P	123	ALA	UNK	SEE REMARK 999	UNP P46406
P	149	CSX	CYS	modified residue	UNP P46406
P	286	ASP	ALA	SEE REMARK 999	UNP P46406
Q	123	ALA	UNK	SEE REMARK 999	UNP P46406
Q	149	CSX	CYS	modified residue	UNP P46406
Q	286	ASP	ALA	SEE REMARK 999	UNP P46406
R	123	ALA	UNK	SEE REMARK 999	UNP P46406
R	149	CSX	CYS	modified residue	UNP P46406
R	286	ASP	ALA	SEE REMARK 999	UNP P46406

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

NAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	P	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	R	1	44	21	7	14	2	0	0

- Molecule 3 is water.

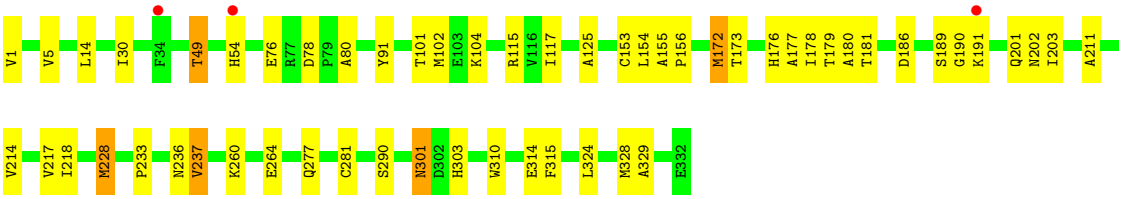
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	O	120	120	120	0	0
			Total	O		
3	P	132	132	132	0	0
			Total	O		
3	Q	108	108	108	0	0
			Total	O		
3	R	113	113	113	0	0

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.

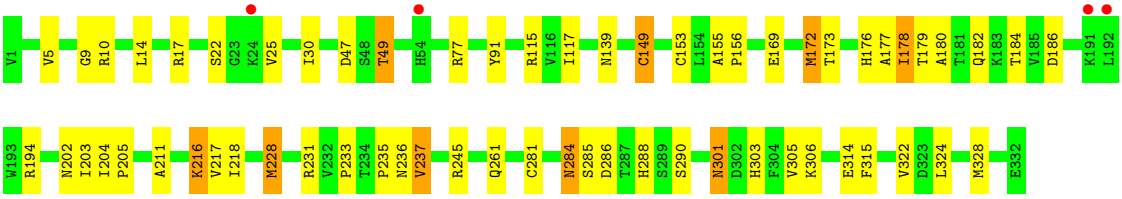
• Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain O:



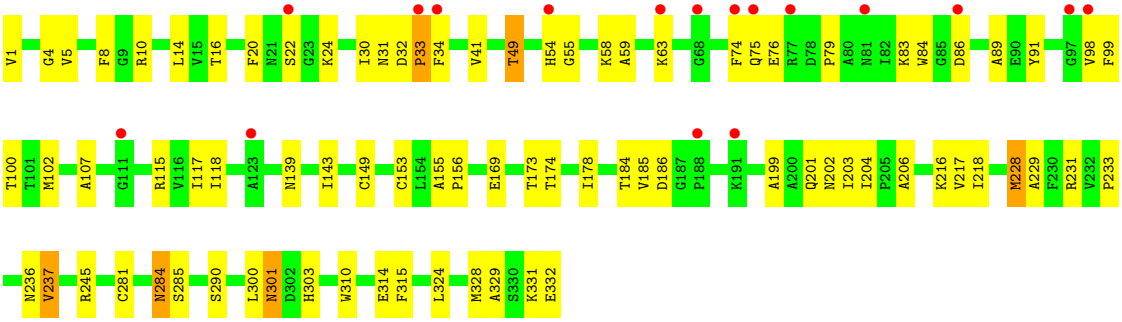
• Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain P:



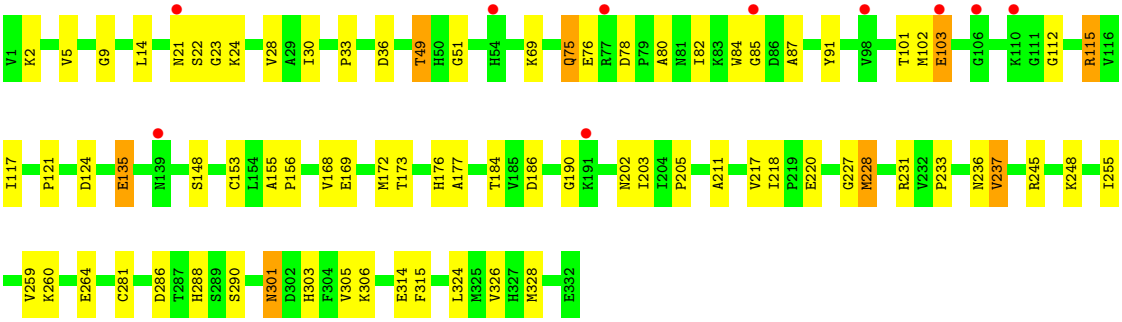
• Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain Q:



• Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain R:


V1
K2
V5
G9
L14
N21
S22
G23
K24
V28
A29
I30
P33
D36
T49
H50
G51
H54
K69
Q75
E76
R77
D78
P79
A80
N81
I82
K83
W84
G85
D86
A87
Y91
V98
T101
M102
E103
G106
K110
G111
G112
R115
V116
I117
P121
D124
E135
N139
S148
C153
L154
A155
P156
V168
E169
M172
T173
H176
A177
T184
V185
D186
G190
K191
N202
I203
I204
P205
A211
V217
I218
P219
E220
G227
M228
R231
V232
P233
N236
V237
R245
K248
I255
V259
K260
E264
C281
D286
T287
H288
S289
S290
N301
D302
H303
F304
V305
K306
E314
F315
L324
M325
V326
H327
M328
E332

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.70Å 98.50Å 183.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.93 – 2.40 17.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (17.93-2.40) 96.3 (17.93-2.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.80 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.239 0.198 , 0.232	Depositor DCC
R_{free} test set	2853 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10605	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, CSX

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	O	0.51	0/2553	0.60	1/3453 (0.0%)
1	P	0.52	0/2553	0.61	1/3453 (0.0%)
1	Q	0.52	0/2553	0.61	1/3453 (0.0%)
1	R	0.51	0/2553	0.60	1/3453 (0.0%)
All	All	0.52	0/10212	0.60	4/13812 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	203	ILE	N-CA-C	-6.61	93.16	111.00
1	O	203	ILE	N-CA-C	-6.52	93.40	111.00
1	Q	203	ILE	N-CA-C	-6.45	93.60	111.00
1	P	203	ILE	N-CA-C	-6.38	93.78	111.00

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	O	2511	0	2510	53	0
1	P	2511	0	2510	65	0
1	Q	2511	0	2510	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2511	0	2510	70	0
2	P	44	0	26	3	0
2	R	44	0	26	1	0
3	O	120	0	0	3	0
3	P	132	0	0	7	0
3	Q	108	0	0	7	0
3	R	113	0	0	5	0
All	All	10605	0	10092	233	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 12.

The worst 5 of 233 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:R:301:ASN:HD22	1:R:303:HIS:H	1.21	0.88
1:Q:178:ILE:HD12	1:Q:199:ALA:HB1	1.53	0.88
1:Q:281:CYS:HB2	1:R:202:ASN:HD21	1.37	0.88
1:O:281:CYS:HB2	1:P:202:ASN:HD21	1.40	0.87
1:Q:281:CYS:H	1:R:202:ASN:HD22	1.24	0.86

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	O	329/332 (99%)	314 (95%)	12 (4%)	3 (1%)	17 25
1	P	329/332 (99%)	314 (95%)	13 (4%)	2 (1%)	25 36
1	Q	329/332 (99%)	308 (94%)	18 (6%)	3 (1%)	17 25
1	R	329/332 (99%)	306 (93%)	18 (6%)	5 (2%)	10 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1316/1328 (99%)	1242 (94%)	61 (5%)	13 (1%)	15 23

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	190	GLY
1	O	237	VAL
1	P	237	VAL
1	Q	237	VAL
1	R	23	GLY

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	O	266/266 (100%)	259 (97%)	7 (3%)	46 66
1	P	266/266 (100%)	257 (97%)	9 (3%)	37 56
1	Q	266/266 (100%)	259 (97%)	7 (3%)	46 66
1	R	266/266 (100%)	256 (96%)	10 (4%)	33 51
All	All	1064/1064 (100%)	1031 (97%)	33 (3%)	40 60

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	115	ARG
1	R	135	GLU
1	R	315	PHE
1	P	261	GLN
1	P	228	MET

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

Mol	Chain	Res	Type
1	R	176	HIS
1	R	202	ASN
1	R	301	ASN
1	P	288	HIS
1	P	202	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSX	R	149	1	3,6,7	0.84	0	1,6,8	1.76	0
1	CSX	O	149	1	3,6,7	0.98	0	1,6,8	1.95	0
1	CSX	P	149	1	3,6,7	0.86	0	1,6,8	2.12	1 (100%)
1	CSX	Q	149	1	3,6,7	0.96	0	1,6,8	2.19	1 (100%)

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
1	CSX	R	149	1	-	0/1/5/7	-
1	CSX	O	149	1	-	0/1/5/7	-
1	CSX	P	149	1	-	0/1/5/7	-
1	CSX	Q	149	1	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	149	CSX	CA-CB-SG	2.19	118.14	113.36
1	P	149	CSX	CA-CB-SG	2.12	117.99	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	149	CSX	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	R	2336	-	42,48,48	2.78	12 (28%)	50,73,73	1.86	8 (16%)
2	NAD	P	1336	-	42,48,48	2.85	11 (26%)	50,73,73	1.85	9 (18%)

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	R	2336	-	-	10/26/62/62	0/5/5/5
2	NAD	P	1336	-	-	11/26/62/62	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1336	NAD	C2N-N1N	9.72	1.46	1.35
2	R	2336	NAD	C2N-N1N	9.36	1.46	1.35
2	R	2336	NAD	C4N-C3N	8.47	1.53	1.39
2	P	1336	NAD	C4N-C3N	8.44	1.53	1.39
2	P	1336	NAD	C5N-C4N	6.72	1.53	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1336	NAD	C5N-C4N-C3N	-7.77	111.15	120.34
2	R	2336	NAD	C5N-C4N-C3N	-7.76	111.17	120.34
2	R	2336	NAD	N3A-C2A-N1A	-4.22	122.08	128.68
2	P	1336	NAD	N3A-C2A-N1A	-4.20	122.12	128.68
2	P	1336	NAD	O2A-PA-O1A	4.10	132.50	112.24

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1336	NAD	C5B-O5B-PA-O1A
2	P	1336	NAD	O4D-C1D-N1N-C2N
2	P	1336	NAD	C2N-C3N-C7N-N7N
2	R	2336	NAD	C5B-O5B-PA-O1A
2	R	2336	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

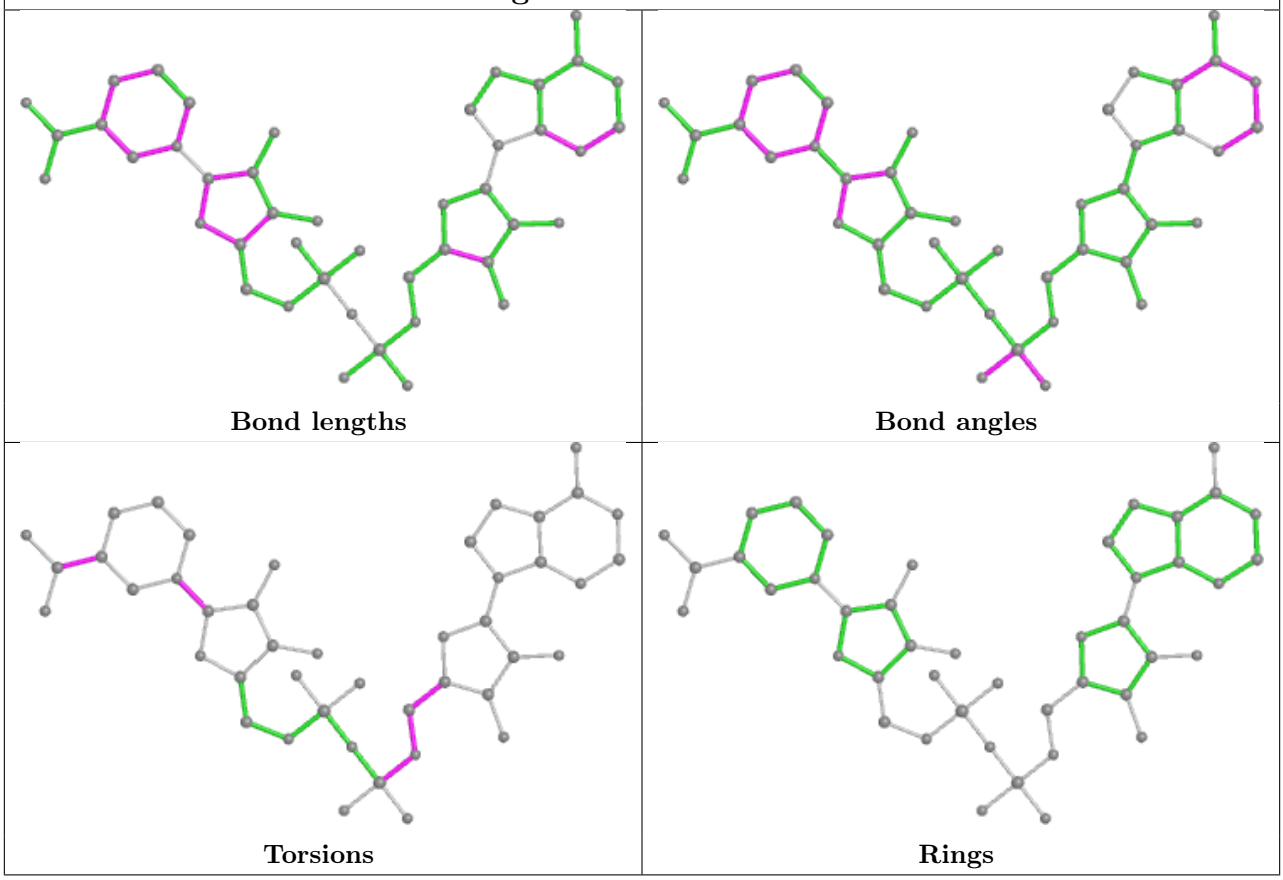
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	2336	NAD	1	0
2	P	1336	NAD	3	0

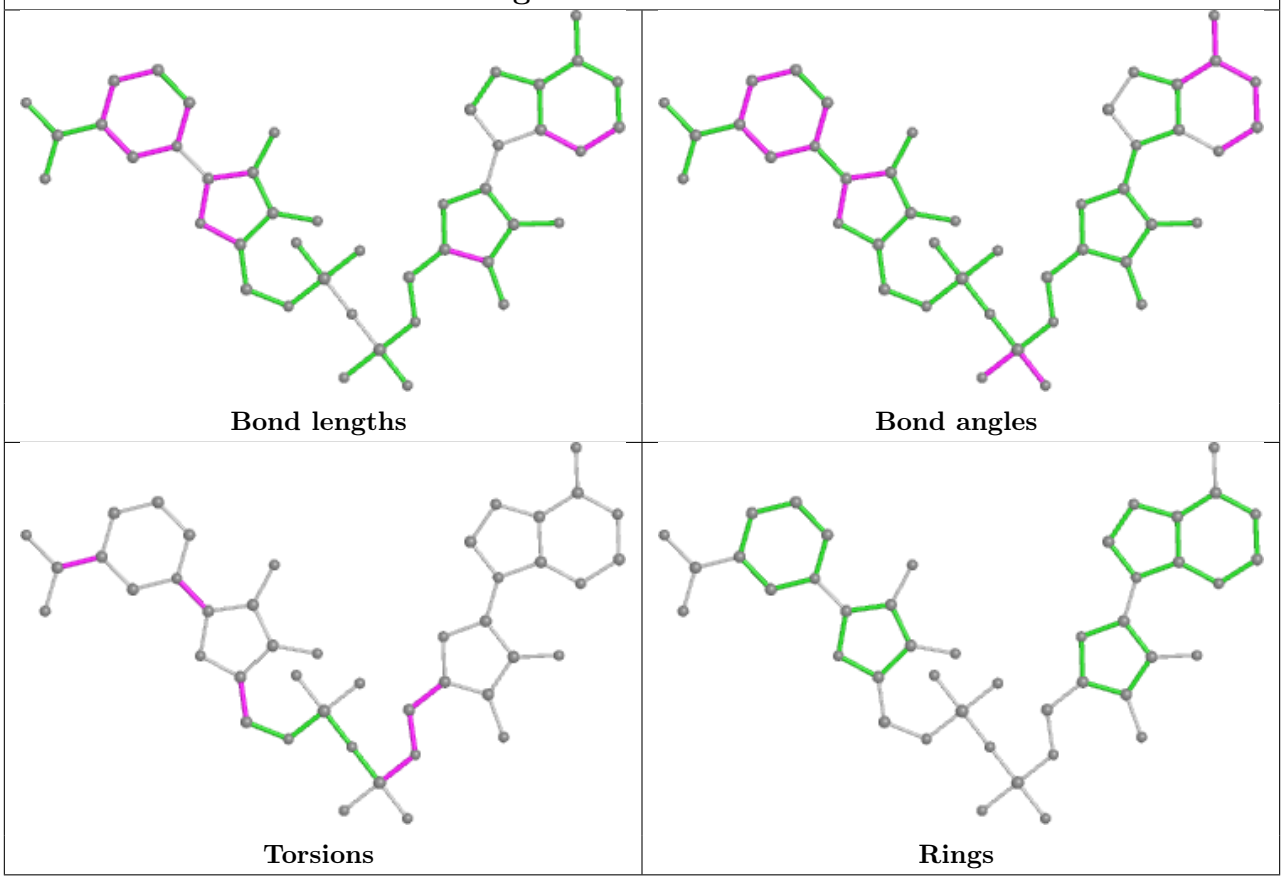
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 R 2336



Ligand NAD P 1336



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	O	331/332 (99%)	-0.31	3 (0%)	84	82	15, 28, 49, 64	0
1	P	331/332 (99%)	-0.32	4 (1%)	79	77	15, 26, 40, 60	0
1	Q	331/332 (99%)	0.04	17 (5%)	28	26	16, 29, 55, 68	0
1	R	331/332 (99%)	-0.19	10 (3%)	50	49	16, 28, 59, 69	0
All	All	1324/1328 (99%)	-0.19	34 (2%)	56	54	15, 28, 53, 69	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	54	HIS	4.9
1	P	24	LYS	4.4
1	P	54	HIS	3.4
1	Q	54	HIS	3.4
1	O	34	PHE	3.3

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSX	Q	149	7/8	0.90	0.13	27,28,42,45	0
1	CSX	P	149	7/8	0.94	0.11	21,24,36,37	0
1	CSX	R	149	7/8	0.94	0.11	25,26,38,40	0
1	CSX	O	149	7/8	0.95	0.10	25,27,36,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

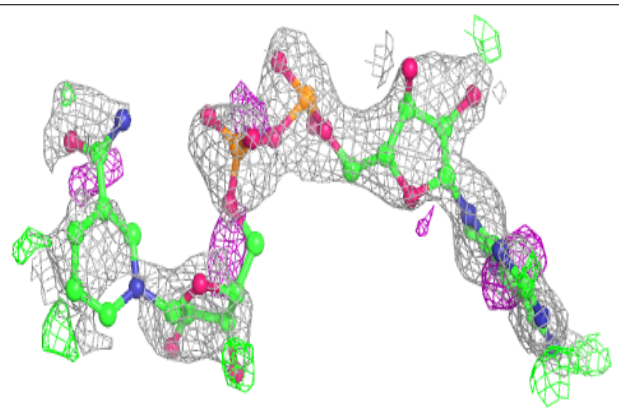
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

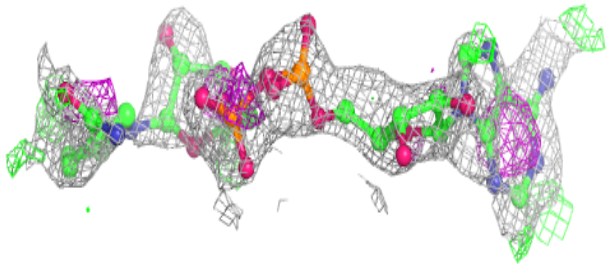
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	P	1336	44/44	0.71	0.37	64,72,77,78	1
2	NAD	R	2336	44/44	0.78	0.31	67,73,77,78	1

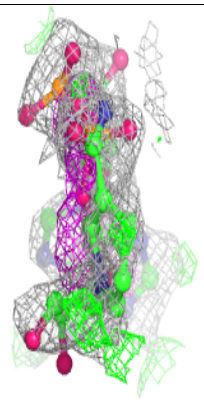
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD P 1336:

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

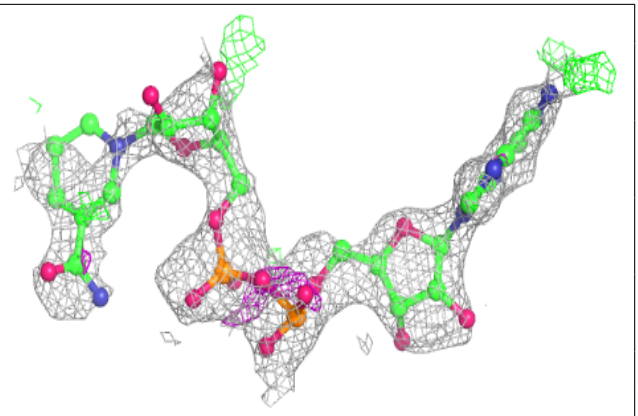


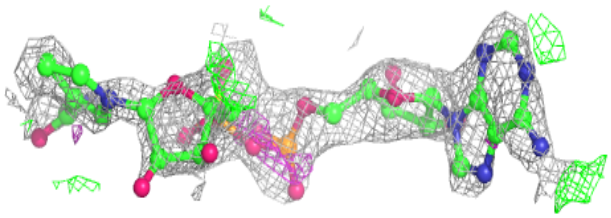


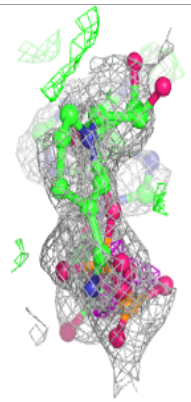


Electron density around NAD R 2336:

$2mF_o$-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.