Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 12:16 AM EDT

PDB ID	:	1NQO
Title	:	Glyceraldehyde-3-Phosphate Dehydrogenase Mutant With Cys 149 Replaced By Ser Complexed With Nad+ and D-Glyceraldehyde-3-Phosphate
Authors	:	Didierjean, C.; Corbier, C.; Fatih, M.; Favier, F.; Boschi-Muller, S.; Branlant, G.; Aubry, A.
Deposited on	:	2003-01-22
Resolution	:	2.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

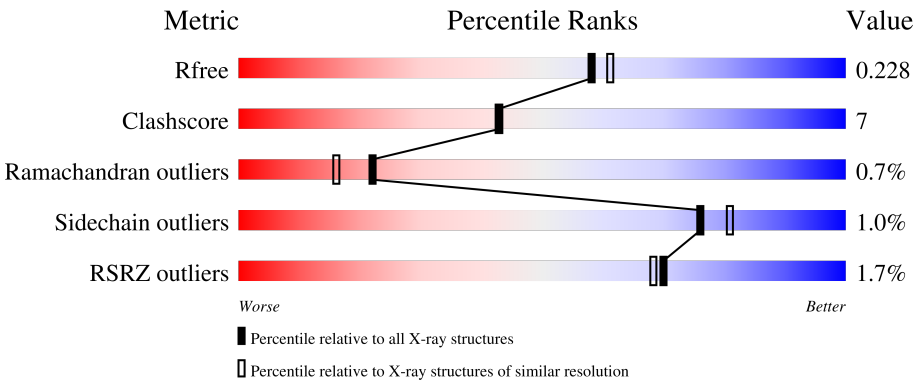
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	334	%, 89%, 10% •
1	C	334	%, 83%, 16% •
1	O	334	3%, 86%, 13% •
1	Q	334	%, 83%, 17% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10991 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.

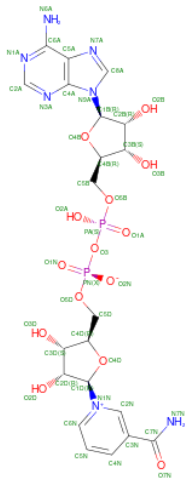
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	334	2525	1582	445	490	8	0	0	0
1	Q	334	2525	1582	445	490	8	0	0	0
1	A	334	2525	1582	445	490	8	0	0	0
1	C	334	2525	1582	445	490	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	149	SER	CYS	engineered mutation	UNP P00362
Q	149	SER	CYS	engineered mutation	UNP P00362
A	149	SER	CYS	engineered mutation	UNP P00362
C	149	SER	CYS	engineered mutation	UNP P00362

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

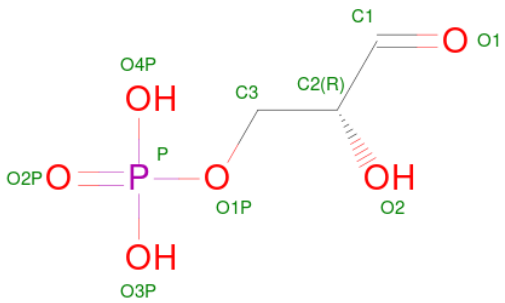
NAD



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

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).

G3H



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	O	1	10	3	6	1	0	0
			Total	C	O	P		
3	Q	1	10	3	6	1	0	0
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
			Total	C	O	P		
3	C	1	10	3	6	1	0	0

- Molecule 4 is water.

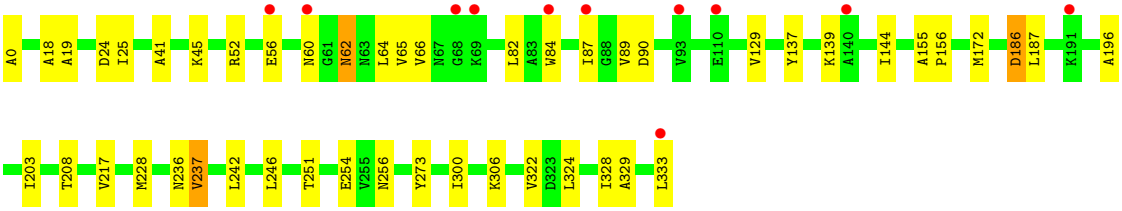
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	O	157	157	157	0	0
			Total	O		
4	Q	183	183	183	0	0
			Total	O		
4	A	170	170	170	0	0
			Total	O		
4	C	165	165	165	0	0

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.

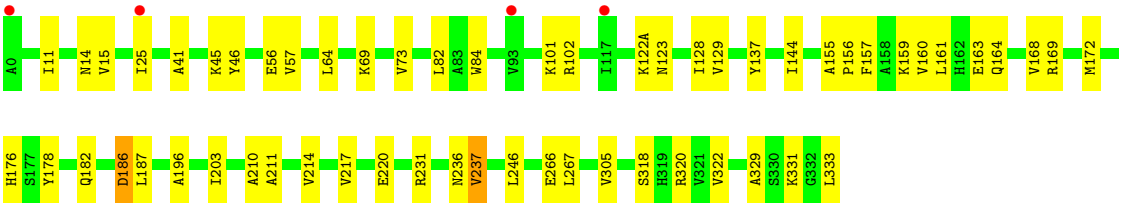
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain O:



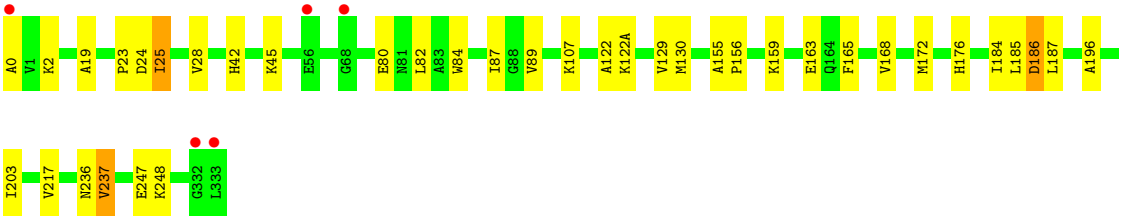
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain Q:



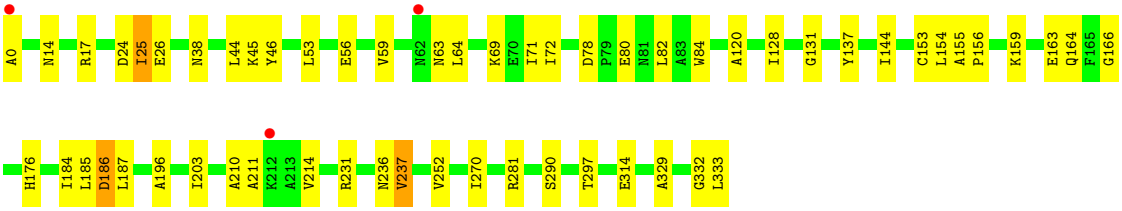
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain A:



• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain C:


A0
N14
R17
D24
I25
E26
N38
L44
K45
Y46
L53
E56
V59
N62
N63
L64
K69
E70
I71
I72
D78
P79
E80
N81
L82
A83
W84
A120
I128
G131
Y137
I144
C153
L154
A155
P156
K159
E163
Q164
F165
G166
H176
I184
L185
D186
L187
A196
I203
A210
A211
K212
A213
V214
R231
N236
V237
V252
I270
R281
S290
T297
E314
A329
G332
L333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.31Å 87.84Å 119.41Å 90.00° 119.05° 90.00°	Depositor
Resolution (Å)	8.00 – 2.01 19.93 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.01) 93.0 (19.93-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.238 0.186 , 0.228	Depositor DCC
R_{free} test set	7933 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 61.3	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	0.93	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: G3H, 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	0.30	0/2561	0.62	1/3474 (0.0%)
1	C	0.30	0/2561	0.62	1/3474 (0.0%)
1	O	0.29	0/2561	0.61	1/3474 (0.0%)
1	Q	0.30	0/2561	0.61	1/3474 (0.0%)
All	All	0.30	0/10244	0.62	4/13896 (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	Q	203	ILE	N-CA-C	-6.13	94.45	111.00
1	C	203	ILE	N-CA-C	-5.68	95.65	111.00
1	A	203	ILE	N-CA-C	-5.48	96.19	111.00
1	O	203	ILE	N-CA-C	-5.25	96.83	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	A	2525	0	2572	25	0
1	C	2525	0	2572	41	0
1	O	2525	0	2572	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2525	0	2572	41	0
2	A	44	0	26	0	0
2	C	44	0	26	1	0
2	O	44	0	26	0	0
2	Q	44	0	26	0	0
3	A	10	0	5	2	0
3	C	10	0	5	0	0
3	O	10	0	5	0	0
3	Q	10	0	5	1	0
4	A	170	0	0	3	0
4	C	165	0	0	3	0
4	O	157	0	0	1	0
4	Q	183	0	0	3	0
All	All	10991	0	10412	141	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 7.

All (141) 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:O:45:LYS:HE3	1:O:52:ARG:HH21	1.20	1.03
1:A:2:LYS:HD3	1:A:28:VAL:HG11	1.55	0.88
1:O:45:LYS:HE3	1:O:52:ARG:NH2	1.88	0.87
1:A:19:ALA:HB1	1:A:25:ILE:HD11	1.58	0.85
1:Q:329:ALA:HA	1:Q:333:LEU:HD21	1.64	0.80
1:C:45:LYS:HE2	4:C:7355:HOH:O	1.81	0.80
1:C:329:ALA:HA	1:C:333:LEU:HD11	1.65	0.78
1:O:329:ALA:HA	1:O:333:LEU:HD11	1.68	0.76
1:C:210:ALA:O	1:C:214:VAL:HG23	1.90	0.71
1:O:90:ASP:HB3	1:O:333:LEU:HD23	1.75	0.69
1:C:329:ALA:HA	1:C:333:LEU:CD1	2.26	0.65
1:Q:101:LYS:HG2	1:Q:122(A):LYS:HD3	1.81	0.63
1:Q:25:ILE:HD13	1:Q:322:VAL:HG13	1.81	0.62
1:C:78:ASP:OD1	1:C:80:GLU:HG2	1.98	0.62
1:O:56:GLU:O	1:O:66:VAL:HA	1.99	0.62
1:C:45:LYS:O	1:C:45:LYS:HD3	1.99	0.61
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.82	0.61
1:C:187:LEU:O	1:C:196:ALA:HB1	2.01	0.61
1:A:159:LYS:O	1:A:163:GLU:HG3	2.01	0.60
1:C:38:ASN:HD22	1:C:59:VAL:HG21	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.84	0.59
1:A:0:ALA:HB3	1:A:24:ASP:O	2.01	0.59
1:Q:129:VAL:HG23	1:Q:217:VAL:HG11	1.84	0.59
1:Q:56:GLU:HG2	1:C:69:LYS:HE3	1.84	0.59
1:Q:331:LYS:HE2	1:A:23:PRO:HG2	1.85	0.58
1:Q:144:ILE:N	1:Q:144:ILE:HD12	2.19	0.58
1:A:187:LEU:O	1:A:196:ALA:HB1	2.04	0.58
1:Q:45:LYS:HE3	1:Q:57:VAL:HB	1.85	0.58
1:A:45:LYS:HZ2	1:A:45:LYS:HB2	1.69	0.57
1:O:87:ILE:HG13	1:O:89:VAL:HG23	1.87	0.56
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.86	0.56
1:O:0:ALA:HB3	1:O:24:ASP:O	2.06	0.56
1:O:60:ASN:HB2	1:O:65:VAL:HG23	1.87	0.56
1:O:18:ALA:HB3	1:O:322:VAL:HG21	1.88	0.56
1:Q:45:LYS:HD2	1:Q:46:TYR:CE2	2.41	0.55
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.87	0.55
1:A:236:ASN:O	1:A:237:VAL:HB	2.07	0.55
1:C:25:ILE:HD12	1:C:26:GLU:N	2.22	0.55
1:C:44:LEU:HG	1:C:53:LEU:HD22	1.89	0.54
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.42	0.54
1:A:45:LYS:HB2	1:A:45:LYS:NZ	2.23	0.54
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.89	0.54
3:Q:3337:G3H:H11	4:Q:3421:HOH:O	2.08	0.53
1:C:144:ILE:HD12	1:C:144:ILE:N	2.23	0.53
1:Q:246:LEU:HD12	1:Q:246:LEU:N	2.24	0.53
1:C:63:ASN:ND2	1:C:72:ILE:HA	2.24	0.53
1:O:144:ILE:HD12	1:O:144:ILE:N	2.24	0.52
1:Q:331:LYS:HE2	1:A:23:PRO:CG	2.40	0.52
1:C:131:GLY:HA3	1:C:270:ILE:CD1	2.40	0.52
1:Q:41:ALA:HB2	1:Q:64:LEU:CD2	2.40	0.52
1:C:131:GLY:HA3	1:C:270:ILE:HD13	1.91	0.52
1:O:52:ARG:HG2	1:O:52:ARG:HH11	1.75	0.52
1:O:187:LEU:O	1:O:196:ALA:HB1	2.09	0.52
1:O:333:LEU:HD12	1:O:333:LEU:N	2.25	0.52
1:Q:25:ILE:CD1	1:Q:322:VAL:HG13	2.40	0.51
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.46	0.51
1:C:0:ALA:HB3	1:C:24:ASP:O	2.10	0.51
1:C:281:ARG:NH1	4:C:7456:HOH:O	2.43	0.50
1:O:60:ASN:HB2	1:O:65:VAL:CG2	2.40	0.50
1:Q:187:LEU:O	1:Q:196:ALA:HB1	2.12	0.50
1:O:41:ALA:HB2	1:O:64:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ASN:ND2	1:O:62:ASN:O	2.45	0.49
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.94	0.49
1:O:129:VAL:CG2	1:O:217:VAL:HG11	2.41	0.49
1:O:137:TYR:OH	1:O:328:ILE:HG23	2.13	0.49
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.48	0.49
1:O:236:ASN:O	1:O:237:VAL:HB	2.12	0.49
1:Q:266:GLU:HG3	1:Q:267:LEU:HG	1.95	0.49
1:C:332:GLY:C	1:C:333:LEU:HD12	2.33	0.49
1:Q:11:ILE:O	1:Q:15:VAL:HG23	2.13	0.49
1:C:45:LYS:HD2	1:C:46:TYR:CE1	2.48	0.49
1:C:236:ASN:O	1:C:237:VAL:HB	2.13	0.49
1:Q:160:VAL:O	1:Q:164:GLN:HB2	2.14	0.48
1:C:25:ILE:HD12	1:C:25:ILE:C	2.33	0.48
1:O:25:ILE:HD13	1:O:322:VAL:HG13	1.95	0.48
1:Q:102:ARG:HD2	1:Q:123:ASN:O	2.13	0.48
1:A:186:ASP:HA	1:A:196:ALA:O	2.14	0.48
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.94	0.47
1:O:300:ILE:HG13	4:O:1465:HOH:O	2.13	0.47
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.15	0.47
1:Q:41:ALA:HB2	1:Q:64:LEU:HD22	1.97	0.47
1:Q:64:LEU:HG	1:Q:73:VAL:CG2	2.44	0.47
1:O:324:LEU:O	1:O:328:ILE:HG13	2.15	0.47
1:Q:246:LEU:HD11	1:Q:305:VAL:HG12	1.97	0.46
1:A:80:GLU:HG2	4:A:5384:HOH:O	2.15	0.46
1:A:176:HIS:NE2	3:A:5337:G3H:O1	2.48	0.46
1:C:64:LEU:HB2	1:C:71:ILE:HB	1.97	0.46
1:O:137:TYR:CZ	1:O:328:ILE:HG23	2.51	0.45
1:A:122:ALA:C	1:A:122(A):LYS:HD3	2.36	0.45
1:Q:168:VAL:HG12	1:Q:169:ARG:HG2	1.98	0.45
1:Q:246:LEU:N	1:Q:246:LEU:CD1	2.80	0.45
1:Q:159:LYS:O	1:Q:163:GLU:HG3	2.17	0.45
1:C:184:ILE:HG22	1:C:185:LEU:HG	1.99	0.45
1:Q:69:LYS:HE3	1:C:56:GLU:OE2	2.17	0.44
1:C:128:ILE:HD11	1:C:137:TYR:HB2	1.98	0.44
1:O:84:TRP:HB3	1:O:89:VAL:HB	2.00	0.44
1:O:19:ALA:CB	1:O:25:ILE:HD11	2.48	0.44
1:Q:56:GLU:CG	1:C:69:LYS:HE3	2.48	0.44
1:O:208:THR:HG22	1:O:228:MET:HA	2.00	0.43
1:C:155:ALA:HB3	1:C:156:PRO:HD3	2.00	0.43
1:Q:182:GLN:HB3	4:Q:3443:HOH:O	2.17	0.43
1:C:159:LYS:O	1:C:163:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:157:PHE:O	1:Q:161:LEU:HG	2.18	0.43
1:A:165:PHE:HA	1:A:248:LYS:HD3	1.99	0.43
3:A:5337:G3H:H11	4:A:5405:HOH:O	2.19	0.43
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.19	0.43
1:C:154:LEU:CD2	1:C:214:VAL:HG21	2.49	0.43
1:A:168:VAL:HG22	1:A:247:GLU:HG2	2.00	0.43
1:C:25:ILE:HG13	1:C:25:ILE:O	2.18	0.43
1:O:186:ASP:HA	1:O:196:ALA:O	2.18	0.43
1:O:41:ALA:HB2	1:O:64:LEU:HD22	2.01	0.42
1:A:80:GLU:HG3	1:A:107:LYS:HD3	2.00	0.42
1:A:184:ILE:HG22	1:A:185:LEU:HG	2.01	0.42
1:Q:211:ALA:HB3	4:Q:3447:HOH:O	2.19	0.42
1:A:80:GLU:HA	4:A:5384:HOH:O	2.20	0.42
1:O:56:GLU:OE1	1:O:56:GLU:HA	2.20	0.42
1:Q:178:TYR:HA	1:Q:182:GLN:OE1	2.19	0.42
1:C:17:ARG:HE	1:C:53:LEU:HD13	1.84	0.42
1:A:42:HIS:HA	1:A:45:LYS:HZ2	1.85	0.42
1:A:87:ILE:HG13	1:A:89:VAL:HG23	2.01	0.42
1:C:186:ASP:HA	1:C:196:ALA:O	2.18	0.42
1:O:256:ASN:HB3	1:O:273:TYR:OH	2.20	0.42
1:Q:333:LEU:HD22	1:Q:333:LEU:N	2.35	0.42
1:Q:186:ASP:HA	1:Q:196:ALA:O	2.20	0.42
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.54	0.42
1:O:139:LYS:N	1:O:139:LYS:HD2	2.35	0.42
1:Q:210:ALA:O	1:Q:214:VAL:HG23	2.20	0.42
1:C:252:VAL:HG13	1:C:297:THR:HG22	2.02	0.42
1:A:236:ASN:O	1:A:237:VAL:CB	2.66	0.41
1:C:120:ALA:HB2	2:C:7336:NAD:H1D	2.01	0.41
1:O:52:ARG:HG2	1:O:52:ARG:NH1	2.36	0.41
1:Q:25:ILE:O	1:Q:25:ILE:HG13	2.20	0.41
1:Q:128:ILE:HD11	1:Q:137:TYR:HB2	2.01	0.41
1:Q:14:ASN:HB3	1:Q:318:SER:OG	2.21	0.41
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.34	0.41
1:C:185:LEU:O	1:C:186:ASP:C	2.58	0.41
1:C:211:ALA:HB3	4:C:7426:HOH:O	2.19	0.41
1:C:153:CYS:HA	1:C:290:SER:HB2	2.03	0.41
1:O:242:LEU:O	1:O:306:LYS:HA	2.21	0.40
1:C:236:ASN:OD1	1:C:314:GLU:HG3	2.22	0.40
1:C:154:LEU:HD23	1:C:214:VAL:HG21	2.02	0.40

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	332/334 (99%)	314 (95%)	16 (5%)	2 (1%)	25	19
1	C	332/334 (99%)	316 (95%)	13 (4%)	3 (1%)	17	11
1	O	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	25	19
1	Q	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	25	19
All	All	1328/1336 (99%)	1260 (95%)	59 (4%)	9 (1%)	22	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	ASP
1	O	186	ASP
1	O	237	VAL
1	Q	186	ASP
1	Q	237	VAL
1	A	186	ASP
1	A	237	VAL
1	C	237	VAL
1	C	166	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	A	272/272 (100%)	269 (99%)	3 (1%)	73	78
1	C	272/272 (100%)	269 (99%)	3 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	272/272 (100%)	269 (99%)	3 (1%)	73	78
1	Q	272/272 (100%)	270 (99%)	2 (1%)	84	88
All	All	1088/1088 (100%)	1077 (99%)	11 (1%)	76	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	172	MET
1	O	246	LEU
1	Q	172	MET
1	Q	220	GLU
1	A	25	ILE
1	A	130	MET
1	A	172	MET
1	C	14	ASN
1	C	25	ILE
1	C	164	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	42	HIS
1	O	62	ASN
1	O	63	ASN
1	O	81	ASN
1	Q	38	ASN
1	Q	42	HIS
1	Q	62	ASN
1	Q	63	ASN
1	Q	81	ASN
1	Q	146	ASN
1	Q	319	HIS
1	A	38	ASN
1	A	60	ASN
1	A	63	ASN
1	A	146	ASN
1	A	164	GLN
1	C	14	ASN
1	C	38	ASN

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Mol	Chain	Res	Type
1	C	63	ASN
1	C	81	ASN
1	C	146	ASN
1	C	164	GLN
1	C	319	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 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	7336	-	42,48,48	1.55	6 (14%)	50,73,73	1.42	5 (10%)
3	G3H	C	7337	-	8,9,9	1.16	0	10,12,12	1.89	3 (30%)
3	G3H	O	1337	-	8,9,9	1.39	1 (12%)	10,12,12	1.87	3 (30%)
2	NAD	A	5336	-	42,48,48	1.51	4 (9%)	50,73,73	1.38	5 (10%)
2	NAD	Q	3336	-	42,48,48	1.69	5 (11%)	50,73,73	1.41	6 (12%)
2	NAD	O	1336	-	42,48,48	1.52	4 (9%)	50,73,73	1.46	5 (10%)
3	G3H	Q	3337	-	8,9,9	1.19	0	10,12,12	1.90	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	G3H	A	5337	-	8,9,9	1.19	0	10,12,12	1.86	3 (30%)

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	7336	-	-	5/26/62/62	0/5/5/5
3	G3H	C	7337	-	-	3/7/8/8	-
3	G3H	O	1337	-	-	3/7/8/8	-
2	NAD	A	5336	-	-	5/26/62/62	0/5/5/5
2	NAD	Q	3336	-	-	5/26/62/62	0/5/5/5
2	NAD	O	1336	-	-	5/26/62/62	0/5/5/5
3	G3H	Q	3337	-	-	3/7/8/8	-
3	G3H	A	5337	-	-	3/7/8/8	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3336	NAD	C2N-N1N	7.91	1.44	1.35
2	O	1336	NAD	C2N-N1N	6.92	1.43	1.35
2	C	7336	NAD	C2N-N1N	6.85	1.43	1.35
2	A	5336	NAD	C2N-N1N	6.77	1.43	1.35
2	O	1336	NAD	C6N-N1N	3.41	1.43	1.35
2	Q	3336	NAD	C6N-N1N	3.23	1.43	1.35
2	A	5336	NAD	C6N-N1N	3.03	1.42	1.35
2	C	7336	NAD	O4D-C1D	3.01	1.45	1.41
2	C	7336	NAD	C6N-N1N	3.01	1.42	1.35
2	Q	3336	NAD	O4D-C1D	2.92	1.45	1.41
2	A	5336	NAD	O4D-C1D	2.91	1.45	1.41
2	Q	3336	NAD	C3N-C7N	2.65	1.54	1.50
3	O	1337	G3H	C3-C2	2.24	1.54	1.51
2	O	1336	NAD	O4B-C1B	2.19	1.44	1.41
2	C	7336	NAD	C2A-N3A	2.18	1.35	1.32
2	C	7336	NAD	C5A-N7A	-2.15	1.31	1.39
2	O	1336	NAD	O4D-C1D	2.15	1.44	1.41
2	Q	3336	NAD	C4N-C3N	2.09	1.42	1.39
2	A	5336	NAD	C2A-N3A	2.07	1.35	1.32
2	C	7336	NAD	O4B-C1B	2.03	1.43	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1336	NAD	N3A-C2A-N1A	-6.23	118.94	128.68
2	Q	3336	NAD	N3A-C2A-N1A	-6.16	119.05	128.68
2	A	5336	NAD	N3A-C2A-N1A	-6.09	119.15	128.68
2	C	7336	NAD	N3A-C2A-N1A	-5.94	119.39	128.68
3	O	1337	G3H	O1P-C3-C2	3.70	118.13	108.33
3	A	5337	G3H	O1P-C3-C2	3.57	117.80	108.33
3	Q	3337	G3H	O1P-C3-C2	3.42	117.38	108.33
3	C	7337	G3H	O1P-C3-C2	3.34	117.17	108.33
2	O	1336	NAD	C1B-N9A-C4A	-3.13	121.14	126.64
2	O	1336	NAD	C4A-C5A-N7A	3.09	112.62	109.40
2	Q	3336	NAD	C4A-C5A-N7A	2.88	112.40	109.40
2	O	1336	NAD	C2A-N1A-C6A	2.84	123.61	118.75
3	O	1337	G3H	O2-C2-C1	-2.75	103.75	109.17
2	Q	3336	NAD	C2A-N1A-C6A	2.73	123.43	118.75
3	C	7337	G3H	P-O1P-C3	2.73	125.80	118.30
3	Q	3337	G3H	P-O1P-C3	2.70	125.74	118.30
2	A	5336	NAD	C2A-N1A-C6A	2.69	123.35	118.75
3	Q	3337	G3H	O2-C2-C1	-2.66	103.92	109.17
2	C	7336	NAD	C2A-N1A-C6A	2.65	123.29	118.75
3	C	7337	G3H	O2-C2-C1	-2.62	104.01	109.17
3	O	1337	G3H	P-O1P-C3	2.60	125.45	118.30
2	C	7336	NAD	C4A-C5A-N7A	2.57	112.08	109.40
2	C	7336	NAD	C5N-C4N-C3N	2.56	123.37	120.34
2	O	1336	NAD	C5N-C4N-C3N	2.53	123.33	120.34
3	A	5337	G3H	O2-C2-C1	-2.51	104.22	109.17
2	A	5336	NAD	C4A-C5A-N7A	2.45	111.96	109.40
2	Q	3336	NAD	C1B-N9A-C4A	-2.44	122.35	126.64
2	C	7336	NAD	C1B-N9A-C4A	-2.35	122.50	126.64
2	A	5336	NAD	C1B-N9A-C4A	-2.29	122.61	126.64
2	Q	3336	NAD	C5N-C4N-C3N	2.21	122.96	120.34
2	Q	3336	NAD	O2D-C2D-C3D	2.15	118.77	111.82
2	A	5336	NAD	C5N-C4N-C3N	2.08	122.81	120.34
3	A	5337	G3H	P-O1P-C3	2.04	123.92	118.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1336	NAD	O4D-C1D-N1N-C2N
2	O	1336	NAD	O4D-C1D-N1N-C6N
2	O	1336	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	O	1336	NAD	C2D-C1D-N1N-C6N
2	Q	3336	NAD	O4D-C1D-N1N-C2N
2	Q	3336	NAD	O4D-C1D-N1N-C6N
2	Q	3336	NAD	C2D-C1D-N1N-C2N
2	Q	3336	NAD	C2D-C1D-N1N-C6N
2	A	5336	NAD	O4D-C1D-N1N-C2N
2	A	5336	NAD	O4D-C1D-N1N-C6N
2	A	5336	NAD	C2D-C1D-N1N-C2N
2	A	5336	NAD	C2D-C1D-N1N-C6N
2	C	7336	NAD	O4D-C1D-N1N-C2N
2	C	7336	NAD	O4D-C1D-N1N-C6N
2	C	7336	NAD	C2D-C1D-N1N-C2N
2	C	7336	NAD	C2D-C1D-N1N-C6N
3	O	1337	G3H	C3-O1P-P-O2P
3	O	1337	G3H	C3-O1P-P-O3P
3	O	1337	G3H	C3-O1P-P-O4P
3	Q	3337	G3H	C3-O1P-P-O2P
3	Q	3337	G3H	C3-O1P-P-O3P
3	Q	3337	G3H	C3-O1P-P-O4P
3	A	5337	G3H	C3-O1P-P-O2P
3	A	5337	G3H	C3-O1P-P-O3P
3	A	5337	G3H	C3-O1P-P-O4P
3	C	7337	G3H	C3-O1P-P-O2P
3	C	7337	G3H	C3-O1P-P-O3P
3	C	7337	G3H	C3-O1P-P-O4P
2	C	7336	NAD	O4B-C4B-C5B-O5B
2	A	5336	NAD	O4B-C4B-C5B-O5B
2	O	1336	NAD	O4B-C4B-C5B-O5B
2	Q	3336	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

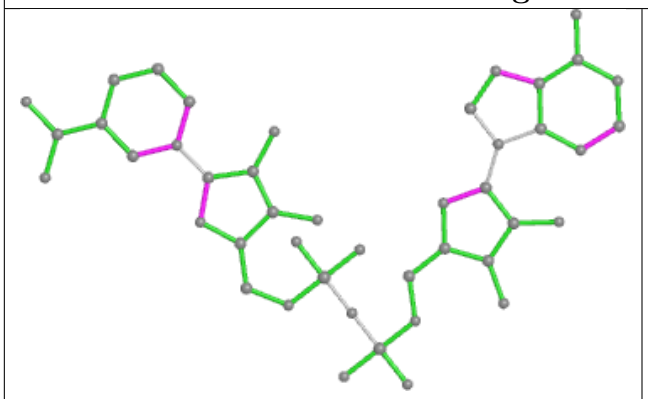
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7336	NAD	1	0
3	Q	3337	G3H	1	0
3	A	5337	G3H	2	0

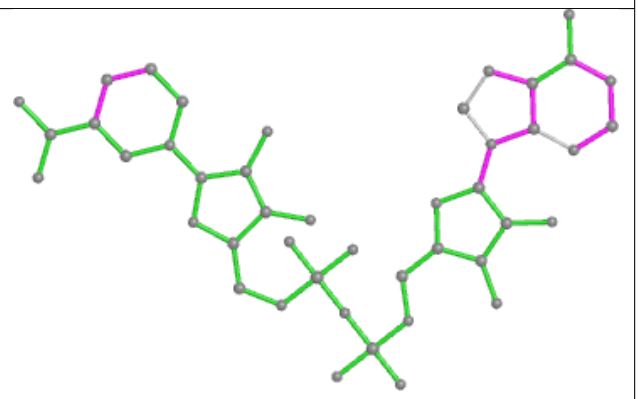
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

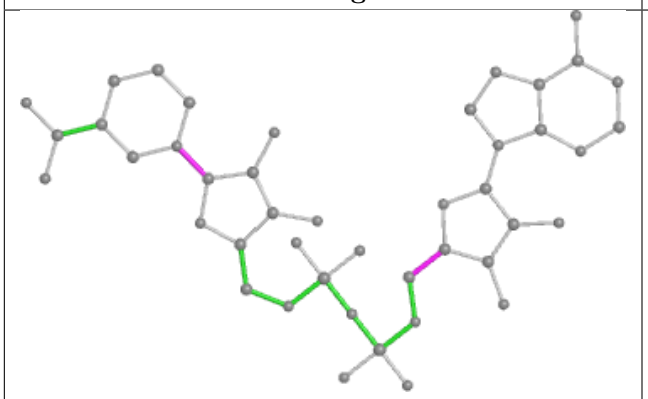
Ligand NAD C 7336



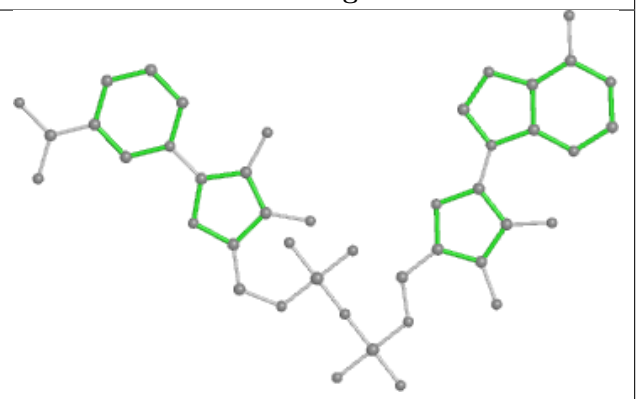
Bond lengths



Bond angles

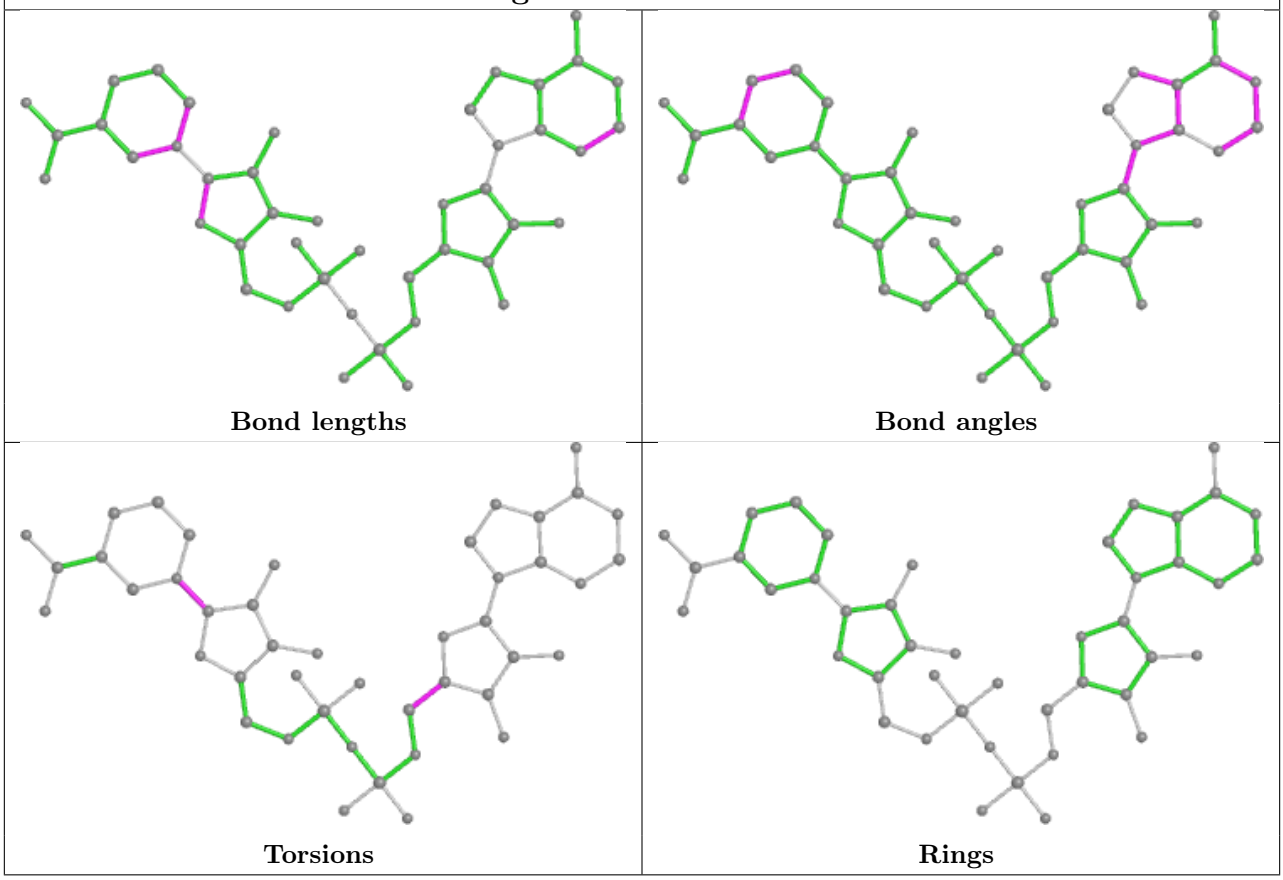


Torsions

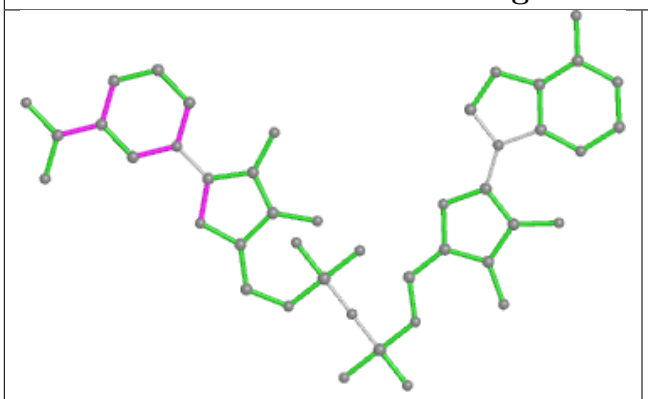


Rings

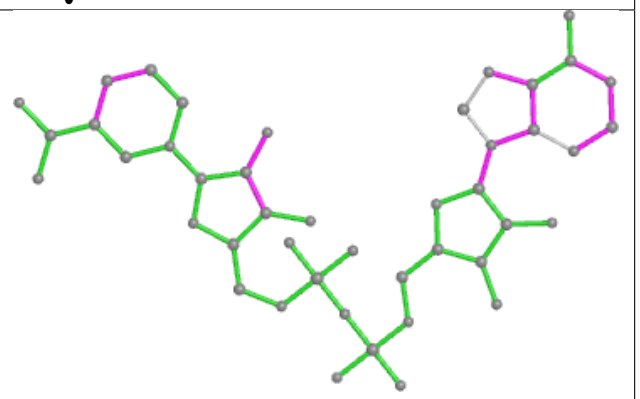
Ligand NAD A 5336



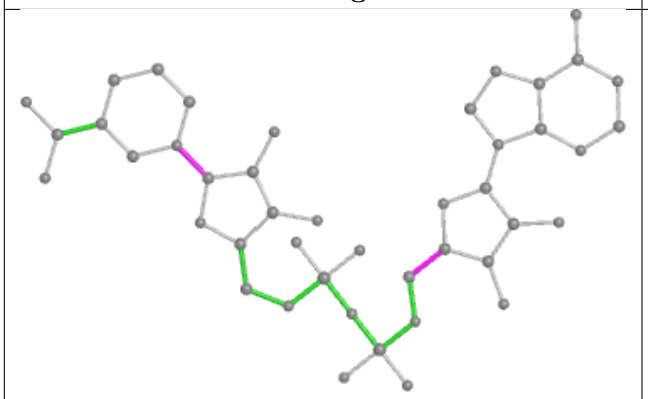
Ligand NAD Q 3336



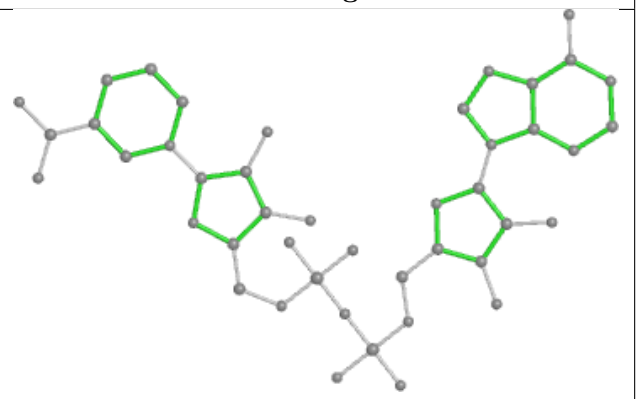
Bond lengths



Bond angles

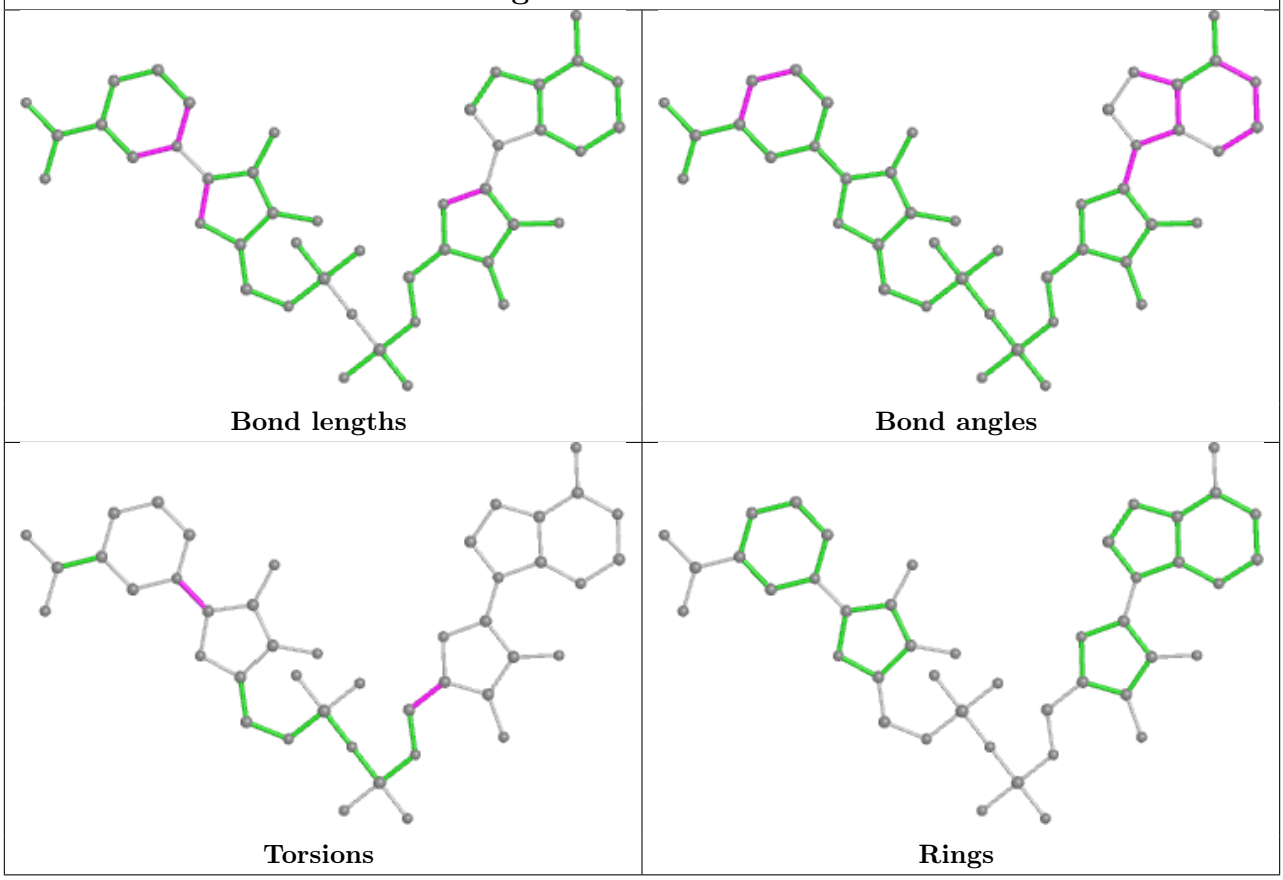


Torsions



Rings

Ligand NAD O 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	A	334/334 (100%)	-0.20	5 (1%)	73	72	8, 15, 28, 37	0
1	C	334/334 (100%)	-0.24	3 (0%)	84	83	8, 16, 28, 35	0
1	O	334/334 (100%)	-0.06	11 (3%)	46	45	6, 18, 35, 45	0
1	Q	334/334 (100%)	-0.18	4 (1%)	79	78	8, 15, 28, 33	0
All	All	1336/1336 (100%)	-0.17	23 (1%)	70	68	6, 16, 30, 45	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	GLY	3.0
1	C	0	ALA	3.0
1	A	333	LEU	2.7
1	O	60	ASN	2.6
1	O	333	LEU	2.6
1	A	0	ALA	2.6
1	O	69	LYS	2.5
1	O	93	VAL	2.5
1	A	56	GLU	2.5
1	Q	25	ILE	2.5
1	Q	0	ALA	2.4
1	A	68	GLY	2.4
1	O	191	LYS	2.3
1	Q	93	VAL	2.2
1	C	62	ASN	2.2
1	C	212	LYS	2.2
1	Q	117	ILE	2.2
1	O	110	GLU	2.2
1	O	87	ILE	2.1
1	O	140	ALA	2.1
1	O	68	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	84	TRP	2.1
1	O	56	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

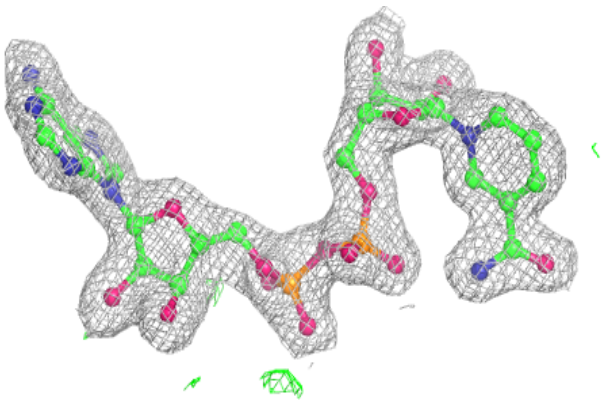
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

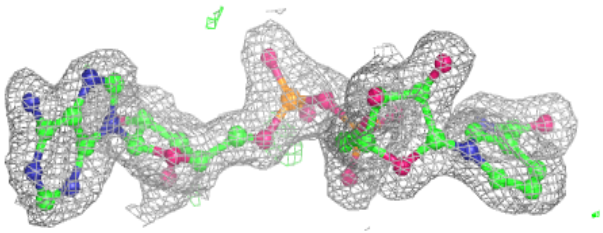
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	G3H	Q	3337	10/10	0.60	0.32	43,49,54,54	0
3	G3H	A	5337	10/10	0.68	0.29	42,46,48,48	0
3	G3H	C	7337	10/10	0.70	0.32	42,47,49,51	0
3	G3H	O	1337	10/10	0.76	0.21	26,37,46,46	0
2	NAD	A	5336	44/44	0.97	0.08	6,12,14,15	0
2	NAD	C	7336	44/44	0.97	0.08	8,11,13,14	0
2	NAD	O	1336	44/44	0.97	0.07	7,13,16,18	0
2	NAD	Q	3336	44/44	0.98	0.07	5,10,12,14	0

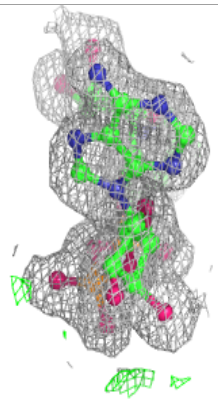
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 5336:

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

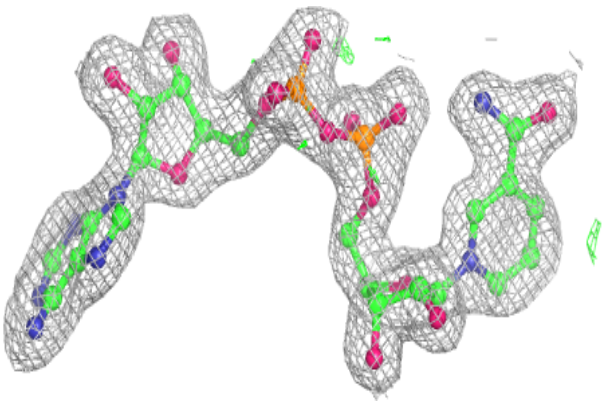


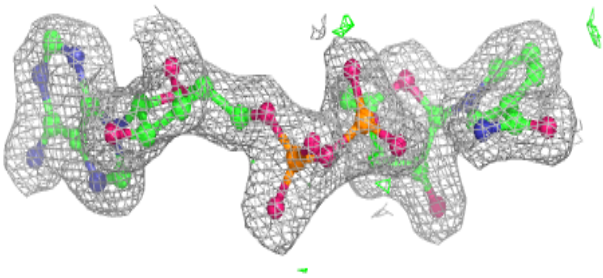


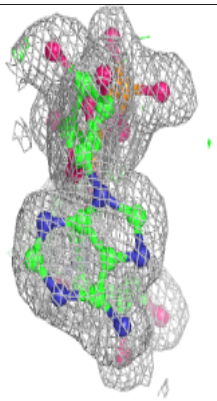


Electron density around NAD C 7336:

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

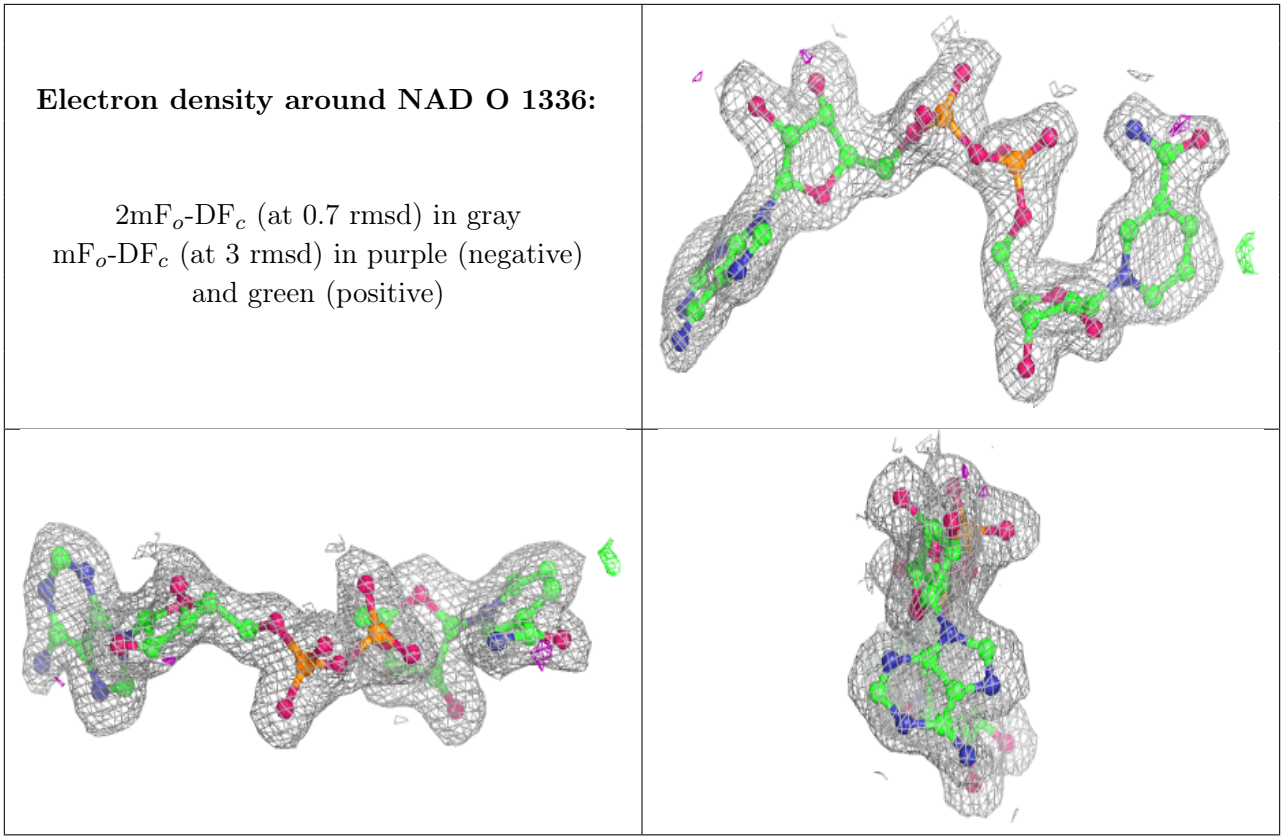






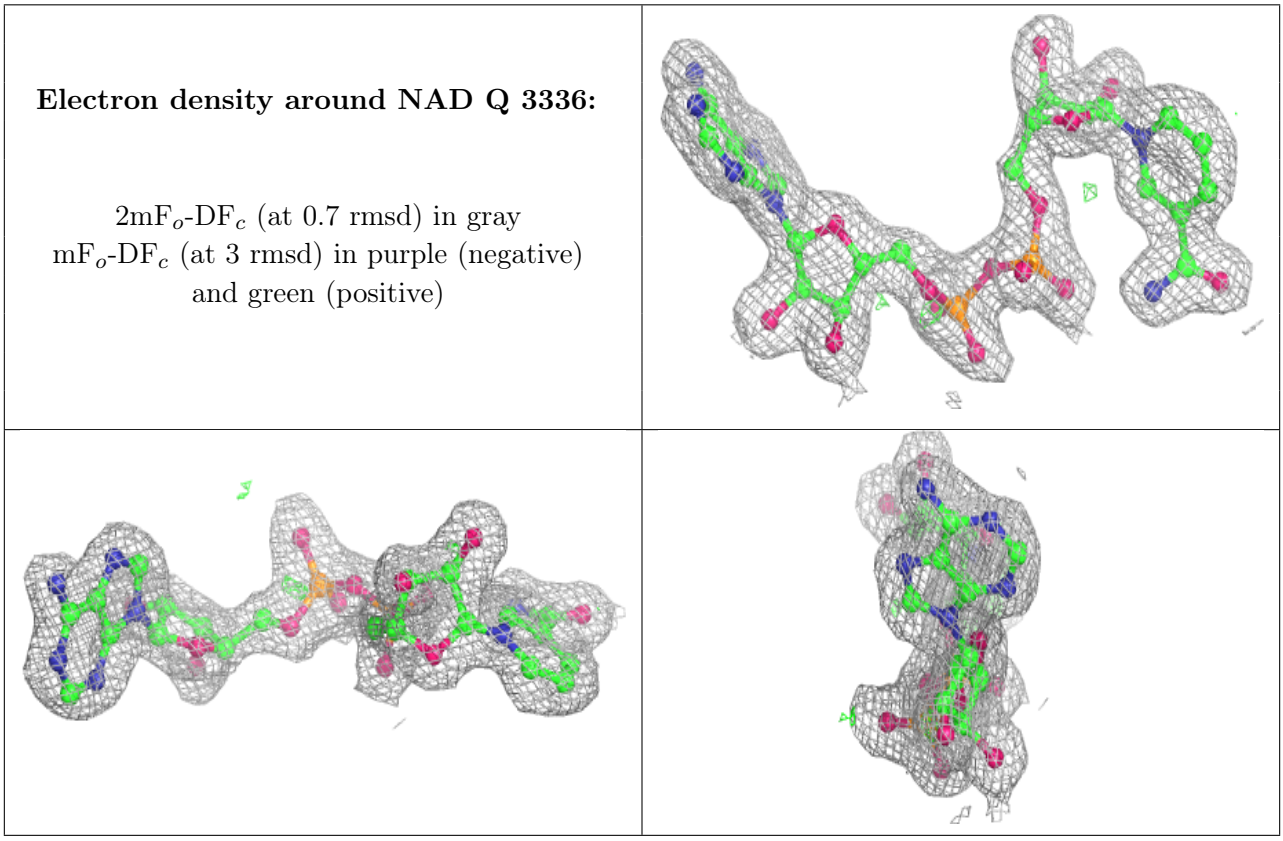
Electron density around NAD O 1336:

$2mF_o$-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 Q 3336:

$2mF_o$-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.